



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 11:02 am BST

PDB ID : 7QGG / pdb_00007qgg
EMDB ID : EMD-13954
Title : Neuronal RNA granules are ribosome complexes stalled at the pre-translocation state
Authors : Pulk, A.; Kipper, K.; Mansour, A.
Deposited on : 2021-12-08
Resolution : 2.86 Å(reported)
Based on initial model : 6OLE

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 : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
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

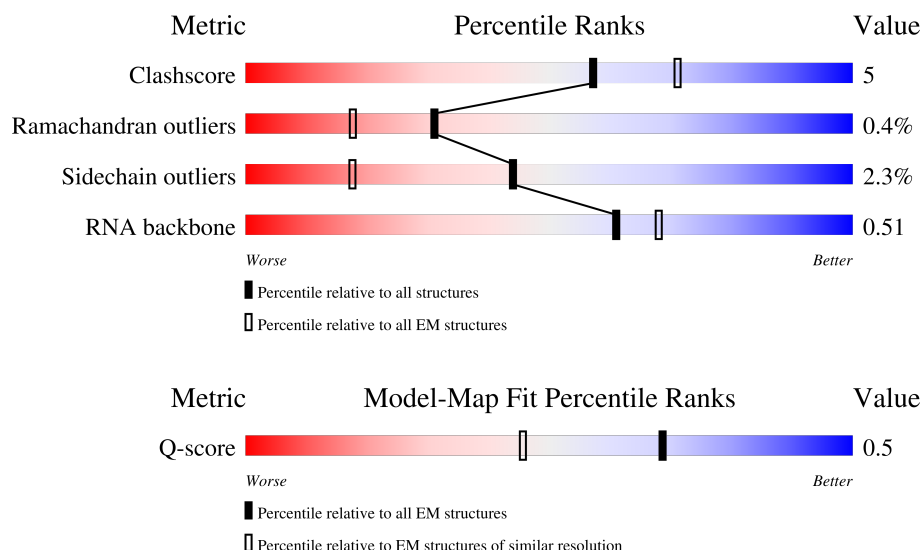
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.86 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.



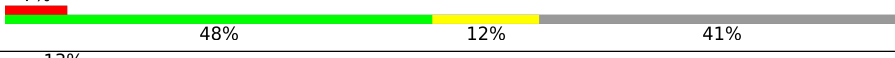
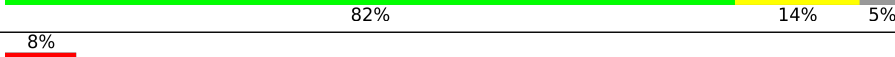
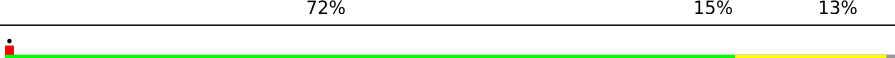
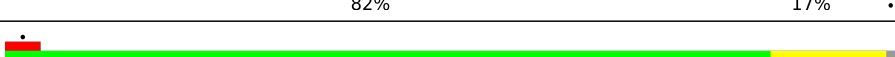
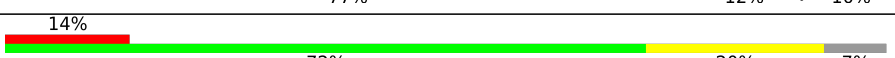
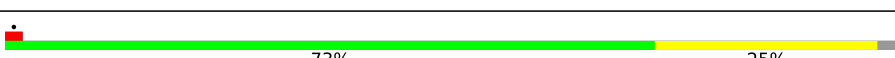
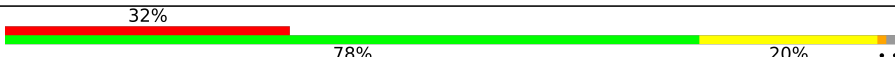
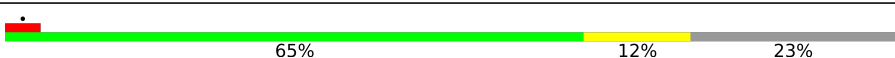
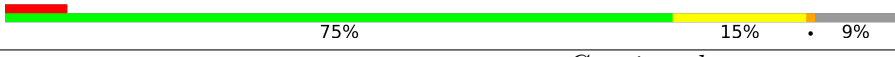
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12017 (2.36 - 3.36)

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	1872	
2	SA	295	
3	SB	264	

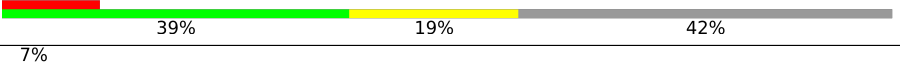
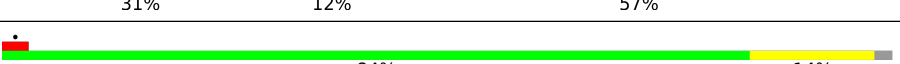
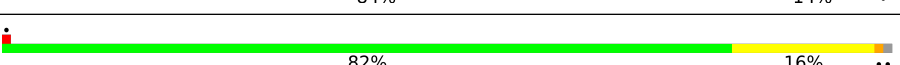
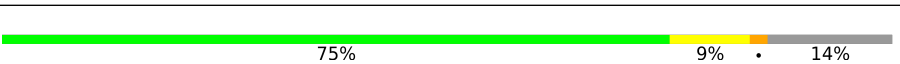
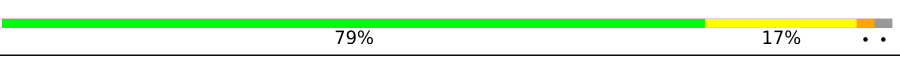
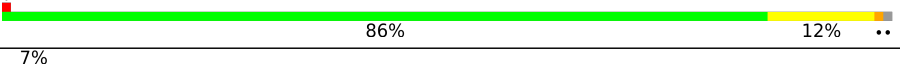
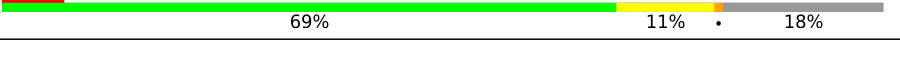
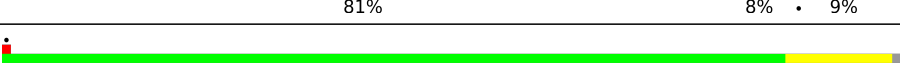
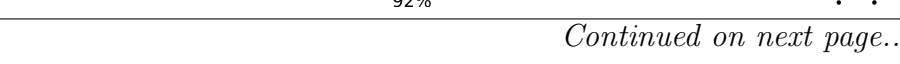
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Mol	Chain	Length	Quality of chain
4	SD	243	
5	SE	263	
6	SF	204	
7	SH	194	
8	SI	208	
9	SK	165	
10	SL	158	
11	SP	145	
12	SQ	146	
13	SR	135	
14	SS	152	
15	ST	145	
16	SU	119	
17	SV	83	
18	SX	143	
19	Sa	115	
20	Sc	69	
21	Sd	56	
22	Sg	317	
23	SC	293	
24	SG	249	
25	SJ	194	
26	SM	132	
27	SN	151	
28	SO	151	

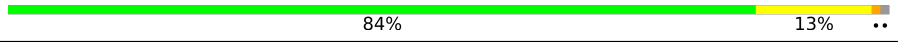
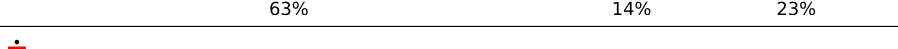
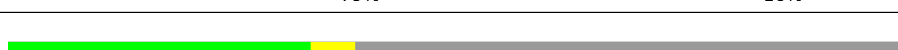
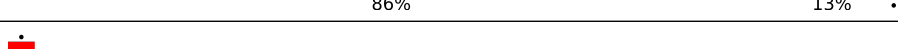
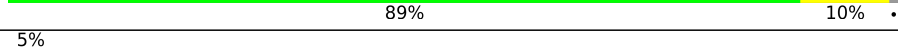
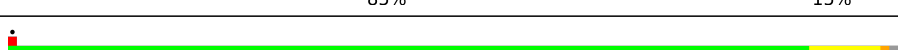
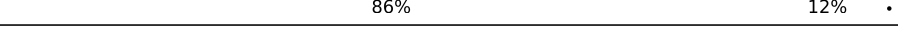
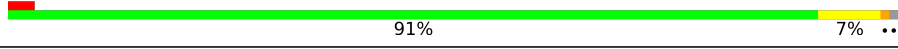
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Mol	Chain	Length	Quality of chain
29	SW	130	
30	SY	133	
31	SZ	125	
32	Sb	84	
33	Se	59	
34	Sf	156	
35	A	257	
36	B	403	
37	C	421	
38	D	157	
39	E	121	
40	F	297	
41	G	298	
42	H	260	
43	I	266	
44	J	192	
45	K	214	
46	L	178	
47	M	211	
48	N	214	
49	O	204	
50	P	203	
51	Q	184	
52	R	188	
53	S	196	

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Mol	Chain	Length	Quality of chain
54	T	176	
55	U	160	
56	V	128	
57	W	140	
58	X	157	
59	Y	156	
60	Z	145	
61	a	136	
62	b	148	
63	c	156	
64	d	115	
65	e	125	
66	f	135	
67	g	110	
68	h	117	
69	i	123	
70	j	105	
71	k	97	
72	l	70	
73	m	51	
74	n	128	
75	o	25	
76	p	106	
77	q	92	
78	r	137	

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Mol	Chain	Length	Quality of chain
79	t	4803	
80	u	76	
81	v	76	
82	w	20	
83	Cz	217	
84	y	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	6MZ	S2	1835	-	X	-	-

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 218574 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 RNA (1872-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S2	1714	Total	C	N	O	P	0	0
			36502	16306	6533	11950	1713		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SA	214	Total	C	N	O	S	0	0
			1693	1076	297	312	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
			1756	1119	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	150	Total	C	N	O	S	0	0
			1220	776	228	210	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SP	130	Total	C	N	O	S	0	0
			1073	681	205	180	7		

- Molecule 12 is a protein called Rps16 protein.

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
			1079	676	201	198	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
			1115	698	217	198	2		

- 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
			822	514	156	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
			626	382	118	121	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	103	Total	C	N	O	S	0	0
			826	515	172	134	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	225	Total	C	N	O	S	1	0
			1755	1134	303	309	9		

- 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	574	160	171	7		

- 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 Ubiquitin-like domain-containing protein.

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 Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Sf	67	Total	C	N	O	S	0	0
			547	345	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
			3204	2041	603	546	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
			2889	1817	575	481	16		

- Molecule 38 is a RNA chain called RNA (157-MER).

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 RNA (121-MER).

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
			2399	1511	442	432	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	G	243	Total	C	N	O	S	0	0
			1960	1251	375	330	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
			1865	1199	357	301	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	I	241	Total	C	N	O	S	0	0
			1935	1232	372	327	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
			1528	961	285	276	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	170	Total	C	N	O	S	0	0
			1362	861	254	241	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
			1659	1036	342	276	5		

- 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
			1142	732	221	182	7		

- Molecule 49 is a protein called 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	197	Total	C	N	O	S	0	0
			1611	1038	316	252	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Q	158	Total	C	N	O	S	0	0
			1282	804	248	221	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
			1516	949	314	249	4		

- Molecule 53 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S	188	Total	C	N	O	S	0	0
			1572	974	337	252	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	T	176	Total	C	N	O	S	0	0
			1458	929	284	234	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	U	158	Total	C	N	O	S	0	0
			1293	821	251	215	6		

- 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	134	Total	C	N	O	S	0	0
			993	625	187	176	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	120	Total	C	N	O	S	0	0
			984	630	185	168	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
			1116	700	227	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
			1165	736	240	185	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
63	c	95	Total	C	N	O	S	0	0
			781	487	171	120	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
64	d	101	Total	C	N	O	S	0	0
			785	498	138	142	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	143	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
68	h	116	Total	C	N	O	S	0	0
			920	575	190	149	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	643	204	167	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
70	j	104	Total	C	N	O	S	0	0
			849	531	180	133	5		

- Molecule 71 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	k	86	Total	C	N	O	S	0	0
			705	434	155	111	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 Ubiquitin-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 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	444	135	122	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	87	GLU	LYS	conflict	UNP A0A6J2LF66

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

Mol	Chain	Residues	Atoms					AltConf	Trace
78	r	131	Total	C	N	O	S	0	0
			1059	655	224	175	5		

- Molecule 79 is a RNA chain called RNA (4803-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
79	t	3679	Total	C	N	O	P	0	0
			78855	35119	14410	25647	3679		

- Molecule 80 is a RNA chain called RNA (76-MER).

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	34	C	G	conflict	GB 1851728667
u	35	C	A	conflict	GB 1851728667
u	36	G	A	conflict	GB 1851728667
u	37	U	A	conflict	GB 1851728667

- Molecule 81 is a RNA chain called RNA (76-MER).

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	?	-	A	deletion	GB 1879656365
v	12	C	U	conflict	GB 1879656365
v	14	C	A	conflict	GB 1879656365
v	16	A	U	conflict	GB 1879656365
v	34	C	G	conflict	GB 1879656365
v	35	C	A	conflict	GB 1879656365
v	36	G	A	conflict	GB 1879656365

- Molecule 82 is a RNA chain called RNA (5'-D(P*($\emptyset$)P*($\emptyset$)P*($\emptyset$)P*($\emptyset$))-R(P*UP*UP*AP*CP*GP*GP*CP*GP*GP*UP*($\emptyset$)P*($\emptyset$)P*($\emptyset$)P*($\emptyset$)P*($\emptyset$))-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
82	w	20	Total	C	N	O	P	0	0
			423	189	72	142	20		

- Molecule 83 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Cz	217	Total	C	N	O	S	0	0
			1741	1113	312	307	9		

- Molecule 84 is a protein called ALA-ALA-LYS-ALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
84	y	4	Total	C	N	O	0	0
			24	15	5	4		

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

Mol	Chain	Residues	Atoms		AltConf
85	S2	3	Total 3	Mg 3	0
85	B	1	Total 1	Mg 1	0
85	D	6	Total 6	Mg 6	0
85	E	9	Total 9	Mg 9	0
85	Z	1	Total 1	Mg 1	0
85	t	13	Total 13	Mg 13	0

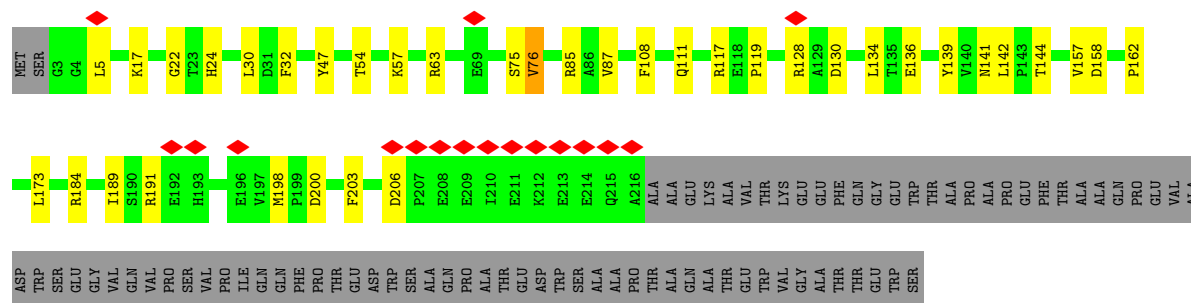
- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

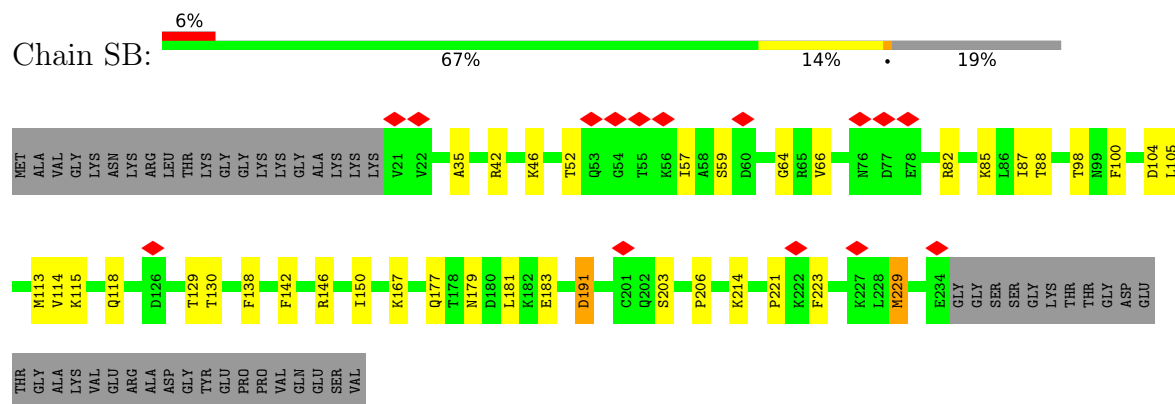
- Molecule 87 is water.

Mol	Chain	Residues	Atoms		AltConf
87	S2	5	Total 5	O 5	0
87	SS	1	Total 1	O 1	0
87	Sf	1	Total 1	O 1	0
87	u	1	Total 1	O 1	0

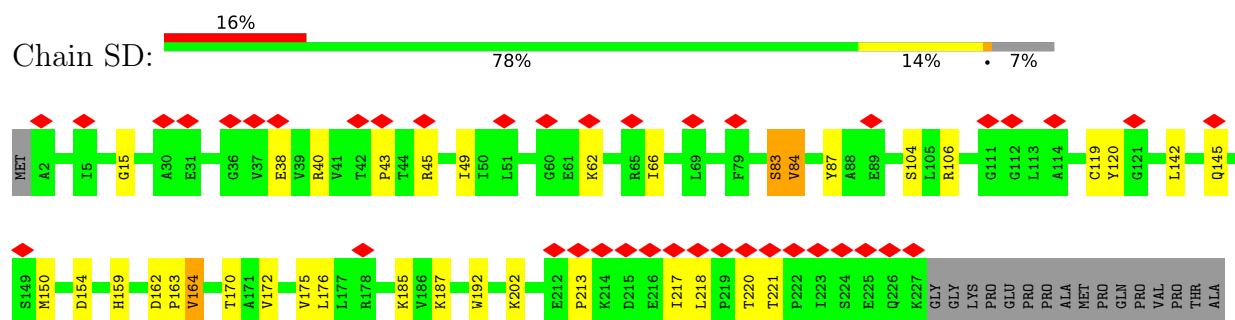




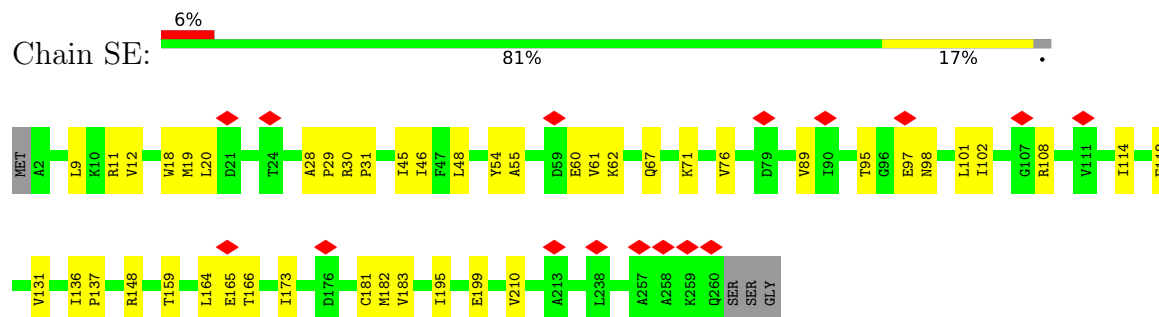
• Molecule 3: 40S ribosomal protein S3a



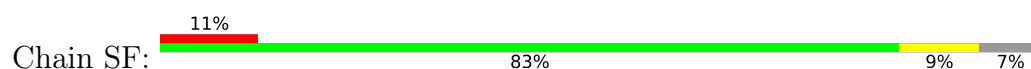
• Molecule 4: 40S ribosomal protein S3

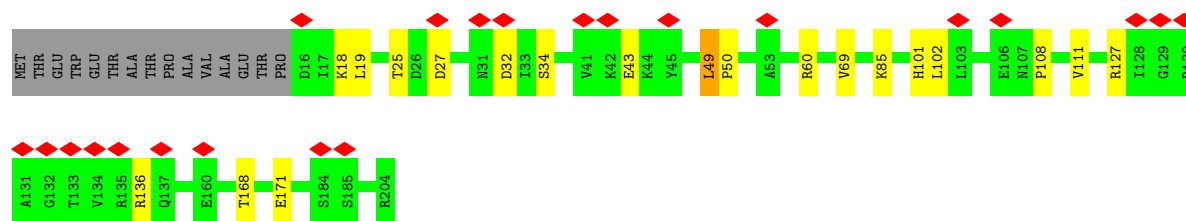


• Molecule 5: 40S ribosomal protein S4, X isoform

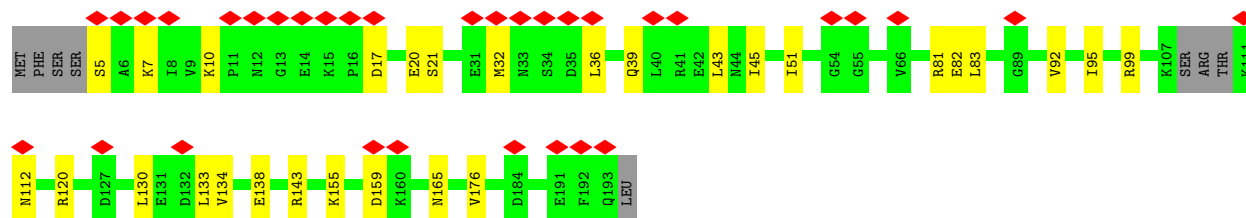
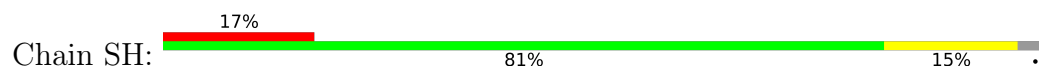


• Molecule 6: 40S ribosomal protein S5

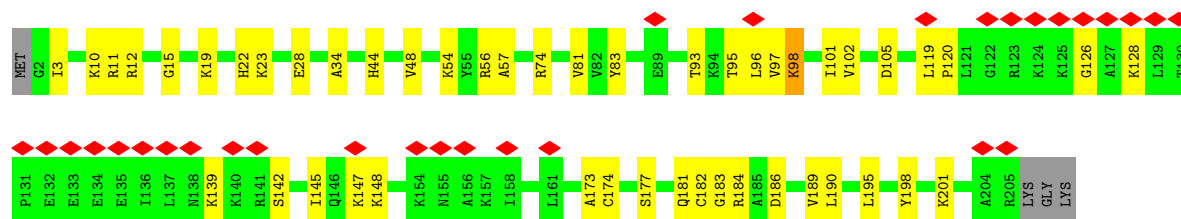
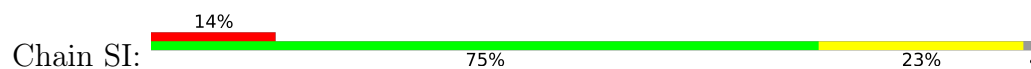




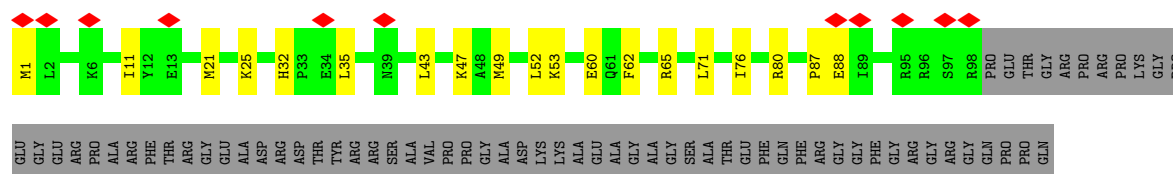
• Molecule 7: 40S ribosomal protein S7



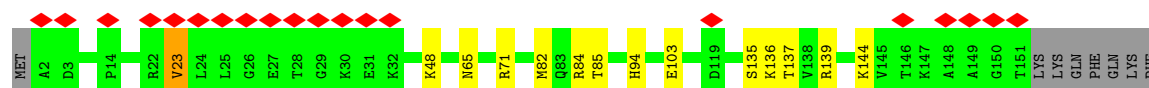
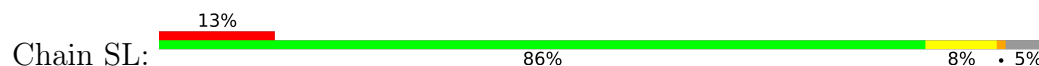
• Molecule 8: 40S ribosomal protein S8



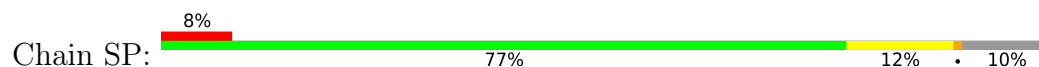
• Molecule 9: 40S ribosomal protein S10



• Molecule 10: 40S ribosomal protein S11

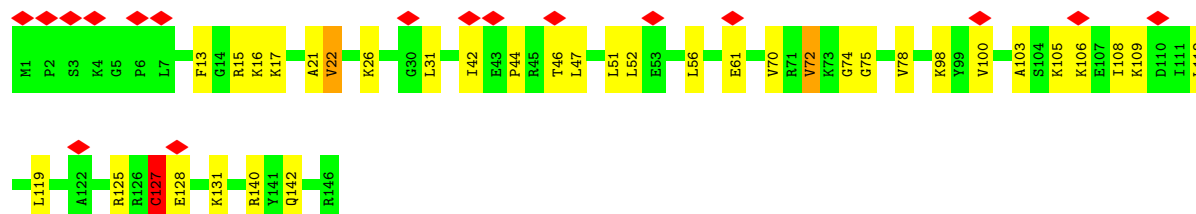
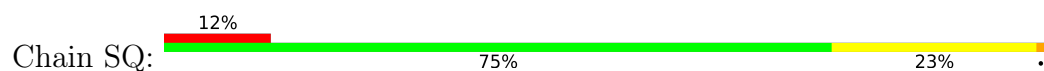


• Molecule 11: 40S ribosomal protein S15

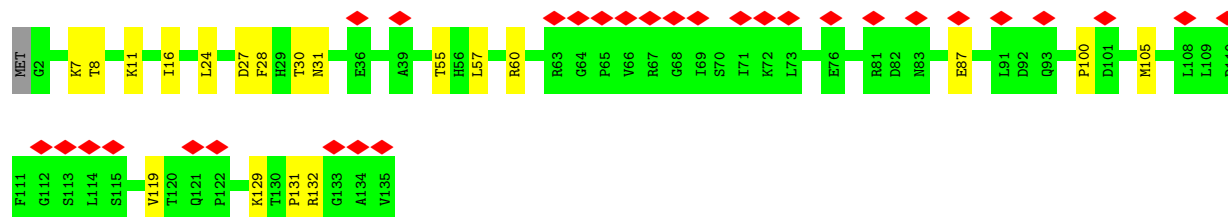
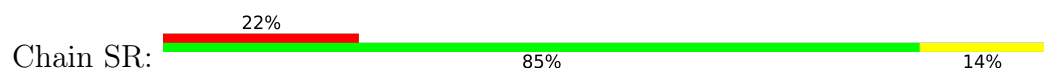




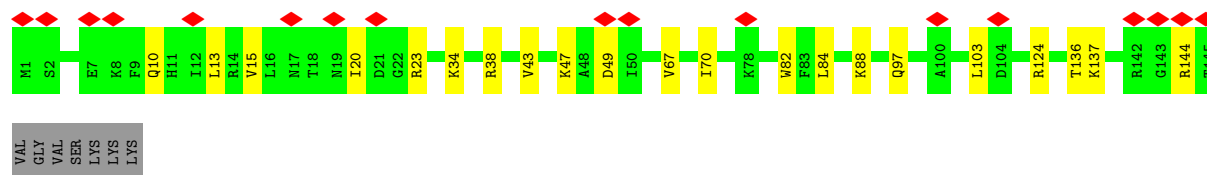
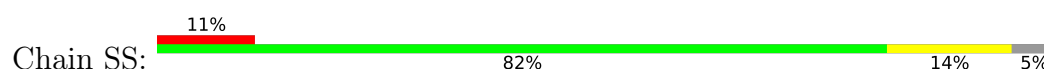
- Molecule 12: Rps16 protein



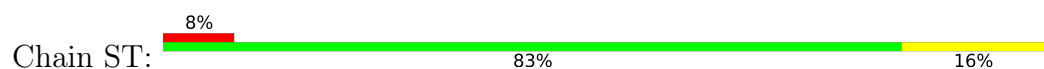
- Molecule 13: 40S ribosomal protein S17



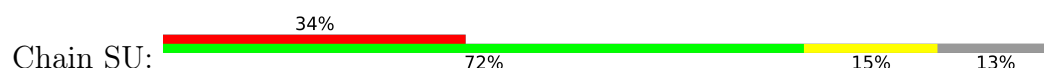
- Molecule 14: 40S ribosomal protein S18

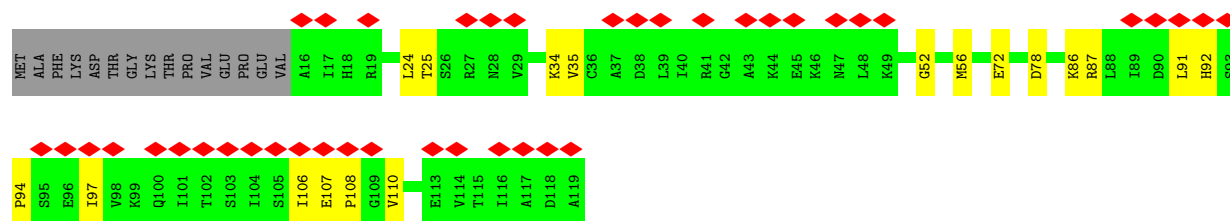


- Molecule 15: 40S ribosomal protein S19

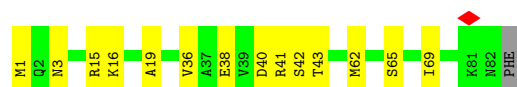
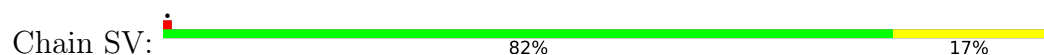


- Molecule 16: 40S ribosomal protein S20





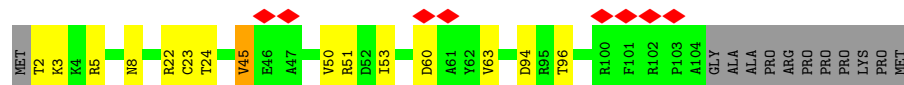
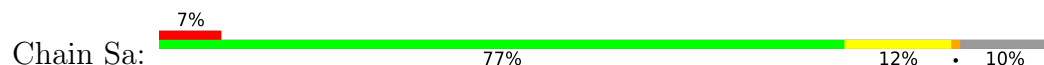
- Molecule 17: 40S ribosomal protein S21



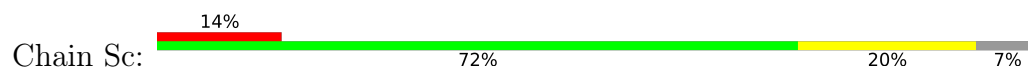
- Molecule 18: 40S ribosomal protein S23



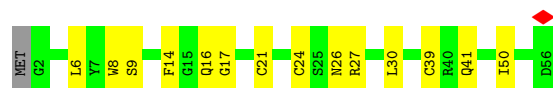
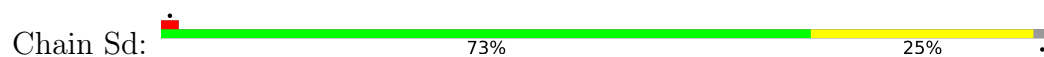
- Molecule 19: 40S ribosomal protein S26



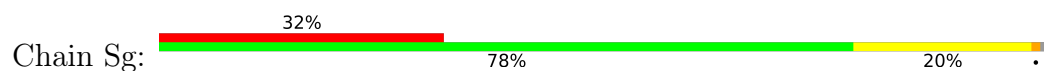
- Molecule 20: 40S ribosomal protein S28

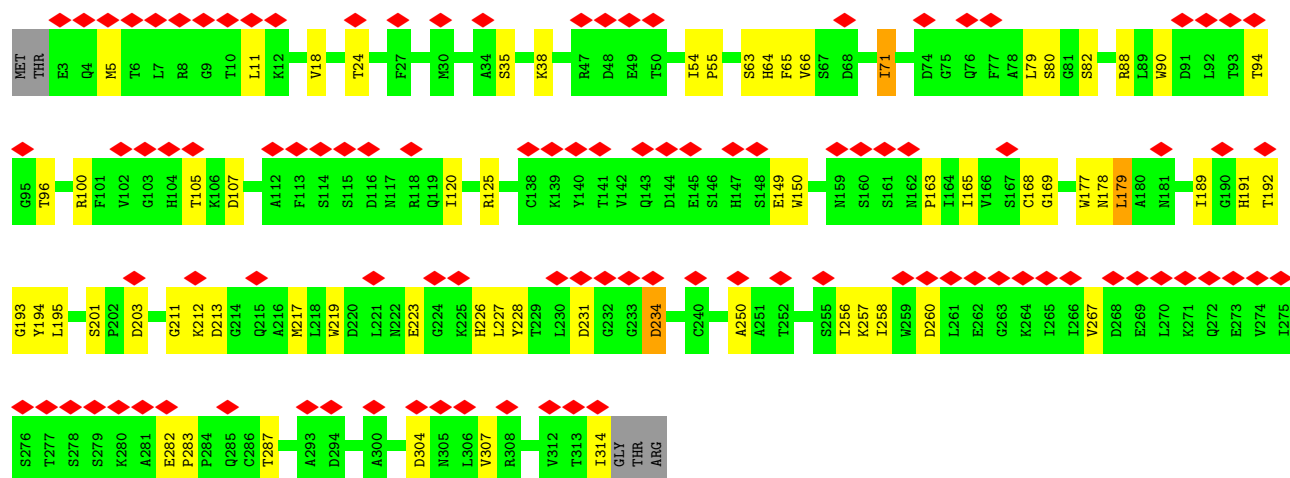


- Molecule 21: 40S ribosomal protein S29

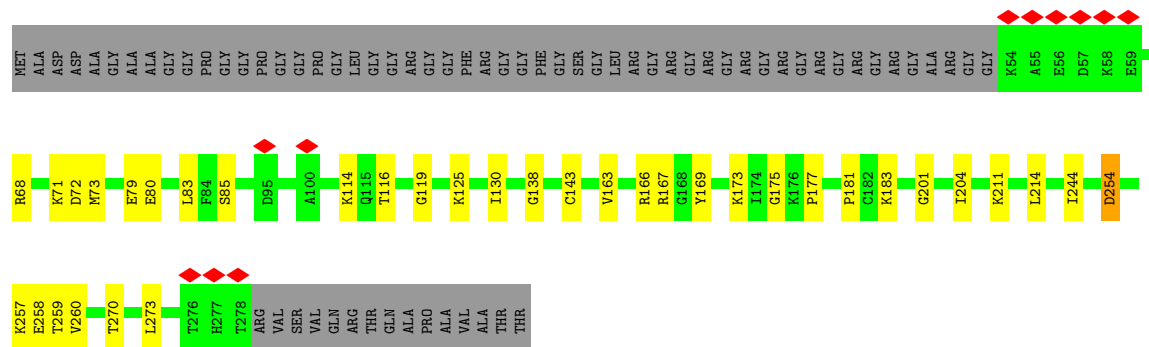


- Molecule 22: Receptor of activated protein C kinase 1

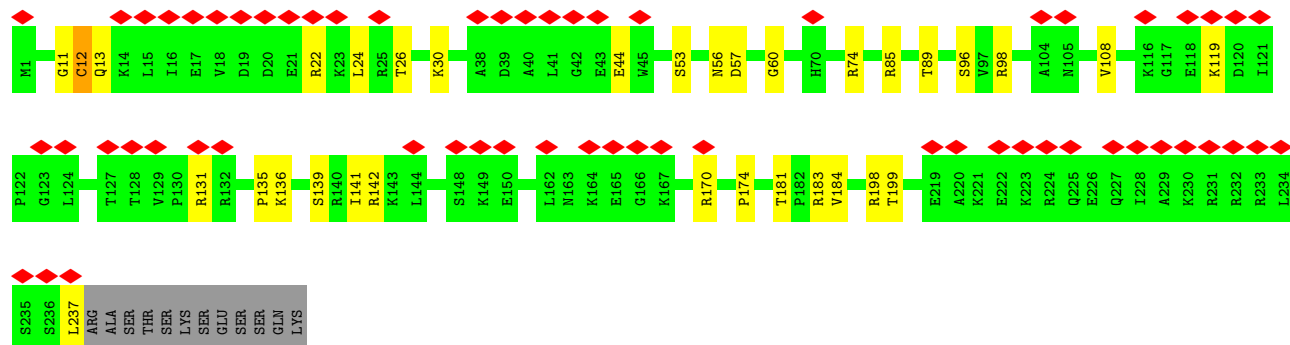
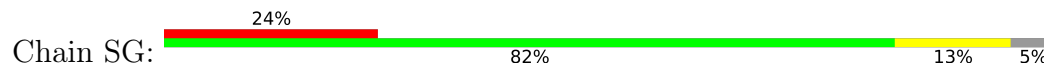




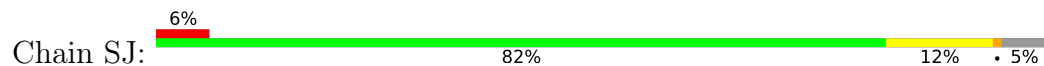
- Molecule 23: 40S ribosomal protein S2

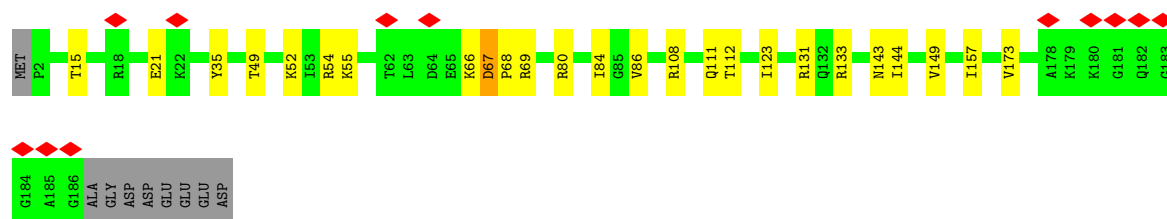


- Molecule 24: 40S ribosomal protein S6

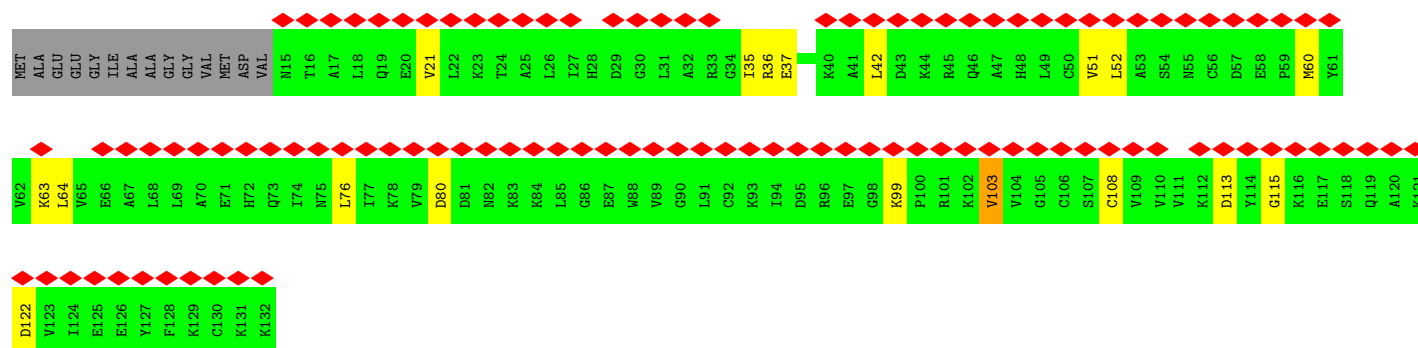
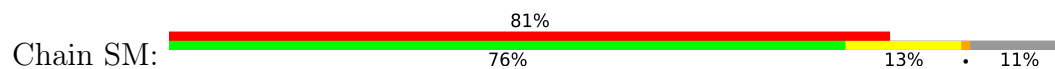


- Molecule 25: 40S ribosomal protein S9

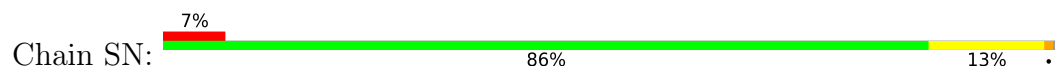




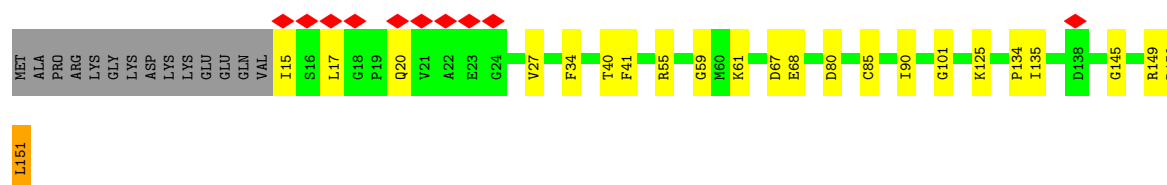
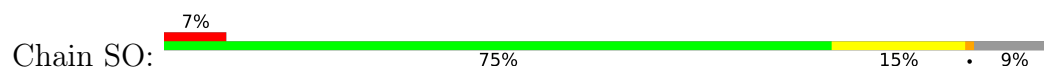
- Molecule 26: 40S ribosomal protein S12



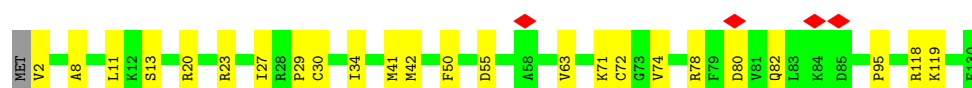
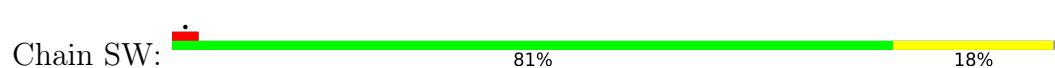
- Molecule 27: 40S ribosomal protein S13



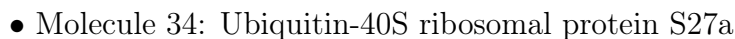
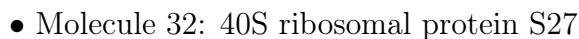
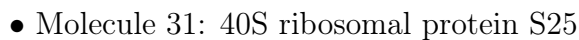
- Molecule 28: 40S ribosomal protein S14



- Molecule 29: 40S ribosomal protein S15a



- Molecule 30: 40S ribosomal protein S24





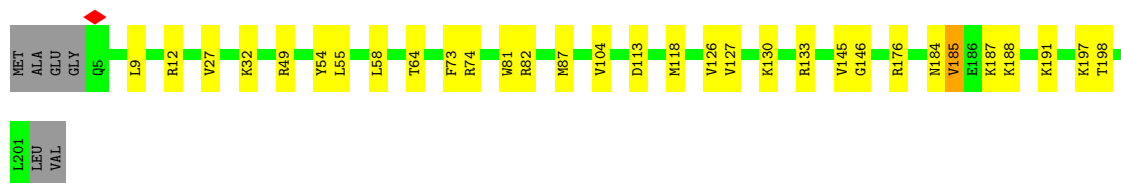
- Molecule 49: Ribosomal protein L15

Chain O:  87% 12%



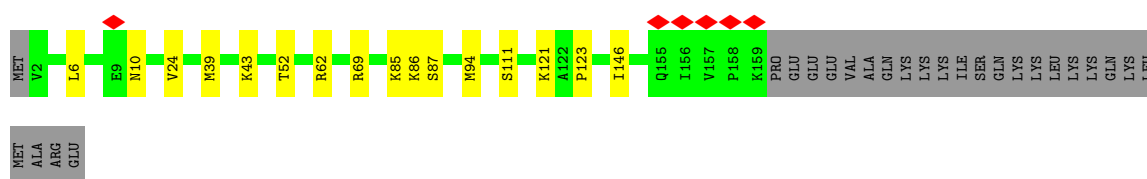
- Molecule 50: 60S ribosomal protein L13a

Chain P:  82% 15%



- Molecule 51: 60S ribosomal protein L17

Chain Q:  77% 9% 14%



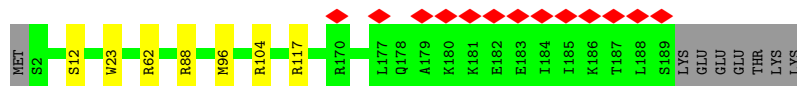
- Molecule 52: 60S ribosomal protein L18

Chain R:  87% 12%



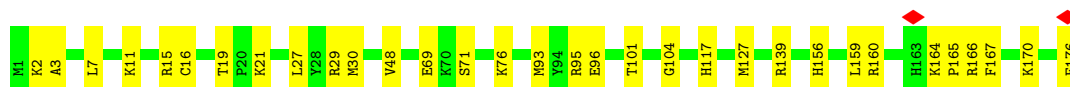
- Molecule 53: Ribosomal protein L19

Chain S:  7% 92%



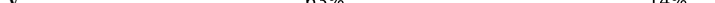
- Molecule 54: 60S ribosomal protein L18a

Chain T:  82% 18%

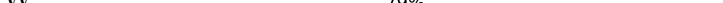


- Molecule 55: 60S ribosomal protein L21

ME1	T2	N3	T4	K7	P18	K21	R32	D41	I42	V48	T68	V80	K100	S101	R102	R108	K116	W125	V126	K129	P132	A133	P148	L151	E152	P153	P159	A174
-----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

- Chain V:  63% 14% 23%

ASP	MET
GLU	ALA
ASP	PRO
	VAL
	LYS
	LYS
	LEU
	VAL
	ALA
	LYS
	GLY
	GLY
	LYS
	LYS
	LYS
	GLN
	V18
	C25
	P28
	E45
	R46
	T62
	T63
	R64
	R65
	S66
	K67
	T73
	V76
	S79
	L86
	D98
	N99
	L100
	S106
	K107
	L112
	Q116
	T1E
	ASN
	GLN
	ASP
	GLU
	GLU
	GLU
	GLU

- Chain W:  79% 16% ..

MET	SER	LYS	ARG	GLY	ARG	G7	K13	F14	R15	C28	A29	D30	G33	N50	R51	V57	K69	I82	R83	K91	L96	E99	V104	M107	E111	M112	K113	I117	T118	G119	P120	V121	A136	V140
-----	-----	-----	-----	-----	-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------

- Chain X: 34% 5% 61%

[illegible]

- Chain Y: 67% 9% 23%

- Chain Z: 77% 15% 8%

M1	T8	S9	D10	R11	H18	S31	S32	E37	R45	P48	D52	V55	Y74	E83	R84	R87	V95	P101	K110	R126	Q127	K130	E131	G132	K133	K134	TYR	LYS	GLU	GLU	THR	ILE	GLU	LYS	MET	GLN	TIU
----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 61: 60S ribosomal protein L27

Chain a:  85% 14% .



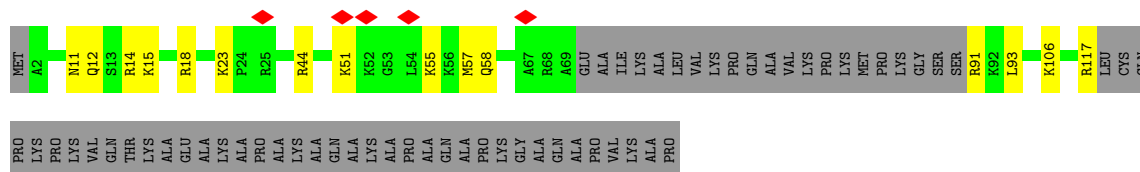
- Molecule 62: 60S ribosomal protein L27a

Chain b:  86% 13% .



- Molecule 63: 60S ribosomal protein L29

Chain c:  51% 10% 39%



- Molecule 64: 60S ribosomal protein L30

Chain d:  5% 75% 11% 12%



- Molecule 65: 60S ribosomal protein L31

Chain e:  74% 10% 15%



- Molecule 66: 60S ribosomal protein L32

Chain f:  82% 13% .

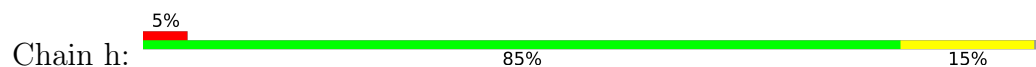


- Molecule 67: 60S ribosomal protein L35a

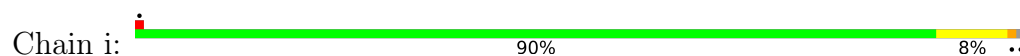
Chain g:  89% 10% .



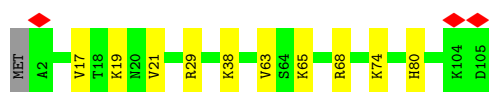
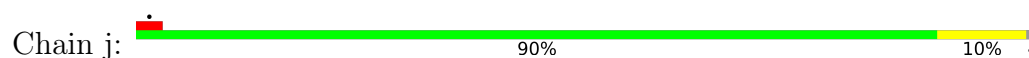
- Molecule 68: 60S ribosomal protein L34



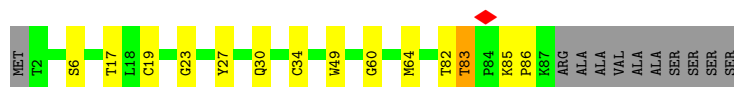
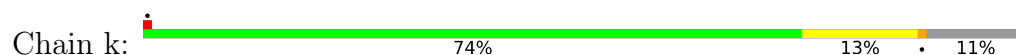
- Molecule 69: 60S ribosomal protein L35



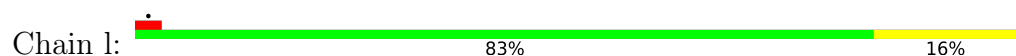
- Molecule 70: 60S ribosomal protein L36



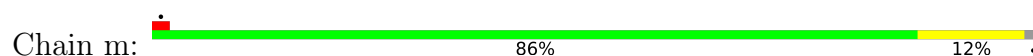
- Molecule 71: Ribosomal protein L37



- Molecule 72: 60S ribosomal protein L38

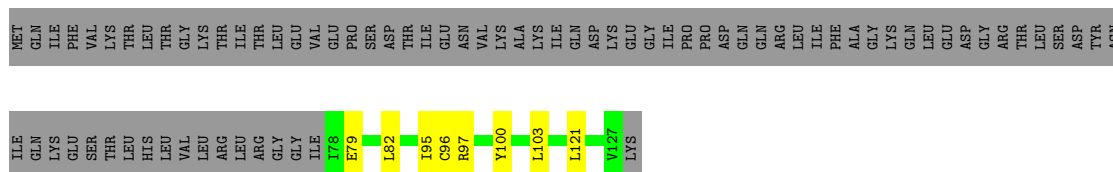


- Molecule 73: 60S ribosomal protein L39



- Molecule 74: Ubiquitin-60S ribosomal protein L40

Chain n:  33% 6% 61%



- Molecule 75: 60S ribosomal protein L41

Chain o:  80% 20%



- Molecule 76: Ribosomal protein L36a

Chain p:  86% 13% .



- Molecule 77: 60S ribosomal protein L37a

Chain q:  91% 7% ..



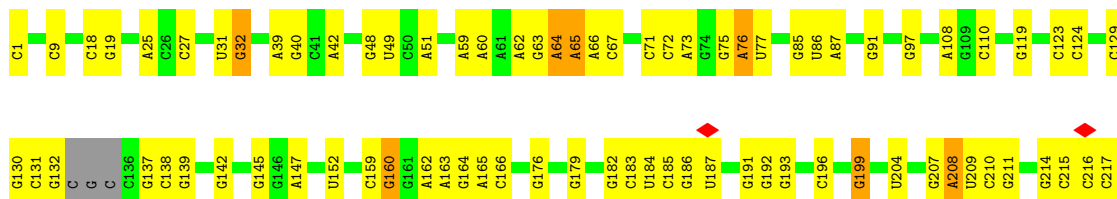
- Molecule 78: 60S ribosomal protein L28

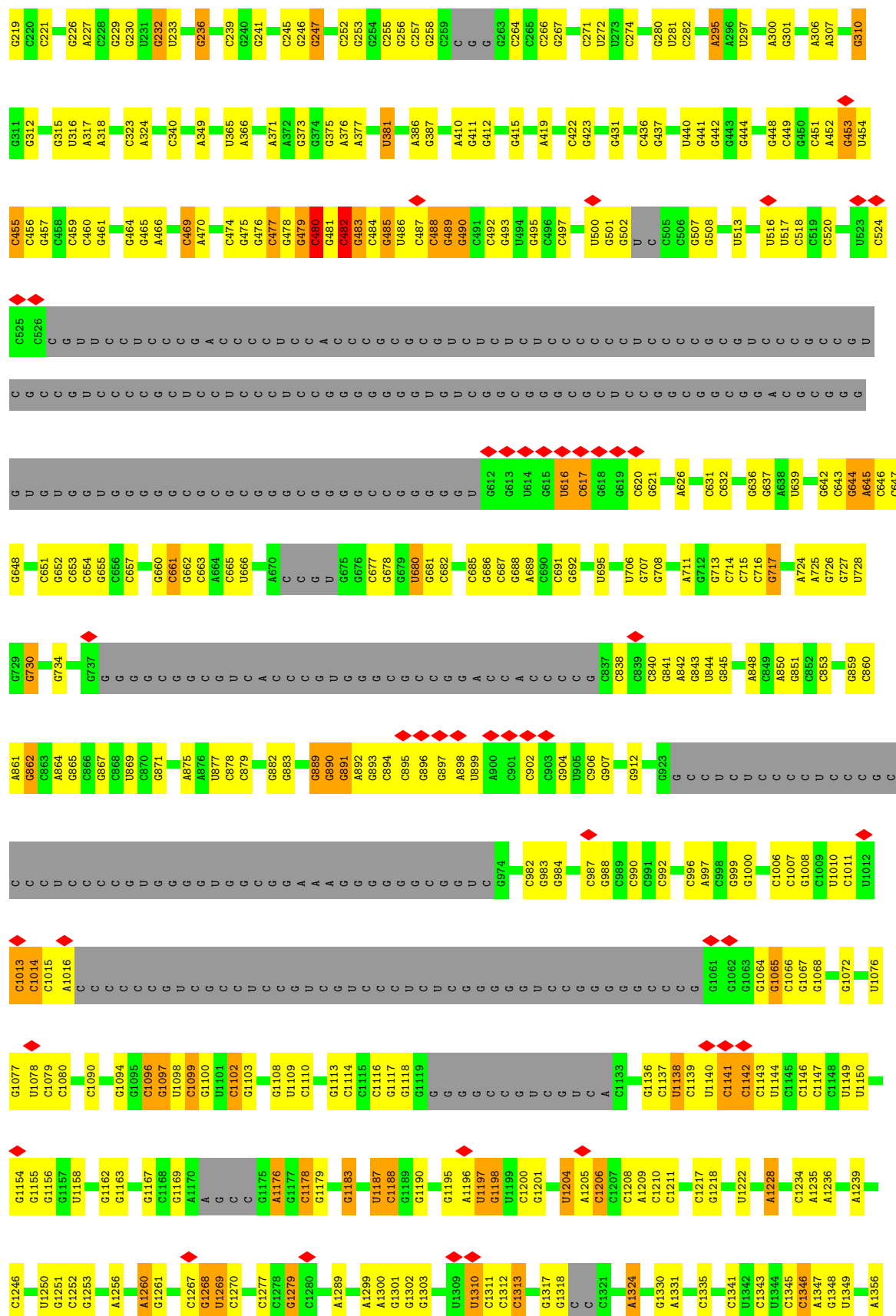
Chain r:  7% 82% 14% .



- Molecule 79: RNA (4803-MER)

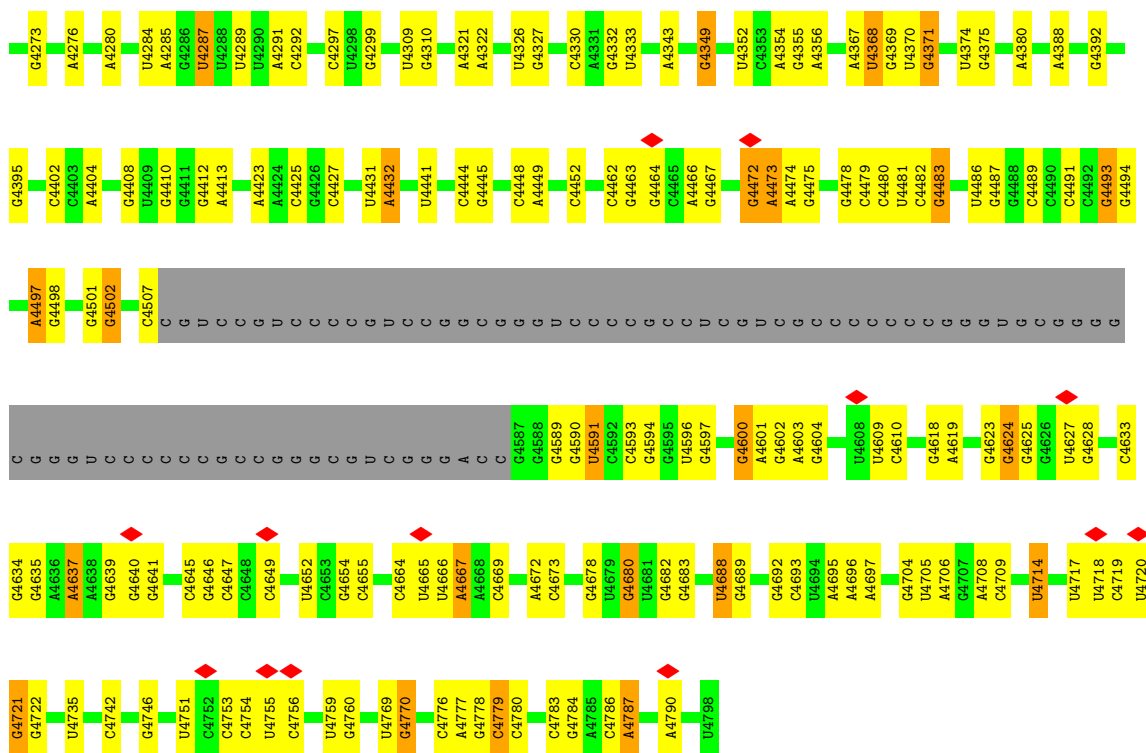
Chain t:  49% 24% 23%



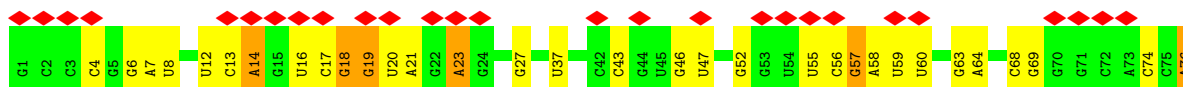




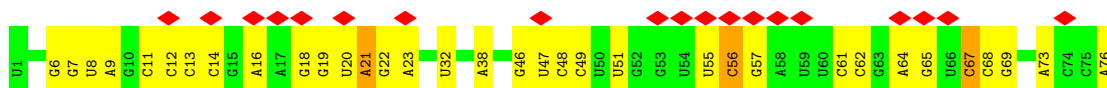




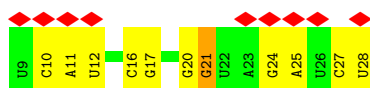
• Molecule 80: RNA (76-MER)



• Molecule 81: RNA (76-MER)

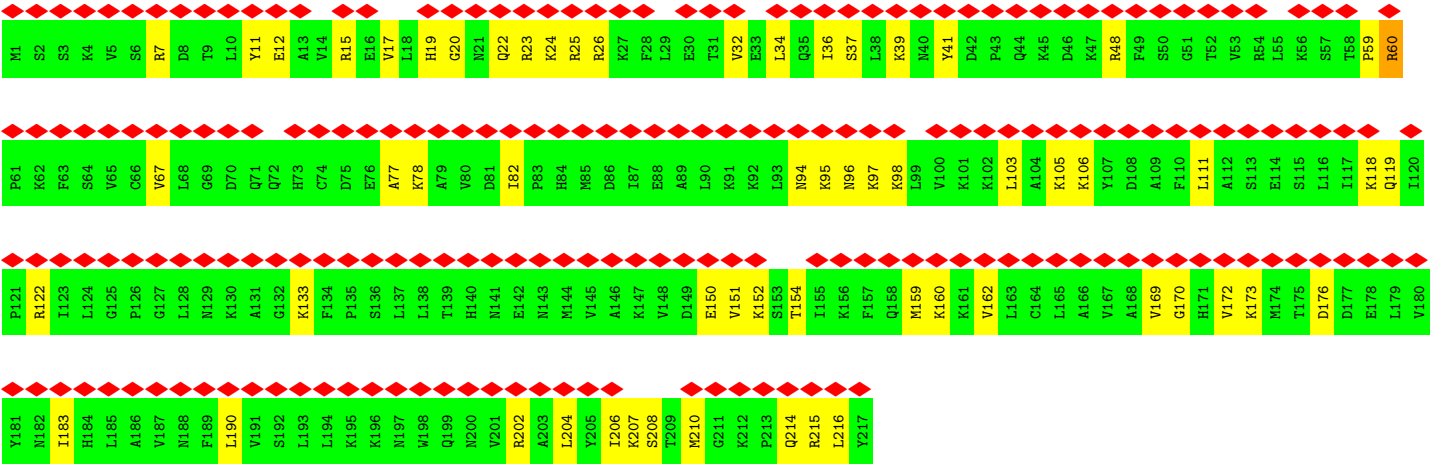


• Molecule 82: RNA (5'-D(P*()P*()P*()P*())-R(P*UP*UP*AP*CP*GP*GP*CP*GP*GP*UP*()P*()P*()P*()P*())-3')

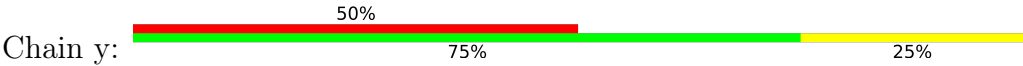


• Molecule 83: 60S ribosomal protein L10a





● Molecule 84: ALA-ALA-LYS-ALA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	62369	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.703	Depositor
Minimum map value	-0.357	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.0475	Depositor
Map size ($\text{\AA}$)	420.18, 420.18, 420.18	wwPDB
Map dimensions	298, 298, 298	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.41, 1.41, 1.41	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.16	2/39984 (0.0%)	0.30	4/62292 (0.0%)
2	SA	0.21	0/1730	0.49	0/2350
3	SB	0.28	0/1765	0.52	1/2362 (0.0%)
4	SD	0.60	5/1784 (0.3%)	0.66	3/2402 (0.1%)
5	SE	0.36	2/2101 (0.1%)	0.52	1/2828 (0.0%)
6	SF	0.27	0/1516	0.51	1/2037 (0.0%)
7	SH	0.30	0/1519	0.52	0/2033
8	SI	0.27	0/1702	0.43	0/2271
9	SK	0.17	0/851	0.45	0/1147
10	SL	0.27	0/1241	0.50	0/1662
11	SP	0.37	0/1094	0.66	2/1460 (0.1%)
12	SQ	0.41	0/1177	0.68	0/1575
13	SR	0.39	0/1093	0.73	0/1469
14	SS	0.32	0/1216	0.58	1/1628 (0.1%)
15	ST	0.16	0/1134	0.42	0/1519
16	SU	0.24	0/832	0.50	0/1117
17	SV	0.20	0/632	0.53	0/845
18	SX	0.27	0/1116	0.56	0/1490
19	Sa	0.16	0/841	0.44	0/1128
20	Sc	0.20	0/508	0.59	0/680
21	Sd	0.14	0/470	0.40	0/623
22	Sg	0.19	0/2486	0.51	0/3384
23	SC	0.19	0/1795	0.48	0/2424
24	SG	0.16	0/1946	0.45	0/2590
25	SJ	0.17	0/1561	0.49	0/2083
26	SM	0.11	0/922	0.32	0/1237
27	SN	0.11	0/1232	0.29	0/1656
28	SO	0.12	0/1037	0.36	0/1391
29	SW	0.16	0/1051	0.40	0/1406
30	SY	0.14	0/1094	0.39	0/1452
31	SZ	0.30	0/585	0.68	0/785
32	Sb	0.17	0/653	0.42	0/876

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Se	0.19	0/458	0.49	0/604
34	Sf	0.15	0/559	0.42	0/743
35	A	0.20	0/1968	0.37	0/2639
36	B	0.15	0/3272	0.40	1/4380 (0.0%)
37	C	0.31	0/2943	0.52	3/3951 (0.1%)
38	D	0.13	0/3726	0.29	0/5804
39	E	0.12	0/2839	0.28	0/4425
40	F	0.13	0/2444	0.36	0/3272
41	G	0.15	0/1998	0.40	0/2676
42	H	0.14	0/1900	0.33	0/2534
43	I	0.16	0/1968	0.42	1/2649 (0.0%)
44	J	0.28	0/1547	0.55	2/2080 (0.1%)
45	K	0.13	0/1730	0.35	0/2311
46	L	0.18	0/1385	0.48	0/1852
47	M	0.17	0/1690	0.46	1/2261 (0.0%)
48	N	0.25	0/1164	0.54	2/1556 (0.1%)
49	O	0.12	0/1746	0.33	0/2338
50	P	0.23	0/1641	0.45	0/2195
51	Q	0.12	0/1309	0.31	0/1756
52	R	0.13	0/1540	0.37	0/2054
53	S	0.17	0/1588	0.47	0/2099
54	T	0.15	0/1498	0.42	1/2010 (0.0%)
55	U	0.23	0/1321	0.46	0/1764
56	V	0.22	0/822	0.54	0/1103
57	W	0.15	0/1007	0.40	0/1350
58	X	0.17	0/524	0.43	0/698
59	Y	0.13	0/1001	0.36	0/1345
60	Z	0.16	0/1132	0.40	0/1503
61	a	0.19	0/1126	0.47	0/1502
62	b	0.11	0/1194	0.33	0/1594
63	c	0.12	0/794	0.32	0/1045
64	d	0.13	0/796	0.37	0/1068
65	e	0.14	0/894	0.37	0/1204
66	f	0.13	0/1082	0.39	0/1443
67	g	0.14	0/895	0.34	0/1198
68	h	0.13	0/930	0.35	0/1238
69	i	0.13	0/1023	0.38	0/1350
70	j	0.15	0/860	0.44	0/1137
71	k	0.13	0/720	0.36	0/952
72	l	0.17	0/575	0.45	0/761
73	m	0.13	0/454	0.36	0/599
74	n	0.16	0/417	0.41	0/553
75	o	0.19	0/241	0.41	0/305

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	p	0.20	0/877	0.51	0/1156
77	q	0.15	0/718	0.45	0/954
78	r	0.18	0/1074	0.47	0/1437
79	t	0.18	7/88201 (0.0%)	0.34	28/137564 (0.0%)
80	u	0.14	0/1800	0.33	0/2804
81	v	0.16	0/1806	0.37	0/2813
82	w	0.13	0/471	0.36	0/731
83	Cz	0.20	0/1769	0.48	0/2371
84	y	0.15	0/23	0.45	0/29
All	All	0.19	16/234128 (0.0%)	0.38	52/343962 (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
12	SQ	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	SD	163	PRO	C-N	17.61	1.55	1.34
5	SE	101	LEU	C-N	-9.69	1.20	1.33
79	t	479	G	O3'-P	-9.28	1.47	1.61
1	S2	1833	UR3	O3'-P	-7.71	1.48	1.56
79	t	1990	G	O5'-C5'	-7.11	1.32	1.42
4	SD	164	VAL	C-N	-6.62	1.25	1.33
4	SD	104	SER	C-N	6.22	1.42	1.34
4	SD	83	SER	C-N	6.09	1.41	1.33
79	t	490	G	O3'-P	5.81	1.69	1.61
79	t	2095	C	C1'-N1	5.71	1.57	1.48
79	t	480	C	P-OP2	-5.65	1.37	1.49
5	SE	102	ILE	C-N	-5.44	1.25	1.33
4	SD	84	VAL	C-N	5.33	1.40	1.33
79	t	478	G	O3'-P	-5.26	1.53	1.61
1	S2	671	A2M	O3'-P	5.06	1.61	1.56
79	t	480	C	P-OP1	-5.02	1.39	1.49

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	t	4473	A	O5'-P-OP1	-22.77	39.70	108.00
79	t	479	G	C1'-C2'-O2'	-19.39	79.32	108.40
79	t	3797	G	O5'-P-OP2	-17.37	55.89	108.00
79	t	480	C	C1'-C2'-O2'	-12.82	89.17	108.40
79	t	3797	G	O5'-P-OP1	-12.71	69.89	108.00
79	t	4473	A	O5'-P-OP2	10.75	140.25	108.00
1	S2	1834	A	C2'-C3'-O3'	-10.61	97.79	113.70
11	SP	68	PRO	CA-N-CD	-10.48	97.33	112.00
1	S2	1834	A	C1'-C2'-O2'	-8.98	94.94	108.40
79	t	477	C	C1'-C2'-O2'	-8.31	95.93	108.40
4	SD	43	PRO	CA-N-CD	-8.26	100.44	112.00
4	SD	163	PRO	O-C-N	8.10	133.09	122.24
37	C	59	GLY	N-CA-C	-6.93	96.75	113.18
79	t	490	G	C1'-C2'-O2'	-6.82	98.17	108.40
1	S2	1834	A	C5'-C4'-O4'	-6.79	99.61	109.80
79	t	1361	G	C1'-C2'-O2'	-6.70	98.35	108.40
79	t	4472	G	O3'-P-O5'	-6.41	94.39	104.00
4	SD	83	SER	O-C-N	6.38	128.42	121.85
79	t	478	G	C2'-C3'-O3'	-6.37	104.15	113.70
79	t	477	C	O4'-C4'-C3'	-6.37	97.63	104.00
79	t	482	C	C3'-C2'-O2'	6.35	120.23	110.70
79	t	4473	A	OP1-P-OP2	-6.35	100.55	119.60
54	T	159	LEU	CA-CB-CG	6.27	138.26	116.30
79	t	480	C	N1-C1'-C2'	6.12	121.17	112.00
79	t	1990	G	O5'-C5'-C4'	-6.07	102.60	111.70
79	t	1990	G	C1'-C2'-O2'	-6.05	102.73	111.80
5	SE	101	LEU	O-C-N	-6.01	116.22	123.13
79	t	478	G	C1'-C2'-O2'	-6.01	99.39	108.40
79	t	644	G	C2'-C3'-O3'	-6.00	104.71	113.70
14	SS	23	ARG	CA-CB-CG	5.93	125.95	114.10
79	t	1990	G	O4'-C1'-C2'	-5.85	99.95	105.80
79	t	479	G	C3'-C2'-O2'	5.82	119.42	110.70
79	t	1361	G	P-O5'-C5'	-5.81	112.19	120.90
48	N	101	LYS	CA-C-N	-5.81	112.50	120.28
48	N	101	LYS	C-N-CA	-5.81	112.50	120.28
43	I	217	LYS	CB-CG-CD	5.67	124.35	111.30
79	t	1346	C	C2'-C3'-O3'	5.63	117.95	109.50
79	t	1990	G	C4'-C3'-O3'	-5.59	101.02	109.40
1	S2	1834	A	C4'-C3'-O3'	5.57	121.35	113.00
6	SF	43	GLU	CB-CA-C	-5.50	109.75	117.23
79	t	3684	A	C3'-C2'-O2'	5.40	118.81	110.70
47	M	155	MET	CB-CG-SD	5.38	128.84	112.70
79	t	480	C	O4'-C4'-C3'	-5.35	98.65	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	B	360	LEU	CA-CB-CG	5.34	134.99	116.30
44	J	29	GLY	CA-C-N	5.32	124.83	119.19
44	J	29	GLY	C-N-CA	5.32	124.83	119.19
3	SB	229	MET	CB-CG-SD	5.32	128.65	112.70
79	t	644	G	C4'-C3'-O3'	5.21	120.81	113.00
79	t	486	U	C4'-C3'-O3'	5.15	120.72	113.00
11	SP	70	MET	CA-CB-CG	5.08	124.26	114.10
37	C	52	TYR	CA-C-N	-5.05	111.89	121.54
37	C	52	TYR	C-N-CA	-5.05	111.89	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	SQ	75	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S2	36502	0	18416	301	0
2	SA	1693	0	1694	26	0
3	SB	1738	0	1809	23	0
4	SD	1756	0	1851	20	0
5	SE	2059	0	2164	26	0
6	SF	1495	0	1549	13	0
7	SH	1497	0	1590	16	0
8	SI	1673	0	1756	35	0
9	SK	827	0	854	12	0
10	SL	1220	0	1289	11	0
11	SP	1073	0	1128	11	0
12	SQ	1158	0	1232	23	0
13	SR	1079	0	1128	12	0
14	SS	1198	0	1261	15	0
15	ST	1115	0	1150	16	0
16	SU	822	0	887	12	0
17	SV	626	0	624	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	SX	1098	0	1167	12	0
19	Sa	826	0	875	9	0
20	Sc	506	0	536	8	0
21	Sd	459	0	449	9	0
22	Sg	2429	0	2386	34	0
23	SC	1755	0	1847	22	0
24	SG	1923	0	2089	25	0
25	SJ	1533	0	1653	15	0
26	SM	912	0	940	19	0
27	SN	1208	0	1294	14	0
28	SO	1024	0	1050	16	0
29	SW	1034	0	1080	16	0
30	SY	1073	0	1155	17	0
31	SZ	579	0	639	13	0
32	Sb	640	0	665	6	0
33	Se	452	0	498	5	0
34	Sf	547	0	549	15	0
35	A	1930	0	2030	23	0
36	B	3204	0	3349	41	0
37	C	2889	0	3064	33	0
38	D	3337	0	1692	25	0
39	E	2541	0	1285	10	0
40	F	2399	0	2425	23	0
41	G	1960	0	2112	23	0
42	H	1865	0	1991	14	0
43	I	1935	0	2081	13	0
44	J	1528	0	1607	14	0
45	K	1692	0	1744	19	0
46	L	1362	0	1399	7	0
47	M	1659	0	1758	22	0
48	N	1142	0	1219	11	0
49	O	1701	0	1749	16	0
50	P	1611	0	1765	21	0
51	Q	1282	0	1322	9	0
52	R	1516	0	1641	20	0
53	S	1572	0	1734	5	0
54	T	1458	0	1500	22	0
55	U	1293	0	1363	17	0
56	V	808	0	831	9	0
57	W	993	0	1050	13	0
58	X	511	0	521	6	0
59	Y	984	0	1066	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	Z	1116	0	1211	13	0
61	a	1103	0	1179	13	0
62	b	1165	0	1212	16	0
63	c	781	0	846	12	0
64	d	785	0	825	9	0
65	e	879	0	924	7	0
66	f	1064	0	1160	13	0
67	g	876	0	912	5	0
68	h	920	0	1020	12	0
69	i	1015	0	1156	10	0
70	j	849	0	934	6	0
71	k	705	0	737	7	0
72	l	569	0	637	6	0
73	m	444	0	483	5	0
74	n	411	0	443	7	0
75	o	240	0	289	2	0
76	p	863	0	929	10	0
77	q	708	0	750	4	0
78	r	1059	0	1138	12	0
79	t	78855	0	39846	599	0
80	u	1613	0	821	13	0
81	v	1618	0	822	8	0
82	w	423	0	215	3	0
83	Cz	1741	0	1854	42	0
84	y	24	0	27	1	0
85	B	1	0	0	0	0
85	D	6	0	0	0	0
85	E	9	0	0	0	0
85	S2	3	0	0	0	0
85	Z	1	0	0	0	0
85	t	13	0	0	0	0
86	S2	1	0	0	0	0
86	Sa	1	0	0	0	0
86	Sf	1	0	0	0	0
86	k	1	0	0	0	0
86	p	1	0	0	0	0
86	q	1	0	0	0	0
87	S2	5	0	0	1	0
87	SS	1	0	0	0	0
87	Sf	1	0	0	0	0
87	u	1	0	0	0	0
All	All	218574	0	161922	1743	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 (1743) 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:S2:1835:6MZ:C3'	1:S2:1835:6MZ:O3'	1.71	1.37
79:t:1708:G:H1	79:t:1734:C:N4	1.26	1.32
26:SM:52:LEU:CD2	26:SM:108:CYS:HB2	1.75	1.16
79:t:1708:G:N1	79:t:1734:C:N4	1.88	1.12
79:t:1708:G:C6	79:t:1734:C:N4	2.22	1.07
26:SM:52:LEU:HD21	26:SM:108:CYS:HB2	1.36	1.05
79:t:1303:G:H22	79:t:1318:G:N2	1.60	1.00
79:t:1303:G:N2	79:t:1318:G:H22	1.60	0.98
79:t:479:G:N2	79:t:652:G:H22	1.65	0.94
79:t:479:G:H22	79:t:652:G:H22	1.04	0.94
26:SM:52:LEU:HD21	26:SM:108:CYS:CB	1.97	0.94
26:SM:52:LEU:CD2	26:SM:108:CYS:CB	2.46	0.93
79:t:477:C:H42	79:t:654:C:H42	1.11	0.92
79:t:1303:G:H22	79:t:1318:G:H22	0.92	0.92
79:t:1708:G:O6	79:t:1734:C:N4	2.00	0.92
79:t:479:G:H22	79:t:652:G:N2	1.67	0.91
79:t:493:G:H1	79:t:639:U:H3	1.19	0.90
26:SM:52:LEU:HD23	26:SM:108:CYS:HA	1.56	0.87
79:t:1359:G:H2'	79:t:1361:G:H5''	1.55	0.87
79:t:489:G:H1	79:t:645:A:H2	1.26	0.83
79:t:1303:G:H1	79:t:1318:G:H1	1.26	0.82
79:t:466:A:H61	79:t:665:C:H42	1.29	0.80
79:t:165:A:H61	79:t:271:C:H42	1.27	0.79
79:t:1706:A:C5	79:t:1736:U:O2'	2.37	0.78
79:t:479:G:H1	79:t:652:G:H1	1.32	0.78
1:S2:1835:6MZ:O3'	1:S2:1835:6MZ:H3'	1.78	0.78
1:S2:1835:6MZ:H3'	1:S2:1836:C:OP2	1.86	0.75
3:SB:129:THR:HA	3:SB:177:GLN:HA	1.68	0.75
1:S2:1327:G:H1	1:S2:1507:U:H3	1.36	0.73
79:t:730:G:H1	79:t:844:U:H3	1.37	0.73
79:t:1706:A:N7	79:t:1736:U:O2'	2.21	0.73
79:t:1732:G:H2'	79:t:1733:G:H8	1.54	0.72
1:S2:1746:G:H21	1:S2:1794:A:H62	1.37	0.72
79:t:1149:U:H3	79:t:1162:G:H22	1.38	0.72
79:t:636:G:H2'	79:t:637:G:H8	1.55	0.71
31:SZ:69:THR:HG22	31:SZ:72:VAL:HG12	1.72	0.71
79:t:1876:U:H4'	79:t:1877:G:H3'	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:2013:G:H5''	79:t:2095:C:H5	1.55	0.71
37:C:53:ALA:O	37:C:54:VAL:C	2.33	0.70
55:U:116:LYS:HG2	79:t:1735:G:O6	1.91	0.70
79:t:1732:G:H2'	79:t:1733:G:C8	2.26	0.70
12:SQ:105:LYS:HE3	12:SQ:109:LYS:HE3	1.74	0.70
26:SM:52:LEU:HD21	26:SM:108:CYS:SG	2.31	0.70
79:t:455:C:H42	79:t:680:U:H3	1.39	0.70
79:t:465:G:H22	79:t:666:U:H3	1.39	0.68
1:S2:1094:C:HO2'	29:SW:2:VAL:N	1.92	0.68
22:Sg:195:LEU:HA	22:Sg:211:GLY:HA3	1.74	0.68
79:t:457:G:H22	79:t:678:G:H1	1.42	0.68
79:t:1706:A:C2	79:t:1734:C:C5	2.82	0.67
79:t:4751:U:H3	79:t:4754:C:N4	1.90	0.67
47:M:21:ARG:HB3	49:O:197:THR:HG22	1.75	0.67
47:M:37:LYS:HE3	79:t:1268:G:H22	1.58	0.67
1:S2:1225:G:H4'	1:S2:1679:U:H3	1.60	0.67
37:C:54:VAL:HG21	37:C:107:THR:HG23	1.75	0.67
1:S2:1306:C:O2	34:Sf:92:LYS:NZ	2.28	0.66
5:SE:11:ARG:HE	5:SE:20:LEU:HD23	1.60	0.66
31:SZ:46:ASN:HD22	31:SZ:80:ARG:HA	1.60	0.66
79:t:1706:A:C2	79:t:1734:C:C4	2.83	0.66
48:N:104:MET:HG2	50:P:197:LYS:CE	2.26	0.66
79:t:1990:G:H4'	79:t:1991:U:H5''	1.77	0.66
79:t:123:C:H42	79:t:147:A:H61	1.43	0.66
1:S2:110:U:H3	1:S2:354:G:H1	1.42	0.66
53:S:96:MET:HE1	79:t:2451:C:H5''	1.78	0.65
1:S2:1660:G:H1	1:S2:1670:U:H3	1.45	0.65
26:SM:52:LEU:HD22	26:SM:108:CYS:HB2	1.76	0.65
79:t:1997:C:H2'	79:t:1998:G:H4'	1.79	0.65
26:SM:52:LEU:HD23	26:SM:108:CYS:CA	2.25	0.65
79:t:2296:G:H21	79:t:2351:A:H62	1.43	0.65
35:A:117:GLU:HG2	35:A:124:GLY:H	1.61	0.65
79:t:1011:C:N3	79:t:1094:G:N2	2.45	0.65
83:Cz:98:LYS:HG3	83:Cz:103:LEU:HB3	1.78	0.65
79:t:4478:G:H22	79:t:4683:G:H1	1.45	0.64
1:S2:380:G:H5''	8:SI:98:LYS:HB3	1.79	0.64
30:SY:20:ARG:HB2	30:SY:74:MET:HE1	1.80	0.64
55:U:129:LYS:HG2	79:t:1739:A:H5'	1.79	0.64
79:t:192:G:H1	79:t:247:G:H22	1.46	0.64
81:v:64:A:N1	81:v:65:G:O6	2.31	0.64
50:P:81:TRP:HB2	50:P:104:VAL:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:u:12:U:H3	80:u:23:A:H61	1.46	0.64
5:SE:136:ILE:HD11	5:SE:148:ARG:HB3	1.79	0.63
68:h:26:PRO:O	79:t:2482:G:N2	2.32	0.63
38:D:128:C:H4'	79:t:2386:G:H4'	1.81	0.63
11:SP:100:LYS:HG3	11:SP:101:THR:HG23	1.80	0.63
79:t:1987:G:N2	79:t:2114:G:H22	1.96	0.63
79:t:3869:C:N4	79:t:3880:G:N7	2.46	0.63
79:t:4481:U:H3	79:t:4680:G:H1	1.47	0.63
79:t:193:G:H22	79:t:246:G:H1	1.45	0.63
79:t:861:A:H2'	79:t:862:G:H8	1.64	0.63
78:r:58:LYS:HG2	78:r:83:ASN:HD21	1.64	0.63
62:b:132:ARG:NH1	79:t:1372:C:OP1	2.33	0.62
79:t:695:U:H3	79:t:883:G:H1	1.46	0.62
79:t:1330:G:H2'	79:t:1361:G:N2	2.13	0.62
1:S2:1835:6MZ:C3'	1:S2:1836:C:P	2.86	0.62
22:Sg:227:LEU:HD12	22:Sg:228:TYR:HB2	1.82	0.62
79:t:1239:A:H62	79:t:2190:C:H5	1.47	0.62
48:N:104:MET:HG2	50:P:197:LYS:HE3	1.82	0.62
38:D:102:G:OP1	38:D:109:C:N4	2.33	0.62
1:S2:1412:A:OP1	12:SQ:26:LYS:NZ	2.32	0.62
79:t:4498:G:H22	79:t:4594:G:H1	1.44	0.62
36:B:250:LYS:NZ	79:t:3632:G:OP1	2.30	0.62
79:t:3448:U:H2'	79:t:3449:G:H8	1.65	0.61
4:SD:220:THR:OG1	4:SD:221:THR:N	2.32	0.61
35:A:198:ARG:NH2	79:t:3422:A:OP2	2.34	0.61
52:R:72:LEU:HD13	79:t:1361:G:O5'	2.00	0.61
62:b:26:ARG:NH2	79:t:1560:U:OP2	2.34	0.61
1:S2:1404:A:H4'	16:SU:52:GLY:HA3	1.81	0.61
19:Sa:51:ARG:HH21	20:Sc:40:ARG:HG2	1.66	0.61
42:H:117:VAL:HG13	42:H:148:VAL:HG12	1.82	0.61
79:t:245:C:H2'	79:t:246:G:H8	1.65	0.61
79:t:4751:U:N3	79:t:4754:C:N4	2.49	0.61
1:S2:698:C:H3'	1:S2:739:C:H42	1.66	0.61
79:t:1335:C:H42	79:t:1356:A:H61	1.49	0.61
79:t:3603:G:H22	79:t:3635:G:H1'	1.66	0.61
1:S2:26:U:H2'	1:S2:27:A2M:H8	1.83	0.60
50:P:113:ASP:N	50:P:113:ASP:OD1	2.34	0.60
44:J:94:SER:HB3	44:J:142:ASP:HB3	1.83	0.60
79:t:3695:A:N6	79:t:3700:A:N7	2.49	0.60
79:t:1331:A:OP2	79:t:1361:G:N2	2.34	0.60
79:t:1495:U:N3	79:t:4287:U:OP1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:3427:A:H62	79:t:3558:G:H21	1.50	0.60
1:S2:989:G:OP2	1:S2:991:C:N4	2.35	0.60
5:SE:29:PRO:HG2	5:SE:46:ILE:HD11	1.83	0.60
79:t:477:C:N4	79:t:654:C:H42	1.93	0.60
25:SJ:49:THR:HA	25:SJ:52:LYS:HE3	1.84	0.60
62:b:59:ARG:HH12	76:p:36:GLN:HE21	1.49	0.60
79:t:1208:C:H2'	79:t:1209:A:H8	1.67	0.59
1:S2:847:U:H2'	1:S2:848:G:H8	1.67	0.59
31:SZ:69:THR:HG23	31:SZ:71:ALA:H	1.67	0.59
47:M:49:ARG:NH1	69:i:117:ARG:O	2.35	0.59
50:P:87:MET:SD	79:t:1814:G:N2	2.75	0.59
1:S2:499:C:H5''	5:SE:29:PRO:HA	1.84	0.59
1:S2:1661:G:OP2	1:S2:1663:C:N4	2.36	0.59
79:t:1887:G:H1	79:t:1908:G:H1	1.49	0.59
79:t:2441:G:H1	79:t:2592:C:H5	1.49	0.59
79:t:4479:C:H2'	79:t:4480:C:O4'	2.03	0.59
2:SA:76:VAL:HG13	2:SA:87:VAL:HB	1.84	0.59
79:t:482:C:H2'	79:t:485:G:N2	2.17	0.59
1:S2:1242:U:H4'	11:SP:124:LYS:HD3	1.85	0.59
1:S2:1502:U:H4'	4:SD:176:LEU:HD21	1.85	0.59
1:S2:382:C:OP1	8:SI:56:ARG:NH2	2.36	0.59
2:SA:54:THR:HG22	2:SA:162:PRO:HG2	1.83	0.59
43:I:108:GLN:NE2	79:t:145:G:OP1	2.36	0.59
1:S2:1099:G:H1	1:S2:1139:U:H3	1.51	0.58
54:T:101:THR:HG22	54:T:104:GLY:H	1.68	0.58
79:t:199:G:N2	79:t:209:U:OP1	2.34	0.58
1:S2:28:U:H2'	1:S2:29:G:H8	1.68	0.58
45:K:102:MET:HE3	45:K:112:GLN:HG3	1.85	0.58
79:t:3435:C:O2'	79:t:3509:A:N3	2.34	0.58
5:SE:62:LYS:O	5:SE:62:LYS:NZ	2.30	0.58
16:SU:25:THR:OG1	16:SU:86:LYS:NZ	2.36	0.58
1:S2:1286:C:H41	26:SM:103:VAL:HA	1.68	0.58
7:SH:133:LEU:HD12	7:SH:134:VAL:HG13	1.85	0.58
47:M:47:ALA:HB3	47:M:49:ARG:HG3	1.85	0.58
79:t:2239:A:N6	79:t:2664:C:O2	2.36	0.58
1:S2:15:U:O2'	1:S2:672:A:N6	2.36	0.58
38:D:87:G:OP1	69:i:7:ARG:NH2	2.37	0.58
1:S2:16:G:H21	1:S2:1198:A:H62	1.52	0.58
36:B:246:ARG:NH1	79:t:4257:C:OP1	2.37	0.58
40:F:62:CYS:HB3	40:F:105:LEU:HD22	1.85	0.58
44:J:71:ARG:HG2	79:t:4423:A:H4'	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:833:A:OP2	1:S2:849:G:N2	2.37	0.58
9:SK:53:LYS:NZ	9:SK:60:GLU:OE1	2.37	0.58
35:A:8:GLN:NE2	79:t:3403:C:OP1	2.37	0.58
36:B:253:CYS:SG	79:t:4252:G:N2	2.77	0.58
61:a:124:THR:O	61:a:126:LYS:NZ	2.36	0.58
10:SL:136:LYS:HG3	10:SL:137:THR:HG23	1.85	0.58
37:C:293:LEU:HD13	79:t:1988:C:O2'	2.03	0.58
39:E:77:A:H62	39:E:99:G:H21	1.51	0.58
41:G:167:HIS:HB3	41:G:170:LYS:HD2	1.86	0.58
43:I:58:PRO:HD2	43:I:61:ILE:HD12	1.85	0.58
79:t:460:C:H2'	79:t:461:G:H8	1.69	0.58
79:t:1234:C:H2'	79:t:1235:A:H8	1.68	0.58
18:SX:68:LYS:HB3	18:SX:91:LEU:HD13	1.86	0.57
37:C:121:ARG:NH1	79:t:1277:C:OP1	2.38	0.57
1:S2:821:A:OP1	25:SJ:80:ARG:NH2	2.37	0.57
1:S2:1593:C:O2'	6:SF:85:LYS:NZ	2.38	0.57
14:SS:10:GLN:HE21	14:SS:13:LEU:HD11	1.69	0.57
27:SN:37:ILE:HG23	27:SN:50:ILE:HG21	1.86	0.57
55:U:116:LYS:CG	79:t:1735:G:O6	2.52	0.57
79:t:196:C:O2	79:t:221:C:O2'	2.22	0.57
5:SE:164:LEU:O	5:SE:166:THR:N	2.36	0.57
22:Sg:250:ALA:HB3	22:Sg:257:LYS:HB2	1.87	0.57
29:SW:55:ASP:OD1	29:SW:55:ASP:N	2.37	0.57
4:SD:38:GLU:HB3	4:SD:49:ILE:HB	1.85	0.57
3:SB:150:ILE:HG23	13:SR:131:PRO:HA	1.86	0.57
31:SZ:60:LYS:O	31:SZ:64:ASN:ND2	2.37	0.57
38:D:133:G:OP1	59:Y:67:ARG:NH1	2.38	0.57
79:t:1921:U:H2'	79:t:1922:G:H8	1.69	0.57
8:SI:190:LEU:HD23	8:SI:195:LEU:HA	1.86	0.57
22:Sg:165:ILE:HG13	22:Sg:177:TRP:HB2	1.87	0.57
79:t:162:A:H61	79:t:274:C:H42	1.52	0.57
15:ST:22:LEU:HD13	15:ST:28:LEU:HD11	1.87	0.56
1:S2:1033:A:H2'	1:S2:1034:A2M:H8	1.86	0.56
22:Sg:234:ASP:OD1	22:Sg:234:ASP:N	2.36	0.56
49:O:68:ARG:NH1	49:O:124:ASP:O	2.39	0.56
72:l:17:ARG:NH1	79:t:2616:C:O2'	2.39	0.56
79:t:196:C:H41	79:t:241:G:H1	1.52	0.56
79:t:642:G:N2	79:t:643:C:O2'	2.39	0.56
41:G:232:LEU:HD12	41:G:248:GLU:HG2	1.88	0.56
52:R:144:LYS:HG3	79:t:1364:C:H5''	1.88	0.56
61:a:11:VAL:HG12	61:a:82:PRO:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:1096:C:H3'	79:t:1097:G:C8	2.41	0.56
79:t:4502:G:H22	79:t:4590:G:H22	1.53	0.56
81:v:64:A:C6	81:v:65:G:O6	2.59	0.56
4:SD:40:ARG:HD2	16:SU:108:PRO:HG3	1.88	0.56
50:P:126:VAL:HG13	50:P:127:VAL:HG13	1.87	0.56
78:r:107:ARG:NH2	79:t:2107:A:OP1	2.36	0.56
79:t:1987:G:H22	79:t:2114:G:H1	1.51	0.56
1:S2:446:U:H3	1:S2:450:A:H62	1.54	0.56
47:M:50:PRO:HB3	47:M:149:GLN:HB3	1.88	0.56
79:t:4367:A:H2	79:t:4395:G:H21	1.52	0.56
1:S2:576:U:N3	1:S2:579:A:OP2	2.39	0.56
29:SW:30:CYS:HA	29:SW:34:ILE:HD11	1.88	0.56
35:A:72:ARG:NH2	79:t:3816:G:O6	2.38	0.56
59:Y:125:ASN:HB2	59:Y:137:TYR:HB2	1.88	0.56
3:SB:66:VAL:HG11	3:SB:85:LYS:HE2	1.88	0.56
79:t:495:G:H22	79:t:637:G:H1	1.52	0.56
1:S2:584:U:OP1	25:SJ:133:ARG:NH2	2.39	0.56
14:SS:15:VAL:HG23	14:SS:20:ILE:HG13	1.88	0.56
29:SW:11:LEU:HD12	29:SW:74:VAL:HB	1.87	0.56
42:H:214:LYS:NZ	79:t:1742:G:OP2	2.39	0.56
44:J:31:ARG:NH1	44:J:149:ASN:OD1	2.39	0.56
54:T:164:LYS:O	54:T:166:ARG:N	2.34	0.56
79:t:67:C:OP2	79:t:312:G:N2	2.36	0.56
79:t:1706:A:H2	79:t:1734:C:C5	2.23	0.56
79:t:2419:U:O2	79:t:2602:G:N2	2.39	0.56
66:f:65:LYS:NZ	79:t:890:G:OP1	2.39	0.56
79:t:871:G:N2	79:t:871:G:OP2	2.38	0.56
2:SA:85:ARG:NH1	2:SA:203:PHE:O	2.39	0.55
37:C:56:GLU:OE1	37:C:58:ALA:HB3	2.06	0.55
79:t:912:G:H1	79:t:1179:G:H22	1.52	0.55
36:B:358:ARG:NH2	79:t:4349:G:OP2	2.40	0.55
37:C:62:THR:OG1	79:t:375:G:OP1	2.23	0.55
42:H:257:ARG:NH2	79:t:875:A:OP1	2.39	0.55
66:f:117:GLN:O	78:r:119:ARG:NH2	2.39	0.55
67:g:7:CYS:HB2	67:g:103:VAL:HB	1.89	0.55
67:g:33:VAL:HG13	67:g:38:GLU:HB2	1.88	0.55
79:t:323:C:H2'	79:t:324:A:H8	1.72	0.55
79:t:2237:C:OP2	79:t:2238:G:N2	2.39	0.55
1:S2:1676:U:H5''	12:SQ:78:VAL:HG12	1.88	0.55
79:t:1183:G:OP1	79:t:1183:G:N2	2.34	0.55
81:v:7:G:N2	81:v:67:C:O2'	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1565:C:H5''	15:ST:71:GLY:HA3	1.89	0.55
21:Sd:6:LEU:HA	21:Sd:9:SER:HB3	1.88	0.55
68:h:41:ALA:HB3	68:h:52:ARG:HB3	1.88	0.55
79:t:2251:G:OP2	79:t:2251:G:N2	2.37	0.55
1:S2:1133:G:OP2	1:S2:1133:G:N2	2.39	0.55
5:SE:20:LEU:HD11	5:SE:46:ILE:HD12	1.89	0.55
7:SH:138:GLU:H	7:SH:159:ASP:HB2	1.72	0.55
8:SI:142:SER:HB2	8:SI:145:ILE:HG12	1.88	0.55
79:t:295:A:N6	79:t:4093:U:O2'	2.36	0.55
1:S2:42:A:N1	1:S2:429:A:N6	2.54	0.55
37:C:94:ASN:OD1	37:C:94:ASN:N	2.37	0.55
41:G:127:PRO:O	78:r:112:ARG:NH1	2.39	0.55
79:t:3495:A:N1	80:u:37:U:O2'	2.38	0.55
12:SQ:13:PHE:HA	12:SQ:22:VAL:HA	1.88	0.55
23:SC:201:GLY:O	25:SJ:54:ARG:NH2	2.39	0.55
36:B:281:ASN:ND2	79:t:4408:G:OP1	2.39	0.55
50:P:9:LEU:HD23	50:P:118:MET:HB2	1.88	0.55
68:h:76:ARG:NH2	79:t:2427:C:OP2	2.40	0.55
3:SB:88:THR:HG22	3:SB:98:THR:HG22	1.87	0.55
5:SE:199:GLU:OE1	5:SE:199:GLU:N	2.40	0.55
8:SI:34:ALA:HB2	8:SI:56:ARG:HH21	1.72	0.55
22:Sg:168:CYS:SG	22:Sg:169:GLY:N	2.80	0.55
37:C:204:ARG:NH1	37:C:205:ARG:O	2.40	0.55
74:n:79:GLU:HB3	74:n:82:LEU:HB2	1.89	0.55
79:t:307:A:N3	79:t:310:G:O2'	2.39	0.55
79:t:1987:G:N2	79:t:2114:G:H1	2.04	0.55
79:t:2434:G:H21	79:t:2599:A:H62	1.54	0.55
1:S2:612:U:H2'	1:S2:613:G:H8	1.71	0.55
1:S2:854:C:H5''	1:S2:855:G:H5'	1.88	0.55
79:t:1204:U:O2'	79:t:1206:C:OP1	2.23	0.55
83:Cz:24:LYS:HB2	83:Cz:172:VAL:HG11	1.88	0.55
1:S2:1127:C:H5''	3:SB:150:ILE:HD12	1.89	0.54
4:SD:66:ILE:HD11	4:SD:87:TYR:HA	1.89	0.54
5:SE:114:ILE:HD11	5:SE:118:GLU:HG3	1.89	0.54
26:SM:60:MET:HA	26:SM:63:LYS:HE2	1.89	0.54
79:t:208:A:N6	79:t:232:G:N7	2.55	0.54
79:t:616:U:H4'	79:t:617:C:H5'	1.89	0.54
79:t:4487:G:H1	79:t:4604:G:H22	1.55	0.54
1:S2:1835:6MZ:H3'	1:S2:1836:C:P	2.45	0.54
20:Sc:18:LEU:HB2	20:Sc:29:GLN:HB2	1.89	0.54
42:H:242:GLY:HA3	54:T:2:LYS:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:J:41:ILE:HG21	44:J:73:ILE:HD11	1.89	0.54
70:j:68:ARG:NH1	79:t:3457:G:OP1	2.41	0.54
34:Sf:97:LYS:HB3	34:Sf:99:LYS:HG2	1.88	0.54
37:C:103:ALA:HA	79:t:1421:G:H22	1.71	0.54
50:P:130:LYS:HB2	50:P:133:ARG:HG2	1.90	0.54
79:t:2101:C:N4	79:t:2104:C:N3	2.55	0.54
1:S2:684:U:H4'	18:SX:9:THR:HG22	1.90	0.54
1:S2:858:G:O2'	10:SL:71:ARG:NH1	2.40	0.54
1:S2:1746:G:N2	1:S2:1794:A:H62	2.05	0.54
2:SA:158:ASP:HB2	17:SV:69:ILE:HD12	1.88	0.54
30:SY:14:THR:HG22	30:SY:21:LYS:HB3	1.89	0.54
35:A:5:ILE:HG12	35:A:232:GLY:HA2	1.89	0.54
54:T:95:ARG:HH12	79:t:1853:G:HO2'	1.55	0.54
79:t:2568:G:O2'	79:t:2570:G:OP2	2.26	0.54
1:S2:866:U:O2'	29:SW:78:ARG:NH1	2.40	0.54
20:Sc:61:SER:OG	20:Sc:62:GLU:N	2.40	0.54
23:SC:254:ASP:OD1	23:SC:254:ASP:N	2.34	0.54
36:B:37:PRO:HA	36:B:188:GLY:HA2	1.89	0.54
40:F:126:ASN:OD1	40:F:126:ASN:N	2.41	0.54
83:Cz:32:VAL:HA	83:Cz:208:SER:HA	1.89	0.54
43:I:167:VAL:HG12	43:I:170:LEU:HD12	1.89	0.54
1:S2:1216:C:H2'	1:S2:1217:A:H8	1.73	0.54
1:S2:1659:G:H1	1:S2:1671:U:H3	1.54	0.54
11:SP:123:TYR:OH	14:SS:124:ARG:NH1	2.40	0.54
22:Sg:191:HIS:ND1	22:Sg:213:ASP:OD2	2.41	0.54
36:B:19:ARG:NH2	79:t:4355:G:OP1	2.41	0.54
39:E:6:C:O2'	40:F:50:ARG:NH2	2.41	0.54
79:t:4502:G:H1	79:t:4590:G:H1	1.56	0.54
35:A:183:GLY:HA3	79:t:1517:A:H5''	1.90	0.54
79:t:4371:G:H1	79:t:4392:G:H22	1.55	0.54
35:A:118:GLU:HG3	35:A:126:LEU:HD11	1.90	0.54
36:B:325:GLU:OE1	79:t:4780:C:O2'	2.25	0.54
46:L:97:ASN:ND2	79:t:3982:G:OP1	2.41	0.54
1:S2:177:G:H22	1:S2:316:A:H5'	1.73	0.54
1:S2:946:U:H2'	1:S2:947:A:H8	1.73	0.54
1:S2:1591:A:H2'	1:S2:1592:A:C8	2.43	0.54
9:SK:43:LEU:HD21	9:SK:47:LYS:HZ2	1.73	0.54
13:SR:87:GLU:OE2	13:SR:87:GLU:N	2.36	0.54
34:Sf:120:GLU:HA	34:Sf:131:PHE:HA	1.90	0.54
35:A:193:ARG:NH2	79:t:3420:C:OP1	2.40	0.54
79:t:997:A:H2	79:t:1108:G:H22	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:Cz:7:ARG:NH2	83:Cz:12:GLU:OE2	2.41	0.54
1:S2:874:U:OP2	27:SN:76:LYS:NZ	2.40	0.53
48:N:35:ARG:HA	48:N:51:PRO:HA	1.89	0.53
51:Q:86:LYS:HB2	79:t:3592:G:H5''	1.91	0.53
79:t:4128:A:H62	79:t:4179:C:H42	1.56	0.53
63:c:117:ARG:NH1	79:t:1176:A:OP2	2.41	0.53
79:t:2689:A:H61	79:t:3578:C:H42	1.55	0.53
1:S2:849:G:OP2	5:SE:108:ARG:NH1	2.41	0.53
3:SB:179:ASN:HB3	3:SB:183:GLU:HB2	1.90	0.53
11:SP:37:TYR:HB3	11:SP:41:GLN:HB2	1.90	0.53
12:SQ:52:LEU:HB3	12:SQ:56:LEU:HD13	1.90	0.53
62:b:95:ASN:OD1	62:b:95:ASN:N	2.40	0.53
68:h:37:LYS:NZ	79:t:2359:G:OP1	2.40	0.53
79:t:661:C:O2	79:t:663:C:N4	2.41	0.53
21:Sd:21:CYS:SG	21:Sd:24:CYS:N	2.74	0.53
79:t:164:G:H1	79:t:272:U:H3	1.56	0.53
79:t:3500:G:O2'	79:t:3502:C:N4	2.41	0.53
37:C:80:ARG:NH2	79:t:1549:C:OP1	2.42	0.53
2:SA:108:PHE:HB2	2:SA:136:GLU:HG2	1.90	0.53
43:I:232:GLU:OE2	43:I:232:GLU:N	2.39	0.53
67:g:89:ARG:NH2	79:t:686:G:OP1	2.42	0.53
79:t:422:C:H2'	79:t:423:G:H8	1.73	0.53
8:SI:105:ASP:OD1	8:SI:105:ASP:N	2.41	0.53
54:T:165:PRO:O	54:T:167:PHE:N	2.41	0.53
79:t:229:G:O6	79:t:230:G:N2	2.41	0.53
79:t:1317:G:H2'	79:t:1318:G:C8	2.43	0.53
79:t:2329:U:H2'	79:t:2330:G:C8	2.43	0.53
79:t:3424:G:O2'	79:t:3553:U:OP2	2.27	0.53
1:S2:104:A:OP1	8:SI:12:ARG:NH1	2.42	0.53
1:S2:1207:A:O2'	1:S2:1703:C:OP2	2.26	0.53
1:S2:1600:C:OP2	31:SZ:85:ARG:NH2	2.41	0.53
42:H:44:ARG:NH1	79:t:897:G:N7	2.56	0.53
67:g:43:LEU:O	67:g:109:ARG:NH1	2.42	0.53
79:t:1808:U:H2'	79:t:1809:A:H8	1.73	0.53
79:t:1996:A:H5'	79:t:1997:C:H5'	1.90	0.53
79:t:4501:G:H1	79:t:4591:U:H3	1.55	0.53
1:S2:106:C:OP1	1:S2:434:G:O2'	2.27	0.53
1:S2:834:G:H2'	1:S2:835:G:C8	2.44	0.53
18:SX:67:ARG:HG3	18:SX:115:ILE:HG12	1.90	0.53
19:Sa:22:ARG:NH2	28:SO:145:GLY:O	2.42	0.53
47:M:18:TRP:NE1	79:t:1420:G:O2'	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:R:155:ALA:O	52:R:158:THR:OG1	2.27	0.53
79:t:2502:G:N2	79:t:2502:G:OP2	2.39	0.53
57:W:50:ASN:ND2	79:t:4189:U:OP1	2.38	0.53
71:k:30:GLN:NE2	79:t:1525:A:OP2	2.42	0.53
79:t:2483:U:HO2'	79:t:2538:G:H1	1.55	0.53
79:t:2589:A:H2'	79:t:2590:A:H8	1.74	0.53
83:Cz:151:VAL:HG23	83:Cz:152:LYS:HD3	1.90	0.53
26:SM:21:VAL:HG21	26:SM:122:ASP:HB2	1.90	0.52
21:Sd:21:CYS:HB3	21:Sd:26:ASN:H	1.74	0.52
40:F:209:ARG:NH1	40:F:233:PRO:O	2.42	0.52
57:W:51:ARG:NH1	79:t:4352:U:OP1	2.42	0.52
79:t:204:U:H3	79:t:208:A:H2	1.56	0.52
1:S2:1185:A:OP1	75:o:18:ARG:NH2	2.36	0.52
1:S2:1239:G:O6	14:SS:137:LYS:NZ	2.43	0.52
1:S2:565:U:H2'	1:S2:566:G:H8	1.74	0.52
1:S2:1310:U:H5	34:Sf:138:ARG:HH22	1.57	0.52
22:Sg:149:GLU:HG2	22:Sg:150:TRP:H	1.74	0.52
29:SW:8:ALA:HA	29:SW:74:VAL:HG11	1.91	0.52
29:SW:41:MET:HE1	29:SW:72:CYS:HB3	1.91	0.52
36:B:28:LYS:HD3	36:B:30:LYS:HD3	1.92	0.52
41:G:133:ARG:O	79:t:891:G:O2'	2.27	0.52
79:t:1228:A:OP2	79:t:4177:U:O2'	2.27	0.52
81:v:32:U:H3	81:v:38:A:H61	1.57	0.52
1:S2:1123:U:OP1	32:Sb:72:ARG:NH1	2.43	0.52
3:SB:57:ILE:HG22	3:SB:59:SER:H	1.74	0.52
19:Sa:60:ASP:OD1	19:Sa:60:ASP:N	2.41	0.52
22:Sg:193:GLY:N	22:Sg:213:ASP:OD1	2.43	0.52
24:SG:22:ARG:NE	24:SG:22:ARG:O	2.43	0.52
30:SY:76:TYR:OH	30:SY:85:ASN:O	2.28	0.52
37:C:97:ARG:NH2	79:t:377:A:OP1	2.42	0.52
38:D:156:U:H3	79:t:1:C:H42	1.58	0.52
64:d:38:ILE:HD11	64:d:46:VAL:HG21	1.90	0.52
78:r:90:LEU:HG	78:r:111:ILE:HG23	1.91	0.52
79:t:470:A:H61	79:t:660:G:H2'	1.74	0.52
79:t:488:C:H2'	79:t:489:G:C8	2.44	0.52
79:t:2445:A:N6	79:t:2588:A:OP2	2.38	0.52
79:t:3683:C:H2'	79:t:3684:A:C8	2.44	0.52
1:S2:443:G:OP1	1:S2:1801:C:O2'	2.28	0.52
79:t:4206:A:OP2	79:t:4208:C:N4	2.43	0.52
8:SI:177:SER:OG	8:SI:182:CYS:SG	2.68	0.52
22:Sg:304:ASP:OD1	22:Sg:304:ASP:N	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:33:ASP:N	35:A:33:ASP:OD1	2.42	0.52
36:B:240:LEU:HB3	36:B:244:THR:HG21	1.92	0.52
43:I:73:ARG:NH1	79:t:3808:G:OP1	2.42	0.52
47:M:46:ILE:HG22	47:M:49:ARG:HE	1.74	0.52
54:T:29:ARG:HB2	55:U:148:PRO:HB2	1.92	0.52
60:Z:45:ARG:HB2	60:Z:126:ARG:HH22	1.73	0.52
72:l:23:VAL:HG22	72:l:36:VAL:HG22	1.92	0.52
79:t:1558:G:N2	79:t:1582:C:OP1	2.42	0.52
79:t:2423:G:N2	79:t:2426:A:OP2	2.39	0.52
2:SA:63:ARG:HH21	17:SV:38:GLU:HA	1.75	0.52
10:SL:135:SER:O	10:SL:139:ARG:NH1	2.42	0.52
36:B:54:THR:OG1	36:B:55:HIS:N	2.42	0.52
52:R:18:PRO:HG3	52:R:29:VAL:HG21	1.92	0.52
79:t:2339:U:H2'	79:t:2340:G:H8	1.75	0.52
79:t:2455:A:H5'	79:t:2532:G:H4'	1.92	0.52
83:Cz:77:ALA:HB1	83:Cz:82:ILE:HD13	1.91	0.52
1:S2:1872:A:N6	3:SB:114:VAL:O	2.42	0.52
15:ST:76:THR:HB	15:ST:94:ARG:HB2	1.92	0.52
25:SJ:84:ILE:HG13	25:SJ:108:ARG:HD3	1.92	0.52
26:SM:52:LEU:CD2	26:SM:108:CYS:CA	2.86	0.52
31:SZ:99:LEU:HD11	31:SZ:102:LYS:HB2	1.91	0.52
37:C:239:LYS:O	37:C:248:ARG:NH1	2.40	0.52
40:F:116:ASP:N	40:F:116:ASP:OD1	2.39	0.52
47:M:28:GLN:OE1	49:O:202:ARG:NH1	2.42	0.52
47:M:101:ARG:NH1	79:t:75:G:O2'	2.43	0.52
55:U:41:ASP:OD1	55:U:41:ASP:N	2.41	0.52
74:n:100:TYR:O	79:t:4204:G:O2'	2.27	0.52
79:t:636:G:H2'	79:t:637:G:C8	2.42	0.52
79:t:2399:G:OP2	79:t:2606:G:N2	2.43	0.52
79:t:4444:C:H2'	79:t:4445:G:H8	1.75	0.52
1:S2:549:G:H2'	1:S2:550:G:C8	2.45	0.52
1:S2:1231:A:H2'	1:S2:1232:G:C8	2.45	0.52
30:SY:57:VAL:HB	30:SY:60:PHE:HE2	1.75	0.52
36:B:174:ARG:NH2	79:t:4714:U:O2	2.43	0.52
46:L:41:GLU:HB2	46:L:48:PRO:HD3	1.92	0.52
47:M:130:LYS:HD2	47:M:131:PRO:HD2	1.90	0.52
79:t:2012:C:H41	79:t:2096:G:H21	1.58	0.52
1:S2:115:U:H2'	1:S2:116:OMU:H6	1.92	0.51
1:S2:221:U:O2	8:SI:184:ARG:NH2	2.43	0.51
11:SP:18:ARG:HH11	14:SS:88:LYS:HE2	1.75	0.51
22:Sg:18:VAL:O	22:Sg:287:THR:OG1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:1636:G:N2	79:t:1637:U:O4	2.41	0.51
79:t:1813:C:H1'	79:t:1819:A:H2'	1.91	0.51
79:t:2621:G:H5''	79:t:2622:G:H5'	1.92	0.51
79:t:4180:G:H5''	79:t:4181:A:H5''	1.92	0.51
1:S2:888:U:H3	1:S2:904:G:H1	1.58	0.51
1:S2:1531:G:O2'	1:S2:1669:C:OP1	2.28	0.51
40:F:83:LEU:HB3	40:F:88:VAL:HB	1.92	0.51
42:H:196:ILE:HG23	42:H:201:ASP:HB2	1.91	0.51
79:t:983:G:H1	79:t:1138:U:H5	1.58	0.51
1:S2:10:G:H21	23:SC:114:LYS:HA	1.74	0.51
1:S2:1832:G:H1'	1:S2:1853:MA6:H2	1.92	0.51
8:SI:57:ALA:HB2	8:SI:183:GLY:HA2	1.92	0.51
52:R:184:ARG:NH1	62:b:55:LYS:O	2.44	0.51
79:t:1759:C:H2'	79:t:1760:A:H8	1.74	0.51
79:t:1993:G:O2'	79:t:2106:G:N2	2.43	0.51
79:t:4259:G:OP2	79:t:4259:G:N2	2.37	0.51
4:SD:170:THR:HG23	4:SD:187:LYS:HG2	1.92	0.51
44:J:23:ARG:NH1	79:t:4497:A:OP1	2.42	0.51
59:Y:82:THR:HG21	69:i:37:THR:HG22	1.92	0.51
66:f:130:ARG:NH1	79:t:2149:U:O2	2.44	0.51
79:t:227:A:H61	79:t:239:C:H42	1.58	0.51
79:t:1990:G:H5''	79:t:1991:U:H3'	1.92	0.51
79:t:4326:U:H2'	79:t:4327:G:H8	1.74	0.51
1:S2:57:U:O2'	1:S2:502:G:N3	2.44	0.51
3:SB:191:ASP:OD1	3:SB:191:ASP:N	2.42	0.51
7:SH:5:SER:OG	7:SH:7:LYS:NZ	2.44	0.51
26:SM:64:LEU:HA	34:Sf:108:VAL:HG21	1.92	0.51
48:N:5:ARG:HD2	54:T:176:PHE:HZ	1.76	0.51
60:Z:31:SER:HA	60:Z:48:PRO:HA	1.91	0.51
66:f:107:ASN:ND2	79:t:2147:C:OP1	2.42	0.51
79:t:647:C:H2'	79:t:648:G:C8	2.46	0.51
79:t:1162:G:H2'	79:t:1163:G:C8	2.46	0.51
79:t:1874:G:H2'	79:t:1875:G:C8	2.46	0.51
80:u:18:G:H1	80:u:55:U:H6	1.59	0.51
3:SB:46:LYS:NZ	28:SO:20:GLN:O	2.43	0.51
12:SQ:103:ALA:O	12:SQ:106:LYS:NZ	2.43	0.51
13:SR:28:PHE:HA	13:SR:55:THR:HG21	1.92	0.51
72:l:7:GLU:OE1	72:l:9:LYS:N	2.42	0.51
79:t:4273:G:N2	79:t:4276:A:OP2	2.37	0.51
1:S2:106:C:H2'	1:S2:107:A:H8	1.75	0.51
1:S2:320:C:OP2	24:SG:183:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1159:U:OP1	29:SW:71:LYS:NZ	2.43	0.51
1:S2:1376:C:OP1	13:SR:7:LYS:NZ	2.40	0.51
1:S2:1530:C:H5'	12:SQ:142:GLN:HB3	1.93	0.51
1:S2:1596:C:O2	15:ST:12:GLN:NE2	2.43	0.51
5:SE:9:LEU:HB3	5:SE:28:ALA:HB3	1.93	0.51
15:ST:50:GLU:OE1	15:ST:50:GLU:N	2.44	0.51
23:SC:183:LYS:HE2	29:SW:95:PRO:HA	1.93	0.51
37:C:266:THR:OG1	37:C:267:TRP:N	2.43	0.51
52:R:39:THR:O	52:R:40:ASN:ND2	2.44	0.51
79:t:4654:G:OP2	79:t:4654:G:N2	2.37	0.51
1:S2:807:U:OP1	29:SW:82:GLN:NE2	2.43	0.51
79:t:2482:G:H1	79:t:2541:A:H61	1.57	0.51
1:S2:146:G:H1	1:S2:173:A:H61	1.58	0.51
8:SI:11:ARG:NH1	8:SI:15:GLY:O	2.44	0.51
22:Sg:24:THR:HG23	22:Sg:71:ILE:HD13	1.93	0.51
1:S2:144:U:H2'	1:S2:145:G:H8	1.76	0.50
1:S2:1335:A:O2'	4:SD:145:GLN:O	2.25	0.50
35:A:223:SER:HG	79:t:3483:A:HO2'	1.58	0.50
57:W:99:GLU:OE1	58:X:21:TYR:OH	2.24	0.50
79:t:3583:U:H2'	79:t:3584:A:H8	1.76	0.50
79:t:4625:G:H1	79:t:4649:C:H42	1.59	0.50
40:F:208:MET:HE3	40:F:233:PRO:HB3	1.92	0.50
51:Q:69:ARG:NH2	79:t:4709:C:N3	2.59	0.50
53:S:88:ARG:O	79:t:2569:A:N6	2.44	0.50
79:t:3574:G:N2	79:t:3578:C:O2'	2.45	0.50
79:t:3590:C:H2'	79:t:3591:A:H8	1.76	0.50
1:S2:206:G:OP1	8:SI:147:LYS:NZ	2.42	0.50
6:SF:127:ARG:HB3	6:SF:136:ARG:H	1.76	0.50
19:Sa:94:ASP:OD1	19:Sa:96:THR:OG1	2.30	0.50
27:SN:70:LYS:HB2	27:SN:73:ARG:HG3	1.92	0.50
45:K:91:LEU:HD12	45:K:135:ILE:HG23	1.91	0.50
50:P:185:VAL:HG23	50:P:187:LYS:HD3	1.94	0.50
79:t:711:A:H62	79:t:865:G:H22	1.59	0.50
79:t:4482:C:H42	79:t:4678:G:H1	1.59	0.50
28:SO:101:GLY:HA3	28:SO:134:PRO:HD2	1.94	0.50
35:A:208:GLU:HG2	79:t:1533:G:H1	1.76	0.50
38:D:13:G:O2'	51:Q:121:LYS:O	2.30	0.50
55:U:108:ARG:NH2	79:t:1704:A:O2'	2.45	0.50
60:Z:83:GLU:OE2	60:Z:84:ARG:NH2	2.44	0.50
63:c:57:MET:HE2	79:t:1714:C:H5''	1.92	0.50
7:SH:83:LEU:HB3	7:SH:92:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:SQ:42:ILE:HG13	12:SQ:51:LEU:HD21	1.93	0.50
36:B:261:ARG:HB2	50:P:64:THR:HG21	1.94	0.50
50:P:49:ARG:NH1	79:t:1832:U:OP2	2.38	0.50
1:S2:1175:U:H2'	1:S2:1176:A:H8	1.76	0.50
1:S2:1853:MA6:OP2	1:S2:1853:MA6:H8	2.11	0.50
4:SD:142:LEU:HD13	4:SD:150:MET:HE3	1.94	0.50
41:G:191:LEU:HD23	41:G:281:LEU:HB2	1.92	0.50
45:K:36:LEU:HD11	45:K:69:ARG:HD2	1.93	0.50
54:T:30:MET:HE2	55:U:151:LEU:HB2	1.94	0.50
59:Y:89:LYS:HD2	59:Y:93:ASN:HD22	1.76	0.50
79:t:3778:A:N7	81:v:56:C:N4	2.60	0.50
3:SB:115:LYS:H	3:SB:118:GLN:HE21	1.60	0.50
38:D:51:U:OP2	73:m:21:ARG:NH2	2.45	0.50
39:E:35:U:O2	39:E:45:U:O2'	2.30	0.50
60:Z:18:HIS:NE2	79:t:229:G:O2'	2.40	0.50
66:f:26:ASP:OD1	66:f:26:ASP:N	2.45	0.50
79:t:3969:C:H1'	79:t:4053:U:H1'	1.94	0.50
8:SI:177:SER:HB3	8:SI:186:ASP:H	1.76	0.50
13:SR:27:ASP:OD2	13:SR:30:THR:OG1	2.30	0.50
17:SV:16:LYS:H	23:SC:259:THR:HG21	1.77	0.50
27:SN:19:ARG:NH2	32:Sb:83:GLN:OE1	2.45	0.50
43:I:160:ASP:OD1	43:I:160:ASP:N	2.39	0.50
45:K:52:MET:HG2	45:K:152:LEU:HD22	1.94	0.50
52:R:2:GLY:N	79:t:1799:A:OP1	2.45	0.50
54:T:95:ARG:NH1	79:t:1853:G:O2'	2.40	0.50
59:Y:73:HIS:H	59:Y:73:HIS:CD2	2.29	0.50
68:h:15:THR:O	68:h:19:LYS:NZ	2.45	0.50
79:t:3628:C:O2'	79:t:4708:A:N1	2.44	0.50
2:SA:206:ASP:OD1	2:SA:206:ASP:N	2.45	0.50
4:SD:119:CYS:SG	4:SD:120:TYR:N	2.85	0.50
18:SX:61:GLN:NE2	82:w:21:G:OP1	2.45	0.50
28:SO:59:GLY:HA2	28:SO:68:GLU:HG2	1.94	0.50
34:Sf:116:ARG:NH2	34:Sf:118:ARG:O	2.44	0.50
36:B:168:MET:HA	36:B:171:LEU:HD12	1.93	0.50
49:O:90:ASN:ND2	79:t:3664:G:OP2	2.45	0.50
50:P:12:ARG:NH1	79:t:4494:G:OP2	2.44	0.50
83:Cz:202:ARG:O	83:Cz:215:ARG:NH2	2.45	0.50
1:S2:1571:C:O2	1:S2:1630:C:O2'	2.30	0.49
5:SE:55:ALA:HB1	5:SE:60:GLU:HG3	1.94	0.49
30:SY:78:SER:OG	30:SY:80:ASP:OD1	2.30	0.49
35:A:241:ARG:NH1	79:t:3394:G:OP1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:H:175:ASN:HD21	79:t:1601:G:H21	1.60	0.49
50:P:74:ARG:HG3	50:P:145:VAL:HG12	1.94	0.49
56:V:28:PRO:HB3	56:V:100:LEU:HD11	1.94	0.49
62:b:134:GLU:OE1	62:b:138:LYS:NZ	2.45	0.49
79:t:688:G:H2'	79:t:689:A:C8	2.47	0.49
79:t:2303:G:N2	79:t:2306:U:OP2	2.45	0.49
1:S2:1104:U:H2'	1:S2:1105:G:H8	1.77	0.49
12:SQ:44:PRO:O	12:SQ:46:THR:N	2.45	0.49
41:G:120:ARG:HH12	79:t:459:C:H4'	1.77	0.49
43:I:28:VAL:O	43:I:29:ASN:ND2	2.45	0.49
49:O:157:LYS:O	49:O:162:ARG:NH1	2.43	0.49
79:t:3376:U:OP2	79:t:3381:A:N6	2.45	0.49
5:SE:71:LYS:HB3	5:SE:76:VAL:HG22	1.94	0.49
29:SW:50:PHE:HB3	29:SW:63:VAL:HG13	1.94	0.49
54:T:3:ALA:HA	54:T:7:LEU:HD21	1.94	0.49
54:T:96:GLU:HG3	54:T:139:ARG:HG2	1.94	0.49
57:W:15:ARG:NH2	79:t:4404:A:OP1	2.46	0.49
79:t:2363:U:O2'	79:t:2374:U:O2	2.30	0.49
1:S2:1036:G:N1	1:S2:1083:A:O2'	2.40	0.49
1:S2:1289:G:H1'	26:SM:35:ILE:HB	1.93	0.49
4:SD:172:VAL:HG22	4:SD:185:LYS:HG2	1.94	0.49
25:SJ:67:ASP:O	25:SJ:69:ARG:NH1	2.45	0.49
26:SM:35:ILE:HG13	26:SM:36:ARG:HG2	1.94	0.49
27:SN:119:GLU:O	27:SN:123:HIS:ND1	2.45	0.49
42:H:225:LEU:O	79:t:1973:C:O2'	2.31	0.49
45:K:53:VAL:HG21	55:U:159:MET:HG3	1.94	0.49
59:Y:96:LEU:HD12	59:Y:140:LEU:HD21	1.93	0.49
63:c:44:ARG:NH1	79:t:1369:G:OP1	2.45	0.49
76:p:11:PHE:O	76:p:81:ARG:NH2	2.44	0.49
79:t:27:C:O2'	79:t:60:A:N3	2.46	0.49
79:t:1268:G:H1'	79:t:1269:U:H5'	1.94	0.49
79:t:1986:G:H2'	79:t:1987:G:C8	2.46	0.49
1:S2:1544:G:OP1	15:ST:56:ARG:NE	2.41	0.49
49:O:169:ARG:NH2	79:t:63:G:OP1	2.45	0.49
51:Q:62:ARG:NH1	79:t:423:G:OP1	2.45	0.49
61:a:46:ILE:HG23	61:a:68:ILE:HG23	1.94	0.49
79:t:1234:C:H2'	79:t:1235:A:C8	2.47	0.49
79:t:2584:U:O2'	79:t:2586:G:N2	2.46	0.49
79:t:4696:A:H2'	79:t:4697:A:H8	1.78	0.49
1:S2:1283:G:OP1	26:SM:99:LYS:HE3	2.13	0.49
23:SC:68:ARG:HH21	23:SC:71:LYS:HD3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:224:THR:HG21	79:t:3440:G:H21	1.76	0.49
38:D:148:A:H2'	38:D:149:G:C8	2.47	0.49
79:t:2412:C:H2'	79:t:2413:G:H8	1.77	0.49
1:S2:1833:UR3:H6	1:S2:1834:A:H62	1.78	0.49
12:SQ:98:LYS:O	22:Sg:94:THR:OG1	2.30	0.49
23:SC:125:LYS:HD3	23:SC:143:CYS:HB3	1.94	0.49
23:SC:204:ILE:O	23:SC:211:LYS:NZ	2.46	0.49
30:SY:27:VAL:HB	30:SY:69:THR:HB	1.94	0.49
43:I:106:THR:OG1	43:I:109:GLU:OE2	2.30	0.49
79:t:219:G:H1	79:t:236:G:H1	1.61	0.49
79:t:1863:G:C2	79:t:1926:A:N7	2.81	0.49
79:t:4759:U:H2'	79:t:4760:G:H8	1.78	0.49
1:S2:433:C:H2'	1:S2:434:G:H8	1.77	0.49
1:S2:1717:U:H2'	1:S2:1718:A:C8	2.48	0.49
4:SD:45:ARG:HG2	4:SD:83:SER:HA	1.94	0.49
50:P:176:ARG:HD2	79:t:4501:G:H5'	1.93	0.49
79:t:3709:G:H4'	83:Cz:210:MET:HE1	1.95	0.49
79:t:4018:C:H2'	79:t:4019:G:H8	1.78	0.49
37:C:52:TYR:O	37:C:54:VAL:HG13	2.13	0.49
37:C:54:VAL:HA	37:C:105:THR:OG1	2.13	0.49
37:C:55:SER:O	37:C:56:GLU:HB2	2.12	0.49
41:G:219:PRO:HG2	41:G:222:LEU:HG	1.95	0.49
54:T:71:SER:O	54:T:76:LYS:NZ	2.45	0.49
79:t:1162:G:H2'	79:t:1163:G:H8	1.78	0.49
79:t:1863:G:N2	79:t:1926:A:C5	2.81	0.49
79:t:4332:G:H1'	79:t:4333:U:H5	1.78	0.49
1:S2:110:U:O2	1:S2:354:G:N2	2.37	0.49
8:SI:83:TYR:HB3	8:SI:101:ILE:HD11	1.95	0.49
18:SX:124:LYS:HA	18:SX:129:SER:HA	1.94	0.49
27:SN:47:PRO:HG3	27:SN:72:LEU:HD13	1.94	0.49
73:m:3:SER:O	79:t:2625:G:O2'	2.30	0.49
79:t:1411:U:H2'	79:t:1412:A:H8	1.78	0.49
79:t:1950:G:HO2'	79:t:3619:U:HO2'	1.61	0.49
24:SG:139:SER:OG	24:SG:142:ARG:NH2	2.46	0.48
35:A:40:TYR:HA	35:A:91:GLY:HA3	1.95	0.48
38:D:55:U:H3	38:D:62:A:H2	1.60	0.48
66:f:12:ILE:HG23	66:f:66:THR:HB	1.95	0.48
1:S2:523:A:O2'	1:S2:828:A:N3	2.39	0.48
1:S2:584:U:H1'	30:SY:34:THR:HG23	1.94	0.48
1:S2:1553:G:H3'	1:S2:1582:A:H61	1.78	0.48
3:SB:52:THR:HG23	3:SB:57:ILE:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SB:100:PHE:HB3	3:SB:181:LEU:HD21	1.95	0.48
18:SX:95:GLU:OE1	18:SX:95:GLU:N	2.43	0.48
79:t:444:G:H21	79:t:2157:A:H8	1.61	0.48
79:t:1013:C:H5''	79:t:1014:C:H5	1.78	0.48
79:t:1466:G:N2	79:t:1469:A:OP2	2.45	0.48
4:SD:106:ARG:HG3	4:SD:175:VAL:HG13	1.95	0.48
8:SI:81:VAL:HG12	8:SI:102:VAL:HG12	1.94	0.48
18:SX:63:ASN:ND2	18:SX:114:ASP:OD2	2.40	0.48
71:k:60:GLY:HA2	71:k:64:MET:HE2	1.94	0.48
79:t:483:G:H5'	79:t:485:G:H5''	1.95	0.48
79:t:687:C:H2'	79:t:688:G:H8	1.76	0.48
79:t:996:C:H2'	79:t:997:A:H8	1.79	0.48
79:t:1681:U:H2'	79:t:1682:A:C8	2.49	0.48
79:t:3820:C:H2'	79:t:3821:G:H8	1.79	0.48
7:SH:51:ILE:HD11	7:SH:176:VAL:HG22	1.95	0.48
78:r:32:LEU:O	78:r:113:ARG:NH1	2.46	0.48
79:t:1096:C:H3'	79:t:1097:G:H8	1.78	0.48
79:t:1797:G:O2'	79:t:1809:A:N3	2.41	0.48
79:t:3785:A:H4'	83:Cz:207:LYS:HE3	1.95	0.48
1:S2:691:U:O2	1:S2:693:G:N2	2.41	0.48
1:S2:1631:C:OP1	15:ST:38:LYS:NZ	2.43	0.48
18:SX:134:TYR:O	33:Se:13:ARG:NH2	2.46	0.48
28:SO:149:ARG:HH21	28:SO:151:LEU:HD23	1.78	0.48
35:A:112:ILE:HD13	35:A:135:THR:HB	1.95	0.48
64:d:40:GLN:HE21	64:d:42:LYS:HE2	1.79	0.48
71:k:27:TYR:HA	71:k:34:CYS:HA	1.95	0.48
79:t:2296:G:N2	79:t:2351:A:H62	2.12	0.48
79:t:3869:C:H3'	79:t:3878:G:H1	1.78	0.48
79:t:4269:C:H2'	79:t:4270:G:H8	1.77	0.48
1:S2:1115:U:O2	1:S2:1124:G:O6	2.30	0.48
1:S2:1447:U:OP1	12:SQ:15:ARG:NH2	2.45	0.48
1:S2:1524:C:OP2	14:SS:136:THR:OG1	2.31	0.48
49:O:144:ARG:NH1	79:t:124:C:OP1	2.47	0.48
49:O:146:PRO:HG2	69:i:104:THR:HG23	1.94	0.48
79:t:882:G:H2'	79:t:883:G:H8	1.78	0.48
79:t:889:G:H1'	79:t:1977:G:H5''	1.94	0.48
79:t:1260:A:H62	79:t:1279:G:H22	1.61	0.48
9:SK:25:LYS:HB2	9:SK:62:PHE:HZ	1.79	0.48
48:N:4:ARG:HH22	79:t:4497:A:H61	1.62	0.48
54:T:69:GLU:HG3	54:T:71:SER:H	1.78	0.48
63:c:15:LYS:HA	63:c:18:ARG:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:4688:U:H2'	79:t:4689:G:H8	1.79	0.48
81:v:6:G:N2	81:v:68:C:O2'	2.43	0.48
1:S2:1467:C:H5''	13:SR:60:ARG:HE	1.79	0.48
1:S2:1753:C:N3	1:S2:1785:G:N2	2.60	0.48
66:f:48:ARG:NH2	79:t:2123:A:O2'	2.46	0.48
68:h:60:ARG:NH2	79:t:2360:G:OP1	2.45	0.48
79:t:474:C:H2'	79:t:475:G:H8	1.79	0.48
1:S2:148:U:H2'	1:S2:149:A:H8	1.79	0.48
11:SP:130:ARG:HH11	11:SP:131:PRO:HD2	1.78	0.48
21:Sd:17:GLY:O	21:Sd:27:ARG:NH2	2.47	0.48
22:Sg:217:MET:SD	22:Sg:226:HIS:NE2	2.87	0.48
34:Sf:86:THR:OG1	34:Sf:87:THR:N	2.42	0.48
40:F:184:ASP:OD1	40:F:184:ASP:N	2.41	0.48
53:S:104:ARG:NH1	79:t:2742:G:OP1	2.46	0.48
79:t:300:A:H2'	79:t:301:G:H8	1.79	0.48
79:t:3787:U:H2'	79:t:3788:A:H8	1.78	0.48
1:S2:538:G:O2'	1:S2:552:C:N3	2.43	0.48
1:S2:1208:C:H2'	1:S2:1209:G:H8	1.79	0.48
5:SE:67:GLN:OE1	30:SY:84:LYS:NZ	2.46	0.48
22:Sg:201:SER:OG	22:Sg:203:ASP:O	2.32	0.48
57:W:82:ILE:HD12	57:W:121:VAL:HG12	1.96	0.48
71:k:49:TRP:O	79:t:1550:A:O2'	2.27	0.48
79:t:840:C:H2'	79:t:841:G:H8	1.79	0.48
79:t:1235:A:H2'	79:t:1236:A:H8	1.79	0.48
79:t:2255:C:H2'	79:t:2256:A:H8	1.79	0.48
83:Cz:36:ILE:HG22	83:Cz:204:LEU:HD12	1.95	0.48
7:SH:20:GLU:OE1	7:SH:20:GLU:N	2.47	0.47
14:SS:47:LYS:NZ	15:ST:35:ASP:OD2	2.46	0.47
28:SO:85:CYS:HB3	28:SO:90:ILE:HB	1.96	0.47
37:C:52:TYR:C	37:C:54:VAL:H	2.21	0.47
45:K:47:PRO:HD2	45:K:141:LYS:HA	1.96	0.47
61:a:133:LYS:NZ	79:t:2598:G:OP2	2.42	0.47
62:b:77:LYS:HZ1	79:t:1406:G:H1	1.61	0.47
66:f:104:SER:HB3	79:t:2147:C:H5''	1.96	0.47
69:i:82:ASP:OD1	69:i:82:ASP:N	2.38	0.47
79:t:4004:G:H22	79:t:4068:A:H2	1.62	0.47
1:S2:1182:G:N2	1:S2:1185:A:OP2	2.42	0.47
1:S2:1302:A:OP1	11:SP:59:ARG:NH1	2.46	0.47
2:SA:119:PRO:HG2	2:SA:142:LEU:HD11	1.95	0.47
9:SK:11:ILE:HB	9:SK:21:MET:HE1	1.95	0.47
24:SG:74:ARG:HG2	24:SG:96:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:SJ:35:TYR:O	25:SJ:111:GLN:NE2	2.47	0.47
39:E:11:A:N6	40:F:16:TYR:O	2.47	0.47
41:G:207:THR:HG22	41:G:209:THR:H	1.79	0.47
49:O:116:LEU:HD22	49:O:135:ILE:HD11	1.96	0.47
55:U:116:LYS:HD3	79:t:1735:G:N7	2.29	0.47
79:t:381:U:H4'	79:t:415:G:H5'	1.96	0.47
79:t:1659:U:H2'	79:t:1660:G:H8	1.79	0.47
22:Sg:260:ASP:OD1	22:Sg:260:ASP:N	2.45	0.47
29:SW:27:ILE:HG22	29:SW:29:PRO:HD2	1.97	0.47
57:W:117:ILE:HB	57:W:136:ALA:HA	1.95	0.47
79:t:896:G:OP1	79:t:1996:A:N6	2.38	0.47
79:t:1987:G:N2	79:t:2114:G:N2	2.63	0.47
79:t:2364:C:H2'	79:t:2365:G:H8	1.80	0.47
1:S2:109:U:O2	10:SL:71:ARG:NH2	2.47	0.47
1:S2:506:C:H3'	1:S2:507:G:H8	1.78	0.47
1:S2:1297:G:N1	1:S2:1309:U:O4	2.48	0.47
64:d:48:LEU:HD11	64:d:60:ILE:HG21	1.95	0.47
83:Cz:94:ASN:ND2	83:Cz:96:ASN:OD1	2.48	0.47
1:S2:1320:C:H2'	1:S2:1321:G:H8	1.79	0.47
24:SG:57:ASP:HB3	24:SG:98:ARG:HD2	1.95	0.47
28:SO:15:ILE:HG12	28:SO:17:LEU:H	1.79	0.47
38:D:67:U:H2'	38:D:68:G:H8	1.79	0.47
39:E:63:C:H5'	39:E:64:G:H5''	1.95	0.47
44:J:50:LYS:HG2	79:t:734:G:H5''	1.96	0.47
47:M:8:MET:HE3	79:t:1246:C:H4'	1.96	0.47
47:M:91:ALA:HB1	47:M:96:ILE:HB	1.95	0.47
70:j:63:VAL:HG23	70:j:65:LYS:HG3	1.96	0.47
79:t:1651:A:H2'	79:t:1652:G:C8	2.49	0.47
79:t:1946:G:O6	79:t:3605:C:O2'	2.32	0.47
1:S2:355:U:O2	10:SL:71:ARG:NE	2.47	0.47
1:S2:566:G:H2'	1:S2:567:A:H8	1.80	0.47
1:S2:1620:G:N1	1:S2:1623:A:OP2	2.45	0.47
7:SH:17:ASP:OD1	7:SH:17:ASP:N	2.38	0.47
40:F:225:GLN:O	40:F:229:ASN:ND2	2.46	0.47
64:d:78:ASN:OD1	64:d:78:ASN:N	2.43	0.47
83:Cz:34:LEU:HD12	83:Cz:206:ILE:HB	1.96	0.47
1:S2:28:U:H2'	1:S2:29:G:C8	2.47	0.47
1:S2:125:C:H5''	24:SG:198:ARG:HE	1.80	0.47
1:S2:951:C:H2'	1:S2:952:G:H8	1.78	0.47
1:S2:1086:A:N7	1:S2:1844:C:O2'	2.44	0.47
1:S2:1526:C:H2'	1:S2:1527:G:H8	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:SA:5:LEU:HB3	17:SV:41:ARG:HH22	1.80	0.47
6:SF:102:LEU:HD22	31:SZ:67:LEU:HD23	1.96	0.47
7:SH:39:GLN:HA	7:SH:43:LEU:HB2	1.95	0.47
13:SR:100:PRO:HG3	13:SR:119:VAL:HG13	1.96	0.47
14:SS:38:ARG:HB3	15:ST:45:LEU:HD21	1.96	0.47
20:Sc:8:PRO:O	20:Sc:10:LYS:NZ	2.47	0.47
28:SO:34:PHE:HB3	28:SO:41:PHE:HB2	1.97	0.47
31:SZ:74:SER:HA	31:SZ:79:ILE:HG23	1.97	0.47
34:Sf:109:ASP:OD1	34:Sf:109:ASP:N	2.46	0.47
36:B:250:LYS:HZ1	79:t:3631:C:H5'	1.80	0.47
39:E:52:C:O2'	39:E:54:A:N7	2.47	0.47
40:F:257:PRO:O	40:F:259:ARG:N	2.46	0.47
47:M:153:PRO:HB3	69:i:121:VAL:HG11	1.96	0.47
51:Q:111:SER:O	51:Q:111:SER:OG	2.31	0.47
60:Z:8:THR:O	79:t:226:G:N2	2.48	0.47
61:a:54:THR:H	61:a:57:MET:HE3	1.79	0.47
74:n:97:ARG:NH1	79:t:4156:A:OP1	2.47	0.47
79:t:318:A:O2'	79:t:3462:A:N3	2.41	0.47
79:t:1217:C:N4	79:t:1218:G:O6	2.48	0.47
79:t:1752:A:N3	79:t:2127:G:O2'	2.47	0.47
1:S2:3:C:N4	87:S2:2003:HOH:O	2.45	0.47
1:S2:5:U:H2'	1:S2:6:G:C8	2.50	0.47
1:S2:74:G:H4'	1:S2:75:G:H5'	1.96	0.47
1:S2:620:G:N7	18:SX:67:ARG:NH1	2.56	0.47
1:S2:841:G:H1'	1:S2:843:C:H5'	1.97	0.47
1:S2:1066:C:O2'	28:SO:150:ARG:O	2.32	0.47
12:SQ:112:LEU:HD22	12:SQ:119:LEU:HD13	1.96	0.47
25:SJ:55:LYS:O	25:SJ:55:LYS:NZ	2.32	0.47
31:SZ:91:LEU:HD22	31:SZ:96:LEU:HD12	1.97	0.47
63:c:14:ARG:NH2	79:t:1780:G:OP2	2.48	0.47
64:d:20:LEU:O	64:d:24:SER:OG	2.29	0.47
72:l:26:LYS:HB2	72:l:69:LEU:HD12	1.97	0.47
79:t:492:C:H2'	79:t:493:G:H8	1.80	0.47
79:t:3399:G:H2'	79:t:3400:G:H8	1.80	0.47
1:S2:223:U:H2'	1:S2:224:A:H8	1.79	0.47
1:S2:615:PSU:O2'	33:Se:11:LYS:NZ	2.48	0.47
5:SE:54:TYR:OH	5:SE:97:GLU:OE1	2.33	0.47
16:SU:78:ASP:OD1	16:SU:78:ASP:N	2.42	0.47
62:b:59:ARG:NH2	62:b:61:TYR:OH	2.48	0.47
65:e:64:ILE:HG23	65:e:68:LEU:HD23	1.96	0.47
79:t:165:A:N6	79:t:271:C:H42	2.05	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:2322:C:O2	79:t:2435:A:O2'	2.29	0.47
1:S2:475:C:O2'	1:S2:477:G:OP1	2.32	0.47
1:S2:1746:G:H21	1:S2:1794:A:N6	2.11	0.47
45:K:76:MET:HE3	45:K:76:MET:HB3	1.85	0.47
73:m:10:LYS:HA	73:m:13:LEU:HD12	1.96	0.47
79:t:1006:C:H2'	79:t:1007:C:C6	2.50	0.47
79:t:1706:A:C4	79:t:1736:U:H1'	2.49	0.47
79:t:4256:G:OP1	79:t:4291:A:N6	2.45	0.47
83:Cz:20:GLY:HA2	83:Cz:23:ARG:HG2	1.97	0.47
1:S2:1602:U:OP1	31:SZ:80:ARG:NE	2.39	0.46
5:SE:181:CYS:SG	5:SE:182:MET:N	2.87	0.46
36:B:92:TYR:HB2	36:B:159:VAL:HB	1.97	0.46
61:a:16:GLY:O	61:a:18:TYR:N	2.46	0.46
79:t:1302:G:H2'	79:t:1303:G:C8	2.50	0.46
83:Cz:34:LEU:HB2	83:Cz:206:ILE:HD13	1.97	0.46
1:S2:946:U:O2'	28:SO:135:ILE:O	2.33	0.46
19:Sa:3:LYS:NZ	19:Sa:8:ASN:OD1	2.49	0.46
36:B:268:ARG:NH2	79:t:4297:C:O2	2.43	0.46
41:G:211:VAL:HG11	41:G:271:ILE:HG22	1.98	0.46
52:R:68:ARG:HH21	79:t:1405:C:H6	1.63	0.46
52:R:75:ARG:HH12	79:t:1361:G:C4'	2.28	0.46
54:T:170:LYS:NZ	79:t:4600:G:O2'	2.36	0.46
83:Cz:15:ARG:HA	83:Cz:15:ARG:HD2	1.75	0.46
1:S2:376:G:H4'	10:SL:85:THR:HG21	1.97	0.46
1:S2:1314:C:OP1	34:Sf:143:LYS:NZ	2.48	0.46
1:S2:1455:A:O2'	1:S2:1478:G:N2	2.49	0.46
22:Sg:80:SER:OG	22:Sg:90:TRP:NE1	2.47	0.46
47:M:145:LYS:HD2	69:i:123:ALA:HA	1.97	0.46
50:P:32:LYS:HE3	50:P:32:LYS:HB3	1.78	0.46
1:S2:511:A:H3'	1:S2:512:OMG:H8	1.80	0.46
1:S2:881:G:H22	1:S2:911:A:H2	1.63	0.46
1:S2:1280:C:H2'	1:S2:1281:A:H8	1.80	0.46
2:SA:189:ILE:HG22	2:SA:191:ARG:H	1.80	0.46
14:SS:67:VAL:HA	14:SS:70:ILE:HB	1.97	0.46
23:SC:270:THR:HA	23:SC:273:LEU:HD12	1.97	0.46
30:SY:56:PHE:O	30:SY:74:MET:N	2.46	0.46
46:L:101:ASP:OD1	46:L:101:ASP:N	2.49	0.46
74:n:100:TYR:OH	79:t:4157:G:OP1	2.34	0.46
79:t:456:C:H2'	79:t:457:G:C8	2.51	0.46
79:t:2554:C:H5'	79:t:2555:G:H5''	1.98	0.46
79:t:2692:G:O2'	79:t:3573:U:O4	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:4431:U:H1'	79:t:4432:A:H5''	1.97	0.46
1:S2:65:C:OP1	24:SG:136:LYS:NZ	2.42	0.46
9:SK:53:LYS:HB2	9:SK:53:LYS:HE3	1.73	0.46
19:Sa:45:VAL:HG11	19:Sa:53:ILE:HG13	1.97	0.46
40:F:133:GLU:OE2	40:F:133:GLU:N	2.48	0.46
41:G:120:ARG:NH1	79:t:459:C:O2'	2.49	0.46
45:K:60:LEU:HD22	45:K:129:VAL:HG21	1.97	0.46
46:L:163:MET:HG2	46:L:174:ILE:HD12	1.98	0.46
60:Z:32:SER:OG	60:Z:101:PRO:O	2.27	0.46
79:t:2206:U:H2'	79:t:2207:A:H8	1.80	0.46
79:t:3652:A:H2'	79:t:3653:G:H8	1.80	0.46
1:S2:471:A:OP1	24:SG:74:ARG:NH1	2.47	0.46
1:S2:1186:A:H2'	1:S2:1187:G:H8	1.81	0.46
1:S2:1548:A:H4'	12:SQ:74:GLY:HA2	1.97	0.46
1:S2:1723:U:O2'	79:t:3531:U:O2'	2.29	0.46
7:SH:81:ARG:NH1	7:SH:82:GLU:OE2	2.49	0.46
30:SY:83:LYS:HD2	30:SY:96:LEU:HD21	1.97	0.46
38:D:76:C:H2'	38:D:77:A:C8	2.49	0.46
40:F:223:PHE:HB3	40:F:226:TYR:HB2	1.96	0.46
47:M:25:TRP:HE1	49:O:199:GLN:HG3	1.80	0.46
54:T:139:ARG:NE	79:t:1854:G:OP1	2.41	0.46
56:V:64:GLU:N	56:V:64:GLU:OE2	2.48	0.46
61:a:35:ASP:OD1	61:a:35:ASP:N	2.45	0.46
79:t:31:U:H3	79:t:51:A:H61	1.63	0.46
79:t:1310:U:O2'	79:t:1313:C:N4	2.49	0.46
79:t:1986:G:H2'	79:t:1987:G:H8	1.80	0.46
1:S2:104:A:H62	1:S2:359:C:H5	1.63	0.46
1:S2:120:U:H2'	1:S2:121:OMU:C6	2.45	0.46
1:S2:1015:A:OP1	27:SN:3:ARG:NH1	2.48	0.46
1:S2:1247:U:H2'	1:S2:1248:G:H8	1.81	0.46
1:S2:1650:A:HO2'	12:SQ:125:ARG:HH21	1.62	0.46
3:SB:229:MET:HA	3:SB:229:MET:HE3	1.98	0.46
5:SE:95:THR:HG23	30:SY:16:ARG:HD3	1.98	0.46
45:K:38:ARG:HD2	45:K:41:ALA:HB2	1.97	0.46
51:Q:52:THR:HG22	51:Q:85:LYS:HB2	1.98	0.46
62:b:41:HIS:NE2	79:t:1585:G:O2'	2.45	0.46
64:d:80:GLU:HA	64:d:83:THR:HB	1.98	0.46
67:g:14:TYR:OH	67:g:92:LEU:O	2.30	0.46
79:t:2255:C:O2'	79:t:2370:C:O2	2.33	0.46
79:t:4769:U:H4'	79:t:4770:G:H5'	1.97	0.46
12:SQ:21:ALA:HB2	12:SQ:72:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B:218:ASP:OD2	36:B:348:ARG:NH2	2.43	0.46
38:D:130:C:H2'	38:D:131:G:H8	1.80	0.46
49:O:63:ARG:NH1	49:O:131:GLU:OE2	2.49	0.46
53:S:62:ARG:NH1	79:t:4380:A:OP1	2.49	0.46
79:t:475:G:H2'	79:t:476:G:C8	2.51	0.46
79:t:1301:G:H2'	79:t:1302:G:H8	1.80	0.46
79:t:1908:G:O2'	79:t:1913:A:N6	2.45	0.46
79:t:3467:A:H2'	79:t:3468:A:H8	1.80	0.46
83:Cz:78:LYS:HA	83:Cz:82:ILE:HG22	1.97	0.46
1:S2:931:G:H2'	1:S2:932:G:C8	2.51	0.46
37:C:57:LEU:O	37:C:58:ALA:HB2	2.14	0.46
40:F:17:GLN:O	79:t:3997:U:N3	2.43	0.46
45:K:35:ASP:N	45:K:35:ASP:OD1	2.49	0.46
47:M:103:ARG:NH1	79:t:73:A:N7	2.64	0.46
52:R:66:MET:HE2	52:R:66:MET:HB3	1.82	0.46
79:t:479:G:N2	79:t:652:G:N2	2.41	0.46
79:t:1330:G:H2'	79:t:1361:G:H22	1.79	0.46
79:t:1835:G:H2'	79:t:1836:A:C8	2.51	0.46
79:t:4330:C:H2'	79:t:4343:A:H61	1.80	0.46
83:Cz:22:GLN:O	83:Cz:25:ARG:NH1	2.48	0.46
83:Cz:97:LYS:H	83:Cz:97:LYS:HD3	1.81	0.46
1:S2:146:G:H2'	1:S2:147:A:H8	1.80	0.46
1:S2:383:G:OP2	8:SI:181:GLN:NE2	2.48	0.46
1:S2:447:G:O2'	1:S2:449:G:O6	2.31	0.46
1:S2:565:U:H2'	1:S2:566:G:C8	2.51	0.46
1:S2:1117:U:H3'	1:S2:1118:U:H2'	1.97	0.46
17:SV:40:ASP:OD1	17:SV:41:ARG:N	2.49	0.46
37:C:228:THR:OG1	37:C:248:ARG:NH2	2.48	0.46
47:M:155:MET:HE3	47:M:155:MET:HA	1.98	0.46
70:j:74:LYS:HE3	70:j:80:HIS:HB2	1.97	0.46
79:t:163:A:H2'	79:t:164:G:H8	1.81	0.46
79:t:1141:C:H5'	79:t:1142:C:H5''	1.97	0.46
79:t:1642:C:O2	79:t:1688:A:N6	2.48	0.46
1:S2:5:U:H2'	1:S2:6:G:H8	1.81	0.45
1:S2:1149:C:O2'	1:S2:1153:A:N1	2.44	0.45
2:SA:17:LYS:HB3	2:SA:173:LEU:HD11	1.98	0.45
2:SA:157:VAL:O	17:SV:65:SER:OG	2.34	0.45
3:SB:104:ASP:OD1	3:SB:105:LEU:N	2.49	0.45
18:SX:41:PHE:HB3	18:SX:44:ALA:HB3	1.97	0.45
36:B:358:ARG:HA	36:B:358:ARG:HD3	1.78	0.45
68:h:49:CYS:O	68:h:51:GLY:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:n:95:ILE:HG21	79:t:4205:A:H4'	1.98	0.45
78:r:132:ARG:NH2	79:t:453:G:N7	2.64	0.45
79:t:1907:U:H3'	79:t:1908:G:H8	1.81	0.45
79:t:4136:U:O2'	79:t:4138:U:O4	2.31	0.45
83:Cz:95:LYS:HA	83:Cz:98:LYS:HD3	1.97	0.45
1:S2:699:G:O4'	1:S2:739:C:N4	2.50	0.45
1:S2:1230:G:N2	1:S2:1638:C:O2'	2.49	0.45
1:S2:1525:A:OP2	14:SS:144:ARG:NH1	2.50	0.45
22:Sg:11:LEU:HB2	22:Sg:307:VAL:HB	1.97	0.45
29:SW:118:ARG:HG3	29:SW:119:LYS:HG2	1.97	0.45
35:A:58:LEU:HD13	35:A:75:LEU:HD21	1.98	0.45
40:F:119:TYR:OH	40:F:139:PRO:O	2.32	0.45
63:c:58:GLN:NE2	79:t:1713:G:H21	2.14	0.45
63:c:91:ARG:HD3	63:c:93:LEU:H	1.80	0.45
68:h:50:PRO:HD3	77:q:61:MET:HE2	1.97	0.45
79:t:159:C:H5''	79:t:160:G:H2'	1.97	0.45
79:t:191:G:H2'	79:t:192:G:H8	1.81	0.45
79:t:4645:C:H2'	79:t:4646:G:C8	2.51	0.45
1:S2:226:C:H2'	1:S2:227:A:C8	2.52	0.45
1:S2:591:G:OP2	1:S2:591:G:N2	2.48	0.45
1:S2:965:A:N1	1:S2:1058:A:O2'	2.49	0.45
22:Sg:107:ASP:HB3	22:Sg:125:ARG:HB2	1.97	0.45
31:SZ:48:VAL:HG22	31:SZ:49:LEU:HG	1.98	0.45
34:Sf:108:VAL:HG13	34:Sf:112:GLY:HA2	1.99	0.45
79:t:2689:A:H61	79:t:3578:C:N4	2.14	0.45
79:t:3605:C:H2'	79:t:3606:A:H8	1.80	0.45
79:t:3708:G:H2'	79:t:3709:G:C8	2.50	0.45
82:w:20:G:H2'	82:w:21:G:C8	2.51	0.45
83:Cz:105:LYS:O	83:Cz:133:LYS:NZ	2.49	0.45
5:SE:9:LEU:O	5:SE:28:ALA:N	2.44	0.45
6:SF:101:HIS:HB2	6:SF:108:PRO:HG3	1.99	0.45
7:SH:32:MET:HE1	7:SH:36:LEU:H	1.82	0.45
37:C:269:LYS:HB3	79:t:631:C:H4'	1.98	0.45
79:t:62:A:N3	79:t:77:U:O2'	2.44	0.45
79:t:906:C:H2'	79:t:907:G:H8	1.81	0.45
79:t:1689:A:N3	79:t:3942:U:O2'	2.49	0.45
79:t:4618:G:H2'	79:t:4619:A:H8	1.81	0.45
80:u:68:C:H2'	80:u:69:G:C8	2.51	0.45
1:S2:922:A:OP2	27:SN:64:ARG:NH1	2.40	0.45
1:S2:1680:U:H2'	1:S2:1681:A2M:H8	1.99	0.45
7:SH:143:ARG:HB2	7:SH:155:LYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:ST:137:GLN:O	15:ST:141:ALA:N	2.48	0.45
34:Sf:118:ARG:HH11	34:Sf:131:PHE:HE2	1.64	0.45
35:A:179:ILE:HB	79:t:3388:A:H4'	1.99	0.45
48:N:118:MET:HA	48:N:118:MET:HE2	1.99	0.45
52:R:161:SER:OG	52:R:162:HIS:N	2.49	0.45
57:W:113:LYS:HE2	57:W:113:LYS:HB3	1.82	0.45
79:t:2124:G:N2	79:t:2125:U:O4	2.49	0.45
12:SQ:127:CYS:O	12:SQ:128:GLU:HG2	2.16	0.45
36:B:50:LYS:HB2	36:B:345:LEU:HD11	1.98	0.45
38:D:75:G:OP2	60:Z:74:TYR:OH	2.31	0.45
54:T:11:LYS:HD2	54:T:29:ARG:HD3	1.99	0.45
62:b:42:ARG:NH1	79:t:4108:A:O2'	2.50	0.45
66:f:78:LEU:O	78:r:20:ARG:NH1	2.42	0.45
79:t:475:G:H2'	79:t:476:G:H8	1.81	0.45
79:t:1706:A:C2	79:t:1736:U:H1'	2.52	0.45
79:t:2255:C:H2'	79:t:2256:A:C8	2.50	0.45
79:t:2257:U:H2'	79:t:2258:G:H8	1.82	0.45
1:S2:121:OMU:H2'	1:S2:122:G:C8	2.51	0.45
5:SE:48:LEU:HB3	5:SE:54:TYR:HB2	1.99	0.45
9:SK:88:GLU:OE1	9:SK:88:GLU:N	2.47	0.45
12:SQ:61:GLU:OE1	12:SQ:61:GLU:N	2.41	0.45
22:Sg:219:TRP:HE1	22:Sg:226:HIS:CD2	2.35	0.45
28:SO:80:ASP:OD1	28:SO:80:ASP:N	2.48	0.45
30:SY:29:HIS:HE2	30:SY:69:THR:HG1	1.65	0.45
41:G:115:ARG:HH22	79:t:470:A:H2	1.64	0.45
49:O:93:LYS:O	79:t:300:A:O2'	2.27	0.45
54:T:21:LYS:HE2	54:T:21:LYS:N	2.32	0.45
79:t:480:C:H2'	79:t:481:G:C8	2.52	0.45
79:t:4018:C:H2'	79:t:4019:G:C8	2.51	0.45
1:S2:586:A:H3'	1:S2:587:A:H8	1.81	0.45
4:SD:62:LYS:HE2	4:SD:62:LYS:HB2	1.78	0.45
5:SE:45:ILE:HG13	5:SE:61:VAL:HG11	1.99	0.45
5:SE:131:VAL:HA	5:SE:137:PRO:HA	1.99	0.45
22:Sg:163:PRO:HG2	22:Sg:179:LEU:HD11	1.99	0.45
32:Sb:67:THR:OG1	32:Sb:70:LYS:O	2.35	0.45
36:B:220:ILE:HB	36:B:346:THR:HB	1.98	0.45
43:I:43:GLN:HB2	43:I:44:ASP:H	1.61	0.45
56:V:46:ARG:HB3	56:V:86:LEU:HD22	1.99	0.45
60:Z:37:GLU:OE2	60:Z:37:GLU:N	2.47	0.45
79:t:1411:U:H2'	79:t:1412:A:C8	2.52	0.45
79:t:1704:A:O2'	79:t:1739:A:OP1	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:4367:A:H8	79:t:4777:A:H61	1.64	0.45
80:u:13:C:H2'	80:u:14:A:C8	2.52	0.45
83:Cz:60:ARG:HH22	83:Cz:173:LYS:HB2	1.82	0.45
1:S2:94:G:O2'	1:S2:511:A:O2'	2.35	0.45
1:S2:642:C:H2'	1:S2:643:A:C8	2.52	0.45
1:S2:1815:U:O4	1:S2:1816:A:N6	2.49	0.45
8:SI:126:GLY:H	8:SI:128:LYS:NZ	2.15	0.45
23:SC:167:ARG:HB3	23:SC:177:PRO:HB2	1.98	0.45
33:Se:36:MET:HE2	33:Se:36:MET:HB2	1.88	0.45
35:A:101:VAL:HG22	35:A:165:VAL:HG22	1.99	0.45
37:C:322:LEU:O	37:C:324:ILE:N	2.49	0.45
40:F:23:ARG:O	40:F:23:ARG:NH1	2.43	0.45
47:M:7:GLY:O	62:b:49:HIS:NE2	2.42	0.45
77:q:91:ASP:N	77:q:91:ASP:OD1	2.50	0.45
79:t:65:A:H61	79:t:75:G:H1'	1.82	0.45
79:t:214:G:OP2	79:t:214:G:N2	2.36	0.45
79:t:219:G:H22	79:t:236:G:H1	1.65	0.45
79:t:716:C:H2'	79:t:717:G:H8	1.82	0.45
1:S2:1494:G:H1'	16:SU:72:GLU:HG2	1.99	0.45
2:SA:134:LEU:HD22	2:SA:144:THR:HG21	1.98	0.45
9:SK:80:ARG:HD3	9:SK:87:PRO:HA	1.99	0.45
25:SJ:112:THR:HG22	25:SJ:123:ILE:HD11	1.99	0.45
32:Sb:19:HIS:HB3	32:Sb:22:LYS:HG2	1.99	0.45
56:V:100:LEU:HD12	56:V:112:LEU:HB3	1.98	0.45
79:t:1737:G:H5'	79:t:1738:G:OP2	2.16	0.45
79:t:1896:C:H2'	79:t:1897:G:H8	1.81	0.45
79:t:1925:G:H2'	79:t:1926:A:H8	1.81	0.45
1:S2:439:G:OP1	1:S2:474:G:O2'	2.35	0.44
1:S2:440:G:H3'	1:S2:441:G:H21	1.81	0.44
3:SB:35:ALA:HB3	3:SB:42:ARG:HA	1.98	0.44
8:SI:48:VAL:HG11	8:SI:54:LYS:HE3	1.97	0.44
17:SV:15:ARG:NH1	23:SC:83:LEU:O	2.47	0.44
27:SN:31:ASP:OD1	27:SN:31:ASP:N	2.50	0.44
39:E:23:A:N3	39:E:118:C:O2'	2.40	0.44
79:t:1076:U:H2'	79:t:1077:G:C8	2.52	0.44
79:t:1365:C:H2'	79:t:1366:A:H8	1.81	0.44
79:t:4589:G:H2'	79:t:4590:G:C8	2.52	0.44
79:t:4776:C:O2'	79:t:4779:C:OP2	2.35	0.44
1:S2:167:G:O2'	24:SG:131:ARG:NH1	2.46	0.44
1:S2:916:A:H5''	7:SH:120:ARG:HH21	1.82	0.44
1:S2:1833:UR3:H1'	1:S2:1834:A:N7	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SI:119:LEU:HD13	8:SI:120:PRO:HD2	1.99	0.44
8:SI:190:LEU:HD21	8:SI:198:TYR:HD2	1.81	0.44
32:Sb:12:PRO:HA	32:Sb:15:GLU:HG3	1.99	0.44
52:R:94:GLU:OE1	52:R:94:GLU:N	2.50	0.44
55:U:102:ARG:HD3	79:t:1703:A:H4'	1.99	0.44
79:t:1621:C:H5''	79:t:1622:C:C5	2.52	0.44
79:t:4005:A:H2'	79:t:4006:A:C8	2.53	0.44
83:Cz:119:GLN:HA	83:Cz:122:ARG:HH11	1.81	0.44
1:S2:832:C:O2'	1:S2:848:G:N2	2.50	0.44
17:SV:19:ALA:O	29:SW:23:ARG:NH1	2.50	0.44
35:A:5:ILE:HG13	35:A:8:GLN:HG3	1.99	0.44
37:C:13:GLU:OE2	37:C:13:GLU:N	2.43	0.44
37:C:54:VAL:O	37:C:55:SER:C	2.60	0.44
42:H:138:ASN:HB3	55:U:132:PRO:HB2	1.98	0.44
52:R:7:HIS:O	52:R:9:LYS:N	2.49	0.44
57:W:83:ARG:NH1	57:W:120:PRO:O	2.41	0.44
71:k:82:THR:OG1	71:k:83:THR:N	2.51	0.44
79:t:4121:C:H2'	79:t:4122:A:C8	2.53	0.44
79:t:4696:A:H2'	79:t:4697:A:C8	2.53	0.44
83:Cz:11:TYR:HB3	83:Cz:215:ARG:HB3	1.99	0.44
1:S2:95:G:H21	1:S2:477:G:H5'	1.82	0.44
1:S2:107:A:H2'	1:S2:108:G:H8	1.81	0.44
1:S2:1231:A:H2'	1:S2:1232:G:H8	1.81	0.44
16:SU:34:LYS:HD2	16:SU:34:LYS:HA	1.72	0.44
27:SN:83:ASP:OD1	27:SN:83:ASP:N	2.51	0.44
28:SO:67:ASP:OD1	28:SO:67:ASP:N	2.48	0.44
34:Sf:107:LYS:HB3	34:Sf:115:SER:HB2	1.99	0.44
39:E:46:C:H3'	39:E:47:G:H21	1.82	0.44
66:f:98:GLU:OE1	66:f:123:THR:OG1	2.33	0.44
79:t:448:G:H2'	79:t:449:C:C6	2.52	0.44
79:t:459:C:H2'	79:t:460:C:C6	2.53	0.44
79:t:1200:C:H2'	79:t:1201:G:H8	1.82	0.44
79:t:2434:G:N2	79:t:2599:A:H62	2.14	0.44
79:t:4025:U:OP2	79:t:4061:G:O2'	2.33	0.44
1:S2:155:G:H21	24:SG:56:ASN:HD21	1.64	0.44
1:S2:190:G:H5'	8:SI:145:ILE:HD13	1.98	0.44
1:S2:910:G:H2'	1:S2:911:A:H8	1.83	0.44
22:Sg:88:ARG:HG3	22:Sg:100:ARG:HB3	2.00	0.44
36:B:189:THR:HG22	36:B:191:ALA:H	1.81	0.44
41:G:104:LYS:O	41:G:114:THR:OG1	2.35	0.44
56:V:67:LYS:HA	56:V:67:LYS:HD2	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:b:46:ASP:O	62:b:48:TYR:N	2.43	0.44
79:t:85:G:O2'	79:t:97:G:O6	2.32	0.44
79:t:210:C:H2'	79:t:211:G:H8	1.82	0.44
79:t:1536:A:H1'	79:t:3376:U:H1'	1.99	0.44
1:S2:165:G:H4'	24:SG:53:SER:HB3	1.99	0.44
1:S2:391:U:H2'	1:S2:392:A:C8	2.53	0.44
3:SB:146:ARG:HE	3:SB:206:PRO:HG2	1.83	0.44
5:SE:195:ILE:HA	5:SE:210:VAL:HG12	2.00	0.44
11:SP:21:ASP:N	11:SP:21:ASP:OD1	2.50	0.44
20:Sc:10:LYS:HE2	20:Sc:10:LYS:HB2	1.89	0.44
49:O:138:PHE:HA	49:O:143:ARG:HD3	1.99	0.44
50:P:55:LEU:HD23	50:P:58:LEU:HD12	1.99	0.44
62:b:12:ARG:HD3	62:b:12:ARG:HA	1.72	0.44
79:t:1950:G:H2'	79:t:1951:G:C8	2.52	0.44
79:t:2013:G:H5''	79:t:2095:C:C5	2.44	0.44
79:t:2401:G:H1	79:t:2414:U:H3	1.66	0.44
79:t:3507:U:H2'	79:t:3508:U:H2'	2.00	0.44
1:S2:70:G:H1	24:SG:170:ARG:HH22	1.65	0.44
1:S2:189:U:OP1	8:SI:148:LYS:NZ	2.42	0.44
1:S2:347:U:H2'	1:S2:348:U:H6	1.83	0.44
1:S2:535:C:H2'	1:S2:536:A:H8	1.82	0.44
22:Sg:54:ILE:HD12	22:Sg:55:PRO:HD2	2.00	0.44
23:SC:166:ARG:HD3	23:SC:181:PRO:HG3	2.00	0.44
36:B:140:ASP:OD1	36:B:141:THR:N	2.50	0.44
38:D:123:U:H3	79:t:2387:A:H1'	1.82	0.44
49:O:44:ARG:NH2	79:t:280:G:OP2	2.50	0.44
69:i:113:LEU:HD21	79:t:267:G:H4'	1.98	0.44
1:S2:647:OMG:HM23	1:S2:647:OMG:H1'	1.81	0.44
1:S2:1289:G:H8	34:Sf:101:ALA:HA	1.82	0.44
14:SS:82:TRP:CD1	14:SS:82:TRP:H	2.35	0.44
36:B:92:TYR:HB3	36:B:99:LEU:HD22	2.00	0.44
37:C:212:ASN:HD21	37:C:255:SER:HB2	1.82	0.44
44:J:105:ILE:HG12	44:J:112:VAL:HG12	2.00	0.44
57:W:33:GLY:HA3	57:W:69:LYS:HG3	2.00	0.44
70:j:29:ARG:NE	70:j:29:ARG:O	2.51	0.44
71:k:19:CYS:HB3	71:k:23:GLY:H	1.83	0.44
79:t:441:G:H2'	79:t:442:G:H8	1.83	0.44
79:t:480:C:H42	79:t:651:C:H42	1.66	0.44
79:t:1950:G:O2'	79:t:3619:U:O2'	2.30	0.44
79:t:2517:G:H5''	79:t:2518:A:H3'	1.99	0.44
2:SA:30:LEU:HB2	2:SA:47:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SF:18:LYS:HA	6:SF:25:THR:HG23	1.99	0.44
7:SH:17:ASP:HB2	7:SH:21:SER:HB2	1.99	0.44
9:SK:65:ARG:NH1	21:Sd:21:CYS:O	2.51	0.44
16:SU:24:LEU:HB2	16:SU:87:ARG:HB2	2.00	0.44
26:SM:80:ASP:OD1	26:SM:80:ASP:N	2.49	0.44
37:C:289:LEU:HD21	52:R:31:LEU:HB2	1.99	0.44
40:F:107:ARG:NH1	40:F:169:GLY:O	2.51	0.44
41:G:106:VAL:HG12	41:G:108:GLY:H	1.82	0.44
41:G:288:THR:OG1	41:G:289:ASN:N	2.44	0.44
59:Y:47:ARG:HE	59:Y:47:ARG:HB3	1.62	0.44
79:t:207:G:N2	79:t:232:G:O5'	2.51	0.44
79:t:1950:G:H2'	79:t:1951:G:H8	1.83	0.44
79:t:2238:G:O2'	79:t:2663:U:O4	2.33	0.44
83:Cz:103:LEU:HG	83:Cz:106:LYS:HE2	2.00	0.44
2:SA:141:ASN:ND2	23:SC:85:SER:O	2.51	0.43
2:SA:184:ARG:HD3	2:SA:191:ARG:HD3	2.00	0.43
36:B:295:ASP:OD1	36:B:295:ASP:N	2.51	0.43
45:K:30:LYS:HE3	45:K:66:GLU:HG2	2.00	0.43
45:K:183:ASP:OD1	45:K:183:ASP:N	2.50	0.43
79:t:371:A:N3	79:t:1435:U:O2'	2.50	0.43
79:t:422:C:H2'	79:t:423:G:C8	2.53	0.43
79:t:654:C:H2'	79:t:655:G:C8	2.53	0.43
79:t:1015:C:O2'	79:t:1016:A:O4'	2.36	0.43
79:t:1235:A:H2'	79:t:1236:A:C8	2.53	0.43
1:S2:186:C:N4	1:S2:187:G:O6	2.50	0.43
1:S2:376:G:OP1	10:SL:137:THR:OG1	2.32	0.43
1:S2:497:C:H42	1:S2:512:OMG:HN22	1.65	0.43
1:S2:659:G:H21	1:S2:666:C:H5''	1.82	0.43
1:S2:880:C:H2'	1:S2:881:G:C8	2.53	0.43
1:S2:1708:C:H2'	1:S2:1709:G:C8	2.53	0.43
4:SD:217:ILE:HD12	4:SD:217:ILE:HA	1.88	0.43
6:SF:19:LEU:HD11	6:SF:69:VAL:HG11	1.99	0.43
10:SL:94:HIS:O	10:SL:103:GLU:N	2.44	0.43
16:SU:94:PRO:HD2	16:SU:97:ILE:HD11	1.99	0.43
21:Sd:21:CYS:HB2	21:Sd:39:CYS:HB3	1.81	0.43
24:SG:24:LEU:O	24:SG:26:THR:N	2.51	0.43
29:SW:42:MET:HE2	29:SW:42:MET:HB3	1.77	0.43
31:SZ:44:LEU:HB3	31:SZ:45:ASN:H	1.59	0.43
37:C:297:GLU:H	37:C:297:GLU:CD	2.26	0.43
42:H:259:MET:HE2	42:H:259:MET:HB3	1.86	0.43
50:P:87:MET:O	79:t:1815:C:O2'	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Q:39:MET:HE3	51:Q:43:LYS:HG2	2.00	0.43
64:d:20:LEU:HB3	64:d:102:SER:HB3	2.00	0.43
74:n:103:LEU:HD12	74:n:121:LEU:HD11	2.00	0.43
79:t:86:U:H2'	79:t:87:A:H8	1.83	0.43
79:t:455:C:N4	79:t:681:G:N7	2.67	0.43
79:t:1664:C:H42	79:t:1673:U:H3	1.65	0.43
79:t:4051:C:H2'	79:t:4052:G:H8	1.83	0.43
1:S2:126:G:H8	24:SG:199:THR:HG21	1.82	0.43
1:S2:140:U:O2'	1:S2:143:U:OP1	2.35	0.43
1:S2:642:C:H2'	1:S2:643:A:H8	1.82	0.43
1:S2:1450:G:H2'	1:S2:1451:A:H8	1.82	0.43
1:S2:1563:U:H3	1:S2:1578:G:H1	1.66	0.43
1:S2:1682:A:H2'	6:SF:60:ARG:HD2	2.00	0.43
1:S2:1751:G:H1	1:S2:1789:U:H3	1.66	0.43
4:SD:159:HIS:O	4:SD:164:VAL:HG21	2.19	0.43
16:SU:91:LEU:HB3	16:SU:92:HIS:H	1.70	0.43
23:SC:73:MET:HE3	23:SC:73:MET:HB3	1.86	0.43
24:SG:85:ARG:NH2	30:SY:118:ARG:HG2	2.33	0.43
36:B:324:GLY:HA2	79:t:4780:C:H4'	2.00	0.43
43:I:147:VAL:HG12	43:I:177:MET:HG3	2.00	0.43
48:N:24:LEU:HD11	48:N:86:TRP:CG	2.53	0.43
49:O:183:THR:O	49:O:183:THR:OG1	2.29	0.43
55:U:100:LYS:HB2	79:t:1632:U:H4'	1.99	0.43
78:r:85:ASN:O	78:r:87:ARG:N	2.51	0.43
79:t:1099:C:O2	79:t:1099:C:H2'	2.17	0.43
79:t:2602:G:H2'	79:t:2603:G:C5	2.54	0.43
79:t:3342:U:H2'	79:t:3343:A:C8	2.54	0.43
79:t:4284:U:H2'	79:t:4285:A:C8	2.52	0.43
80:u:76:A:O2'	84:y:38:LYS:O	2.34	0.43
1:S2:24:C:H4'	1:S2:418:A:H4'	2.01	0.43
1:S2:326:C:H2'	1:S2:330:G:H22	1.84	0.43
1:S2:549:G:H2'	1:S2:550:G:H8	1.82	0.43
1:S2:815:A:O2'	5:SE:12:VAL:O	2.32	0.43
1:S2:1514:U:H2'	1:S2:1515:C:H6	1.83	0.43
1:S2:1596:C:H1'	15:ST:12:GLN:HE22	1.83	0.43
16:SU:56:MET:HB3	16:SU:56:MET:HE2	1.74	0.43
24:SG:12:CYS:SG	24:SG:13:GLN:N	2.91	0.43
36:B:378:ARG:HE	58:X:32:LEU:HD21	1.82	0.43
41:G:274:VAL:HB	41:G:277:LEU:HB2	2.00	0.43
80:u:68:C:H2'	80:u:69:G:H8	1.83	0.43
83:Cz:26:ARG:HA	83:Cz:26:ARG:HD2	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:Cz:59:PRO:HB3	83:Cz:170:GLY:HA2	2.01	0.43
83:Cz:176:ASP:N	83:Cz:176:ASP:OD1	2.51	0.43
1:S2:877:G:H2'	1:S2:878:A:H8	1.83	0.43
1:S2:1078:C:H2'	1:S2:1079:G:H8	1.83	0.43
1:S2:1101:C:H2'	1:S2:1102:G:C8	2.52	0.43
1:S2:1656:U:H2'	1:S2:1657:G:C8	2.53	0.43
41:G:234:LYS:H	41:G:245:THR:HG23	1.84	0.43
76:p:39:ARG:HD2	79:t:295:A:H5'	2.00	0.43
79:t:495:G:H22	79:t:637:G:H22	1.64	0.43
79:t:1456:G:O2'	79:t:1478:G:N2	2.46	0.43
79:t:3452:A:H2'	79:t:3453:A:H8	1.83	0.43
79:t:4482:C:H2'	79:t:4483:G:C8	2.53	0.43
1:S2:347:U:H2'	1:S2:348:U:C6	2.53	0.43
9:SK:32:HIS:HB3	9:SK:35:LEU:HB2	2.01	0.43
23:SC:79:GLU:OE2	23:SC:79:GLU:N	2.45	0.43
37:C:52:TYR:C	37:C:54:VAL:N	2.76	0.43
37:C:328:LEU:HD22	42:H:199:MET:HG3	2.01	0.43
40:F:140:GLY:O	79:t:1721:G:O2'	2.36	0.43
42:H:139:LYS:HB2	55:U:133:ALA:HB3	2.00	0.43
59:Y:153:ILE:HD11	59:Y:155:ILE:HD11	2.01	0.43
65:e:39:LYS:NZ	79:t:2213:U:O2	2.49	0.43
68:h:83:CYS:O	68:h:85:LYS:N	2.45	0.43
79:t:1200:C:H2'	79:t:1201:G:C8	2.52	0.43
83:Cz:17:VAL:O	83:Cz:23:ARG:NH2	2.52	0.43
1:S2:535:C:H2'	1:S2:536:A:C8	2.54	0.43
1:S2:1622:A:OP1	11:SP:47:ARG:NE	2.52	0.43
4:SD:15:GLY:HA3	21:Sd:50:ILE:HG23	2.01	0.43
6:SF:32:ASP:OD2	6:SF:34:SER:OG	2.33	0.43
8:SI:148:LYS:HE3	8:SI:148:LYS:HB3	1.81	0.43
13:SR:105:MET:HE3	13:SR:105:MET:HB3	1.84	0.43
17:SV:3:ASN:HA	23:SC:173:LYS:HE2	2.00	0.43
23:SC:257:LYS:NZ	23:SC:258:GLU:O	2.52	0.43
24:SG:30:LYS:HD3	24:SG:30:LYS:HA	1.80	0.43
28:SO:61:LYS:HA	28:SO:61:LYS:HD2	1.77	0.43
36:B:36:ASP:HB3	36:B:39:LYS:HG3	2.00	0.43
46:L:68:ILE:HD11	79:t:3990:C:H5'	2.00	0.43
57:W:107:ASN:OD1	57:W:111:GLU:N	2.52	0.43
65:e:93:ASN:OD1	65:e:93:ASN:N	2.51	0.43
66:f:77:PHE:HB2	78:r:23:GLN:HE22	1.83	0.43
79:t:436:C:H2'	79:t:437:G:H8	1.83	0.43
79:t:2412:C:H2'	79:t:2413:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:2452:G:H2'	79:t:2453:G:H8	1.84	0.43
79:t:4374:U:H2'	79:t:4375:G:H8	1.84	0.43
83:Cz:37:SER:HB3	83:Cz:202:ARG:HB3	2.01	0.43
1:S2:442:A:H4'	1:S2:1802:G:H4'	2.01	0.43
1:S2:548:A:H2'	1:S2:549:G:C8	2.54	0.43
1:S2:576:U:H3	1:S2:578:A:H3'	1.83	0.43
1:S2:1082:C:O2'	1:S2:1185:A:N1	2.50	0.43
1:S2:1859:C:H2'	1:S2:1860:G:C8	2.54	0.43
13:SR:8:THR:HA	13:SR:11:LYS:HE3	2.00	0.43
22:Sg:178:ASN:OD1	22:Sg:178:ASN:N	2.47	0.43
37:C:230:LEU:HD12	37:C:230:LEU:HA	1.89	0.43
50:P:82:ARG:HH22	79:t:3621:G:H5''	1.84	0.43
56:V:45:GLU:OE2	56:V:45:GLU:N	2.41	0.43
72:l:47:ILE:HG22	72:l:49:ASP:H	1.84	0.43
79:t:483:G:H5'	79:t:485:G:C5'	2.48	0.43
79:t:1116:C:H2'	79:t:1117:G:C8	2.54	0.43
79:t:1757:G:O6	79:t:1782:G:N2	2.52	0.43
82:w:16:C:H2'	82:w:17:G:H8	1.83	0.43
83:Cz:150:GLU:HA	83:Cz:154:THR:HB	2.01	0.43
1:S2:1103:A:OP1	13:SR:132:ARG:NH1	2.52	0.43
1:S2:1316:A:N6	26:SM:37:GLU:OE2	2.52	0.43
3:SB:221:PRO:O	3:SB:223:PHE:N	2.49	0.43
10:SL:84:ARG:HD3	10:SL:84:ARG:HA	1.74	0.43
45:K:32:ARG:HE	45:K:32:ARG:HB3	1.64	0.43
56:V:66:SER:OG	56:V:67:LYS:N	2.52	0.43
61:a:17:ARG:NH1	79:t:2422:G:N7	2.67	0.43
64:d:34:THR:HG23	64:d:95:ALA:HB2	2.00	0.43
72:l:26:LYS:NZ	72:l:28:ASN:OD1	2.47	0.43
79:t:469:C:H2'	79:t:470:A:H8	1.84	0.43
79:t:3804:C:H2'	79:t:3805:A:H8	1.84	0.43
1:S2:1596:C:H2'	1:S2:1597:A:C8	2.54	0.43
17:SV:42:SER:OG	17:SV:43:THR:N	2.52	0.43
17:SV:62:MET:SD	29:SW:20:ARG:NH2	2.92	0.43
25:SJ:21:GLU:N	25:SJ:21:GLU:OE2	2.51	0.43
38:D:30:U:H2'	38:D:31:G:H8	1.84	0.43
45:K:140:THR:OG1	45:K:141:LYS:N	2.51	0.43
56:V:106:SER:OG	56:V:107:LYS:N	2.49	0.43
76:p:99:ARG:HE	76:p:102:GLN:NE2	2.16	0.43
79:t:1250:U:H2'	79:t:1251:G:H8	1.84	0.43
79:t:4044:U:H2'	79:t:4045:A:C8	2.54	0.43
79:t:4124:G:N2	79:t:4127:U:O2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:4269:C:H2'	79:t:4270:G:C8	2.53	0.43
79:t:4478:G:H22	79:t:4683:G:H22	1.66	0.43
80:u:27:G:H1	80:u:43:C:H41	1.66	0.43
83:Cz:169:VAL:HG11	83:Cz:183:ILE:HG22	2.01	0.43
1:S2:388:G:O2'	8:SI:10:LYS:NZ	2.51	0.42
1:S2:826:PSU:N1	25:SJ:143:ASN:OD1	2.44	0.42
2:SA:22:GLY:O	2:SA:24:HIS:ND1	2.43	0.42
9:SK:49:MET:HA	9:SK:52:LEU:HD13	1.99	0.42
10:SL:48:LYS:HB2	10:SL:48:LYS:HE2	1.83	0.42
22:Sg:192:THR:OG1	22:Sg:193:GLY:N	2.52	0.42
24:SG:181:THR:HG22	24:SG:184:VAL:HG23	2.01	0.42
48:N:97:ALA:O	50:P:198:THR:HG21	2.18	0.42
51:Q:94:MET:HE1	51:Q:146:ILE:HB	2.01	0.42
59:Y:64:SER:OG	59:Y:65:ALA:N	2.52	0.42
65:e:101:LYS:HD3	65:e:101:LYS:HA	1.80	0.42
79:t:1885:A:H4'	79:t:1886:A:H5'	2.00	0.42
79:t:2364:C:H2'	79:t:2365:G:C8	2.54	0.42
79:t:2365:G:H5'	79:t:2484:G:H1'	2.00	0.42
79:t:3885:C:H2'	79:t:3886:G:H8	1.84	0.42
1:S2:983:A:H2'	1:S2:984:A:C8	2.54	0.42
40:F:263:LYS:NZ	40:F:264:LYS:O	2.45	0.42
52:R:73:PRO:O	79:t:1359:G:O2'	2.33	0.42
60:Z:1:MET:HE3	79:t:1270:C:C2	2.53	0.42
79:t:490:G:H8	79:t:490:G:O5'	2.02	0.42
79:t:1734:C:H6	79:t:1734:C:H5''	1.84	0.42
79:t:3562:G:O2'	79:t:3564:G:OP2	2.25	0.42
79:t:3596:A:H2'	79:t:3597:A:H8	1.84	0.42
79:t:3820:C:H2'	79:t:3821:G:C8	2.53	0.42
79:t:4006:A:H2'	79:t:4007:G:C8	2.53	0.42
1:S2:77:A:O2'	24:SG:174:PRO:O	2.37	0.42
1:S2:1867:U:H3'	19:Sa:5:ARG:HH21	1.84	0.42
2:SA:22:GLY:O	2:SA:24:HIS:N	2.51	0.42
3:SB:82:ARG:NH2	3:SB:191:ASP:OD2	2.52	0.42
9:SK:49:MET:HE3	9:SK:49:MET:HB2	1.86	0.42
11:SP:69:PRO:HB2	11:SP:70:MET:HE3	2.00	0.42
40:F:41:LYS:NZ	55:U:32:ARG:O	2.38	0.42
44:J:41:ILE:HD13	44:J:73:ILE:HD11	2.01	0.42
61:a:50:PRO:HD3	61:a:68:ILE:HG12	2.00	0.42
79:t:842:A:H2'	79:t:843:G:H8	1.83	0.42
79:t:2397:A:H2	79:t:2609:A:H62	1.68	0.42
1:S2:345:C:H2'	1:S2:346:A:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:956:C:O2	28:SO:55:ARG:NH1	2.40	0.42
1:S2:1848:A:H2'	1:S2:1849:G:C8	2.54	0.42
3:SB:167:LYS:HA	3:SB:167:LYS:HD3	1.85	0.42
5:SE:159:THR:HB	5:SE:173:ILE:HB	2.01	0.42
8:SI:28:GLU:OE2	8:SI:28:GLU:N	2.53	0.42
8:SI:93:THR:HG23	8:SI:95:THR:HG22	2.00	0.42
23:SC:80:GLU:OE1	23:SC:80:GLU:N	2.41	0.42
27:SN:29:THR:OG1	27:SN:32:ASP:OD2	2.38	0.42
38:D:155:C:OP2	43:I:89:ARG:NH1	2.52	0.42
41:G:174:PHE:HA	41:G:185:VAL:HG23	2.00	0.42
52:R:172:ARG:HD2	62:b:57:GLY:HA3	2.01	0.42
71:k:17:THR:HG23	73:m:51:LEU:HD21	2.02	0.42
74:n:96:CYS:SG	74:n:97:ARG:N	2.91	0.42
79:t:3583:U:H2'	79:t:3584:A:C8	2.54	0.42
1:S2:94:G:HO2'	1:S2:511:A:HO2'	1.64	0.42
1:S2:910:G:H2'	1:S2:911:A:C8	2.54	0.42
1:S2:932:G:N2	1:S2:1107:G:O2'	2.53	0.42
1:S2:1863:A:H3'	19:Sa:8:ASN:HB3	2.01	0.42
16:SU:35:VAL:HG11	16:SU:110:VAL:HG11	2.01	0.42
27:SN:86:GLU:O	27:SN:90:HIS:ND1	2.47	0.42
39:E:35:U:O2'	40:F:155:THR:O	2.35	0.42
41:G:122:MET:HE3	41:G:122:MET:HB3	1.89	0.42
41:G:133:ARG:HH12	79:t:894:C:H41	1.65	0.42
78:r:22:LYS:HD3	78:r:22:LYS:HA	1.72	0.42
79:t:476:G:H1	79:t:655:G:H22	1.66	0.42
79:t:1324:A:OP2	79:t:1405:C:N4	2.46	0.42
79:t:1407:A:H4'	79:t:1408:G:H5'	2.02	0.42
79:t:1409:C:H2'	79:t:1410:G:H8	1.85	0.42
79:t:1720:G:O2'	79:t:1722:C:OP2	2.32	0.42
79:t:1872:A:N6	79:t:1916:U:OP2	2.48	0.42
79:t:3467:A:H2'	79:t:3468:A:C8	2.54	0.42
79:t:4412:G:H2'	79:t:4413:A:C8	2.55	0.42
79:t:4624:G:H2'	79:t:4625:G:H8	1.85	0.42
1:S2:875:A:O2'	1:S2:877:G:OP2	2.38	0.42
9:SK:71:LEU:HD13	9:SK:76:ILE:HG22	2.01	0.42
34:Sf:124:ASP:OD1	34:Sf:124:ASP:N	2.53	0.42
38:D:14:U:H5''	51:Q:123:PRO:HD3	2.01	0.42
38:D:132:G:H2'	38:D:133:G:H8	1.85	0.42
40:F:4:VAL:HG23	40:F:5:LYS:HE2	2.02	0.42
60:Z:52:ASP:HB2	60:Z:110:LYS:HD3	2.01	0.42
62:b:7:LYS:NZ	79:t:2128:G:OP1	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:p:63:THR:OG1	79:t:3961:U:OP1	2.32	0.42
79:t:1252:C:H2'	79:t:1253:G:C8	2.54	0.42
79:t:1772:C:H2'	79:t:1773:A:H8	1.84	0.42
79:t:2435:A:H2'	79:t:2436:U:H6	1.85	0.42
79:t:2601:A:H2'	79:t:2602:G:C8	2.54	0.42
83:Cz:214:GLN:OE1	83:Cz:214:GLN:N	2.52	0.42
1:S2:966:A:H2'	1:S2:967:A:C8	2.54	0.42
1:S2:1450:G:H2'	1:S2:1451:A:C8	2.54	0.42
7:SH:165:ASN:OD1	7:SH:165:ASN:N	2.53	0.42
23:SC:169:TYR:OH	23:SC:175:GLY:O	2.33	0.42
24:SG:44:GLU:HB2	24:SG:119:LYS:HE2	2.00	0.42
25:SJ:67:ASP:HA	25:SJ:68:PRO:HD3	1.87	0.42
35:A:107:MET:HG2	35:A:111:THR:HG21	2.00	0.42
36:B:245:HIS:H	79:t:4257:C:H4'	1.83	0.42
44:J:41:ILE:HG22	44:J:43:VAL:HB	2.01	0.42
45:K:184:MET:HG2	45:K:190:LEU:HG	2.01	0.42
52:R:184:ARG:HA	52:R:184:ARG:HD3	1.94	0.42
63:c:106:LYS:HE3	63:c:106:LYS:HB3	1.86	0.42
66:f:67:LYS:HG2	79:t:2162:G:H5''	2.02	0.42
79:t:3885:C:H2'	79:t:3886:G:C8	2.55	0.42
83:Cz:48:ARG:HB3	83:Cz:159:MET:HE1	2.01	0.42
83:Cz:160:LYS:HA	83:Cz:160:LYS:HD3	1.74	0.42
1:S2:557:A:O2'	1:S2:558:A:N3	2.52	0.42
1:S2:1100:G:H4'	2:SA:32:PHE:CG	2.55	0.42
15:ST:104:LEU:HD13	15:ST:121:ARG:HD3	2.01	0.42
22:Sg:258:ILE:HG23	22:Sg:267:VAL:HB	2.01	0.42
27:SN:102:LEU:HD23	27:SN:102:LEU:HA	1.88	0.42
28:SO:125:LYS:HA	28:SO:125:LYS:HD3	1.87	0.42
33:Se:6:LEU:HD23	33:Se:6:LEU:HA	1.89	0.42
55:U:18:PRO:HG2	55:U:21:LYS:HB2	2.02	0.42
58:X:45:ASN:HB3	58:X:48:GLN:HB2	2.01	0.42
64:d:31:TYR:N	79:t:2518:A:OP2	2.53	0.42
77:q:44:LYS:NZ	79:t:2516:C:OP1	2.42	0.42
79:t:86:U:H2'	79:t:87:A:C8	2.55	0.42
79:t:3668:G:H2'	79:t:3669:G:H8	1.85	0.42
1:S2:160:U:O2'	1:S2:162:C:OP2	2.32	0.42
1:S2:319:G:H3'	24:SG:183:ARG:HH12	1.84	0.42
2:SA:57:LYS:HA	2:SA:57:LYS:HD2	1.94	0.42
6:SF:19:LEU:HD23	6:SF:19:LEU:HA	1.95	0.42
6:SF:168:THR:OG1	6:SF:171:GLU:OE1	2.31	0.42
14:SS:43:VAL:HG22	15:ST:36:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Sg:282:GLU:HA	22:Sg:283:PRO:HD2	1.93	0.42
35:A:117:GLU:OE2	35:A:163:ARG:NH2	2.53	0.42
36:B:39:LYS:HB3	36:B:39:LYS:HE3	1.79	0.42
57:W:96:LEU:HD23	58:X:20:ARG:HG2	2.01	0.42
58:X:21:TYR:HD2	58:X:29:PHE:HB2	1.83	0.42
60:Z:127:GLN:OE1	60:Z:130:LYS:NZ	2.53	0.42
79:t:3509:A:H2'	79:t:3510:A:C8	2.55	0.42
79:t:4448:C:H2'	79:t:4449:A:H8	1.84	0.42
1:S2:1356:A:OP1	2:SA:139:TYR:OH	2.34	0.42
4:SD:40:ARG:HH22	16:SU:106:ILE:HB	1.85	0.42
36:B:224:LYS:HB2	36:B:224:LYS:HE2	1.90	0.42
48:N:32:ASP:O	48:N:34:ASN:N	2.48	0.42
70:j:38:LYS:HB3	70:j:38:LYS:HE3	1.72	0.42
79:t:64:A:H1'	79:t:76:A:H1'	2.01	0.42
79:t:687:C:H2'	79:t:688:G:C8	2.54	0.42
79:t:691:C:H2'	79:t:692:G:H8	1.84	0.42
79:t:1064:G:H2'	79:t:1065:G:H8	1.84	0.42
79:t:1942:A:N7	79:t:4166:C:O2'	2.51	0.42
79:t:2451:C:H2'	79:t:2452:G:H8	1.84	0.42
79:t:4326:U:H2'	79:t:4327:G:C8	2.54	0.42
81:v:21:A:O2'	81:v:46:G:O6	2.33	0.42
2:SA:128:ARG:HA	2:SA:128:ARG:HD3	1.83	0.41
5:SE:18:TRP:HH2	5:SE:31:PRO:HD3	1.85	0.41
7:SH:7:LYS:HB3	7:SH:10:LYS:HB3	2.02	0.41
17:SV:62:MET:HE2	17:SV:62:MET:HB2	1.86	0.41
25:SJ:66:LYS:HE3	25:SJ:66:LYS:HB3	1.83	0.41
44:J:64:ARG:NH2	79:t:4425:C:OP1	2.50	0.41
54:T:127:MET:HA	55:U:153:PRO:HG2	2.02	0.41
56:V:98:ASP:OD1	56:V:98:ASP:N	2.52	0.41
60:Z:10:ASP:OD1	60:Z:11:ARG:N	2.53	0.41
70:j:19:LYS:HZ3	70:j:21:VAL:HG22	1.85	0.41
79:t:1197:U:H4'	79:t:1198:G:O4'	2.19	0.41
79:t:1349:U:H3	79:t:2000:G:H1	1.68	0.41
79:t:1413:C:H2'	79:t:1414:G:H8	1.84	0.41
79:t:1528:G:H4'	79:t:1529:G:H5'	2.01	0.41
79:t:3456:U:H2'	79:t:3457:G:H8	1.84	0.41
79:t:4121:C:H2'	79:t:4122:A:H8	1.85	0.41
81:v:64:A:H2'	81:v:65:G:C8	2.55	0.41
83:Cz:206:ILE:HG22	83:Cz:216:LEU:HD11	2.02	0.41
1:S2:17:C:H2'	1:S2:18:C:C6	2.55	0.41
1:S2:695:G:H2'	1:S2:696:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1395:U:H2'	1:S2:1396:G:H8	1.85	0.41
10:SL:144:LYS:HB3	10:SL:144:LYS:HE3	1.86	0.41
22:Sg:79:LEU:HD12	22:Sg:79:LEU:HA	1.92	0.41
30:SY:105:LYS:HD2	30:SY:105:LYS:HA	1.94	0.41
36:B:139:ASP:OD1	36:B:139:ASP:N	2.53	0.41
36:B:395:ASP:O	36:B:397:ILE:N	2.51	0.41
59:Y:89:LYS:HE3	59:Y:95:THR:HG21	2.03	0.41
79:t:419:A:N3	79:t:1234:C:O2'	2.47	0.41
79:t:492:C:H2'	79:t:493:G:C8	2.55	0.41
79:t:984:G:H22	79:t:1136:G:H1	1.68	0.41
79:t:1102:C:H2'	79:t:1103:G:C8	2.55	0.41
79:t:1187:U:O2'	79:t:1188:C:O5'	2.38	0.41
79:t:4786:C:H2'	79:t:4787:A:C8	2.55	0.41
1:S2:1363:U:O2'	1:S2:1382:A:OP2	2.33	0.41
1:S2:1515:C:H5''	21:Sd:8:TRP:HZ3	1.85	0.41
1:S2:1548:A:H2'	1:S2:1549:G:C8	2.56	0.41
1:S2:1664:A:H8	21:Sd:14:PHE:HB2	1.84	0.41
8:SI:83:TYR:OH	8:SI:201:LYS:NZ	2.49	0.41
15:ST:75:MET:HB3	15:ST:79:TYR:HE1	1.84	0.41
17:SV:1:MET:HE3	17:SV:1:MET:HB3	1.89	0.41
35:A:132:ASN:HD22	35:A:132:ASN:HA	1.69	0.41
41:G:234:LYS:HB2	41:G:245:THR:HA	2.03	0.41
45:K:28:ASP:OD1	45:K:28:ASP:N	2.53	0.41
48:N:103:LYS:HB3	48:N:103:LYS:HE2	1.89	0.41
50:P:54:TYR:OH	50:P:73:PHE:O	2.37	0.41
54:T:21:LYS:HE2	54:T:21:LYS:H	1.86	0.41
65:e:32:ARG:HD3	65:e:48:GLU:HB3	2.02	0.41
65:e:79:ASN:ND2	79:t:4368:U:O4	2.42	0.41
69:i:71:LYS:HE3	69:i:71:LYS:HB3	1.91	0.41
76:p:8:ARG:NH2	79:t:3964:U:O4	2.53	0.41
76:p:98:LYS:HE2	79:t:3965:A:H4'	2.00	0.41
79:t:1634:C:H2'	79:t:1635:G:C8	2.55	0.41
79:t:2108:C:O5'	79:t:2108:C:H6	2.02	0.41
79:t:4487:G:H22	79:t:4604:G:H22	1.69	0.41
79:t:4682:G:H2'	79:t:4683:G:C8	2.55	0.41
1:S2:584:U:O2'	30:SY:32:LYS:O	2.38	0.41
1:S2:1197:A:OP1	18:SX:60:LYS:NZ	2.50	0.41
1:S2:1298:A:H5'	1:S2:1299:U:H5	1.85	0.41
1:S2:1565:C:H2'	1:S2:1566:G:H8	1.85	0.41
13:SR:16:ILE:HG22	13:SR:24:LEU:HD21	2.03	0.41
17:SV:38:GLU:OE2	17:SV:38:GLU:N	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B:57:VAL:HB	36:B:367:PHE:HB3	2.03	0.41
38:D:67:U:H2'	38:D:68:G:C8	2.55	0.41
47:M:149:GLN:HE21	47:M:149:GLN:HB2	1.68	0.41
52:R:2:GLY:N	79:t:1973:C:OP1	2.53	0.41
62:b:13:GLY:HA2	79:t:1564:U:H3'	2.03	0.41
79:t:252:C:N4	79:t:253:G:O6	2.53	0.41
79:t:4704:G:O2'	79:t:4706:A:N6	2.52	0.41
83:Cz:67:VAL:HG13	83:Cz:111:LEU:HD22	2.01	0.41
83:Cz:215:ARG:NH1	83:Cz:216:LEU:O	2.53	0.41
1:S2:528:A:H5'	33:Se:32:ALA:HB2	2.03	0.41
1:S2:554:U:H2'	1:S2:555:G:C8	2.55	0.41
1:S2:603:G:H2'	1:S2:604:G:C8	2.56	0.41
1:S2:947:A:H5''	28:SO:134:PRO:HB3	2.02	0.41
1:S2:1132:G:H2'	1:S2:1133:G:C4	2.55	0.41
1:S2:1682:A:H5''	20:Sc:20:ARG:HH12	1.85	0.41
3:SB:113:MET:HE3	3:SB:142:PHE:HE1	1.85	0.41
8:SI:44:HIS:HB2	8:SI:56:ARG:HB3	2.03	0.41
13:SR:27:ASP:O	13:SR:31:ASN:ND2	2.39	0.41
31:SZ:81:GLY:O	31:SZ:83:LEU:N	2.54	0.41
37:C:54:VAL:CG2	37:C:107:THR:HG23	2.49	0.41
38:D:90:C:H2'	38:D:91:A:C8	2.56	0.41
39:E:82:G:H2'	39:E:83:A:C8	2.55	0.41
61:a:98:LYS:HE2	61:a:98:LYS:HB3	1.81	0.41
79:t:165:A:H61	79:t:271:C:N4	2.04	0.41
79:t:999:G:H2'	79:t:1000:G:C8	2.55	0.41
79:t:2119:G:H2'	79:t:2120:A:C8	2.56	0.41
79:t:3368:C:H2'	79:t:3369:G:C8	2.56	0.41
79:t:4493:G:H2'	79:t:4494:G:C8	2.54	0.41
79:t:4721:G:H2'	79:t:4722:G:C8	2.56	0.41
1:S2:84:A:O2'	30:SY:119:GLY:O	2.38	0.41
1:S2:435:G:H2'	1:S2:436:A:C8	2.54	0.41
1:S2:1467:C:H2'	1:S2:1468:A:C8	2.56	0.41
1:S2:1658:C:H2'	1:S2:1659:G:H8	1.85	0.41
1:S2:1739:G:H2'	1:S2:1740:G:C8	2.56	0.41
1:S2:1805:C:H2'	1:S2:1806:U:C6	2.56	0.41
5:SE:19:MET:HE3	5:SE:19:MET:HB3	1.88	0.41
12:SQ:131:LYS:HB2	12:SQ:140:ARG:HH12	1.85	0.41
15:ST:37:VAL:HG11	15:ST:52:TRP:HZ2	1.85	0.41
22:Sg:256:ILE:HD13	22:Sg:256:ILE:HA	1.94	0.41
27:SN:29:THR:OG1	27:SN:31:ASP:OD1	2.37	0.41
35:A:228:ASP:OD1	35:A:228:ASP:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B:95:THR:HG23	79:t:4637:A:H4'	2.03	0.41
41:G:61:ARG:O	79:t:1183:G:N1	2.39	0.41
41:G:125:TYR:HD1	78:r:115:SER:HB3	1.86	0.41
45:K:208:LYS:HE3	45:K:208:LYS:HB2	1.86	0.41
47:M:8:MET:HE2	47:M:8:MET:HB2	1.86	0.41
49:O:73:ARG:NH2	79:t:32:G:OP2	2.53	0.41
54:T:15:ARG:HD3	54:T:27:LEU:HD12	2.02	0.41
61:a:60:LYS:HE2	61:a:60:LYS:HB2	1.92	0.41
79:t:1621:C:H6	79:t:1621:C:H2'	1.70	0.41
79:t:1844:A:H2'	79:t:1845:A:C8	2.55	0.41
79:t:2179:C:H2'	79:t:2180:G:H8	1.85	0.41
1:S2:17:C:O2'	1:S2:1197:A:N1	2.46	0.41
1:S2:107:A:H2'	1:S2:108:G:C8	2.55	0.41
1:S2:156:G:N2	24:SG:60:GLY:O	2.41	0.41
1:S2:312:G:H21	1:S2:343:C:H1'	1.85	0.41
1:S2:332:G:H2'	1:S2:333:G:H8	1.85	0.41
1:S2:1010:C:H2'	1:S2:1011:A:C8	2.56	0.41
25:SJ:131:ARG:HD2	25:SJ:131:ARG:HA	1.92	0.41
36:B:56:ILE:HG22	36:B:368:ILE:HG12	2.02	0.41
36:B:85:VAL:HG12	36:B:204:GLN:HG2	2.01	0.41
36:B:138:GLN:O	36:B:143:LYS:NZ	2.53	0.41
42:H:39:GLU:OE2	42:H:39:GLU:N	2.49	0.41
44:J:23:ARG:HA	44:J:45:LEU:HD12	2.02	0.41
44:J:50:LYS:HB3	44:J:50:LYS:HE3	1.82	0.41
48:N:104:MET:HE2	48:N:104:MET:HB3	1.97	0.41
63:c:23:LYS:HD2	63:c:23:LYS:HA	1.88	0.41
79:t:1007:C:H2'	79:t:1008:G:C8	2.56	0.41
79:t:1877:G:H5'	79:t:1886:A:H4'	2.02	0.41
80:u:18:G:O2'	80:u:57:G:N1	2.44	0.41
83:Cz:19:HIS:H	83:Cz:19:HIS:CD2	2.38	0.41
83:Cz:32:VAL:HB	83:Cz:206:ILE:HD11	2.02	0.41
1:S2:92:A:H61	1:S2:447:G:H1'	1.85	0.41
1:S2:101:U:H5''	8:SI:19:LYS:HE2	2.02	0.41
1:S2:573:C:O2'	30:SY:34:THR:O	2.35	0.41
1:S2:1177:U:H2'	1:S2:1178:G:H8	1.84	0.41
1:S2:1859:C:H2'	1:S2:1860:G:H8	1.86	0.41
3:SB:64:GLY:HA2	3:SB:87:ILE:HD11	2.02	0.41
4:SD:154:ASP:OD1	4:SD:154:ASP:N	2.53	0.41
23:SC:257:LYS:HE3	23:SC:257:LYS:HB3	1.79	0.41
25:SJ:149:VAL:HG11	25:SJ:157:ILE:HD11	2.03	0.41
38:D:19:C:H2'	38:D:20:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:L:94:LEU:HD21	46:L:107:PHE:HD2	1.86	0.41
54:T:160:ARG:HD2	54:T:160:ARG:HA	1.85	0.41
68:h:65:MET:H	68:h:65:MET:HG2	1.62	0.41
76:p:31:ASP:OD2	79:t:4075:U:O2'	2.39	0.41
77:q:48:LYS:HB2	77:q:48:LYS:HE2	1.76	0.41
79:t:191:G:H2'	79:t:192:G:C8	2.56	0.41
79:t:1252:C:H2'	79:t:1253:G:H8	1.85	0.41
79:t:4152:U:H5''	79:t:4153:C:H5	1.85	0.41
79:t:4309:U:H2'	79:t:4310:G:C8	2.56	0.41
80:u:63:G:H2'	80:u:64:A:H8	1.86	0.41
1:S2:17:C:H4'	1:S2:1169:G:C8	2.56	0.41
1:S2:190:G:OP1	8:SI:139:LYS:NZ	2.43	0.41
1:S2:561:G:H4'	1:S2:562:G:OP1	2.21	0.41
1:S2:1013:G:H2'	1:S2:1014:A:H8	1.86	0.41
4:SD:218:LEU:HD13	22:Sg:189:ILE:HG21	2.02	0.41
7:SH:112:ASN:OD1	7:SH:112:ASN:N	2.54	0.41
12:SQ:16:LYS:O	12:SQ:17:LYS:C	2.64	0.41
12:SQ:105:LYS:HA	12:SQ:108:ILE:HG12	2.02	0.41
14:SS:34:LYS:HE3	14:SS:103:LEU:HD23	2.03	0.41
14:SS:84:LEU:HD22	14:SS:97:GLN:HB2	2.02	0.41
18:SX:139:GLU:OE1	18:SX:140:ARG:N	2.54	0.41
22:Sg:38:LYS:HA	22:Sg:65:PHE:HA	2.03	0.41
22:Sg:223:GLU:OE1	22:Sg:223:GLU:N	2.52	0.41
23:SC:116:THR:OG1	23:SC:119:GLY:O	2.31	0.41
34:Sf:113:LYS:HA	34:Sf:113:LYS:HD3	1.87	0.41
36:B:242:ARG:NH2	79:t:2700:C:O2	2.48	0.41
37:C:69:THR:HB	37:C:70:GLY:H	1.64	0.41
38:D:19:C:H2'	38:D:20:A:H8	1.85	0.41
38:D:78:G:H2'	38:D:79:G:C4	2.56	0.41
38:D:134:G:H5''	59:Y:63:LYS:HE2	2.02	0.41
42:H:175:ASN:HB3	42:H:176:LYS:H	1.70	0.41
58:X:52:THR:HG22	58:X:54:LEU:H	1.86	0.41
60:Z:87:ARG:NH1	79:t:386:A:O2'	2.54	0.41
63:c:51:LYS:HE3	63:c:51:LYS:HB3	1.88	0.41
66:f:14:LYS:O	66:f:16:ARG:N	2.54	0.41
73:m:29:MET:H	73:m:29:MET:HG2	1.69	0.41
75:o:7:LYS:HE3	75:o:11:ARG:HH21	1.86	0.41
76:p:6:LYS:HE3	76:p:94:GLY:HA3	2.01	0.41
76:p:28:LYS:O	79:t:4076:U:O2'	2.38	0.41
79:t:18:C:H2'	79:t:19:G:H8	1.86	0.41
79:t:476:G:H22	79:t:655:G:H22	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:1195:G:OP2	79:t:1195:G:N2	2.38	0.41
79:t:1208:C:H2'	79:t:1209:A:C8	2.52	0.41
79:t:1786:C:O2'	79:t:1970:A:O2'	2.39	0.41
79:t:2589:A:H2'	79:t:2590:A:C8	2.53	0.41
79:t:3337:C:H2'	79:t:3338:G:C8	2.55	0.41
79:t:3701:A:H2'	79:t:3702:G:C8	2.56	0.41
79:t:4053:U:H2'	79:t:4054:G:C8	2.56	0.41
79:t:4054:G:N2	79:t:4057:A:OP2	2.41	0.41
79:t:4370:U:H2'	79:t:4371:G:C8	2.56	0.41
80:u:19:G:O4'	80:u:57:G:N2	2.54	0.41
83:Cz:39:LYS:O	83:Cz:41:TYR:N	2.54	0.41
1:S2:1052:A:O2'	1:S2:1857:U:O2	2.39	0.41
1:S2:1801:C:H2'	1:S2:1802:G:O4'	2.21	0.41
1:S2:1844:C:H2'	1:S2:1845:4AC:H6	2.02	0.41
2:SA:111:GLN:OE1	2:SA:111:GLN:N	2.54	0.41
8:SI:3:ILE:H	8:SI:3:ILE:HG13	1.70	0.41
8:SI:173:ALA:HA	8:SI:189:VAL:HA	2.02	0.41
32:Sb:45:THR:OG1	32:Sb:82:LYS:NZ	2.54	0.41
37:C:52:TYR:O	37:C:54:VAL:N	2.54	0.41
38:D:96:C:H5'	69:i:66:LYS:HG2	2.03	0.41
40:F:50:ARG:NH1	40:F:147:ASP:OD2	2.54	0.41
45:K:101:LYS:HE3	45:K:101:LYS:HB3	1.90	0.41
65:e:59:THR:OG1	65:e:104:THR:OG1	2.36	0.41
79:t:281:U:H2'	79:t:282:C:H6	1.86	0.41
79:t:653:C:H2'	79:t:654:C:C6	2.56	0.41
79:t:1418:U:H2'	79:t:1419:A:C8	2.56	0.41
79:t:3345:A:H2'	79:t:3346:A:H8	1.86	0.41
79:t:3452:A:OP2	79:t:3470:G:N2	2.44	0.41
79:t:3615:G:H2'	79:t:3616:G:C8	2.56	0.41
79:t:3970:G:H2'	79:t:3971:A:H8	1.86	0.41
83:Cz:67:VAL:HG21	83:Cz:82:ILE:HD11	2.03	0.41
1:S2:332:G:H2'	1:S2:333:G:C8	2.56	0.40
1:S2:1571:C:H2'	1:S2:1572:A:C8	2.56	0.40
1:S2:1647:C:H4'	12:SQ:140:ARG:HB2	2.02	0.40
6:SF:49:LEU:HD23	12:SQ:47:LEU:HD12	2.03	0.40
6:SF:49:LEU:HA	6:SF:50:PRO:HD3	1.96	0.40
11:SP:9:LYS:HB3	11:SP:9:LYS:HE3	1.81	0.40
20:Sc:15:THR:OG1	20:Sc:31:ARG:O	2.32	0.40
20:Sc:34:PHE:O	20:Sc:36:ASP:N	2.48	0.40
24:SG:56:ASN:HB2	24:SG:108:VAL:HG12	2.02	0.40
26:SM:113:ASP:OD1	26:SM:115:GLY:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:J:13:PRO:HG2	44:J:16:VAL:HG22	2.02	0.40
52:R:160:HIS:HB2	52:R:161:SER:H	1.62	0.40
54:T:93:MET:HE1	54:T:117:HIS:CE1	2.56	0.40
57:W:30:ASP:HB3	57:W:104:VAL:HG12	2.02	0.40
63:c:11:ASN:ND2	79:t:1573:A:OP1	2.48	0.40
63:c:93:LEU:HD23	63:c:93:LEU:HA	1.92	0.40
1:S2:657:A:OP2	1:S2:658:A:O2'	2.32	0.40
1:S2:1192:A:H2'	1:S2:1193:A:H8	1.86	0.40
2:SA:117:ARG:HG3	2:SA:119:PRO:HD3	2.03	0.40
22:Sg:194:TYR:CE2	22:Sg:212:LYS:HD2	2.56	0.40
24:SG:135:PRO:HG2	24:SG:141:ILE:HG12	2.04	0.40
43:I:30:PRO:HB2	61:a:125:GLY:H	1.86	0.40
52:R:75:ARG:HH12	79:t:1361:G:H5''	1.86	0.40
53:S:117:ARG:NH1	79:t:2504:A:OP1	2.51	0.40
55:U:7:LYS:O	79:t:4066:U:O2'	2.29	0.40
57:W:13:LYS:NZ	57:W:57:VAL:O	2.53	0.40
68:h:60:ARG:HB2	68:h:63:VAL:HG23	2.04	0.40
79:t:1580:C:H41	79:t:4110:A:H2'	1.85	0.40
1:S2:166:A2M:HM'1	24:SG:11:GLY:HA2	2.03	0.40
6:SF:27:ASP:OD1	6:SF:27:ASP:N	2.50	0.40
8:SI:22:HIS:ND1	8:SI:23:LYS:O	2.49	0.40
8:SI:101:ILE:HG22	8:SI:174:CYS:HB2	2.03	0.40
23:SC:130:ILE:O	23:SC:138:GLY:N	2.49	0.40
36:B:257:TRP:HB3	79:t:4250:A:OP2	2.22	0.40
37:C:212:ASN:HB3	37:C:232:VAL:HG12	2.04	0.40
44:J:118:LEU:HD23	44:J:118:LEU:HA	1.92	0.40
45:K:91:LEU:HD23	45:K:91:LEU:HA	1.97	0.40
46:L:80:GLU:OE2	46:L:80:GLU:N	2.43	0.40
47:M:37:LYS:HA	47:M:37:LYS:HD2	1.82	0.40
47:M:42:LYS:HE3	47:M:46:ILE:HD11	2.02	0.40
61:a:17:ARG:H	68:h:76:ARG:HG3	1.85	0.40
79:t:365:U:H2'	79:t:366:A:H8	1.86	0.40
79:t:1178:C:H2'	79:t:1179:G:C8	2.57	0.40
79:t:2302:C:O2	79:t:3406:G:N2	2.54	0.40
80:u:58:A:O2'	80:u:60:U:OP2	2.34	0.40
83:Cz:67:VAL:HG22	83:Cz:111:LEU:HB3	2.03	0.40
1:S2:305:A:OP1	8:SI:74:ARG:NH1	2.54	0.40
1:S2:643:A:H2'	1:S2:644:A:C8	2.56	0.40
1:S2:831:G:N2	1:S2:833:A:O2'	2.53	0.40
1:S2:1524:C:OP1	14:SS:124:ARG:NH2	2.49	0.40
2:SA:63:ARG:HG3	17:SV:36:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:SA:198:MET:HG3	2:SA:200:ASP:H	1.86	0.40
3:SB:138:PHE:HD2	3:SB:214:LYS:HB3	1.86	0.40
15:ST:9:VAL:HG21	15:ST:138:VAL:HG13	2.04	0.40
19:Sa:23:CYS:SG	19:Sa:24:THR:N	2.94	0.40
36:B:13:SER:HB2	79:t:4354:A:H4'	2.03	0.40
43:I:217:LYS:HA	43:I:217:LYS:HE2	2.03	0.40
79:t:620:C:H2'	79:t:621:G:H8	1.86	0.40
79:t:1210:C:H2'	79:t:1211:C:C6	2.56	0.40
79:t:2167:C:H2'	79:t:2168:C:H6	1.87	0.40
79:t:2206:U:H2'	79:t:2207:A:C8	2.56	0.40
79:t:2440:G:H2'	79:t:2441:G:H8	1.87	0.40
79:t:2549:A:H61	79:t:2554:C:H42	1.69	0.40
80:u:19:G:N3	80:u:57:G:N2	2.69	0.40
1:S2:1338:G:OP1	4:SD:185:LYS:NZ	2.42	0.40
12:SQ:131:LYS:HB2	12:SQ:140:ARG:HH22	1.86	0.40
22:Sg:66:VAL:HA	22:Sg:82:SER:HA	2.02	0.40
41:G:193:ARG:NE	79:t:4667:A:OP1	2.37	0.40
50:P:185:VAL:O	50:P:188:LYS:NZ	2.55	0.40
79:t:441:G:H2'	79:t:442:G:C8	2.57	0.40
79:t:1222:U:O2'	79:t:1793:A:N1	2.47	0.40
79:t:1365:C:H2'	79:t:1366:A:C8	2.56	0.40
79:t:1570:C:O2'	79:t:1592:G:OP1	2.33	0.40
79:t:3992:U:H2'	79:t:3993:C:C6	2.57	0.40
79:t:4079:G:H2'	79:t:4080:A:C8	2.56	0.40
79:t:4478:G:N2	79:t:4683:G:H22	2.20	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	212/295 (72%)	196 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	SB	212/264 (80%)	201 (95%)	9 (4%)	2 (1%)	14	28
4	SD	224/243 (92%)	197 (88%)	23 (10%)	4 (2%)	6	15
5	SE	257/263 (98%)	238 (93%)	16 (6%)	3 (1%)	10	22
6	SF	187/204 (92%)	172 (92%)	15 (8%)	0	100	100
7	SH	182/194 (94%)	169 (93%)	12 (7%)	1 (0%)	24	42
8	SI	202/208 (97%)	183 (91%)	17 (8%)	2 (1%)	12	25
9	SK	96/165 (58%)	87 (91%)	9 (9%)	0	100	100
10	SL	148/158 (94%)	140 (95%)	6 (4%)	2 (1%)	9	19
11	SP	128/145 (88%)	121 (94%)	7 (6%)	0	100	100
12	SQ	144/146 (99%)	133 (92%)	9 (6%)	2 (1%)	9	19
13	SR	132/135 (98%)	115 (87%)	16 (12%)	1 (1%)	16	31
14	SS	143/152 (94%)	127 (89%)	15 (10%)	1 (1%)	18	35
15	ST	141/145 (97%)	134 (95%)	7 (5%)	0	100	100
16	SU	102/119 (86%)	95 (93%)	6 (6%)	1 (1%)	12	25
17	SV	80/83 (96%)	75 (94%)	5 (6%)	0	100	100
18	SX	139/143 (97%)	123 (88%)	16 (12%)	0	100	100
19	Sa	101/115 (88%)	95 (94%)	6 (6%)	0	100	100
20	Sc	62/69 (90%)	51 (82%)	11 (18%)	0	100	100
21	Sd	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
22	Sg	310/317 (98%)	273 (88%)	37 (12%)	0	100	100
23	SC	224/293 (76%)	208 (93%)	16 (7%)	0	100	100
24	SG	235/249 (94%)	217 (92%)	18 (8%)	0	100	100
25	SJ	184/194 (95%)	169 (92%)	14 (8%)	1 (0%)	24	42
26	SM	116/132 (88%)	101 (87%)	15 (13%)	0	100	100
27	SN	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
28	SO	135/151 (89%)	120 (89%)	15 (11%)	0	100	100
29	SW	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
30	SY	130/133 (98%)	118 (91%)	12 (9%)	0	100	100
31	SZ	71/125 (57%)	62 (87%)	9 (13%)	0	100	100
32	Sb	80/84 (95%)	75 (94%)	5 (6%)	0	100	100
33	Se	55/59 (93%)	48 (87%)	7 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	Sf	65/156 (42%)	51 (78%)	14 (22%)	0	100	100
35	A	250/257 (97%)	231 (92%)	19 (8%)	0	100	100
36	B	395/403 (98%)	367 (93%)	28 (7%)	0	100	100
37	C	361/421 (86%)	333 (92%)	21 (6%)	7 (2%)	6	14
40	F	292/297 (98%)	275 (94%)	15 (5%)	2 (1%)	18	35
41	G	239/298 (80%)	209 (87%)	28 (12%)	2 (1%)	16	31
42	H	223/260 (86%)	210 (94%)	13 (6%)	0	100	100
43	I	239/266 (90%)	222 (93%)	17 (7%)	0	100	100
44	J	189/192 (98%)	176 (93%)	12 (6%)	1 (0%)	24	42
45	K	204/214 (95%)	193 (95%)	11 (5%)	0	100	100
46	L	168/178 (94%)	159 (95%)	8 (5%)	1 (1%)	21	38
47	M	203/211 (96%)	175 (86%)	25 (12%)	3 (2%)	8	18
48	N	137/214 (64%)	132 (96%)	5 (4%)	0	100	100
49	O	201/204 (98%)	191 (95%)	9 (4%)	1 (0%)	24	42
50	P	195/203 (96%)	189 (97%)	5 (3%)	1 (0%)	24	42
51	Q	156/184 (85%)	151 (97%)	5 (3%)	0	100	100
52	R	185/188 (98%)	172 (93%)	13 (7%)	0	100	100
53	S	186/196 (95%)	180 (97%)	6 (3%)	0	100	100
54	T	174/176 (99%)	160 (92%)	14 (8%)	0	100	100
55	U	156/160 (98%)	149 (96%)	6 (4%)	1 (1%)	21	38
56	V	97/128 (76%)	94 (97%)	3 (3%)	0	100	100
57	W	132/140 (94%)	126 (96%)	6 (4%)	0	100	100
58	X	59/157 (38%)	56 (95%)	3 (5%)	0	100	100
59	Y	118/156 (76%)	114 (97%)	4 (3%)	0	100	100
60	Z	132/145 (91%)	124 (94%)	8 (6%)	0	100	100
61	a	132/136 (97%)	122 (92%)	10 (8%)	0	100	100
62	b	145/148 (98%)	133 (92%)	12 (8%)	0	100	100
63	c	91/156 (58%)	86 (94%)	5 (6%)	0	100	100
64	d	99/115 (86%)	93 (94%)	6 (6%)	0	100	100
65	e	104/125 (83%)	99 (95%)	5 (5%)	0	100	100
66	f	127/135 (94%)	118 (93%)	8 (6%)	1 (1%)	16	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	g	107/110 (97%)	102 (95%)	5 (5%)	0	100	100
68	h	114/117 (97%)	106 (93%)	8 (7%)	0	100	100
69	i	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
70	j	102/105 (97%)	95 (93%)	7 (7%)	0	100	100
71	k	84/97 (87%)	79 (94%)	3 (4%)	2 (2%)	4	10
72	l	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
73	m	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
74	n	48/128 (38%)	46 (96%)	2 (4%)	0	100	100
75	o	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
76	p	103/106 (97%)	93 (90%)	9 (9%)	1 (1%)	12	25
77	q	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
78	r	129/137 (94%)	114 (88%)	15 (12%)	0	100	100
83	Cz	215/217 (99%)	183 (85%)	31 (14%)	1 (0%)	24	42
84	y	2/4 (50%)	2 (100%)	0	0	100	100
All	All	11465/12921 (89%)	10600 (92%)	821 (7%)	44 (0%)	31	48

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	SB	191	ASP
5	SE	165	GLU
10	SL	82	MET
37	C	55	SER
37	C	58	ALA
83	Cz	60	ARG
37	C	54	VAL
37	C	56	GLU
37	C	318	PRO
47	M	46	ILE
55	U	4	THR
71	k	86	PRO
76	p	76	ASN
4	SD	213	PRO
12	SQ	127	CYS
37	C	57	LEU
4	SD	202	LYS
8	SI	98	LYS

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Mol	Chain	Res	Type
16	SU	107	GLU
25	SJ	67	ASP
37	C	319	LEU
41	G	117	VAL
49	O	145	ASN
3	SB	130	THR
4	SD	192	TRP
10	SL	23	VAL
40	F	6	VAL
46	L	111	GLU
47	M	157	ILE
4	SD	162	ASP
5	SE	98	ASN
7	SH	99	ARG
13	SR	129	LYS
14	SS	49	ASP
40	F	253	TYR
44	J	2	LYS
47	M	164	GLU
66	f	19	LYS
8	SI	97	VAL
71	k	85	LYS
5	SE	30	ARG
12	SQ	100	VAL
41	G	116	VAL
50	P	146	GLY

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	179/242 (74%)	176 (98%)	3 (2%)	53	75
3	SB	195/231 (84%)	194 (100%)	1 (0%)	81	90
4	SD	189/202 (94%)	188 (100%)	1 (0%)	81	90
5	SE	222/225 (99%)	220 (99%)	2 (1%)	70	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	SF	159/171 (93%)	157 (99%)	2 (1%)	61	79
7	SH	166/174 (95%)	163 (98%)	3 (2%)	51	73
8	SI	177/180 (98%)	176 (99%)	1 (1%)	78	89
9	SK	89/136 (65%)	88 (99%)	1 (1%)	65	81
10	SL	134/142 (94%)	132 (98%)	2 (2%)	57	77
11	SP	116/130 (89%)	114 (98%)	2 (2%)	53	75
12	SQ	121/121 (100%)	116 (96%)	5 (4%)	27	52
13	SR	120/121 (99%)	119 (99%)	1 (1%)	73	86
14	SS	126/132 (96%)	126 (100%)	0	100	100
15	ST	113/115 (98%)	112 (99%)	1 (1%)	70	84
16	SU	94/107 (88%)	94 (100%)	0	100	100
17	SV	66/67 (98%)	66 (100%)	0	100	100
18	SX	113/115 (98%)	112 (99%)	1 (1%)	70	84
19	Sa	89/98 (91%)	85 (96%)	4 (4%)	24	48
20	Sc	57/62 (92%)	55 (96%)	2 (4%)	32	57
21	Sd	48/49 (98%)	45 (94%)	3 (6%)	16	34
22	Sg	271/275 (98%)	259 (96%)	12 (4%)	25	49
23	SC	191/224 (85%)	185 (97%)	6 (3%)	35	60
24	SG	207/218 (95%)	204 (99%)	3 (1%)	59	78
25	SJ	162/168 (96%)	158 (98%)	4 (2%)	42	66
26	SM	98/108 (91%)	94 (96%)	4 (4%)	27	52
27	SN	130/131 (99%)	128 (98%)	2 (2%)	57	77
28	SO	107/119 (90%)	104 (97%)	3 (3%)	38	62
29	SW	112/113 (99%)	110 (98%)	2 (2%)	51	73
30	SY	114/115 (99%)	113 (99%)	1 (1%)	70	84
31	SZ	64/103 (62%)	61 (95%)	3 (5%)	23	47
32	Sb	74/76 (97%)	74 (100%)	0	100	100
33	Se	46/48 (96%)	45 (98%)	1 (2%)	45	69
34	Sf	60/140 (43%)	60 (100%)	0	100	100
35	A	194/199 (98%)	187 (96%)	7 (4%)	31	56
36	B	345/349 (99%)	332 (96%)	13 (4%)	29	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	C	304/349 (87%)	290 (95%)	14 (5%)	24	48
40	F	248/250 (99%)	242 (98%)	6 (2%)	43	67
41	G	216/256 (84%)	212 (98%)	4 (2%)	50	72
42	H	195/224 (87%)	193 (99%)	2 (1%)	68	83
43	I	205/223 (92%)	197 (96%)	8 (4%)	28	54
44	J	171/172 (99%)	167 (98%)	4 (2%)	44	68
45	K	178/181 (98%)	172 (97%)	6 (3%)	32	58
46	L	143/149 (96%)	138 (96%)	5 (4%)	32	57
47	M	171/177 (97%)	165 (96%)	6 (4%)	32	57
48	N	118/157 (75%)	116 (98%)	2 (2%)	53	75
49	O	171/172 (99%)	166 (97%)	5 (3%)	37	61
50	P	169/173 (98%)	165 (98%)	4 (2%)	43	67
51	Q	139/163 (85%)	135 (97%)	4 (3%)	37	61
52	R	164/165 (99%)	163 (99%)	1 (1%)	78	89
53	S	167/175 (95%)	165 (99%)	2 (1%)	63	80
54	T	156/156 (100%)	152 (97%)	4 (3%)	40	65
55	U	139/140 (99%)	131 (94%)	8 (6%)	18	38
56	V	89/114 (78%)	83 (93%)	6 (7%)	15	31
57	W	102/107 (95%)	98 (96%)	4 (4%)	28	54
58	X	53/126 (42%)	53 (100%)	0	100	100
59	Y	108/133 (81%)	106 (98%)	2 (2%)	50	72
60	Z	124/135 (92%)	122 (98%)	2 (2%)	55	76
61	a	117/118 (99%)	115 (98%)	2 (2%)	53	75
62	b	120/121 (99%)	119 (99%)	1 (1%)	73	86
63	c	80/124 (64%)	78 (98%)	2 (2%)	42	66
64	d	86/97 (89%)	84 (98%)	2 (2%)	44	68
65	e	97/110 (88%)	94 (97%)	3 (3%)	35	60
66	f	115/121 (95%)	114 (99%)	1 (1%)	70	84
67	g	88/89 (99%)	86 (98%)	2 (2%)	44	68
68	h	99/100 (99%)	97 (98%)	2 (2%)	48	71
69	i	109/110 (99%)	107 (98%)	2 (2%)	51	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	j	88/89 (99%)	87 (99%)	1 (1%)	65	81
71	k	73/80 (91%)	71 (97%)	2 (3%)	39	63
72	l	64/65 (98%)	63 (98%)	1 (2%)	55	76
73	m	47/48 (98%)	47 (100%)	0	100	100
74	n	46/116 (40%)	46 (100%)	0	100	100
75	o	24/24 (100%)	22 (92%)	2 (8%)	10	22
76	p	93/94 (99%)	93 (100%)	0	100	100
77	q	74/75 (99%)	70 (95%)	4 (5%)	20	42
78	r	115/121 (95%)	112 (97%)	3 (3%)	40	65
83	Cz	195/196 (100%)	192 (98%)	3 (2%)	57	77
84	y	1/1 (100%)	1 (100%)	0	100	100
All	All	10009/11002 (91%)	9781 (98%)	228 (2%)	44	68

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SA	75	SER
2	SA	76	VAL
2	SA	130	ASP
3	SB	203	SER
4	SD	84	VAL
5	SE	89	VAL
5	SE	183	VAL
6	SF	49	LEU
6	SF	111	VAL
7	SH	45	ILE
7	SH	95	ILE
7	SH	130	LEU
8	SI	96	LEU
9	SK	1	MET
10	SL	23	VAL
10	SL	65	ASN
11	SP	24	GLN
11	SP	96	VAL
12	SQ	22	VAL
12	SQ	31	LEU
12	SQ	70	VAL
12	SQ	72	VAL

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Mol	Chain	Res	Type
12	SQ	127	CYS
13	SR	57	LEU
15	ST	87	VAL
18	SX	125	VAL
19	Sa	2	THR
19	Sa	45	VAL
19	Sa	50	VAL
19	Sa	63	VAL
20	Sc	17	VAL
20	Sc	57	THR
21	Sd	16	GLN
21	Sd	30	LEU
21	Sd	41	GLN
22	Sg	5	MET
22	Sg	35	SER
22	Sg	63	SER
22	Sg	64	HIS
22	Sg	71	ILE
22	Sg	96	THR
22	Sg	105	THR
22	Sg	120	ILE
22	Sg	179	LEU
22	Sg	231	ASP
22	Sg	234	ASP
22	Sg	314	ILE
23	SC	72	ASP
23	SC	163	VAL
23	SC	214	LEU
23	SC	244	ILE
23	SC	254	ASP
23	SC	260	VAL
24	SG	12	CYS
24	SG	89	THR
24	SG	237	LEU
25	SJ	15	THR
25	SJ	86	VAL
25	SJ	144	ILE
25	SJ	173	VAL
26	SM	42	LEU
26	SM	51	VAL
26	SM	76	LEU
26	SM	103	VAL

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Mol	Chain	Res	Type
27	SN	21	SER
27	SN	32	ASP
28	SO	27	VAL
28	SO	40	THR
28	SO	151	LEU
29	SW	13	SER
29	SW	80	ASP
30	SY	120	THR
31	SZ	57	LYS
31	SZ	58	LEU
31	SZ	113	THR
33	Se	46	VAL
35	A	32	VAL
35	A	61	VAL
35	A	102	LEU
35	A	160	SER
35	A	207	VAL
35	A	243	THR
35	A	246	LEU
36	B	60	VAL
36	B	73	VAL
36	B	85	VAL
36	B	90	VAL
36	B	93	VAL
36	B	94	GLU
36	B	168	MET
36	B	181	MET
36	B	302	ASN
36	B	337	VAL
36	B	344	VAL
36	B	350	SER
36	B	395	ASP
37	C	7	LEU
37	C	54	VAL
37	C	69	THR
37	C	94	ASN
37	C	150	LEU
37	C	255	SER
37	C	266	THR
37	C	291	ARG
37	C	313	VAL
37	C	345	ARG

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Mol	Chain	Res	Type
37	C	348	LYS
37	C	350	ARG
37	C	352	LYS
37	C	353	LYS
40	F	118	ILE
40	F	126	ASN
40	F	132	VAL
40	F	136	ASP
40	F	155	THR
40	F	172	SER
41	G	117	VAL
41	G	178	LEU
41	G	268	LEU
41	G	274	VAL
42	H	116	LYS
42	H	189	ARG
43	I	22	GLN
43	I	27	VAL
43	I	28	VAL
43	I	70	LEU
43	I	128	VAL
43	I	167	VAL
43	I	202	VAL
43	I	218	LEU
44	J	6	SER
44	J	24	THR
44	J	84	VAL
44	J	163	GLN
45	K	26	VAL
45	K	31	ILE
45	K	62	SER
45	K	102	MET
45	K	164	LYS
45	K	197	VAL
46	L	39	VAL
46	L	47	THR
46	L	70	VAL
46	L	83	LEU
46	L	150	CYS
47	M	8	MET
47	M	22	VAL
47	M	59	VAL

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Mol	Chain	Res	Type
47	M	105	LYS
47	M	121	ARG
47	M	144	LEU
48	N	16	SER
48	N	118	MET
49	O	5	LYS
49	O	44	ARG
49	O	75	VAL
49	O	92	LEU
49	O	125	SER
50	P	27	VAL
50	P	184	ASN
50	P	185	VAL
50	P	191	LYS
51	Q	6	LEU
51	Q	10	ASN
51	Q	24	VAL
51	Q	87	SER
52	R	183	SER
53	S	12	SER
53	S	23	TRP
54	T	16	CYS
54	T	19	THR
54	T	48	VAL
54	T	156	HIS
55	U	4	THR
55	U	42	ILE
55	U	48	VAL
55	U	68	THR
55	U	80	VAL
55	U	125	TRP
55	U	126	VAL
55	U	129	LYS
56	V	25	CYS
56	V	62	THR
56	V	65	ARG
56	V	73	THR
56	V	76	VAL
56	V	79	SER
57	W	28	CYS
57	W	91	LYS
57	W	99	GLU

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Mol	Chain	Res	Type
57	W	118	THR
59	Y	47	ARG
59	Y	82	THR
60	Z	55	VAL
60	Z	95	VAL
61	a	13	VAL
61	a	119	GLU
62	b	140	VAL
63	c	12	GLN
63	c	55	LYS
64	d	48	LEU
64	d	78	ASN
65	e	84	ILE
65	e	98	SER
65	e	122	VAL
66	f	87	VAL
67	g	84	VAL
67	g	90	SER
68	h	5	LEU
68	h	102	ILE
69	i	18	LEU
69	i	82	ASP
70	j	17	VAL
71	k	6	SER
71	k	83	THR
72	l	46	VAL
75	o	13	LEU
75	o	25	LYS
77	q	8	VAL
77	q	74	THR
77	q	75	SER
77	q	91	ASP
78	r	27	THR
78	r	61	VAL
78	r	80	THR
83	Cz	118	LYS
83	Cz	162	VAL
83	Cz	190	LEU

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

Mol	Chain	Res	Type
2	SA	141	ASN
2	SA	215	GLN
3	SB	157	GLN
3	SB	186	ASN
4	SD	101	GLN
4	SD	165	ASN
5	SE	17	HIS
6	SF	101	HIS
6	SF	118	ASN
7	SH	114	GLN
9	SK	50	GLN
10	SL	65	ASN
10	SL	83	GLN
11	SP	103	ASN
12	SQ	11	GLN
12	SQ	80	GLN
12	SQ	86	GLN
12	SQ	142	GLN
13	SR	116	ASN
13	SR	118	GLN
14	SS	19	ASN
14	SS	72	GLN
14	SS	73	ASN
14	SS	105	ASN
16	SU	92	HIS
17	SV	21	ASN
17	SV	47	ASN
18	SX	16	HIS
18	SX	20	GLN
18	SX	31	HIS
19	Sa	25	ASN
20	Sc	29	GLN
21	Sd	45	GLN
22	Sg	15	ASN
22	Sg	51	ASN
22	Sg	119	GLN
22	Sg	181	ASN
22	Sg	187	ASN
23	SC	115	GLN
23	SC	235	ASN
23	SC	277	HIS
24	SG	56	ASN
24	SG	187	HIS

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Mol	Chain	Res	Type
25	SJ	111	GLN
26	SM	119	GLN
28	SO	38	ASN
28	SO	103	ASN
29	SW	24	GLN
29	SW	90	GLN
29	SW	91	ASN
30	SY	112	ASN
31	SZ	46	ASN
33	Se	44	ASN
34	Sf	93	HIS
35	A	22	HIS
35	A	95	GLN
35	A	140	ASN
35	A	194	ASN
35	A	205	ASN
36	B	121	ASN
36	B	208	ASN
36	B	213	GLN
36	B	289	GLN
36	B	328	ASN
37	C	43	ASN
37	C	223	ASN
37	C	286	ASN
37	C	299	GLN
37	C	329	ASN
37	C	347	HIS
40	F	63	GLN
40	F	138	GLN
40	F	202	GLN
41	G	111	ASN
42	H	111	ASN
42	H	138	ASN
42	H	163	ASN
42	H	175	ASN
42	H	260	ASN
43	I	100	HIS
43	I	112	GLN
43	I	149	ASN
43	I	240	ASN
44	J	39	ASN
44	J	63	ASN

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Mol	Chain	Res	Type
45	K	73	ASN
45	K	144	ASN
46	L	65	ASN
46	L	71	HIS
46	L	97	ASN
47	M	104	ASN
47	M	149	GLN
48	N	66	HIS
49	O	8	GLN
49	O	32	GLN
49	O	99	GLN
49	O	196	ASN
50	P	50	ASN
50	P	96	GLN
51	Q	10	ASN
51	Q	28	ASN
51	Q	116	HIS
51	Q	133	HIS
52	R	40	ASN
52	R	44	ASN
52	R	45	GLN
53	S	30	ASN
53	S	40	GLN
54	T	50	GLN
54	T	108	GLN
55	U	127	GLN
56	V	38	ASN
57	W	27	ASN
57	W	135	ASN
58	X	48	GLN
59	Y	73	HIS
59	Y	93	ASN
60	Z	56	GLN
60	Z	96	HIS
61	a	78	ASN
61	a	97	ASN
61	a	132	GLN
62	b	60	HIS
63	c	12	GLN
63	c	19	ASN
63	c	27	GLN
63	c	58	GLN

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Mol	Chain	Res	Type
64	d	33	GLN
64	d	40	GLN
64	d	51	ASN
66	f	24	GLN
66	f	34	ASN
66	f	52	GLN
66	f	80	HIS
66	f	107	ASN
69	i	65	GLN
69	i	98	HIS
70	j	15	HIS
70	j	80	HIS
74	n	87	GLN
76	p	25	GLN
76	p	36	GLN
76	p	102	GLN
78	r	23	GLN
78	r	30	ASN
78	r	41	ASN
78	r	83	ASN
78	r	85	ASN
78	r	100	ASN
83	Cz	19	HIS
83	Cz	22	GLN
83	Cz	72	GLN
83	Cz	129	ASN
83	Cz	143	ASN
83	Cz	158	GLN
83	Cz	182	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1697/1872 (90%)	392 (23%)	19 (1%)
38	D	156/157 (99%)	32 (20%)	1 (0%)
39	E	118/121 (97%)	11 (9%)	0
79	t	3660/4803 (76%)	691 (18%)	0
80	u	75/76 (98%)	20 (26%)	0
81	v	75/76 (98%)	26 (34%)	0
82	w	19/20 (95%)	8 (42%)	0
All	All	5800/7125 (81%)	1180 (20%)	20 (0%)

All (1180) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	2	A
1	S2	9	U
1	S2	25	A
1	S2	33	G
1	S2	41	G
1	S2	42	A
1	S2	43	U
1	S2	44	U
1	S2	46	A
1	S2	55	U
1	S2	56	G
1	S2	60	A
1	S2	61	A
1	S2	64	A
1	S2	66	G
1	S2	67	C
1	S2	68	A
1	S2	70	G
1	S2	73	C
1	S2	74	G
1	S2	76	U
1	S2	80	G
1	S2	113	G
1	S2	114	G
1	S2	115	U
1	S2	116	OMU
1	S2	125	C
1	S2	126	G
1	S2	142	C
1	S2	143	U
1	S2	155	G
1	S2	159	A2M
1	S2	160	U
1	S2	161	U
1	S2	168	C
1	S2	173	A
1	S2	176	U
1	S2	189	U
1	S2	190	G
1	S2	191	A
1	S2	193	C
1	S2	194	C

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Mol	Chain	Res	Type
1	S2	195	C
1	S2	196	C
1	S2	197	C
1	S2	198	U
1	S2	206	G
1	S2	207	G
1	S2	209	G
1	S2	211	G
1	S2	212	A
1	S2	213	U
1	S2	218	G
1	S2	297	U
1	S2	298	C
1	S2	308	U
1	S2	311	G
1	S2	315	G
1	S2	316	A
1	S2	321	A
1	S2	322	C
1	S2	326	C
1	S2	327	U
1	S2	328	C
1	S2	329	C
1	S2	330	G
1	S2	331	U
1	S2	332	G
1	S2	335	G
1	S2	338	G
1	S2	343	C
1	S2	350	G
1	S2	363	A
1	S2	367	A
1	S2	371	U
1	S2	372	C
1	S2	388	G
1	S2	389	C
1	S2	390	C
1	S2	411	A
1	S2	412	C
1	S2	419	U
1	S2	420	C
1	S2	432	C

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Mol	Chain	Res	Type
1	S2	439	G
1	S2	449	G
1	S2	451	A
1	S2	452	A
1	S2	453	C
1	S2	455	G
1	S2	467	A
1	S2	473	G
1	S2	475	C
1	S2	476	A
1	S2	488	A
1	S2	490	U
1	S2	491	U
1	S2	505	C
1	S2	506	C
1	S2	520	OMC
1	S2	528	A
1	S2	534	A
1	S2	537	G
1	S2	550	G
1	S2	552	C
1	S2	556	U
1	S2	557	A
1	S2	558	A
1	S2	559	U
1	S2	561	G
1	S2	562	G
1	S2	563	A
1	S2	564	A
1	S2	567	A
1	S2	571	MMX
1	S2	573	C
1	S2	579	A
1	S2	581	C
1	S2	582	C
1	S2	586	A
1	S2	591	G
1	S2	592	G
1	S2	593	A
1	S2	594	U
1	S2	603	G
1	S2	607	A

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Mol	Chain	Res	Type
1	S2	610	U
1	S2	611	C
1	S2	617	C
1	S2	620	G
1	S2	629	G
1	S2	630	U
1	S2	631	A
1	S2	632	A
1	S2	646	A
1	S2	658	A
1	S2	663	C
1	S2	666	C
1	S2	671	A2M
1	S2	672	A
1	S2	674	A
1	S2	675	A
1	S2	676	G
1	S2	686	OMG
1	S2	693	G
1	S2	694	G
1	S2	695	G
1	S2	696	A
1	S2	697	G
1	S2	698	C
1	S2	700	G
1	S2	734	G
1	S2	736	C
1	S2	737	C
1	S2	738	C
1	S2	740	G
1	S2	741	C
1	S2	742	C
1	S2	751	C
1	S2	754	G
1	S2	755	G
1	S2	756	C
1	S2	792	G
1	S2	793	C
1	S2	794	C
1	S2	795	C
1	S2	800	C
1	S2	801	G

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Mol	Chain	Res	Type
1	S2	802	U
1	S2	804	U
1	S2	818	U
1	S2	820	G
1	S2	824	G
1	S2	825	PSU
1	S2	833	A
1	S2	834	G
1	S2	838	C
1	S2	839	G
1	S2	840	A
1	S2	841	G
1	S2	842	C
1	S2	844	G
1	S2	845	C
1	S2	850	A
1	S2	861	A
1	S2	862	G
1	S2	872	A
1	S2	873	A
1	S2	875	A
1	S2	876	G
1	S2	890	U
1	S2	891	U
1	S2	893	U
1	S2	894	G
1	S2	897	G
1	S2	898	G
1	S2	900	U
1	S2	906	A
1	S2	908	C
1	S2	910	G
1	S2	916	A
1	S2	917	U
1	S2	920	U
1	S2	923	A
1	S2	936	G
1	S2	958	A
1	S2	972	U
1	S2	973	G
1	S2	974	G
1	S2	976	C

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Mol	Chain	Res	Type
1	S2	993	A
1	S2	995	A
1	S2	1002	G
1	S2	1004	A
1	S2	1005	U
1	S2	1019	U
1	S2	1020	U
1	S2	1024	U
1	S2	1026	A
1	S2	1048	U
1	S2	1052	A
1	S2	1064	U
1	S2	1065	A
1	S2	1086	A
1	S2	1087	A
1	S2	1088	C
1	S2	1091	U
1	S2	1112	C
1	S2	1117	U
1	S2	1118	U
1	S2	1119	C
1	S2	1120	C
1	S2	1122	A
1	S2	1124	G
1	S2	1136	A
1	S2	1141	C
1	S2	1152	A
1	S2	1153	A
1	S2	1157	U
1	S2	1173	A
1	S2	1198	A
1	S2	1210	G
1	S2	1211	A
1	S2	1218	C
1	S2	1220	A
1	S2	1222	C
1	S2	1223	A
1	S2	1227	G
1	S2	1236	G
1	S2	1245	U
1	S2	1246	PSU
1	S2	1254	A

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Mol	Chain	Res	Type
1	S2	1256	A
1	S2	1259	G
1	S2	1260	G
1	S2	1262	A
1	S2	1263	A
1	S2	1268	A
1	S2	1277	G
1	S2	1278	G
1	S2	1286	C
1	S2	1287	A
1	S2	1288	G
1	S2	1289	G
1	S2	1290	A
1	S2	1292	U
1	S2	1298	A
1	S2	1299	U
1	S2	1303	U
1	S2	1304	A
1	S2	1305	G
1	S2	1306	C
1	S2	1312	C
1	S2	1315	G
1	S2	1316	A
1	S2	1325	G
1	S2	1330	G
1	S2	1333	G
1	S2	1336	U
1	S2	1344	C
1	S2	1345	U
1	S2	1374	U
1	S2	1379	A
1	S2	1381	A
1	S2	1400	U
1	S2	1401	G
1	S2	1406	C
1	S2	1407	U
1	S2	1421	C
1	S2	1423	G
1	S2	1424	A
1	S2	1436	C
1	S2	1437	C
1	S2	1439	C

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Mol	Chain	Res	Type
1	S2	1440	C
1	S2	1441	A
1	S2	1442	A
1	S2	1445	U
1	S2	1449	A
1	S2	1450	G
1	S2	1457	A
1	S2	1461	G
1	S2	1465	U
1	S2	1466	U
1	S2	1469	G
1	S2	1473	C
1	S2	1480	U
1	S2	1492	A
1	S2	1493	G
1	S2	1497	U
1	S2	1498	G
1	S2	1500	G
1	S2	1501	A
1	S2	1510	G
1	S2	1511	A
1	S2	1522	U
1	S2	1523	G
1	S2	1524	C
1	S2	1536	A
1	S2	1537	C
1	S2	1539	G
1	S2	1540	A
1	S2	1547	C
1	S2	1548	A
1	S2	1555	G
1	S2	1559	A
1	S2	1560	C
1	S2	1561	C
1	S2	1563	U
1	S2	1571	C
1	S2	1573	G
1	S2	1576	G
1	S2	1583	A
1	S2	1584	C
1	S2	1588	U
1	S2	1589	U

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Mol	Chain	Res	Type
1	S2	1591	A
1	S2	1601	G
1	S2	1602	U
1	S2	1603	G
1	S2	1609	G
1	S2	1624	U
1	S2	1626	A
1	S2	1650	A
1	S2	1651	G
1	S2	1657	G
1	S2	1665	U
1	S2	1668	G
1	S2	1674	G
1	S2	1678	A
1	S2	1679	U
1	S2	1680	U
1	S2	1685	C
1	S2	1689	G
1	S2	1698	A
1	S2	1702	A
1	S2	1725	G
1	S2	1731	U
1	S2	1732	U
1	S2	1752	G
1	S2	1754	C
1	S2	1783	G
1	S2	1784	A
1	S2	1785	G
1	S2	1786	C
1	S2	1787	G
1	S2	1788	C
1	S2	1789	U
1	S2	1794	A
1	S2	1806	U
1	S2	1808	G
1	S2	1817	G
1	S2	1818	A
1	S2	1819	G
1	S2	1827	A
1	S2	1828	A
1	S2	1829	G
1	S2	1832	G

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Mol	Chain	Res	Type
1	S2	1834	A
1	S2	1835	6MZ
1	S2	1838	A
1	S2	1839	G
1	S2	1841	U
1	S2	1843	U
1	S2	1852	G
1	S2	1853	MA6
1	S2	1855	C
1	S2	1864	G
1	S2	1865	G
1	S2	1866	A
1	S2	1868	C
1	S2	1872	A
38	D	16	G
38	D	23	C
38	D	34	U
38	D	35	C
38	D	38	U
38	D	39	G
38	D	59	A
38	D	63	U
38	D	71	A
38	D	72	A
38	D	77	A
38	D	78	G
38	D	79	G
38	D	81	C
38	D	83	C
38	D	84	A
38	D	85	U
38	D	86	U
38	D	87	G
38	D	94	G
38	D	103	A
38	D	105	C
38	D	109	C
38	D	110	U
38	D	111	U
38	D	122	G
38	D	124	U
38	D	125	C

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Mol	Chain	Res	Type
38	D	126	C
38	D	128	C
38	D	129	C
38	D	148	A
39	E	7	G
39	E	22	A
39	E	33	U
39	E	50	A
39	E	51	G
39	E	53	U
39	E	54	A
39	E	63	C
39	E	64	G
39	E	102	U
39	E	110	G
79	t	9	C
79	t	25	A
79	t	32	G
79	t	39	A
79	t	40	G
79	t	42	A
79	t	48	G
79	t	49	U
79	t	59	A
79	t	64	A
79	t	65	A
79	t	66	A
79	t	71	C
79	t	72	C
79	t	76	A
79	t	91	G
79	t	108	A
79	t	110	C
79	t	119	G
79	t	129	C
79	t	130	G
79	t	131	C
79	t	132	G
79	t	137	G
79	t	138	C
79	t	139	G
79	t	142	G

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Mol	Chain	Res	Type
79	t	152	U
79	t	160	G
79	t	166	C
79	t	176	G
79	t	179	G
79	t	182	G
79	t	183	C
79	t	184	U
79	t	185	C
79	t	186	G
79	t	187	U
79	t	199	G
79	t	208	A
79	t	215	C
79	t	216	C
79	t	217	C
79	t	218	A
79	t	232	G
79	t	233	U
79	t	236	G
79	t	247	G
79	t	255	C
79	t	256	G
79	t	257	C
79	t	258	G
79	t	264	C
79	t	266	C
79	t	295	A
79	t	297	U
79	t	306	A
79	t	310	G
79	t	315	G
79	t	316	U
79	t	317	A
79	t	340	C
79	t	349	A
79	t	373	G
79	t	376	A
79	t	381	U
79	t	387	G
79	t	410	A
79	t	411	G

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Mol	Chain	Res	Type
79	t	412	G
79	t	431	G
79	t	440	U
79	t	451	C
79	t	452	A
79	t	453	G
79	t	454	U
79	t	455	C
79	t	464	G
79	t	469	C
79	t	480	C
79	t	482	C
79	t	483	G
79	t	484	C
79	t	485	G
79	t	487	C
79	t	488	C
79	t	489	G
79	t	497	C
79	t	500	U
79	t	501	G
79	t	502	G
79	t	507	G
79	t	508	G
79	t	513	U
79	t	516	U
79	t	517	U
79	t	518	C
79	t	520	C
79	t	524	C
79	t	616	U
79	t	617	C
79	t	626	A
79	t	632	C
79	t	644	G
79	t	645	A
79	t	646	C
79	t	657	C
79	t	661	C
79	t	662	G
79	t	677	C
79	t	680	U

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Mol	Chain	Res	Type
79	t	682	C
79	t	685	C
79	t	706	U
79	t	707	G
79	t	708	G
79	t	713	G
79	t	714	C
79	t	715	C
79	t	717	G
79	t	724	A
79	t	725	A
79	t	726	G
79	t	727	G
79	t	728	U
79	t	730	G
79	t	838	C
79	t	845	G
79	t	848	A
79	t	850	A
79	t	851	G
79	t	853	C
79	t	859	G
79	t	860	C
79	t	862	G
79	t	864	A
79	t	867	G
79	t	869	U
79	t	877	U
79	t	878	C
79	t	879	C
79	t	889	G
79	t	890	G
79	t	891	G
79	t	892	A
79	t	893	G
79	t	895	C
79	t	898	A
79	t	899	U
79	t	902	C
79	t	904	G
79	t	982	C
79	t	987	C

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Mol	Chain	Res	Type
79	t	988	G
79	t	990	C
79	t	992	C
79	t	1010	U
79	t	1013	C
79	t	1014	C
79	t	1065	G
79	t	1066	C
79	t	1067	G
79	t	1068	G
79	t	1072	G
79	t	1078	U
79	t	1079	C
79	t	1080	C
79	t	1090	C
79	t	1096	C
79	t	1097	G
79	t	1098	U
79	t	1099	C
79	t	1100	G
79	t	1102	C
79	t	1109	U
79	t	1110	C
79	t	1113	G
79	t	1114	C
79	t	1118	G
79	t	1137	C
79	t	1138	U
79	t	1139	C
79	t	1140	U
79	t	1141	C
79	t	1142	C
79	t	1143	C
79	t	1144	U
79	t	1146	C
79	t	1147	C
79	t	1150	U
79	t	1154	G
79	t	1155	G
79	t	1156	G
79	t	1158	U
79	t	1167	G

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Mol	Chain	Res	Type
79	t	1169	G
79	t	1176	A
79	t	1178	C
79	t	1183	G
79	t	1187	U
79	t	1188	C
79	t	1190	G
79	t	1196	A
79	t	1197	U
79	t	1198	G
79	t	1204	U
79	t	1205	A
79	t	1206	C
79	t	1228	A
79	t	1256	A
79	t	1260	A
79	t	1261	G
79	t	1267	C
79	t	1268	G
79	t	1269	U
79	t	1279	G
79	t	1289	A
79	t	1299	A
79	t	1300	A
79	t	1310	U
79	t	1311	C
79	t	1312	C
79	t	1313	C
79	t	1324	A
79	t	1341	C
79	t	1343	C
79	t	1345	C
79	t	1346	C
79	t	1347	A
79	t	1348	G
79	t	1361	G
79	t	1379	G
79	t	1385	C
79	t	1386	G
79	t	1387	C
79	t	1388	G
79	t	1390	C

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Mol	Chain	Res	Type
79	t	1401	A
79	t	1402	G
79	t	1406	G
79	t	1427	A
79	t	1429	A
79	t	1438	A
79	t	1451	A
79	t	1467	A
79	t	1470	C
79	t	1478	G
79	t	1482	U
79	t	1495	U
79	t	1500	U
79	t	1505	A
79	t	1511	C
79	t	1516	G
79	t	1517	A
79	t	1528	G
79	t	1529	G
79	t	1535	A
79	t	1537	G
79	t	1538	A
79	t	1542	A
79	t	1545	G
79	t	1558	G
79	t	1565	C
79	t	1574	G
79	t	1595	G
79	t	1598	C
79	t	1603	A
79	t	1606	G
79	t	1607	C
79	t	1608	G
79	t	1609	G
79	t	1618	A
79	t	1619	A
79	t	1633	C
79	t	1643	G
79	t	1666	G
79	t	1667	A
79	t	1668	A
79	t	1674	C

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Mol	Chain	Res	Type
79	t	1675	U
79	t	1683	U
79	t	1689	A
79	t	1696	A
79	t	1705	G
79	t	1706	A
79	t	1723	G
79	t	1735	G
79	t	1736	U
79	t	1737	G
79	t	1738	G
79	t	1739	A
79	t	1744	G
79	t	1757	G
79	t	1771	G
79	t	1791	U
79	t	1793	A
79	t	1794	A
79	t	1800	C
79	t	1817	C
79	t	1820	U
79	t	1823	C
79	t	1824	G
79	t	1833	C
79	t	1842	G
79	t	1849	U
79	t	1850	G
79	t	1859	U
79	t	1860	A
79	t	1862	A
79	t	1863	G
79	t	1864	A
79	t	1878	G
79	t	1881	A
79	t	1882	U
79	t	1884	G
79	t	1885	A
79	t	1887	G
79	t	1889	C
79	t	1895	C
79	t	1900	A
79	t	1904	G

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Mol	Chain	Res	Type
79	t	1905	U
79	t	1909	U
79	t	1914	A
79	t	1927	A
79	t	1932	C
79	t	1935	G
79	t	1947	G
79	t	1949	U
79	t	1956	G
79	t	1957	G
79	t	1970	A
79	t	1971	U
79	t	1985	C
79	t	1992	C
79	t	1993	G
79	t	1994	G
79	t	1995	A
79	t	1996	A
79	t	1997	C
79	t	1998	G
79	t	1999	G
79	t	2002	C
79	t	2003	G
79	t	2005	G
79	t	2008	C
79	t	2009	G
79	t	2011	C
79	t	2012	C
79	t	2013	G
79	t	2096	G
79	t	2098	G
79	t	2099	C
79	t	2100	C
79	t	2102	C
79	t	2106	G
79	t	2112	A
79	t	2133	C
79	t	2143	G
79	t	2144	A
79	t	2145	G
79	t	2150	G
79	t	2157	A

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Mol	Chain	Res	Type
79	t	2173	U
79	t	2175	G
79	t	2176	A
79	t	2192	G
79	t	2194	U
79	t	2195	C
79	t	2204	A
79	t	2205	G
79	t	2239	A
79	t	2240	A
79	t	2246	G
79	t	2254	C
79	t	2261	A
79	t	2262	A
79	t	2265	G
79	t	2266	C
79	t	2269	U
79	t	2291	U
79	t	2294	G
79	t	2307	G
79	t	2314	C
79	t	2315	G
79	t	2323	G
79	t	2332	C
79	t	2333	C
79	t	2334	U
79	t	2337	G
79	t	2338	U
79	t	2347	G
79	t	2348	C
79	t	2349	C
79	t	2350	G
79	t	2357	A
79	t	2388	G
79	t	2389	U
79	t	2390	G
79	t	2391	G
79	t	2397	A
79	t	2398	U
79	t	2410	G
79	t	2425	A
79	t	2430	G

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Mol	Chain	Res	Type
79	t	2431	A
79	t	2433	C
79	t	2435	A
79	t	2445	A
79	t	2450	G
79	t	2462	G
79	t	2471	C
79	t	2482	G
79	t	2484	G
79	t	2504	A
79	t	2513	C
79	t	2517	G
79	t	2531	U
79	t	2538	G
79	t	2539	A
79	t	2540	A
79	t	2552	U
79	t	2554	C
79	t	2555	G
79	t	2556	G
79	t	2565	G
79	t	2570	G
79	t	2584	U
79	t	2587	A
79	t	2591	U
79	t	2603	G
79	t	2604	G
79	t	2605	U
79	t	2606	G
79	t	2608	A
79	t	2610	A
79	t	2613	U
79	t	2631	A
79	t	2632	U
79	t	2634	U
79	t	2640	G
79	t	2641	C
79	t	2643	G
79	t	2650	A
79	t	2658	C
79	t	2670	U
79	t	2671	G

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Mol	Chain	Res	Type
79	t	2687	U
79	t	2699	G
79	t	2725	A
79	t	2741	G
79	t	2746	G
79	t	3334	A
79	t	3336	C
79	t	3340	C
79	t	3341	U
79	t	3353	C
79	t	3360	G
79	t	3361	G
79	t	3370	A
79	t	3376	U
79	t	3397	A
79	t	3399	G
79	t	3407	G
79	t	3408	C
79	t	3433	G
79	t	3445	G
79	t	3446	A
79	t	3447	A
79	t	3464	U
79	t	3471	A
79	t	3483	A
79	t	3492	G
79	t	3494	A
79	t	3495	A
79	t	3508	U
79	t	3509	A
79	t	3511	G
79	t	3512	G
79	t	3513	U
79	t	3515	G
79	t	3519	A
79	t	3545	C
79	t	3546	G
79	t	3547	C
79	t	3549	U
79	t	3552	A
79	t	3553	U
79	t	3554	G

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Mol	Chain	Res	Type
79	t	3559	A
79	t	3564	G
79	t	3573	U
79	t	3574	G
79	t	3575	U
79	t	3612	A
79	t	3614	G
79	t	3627	U
79	t	3632	G
79	t	3636	A
79	t	3641	A
79	t	3642	G
79	t	3644	C
79	t	3650	U
79	t	3658	A
79	t	3674	G
79	t	3685	U
79	t	3690	G
79	t	3695	A
79	t	3696	G
79	t	3697	A
79	t	3698	A
79	t	3699	U
79	t	3701	A
79	t	3708	G
79	t	3769	C
79	t	3773	C
79	t	3775	G
79	t	3779	A
79	t	3780	A
79	t	3781	U
79	t	3794	A
79	t	3796	C
79	t	3797	G
79	t	3808	G
79	t	3825	G
79	t	3826	G
79	t	3827	G
79	t	3828	C
79	t	3829	G
79	t	3833	C
79	t	3834	C

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Mol	Chain	Res	Type
79	t	3835	C
79	t	3836	G
79	t	3837	A
79	t	3842	C
79	t	3844	C
79	t	3846	C
79	t	3847	G
79	t	3851	C
79	t	3869	C
79	t	3894	C
79	t	3895	U
79	t	3896	C
79	t	3902	A
79	t	3915	G
79	t	3916	G
79	t	3923	G
79	t	3928	G
79	t	3935	A
79	t	3944	A
79	t	3946	A
79	t	3957	G
79	t	3961	U
79	t	3965	A
79	t	3966	A
79	t	3981	G
79	t	3983	A
79	t	3986	G
79	t	3987	A
79	t	3998	G
79	t	4000	A
79	t	4004	G
79	t	4006	A
79	t	4013	A
79	t	4036	A
79	t	4037	G
79	t	4038	U
79	t	4046	C
79	t	4062	G
79	t	4064	C
79	t	4081	C
79	t	4086	U
79	t	4100	G

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Mol	Chain	Res	Type
79	t	4103	G
79	t	4104	U
79	t	4108	A
79	t	4109	G
79	t	4110	A
79	t	4111	A
79	t	4119	C
79	t	4125	G
79	t	4126	A
79	t	4128	A
79	t	4137	G
79	t	4153	C
79	t	4154	A
79	t	4169	U
79	t	4176	C
79	t	4185	C
79	t	4196	A
79	t	4198	C
79	t	4207	G
79	t	4225	U
79	t	4226	G
79	t	4244	U
79	t	4245	A
79	t	4250	A
79	t	4251	C
79	t	4256	G
79	t	4280	A
79	t	4287	U
79	t	4289	U
79	t	4292	C
79	t	4299	G
79	t	4321	A
79	t	4322	A
79	t	4349	G
79	t	4356	A
79	t	4368	U
79	t	4369	G
79	t	4371	G
79	t	4388	A
79	t	4402	C
79	t	4410	G
79	t	4427	C

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Mol	Chain	Res	Type
79	t	4432	A
79	t	4441	U
79	t	4452	C
79	t	4462	C
79	t	4463	G
79	t	4464	G
79	t	4466	A
79	t	4467	G
79	t	4472	G
79	t	4473	A
79	t	4474	A
79	t	4475	G
79	t	4483	G
79	t	4486	U
79	t	4489	C
79	t	4491	C
79	t	4493	G
79	t	4497	A
79	t	4502	G
79	t	4507	C
79	t	4591	U
79	t	4593	C
79	t	4596	U
79	t	4597	G
79	t	4600	G
79	t	4601	A
79	t	4602	G
79	t	4603	A
79	t	4609	U
79	t	4610	C
79	t	4623	G
79	t	4624	G
79	t	4627	U
79	t	4628	G
79	t	4633	C
79	t	4634	G
79	t	4635	G
79	t	4637	A
79	t	4639	G
79	t	4640	G
79	t	4641	G
79	t	4647	C

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Mol	Chain	Res	Type
79	t	4652	U
79	t	4655	C
79	t	4664	C
79	t	4665	U
79	t	4666	U
79	t	4667	A
79	t	4669	C
79	t	4672	A
79	t	4673	C
79	t	4680	G
79	t	4688	U
79	t	4692	G
79	t	4693	C
79	t	4695	A
79	t	4705	U
79	t	4714	U
79	t	4717	U
79	t	4718	U
79	t	4719	C
79	t	4720	U
79	t	4721	G
79	t	4735	U
79	t	4742	C
79	t	4746	G
79	t	4753	C
79	t	4755	U
79	t	4756	C
79	t	4770	G
79	t	4778	G
79	t	4779	C
79	t	4783	C
79	t	4784	G
79	t	4787	A
79	t	4790	A
80	u	4	C
80	u	6	G
80	u	7	A
80	u	8	U
80	u	14	A
80	u	16	U
80	u	17	C
80	u	18	G

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Mol	Chain	Res	Type
80	u	19	G
80	u	20	U
80	u	21	A
80	u	23	A
80	u	46	G
80	u	47	U
80	u	52	G
80	u	56	C
80	u	57	G
80	u	59	U
80	u	74	C
80	u	76	A
81	v	8	U
81	v	9	A
81	v	11	C
81	v	12	C
81	v	13	C
81	v	14	C
81	v	16	A
81	v	18	G
81	v	19	G
81	v	20	U
81	v	21	A
81	v	22	G
81	v	23	A
81	v	47	U
81	v	48	C
81	v	49	C
81	v	51	U
81	v	55	U
81	v	56	C
81	v	57	G
81	v	61	C
81	v	62	C
81	v	67	C
81	v	69	G
81	v	73	A
81	v	76	A
82	w	10	C
82	w	11	A
82	w	12	U
82	w	21	G

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Mol	Chain	Res	Type
82	w	24	G
82	w	25	A
82	w	27	C
82	w	28	U

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	42	A
1	S2	60	A
1	S2	196	C
1	S2	307	C
1	S2	320	C
1	S2	448	A
1	S2	561	G
1	S2	562	G
1	S2	566	G
1	S2	673	A
1	S2	871	G
1	S2	875	A
1	S2	1399	A
1	S2	1570	G
1	S2	1575	C
1	S2	1684	U
1	S2	1805	C
1	S2	1818	A
1	S2	1827	A
38	D	86	U

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

33 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	S2	826	1	18,21,22	1.08	1 (5%)	22,30,33	1.66	5 (22%)
1	PSU	S2	1084	1	18,21,22	1.06	1 (5%)	22,30,33	1.71	4 (18%)
1	5MU	S2	817	1	19,22,23	0.40	0	28,32,35	0.91	2 (7%)
1	OMG	S2	686	1	23,26,27	0.48	0	33,38,41	0.53	0
1	UR3	S2	1833	1	19,22,23	3.00	7 (36%)	26,32,35	1.65	4 (15%)
1	B8N	S2	1251	1	24,29,30	3.06	5 (20%)	29,42,45	1.74	5 (17%)
1	OMG	S2	647	1	23,26,27	0.47	0	33,38,41	0.46	0
1	A2M	S2	1034	1	22,25,26	3.18	9 (40%)	31,36,39	2.97	10 (32%)
1	OMC	S2	1706	1	19,22,23	0.50	0	26,31,34	0.66	0
1	A2M	S2	487	1	22,25,26	3.19	9 (40%)	31,36,39	2.95	10 (32%)
1	PSU	S2	615	1	18,21,22	1.02	1 (5%)	22,30,33	1.66	4 (18%)
1	A2M	S2	1681	1	22,25,26	3.16	9 (40%)	31,36,39	2.98	11 (35%)
1	6MZ	S2	1835	1	22,25,26	4.96	15 (68%)	30,36,39	4.58	23 (76%)
1	4AC	S2	1845	1	21,24,25	3.56	10 (47%)	29,34,37	1.13	3 (10%)
1	OMU	S2	116	1	19,22,23	3.10	8 (42%)	26,31,34	1.69	5 (19%)
1	PSU	S2	1246	1	18,21,22	1.08	1 (5%)	22,30,33	1.72	4 (18%)
1	OMG	S2	512	1	23,26,27	0.47	0	33,38,41	0.48	0
1	A2M	S2	166	1	22,25,26	3.18	9 (40%)	31,36,39	3.00	11 (35%)
1	5MC	S2	1377	1	18,22,23	0.53	0	26,32,35	0.75	0
1	MA6	S2	1854	1	23,26,27	1.31	3 (13%)	34,38,41	3.28	12 (35%)
1	PSU	S2	825	1	18,21,22	1.10	1 (5%)	22,30,33	1.70	4 (18%)
1	A2M	S2	159	1	22,25,26	3.19	9 (40%)	31,36,39	3.01	11 (35%)
1	PSU	S2	119	1	18,21,22	1.10	1 (5%)	22,30,33	1.71	4 (18%)
1	MA6	S2	1853	1	23,26,27	1.33	4 (17%)	34,38,41	3.25	11 (32%)
1	A2M	S2	671	1	22,25,26	3.18	9 (40%)	31,36,39	3.00	13 (41%)
1	MMX	S2	571	1	19,23,24	4.00	4 (21%)	22,33,36	2.83	6 (27%)
1	OMC	S2	1713	1	19,22,23	0.51	0	26,31,34	0.67	0
1	OMC	S2	174	1	19,22,23	0.51	0	26,31,34	0.67	0
1	OMC	S2	520	1	19,22,23	0.52	0	26,31,34	0.77	0
1	4AC	S2	1340	1	21,24,25	3.56	10 (47%)	29,34,37	1.12	3 (10%)
1	A2M	S2	27	1	22,25,26	3.19	9 (40%)	31,36,39	2.94	11 (35%)
1	M7A	S2	1809	1	20,25,26	2.07	3 (15%)	28,37,40	4.10	8 (28%)
1	OMU	S2	121	1	19,22,23	1.39	3 (15%)	26,31,34	1.96	7 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	826	1	-	2/7/25/26	0/2/2/2
1	PSU	S2	1084	1	-	0/7/25/26	0/2/2/2
1	5MU	S2	817	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	686	1	-	2/9/27/28	0/3/3/3
1	UR3	S2	1833	1	-	2/7/25/26	0/2/2/2
1	B8N	S2	1251	1	-	2/16/34/35	0/2/2/2
1	OMG	S2	647	1	-	2/9/27/28	0/3/3/3
1	A2M	S2	1034	1	-	0/9/27/28	0/3/3/3
1	OMC	S2	1706	1	-	0/9/27/28	0/2/2/2
1	A2M	S2	487	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	615	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	1681	1	-	2/9/27/28	0/3/3/3
1	6MZ	S2	1835	1	-	1/9/27/28	0/3/3/3
1	4AC	S2	1845	1	-	0/11/29/30	0/2/2/2
1	OMU	S2	116	1	-	2/9/27/28	0/2/2/2
1	PSU	S2	1246	1	-	2/7/25/26	0/2/2/2
1	OMG	S2	512	1	-	0/9/27/28	0/3/3/3
1	A2M	S2	166	1	-	0/9/27/28	0/3/3/3
1	5MC	S2	1377	1	-	0/7/25/26	0/2/2/2
1	MA6	S2	1854	1	-	6/11/29/30	0/3/3/3
1	PSU	S2	825	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	159	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	119	1	-	0/7/25/26	0/2/2/2
1	MA6	S2	1853	1	-	5/11/29/30	0/3/3/3
1	A2M	S2	671	1	-	2/9/27/28	0/3/3/3
1	MMX	S2	571	1	-	4/9/44/45	0/2/2/2
1	OMC	S2	1713	1	-	0/9/27/28	0/2/2/2
1	OMC	S2	174	1	-	0/9/27/28	0/2/2/2
1	OMC	S2	520	1	-	2/9/27/28	0/2/2/2
1	4AC	S2	1340	1	-	0/11/29/30	0/2/2/2
1	A2M	S2	27	1	-	2/9/27/28	0/3/3/3
1	M7A	S2	1809	1	-	1/7/37/38	0/3/3/3
1	OMU	S2	121	1	-	1/9/27/28	0/2/2/2

All (141) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1835	6MZ	O3'-C3'	11.94	1.71	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	571	MMX	C2-N1	10.18	1.50	1.37
1	S2	571	MMX	C4-N3	9.93	1.53	1.45
1	S2	1835	6MZ	C3'-C4'	-8.85	1.30	1.53
1	S2	166	A2M	C3'-C4'	-8.82	1.30	1.53
1	S2	27	A2M	C3'-C4'	-8.76	1.30	1.53
1	S2	1034	A2M	C3'-C4'	-8.74	1.30	1.53
1	S2	1681	A2M	C3'-C4'	-8.73	1.30	1.53
1	S2	487	A2M	C3'-C4'	-8.69	1.30	1.53
1	S2	159	A2M	C3'-C4'	-8.62	1.31	1.53
1	S2	571	MMX	C2-N3	8.56	1.48	1.37
1	S2	671	A2M	C3'-C4'	-8.56	1.31	1.53
1	S2	1251	B8N	C6-N1	7.91	1.56	1.36
1	S2	159	A2M	O4'-C4'	7.72	1.62	1.45
1	S2	27	A2M	O4'-C4'	7.69	1.62	1.45
1	S2	1034	A2M	O4'-C4'	7.66	1.62	1.45
1	S2	671	A2M	O4'-C4'	7.65	1.62	1.45
1	S2	487	A2M	O4'-C4'	7.64	1.62	1.45
1	S2	166	A2M	O4'-C4'	7.62	1.62	1.45
1	S2	1833	UR3	C2-N1	7.61	1.49	1.38
1	S2	1845	4AC	C4-N3	7.48	1.45	1.32
1	S2	1340	4AC	C4-N3	7.46	1.45	1.32
1	S2	1681	A2M	O4'-C4'	7.45	1.61	1.45
1	S2	1251	B8N	C4-N3	-7.39	1.26	1.40
1	S2	116	OMU	C2-N1	7.36	1.50	1.38
1	S2	1835	6MZ	O4'-C1'	-7.20	1.24	1.42
1	S2	116	OMU	C2-N3	6.99	1.50	1.38
1	S2	1835	6MZ	C5-C4	-6.84	1.26	1.39
1	S2	1340	4AC	C6-C5	6.83	1.50	1.35
1	S2	1833	UR3	C6-C5	6.82	1.50	1.35
1	S2	1845	4AC	C6-C5	6.77	1.50	1.35
1	S2	1809	M7A	C4-N9	6.12	1.49	1.38
1	S2	1251	B8N	C2-N1	5.90	1.56	1.39
1	S2	1833	UR3	C2-N3	5.89	1.50	1.39
1	S2	1835	6MZ	O4'-C4'	5.82	1.58	1.45
1	S2	116	OMU	C6-C5	5.69	1.48	1.35
1	S2	1835	6MZ	C5-N7	-5.68	1.28	1.39
1	S2	1845	4AC	C7-N4	5.65	1.47	1.37
1	S2	1340	4AC	C7-N4	5.65	1.47	1.37
1	S2	1251	B8N	C6-C5	5.54	1.42	1.34
1	S2	1340	4AC	C4-N4	5.29	1.47	1.39
1	S2	1845	4AC	C2-N3	5.29	1.47	1.36
1	S2	1845	4AC	C2-N1	5.28	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1340	4AC	C2-N1	5.27	1.51	1.40
1	S2	1845	4AC	C4-N4	5.24	1.47	1.39
1	S2	1340	4AC	C2-N3	5.23	1.47	1.36
1	S2	1835	6MZ	O2'-C2'	-5.17	1.30	1.43
1	S2	1835	6MZ	C6-N1	-5.08	1.27	1.35
1	S2	1835	6MZ	C6-N6	4.80	1.39	1.34
1	S2	487	A2M	O4'-C1'	-4.78	1.30	1.42
1	S2	671	A2M	O4'-C1'	-4.76	1.30	1.42
1	S2	159	A2M	O4'-C1'	-4.71	1.30	1.42
1	S2	166	A2M	C6-N6	4.60	1.45	1.34
1	S2	159	A2M	C6-N6	4.59	1.45	1.34
1	S2	1681	A2M	C6-N6	4.58	1.45	1.34
1	S2	487	A2M	C6-N6	4.58	1.45	1.34
1	S2	671	A2M	C6-N6	4.58	1.45	1.34
1	S2	27	A2M	C6-N6	4.56	1.45	1.34
1	S2	1034	A2M	C6-N6	4.54	1.45	1.34
1	S2	1681	A2M	O4'-C1'	-4.53	1.31	1.42
1	S2	27	A2M	O4'-C1'	-4.49	1.31	1.42
1	S2	1835	6MZ	C8-N9	-4.48	1.29	1.37
1	S2	1034	A2M	O4'-C1'	-4.48	1.31	1.42
1	S2	166	A2M	O4'-C1'	-4.46	1.31	1.42
1	S2	1809	M7A	C6-N6	4.41	1.45	1.34
1	S2	116	OMU	C4-N3	4.36	1.46	1.38
1	S2	571	MMX	C5-C4	-4.22	1.48	1.52
1	S2	1845	4AC	C5-C4	4.18	1.49	1.40
1	S2	1340	4AC	C5-C4	4.12	1.49	1.40
1	S2	1340	4AC	CM7-C7	4.11	1.59	1.50
1	S2	1845	4AC	CM7-C7	4.09	1.59	1.50
1	S2	1809	M7A	C5-N7	4.03	1.49	1.39
1	S2	1251	B8N	C1'-C5	3.97	1.59	1.50
1	S2	1835	6MZ	C4-N9	-3.96	1.28	1.37
1	S2	1853	MA6	C6-N6	3.77	1.48	1.36
1	S2	1854	MA6	C6-N6	3.76	1.47	1.36
1	S2	119	PSU	C6-C5	3.69	1.39	1.35
1	S2	825	PSU	C6-C5	3.65	1.39	1.35
1	S2	1246	PSU	C6-C5	3.62	1.39	1.35
1	S2	826	PSU	C6-C5	3.58	1.39	1.35
1	S2	1833	UR3	C6-N1	3.49	1.46	1.38
1	S2	1084	PSU	C6-C5	3.44	1.39	1.35
1	S2	615	PSU	C6-C5	3.39	1.39	1.35
1	S2	1835	6MZ	C5-C6	-3.38	1.33	1.41
1	S2	121	OMU	C4-N3	-3.32	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	121	OMU	C2-N3	-3.07	1.32	1.38
1	S2	671	A2M	O3'-C3'	3.06	1.50	1.43
1	S2	1835	6MZ	C2-N1	-2.96	1.28	1.33
1	S2	1034	A2M	O3'-C3'	2.92	1.49	1.43
1	S2	159	A2M	O3'-C3'	2.91	1.49	1.43
1	S2	1835	6MZ	C8-N7	-2.91	1.26	1.31
1	S2	27	A2M	O3'-C3'	2.90	1.49	1.43
1	S2	487	A2M	O3'-C3'	2.89	1.49	1.43
1	S2	116	OMU	O4-C4	-2.88	1.18	1.24
1	S2	116	OMU	C6-N1	2.86	1.44	1.38
1	S2	1681	A2M	O3'-C3'	2.84	1.49	1.43
1	S2	166	A2M	O3'-C3'	2.84	1.49	1.43
1	S2	1835	6MZ	C4-N3	-2.73	1.29	1.34
1	S2	166	A2M	C5-C4	-2.73	1.33	1.39
1	S2	159	A2M	C5-C4	-2.66	1.34	1.39
1	S2	27	A2M	C5-C4	-2.66	1.34	1.39
1	S2	487	A2M	C5-C4	-2.65	1.34	1.39
1	S2	1034	A2M	C5-C4	-2.65	1.34	1.39
1	S2	671	A2M	C5-C4	-2.65	1.34	1.39
1	S2	1681	A2M	C5-C4	-2.62	1.34	1.39
1	S2	1854	MA6	C5-C4	-2.59	1.34	1.39
1	S2	1340	4AC	C6-N1	2.58	1.44	1.38
1	S2	1853	MA6	C5-C4	-2.58	1.34	1.39
1	S2	166	A2M	O2'-C2'	-2.57	1.36	1.42
1	S2	27	A2M	O2'-C2'	-2.56	1.36	1.42
1	S2	1034	A2M	O2'-C2'	-2.56	1.36	1.42
1	S2	121	OMU	C5-C4	-2.56	1.38	1.43
1	S2	1845	4AC	C6-N1	2.55	1.44	1.38
1	S2	671	A2M	O2'-C2'	-2.52	1.36	1.42
1	S2	1681	A2M	O2'-C2'	-2.52	1.36	1.42
1	S2	487	A2M	O2'-C2'	-2.50	1.36	1.42
1	S2	159	A2M	O2'-C2'	-2.50	1.36	1.42
1	S2	27	A2M	C8-N9	-2.47	1.33	1.37
1	S2	1681	A2M	C8-N9	-2.39	1.33	1.37
1	S2	116	OMU	C5-C4	2.35	1.48	1.43
1	S2	159	A2M	C8-N9	-2.33	1.33	1.37
1	S2	1034	A2M	C8-N9	-2.33	1.33	1.37
1	S2	1833	UR3	C4-N3	2.29	1.45	1.40
1	S2	166	A2M	C8-N9	-2.28	1.33	1.37
1	S2	487	A2M	C8-N9	-2.27	1.33	1.37
1	S2	1853	MA6	C5-N7	-2.27	1.34	1.39
1	S2	671	A2M	C8-N9	-2.26	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	116	OMU	O2-C2	-2.25	1.18	1.23
1	S2	1681	A2M	C5-N7	-2.23	1.34	1.39
1	S2	1845	4AC	O7-C7	-2.21	1.18	1.23
1	S2	1340	4AC	O7-C7	-2.20	1.18	1.23
1	S2	1833	UR3	C5-C4	2.19	1.49	1.43
1	S2	1854	MA6	C5-N7	-2.18	1.34	1.39
1	S2	27	A2M	C5-N7	-2.16	1.34	1.39
1	S2	159	A2M	C5-N7	-2.15	1.35	1.39
1	S2	487	A2M	C5-N7	-2.14	1.35	1.39
1	S2	1833	UR3	O2-C2	-2.14	1.18	1.22
1	S2	671	A2M	C5-N7	-2.13	1.35	1.39
1	S2	1853	MA6	C8-N9	-2.08	1.33	1.37
1	S2	1034	A2M	C5-N7	-2.07	1.35	1.39
1	S2	166	A2M	C5-N7	-2.04	1.35	1.39

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1809	M7A	C5-C6-N6	13.86	147.41	123.74
1	S2	1854	MA6	N1-C6-N6	-12.80	103.09	117.08
1	S2	1853	MA6	N1-C6-N6	-12.69	103.21	117.08
1	S2	1809	M7A	N6-C6-N1	-11.78	92.55	118.35
1	S2	1835	6MZ	O2'-C2'-C1'	-9.14	79.48	110.02
1	S2	1835	6MZ	C5-C4-N3	-8.98	115.04	126.75
1	S2	571	MMX	N3-C2-N1	8.58	122.47	116.83
1	S2	1835	6MZ	C4-C5-C6	7.13	122.34	116.81
1	S2	1835	6MZ	C3'-C2'-C1'	7.13	114.97	101.43
1	S2	1854	MA6	C5-C6-N6	6.93	137.38	125.30
1	S2	1853	MA6	C5-C6-N6	6.87	137.26	125.30
1	S2	671	A2M	N6-C6-N1	-6.75	103.56	118.35
1	S2	1034	A2M	N6-C6-N1	-6.74	103.59	118.35
1	S2	487	A2M	N6-C6-N1	-6.69	103.70	118.35
1	S2	166	A2M	N6-C6-N1	-6.68	103.72	118.35
1	S2	159	A2M	N6-C6-N1	-6.66	103.76	118.35
1	S2	1809	M7A	C4-N9-C1'	-6.55	111.05	126.60
1	S2	1681	A2M	N6-C6-N1	-6.55	104.01	118.35
1	S2	27	A2M	N6-C6-N1	-6.54	104.03	118.35
1	S2	1835	6MZ	C1'-N9-C8	6.51	141.82	127.14
1	S2	166	A2M	N9-C8-N7	-6.25	105.36	113.91
1	S2	1835	6MZ	C4-N9-C1'	-6.19	111.83	126.59
1	S2	1034	A2M	N9-C8-N7	-6.15	105.50	113.91
1	S2	159	A2M	N9-C8-N7	-6.08	105.60	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	671	A2M	N9-C8-N7	-6.04	105.65	113.91
1	S2	1835	6MZ	O3'-C3'-C4'	6.01	128.43	111.05
1	S2	671	A2M	C5-C6-N6	5.98	136.44	123.43
1	S2	1034	A2M	C5-C6-N6	5.97	136.41	123.43
1	S2	27	A2M	N9-C8-N7	-5.94	105.79	113.91
1	S2	159	A2M	C5-C6-N6	5.93	136.33	123.43
1	S2	166	A2M	C5-C6-N6	5.91	136.29	123.43
1	S2	487	A2M	C5-C6-N6	5.91	136.28	123.43
1	S2	487	A2M	N9-C8-N7	-5.86	105.91	113.91
1	S2	1681	A2M	N9-C8-N7	-5.81	105.96	113.91
1	S2	27	A2M	C5-C6-N6	5.81	136.08	123.43
1	S2	166	A2M	N3-C2-N1	-5.79	119.54	128.60
1	S2	1681	A2M	C5-C6-N6	5.76	135.97	123.43
1	S2	1835	6MZ	O4'-C1'-C2'	-5.70	94.23	106.64
1	S2	1681	A2M	N3-C2-N1	-5.62	119.81	128.60
1	S2	1809	M7A	N3-C2-N1	-5.57	119.89	128.60
1	S2	1034	A2M	N3-C2-N1	-5.53	119.95	128.60
1	S2	487	A2M	N3-C2-N1	-5.53	119.95	128.60
1	S2	1854	MA6	N1-C2-N3	-5.52	119.96	128.60
1	S2	27	A2M	N3-C2-N1	-5.51	119.99	128.60
1	S2	671	A2M	N3-C2-N1	-5.49	120.02	128.60
1	S2	571	MMX	C4-N3-C2	-5.49	116.49	121.62
1	S2	571	MMX	O2-C2-N3	-5.47	115.14	122.07
1	S2	159	A2M	N3-C2-N1	-5.47	120.05	128.60
1	S2	1835	6MZ	N3-C4-N9	5.44	136.05	127.08
1	S2	1853	MA6	N1-C2-N3	-5.41	120.14	128.60
1	S2	166	A2M	C4-N9-C8	5.38	111.55	105.73
1	S2	1835	6MZ	C5-C6-N1	5.32	123.87	118.20
1	S2	1034	A2M	C4-N9-C8	5.29	111.46	105.73
1	S2	121	OMU	C2'-C1'-N1	-5.24	104.05	114.22
1	S2	1853	MA6	C5-C4-N3	-5.20	119.97	126.75
1	S2	27	A2M	C4-N9-C8	5.18	111.34	105.73
1	S2	159	A2M	C4-N9-C8	5.18	111.34	105.73
1	S2	1251	B8N	C5-C4-N3	5.15	125.71	116.17
1	S2	1854	MA6	C5-C4-N3	-5.12	120.08	126.75
1	S2	671	A2M	C4-N9-C8	5.09	111.25	105.73
1	S2	116	OMU	C4-N3-C2	-5.03	119.95	126.58
1	S2	1681	A2M	C5-C4-N3	-5.02	120.20	126.75
1	S2	1681	A2M	C4-N9-C8	4.95	111.09	105.73
1	S2	1835	6MZ	O4'-C4'-C5'	-4.88	93.31	109.37
1	S2	487	A2M	C4-N9-C8	4.84	110.98	105.73
1	S2	159	A2M	C5-C4-N3	-4.74	120.57	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	487	A2M	C5-C4-N3	-4.71	120.60	126.75
1	S2	27	A2M	C5-C4-N3	-4.68	120.64	126.75
1	S2	671	A2M	C5-C4-N3	-4.65	120.68	126.75
1	S2	1034	A2M	C5-C4-N3	-4.64	120.69	126.75
1	S2	1809	M7A	N3-C4-N9	4.63	132.72	126.87
1	S2	166	A2M	C5-C4-N3	-4.51	120.87	126.75
1	S2	1681	A2M	C1'-N9-C8	-4.50	116.97	127.14
1	S2	1084	PSU	C4-N3-C2	-4.48	119.88	126.34
1	S2	1251	B8N	C4-N3-C2	-4.45	119.83	125.46
1	S2	1246	PSU	N1-C2-N3	4.44	120.16	115.13
1	S2	119	PSU	C4-N3-C2	-4.44	119.95	126.34
1	S2	1854	MA6	N9-C8-N7	-4.42	107.87	113.91
1	S2	1835	6MZ	C2-N3-C4	4.42	122.18	111.75
1	S2	825	PSU	C4-N3-C2	-4.41	119.99	126.34
1	S2	571	MMX	C5-C6-N1	4.40	117.94	110.71
1	S2	119	PSU	N1-C2-N3	4.38	120.09	115.13
1	S2	825	PSU	N1-C2-N3	4.36	120.08	115.13
1	S2	1246	PSU	C4-N3-C2	-4.33	120.10	126.34
1	S2	1833	UR3	C1'-N1-C2	4.33	124.30	116.99
1	S2	826	PSU	C4-N3-C2	-4.31	120.13	126.34
1	S2	615	PSU	N1-C2-N3	4.30	120.00	115.13
1	S2	1084	PSU	N1-C2-N3	4.30	120.00	115.13
1	S2	1681	A2M	N3-C4-N9	4.23	134.05	127.08
1	S2	826	PSU	N1-C2-N3	4.21	119.91	115.13
1	S2	1833	UR3	C4-N3-C2	-4.20	120.61	124.56
1	S2	615	PSU	C4-N3-C2	-4.18	120.31	126.34
1	S2	27	A2M	C1'-N9-C8	-4.16	117.74	127.14
1	S2	1853	MA6	N9-C8-N7	-4.11	108.29	113.91
1	S2	1835	6MZ	N1-C2-N3	-4.05	122.27	128.60
1	S2	1835	6MZ	C4'-O4'-C1'	4.04	118.39	109.47
1	S2	121	OMU	N3-C2-N1	4.02	120.22	114.89
1	S2	27	A2M	N3-C4-N9	3.99	133.66	127.08
1	S2	159	A2M	C1'-N9-C8	-3.97	118.17	127.14
1	S2	1835	6MZ	N9-C8-N7	-3.95	108.50	113.91
1	S2	1853	MA6	C4-C5-C6	3.95	120.30	115.88
1	S2	159	A2M	N3-C4-N9	3.94	133.58	127.08
1	S2	1034	A2M	C1'-N9-C8	-3.91	118.31	127.14
1	S2	1809	M7A	C71-N7-C5	-3.87	109.15	124.01
1	S2	1034	A2M	N3-C4-N9	3.87	133.45	127.08
1	S2	487	A2M	N3-C4-N9	3.81	133.37	127.08
1	S2	671	A2M	N3-C4-N9	3.78	133.31	127.08
1	S2	166	A2M	C5-N7-C8	3.77	108.87	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1034	A2M	C5-N7-C8	3.76	108.85	103.51
1	S2	166	A2M	N3-C4-N9	3.75	133.26	127.08
1	S2	159	A2M	C5-N7-C8	3.75	108.84	103.51
1	S2	671	A2M	C5-N7-C8	3.71	108.78	103.51
1	S2	1854	MA6	C4-C5-C6	3.71	120.03	115.88
1	S2	487	A2M	C5-N7-C8	3.68	108.74	103.51
1	S2	1833	UR3	C6-N1-C2	-3.68	118.50	121.79
1	S2	1854	MA6	C2-N1-C6	3.67	120.42	111.75
1	S2	166	A2M	C1'-N9-C8	-3.67	118.86	127.14
1	S2	671	A2M	C1'-N9-C8	-3.63	118.94	127.14
1	S2	116	OMU	N3-C2-N1	3.62	119.70	114.89
1	S2	487	A2M	C1'-N9-C8	-3.61	118.97	127.14
1	S2	121	OMU	C4-N3-C2	-3.61	121.82	126.58
1	S2	27	A2M	C5-N7-C8	3.60	108.62	103.51
1	S2	1681	A2M	C5-N7-C8	3.60	108.62	103.51
1	S2	1853	MA6	C2-N1-C6	3.58	120.22	111.75
1	S2	1681	A2M	C2-N3-C4	3.52	120.06	111.75
1	S2	1809	M7A	C2-N3-C4	3.52	120.06	111.75
1	S2	1854	MA6	C2-N3-C4	3.49	119.98	111.75
1	S2	166	A2M	C2-N3-C4	3.43	119.84	111.75
1	S2	1853	MA6	C2-N3-C4	3.43	119.84	111.75
1	S2	487	A2M	C2-N3-C4	3.35	119.68	111.75
1	S2	121	OMU	C5-C4-N3	3.34	119.84	114.84
1	S2	159	A2M	C2-N3-C4	3.33	119.63	111.75
1	S2	671	A2M	C2-N3-C4	3.33	119.62	111.75
1	S2	1835	6MZ	C5-N7-C8	3.33	108.24	103.51
1	S2	1034	A2M	C2-N3-C4	3.33	119.62	111.75
1	S2	27	A2M	C2-N3-C4	3.31	119.57	111.75
1	S2	116	OMU	C5-C4-N3	3.24	119.69	114.84
1	S2	1853	MA6	N3-C4-N9	3.21	132.38	127.08
1	S2	1854	MA6	C5-N7-C8	3.21	108.08	103.51
1	S2	1854	MA6	N3-C4-N9	3.13	132.24	127.08
1	S2	116	OMU	O4-C4-C5	-3.05	119.79	125.16
1	S2	1853	MA6	C5-N7-C8	3.01	107.79	103.51
1	S2	571	MMX	C6-C5-C4	2.99	117.32	110.92
1	S2	1835	6MZ	C2'-C3'-C4'	-2.98	96.84	102.64
1	S2	1251	B8N	N3-C2-N1	2.95	120.92	116.76
1	S2	571	MMX	C31-N3-C2	2.93	121.21	117.44
1	S2	1835	6MZ	O3'-C3'-C2'	2.93	121.29	111.82
1	S2	1845	4AC	C6-C5-C4	2.82	120.42	116.96
1	S2	166	A2M	C2'-C1'-N9	-2.82	108.78	113.53
1	S2	1833	UR3	O2-C2-N3	-2.80	117.39	121.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1340	4AC	C6-C5-C4	2.75	120.33	116.96
1	S2	1809	M7A	C5-C4-N3	-2.73	120.21	126.62
1	S2	1835	6MZ	C5-C4-N9	2.66	108.88	105.78
1	S2	1246	PSU	O2-C2-N1	-2.64	119.89	122.79
1	S2	119	PSU	O2-C2-N1	-2.62	119.91	122.79
1	S2	817	5MU	C1'-N1-C2	2.61	122.29	117.57
1	S2	121	OMU	O4-C4-C5	-2.58	120.62	125.16
1	S2	615	PSU	O2-C2-N1	-2.57	119.96	122.79
1	S2	825	PSU	O2-C2-N1	-2.57	119.96	122.79
1	S2	121	OMU	O2'-C2'-C1'	2.54	114.03	109.08
1	S2	1845	4AC	C5-C4-N3	-2.53	118.53	122.59
1	S2	1340	4AC	C5-C4-N3	-2.52	118.53	122.59
1	S2	1084	PSU	O2-C2-N1	-2.50	120.04	122.79
1	S2	1835	6MZ	C6-C5-N7	-2.49	129.69	132.39
1	S2	826	PSU	O2-C2-N1	-2.46	120.08	122.79
1	S2	1251	B8N	O4-C4-N3	-2.46	115.81	119.98
1	S2	1246	PSU	C6-N1-C2	-2.39	120.24	122.68
1	S2	1854	MA6	C4-N9-C8	2.37	108.30	105.73
1	S2	615	PSU	C6-N1-C2	-2.33	120.30	122.68
1	S2	1835	6MZ	O5'-C5'-C4'	2.30	116.83	108.99
1	S2	1251	B8N	O4'-C1'-C2'	2.29	108.38	105.14
1	S2	159	A2M	C2'-C3'-C4'	2.29	106.96	101.99
1	S2	119	PSU	C6-N1-C2	-2.26	120.37	122.68
1	S2	1681	A2M	C4-N9-C1'	2.22	131.88	126.59
1	S2	825	PSU	C6-N1-C2	-2.19	120.44	122.68
1	S2	826	PSU	C6-N1-C2	-2.18	120.46	122.68
1	S2	1835	6MZ	C4-C5-N7	-2.17	107.97	110.62
1	S2	671	A2M	C3'-C2'-C1'	2.17	106.96	102.89
1	S2	817	5MU	C1'-N1-C6	-2.15	117.54	121.12
1	S2	1835	6MZ	O4'-C1'-N9	-2.15	103.83	108.06
1	S2	1853	MA6	C4-N9-C8	2.14	108.05	105.73
1	S2	116	OMU	C1'-N1-C2	2.14	121.45	117.57
1	S2	671	A2M	C2'-C3'-C4'	2.12	106.59	101.99
1	S2	671	A2M	O4'-C4'-C3'	2.11	109.29	105.11
1	S2	1854	MA6	C4-C5-N7	-2.09	108.07	110.62
1	S2	1340	4AC	N4-C4-N3	2.09	117.36	113.85
1	S2	1084	PSU	C6-N1-C2	-2.08	120.56	122.68
1	S2	1845	4AC	N4-C4-N3	2.06	117.31	113.85
1	S2	826	PSU	O4'-C1'-C2'	2.05	108.04	105.14
1	S2	121	OMU	O4'-C1'-N1	2.01	112.95	108.36
1	S2	27	A2M	C2'-C1'-N9	-2.00	110.16	113.53

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S2	27	A2M	C3'-C4'-C5'-O5'
1	S2	116	OMU	C3'-C4'-C5'-O5'
1	S2	116	OMU	O4'-C4'-C5'-O5'
1	S2	121	OMU	C1'-C2'-O2'-CM2
1	S2	520	OMC	O4'-C4'-C5'-O5'
1	S2	571	MMX	O4'-C1'-N1-C2
1	S2	571	MMX	O4'-C1'-N1-C6
1	S2	686	OMG	C3'-C4'-C5'-O5'
1	S2	826	PSU	O4'-C1'-C5-C4
1	S2	826	PSU	O4'-C1'-C5-C6
1	S2	1251	B8N	N3-C31-C32-C33
1	S2	1833	UR3	O4'-C1'-N1-C6
1	S2	1833	UR3	O4'-C1'-N1-C2
1	S2	1853	MA6	O4'-C4'-C5'-O5'
1	S2	1853	MA6	C3'-C4'-C5'-O5'
1	S2	1853	MA6	C5-C6-N6-C9
1	S2	1853	MA6	C5-C6-N6-C10
1	S2	1854	MA6	C5-C6-N6-C10
1	S2	27	A2M	O4'-C4'-C5'-O5'
1	S2	520	OMC	C3'-C4'-C5'-O5'
1	S2	571	MMX	C3'-C4'-C5'-O5'
1	S2	571	MMX	O4'-C4'-C5'-O5'
1	S2	1246	PSU	C3'-C4'-C5'-O5'
1	S2	1854	MA6	O4'-C4'-C5'-O5'
1	S2	1246	PSU	O4'-C4'-C5'-O5'
1	S2	1854	MA6	C3'-C4'-C5'-O5'
1	S2	1853	MA6	N1-C6-N6-C9
1	S2	1854	MA6	N1-C6-N6-C10
1	S2	1835	6MZ	O4'-C4'-C5'-O5'
1	S2	686	OMG	O4'-C4'-C5'-O5'
1	S2	1681	A2M	O4'-C4'-C5'-O5'
1	S2	1854	MA6	C5-C6-N6-C9
1	S2	1809	M7A	C2'-C1'-N9-C8
1	S2	159	A2M	C4'-C5'-O5'-P
1	S2	671	A2M	C4'-C5'-O5'-P
1	S2	671	A2M	C2'-C1'-N9-C8
1	S2	1251	B8N	N34-C33-C34-O35
1	S2	1854	MA6	C4'-C5'-O5'-P
1	S2	1681	A2M	C3'-C4'-C5'-O5'
1	S2	647	OMG	C3'-C4'-C5'-O5'
1	S2	647	OMG	C4'-C5'-O5'-P

There are no ring outliers.

14 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	826	PSU	1	0
1	S2	1833	UR3	2	0
1	S2	647	OMG	1	0
1	S2	1034	A2M	1	0
1	S2	615	PSU	1	0
1	S2	1681	A2M	1	0
1	S2	1835	6MZ	5	0
1	S2	1845	4AC	1	0
1	S2	116	OMU	1	0
1	S2	512	OMG	2	0
1	S2	166	A2M	1	0
1	S2	1853	MA6	2	0
1	S2	27	A2M	1	0
1	S2	121	OMU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 39 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

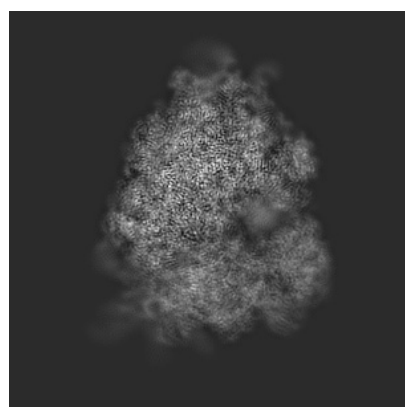
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13954. These allow visual inspection of the internal detail of the map and identification of artifacts.

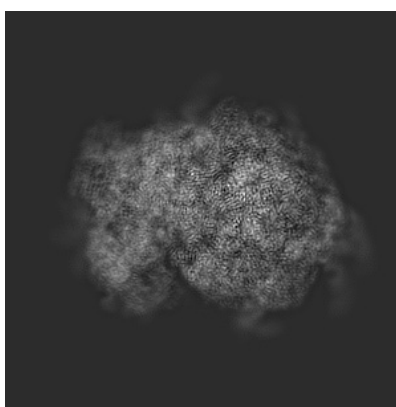
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

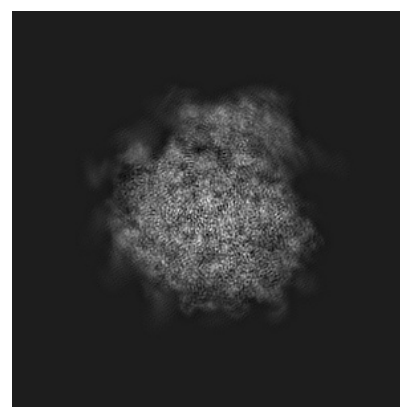
6.1.1 Primary map



X



Y

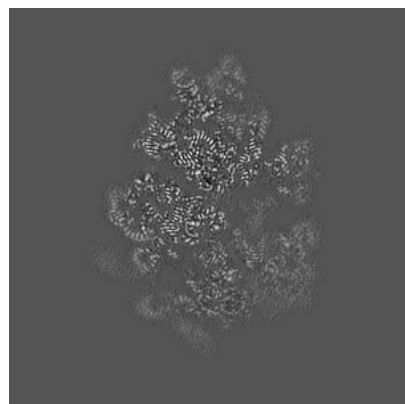


Z

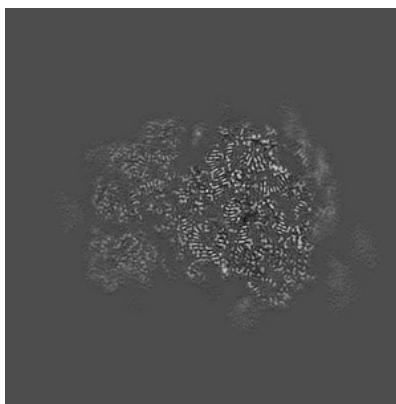
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

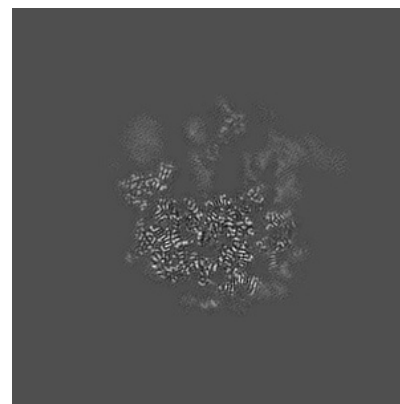
6.2.1 Primary map



X Index: 149



Y Index: 149

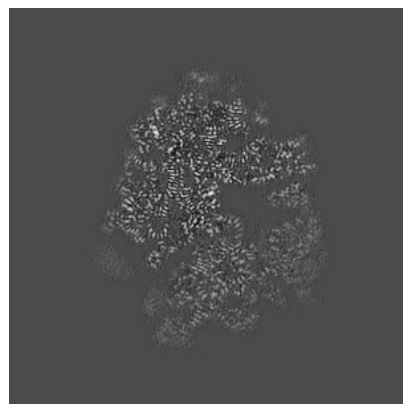


Z Index: 149

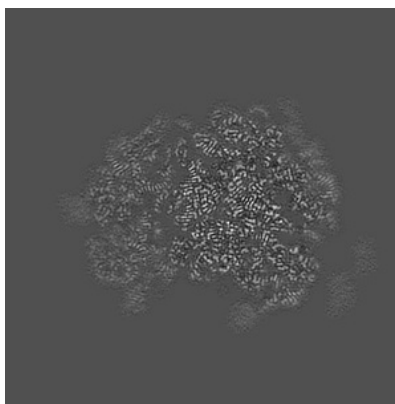
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

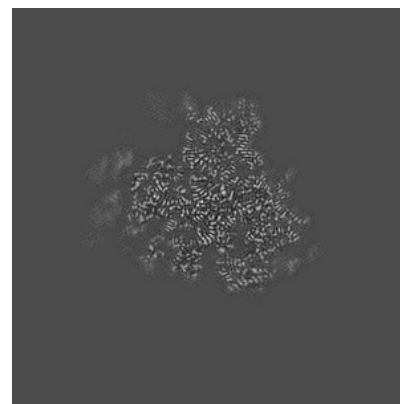
6.3.1 Primary map



X Index: 162



Y Index: 141

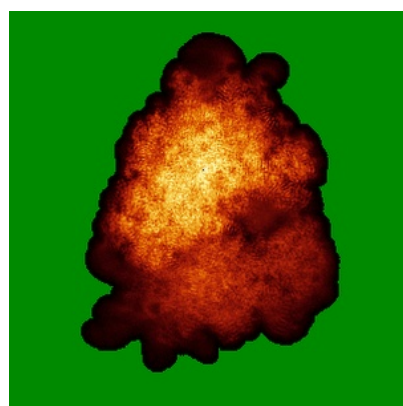


Z Index: 183

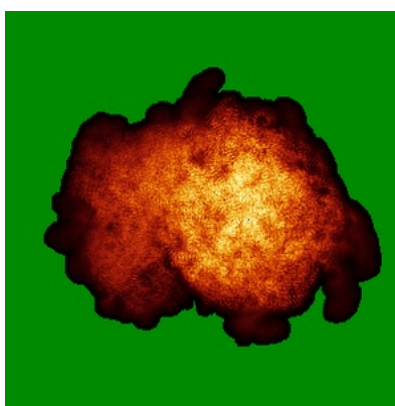
The images above show the largest variance slices of the map in three orthogonal directions.

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

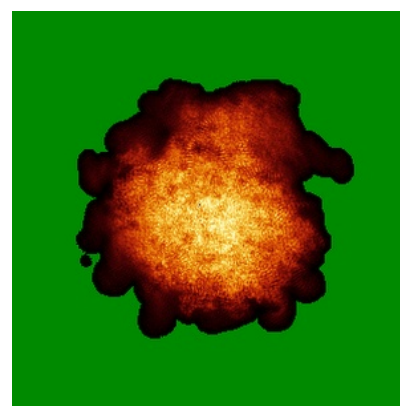
6.4.1 Primary map



X



Y

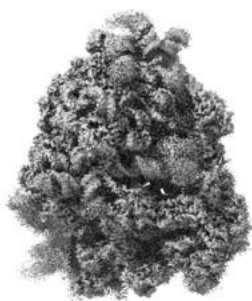


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0475. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

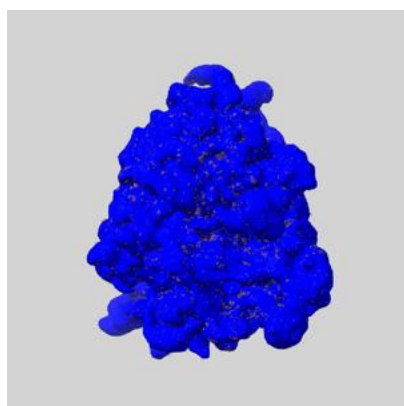
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

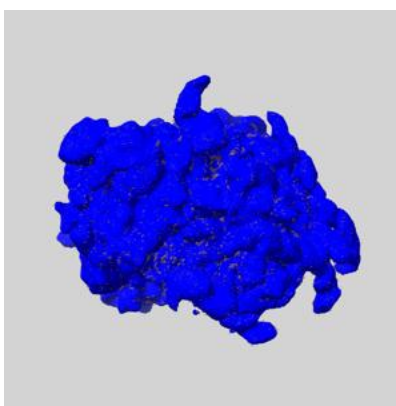
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

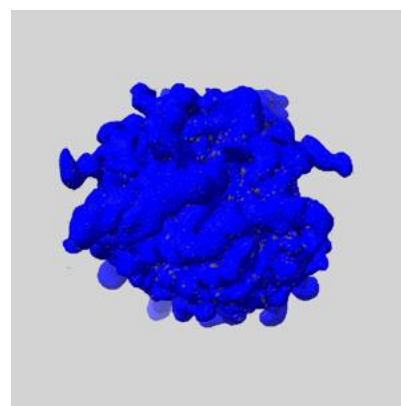
6.6.1 emd_13954_msk_1.map [i](#)



X



Y

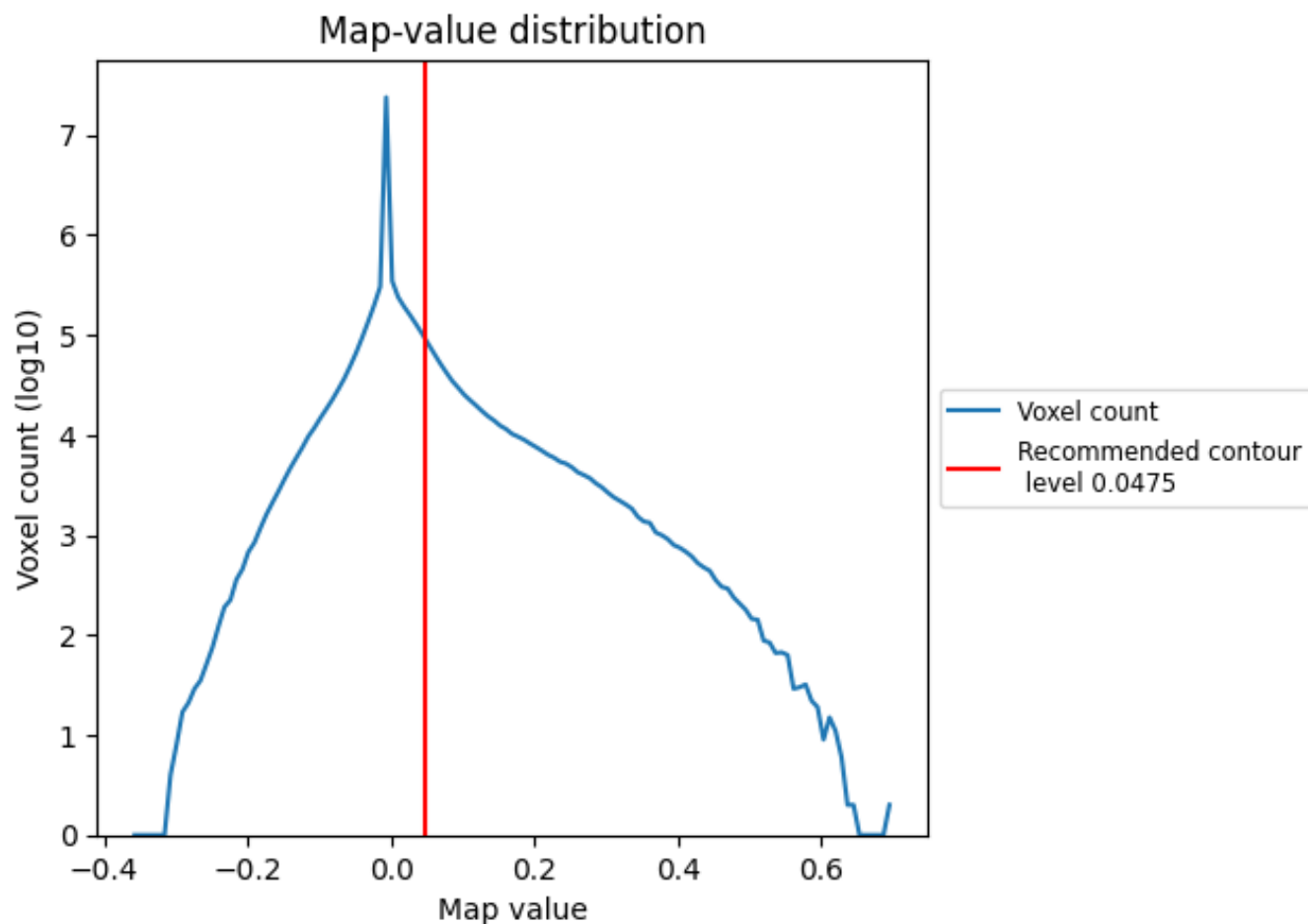


Z

7 Map analysis [i](#)

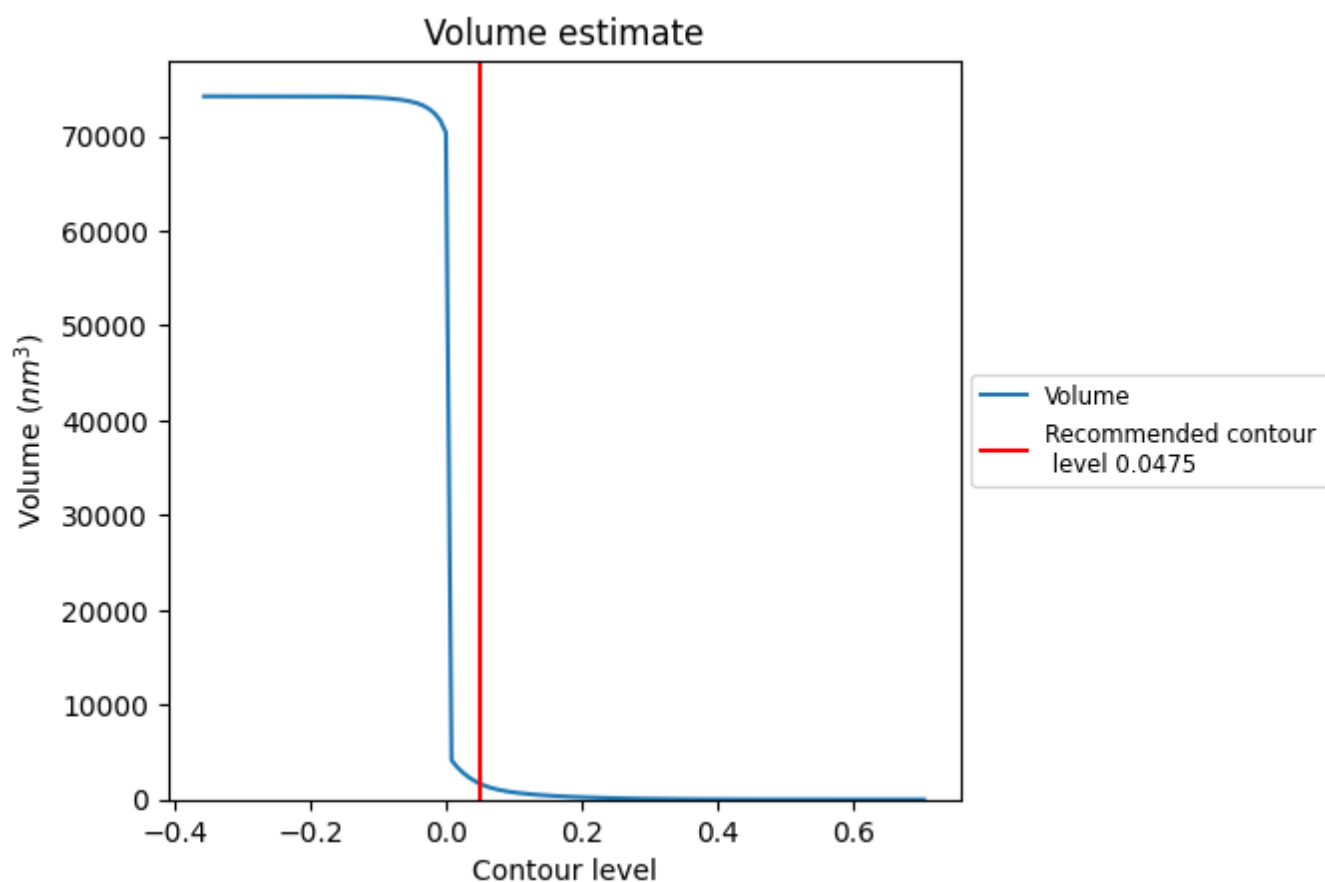
This section contains the results of statistical analysis of the map.

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.

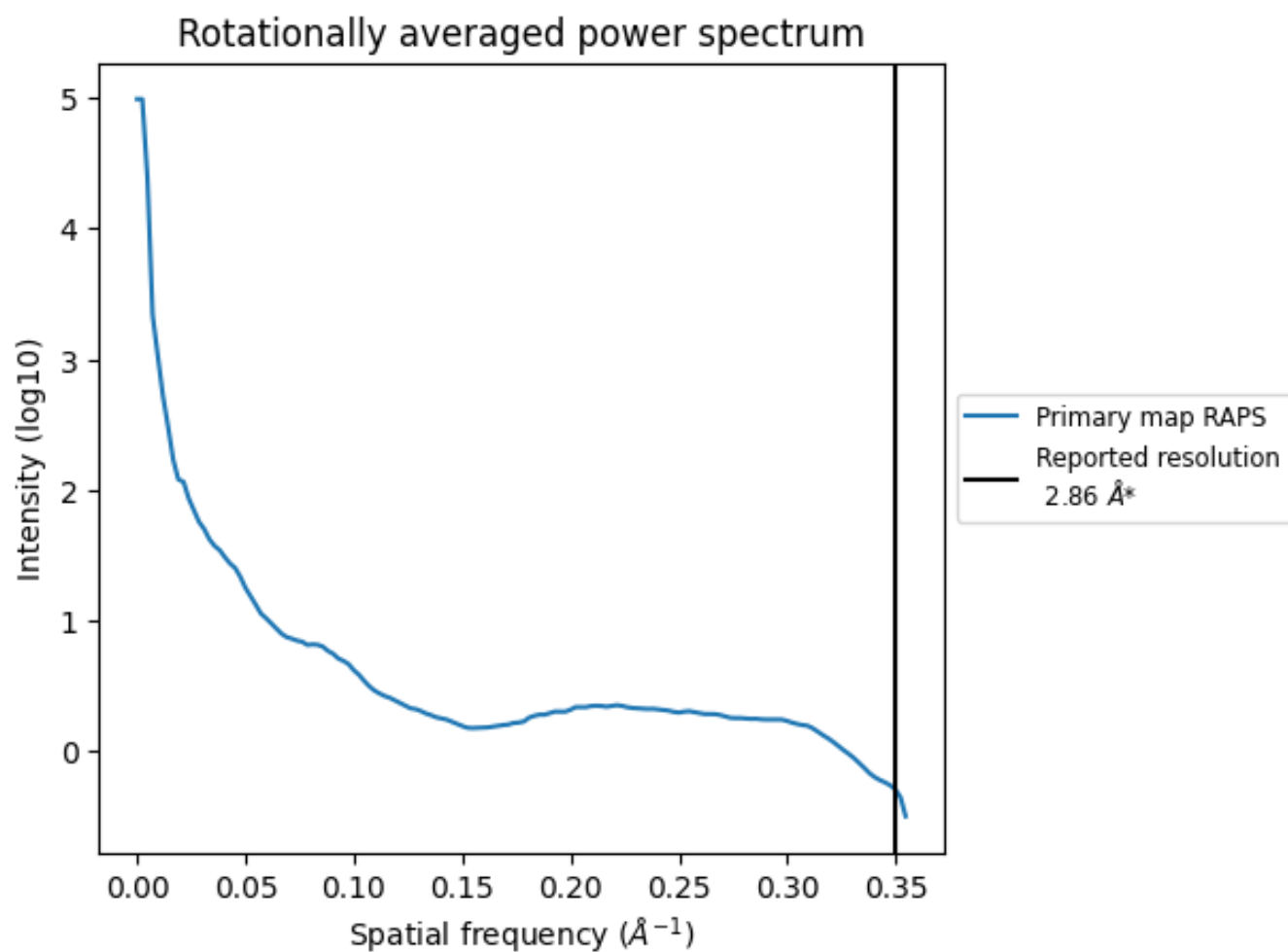
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1728 nm³; this corresponds to an approximate mass of 1561 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 [i](#)

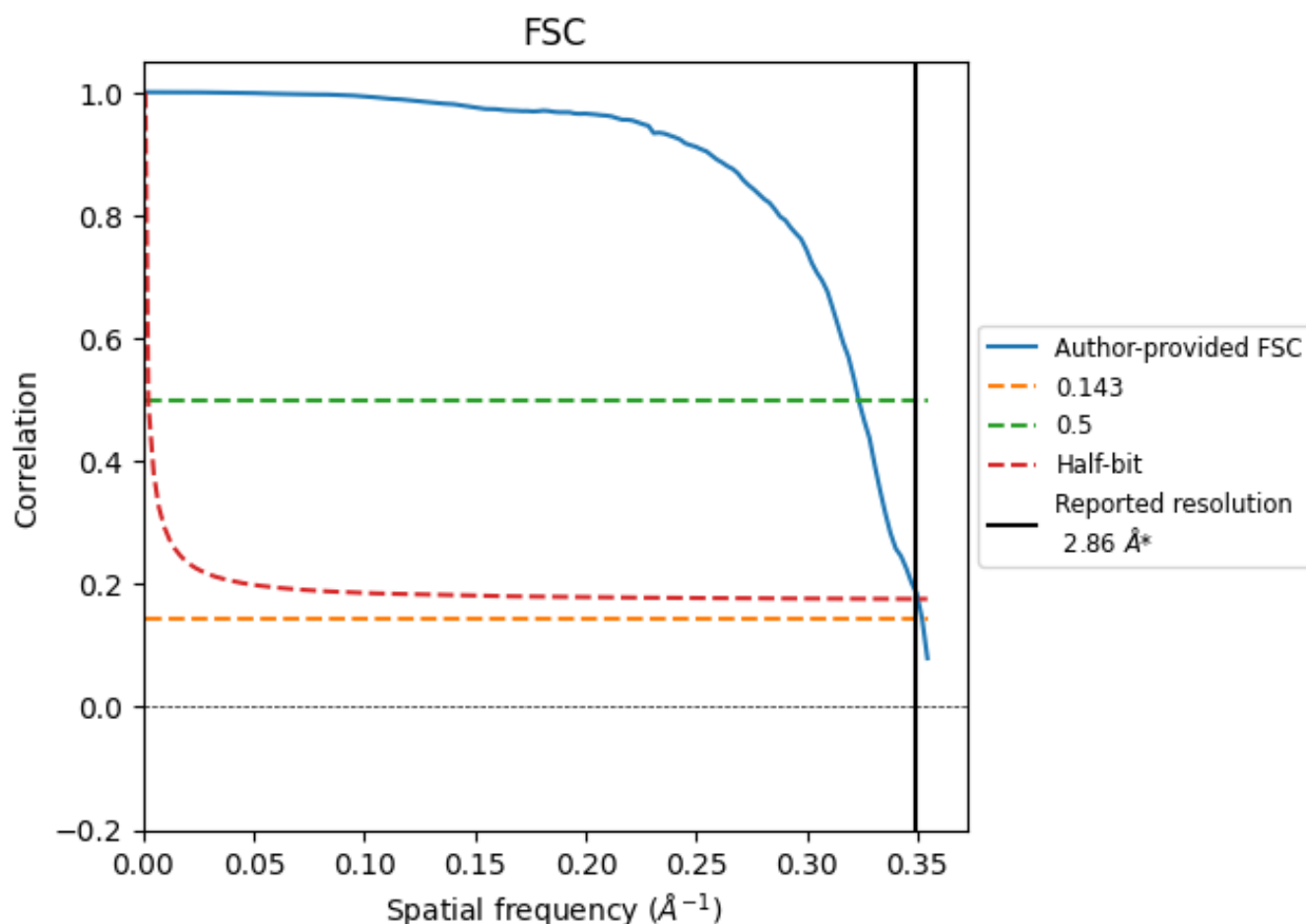


*Reported resolution corresponds to spatial frequency of 0.350 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.350 Å⁻¹

8.2 Resolution estimates [i](#)

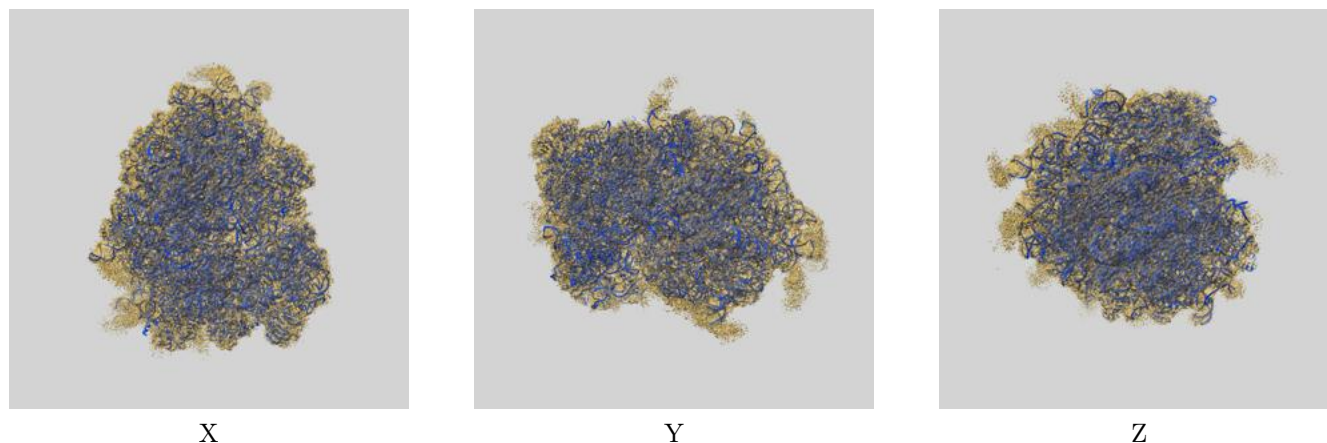
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.84	3.09	2.85
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

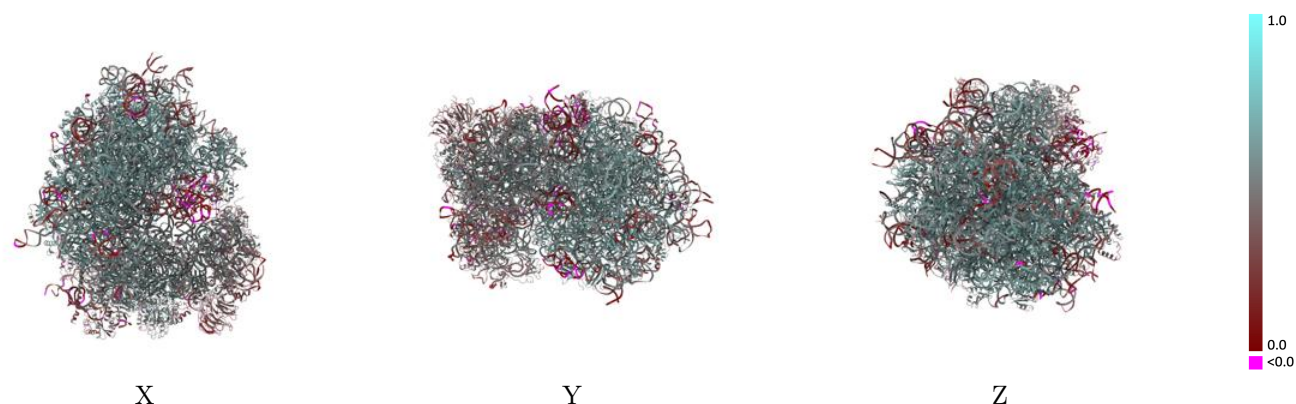
This section contains information regarding the fit between EMDB map EMD-13954 and PDB model 7QGG. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



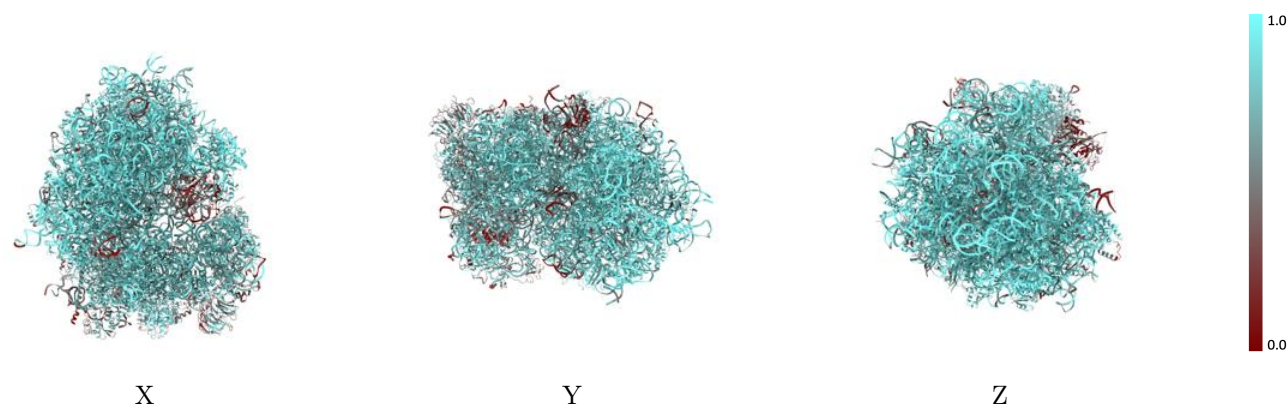
The images above show the 3D surface view of the map at the recommended contour level 0.0475 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



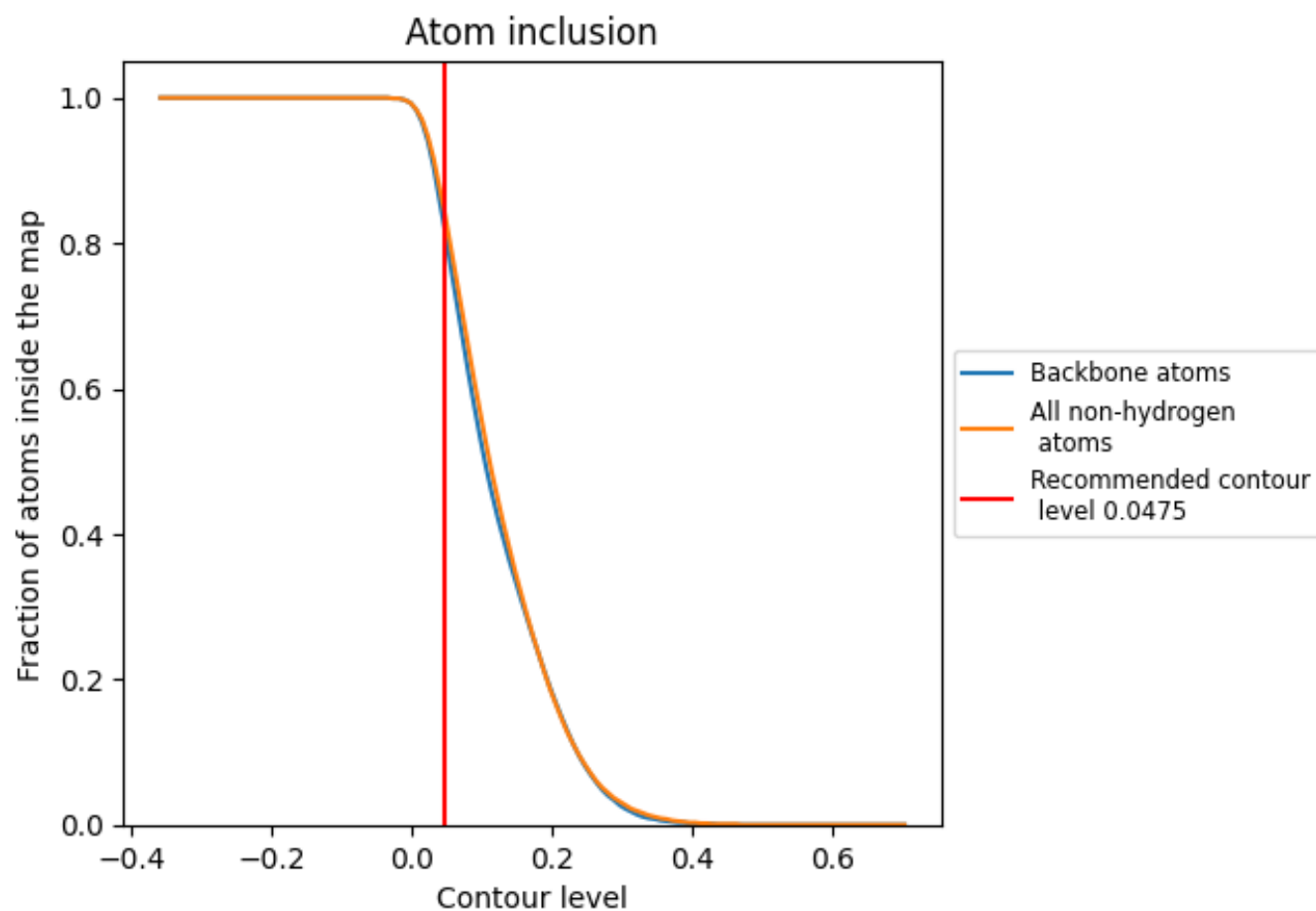
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0475).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 84% 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 (0.0475) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.5000
A	 0.9150	 0.6060
B	 0.9330	 0.5960
C	 0.9360	 0.5990
Cz	 0.1280	 0.1170
D	 0.9130	 0.5300
E	 0.9860	 0.5870
F	 0.9260	 0.5610
G	 0.8330	 0.5180
H	 0.9470	 0.6150
I	 0.8110	 0.5150
J	 0.9190	 0.5800
K	 0.8980	 0.5820
L	 0.8630	 0.5240
M	 0.8610	 0.5390
N	 0.9340	 0.5880
O	 0.9640	 0.6240
P	 0.9300	 0.5940
Q	 0.9250	 0.5960
R	 0.9300	 0.6150
S	 0.8290	 0.5400
S2	 0.8380	 0.4570
SA	 0.7690	 0.4890
SB	 0.7510	 0.4850
SC	 0.7840	 0.5210
SD	 0.6230	 0.4060
SE	 0.7740	 0.4790
SF	 0.6770	 0.4500
SG	 0.6170	 0.3890
SH	 0.6220	 0.3970
SI	 0.7000	 0.4390
SJ	 0.7850	 0.4560
SK	 0.6840	 0.3910
SL	 0.7170	 0.4950
SM	 0.1180	 0.1860



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Chain	Atom inclusion	Q-score
SN	 0.7680	 0.5080
SO	 0.7890	 0.5040
SP	 0.7560	 0.4500
SQ	 0.7110	 0.4330
SR	 0.6250	 0.4020
SS	 0.7270	 0.4630
ST	 0.7430	 0.4590
SU	 0.5020	 0.3760
SV	 0.7870	 0.4980
SW	 0.8580	 0.5550
SX	 0.8030	 0.5330
SY	 0.7040	 0.4200
SZ	 0.5950	 0.3790
Sa	 0.8220	 0.5210
Sb	 0.7370	 0.4730
Sc	 0.6280	 0.4060
Sd	 0.8120	 0.4640
Se	 0.6220	 0.4270
Sf	 0.1460	 0.2010
Sg	 0.5340	 0.3160
T	 0.9330	 0.5910
U	 0.9170	 0.5790
V	 0.8730	 0.5120
W	 0.8990	 0.5960
X	 0.9230	 0.5950
Y	 0.9100	 0.5880
Z	 0.9230	 0.5890
a	 0.9200	 0.5730
b	 0.9520	 0.6140
c	 0.8700	 0.5450
d	 0.8700	 0.5460
e	 0.9200	 0.5860
f	 0.9280	 0.6010
g	 0.9550	 0.6230
h	 0.8750	 0.5660
i	 0.9090	 0.5820
j	 0.8920	 0.5700
k	 0.9390	 0.5960
l	 0.8280	 0.5250
m	 0.9170	 0.6110
n	 0.9600	 0.5870
o	 0.8080	 0.5540

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Chain	Atom inclusion	Q-score
p	 0.8900	 0.5700
q	 0.8870	 0.5890
r	 0.8950	 0.5690
t	 0.9050	 0.5110
u	 0.5060	 0.3080
v	 0.6020	 0.3140
w	 0.5650	 0.3760
y	 0.4580	 0.3900