



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:43 PM UTC

PDB ID : 5M1J / pdb_00005m1j
EMDB ID : EMD-4140
Title : Nonstop ribosomal complex bound with Dom34 and Hbs1
Authors : Hilal, T.; Yamamoto, H.; Loerke, J.; Buerger, J.; Mielke, T.; Spahn, C.M.T.
Deposited on : 2016-10-07
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

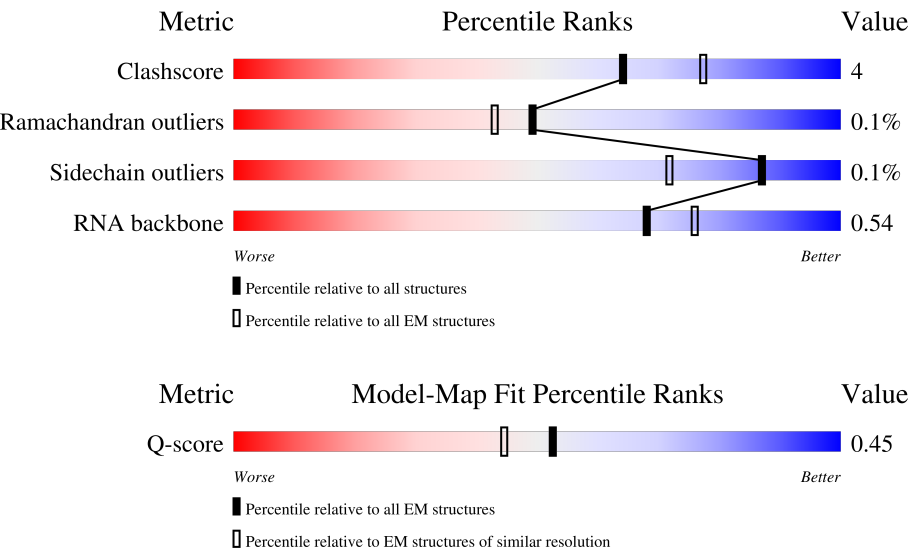
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	A1	381	
2	A2	207	
3	a2	98	

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Mol	Chain	Length	Quality of chain
4	B2	214	
5	b2	81	
6	C2	217	
7	c2	63	
8	D2	223	
9	d2	53	
10	E2	260	
11	e2	60	
12	F2	206	
13	G2	226	
14	g2	318	
15	H2	184	
16	I2	199	
17	J2	185	
18	K2	96	
19	L2	155	
20	M2	124	
21	N2	150	
22	O2	127	
23	P2	124	
24	Q2	141	
25	R2	125	
26	S2	145	
27	T2	143	
28	U2	107	

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Mol	Chain	Length	Quality of chain
29	V2	87	
30	W2	129	
31	X2	144	
32	Y2	134	
33	Z2	70	
34	22	1798	
35	f2	71	
36	14	3396	
37	34	121	
38	44	158	
39	a5	148	
40	A5	252	
41	b5	58	
42	B5	386	
43	c5	97	
44	C5	361	
45	D5	296	
46	d5	109	
47	e5	127	
48	f5	106	
49	F5	222	
50	g5	112	
51	G5	233	
52	h5	119	
53	H5	191	

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Mol	Chain	Length	Quality of chain
54	i5	99	
55	I5	220	
56	J5	169	
57	j5	87	
58	k5	77	
59	l5	50	
60	L5	193	
61	m5	52	
62	M5	136	
63	N5	203	
64	o5	105	
65	p5	91	
66	P5	183	
67	Q5	185	
68	S5	172	
69	U5	100	
70	V5	136	
71	Z5	135	
72	K5	197	
73	n5	25	
74	R5	188	
75	X5	121	
76	Y5	126	
77	T5	159	
78	E5	175	

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Mol	Chain	Length	Quality of chain
79	W5	98	41% 94% 6%
80	A6	611	64% 74% 14% 12%
81	X7	20	25% 15% 30% 15% 40%
82	A3	76	50% 30% 17%

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 212865 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 protein called Protein DOM34.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	381	Total	C	N	O	S	0	0
			3058	1976	478	589	15		

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A2	207	Total	C	N	O	S	0	0
			1621	1039	286	294	2		

- Molecule 3 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a2	98	Total	C	N	O	S	0	0
			778	480	162	131	5		

- Molecule 4 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B2	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 5 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	b2	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 6 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C2	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 7 is a protein called 40S ribosomal protein S28-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c2	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 8 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D2	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 9 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	d2	53	Total	C	N	O	S	0	0
			443	275	92	72	4		

- Molecule 10 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E2	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 11 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	e2	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 12 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F2	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 13 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G2	226	Total	C	N	O	S	0	0
			1820	1142	350	325	3		

- Molecule 14 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	g2	318	Total	C	N	O	S	0	0
			2445	1546	419	472	8		

- Molecule 15 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H2	184	Total	C	N	O	S	0	0
			1481	951	265	265			

- Molecule 16 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I2	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 17 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J2	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 18 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K2	96	Total	C	N	O	S	0	0
			817	529	133	153	2		

- Molecule 19 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L2	155	Total	C	N	O	S	0	0
			1244	798	235	208	3		

- Molecule 20 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M2	124	Total	C	N	O	S	0	0
			934	587	165	180	2		

- Molecule 21 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N2	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 22 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O2	127	Total	C	N	O	S	0	0
			941	578	186	174	3		

- Molecule 23 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P2	124	Total	C	N	O	S	0	0
			991	631	187	166	7		

- Molecule 24 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q2	141	Total	C	N	O		0	0
			1105	708	203	194			

- Molecule 25 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R2	125	Total	C	N	O	S	0	0
			1000	625	188	185	2		

- Molecule 26 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S2	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 27 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T2	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 28 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U2	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 29 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V2	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 30 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W2	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 31 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X2	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 32 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Y2	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 33 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Z2	70	Total	C	N	O	0	0
			563	360	104	99		

- Molecule 34 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	22	1781	Total	C	N	O	P	0	0
			37948	16965	6715	12487	1781		

- Molecule 35 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f2	71	Total	C	N	O	S	0	0
			497	309	93	91	4		

- Molecule 36 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	14	3295	Total	C	N	O	P	0	0
			70476	31477	12696	23008	3295		

- Molecule 37 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	34	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	44	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 39 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	a5	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 40 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A5	252	Total	C	N	O	S	0	0
			1918	1193	389	335	1		

- Molecule 41 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	b5	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 42 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	B5	386	Total	C	N	O	S	0	0
			3081	1956	584	533	8		

- Molecule 43 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	c5	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 44 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	C5	361	Total	C	N	O	S	0	0
			2749	1730	522	494	3		

- Molecule 45 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	D5	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 46 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	d5	109	Total	C	N	O	S	0	0
			890	565	168	156	1		

- Molecule 47 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	e5	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 48 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	f5	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 49 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	F5	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 50 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	g5	112	Total	C	N	O	S	0	0
			881	546	179	152	4		

- Molecule 51 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	G5	233	Total	C	N	O	S	0	0
			1817	1159	326	329	3		

- Molecule 52 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	h5	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 53 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	H5	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 54 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	i5	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 55 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	I5	211	Total	C	N	O	S	0	0
			1717	1089	325	297	6		

- Molecule 56 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	J5	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 57 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	j5	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 58 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	k5	77	Total	C	N	O		0	0
			612	391	115	106			

- Molecule 59 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	l5	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	L5	193	Total	C	N	O		0	0
			1543	962	315	266			

- Molecule 61 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	m5	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 62 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	M5	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 63 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	N5	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 64 is a protein called 60S ribosomal protein L42-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	o5	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 65 is a protein called 60S ribosomal protein L43-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	p5	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 66 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	P5	183	Total	C	N	O	S	0	0
			1442	896	287	259			

- Molecule 67 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Q5	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 68 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	S5	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 69 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	U5	100	Total	C	N	O	S	0	0
			796	516	131	149			

- Molecule 70 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	V5	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 71 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Z5	135	Total	C	N	O		0	0
			1092	710	202	180			

- Molecule 72 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	K5	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 73 is a protein called 60S ribosomal protein L41-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	n5	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 74 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	R5	188	Total	C	N	O		0	0
			1521	935	326	260			

- Molecule 75 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	X5	121	Total	C	N	O	S	0	0
			968	623	170	173	2		

- Molecule 76 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Y5	126	Total	C	N	O		0	0
			993	625	192	176			

- Molecule 77 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	T5	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 78 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	E5	157	Total	C	N	O	S	0	0
			1248	806	224	217	1		

- Molecule 79 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	W5	98	Total	C	N	O	S	0	0
			800	508	159	132	1		

- Molecule 80 is a protein called Protein HBS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	A6	539	Total	C	N	O	S	0	0
			4279	2712	723	827	17		

- Molecule 81 is a RNA chain called nonstop mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	X7	12	Total	C	N	O	P	0	0
			259	116	49	82	12		

- Molecule 82 is a RNA chain called yeast Phe-tRNA-Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	A3	76	Total	C	N	O	P	0	0
			1651	745	294	536	76		

- Molecule 83 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
83	a2	1	Total	Zn	0
			1	1	
83	b2	1	Total	Zn	0
			1	1	
83	d2	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
83	f2	1	Total 1	Zn 1	0
83	j5	1	Total 1	Zn 1	0
83	m5	1	Total 1	Zn 1	0
83	o5	1	Total 1	Zn 1	0
83	p5	1	Total 1	Zn 1	0

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

Mol	Chain	Residues	Atoms		AltConf
84	B2	1	Total 1	Mg 1	0
84	C2	2	Total 2	Mg 2	0
84	d2	1	Total 1	Mg 1	0
84	E2	2	Total 2	Mg 2	0
84	F2	2	Total 2	Mg 2	0
84	I2	2	Total 2	Mg 2	0
84	J2	1	Total 1	Mg 1	0
84	L2	1	Total 1	Mg 1	0
84	N2	2	Total 2	Mg 2	0
84	Q2	1	Total 1	Mg 1	0
84	S2	4	Total 4	Mg 4	0
84	T2	1	Total 1	Mg 1	0
84	U2	1	Total 1	Mg 1	0
84	X2	3	Total 3	Mg 3	0

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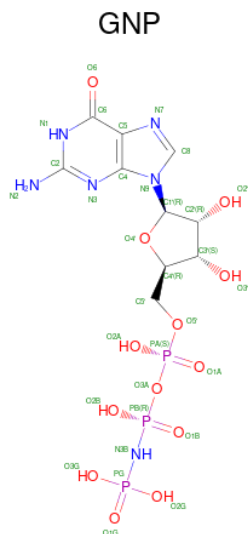
Mol	Chain	Residues	Atoms		AltConf
84	Y2	1	Total 1	Mg 1	0
84	22	177	Total 177	Mg 177	0
84	14	701	Total 701	Mg 701	0
84	34	16	Total 16	Mg 16	0
84	44	34	Total 34	Mg 34	0
84	a5	3	Total 3	Mg 3	0
84	A5	6	Total 6	Mg 6	0
84	b5	1	Total 1	Mg 1	0
84	B5	5	Total 5	Mg 5	0
84	C5	8	Total 8	Mg 8	0
84	D5	1	Total 1	Mg 1	0
84	d5	3	Total 3	Mg 3	0
84	e5	3	Total 3	Mg 3	0
84	f5	1	Total 1	Mg 1	0
84	F5	4	Total 4	Mg 4	0
84	I5	4	Total 4	Mg 4	0
84	J5	2	Total 2	Mg 2	0
84	j5	7	Total 7	Mg 7	0
84	l5	1	Total 1	Mg 1	0
84	L5	4	Total 4	Mg 4	0
84	m5	3	Total 3	Mg 3	0

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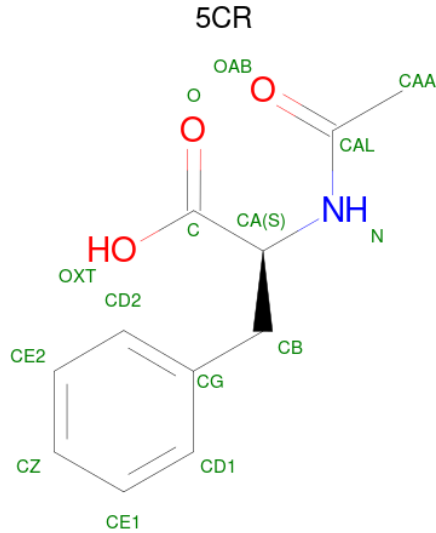
Mol	Chain	Residues	Atoms		AltConf
84	M5	1	Total 1	Mg 1	0
84	N5	7	Total 7	Mg 7	0
84	o5	3	Total 3	Mg 3	0
84	P5	7	Total 7	Mg 7	0
84	Q5	4	Total 4	Mg 4	0
84	S5	4	Total 4	Mg 4	0
84	V5	3	Total 3	Mg 3	0
84	K5	5	Total 5	Mg 5	0
84	R5	3	Total 3	Mg 3	0
84	Y5	2	Total 2	Mg 2	0
84	T5	1	Total 1	Mg 1	0
84	E5	1	Total 1	Mg 1	0
84	A6	2	Total 2	Mg 2	0
84	A3	6	Total 6	Mg 6	0

- Molecule 85 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
85	A6	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 86 is N-acetyl-L-phenylalanine (CCD ID: 5CR) (formula: $C_{11}H_{13}NO_3$).



Mol	Chain	Residues	Atoms				AltConf
86	A3	1	Total	C	N	O	0
			14	11	1	2	

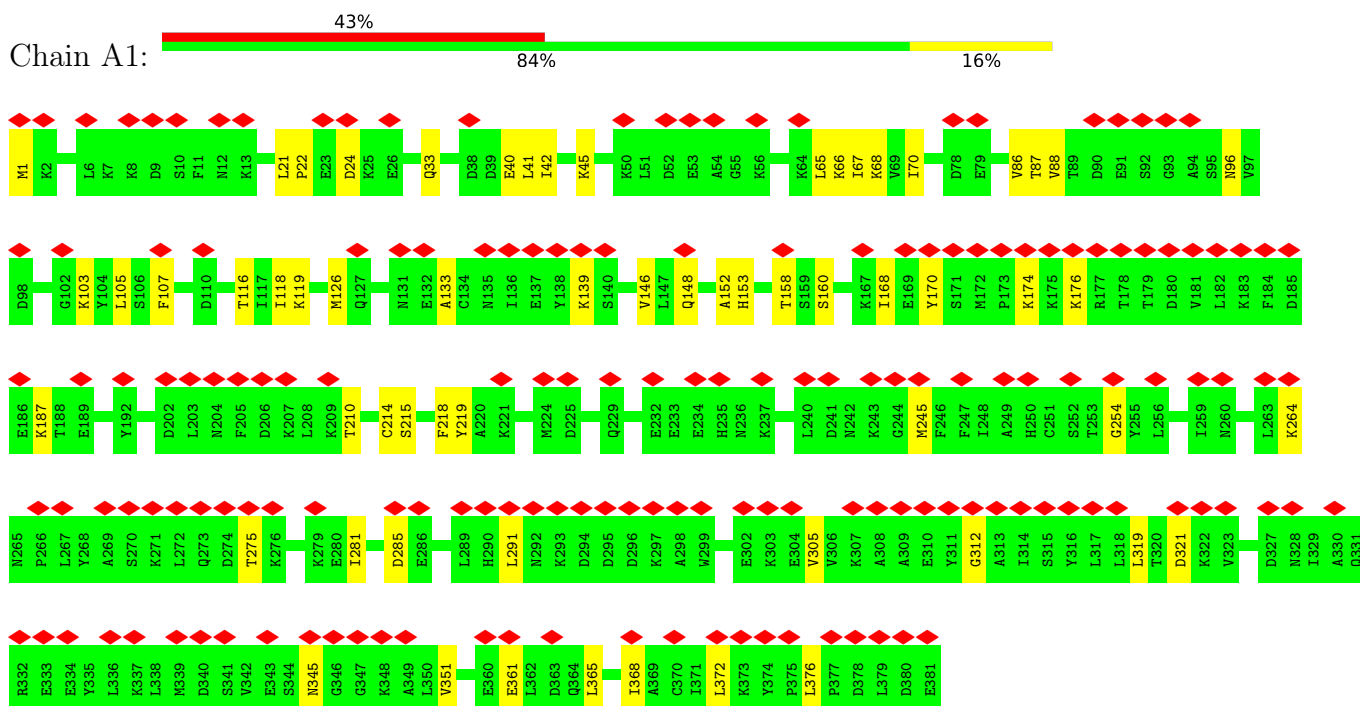
- Molecule 87 is water.

Mol	Chain	Residues	Atoms		AltConf
87	A1	7	Total 7	O 7	0
87	A6	6	Total 6	O 6	0

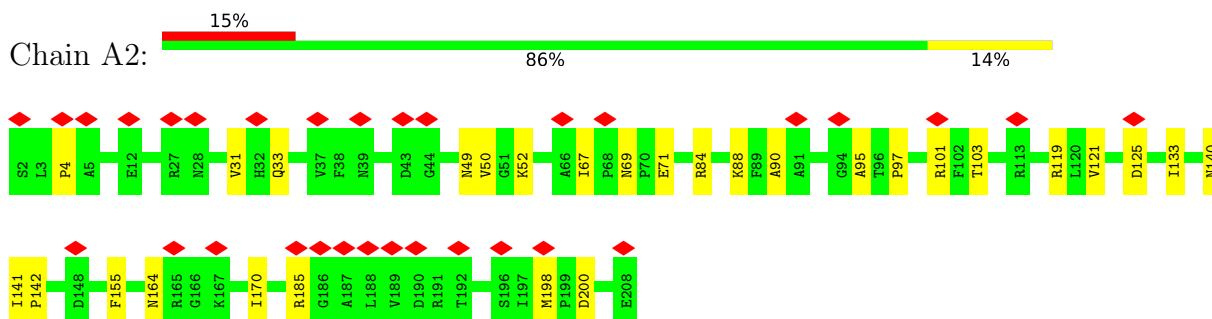
3 Residue-property plots

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

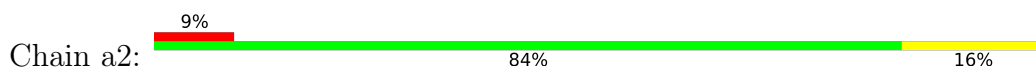
• Molecule 1: Protein DOM34

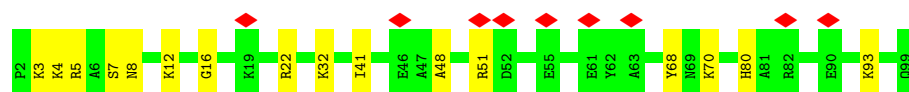


• Molecule 2: 40S ribosomal protein S0-A

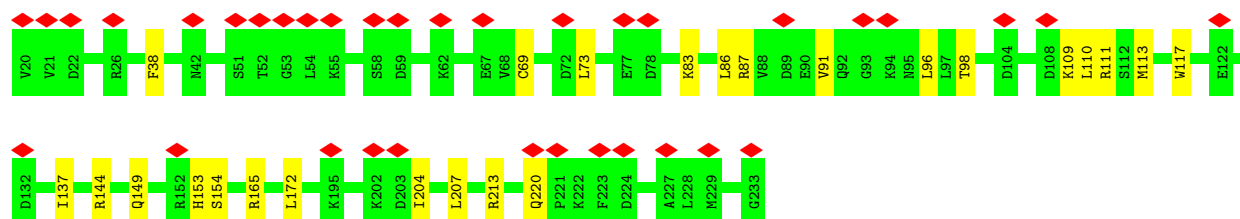
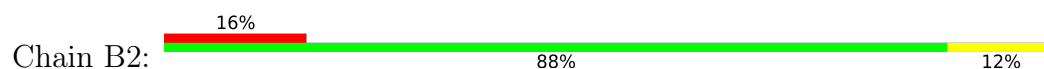


• Molecule 3: 40S ribosomal protein S26-B

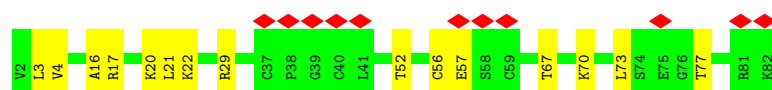
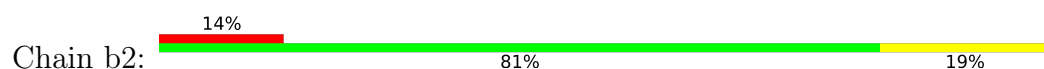




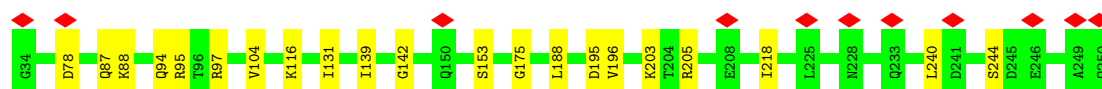
- Molecule 4: 40S ribosomal protein S1-A



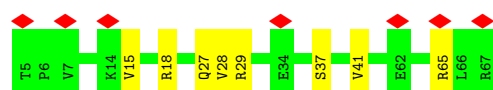
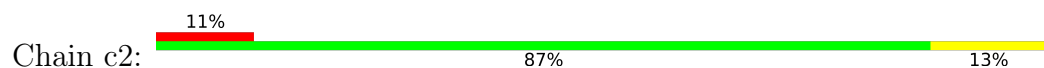
- Molecule 5: 40S ribosomal protein S27-A



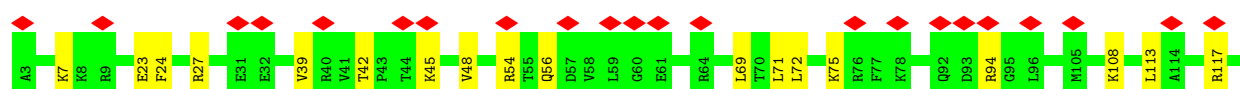
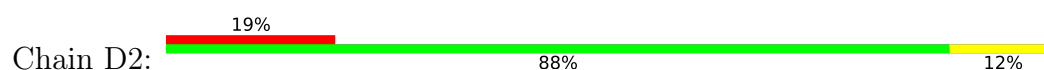
- Molecule 6: 40S ribosomal protein S2



- Molecule 7: 40S ribosomal protein S28-B

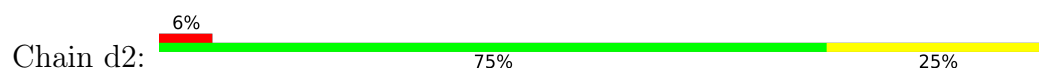


- Molecule 8: 40S ribosomal protein S3

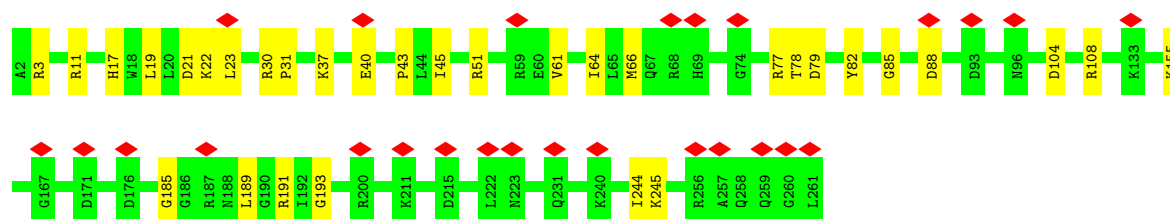
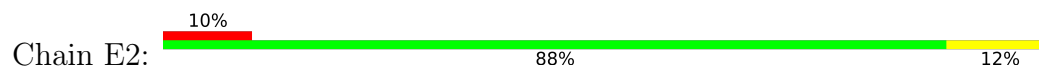


- Molecule 9: 40S ribosomal protein S29-A

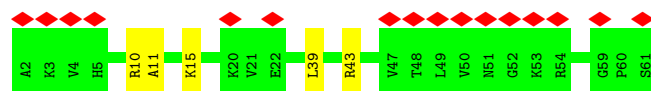




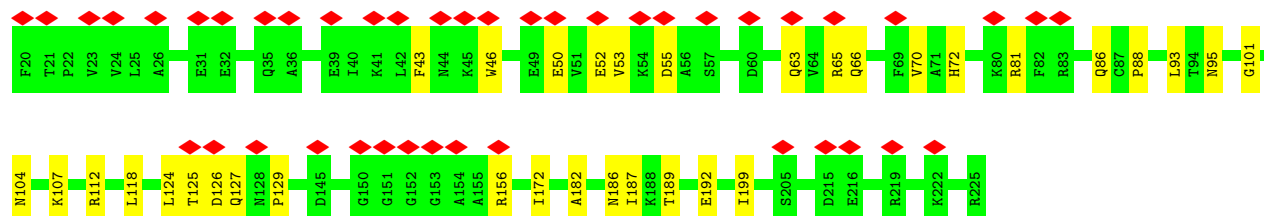
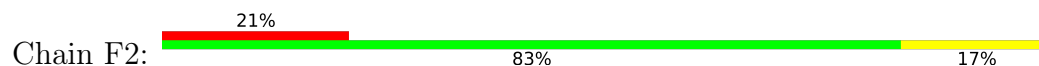
- Molecule 10: 40S ribosomal protein S4-A



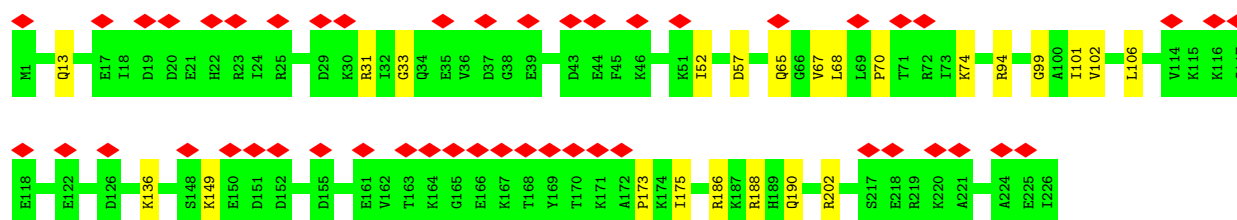
- Molecule 11: 40S ribosomal protein S30-A



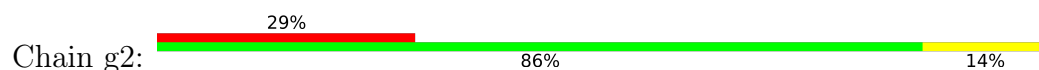
- Molecule 12: 40S ribosomal protein S5

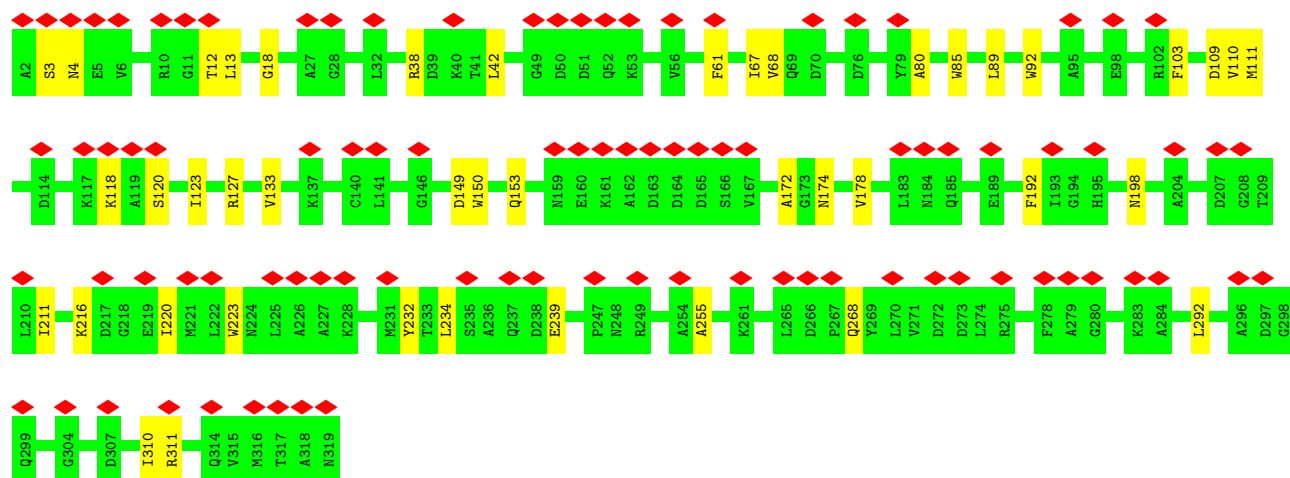


- Molecule 13: 40S ribosomal protein S6-A

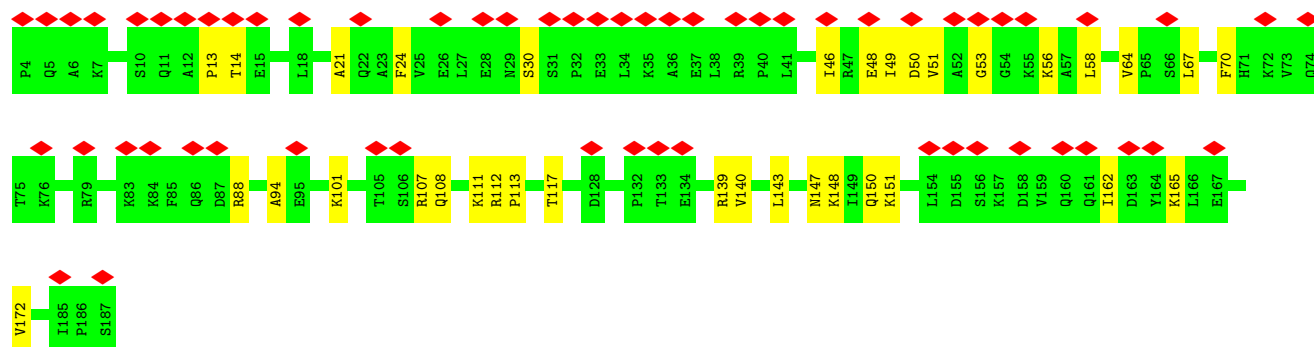
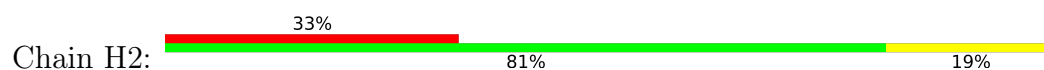


- Molecule 14: Guanine nucleotide-binding protein subunit beta-like protein

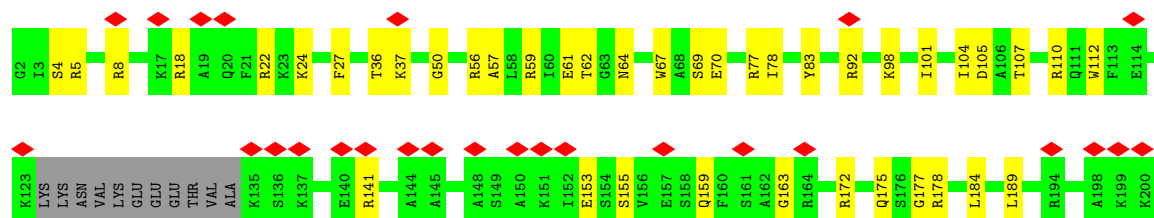
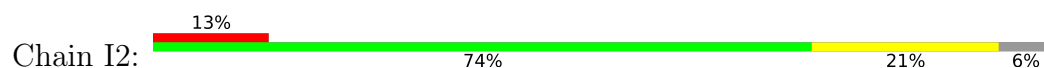




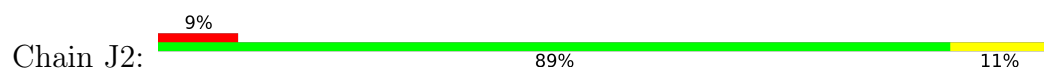
- Molecule 15: 40S ribosomal protein S7-A



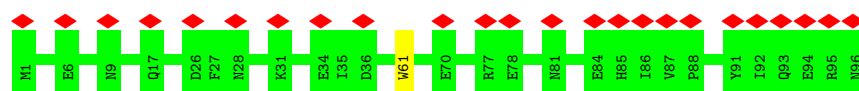
- Molecule 16: 40S ribosomal protein S8-A



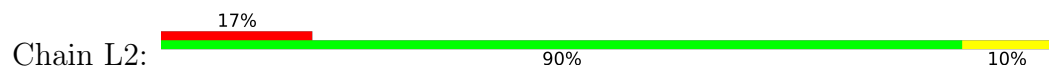
- Molecule 17: 40S ribosomal protein S9-A



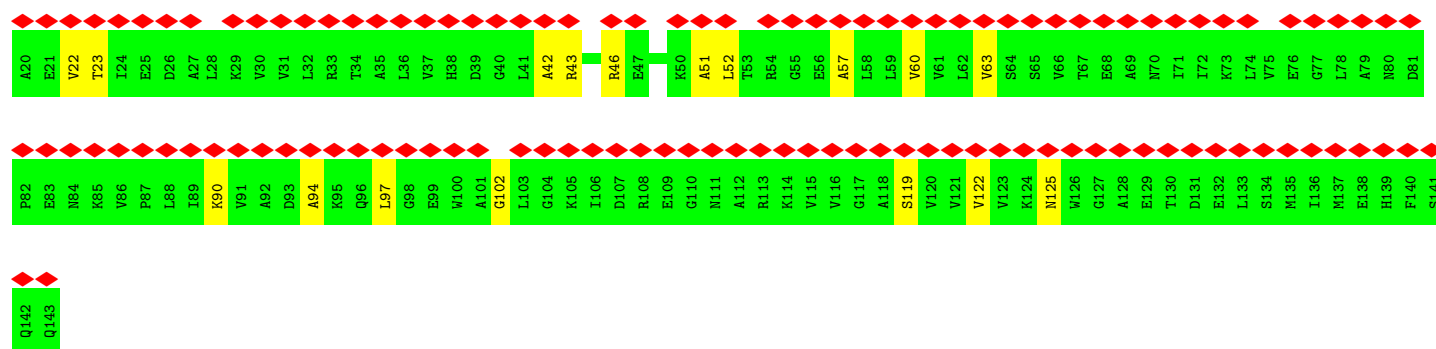
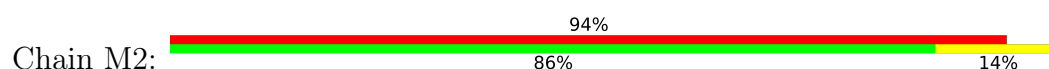
- Molecule 18: 40S ribosomal protein S10-A



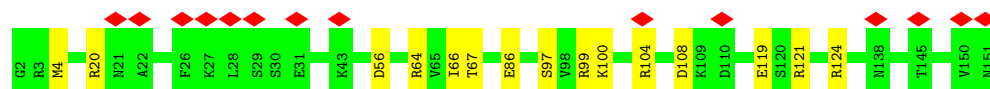
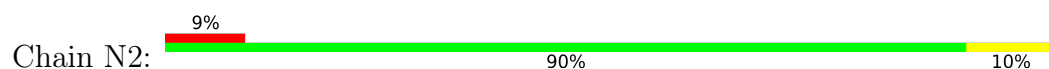
• Molecule 19: 40S ribosomal protein S11-A



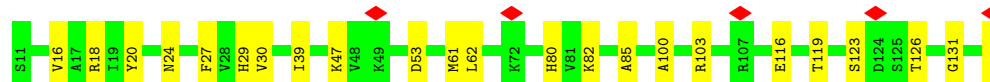
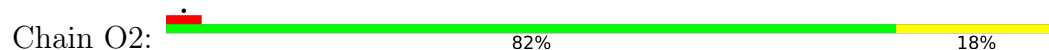
• Molecule 20: 40S ribosomal protein S12



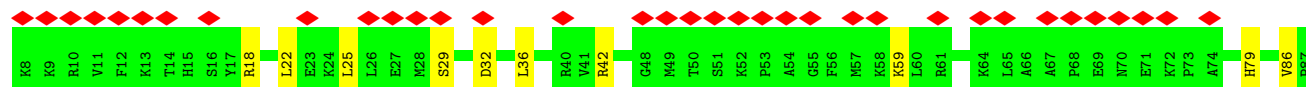
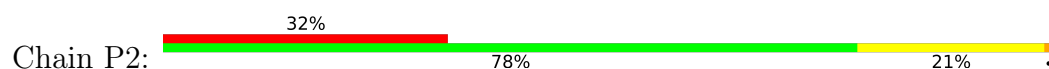
• Molecule 21: 40S ribosomal protein S13



• Molecule 22: 40S ribosomal protein S14-A

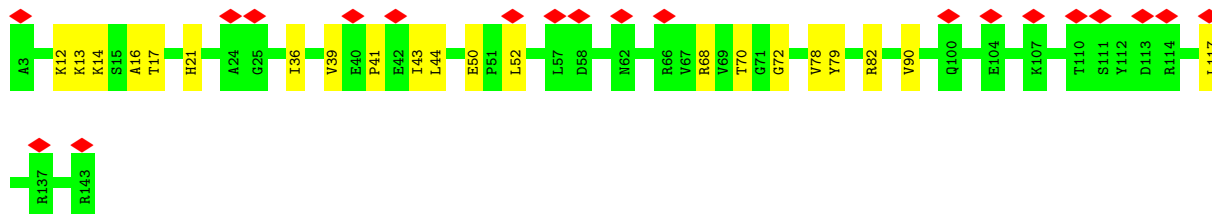
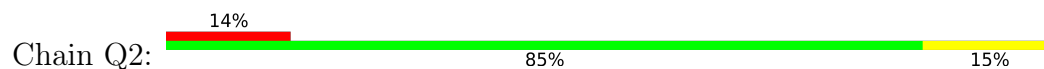


• Molecule 23: 40S ribosomal protein S15

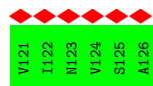
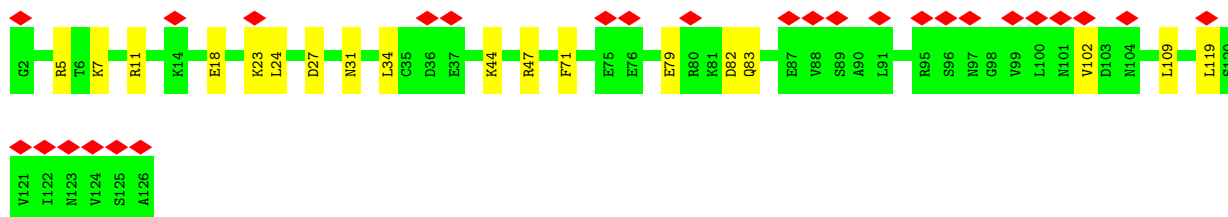
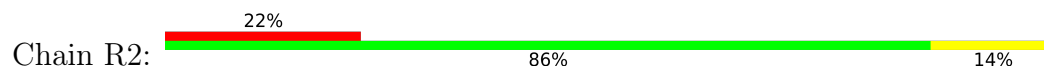




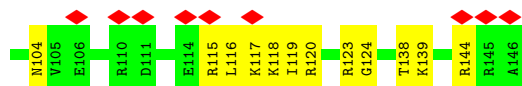
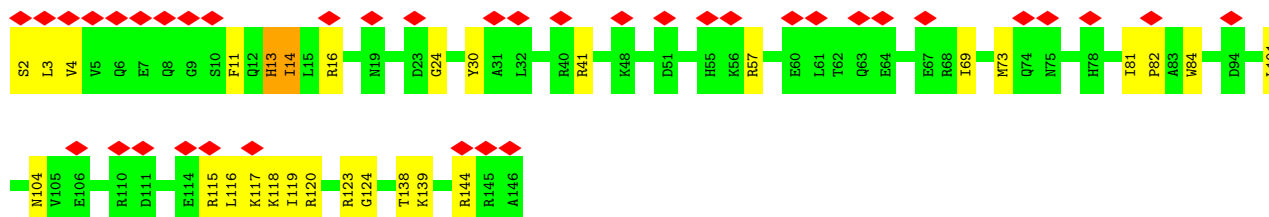
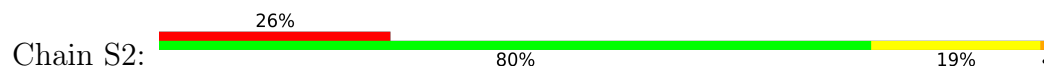
- Molecule 24: 40S ribosomal protein S16-A



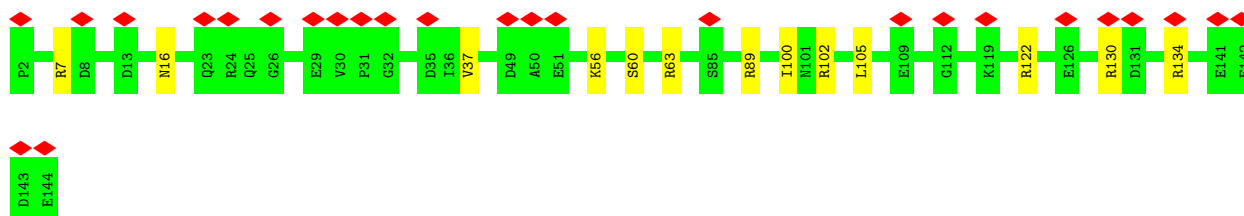
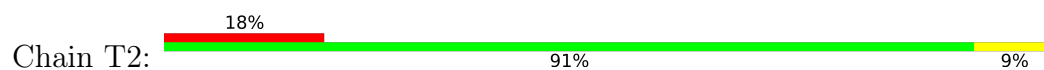
- Molecule 25: 40S ribosomal protein S17-B



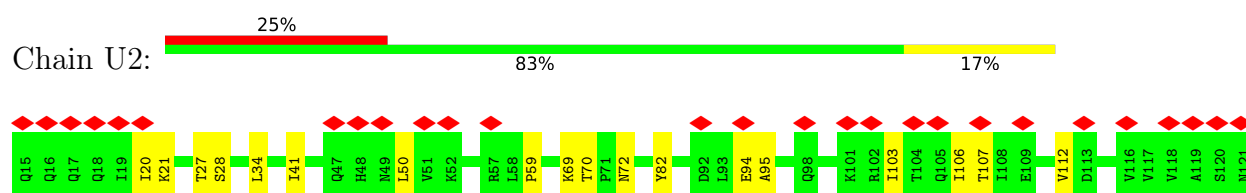
- Molecule 26: 40S ribosomal protein S18-A



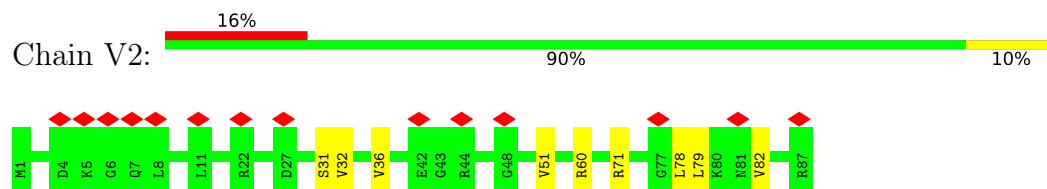
- Molecule 27: 40S ribosomal protein S19-A



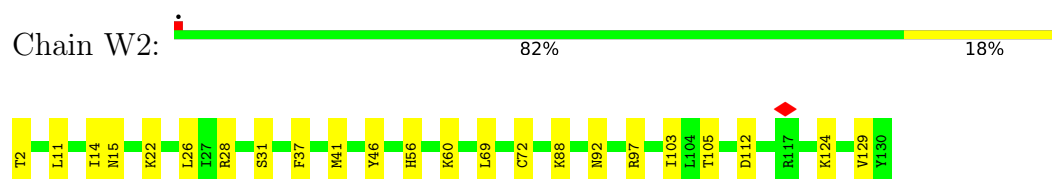
- Molecule 28: 40S ribosomal protein S20



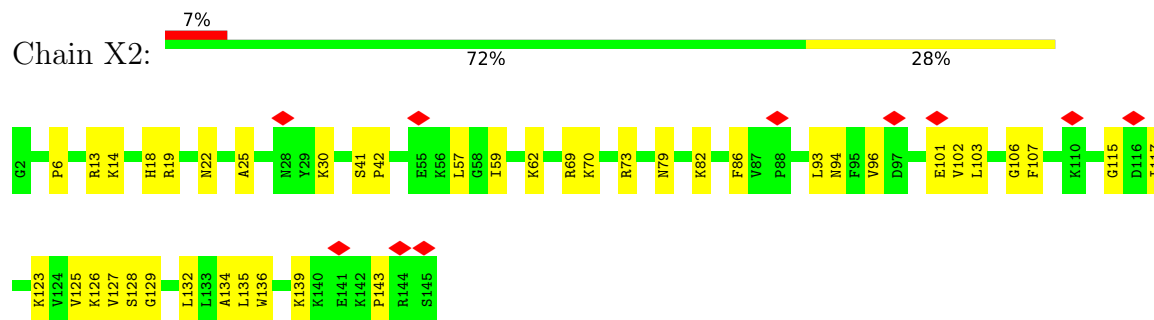
- Molecule 29: 40S ribosomal protein S21-A



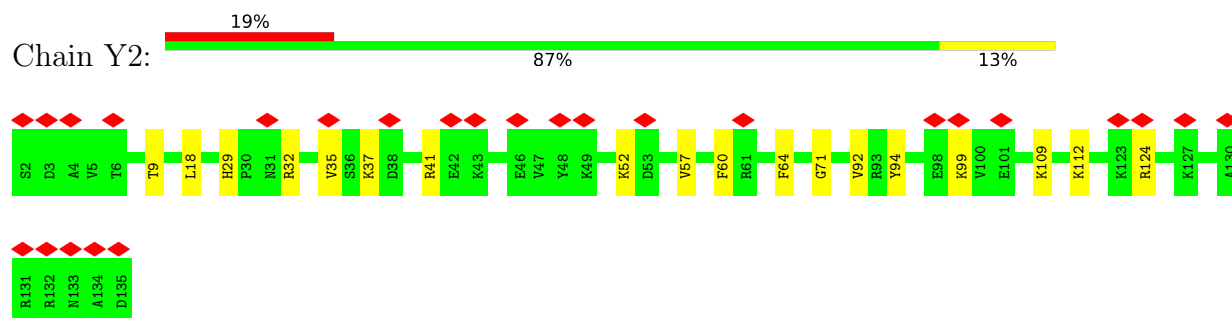
- Molecule 30: 40S ribosomal protein S22-A



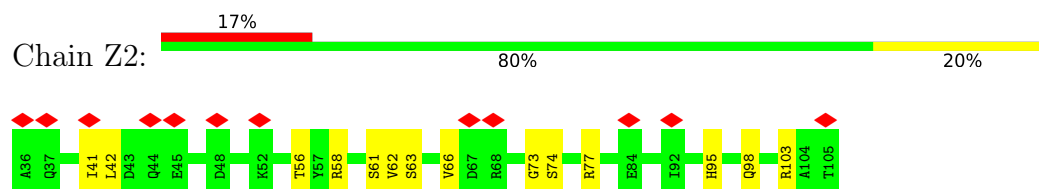
- Molecule 31: 40S ribosomal protein S23-A



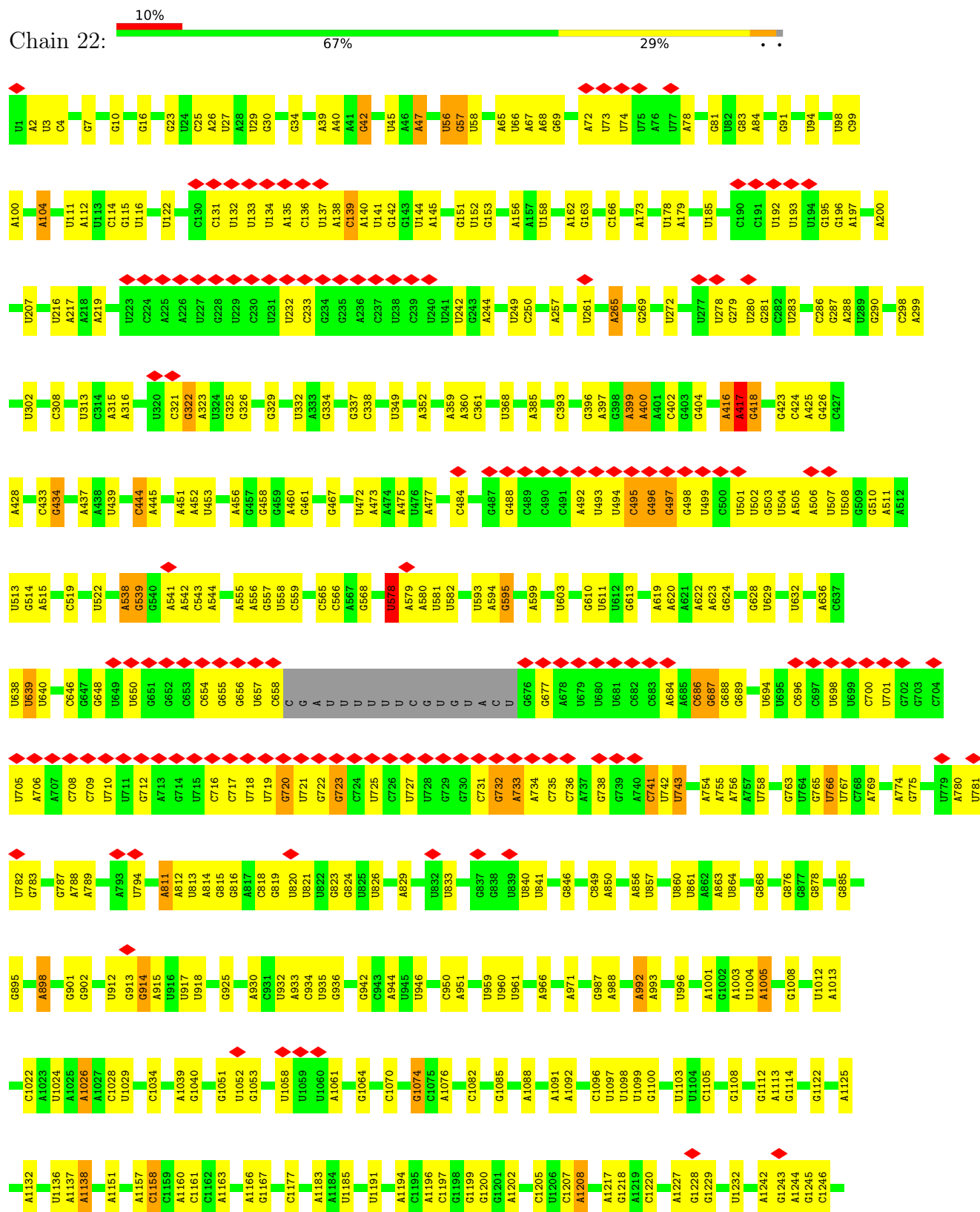
- Molecule 32: 40S ribosomal protein S24-A



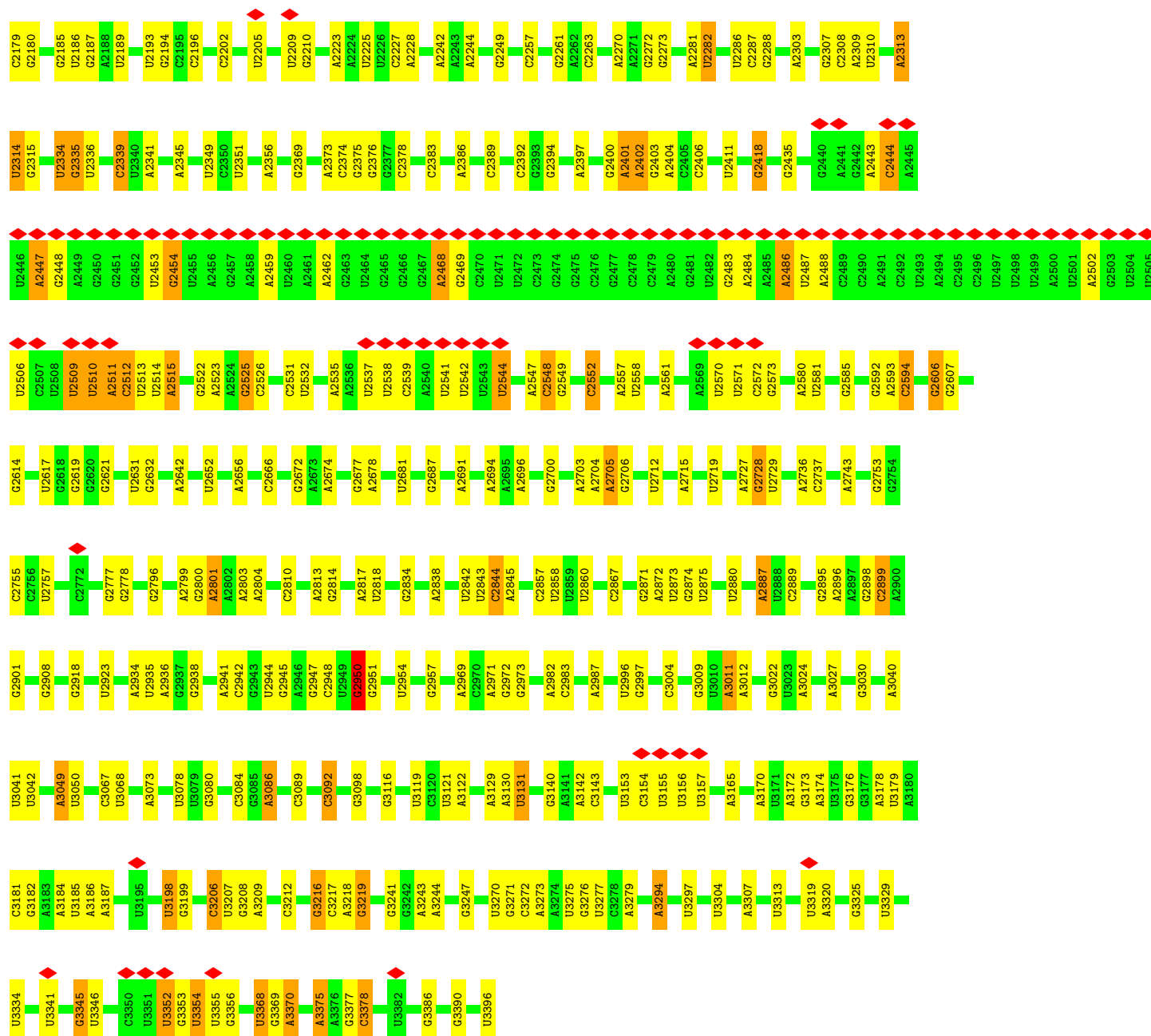
- Molecule 33: 40S ribosomal protein S25-A



• Molecule 34: 18S ribosomal RNA

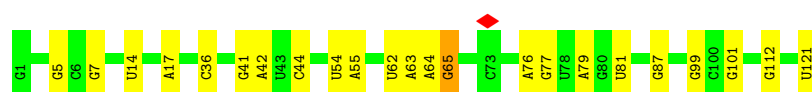


U2085	A2086	C2087	A2088	A2089	U2090	U2091	A2092	C2093	C2094	G2095	C2098	A2099	A2107	G2110	G2111	U2112	A2113	C2114	G2115	A2117	C2118	G2121	G2122	A2131	U2137	A2138	A2139	U2056	G2057	A2141	A2142	A2143	A2144	A2145	C2146	A2149	G2150	U2159	G2160	C2163	A2168	G2169	U2170	G2174	U2175	U2176	G2177	A2178																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
G	A	C	U	A	C	U	U	G	C2034	G2035	U2036	G2037	C2038	C2039	U2040	U2041	U2042	U2043	U2044	G2045	U2046	A2047	G2048	A2049	C2050	G2051	C2052	C2053	C2054	U2055	U2056	G2057	A2058	U2059	A2060	G2061	G2062	U2063	C2064	U2065	C2066	U2067	U2068	G2069	U2070	A2071	G2072	A2073	C2074	C2075	G2076	U2077	C2078	G2079	C2080	U2081	U2082	C2083																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
C1965	U1966	U1967	G1968	G1969	U1970	C1971	A1972	G1973	A1974	C1975	G1976	C1977	A1978	C1979	G1980	G1981	G1982	G1983	G1984	G1985	U1986	G1987	C	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U



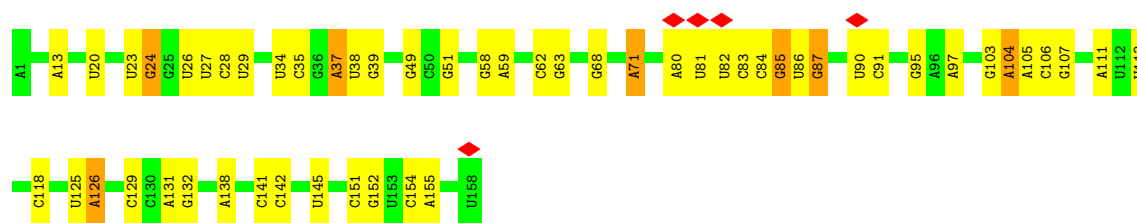
• Molecule 37: 5S ribosomal RNA

Chain 34: 81% 18%

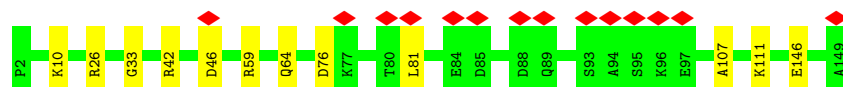


• Molecule 38: 5.8S ribosomal RNA

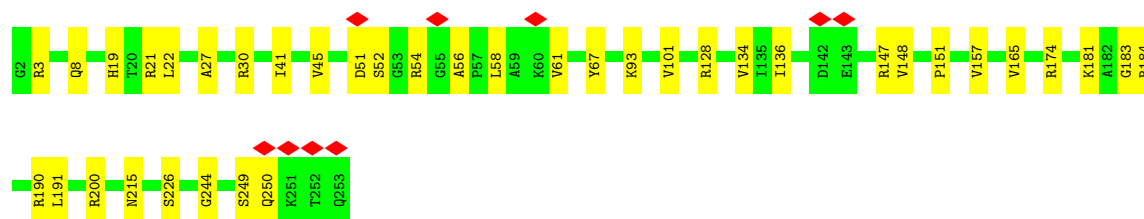
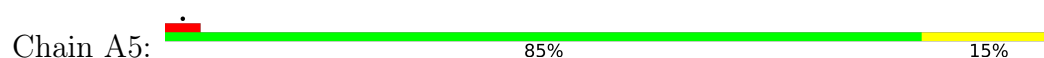
Chain 44: 66% 30%



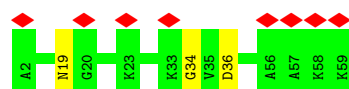
- Molecule 39: 60S ribosomal protein L28



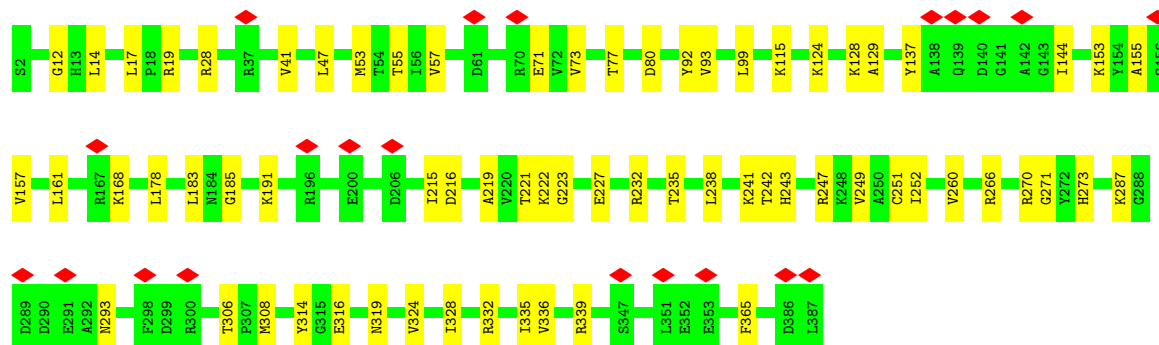
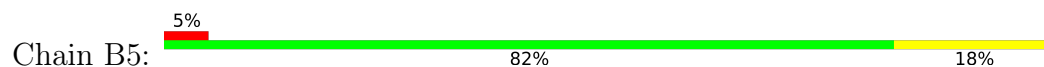
- Molecule 40: 60S ribosomal protein L2-A



- Molecule 41: 60S ribosomal protein L29



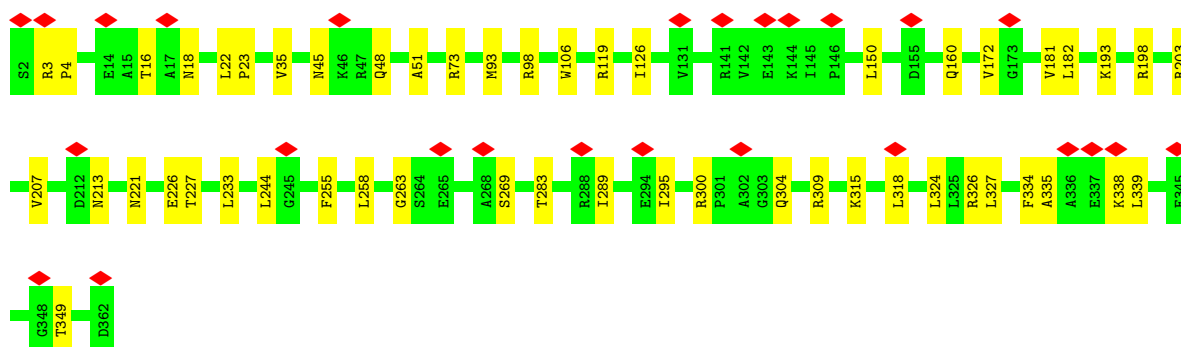
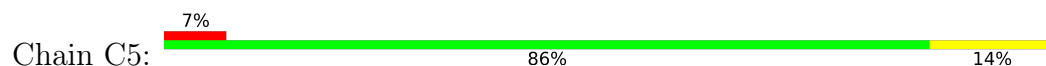
- Molecule 42: 60S ribosomal protein L3



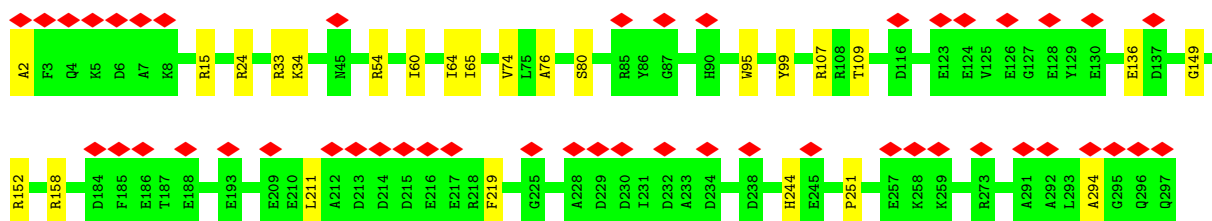
- Molecule 43: 60S ribosomal protein L30



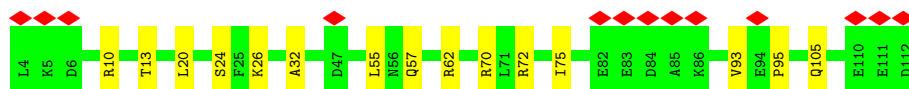
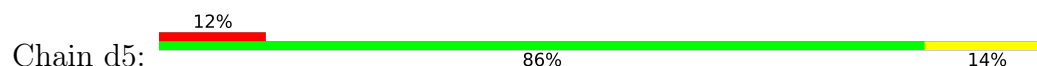
- Molecule 44: 60S ribosomal protein L4-A



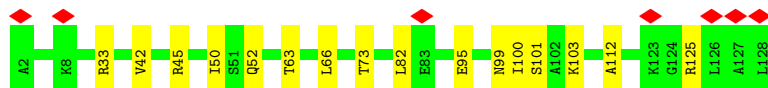
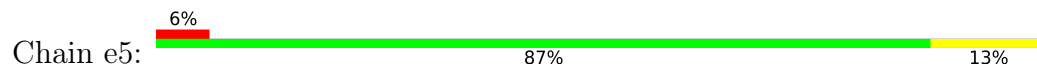
- Molecule 45: 60S ribosomal protein L5



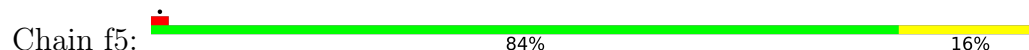
- Molecule 46: 60S ribosomal protein L31-A

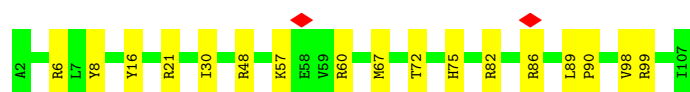


- Molecule 47: 60S ribosomal protein L32

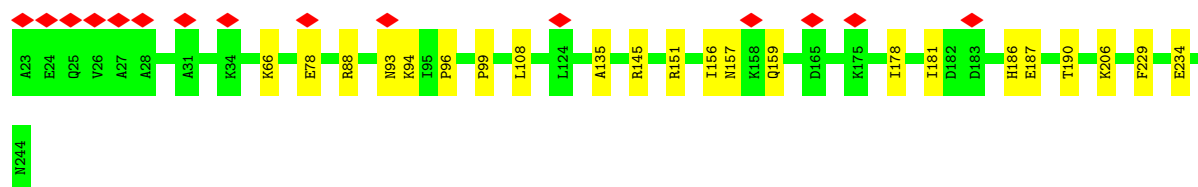
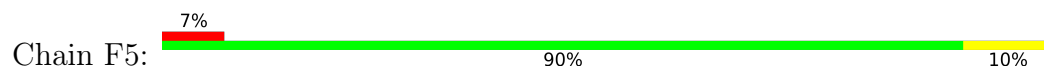


- Molecule 48: 60S ribosomal protein L33-A

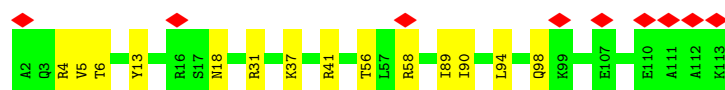
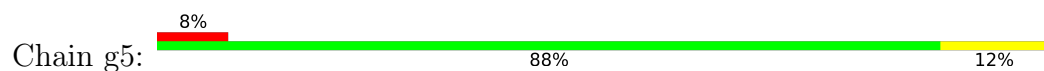




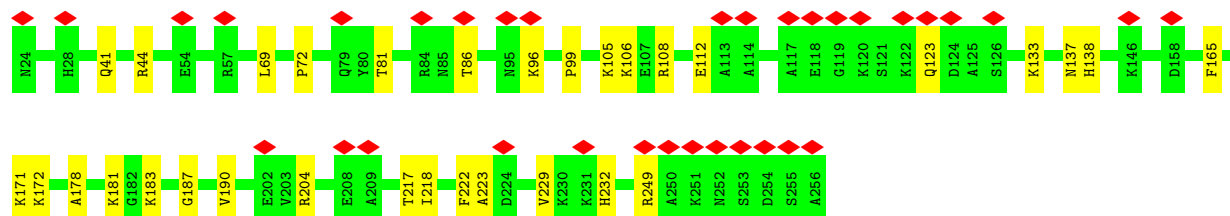
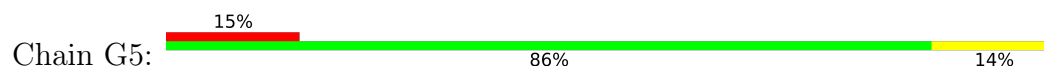
- Molecule 49: 60S ribosomal protein L7-A



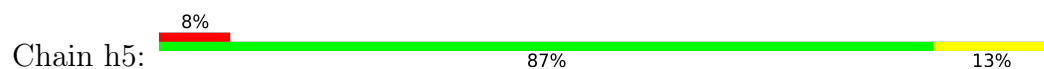
- Molecule 50: 60S ribosomal protein L34-A



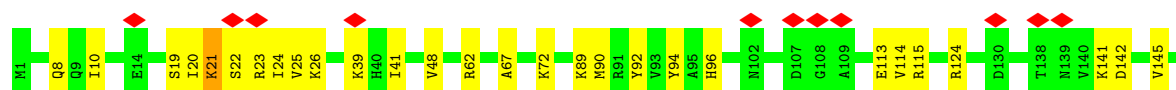
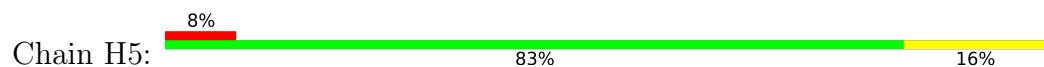
- Molecule 51: 60S ribosomal protein L8-A

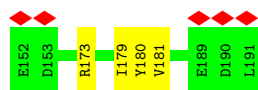


- Molecule 52: 60S ribosomal protein L35-A

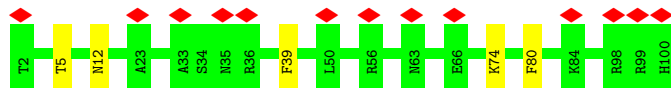


- Molecule 53: 60S ribosomal protein L9-A

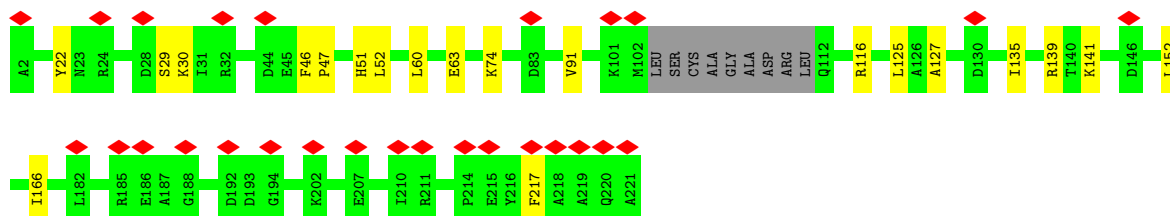
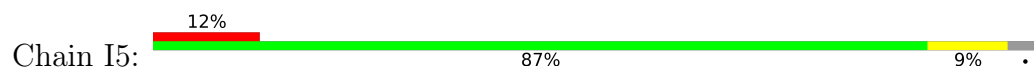




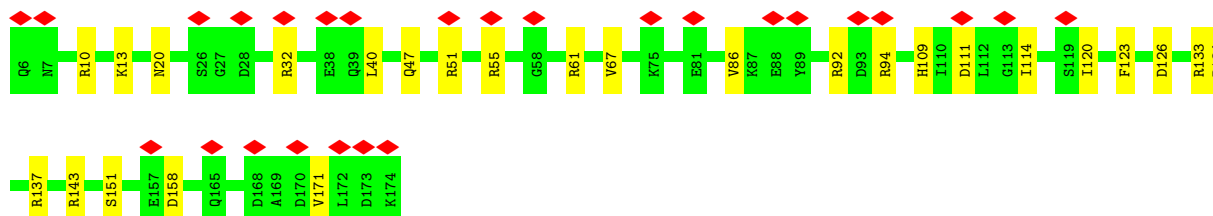
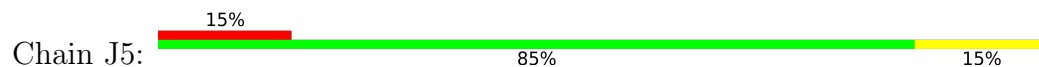
- Molecule 54: 60S ribosomal protein L36-A



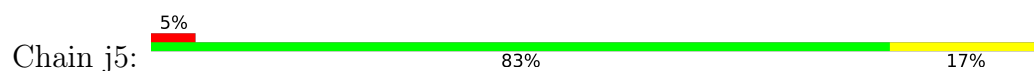
- Molecule 55: 60S ribosomal protein L10



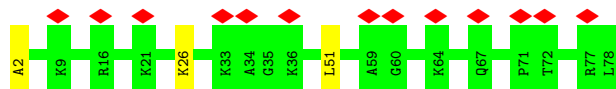
- Molecule 56: 60S ribosomal protein L11-A



- Molecule 57: 60S ribosomal protein L37-A



- Molecule 58: 60S ribosomal protein L38

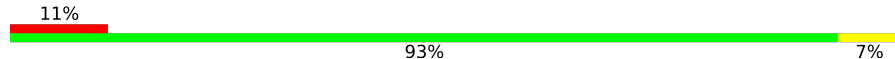


- Molecule 59: 60S ribosomal protein L39

Chain l5:  92% 8%



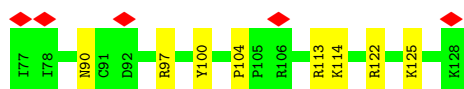
- Molecule 60: 60S ribosomal protein L13-A

Chain L5:  11% 93% 7%



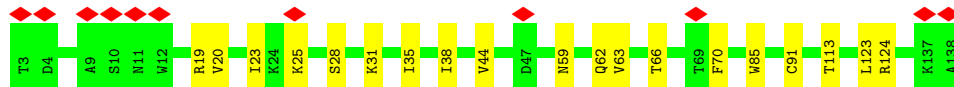
- Molecule 61: Ubiquitin-60S ribosomal protein L40

Chain m5:  10% 85% 15%



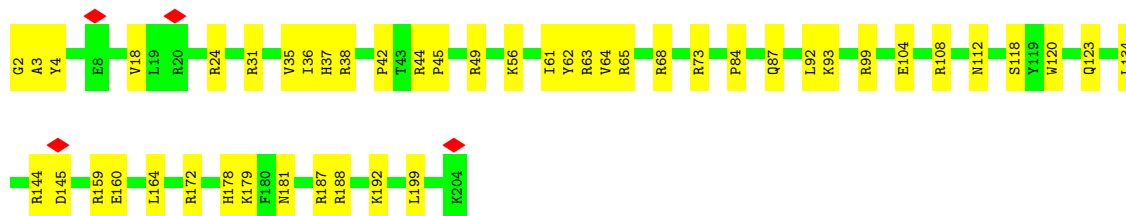
- Molecule 62: 60S ribosomal protein L14-A

Chain M5:  8% 86% 14%

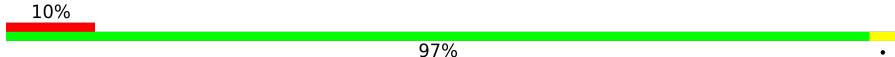


- Molecule 63: 60S ribosomal protein L15-A

Chain N5:  77% 23%

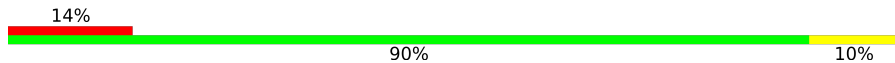


- Molecule 64: 60S ribosomal protein L42-B

Chain o5:  10% 97%

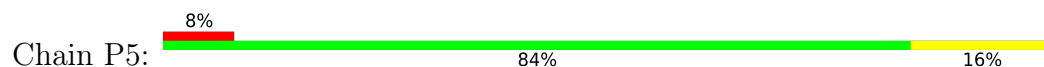


- Molecule 65: 60S ribosomal protein L43-B

Chain p5:  14% 90% 10%



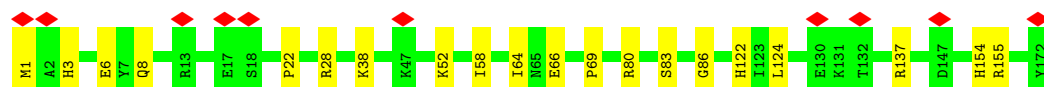
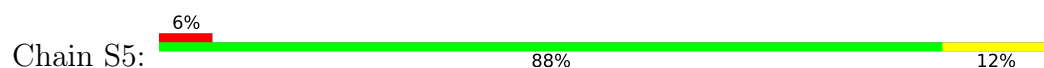
- Molecule 66: 60S ribosomal protein L17-A



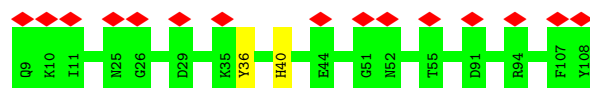
- Molecule 67: 60S ribosomal protein L18-A



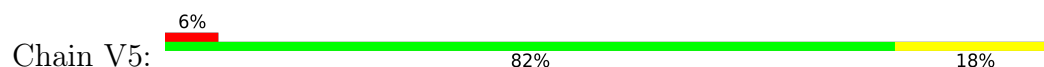
- Molecule 68: 60S ribosomal protein L20-A



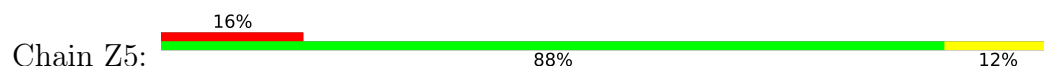
- Molecule 69: 60S ribosomal protein L22-A

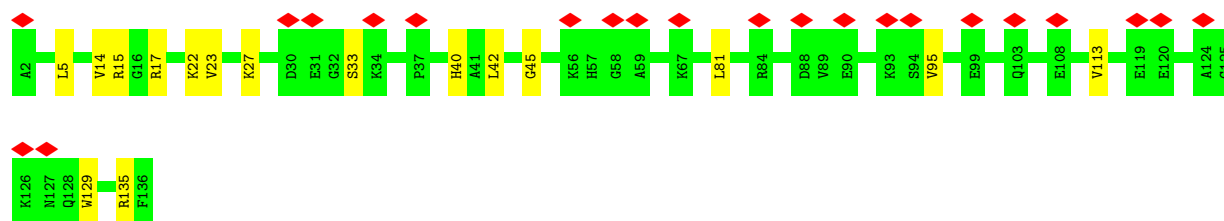


- Molecule 70: 60S ribosomal protein L23-A



- Molecule 71: 60S ribosomal protein L27-A

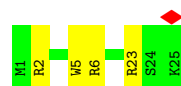
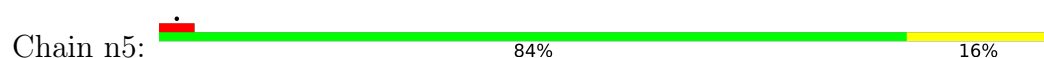




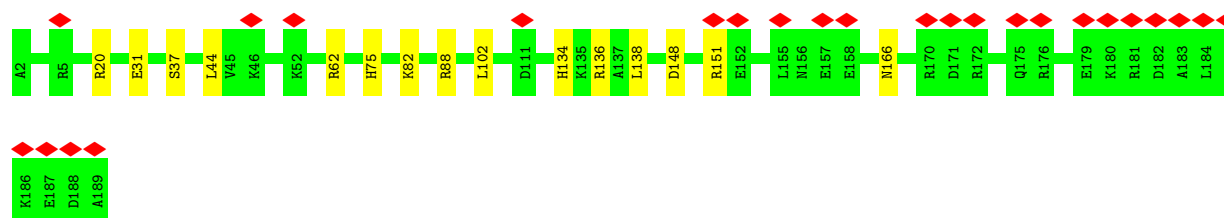
- Molecule 72: 60S ribosomal protein L16-A



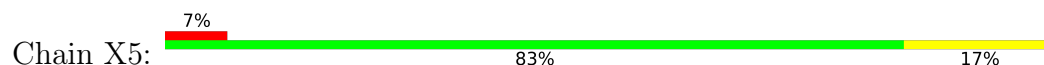
- Molecule 73: 60S ribosomal protein L41-B



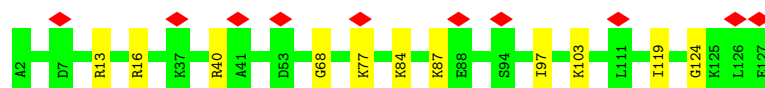
- Molecule 74: 60S ribosomal protein L19-A



- Molecule 75: 60S ribosomal protein L25



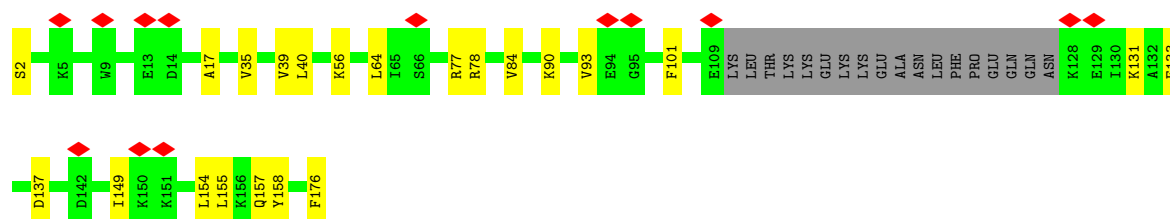
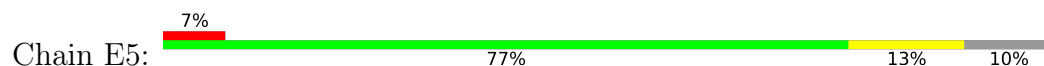
- Molecule 76: 60S ribosomal protein L26-A



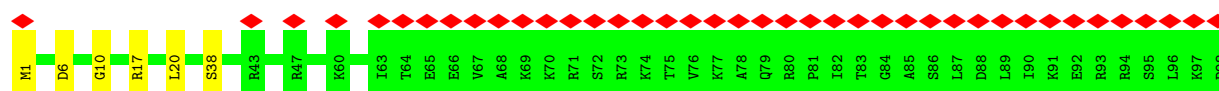
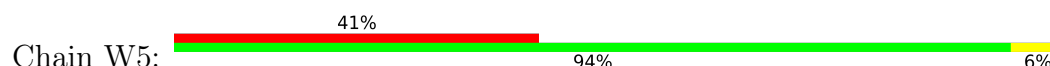
- Molecule 77: 60S ribosomal protein L21-A



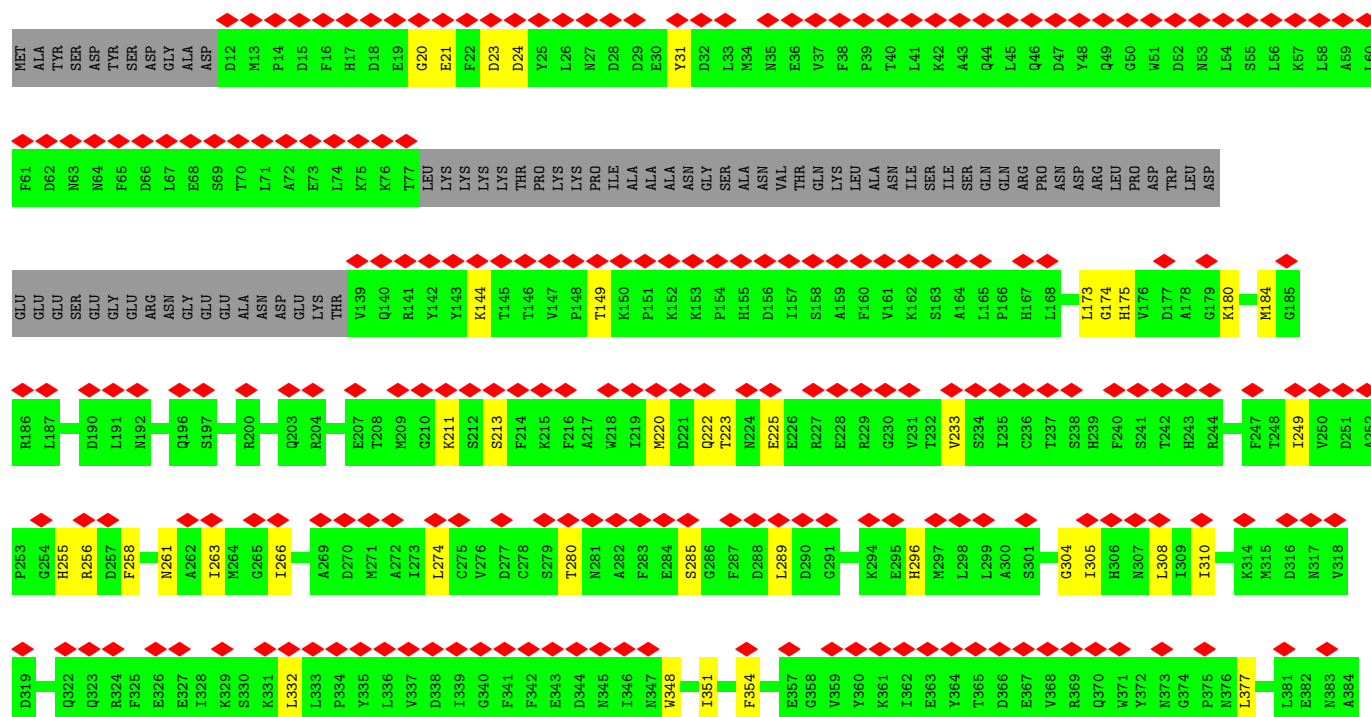
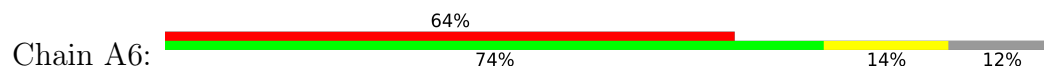
• Molecule 78: 60S ribosomal protein L6-A

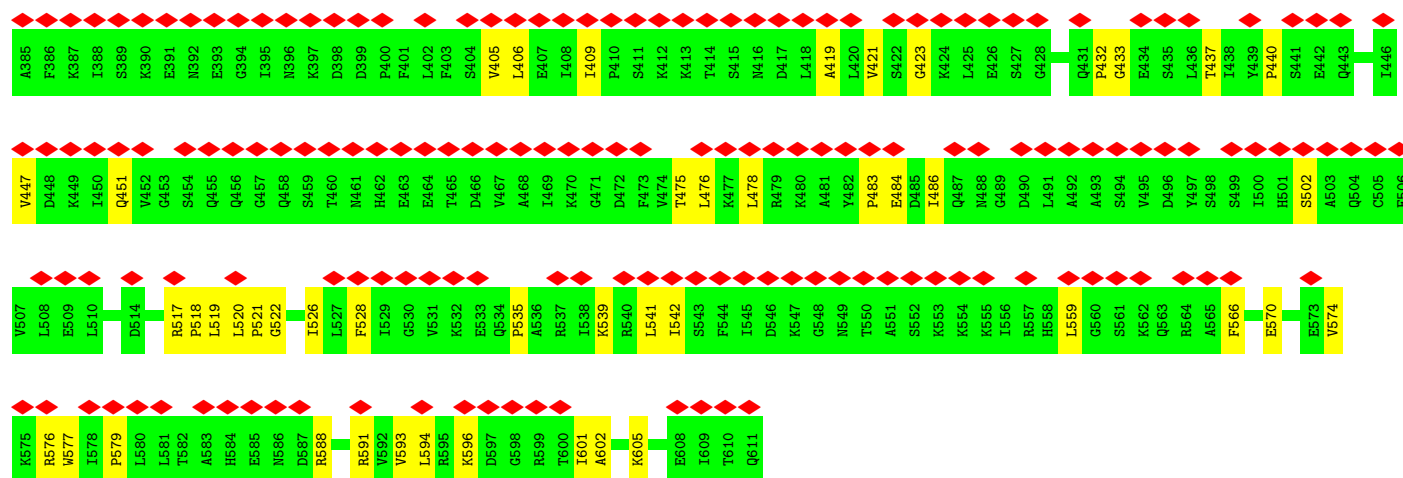


• Molecule 79: 60S ribosomal protein L24-A

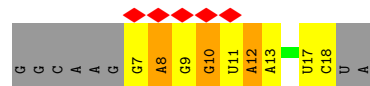


• Molecule 80: Protein HBS1

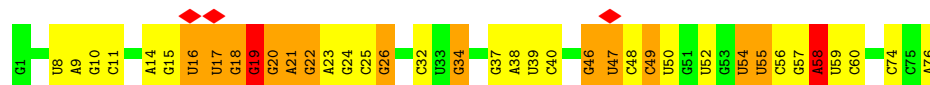




- Molecule 81: nonstop mRNA



- Molecule 82: yeast Phe-tRNA-Phe



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	73391	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	80645	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	21.317	Depositor
Minimum map value	-12.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	409.528, 409.528, 409.528	wwPDB
Map dimensions	412, 412, 412	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.994, 0.994, 0.994	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: M2G, YYG, 7MG, OMC, 5MU, H2U, MG, 5CR, OMG, ZN, 2MG, PSU, 5MC, GNP, 1MA

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	A1	0.17	0/3110	0.53	2/4179 (0.0%)
2	A2	0.20	0/1662	0.61	0/2273
3	a2	0.18	0/791	0.60	2/1059 (0.2%)
4	B2	0.22	0/1735	0.65	0/2335
5	b2	0.17	0/620	0.49	0/838
6	C2	0.19	0/1665	0.52	0/2263
7	c2	0.18	0/499	0.45	0/670
8	D2	0.23	1/1759 (0.1%)	0.55	0/2368
9	d2	0.19	0/453	0.50	0/602
10	E2	0.19	0/2109	0.60	1/2839 (0.0%)
11	e2	0.18	0/483	0.48	0/643
12	F2	0.20	0/1629	0.61	0/2202
13	G2	0.18	0/1844	0.55	0/2464
14	g2	0.15	0/2498	0.45	0/3398
15	H2	0.22	0/1506	0.59	2/2028 (0.1%)
16	I2	0.20	0/1514	0.59	0/2021
17	J2	0.19	0/1519	0.58	0/2035
18	K2	0.18	0/837	0.57	0/1131
19	L2	0.22	0/1272	0.54	0/1712
20	M2	0.25	0/942	0.79	2/1274 (0.2%)
21	N2	0.19	0/1215	0.58	0/1638
22	O2	0.22	0/952	0.64	2/1279 (0.2%)
23	P2	0.36	1/1012 (0.1%)	0.67	1/1356 (0.1%)
24	Q2	0.20	0/1125	0.61	0/1510
25	R2	0.20	0/1010	0.60	0/1355
26	S2	0.22	0/1211	0.66	2/1628 (0.1%)
27	T2	0.20	0/1130	0.55	0/1517
28	U2	0.19	0/865	0.51	0/1169
29	V2	0.18	0/693	0.59	0/935
30	W2	0.19	0/1038	0.54	0/1395
31	X2	0.21	0/1139	0.64	2/1518 (0.1%)
32	Y2	0.17	0/1087	0.55	0/1449

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Z2	0.16	0/571	0.50	0/768
34	22	0.12	0/42444	0.30	7/66138 (0.0%)
35	f2	0.20	0/504	0.66	0/682
36	14	0.12	0/78885	0.29	10/122992 (0.0%)
37	34	0.10	0/2883	0.19	0/4491
38	44	0.11	0/3746	0.26	0/5832
39	a5	0.18	0/1204	0.57	0/1612
40	A5	0.21	0/1952	0.60	0/2622
41	b5	0.18	0/473	0.53	0/629
42	B5	0.18	0/3152	0.53	0/4239
43	c5	0.17	0/751	0.45	0/1008
44	C5	0.20	0/2801	0.59	2/3792 (0.1%)
45	D5	0.17	0/2425	0.56	2/3271 (0.1%)
46	d5	0.22	0/904	0.49	0/1213
47	e5	0.17	0/1041	0.52	0/1394
48	f5	0.17	0/868	0.46	0/1168
49	F5	0.21	0/1821	0.58	0/2451
50	g5	0.17	0/891	0.54	1/1191 (0.1%)
51	G5	0.20	0/1849	0.61	2/2495 (0.1%)
52	h5	0.17	0/978	0.56	2/1301 (0.2%)
53	H5	0.19	0/1539	0.57	2/2073 (0.1%)
54	i5	0.19	0/778	0.61	0/1034
55	I5	0.16	0/1753	0.48	0/2350
56	J5	0.20	0/1374	0.57	0/1842
57	j5	0.20	0/696	0.58	0/923
58	k5	0.17	0/618	0.51	0/826
59	l5	0.19	0/443	0.56	0/588
60	L5	0.20	0/1568	0.62	0/2106
61	m5	0.19	0/423	0.52	0/562
62	M5	0.17	0/1068	0.53	0/1438
63	N5	0.19	0/1757	0.53	0/2354
64	o5	0.16	0/860	0.52	0/1136
65	p5	0.19	0/701	0.57	0/934
66	P5	0.19	0/1465	0.54	0/1968
67	Q5	0.17	0/1465	0.53	0/1965
68	S5	0.18	0/1481	0.55	0/1990
69	U5	0.25	0/812	0.60	0/1099
70	V5	0.18	0/1018	0.46	0/1369
71	Z5	0.18	0/1118	0.51	0/1497
72	K5	0.18	0/1585	0.48	0/2128
73	n5	0.16	0/234	0.52	0/300
74	R5	0.17	0/1538	0.57	0/2050
75	X5	0.17	0/983	0.48	0/1325

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Y5	0.17	0/1004	0.49	0/1341
77	T5	0.18	0/1300	0.53	0/1743
78	E5	0.17	0/1269	0.51	1/1705 (0.1%)
79	W5	0.22	0/814	0.59	0/1081
80	A6	0.17	0/4364	0.46	1/5898 (0.0%)
81	X7	0.33	0/290	0.39	0/450
82	A3	0.38	0/1487	0.48	1/2315 (0.0%)
All	All	0.16	2/226872 (0.0%)	0.42	47/332762 (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	F2	0	1
17	J2	0	2
20	M2	0	1
26	S2	0	1
31	X2	0	1
49	F5	0	1
60	L5	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P2	120	SER	N-CA	7.88	1.55	1.46
8	D2	162	GLN	C-N	5.05	1.39	1.34

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	14	2509	U	C2'-C3'-O3'	8.70	122.55	109.50
36	14	1795	U	N1-C1'-C2'	6.31	121.46	112.00
26	S2	13	HIS	CA-C-N	6.03	132.82	121.97
26	S2	13	HIS	C-N-CA	6.03	132.82	121.97
78	E5	93	VAL	N-CA-C	-5.96	107.48	113.20
51	G5	123	GLN	CA-C-N	5.67	132.37	121.54
51	G5	123	GLN	C-N-CA	5.67	132.37	121.54
82	A3	19	G	P-O3'-C3'	5.59	128.59	120.20
44	C5	304	GLN	CA-C-N	5.53	132.11	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	C5	304	GLN	C-N-CA	5.53	132.11	121.54
50	g5	89	ILE	N-CA-C	-5.51	107.07	111.81
52	h5	84	LYS	CA-C-N	5.48	132.00	121.54
52	h5	84	LYS	C-N-CA	5.48	132.00	121.54
36	14	2950	G	C4'-C3'-O3'	5.43	117.55	109.40
20	M2	125	ASN	CA-C-N	5.37	131.80	121.54
20	M2	125	ASN	C-N-CA	5.37	131.80	121.54
34	22	417	A	C2'-C3'-O3'	5.37	117.56	109.50
36	14	979	U	P-O3'-C3'	5.37	128.25	120.20
36	14	1715	A	P-O3'-C3'	5.35	128.23	120.20
36	14	2468	A	P-O3'-C3'	5.30	128.16	120.20
34	22	578	U	P-O3'-C3'	5.28	128.12	120.20
34	22	686	C	P-O3'-C3'	5.27	128.11	120.20
23	P2	122	THR	N-CA-C	5.26	117.10	111.36
36	14	1815	U	P-O3'-C3'	5.25	128.08	120.20
34	22	1761	U	P-O3'-C3'	5.23	128.04	120.20
80	A6	233	VAL	N-CA-C	-5.21	108.42	113.53
45	D5	136	GLU	CA-C-N	5.19	131.46	121.54
45	D5	136	GLU	C-N-CA	5.19	131.46	121.54
36	14	2447	A	P-O3'-C3'	5.18	127.97	120.20
34	22	444	C	C4'-C3'-O3'	5.18	120.77	113.00
34	22	139	C	P-O3'-C3'	5.16	127.94	120.20
34	22	497	G	P-O3'-C3'	5.16	127.94	120.20
10	E2	193	GLY	N-CA-C	5.15	125.39	113.18
3	a2	7	SER	CA-C-N	5.15	131.37	121.54
3	a2	7	SER	C-N-CA	5.15	131.37	121.54
36	14	2093	A	P-O3'-C3'	5.12	127.87	120.20
53	H5	21	LYS	CA-C-N	5.08	131.24	121.54
53	H5	21	LYS	C-N-CA	5.08	131.24	121.54
1	A1	275	THR	CA-C-N	5.06	131.20	121.54
1	A1	275	THR	C-N-CA	5.06	131.20	121.54
36	14	2112	U	P-O3'-C3'	5.05	127.77	120.20
22	O2	126	THR	CA-C-N	5.03	129.41	121.56
22	O2	126	THR	C-N-CA	5.03	129.41	121.56
31	X2	115	GLY	CA-C-N	5.02	131.12	121.54
31	X2	115	GLY	C-N-CA	5.02	131.12	121.54
15	H2	30	SER	CA-C-N	5.01	128.38	120.97
15	H2	30	SER	C-N-CA	5.01	128.38	120.97

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	F2	126	ASP	Peptide
49	F5	156	ILE	Peptide
17	J2	133	HIS	Peptide
17	J2	163	PRO	Peptide
60	L5	47	ALA	Peptide
20	M2	90	LYS	Peptide
26	S2	13	HIS	Peptide
31	X2	41	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	3058	0	3134	56	0
2	A2	1621	0	1629	21	0
3	a2	778	0	823	16	0
4	B2	1709	0	1784	14	0
5	b2	610	0	631	11	0
6	C2	1635	0	1723	15	0
7	c2	497	0	535	7	0
8	D2	1734	0	1817	19	0
9	d2	443	0	434	13	0
10	E2	2068	0	2154	22	0
11	e2	475	0	525	4	0
12	F2	1609	0	1674	38	0
13	G2	1820	0	1918	16	0
14	g2	2445	0	2401	24	0
15	H2	1481	0	1572	22	0
16	I2	1489	0	1525	29	0
17	J2	1494	0	1573	13	0
18	K2	817	0	804	2	0
19	L2	1244	0	1314	11	0
20	M2	934	0	975	10	0
21	N2	1192	0	1255	11	0
22	O2	941	0	979	17	0
23	P2	991	0	1035	29	0
24	Q2	1105	0	1166	12	0
25	R2	1000	0	1063	13	0
26	S2	1192	0	1222	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	T2	1112	0	1124	11	0
28	U2	855	0	917	13	0
29	V2	684	0	672	8	0
30	W2	1021	0	1060	16	0
31	X2	1121	0	1196	28	0
32	Y2	1073	0	1132	12	0
33	Z2	563	0	602	68	0
34	22	37948	0	19089	245	0
35	f2	497	0	439	4	0
36	14	70476	0	35381	334	0
37	34	2579	0	1304	13	0
38	44	3353	0	1693	22	0
39	a5	1173	0	1214	11	0
40	A5	1918	0	1986	29	0
41	b5	462	0	491	3	0
42	B5	3081	0	3165	47	0
43	c5	743	0	797	4	0
44	C5	2749	0	2863	38	0
45	D5	2375	0	2324	16	0
46	d5	890	0	938	11	0
47	e5	1020	0	1090	11	0
48	f5	850	0	880	12	0
49	F5	1784	0	1862	13	0
50	g5	881	0	949	8	0
51	G5	1817	0	1908	21	0
52	h5	969	0	1078	11	0
53	H5	1518	0	1587	27	0
54	i5	771	0	849	3	0
55	I5	1717	0	1753	12	0
56	J5	1353	0	1383	40	0
57	j5	681	0	683	13	0
58	k5	612	0	682	3	0
59	l5	436	0	475	5	0
60	L5	1543	0	1608	9	0
61	m5	417	0	455	8	0
62	M5	1053	0	1149	12	0
63	N5	1720	0	1778	36	0
64	o5	847	0	915	2	0
65	p5	694	0	735	5	0
66	P5	1442	0	1485	20	0
67	Q5	1441	0	1542	12	0
68	S5	1445	0	1487	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	U5	796	0	812	1	0
70	V5	1003	0	1048	17	0
71	Z5	1092	0	1155	10	0
72	K5	1555	0	1659	10	0
73	n5	233	0	284	3	0
74	R5	1521	0	1617	13	0
75	X5	968	0	1036	14	0
76	Y5	993	0	1081	8	0
77	T5	1276	0	1323	16	0
78	E5	1248	0	1339	13	0
79	W5	800	0	865	5	0
80	A6	4279	0	4232	80	0
81	X7	259	0	130	8	0
82	A3	1651	0	856	38	0
83	a2	1	0	0	0	0
83	b2	1	0	0	0	0
83	d2	1	0	0	0	0
83	f2	1	0	0	0	0
83	j5	1	0	0	0	0
83	m5	1	0	0	0	0
83	o5	1	0	0	0	0
83	p5	1	0	0	0	0
84	14	701	0	0	0	0
84	22	177	0	0	0	0
84	34	16	0	0	0	0
84	44	34	0	0	0	0
84	A3	6	0	0	0	0
84	A5	6	0	0	0	0
84	A6	2	0	0	0	0
84	B2	1	0	0	0	0
84	B5	5	0	0	0	0
84	C2	2	0	0	0	0
84	C5	8	0	0	0	0
84	D5	1	0	0	0	0
84	E2	2	0	0	0	0
84	E5	1	0	0	0	0
84	F2	2	0	0	0	0
84	F5	4	0	0	0	0
84	I2	2	0	0	0	0
84	I5	4	0	0	0	0
84	J2	1	0	0	0	0
84	J5	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	K5	5	0	0	0	0
84	L2	1	0	0	0	0
84	L5	4	0	0	0	0
84	M5	1	0	0	0	0
84	N2	2	0	0	0	0
84	N5	7	0	0	0	0
84	P5	7	0	0	0	0
84	Q2	1	0	0	0	0
84	Q5	4	0	0	0	0
84	R5	3	0	0	0	0
84	S2	4	0	0	0	0
84	S5	4	0	0	0	0
84	T2	1	0	0	0	0
84	T5	1	0	0	0	0
84	U2	1	0	0	0	0
84	V5	3	0	0	0	0
84	X2	3	0	0	0	0
84	Y2	1	0	0	0	0
84	Y5	2	0	0	0	0
84	a5	3	0	0	0	0
84	b5	1	0	0	0	0
84	d2	1	0	0	0	0
84	d5	3	0	0	0	0
84	e5	3	0	0	0	0
84	f5	1	0	0	0	0
84	j5	7	0	0	0	0
84	l5	1	0	0	0	0
84	m5	3	0	0	0	0
84	o5	3	0	0	0	0
85	A6	32	0	13	1	0
86	A3	14	0	0	3	0
87	A1	7	0	0	0	0
87	A6	6	0	0	0	0
All	All	212865	0	157835	1395	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 4.

All (1395) 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)
26:S2:4:VAL:CG1	33:Z2:42:LEU:HD22	1.12	1.52
56:J5:55:ARG:CD	82:A3:20:G:H22	1.25	1.47
12:F2:125:THR:N	33:Z2:58:ARG:NH2	1.64	1.45
26:S2:4:VAL:HG11	33:Z2:42:LEU:CD2	0.99	1.44
1:A1:218:PHE:CD2	80:A6:225:GLU:OE2	1.75	1.40
56:J5:55:ARG:HD3	82:A3:20:G:N2	1.03	1.32
56:J5:55:ARG:CD	82:A3:20:G:H1	1.41	1.31
26:S2:4:VAL:HG11	33:Z2:42:LEU:CG	1.68	1.24
56:J5:55:ARG:CD	82:A3:20:G:N2	1.87	1.23
56:J5:55:ARG:CD	82:A3:20:G:N1	2.01	1.23
23:P2:128:HIS:NE2	34:22:1459:C:O2'	1.68	1.22
1:A1:218:PHE:CE2	80:A6:225:GLU:OE1	1.95	1.18
56:J5:55:ARG:CD	82:A3:20:G:C2	2.27	1.17
33:Z2:73:GLY:N	34:22:1534:G:O2'	1.75	1.17
33:Z2:77:ARG:NH1	34:22:1533:C:C5	2.12	1.15
56:J5:55:ARG:HD2	82:A3:20:G:N1	1.62	1.14
53:H5:96:HIS:CD2	80:A6:280:THR:HG23	1.83	1.13
56:J5:55:ARG:NE	82:A3:20:G:H1	1.48	1.12
26:S2:4:VAL:HG13	33:Z2:42:LEU:HD13	1.22	1.12
33:Z2:77:ARG:CZ	34:22:1533:C:H5	1.62	1.11
56:J5:55:ARG:HD3	82:A3:20:G:C2	1.85	1.10
12:F2:112:ARG:NH1	33:Z2:95:HIS:CD2	2.20	1.09
33:Z2:77:ARG:NH1	34:22:1534:G:N7	2.00	1.09
33:Z2:77:ARG:CZ	34:22:1533:C:C5	2.38	1.06
56:J5:55:ARG:HD2	82:A3:20:G:H1	1.08	1.05
56:J5:55:ARG:NE	82:A3:20:G:N1	2.03	1.05
1:A1:218:PHE:CD2	80:A6:225:GLU:CD	2.33	1.04
1:A1:218:PHE:CE2	80:A6:225:GLU:CD	2.35	1.03
23:P2:130:ARG:H	23:P2:130:ARG:HD3	1.21	1.03
12:F2:112:ARG:NH1	33:Z2:95:HIS:NE2	2.07	1.02
33:Z2:73:GLY:CA	34:22:1534:G:O2'	2.07	1.02
12:F2:112:ARG:HH11	33:Z2:95:HIS:CD2	1.77	1.01
26:S2:4:VAL:CB	33:Z2:42:LEU:HD22	1.93	0.98
26:S2:4:VAL:CG1	33:Z2:42:LEU:HD13	1.95	0.96
36:14:2954:U:C1'	86:A3:101:5CR:OAB	2.15	0.94
33:Z2:73:GLY:HA3	34:22:1534:G:O2'	1.68	0.93
36:14:2954:U:O4'	86:A3:101:5CR:OAB	1.91	0.89
26:S2:4:VAL:CG1	33:Z2:42:LEU:CD2	1.94	0.88
26:S2:4:VAL:CG1	33:Z2:42:LEU:CD1	2.52	0.88
1:A1:176:LYS:HD2	80:A6:222:GLN:HG3	1.54	0.88
36:14:2954:U:H1'	86:A3:101:5CR:OAB	1.72	0.87
30:W2:2:THR:N	34:22:1034:C:HO2'	1.71	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:174:LYS:HD3	80:A6:409:ILE:HG12	1.57	0.87
33:Z2:74:SER:OG	34:22:1534:G:OP2	1.90	0.87
26:S2:4:VAL:HG13	33:Z2:42:LEU:CD1	2.04	0.86
23:P2:128:HIS:CE1	34:22:1459:C:O2'	2.29	0.85
1:A1:291:LEU:CB	80:A6:518:PRO:HG2	2.07	0.84
1:A1:291:LEU:HB2	80:A6:518:PRO:HG2	1.60	0.84
23:P2:128:HIS:CE1	34:22:1459:C:HO2'	1.97	0.81
1:A1:285:ASP:OD1	80:A6:517:ARG:NH2	2.14	0.81
56:J5:55:ARG:NH1	82:A3:19:G:H1'	1.97	0.80
1:A1:176:LYS:NZ	80:A6:223:THR:OG1	2.13	0.80
36:14:2138:A:HO2'	57:j5:2:GLY:N	1.81	0.79
26:S2:4:VAL:CG1	33:Z2:42:LEU:CG	2.45	0.79
12:F2:112:ARG:NH1	33:Z2:95:HIS:HE2	1.78	0.78
22:O2:137:LEU:HD13	81:X7:12:A:O2'	1.83	0.77
1:A1:218:PHE:HE2	80:A6:225:GLU:OE1	1.63	0.76
56:J5:55:ARG:NE	82:A3:20:G:C2	2.50	0.76
23:P2:97:TYR:HB2	23:P2:102:PHE:CD1	2.21	0.75
56:J5:55:ARG:NH2	82:A3:20:G:N2	2.34	0.75
36:14:412:G:H5''	66:P5:30:ARG:HE	1.52	0.74
12:F2:124:LEU:HA	33:Z2:58:ARG:HE	1.51	0.74
1:A1:218:PHE:CG	80:A6:225:GLU:OE2	2.38	0.73
26:S2:4:VAL:HG12	33:Z2:42:LEU:HD22	1.57	0.73
33:Z2:73:GLY:HA3	34:22:1534:G:C2'	2.18	0.73
33:Z2:73:GLY:H	34:22:1534:G:C2'	2.01	0.72
33:Z2:73:GLY:C	34:22:1534:G:C8	2.67	0.72
1:A1:218:PHE:HD2	80:A6:225:GLU:OE2	1.62	0.72
56:J5:55:ARG:NE	82:A3:20:G:N2	2.38	0.72
12:F2:125:THR:CA	33:Z2:58:ARG:NH2	2.53	0.71
56:J5:55:ARG:HH21	82:A3:20:G:N2	1.87	0.71
36:14:1158:A:N7	49:F5:93:ASN:ND2	2.38	0.71
26:S2:4:VAL:HG21	33:Z2:42:LEU:HD21	1.72	0.70
1:A1:176:LYS:HZ1	80:A6:223:THR:HG1	1.36	0.70
53:H5:96:HIS:NE2	80:A6:280:THR:HG23	2.07	0.70
12:F2:187:ILE:HG12	33:Z2:66:VAL:HG11	1.73	0.69
23:P2:122:THR:HG21	34:22:1454:G:O3'	1.93	0.69
33:Z2:77:ARG:NH1	34:22:1533:C:H5	1.66	0.69
36:14:1981:G:H1	36:14:2041:U:H3	1.40	0.68
8:D2:56:GLN:N	80:A6:31:TYR:OH	2.25	0.68
12:F2:125:THR:N	33:Z2:58:ARG:HH22	1.81	0.68
36:14:1385:C:H42	36:14:1421:G:H1	1.42	0.67
23:P2:100:LYS:HD3	34:22:1183:A:C4	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z2:77:ARG:NH2	34:22:1533:C:C6	2.63	0.67
22:O2:85:ALA:H	22:O2:119:THR:HG22	1.60	0.66
23:P2:100:LYS:HD3	34:22:1183:A:N9	2.11	0.66
42:B5:227:GLU:HG2	42:B5:270:ARG:HE	1.61	0.66
26:S2:4:VAL:HG11	33:Z2:42:LEU:CD1	2.19	0.65
12:F2:81:ARG:HD2	34:22:1615:C:H2'	1.78	0.65
13:G2:202:ARG:HH22	34:22:179:A:H61	1.44	0.65
33:Z2:77:ARG:NH2	34:22:1533:C:OP2	2.29	0.65
1:A1:176:LYS:HE3	80:A6:222:GLN:H	1.62	0.64
56:J5:55:ARG:CZ	82:A3:20:G:N2	2.60	0.64
3:a2:8:ASN:HB3	34:22:1791:A:H3'	1.80	0.64
12:F2:112:ARG:HH12	33:Z2:95:HIS:HE2	1.46	0.64
23:P2:79:HIS:CD2	23:P2:102:PHE:HE1	2.15	0.64
3:a2:68:TYR:HB2	4:B2:111:ARG:HB3	1.80	0.63
12:F2:53:VAL:HG12	12:F2:55:ASP:H	1.64	0.63
33:Z2:73:GLY:CA	34:22:1534:G:C2'	2.76	0.63
36:14:1634:G:N7	71:Z5:17:ARG:NH1	2.46	0.63
44:C5:318:LEU:H	44:C5:324:LEU:HD13	1.64	0.63
1:A1:176:LYS:HD2	80:A6:222:GLN:CG	2.27	0.62
8:D2:94:ARG:HD3	80:A6:24:ASP:HB3	1.80	0.62
33:Z2:74:SER:HG	34:22:1534:G:P	2.20	0.62
34:22:1220:C:H42	34:22:1263:G:H1	1.47	0.62
22:O2:20:TYR:HB3	22:O2:27:PHE:HB2	1.80	0.62
36:14:170:G:H1	36:14:248:U:H3	1.48	0.62
48:f5:60:ARG:NH1	66:P5:169:THR:OG1	2.33	0.62
63:N5:36:ILE:HG12	63:N5:64:VAL:HG23	1.82	0.62
3:a2:93:LYS:HG2	34:22:1796:C:H42	1.65	0.61
63:N5:42:PRO:HG3	63:N5:61:ILE:HG13	1.81	0.61
12:F2:112:ARG:HH12	33:Z2:95:HIS:CD2	2.16	0.61
26:S2:116:LEU:HD21	26:S2:123:ARG:HE	1.63	0.61
15:H2:140:VAL:HG22	15:H2:150:GLN:HG2	1.82	0.61
24:Q2:50:GLU:OE1	24:Q2:82:ARG:NH2	2.33	0.61
30:W2:31:SER:HB2	34:22:636:A:H5''	1.82	0.61
36:14:1841:A:H1'	36:14:1848:G:H1'	1.82	0.61
78:E5:56:LYS:HB3	78:E5:64:LEU:HD12	1.82	0.61
34:22:1680:G:O2'	34:22:1721:A:N6	2.33	0.61
14:g2:42:LEU:HB2	14:g2:61:PHE:HB2	1.82	0.60
42:B5:235:THR:HG21	42:B5:249:VAL:HG22	1.83	0.60
53:H5:96:HIS:CG	80:A6:280:THR:HG23	2.35	0.60
36:14:2193:U:H5'	36:14:2194:G:H5'	1.82	0.60
56:J5:40:LEU:HD13	56:J5:114:ILE:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S2:4:VAL:CB	33:Z2:42:LEU:CD2	2.68	0.60
44:C5:106:TRP:HB2	63:N5:199:LEU:HD22	1.83	0.60
53:H5:96:HIS:NE2	80:A6:280:THR:CG2	2.65	0.60
2:A2:88:LYS:NZ	25:R2:82:ASP:OD2	2.34	0.60
3:a2:12:LYS:HD3	3:a2:16:GLY:H	1.66	0.60
16:I2:57:ALA:HB2	16:I2:177:GLY:HA2	1.83	0.60
74:R5:102:LEU:HD22	74:R5:138:LEU:HD13	1.84	0.60
1:A1:291:LEU:CD1	80:A6:520:LEU:HD21	2.32	0.60
1:A1:291:LEU:HD13	80:A6:520:LEU:HD21	1.83	0.60
23:P2:95:GLY:HA2	23:P2:103:ASN:O	2.02	0.59
26:S2:4:VAL:CG1	33:Z2:42:LEU:HB2	2.31	0.59
26:S2:14:ILE:HD12	26:S2:24:GLY:H	1.66	0.59
31:X2:70:LYS:HB3	31:X2:93:LEU:HD22	1.83	0.59
20:M2:22:VAL:HG12	20:M2:23:THR:HG23	1.84	0.59
33:Z2:77:ARG:NH2	34:22:1533:C:H6	2.00	0.59
16:I2:172:ARG:HE	16:I2:175:GLN:HG3	1.65	0.59
53:H5:92:TYR:HB2	53:H5:142:ASP:HB3	1.83	0.59
33:Z2:73:GLY:N	34:22:1534:G:C2'	2.64	0.59
16:I2:61:GLU:HG3	16:I2:62:THR:HG23	1.85	0.59
23:P2:130:ARG:HD3	23:P2:130:ARG:N	2.02	0.59
36:14:2557:A:H5'	71:Z5:135:ARG:HE	1.67	0.59
8:D2:137:VAL:HB	8:D2:185:LYS:HB2	1.84	0.59
14:g2:178:VAL:HB	14:g2:192:PHE:HB2	1.84	0.59
34:22:1542:G:H22	34:22:1568:C:HO2'	1.49	0.59
36:14:2402:A:N7	44:C5:73:ARG:NH2	2.50	0.59
36:14:117:U:OP2	63:N5:2:GLY:N	2.36	0.58
27:T2:102:ARG:NH2	34:22:1502:G:N7	2.50	0.58
31:X2:125:VAL:HG12	31:X2:126:LYS:HG3	1.85	0.58
33:Z2:74:SER:OG	34:22:1533:C:H3'	2.03	0.58
9:d2:44:ARG:NH1	28:U2:69:LYS:O	2.37	0.58
19:L2:71:LEU:HB3	19:L2:88:ARG:HH12	1.69	0.58
36:14:1408:G:OP1	47:e5:33:ARG:NH2	2.37	0.58
22:O2:137:LEU:CD1	81:X7:12:A:O2'	2.52	0.58
27:T2:89:ARG:NH2	34:22:1562:G:OP1	2.37	0.58
31:X2:102:VAL:HG12	31:X2:127:VAL:HG12	1.86	0.58
60:L5:91:ARG:HH21	60:L5:97:VAL:HB	1.68	0.58
10:E2:191:ARG:HH11	10:E2:245:LYS:HB3	1.68	0.58
16:I2:5:ARG:NH2	34:22:334:G:O6	2.37	0.58
19:L2:17:PRO:HG2	34:22:249:U:H3	1.69	0.58
20:M2:42:ALA:HB3	20:M2:122:VAL:HB	1.85	0.58
36:14:2858:U:O2'	36:14:2887:A:N6	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:J5:20:ASN:HB3	56:J5:126:ASP:HB2	1.86	0.58
56:J5:47:GLN:HG2	56:J5:67:VAL:HG12	1.85	0.58
3:a2:3:LYS:HE3	3:a2:8:ASN:HD21	1.69	0.58
29:V2:36:VAL:HB	29:V2:51:VAL:HB	1.86	0.58
36:14:2137:U:OP2	36:14:2142:A:N6	2.37	0.58
36:14:2736:A:OP1	77:T5:92:ARG:NH1	2.37	0.58
2:A2:67:ILE:O	2:A2:185:ARG:NH1	2.37	0.57
23:P2:128:HIS:CD2	34:22:1459:C:HO2'	2.07	0.57
33:Z2:77:ARG:CZ	34:22:1533:C:C6	2.87	0.57
56:J5:55:ARG:NE	82:A3:20:G:H22	1.92	0.57
26:S2:144:ARG:HH12	34:22:1570:A:H4'	1.69	0.57
36:14:284:A:OP2	64:o5:41:ARG:NH1	2.37	0.57
36:14:2898:G:OP2	53:H5:173:ARG:NH2	2.38	0.57
36:14:804:C:OP1	44:C5:98:ARG:NH2	2.38	0.57
79:W5:6:ASP:HB3	79:W5:10:GLY:H	1.69	0.57
36:14:1491:A:OP1	57:j5:14:LYS:NZ	2.38	0.57
67:Q5:86:THR:HG22	67:Q5:105:ARG:HB3	1.85	0.57
65:p5:36:ARG:HG3	65:p5:45:LYS:HG2	1.86	0.57
81:X7:9:G:O2'	81:X7:10:G:N2	2.37	0.57
1:A1:176:LYS:CD	80:A6:222:GLN:HG3	2.29	0.57
19:L2:128:CYS:SG	19:L2:129:ARG:N	2.76	0.57
31:X2:30:LYS:NZ	34:22:1132:A:OP1	2.37	0.57
42:B5:238:LEU:HB3	42:B5:242:THR:HG21	1.86	0.57
23:P2:97:TYR:HB2	23:P2:102:PHE:CE1	2.39	0.57
36:14:1523:U:H5'	75:X5:113:LEU:HB3	1.87	0.57
1:A1:152:ALA:HB3	1:A1:168:ILE:HB	1.87	0.56
5:b2:4:VAL:HG11	29:V2:71:ARG:HD3	1.86	0.56
36:14:712:G:OP1	60:L5:174:ARG:NH1	2.38	0.56
36:14:2799:A:O2'	39:a5:42:ARG:NH1	2.38	0.56
54:i5:5:THR:HG23	54:i5:12:ASN:HB2	1.87	0.56
10:E2:79:ASP:HB3	10:E2:82:TYR:HB2	1.86	0.56
16:I2:37:LYS:HB2	16:I2:59:ARG:HG2	1.86	0.56
21:N2:4:MET:SD	21:N2:124:ARG:NH1	2.78	0.56
34:22:1588:G:H1	34:22:1608:U:H3	1.52	0.56
38:44:141:C:O2	63:N5:112:ASN:ND2	2.38	0.56
36:14:129:U:OP1	75:X5:45:LYS:NZ	2.37	0.56
36:14:1796:G:H5'	40:A5:22:LEU:HD21	1.88	0.56
56:J5:133:ARG:NH2	56:J5:158:ASP:OD2	2.39	0.56
12:F2:63:GLN:NE2	12:F2:86:GLN:O	2.38	0.56
36:14:1447:G:N2	36:14:2356:A:OP2	2.38	0.56
36:14:3041:U:OP1	70:V5:12:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:125:ASP:OD1	2:A2:164:ASN:ND2	2.39	0.56
2:A2:198:MET:HE3	2:A2:200:ASP:HB2	1.86	0.56
22:O2:82:LYS:NZ	22:O2:116:GLU:OE2	2.38	0.56
36:14:969:C:OP1	41:b5:19:ASN:ND2	2.39	0.56
50:g5:41:ARG:HG2	50:g5:56:THR:HG21	1.86	0.56
53:H5:96:HIS:CD2	80:A6:280:THR:CG2	2.74	0.56
36:14:200:C:N4	36:14:219:A:OP2	2.39	0.56
70:V5:81:GLN:O	70:V5:98:ASN:ND2	2.38	0.56
36:14:813:G:O2'	57:j5:45:ARG:NH2	2.39	0.56
36:14:1302:A:N7	36:14:2857:C:O2'	2.38	0.56
37:34:7:G:OP1	45:D5:33:ARG:NH1	2.38	0.56
70:V5:21:ALA:HB3	70:V5:36:ILE:HD12	1.88	0.56
80:A6:591:ARG:HG2	80:A6:605:LYS:HG2	1.88	0.56
6:C2:94:GLN:NE2	34:22:10:G:O2'	2.38	0.56
17:J2:133:HIS:HD2	17:J2:162:SER:HB2	1.70	0.56
36:14:1390:A:O4'	36:14:1418:A:N6	2.38	0.56
50:g5:94:LEU:O	50:g5:98:GLN:NE2	2.39	0.56
52:h5:27:GLU:HG2	52:h5:47:VAL:HG21	1.88	0.56
2:A2:52:LYS:HG2	29:V2:82:VAL:HG22	1.88	0.55
12:F2:112:ARG:HE	24:Q2:43:ILE:HD11	1.71	0.55
36:14:1428:A:O2'	36:14:1430:U:OP2	2.24	0.55
42:B5:137:TYR:HA	42:B5:144:ILE:HD11	1.87	0.55
1:A1:291:LEU:HB3	80:A6:518:PRO:HG2	1.84	0.55
6:C2:88:LYS:HA	34:22:10:G:H21	1.72	0.55
14:g2:198:ASN:HD21	25:R2:23:LYS:H	1.54	0.55
34:22:152:U:H3	34:22:162:A:H61	1.54	0.55
45:D5:65:ILE:HG12	45:D5:74:VAL:HG22	1.87	0.55
1:A1:42:ILE:HB	1:A1:116:THR:HB	1.88	0.55
8:D2:108:LYS:NZ	80:A6:21:GLU:OE2	2.30	0.55
25:R2:79:GLU:O	25:R2:83:GLN:NE2	2.39	0.55
42:B5:168:LYS:O	42:B5:319:ASN:ND2	2.40	0.55
63:N5:73:ARG:HH21	63:N5:92:LEU:HD21	1.71	0.55
80:A6:440:PRO:HD3	80:A6:579:PRO:HD3	1.88	0.55
36:14:55:G:OP1	57:j5:43:LYS:NZ	2.40	0.55
36:14:3329:U:H5''	42:B5:308:MET:HE2	1.88	0.55
66:P5:109:ALA:HA	66:P5:112:LEU:HD13	1.87	0.55
16:I2:98:LYS:HB3	34:22:329:G:H5''	1.88	0.55
28:U2:21:LYS:HG2	28:U2:94:GLU:HG2	1.87	0.55
35:f2:108:VAL:HG23	35:f2:114:VAL:HG22	1.89	0.55
36:14:216:G:OP1	76:Y5:16:ARG:NH1	2.40	0.55
14:g2:216:LYS:HA	14:g2:239:GLU:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:T2:7:ARG:NH1	34:22:1366:U:O2'	2.40	0.55
36:14:1374:G:O6	39:a5:10:LYS:NZ	2.39	0.55
36:14:2116:G:OP1	36:14:2118:C:N4	2.39	0.55
80:A6:519:LEU:HD12	80:A6:559:LEU:HD23	1.87	0.55
34:22:1584:G:N2	34:22:1611:A:OP2	2.39	0.55
36:14:140:C:OP1	51:G5:106:LYS:NZ	2.38	0.55
42:B5:53:MET:HG2	42:B5:77:THR:HG22	1.89	0.55
1:A1:361:GLU:HG3	80:A6:522:GLY:O	2.07	0.55
36:14:1334:U:H5''	49:F5:206:LYS:HB3	1.89	0.55
36:14:2950:G:OP2	36:14:2950:G:N2	2.39	0.55
37:34:41:G:O2'	37:34:44:C:N4	2.40	0.55
53:H5:113:GLU:OE2	53:H5:115:ARG:NH2	2.39	0.55
72:K5:22:VAL:HG21	72:K5:120:VAL:HG11	1.89	0.55
14:g2:118:LYS:NZ	14:g2:120:SER:OG	2.39	0.55
34:22:434:G:N1	34:22:437:A:OP2	2.38	0.55
34:22:1191:U:O2	82:A3:34:OMG:H5'	2.07	0.55
36:14:668:G:O2'	67:Q5:164:ARG:NH1	2.40	0.55
36:14:2341:A:OP2	42:B5:247:ARG:NH1	2.40	0.55
36:14:2535:A:H61	36:14:2544:U:H3	1.54	0.55
51:G5:72:PRO:HG3	63:N5:18:VAL:HA	1.89	0.55
4:B2:69:CYS:HA	4:B2:83:LYS:HA	1.88	0.54
36:14:1390:A:OP1	47:e5:103:LYS:NZ	2.40	0.54
36:14:3140:G:N7	42:B5:28:ARG:NH2	2.55	0.54
38:44:71:A:N6	38:44:87:G:O2'	2.40	0.54
6:C2:88:LYS:HE2	6:C2:95:ARG:HE	1.72	0.54
15:H2:113:PRO:HD3	34:22:811:A:H61	1.71	0.54
36:14:190:U:OP1	76:Y5:40:ARG:NH1	2.40	0.54
36:14:959:C:H41	36:14:2801:A:H5''	1.72	0.54
34:22:67:A:N6	34:22:83:G:O2'	2.40	0.54
36:14:2896:A:O2'	61:m5:122:ARG:NH2	2.41	0.54
36:14:3297:U:O4	42:B5:124:LYS:NZ	2.40	0.54
3:a2:12:LYS:NZ	34:22:1029:U:OP2	2.40	0.54
13:G2:136:LYS:NZ	34:22:66:U:OP2	2.40	0.54
19:L2:67:ARG:NH1	34:22:112:A:O2'	2.41	0.54
66:P5:23:ARG:HH22	66:P5:125:GLN:HG3	1.72	0.54
36:14:75:G:OP1	60:L5:101:ARG:NH2	2.41	0.54
36:14:126:U:OP1	63:N5:144:ARG:NH1	2.41	0.54
36:14:98:G:N7	60:L5:13:HIS:NE2	2.55	0.54
36:14:609:G:OP2	44:C5:315:LYS:NZ	2.40	0.54
36:14:2303:A:OP1	73:n5:23:ARG:NH2	2.41	0.54
55:I5:47:PRO:HD2	55:I5:141:LYS:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:W2:103:ILE:HA	30:W2:112:ASP:HA	1.89	0.54
31:X2:132:LEU:HD23	31:X2:135:LEU:HD12	1.89	0.54
36:14:1084:A:H5''	77:T5:35:LYS:HE3	1.90	0.54
1:A1:88:VAL:O	1:A1:96:ASN:ND2	2.41	0.54
12:F2:104:ASN:ND2	34:22:1587:A:O2'	2.39	0.54
24:Q2:44:LEU:HB3	24:Q2:78:VAL:HG11	1.88	0.54
34:22:156:A:O2'	34:22:416:A:N6	2.41	0.54
10:E2:191:ARG:NH1	10:E2:244:ILE:O	2.41	0.54
36:14:2899:C:N3	53:H5:173:ARG:NH1	2.53	0.54
39:a5:146:GLU:OE1	60:L5:157:ARG:NH2	2.41	0.54
3:a2:41:ILE:HD11	81:X7:7:G:O2'	2.09	0.54
10:E2:108:ARG:NH1	34:22:788:A:OP2	2.41	0.54
11:e2:39:LEU:HD11	11:e2:43:ARG:HH21	1.73	0.54
12:F2:125:THR:CA	33:Z2:58:ARG:HH22	2.18	0.54
33:Z2:77:ARG:HH22	34:22:1533:C:H6	1.56	0.54
36:14:2202:C:H5''	40:A5:226:SER:HB2	1.90	0.54
36:14:3089:C:OP1	42:B5:222:LYS:NZ	2.41	0.54
40:A5:30:ARG:HH12	40:A5:41:ILE:HD13	1.73	0.54
21:N2:121:ARG:NH1	34:22:868:G:OP1	2.41	0.53
36:14:1150:A:N6	36:14:2369:G:O2'	2.41	0.53
36:14:3182:G:OP1	72:K5:117:ARG:NH2	2.40	0.53
66:P5:129:THR:HG23	66:P5:139:TYR:HB2	1.90	0.53
71:Z5:14:VAL:HG13	71:Z5:15:ARG:HG2	1.89	0.53
80:A6:451:GLN:HB2	80:A6:475:THR:HB	1.90	0.53
1:A1:40:GLU:HB2	1:A1:118:ILE:HB	1.90	0.53
36:14:664:U:H3	36:14:798:G:H1	1.55	0.53
20:M2:43:ARG:NH1	20:M2:102:GLY:O	2.41	0.53
36:14:1389:G:H5''	47:e5:101:SER:HB3	1.89	0.53
50:g5:37:LYS:HB2	50:g5:58:ARG:HH22	1.73	0.53
56:J5:51:ARG:O	56:J5:61:ARG:NH2	2.41	0.53
57:j5:52:LYS:HG2	57:j5:55:ARG:HH21	1.71	0.53
80:A6:539:LYS:HD2	80:A6:570:GLU:HB2	1.88	0.53
27:T2:122:ARG:NH1	34:22:1499:G:OP1	2.41	0.53
42:B5:221:THR:HB	42:B5:273:HIS:H	1.72	0.53
63:N5:56:LYS:NZ	63:N5:145:ASP:OD2	2.41	0.53
68:S5:154:HIS:HE1	72:K5:126:VAL:HG22	1.73	0.53
31:X2:42:PRO:O	31:X2:79:ASN:ND2	2.41	0.53
32:Y2:112:LYS:NZ	34:22:57:G:OP1	2.42	0.53
34:22:716:C:H41	34:22:723:G:H21	1.55	0.53
36:14:590:G:O2'	44:C5:309:ARG:NH1	2.41	0.53
51:G5:86:THR:HG21	51:G5:217:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:A6:526:ILE:HA	80:A6:535:PRO:HA	1.90	0.53
1:A1:41:LEU:HD12	1:A1:67:ILE:HD11	1.90	0.53
15:H2:64:VAL:HB	34:22:856:A:H1'	1.89	0.53
35:f2:121:CYS:SG	35:f2:122:SER:N	2.82	0.53
36:14:1483:G:O6	50:g5:4:ARG:NH2	2.39	0.53
36:14:1528:G:O2'	59:l5:4:GLN:NE2	2.41	0.53
36:14:3206:C:H1'	68:S5:155:ARG:HH12	1.73	0.53
63:N5:44:ARG:NH1	63:N5:120:TRP:O	2.42	0.53
23:P2:128:HIS:CD2	34:22:1459:C:O2'	2.55	0.53
40:A5:21:ARG:HH21	40:A5:22:LEU:HD12	1.73	0.53
56:J5:55:ARG:NH2	82:A3:19:G:O2'	2.41	0.53
80:A6:304:GLY:O	80:A6:588:ARG:NH1	2.42	0.53
34:22:1202:A:N6	34:22:1457:C:OP1	2.35	0.53
80:A6:173:LEU:HD13	80:A6:296:HIS:HB3	1.90	0.53
11:e2:15:LYS:NZ	31:X2:136:TRP:O	2.41	0.53
36:14:1192:C:OP1	61:m5:113:ARG:NH2	2.38	0.53
36:14:3040:A:H5''	70:V5:12:ARG:HB2	1.91	0.53
42:B5:287:LYS:O	42:B5:293:ASN:ND2	2.41	0.53
44:C5:3:ARG:HE	44:C5:22:LEU:HB2	1.72	0.53
6:C2:87:GLN:OE1	6:C2:94:GLN:NE2	2.42	0.53
6:C2:203:LYS:NZ	34:22:16:G:O6	2.42	0.53
9:d2:52:PHE:HB3	28:U2:82:TYR:HB3	1.91	0.53
13:G2:65:GLN:NE2	34:22:1682:U:O2'	2.42	0.53
26:S2:4:VAL:CG1	33:Z2:42:LEU:CB	2.85	0.53
37:34:5:G:OP1	56:J5:143:ARG:NH2	2.42	0.53
45:D5:64:ILE:HD13	45:D5:109:THR:HG21	1.90	0.53
68:S5:22:PRO:O	77:T5:146:ASN:ND2	2.39	0.53
17:J2:77:ILE:HD11	17:J2:93:LEU:HB2	1.92	0.52
36:14:938:C:OP2	39:a5:26:ARG:NH1	2.41	0.52
36:14:1900:A:H61	36:14:1908:A:H61	1.57	0.52
36:14:2880:U:OP1	70:V5:47:ASN:ND2	2.41	0.52
36:14:2908:G:O2'	61:m5:114:LYS:NZ	2.42	0.52
10:E2:104:ASP:HB2	10:E2:108:ARG:H	1.73	0.52
36:14:2548:C:OP2	40:A5:93:LYS:NZ	2.42	0.52
36:14:3011:A:N6	42:B5:12:GLY:O	2.42	0.52
38:44:24:G:O6	76:Y5:13:ARG:NH2	2.43	0.52
43:c5:35:ARG:HD2	71:Z5:5:LEU:HD11	1.91	0.52
67:Q5:75:GLY:O	67:Q5:79:LYS:NZ	2.42	0.52
1:A1:67:ILE:HA	1:A1:87:THR:HA	1.90	0.52
1:A1:264:LYS:HD2	80:A6:517:ARG:HH12	1.73	0.52
1:A1:312:GLY:HA3	1:A1:345:ASN:HD22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B2:86:LEU:HD23	4:B2:98:THR:HG21	1.91	0.52
9:d2:36:LEU:HD12	9:d2:38:ILE:H	1.73	0.52
34:22:42:G:H1	34:22:433:C:H42	1.55	0.52
36:14:1214:U:OP2	68:S5:137:ARG:NH2	2.42	0.52
36:14:3027:A:H1'	80:A6:256:ARG:NH2	2.24	0.52
36:14:3049:A:N3	42:B5:55:THR:OG1	2.39	0.52
63:N5:37:HIS:HE1	63:N5:63:ARG:HH11	1.55	0.52
12:F2:156:ARG:NH1	22:O2:53:ASP:OD2	2.41	0.52
34:22:1112:G:OP1	73:n5:6:ARG:NH2	2.43	0.52
36:14:777:U:HO2'	36:14:2719:U:HO2'	1.57	0.52
1:A1:103:LYS:NZ	34:22:578:U:OP2	2.41	0.52
36:14:2969:A:N7	40:A5:215:ASN:ND2	2.57	0.52
66:P5:30:ARG:HH12	66:P5:62:ARG:HH11	1.56	0.52
72:K5:61:ALA:HA	72:K5:70:PRO:HD2	1.91	0.52
9:d2:12:ARG:NH1	34:22:1205:C:O2'	2.43	0.52
34:22:1594:G:OP2	34:22:1596:C:N4	2.42	0.52
36:14:1189:C:N4	36:14:1315:U:O2'	2.43	0.52
36:14:1900:A:O2'	36:14:1902:G:N7	2.41	0.52
36:14:3275:U:O2'	48:f5:99:ARG:NH1	2.43	0.52
37:34:44:C:OP2	56:J5:137:ARG:NH2	2.41	0.52
38:44:29:U:H5''	60:L5:27:ASP:HB3	1.92	0.52
42:B5:219:ALA:HB2	42:B5:336:VAL:HG23	1.92	0.52
47:e5:63:THR:HA	47:e5:66:LEU:HD12	1.89	0.52
12:F2:63:GLN:HG2	12:F2:88:PRO:HB3	1.92	0.52
25:R2:5:ARG:NH2	34:22:1390:U:OP1	2.43	0.52
36:14:1245:A:N6	36:14:1272:C:O2'	2.38	0.52
52:h5:33:VAL:HG22	75:X5:66:PRO:HG2	1.92	0.52
33:Z2:56:THR:O	33:Z2:103:ARG:NH1	2.42	0.52
36:14:1603:A:H61	75:X5:71:THR:HG21	1.74	0.52
49:F5:66:LYS:NZ	49:F5:78:GLU:OE2	2.43	0.52
56:J5:55:ARG:HE	82:A3:20:G:H1	1.46	0.52
80:A6:274:LEU:HB3	80:A6:310:ILE:HG23	1.92	0.52
4:B2:204:ILE:O	34:22:1064:G:O2'	2.28	0.52
9:d2:44:ARG:HH12	34:22:1280:C:H5'	1.75	0.52
12:F2:125:THR:HA	33:Z2:58:ARG:HH22	1.75	0.52
15:H2:46:ILE:HD11	15:H2:58:LEU:HB3	1.90	0.52
26:S2:117:LYS:O	26:S2:120:ARG:NH2	2.43	0.52
36:14:40:A:O2'	36:14:937:G:O6	2.28	0.52
36:14:116:A:OP2	63:N5:2:GLY:N	2.42	0.52
23:P2:59:LYS:NZ	34:22:1242:A:OP1	2.42	0.52
34:22:16:G:H21	34:22:1138:A:H62	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:22:815:G:OP2	74:R5:166:ASN:ND2	2.43	0.52
36:14:119:U:H4'	36:14:120:G:H3'	1.91	0.52
36:14:2727:A:OP2	36:14:2728:G:N2	2.43	0.52
31:X2:14:LYS:NZ	34:22:1105:C:OP2	2.43	0.51
36:14:13:A:H61	38:44:145:U:H3	1.58	0.51
36:14:374:A:OP1	76:Y5:77:LYS:NZ	2.44	0.51
36:14:608:A:O2'	44:C5:326:ARG:NH1	2.43	0.51
36:14:784:A:H2'	67:Q5:69:ARG:HE	1.75	0.51
36:14:1160:C:OP1	67:Q5:2:GLY:N	2.43	0.51
36:14:1361:U:O2	49:F5:159:GLN:NE2	2.44	0.51
45:D5:54:ARG:HH12	45:D5:149:GLY:HA3	1.75	0.51
51:G5:137:ASN:HD21	63:N5:4:TYR:HE2	1.58	0.51
75:X5:100:LYS:NZ	75:X5:106:ASP:OD1	2.43	0.51
5:b2:3:LEU:HA	30:W2:22:LYS:HD3	1.92	0.51
8:D2:27:ARG:NH2	34:22:1436:A:OP2	2.43	0.51
9:d2:19:ARG:NH2	34:22:1596:C:OP2	2.43	0.51
36:14:394:G:N1	36:14:397:A:OP2	2.43	0.51
36:14:2335:G:N2	36:14:2339:C:O2'	2.43	0.51
44:C5:16:THR:HG22	44:C5:18:ASN:H	1.75	0.51
44:C5:300:ARG:O	67:Q5:39:ARG:NH2	2.43	0.51
12:F2:52:GLU:OE2	12:F2:65:ARG:NH1	2.43	0.51
19:L2:123:VAL:HG23	19:L2:142:VAL:HG22	1.93	0.51
30:W2:15:ASN:HD21	30:W2:72:CYS:H	1.57	0.51
36:14:874:U:OP2	42:B5:241:LYS:NZ	2.40	0.51
36:14:1324:U:H5''	68:S5:1:MET:HA	1.91	0.51
38:44:103:G:OP2	38:44:105:A:O2'	2.29	0.51
40:A5:181:LYS:HG3	40:A5:184:ARG:H	1.75	0.51
64:o5:2:VAL:N	64:o5:90:HIS:O	2.44	0.51
68:S5:38:LYS:HD3	68:S5:58:ILE:HG21	1.93	0.51
3:a2:48:ALA:O	22:O2:103:ARG:NH2	2.43	0.51
8:D2:42:THR:OG1	8:D2:45:LYS:O	2.29	0.51
14:g2:123:ILE:HG22	14:g2:133:VAL:HG22	1.92	0.51
14:g2:150:TRP:HB2	14:g2:174:ASN:HD22	1.75	0.51
16:I2:67:TRP:NE1	16:I2:69:SER:OG	2.44	0.51
36:14:1547:G:OP1	63:N5:108:ARG:NH2	2.43	0.51
36:14:2712:U:O2'	36:14:2743:A:O2'	2.28	0.51
1:A1:158:THR:HG22	1:A1:160:SER:H	1.76	0.51
34:22:91:G:OP1	34:22:397:A:N6	2.42	0.51
36:14:1481:A:O2'	36:14:1858:A:N3	2.42	0.51
36:14:3198:U:H1'	53:H5:21:LYS:HB2	1.92	0.51
41:b5:34:GLY:O	77:T5:66:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:H5:8:GLN:HB3	53:H5:72:LYS:HD2	1.93	0.51
80:A6:502:SER:HB3	80:A6:577:TRP:HB3	1.91	0.51
82:A3:47:U:O2'	82:A3:50:U:OP1	2.27	0.51
12:F2:95:ASN:OD1	12:F2:107:LYS:NZ	2.43	0.51
34:22:472:U:O2'	34:22:769:A:N3	2.42	0.51
51:G5:108:ARG:NH2	51:G5:112:GLU:OE2	2.44	0.51
4:B2:149:GLN:HE22	4:B2:154:SER:HB2	1.75	0.51
16:I2:105:ASP:OD2	16:I2:107:THR:OG1	2.26	0.51
23:P2:86:VAL:HG13	23:P2:88:GLU:H	1.76	0.51
36:14:32:U:O4	63:N5:188:ARG:NH2	2.43	0.51
44:C5:4:PRO:HD2	44:C5:22:LEU:HD12	1.93	0.51
48:f5:75:HIS:HB2	48:f5:82:ARG:HG3	1.93	0.51
8:D2:191:ASP:HB3	8:D2:194:LYS:HG2	1.93	0.51
13:G2:70:PRO:HD3	13:G2:101:ILE:HD12	1.93	0.51
15:H2:111:LYS:HB3	34:22:811:A:H62	1.74	0.51
15:H2:143:LEU:HB2	15:H2:147:ASN:HB2	1.93	0.51
16:I2:56:ARG:NH2	34:22:332:U:OP1	2.44	0.51
36:14:86:G:N2	36:14:99:A:OP2	2.44	0.51
37:34:101:G:OP2	68:S5:52:LYS:NZ	2.44	0.51
47:e5:42:VAL:HG12	47:e5:52:GLN:HE21	1.76	0.51
70:V5:102:ILE:HG23	70:V5:110:LYS:HB3	1.92	0.51
2:A2:119:ARG:HH22	6:C2:240:LEU:HB3	1.76	0.51
6:C2:78:ASP:HA	6:C2:104:VAL:HG12	1.93	0.51
21:N2:99:ARG:NH2	21:N2:119:GLU:OE2	2.43	0.51
22:O2:18:ARG:NH1	34:22:918:U:O2'	2.44	0.51
36:14:2552:C:H2'	43:c5:50:VAL:HG11	1.92	0.51
40:A5:54:ARG:HG2	40:A5:56:ALA:H	1.76	0.51
53:H5:24:ILE:HD11	53:H5:39:LYS:HE2	1.92	0.51
14:g2:13:LEU:HB2	14:g2:310:ILE:HB	1.93	0.51
17:J2:3:ARG:NH2	34:22:39:A:OP1	2.44	0.51
23:P2:86:VAL:HG12	23:P2:89:MET:HE3	1.93	0.51
28:U2:28:SER:HB3	28:U2:34:LEU:HD12	1.93	0.51
32:Y2:41:ARG:NH2	32:Y2:52:LYS:O	2.41	0.51
34:22:65:A:H2	34:22:84:A:H62	1.59	0.51
36:14:68:C:N4	36:14:314:U:O2'	2.44	0.51
36:14:292:U:OP2	63:N5:68:ARG:NH2	2.44	0.51
36:14:911:C:H42	40:A5:3:ARG:HD3	1.75	0.51
36:14:1724:U:O2'	36:14:1725:C:O4'	2.29	0.51
67:Q5:8:LYS:HB3	67:Q5:11:LYS:HD3	1.92	0.51
14:g2:89:LEU:HB2	14:g2:103:PHE:HB2	1.93	0.50
16:I2:77:ARG:NH2	36:14:3354:U:O2'	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:22:936:G:OP1	34:22:1074:G:N2	2.42	0.50
36:14:1213:G:OP2	68:S5:137:ARG:NH1	2.44	0.50
36:14:1354:G:N7	36:14:1357:G:O2'	2.44	0.50
65:p5:46:THR:HB	65:p5:58:SER:HB2	1.93	0.50
16:I2:92:ARG:HE	36:14:3345:G:H4'	1.76	0.50
36:14:347:G:N2	36:14:352:A:O2'	2.42	0.50
22:O2:29:HIS:NE2	34:22:917:U:O2'	2.38	0.50
24:Q2:36:ILE:HD13	24:Q2:52:LEU:HD11	1.94	0.50
34:22:142:G:H22	34:22:173:A:H2	1.59	0.50
36:14:2549:G:N2	36:14:2549:G:OP2	2.44	0.50
48:f5:30:ILE:HD12	48:f5:98:VAL:HG11	1.93	0.50
49:F5:88:ARG:NH1	49:F5:108:LEU:O	2.44	0.50
56:J5:109:HIS:HD2	56:J5:123:PHE:H	1.60	0.50
68:S5:6:GLU:OE2	68:S5:28:ARG:NH1	2.43	0.50
2:A2:142:PRO:HG3	29:V2:32:VAL:HG13	1.93	0.50
9:d2:42:CYS:SG	34:22:1433:G:N2	2.77	0.50
26:S2:4:VAL:HG11	33:Z2:42:LEU:CB	2.35	0.50
34:22:58:U:O2'	34:22:451:A:N3	2.44	0.50
36:14:218:G:H1'	36:14:372:A:H1'	1.93	0.50
36:14:2345:A:OP1	46:d5:24:SER:OG	2.30	0.50
36:14:3377:G:H21	42:B5:332:ARG:HH21	1.59	0.50
7:c2:18:ARG:NH1	34:22:1616:G:O2'	2.44	0.50
77:T5:50:LYS:HB3	77:T5:92:ARG:HH11	1.77	0.50
21:N2:64:ARG:NH2	34:22:861:U:OP2	2.45	0.50
36:14:3178:A:H2'	72:K5:115:LYS:HD2	1.93	0.50
34:22:1026:A:N7	34:22:1772:C:O2'	2.42	0.50
36:14:63:A:N3	36:14:78:U:O2'	2.43	0.50
45:D5:76:ALA:HB3	45:D5:109:THR:HG22	1.94	0.50
26:S2:41:ARG:NH1	34:22:1565:C:OP1	2.45	0.50
27:T2:130:ARG:HH12	27:T2:134:ARG:HD3	1.77	0.50
31:X2:19:ARG:HH12	34:22:610:G:H21	1.60	0.50
36:14:691:A:N1	38:44:28:C:O2'	2.44	0.50
36:14:1985:G:H1	36:14:2036:U:H3	1.59	0.50
44:C5:160:GLN:NE2	44:C5:213:ASN:O	2.45	0.50
58:k5:2:ALA:N	58:k5:51:LEU:O	2.45	0.50
63:N5:4:TYR:HE1	63:N5:45:PRO:HB2	1.77	0.50
44:C5:334:PHE:HA	44:C5:339:LEU:HD12	1.93	0.50
69:U5:36:TYR:O	69:U5:40:HIS:ND1	2.44	0.50
4:B2:110:LEU:HD21	4:B2:213:ARG:HD2	1.93	0.49
53:H5:114:VAL:HB	53:H5:124:ARG:HB2	1.93	0.49
10:E2:19:LEU:HD11	10:E2:108:ARG:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E2:104:ASP:N	10:E2:108:ARG:O	2.46	0.49
13:G2:67:VAL:HG23	13:G2:99:GLY:HA2	1.93	0.49
22:O2:18:ARG:HA	22:O2:82:LYS:HB2	1.94	0.49
31:X2:134:ALA:HB1	31:X2:139:LYS:HB2	1.92	0.49
80:A6:432:PRO:HA	80:A6:447:VAL:HG13	1.94	0.49
2:A2:155:PHE:HA	29:V2:60:ARG:HB3	1.93	0.49
9:d2:44:ARG:NH2	34:22:1280:C:OP1	2.45	0.49
17:J2:134:ILE:HG22	17:J2:158:PHE:HA	1.95	0.49
26:S2:138:THR:OG1	34:22:1459:C:OP2	2.30	0.49
27:T2:16:ASN:OD1	27:T2:56:LYS:NZ	2.45	0.49
31:X2:96:VAL:HG12	31:X2:127:VAL:HG21	1.94	0.49
36:14:197:G:N2	36:14:218:G:O2'	2.46	0.49
36:14:286:U:O2'	63:N5:179:LYS:O	2.29	0.49
52:h5:25:LYS:NZ	75:X5:58:ASP:OD2	2.43	0.49
16:I2:141:ARG:NH2	34:22:196:G:O6	2.44	0.49
16:I2:153:GLU:HG2	16:I2:155:SER:H	1.78	0.49
28:U2:106:ILE:HG23	28:U2:107:THR:HG23	1.93	0.49
34:22:1022:C:O2'	34:22:1125:A:N1	2.45	0.49
36:14:217:U:O2	76:Y5:103:LYS:NZ	2.44	0.49
36:14:1747:G:H21	58:k5:2:ALA:HB1	1.77	0.49
40:A5:52:SER:HB3	40:A5:191:LEU:HD23	1.94	0.49
62:M5:85:TRP:NE1	62:M5:91:CYS:SG	2.85	0.49
76:Y5:87:LYS:HB2	76:Y5:97:ILE:HD11	1.94	0.49
1:A1:146:VAL:HA	1:A1:214:CYS:HB2	1.95	0.49
36:14:2945:G:O2'	36:14:2948:C:OP2	2.31	0.49
42:B5:14:LEU:HA	42:B5:17:LEU:HD13	1.94	0.49
52:h5:118:ILE:HG12	60:L5:123:ILE:HG22	1.94	0.49
82:A3:8:U:O2'	82:A3:21:A:N1	2.38	0.49
82:A3:22:G:H2'	82:A3:23:A:H8	1.78	0.49
3:a2:41:ILE:HG13	81:X7:8:A:OP1	2.12	0.49
36:14:3067:C:H3'	74:R5:62:ARG:HH12	1.78	0.49
16:I2:5:ARG:NH1	34:22:332:U:O2'	2.43	0.49
17:J2:52:ILE:HG23	17:J2:76:LEU:HD11	1.94	0.49
28:U2:72:ASN:ND2	34:22:1429:G:N3	2.59	0.49
34:22:368:U:O2'	34:22:603:U:O2'	2.29	0.49
36:14:1521:G:O6	59:l5:17:LYS:NZ	2.45	0.49
36:14:3119:U:H4'	61:m5:104:PRO:HG2	1.95	0.49
44:C5:327:LEU:HD23	49:F5:181:ILE:HG21	1.95	0.49
72:K5:34:VAL:HG12	72:K5:103:LYS:HB2	1.95	0.49
34:22:396:G:N2	34:22:399:A:OP2	2.43	0.49
34:22:1488:G:H3'	34:22:1515:A:H61	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:14:3092:C:H2'	70:V5:12:ARG:HH21	1.75	0.49
80:A6:308:LEU:HD12	80:A6:310:ILE:HD11	1.93	0.49
8:D2:54:ARG:HD3	80:A6:20:GLY:HA2	1.93	0.49
15:H2:112:ARG:NH1	34:22:638:U:O2'	2.46	0.49
34:22:393:C:H41	34:22:400:A:H1'	1.77	0.49
34:22:514:G:H2'	34:22:515:A:H8	1.78	0.49
36:14:1048:A:HO2'	36:14:2632:G:HO2'	1.58	0.49
36:14:1794:G:O2'	36:14:1796:G:N2	2.46	0.49
71:Z5:22:LYS:NZ	71:Z5:129:TRP:O	2.43	0.49
1:A1:24:ASP:OD2	1:A1:139:LYS:NZ	2.42	0.49
34:22:701:U:O2	34:22:738:G:N2	2.46	0.49
36:14:2185:G:O2'	36:14:2314:U:OP2	2.29	0.49
36:14:2349:U:O2'	36:14:3307:A:N3	2.46	0.49
36:14:2947:G:OP1	36:14:2982:A:N6	2.44	0.49
36:14:3325:G:OP1	46:d5:70:ARG:NH2	2.46	0.49
62:M5:19:ARG:HB3	62:M5:35:ILE:HD12	1.94	0.49
71:Z5:23:VAL:HG12	71:Z5:45:GLY:HA3	1.95	0.49
74:R5:148:ASP:OD1	74:R5:151:ARG:NH1	2.46	0.49
8:D2:132:LYS:HG3	8:D2:156:PHE:HB3	1.95	0.48
26:S2:69:ILE:HG22	26:S2:73:MET:HE2	1.94	0.48
28:U2:59:PRO:HG3	34:22:1381:U:H4'	1.94	0.48
34:22:1191:U:C2	82:A3:34:OMG:H5'	2.48	0.48
52:h5:38:ARG:HD2	52:h5:41:LEU:HD13	1.95	0.48
27:T2:105:LEU:HD13	27:T2:122:ARG:HD2	1.95	0.48
34:22:1640:C:N4	81:X7:18:C:OP1	2.46	0.48
36:14:1385:C:O2	78:E5:2:SER:N	2.46	0.48
65:p5:46:THR:OG1	65:p5:57:CYS:SG	2.70	0.48
1:A1:1:MET:N	1:A1:133:ALA:O	2.46	0.48
9:d2:19:ARG:HE	9:d2:30:LEU:HD22	1.79	0.48
14:g2:80:ALA:HB3	14:g2:92:TRP:HB2	1.95	0.48
16:I2:5:ARG:NH2	16:I2:27:PHE:O	2.46	0.48
36:14:633:C:O2'	48:f5:21:ARG:O	2.31	0.48
36:14:2617:U:O2'	55:I5:116:ARG:NH2	2.46	0.48
12:F2:187:ILE:HG21	33:Z2:66:VAL:HB	1.96	0.48
34:22:542:A:O2'	34:22:543:C:O2	2.32	0.48
37:34:36:C:H42	37:34:41:G:H1	1.60	0.48
42:B5:93:VAL:HG22	42:B5:155:ALA:H	1.78	0.48
44:C5:203:ARG:NH2	44:C5:226:GLU:OE1	2.45	0.48
62:M5:123:LEU:HD22	72:K5:190:VAL:HG23	1.95	0.48
78:E5:131:LYS:HG3	78:E5:133:GLU:H	1.78	0.48
82:A3:23:A:H2'	82:A3:24:G:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:84:ARG:NH2	25:R2:82:ASP:O	2.47	0.48
7:c2:27:GLN:HE22	7:c2:65:ARG:HG2	1.79	0.48
13:G2:31:ARG:HE	13:G2:68:LEU:HD21	1.77	0.48
16:I2:83:TYR:HB3	16:I2:101:ILE:HB	1.94	0.48
38:44:13:A:O2'	66:P5:121:GLN:O	2.32	0.48
46:d5:55:LEU:HB2	46:d5:95:PRO:HD3	1.96	0.48
53:H5:41:ILE:HD11	53:H5:67:ALA:HB1	1.94	0.48
24:Q2:12:LYS:HG2	24:Q2:17:THR:HG22	1.95	0.48
24:Q2:39:VAL:HG12	24:Q2:41:PRO:HD2	1.95	0.48
36:14:21:G:O2'	38:44:37:A:N6	2.47	0.48
36:14:289:A:O2'	63:N5:93:LYS:O	2.27	0.48
36:14:1447:G:OP1	66:P5:65:SER:OG	2.27	0.48
38:44:27:U:H4'	44:C5:51:ALA:HB3	1.95	0.48
38:44:58:G:O6	57:j5:63:ARG:NH2	2.46	0.48
5:b2:73:LEU:HB3	5:b2:77:THR:HG21	1.94	0.48
13:G2:57:ASP:HB3	13:G2:106:LEU:HD23	1.96	0.48
26:S2:16:ARG:NH2	56:J5:111:ASP:OD1	2.33	0.48
30:W2:105:THR:N	30:W2:124:LYS:O	2.47	0.48
34:22:104:A:OP2	34:22:308:C:N4	2.43	0.48
34:22:1122:G:N2	34:22:1125:A:OP2	2.44	0.48
40:A5:249:SER:OG	40:A5:250:GLN:N	2.46	0.48
63:N5:99:ARG:NH2	63:N5:118:SER:O	2.45	0.48
70:V5:23:MET:HE1	70:V5:78:VAL:HG22	1.96	0.48
3:a2:32:LYS:NZ	34:22:932:U:O2	2.47	0.48
34:22:322:G:N2	34:22:325:G:O6	2.42	0.48
34:22:1362:U:O2	34:22:1363:U:N3	2.45	0.48
36:14:1145:G:O2'	47:e5:45:ARG:O	2.30	0.48
36:14:1635:G:N2	36:14:1638:A:OP2	2.42	0.48
46:d5:72:ARG:NH1	46:d5:105:GLN:O	2.47	0.48
68:S5:1:MET:HG2	68:S5:3:HIS:H	1.79	0.48
80:A6:574:VAL:HG22	80:A6:576:ARG:H	1.79	0.48
1:A1:65:LEU:HD13	1:A1:105:LEU:HD21	1.96	0.48
5:b2:20:LYS:HG3	5:b2:21:LEU:HD12	1.96	0.48
9:d2:22:ARG:HH21	9:d2:37:ASN:HD22	1.60	0.48
15:H2:108:GLN:NE2	34:22:743:U:O4'	2.47	0.48
21:N2:104:ARG:NH1	34:22:950:C:O2'	2.46	0.48
30:W2:28:ARG:HD3	30:W2:60:LYS:HE2	1.95	0.48
31:X2:101:GLU:O	31:X2:128:SER:N	2.46	0.48
33:Z2:77:ARG:NH2	34:22:1533:C:C5	2.76	0.48
36:14:1836:C:H41	59:l5:3:ALA:HB2	1.78	0.48
40:A5:51:ASP:HB2	40:A5:58:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:V5:14:SER:O	70:V5:81:GLN:NE2	2.47	0.48
4:B2:165:ARG:HH12	34:22:946:U:H5''	1.79	0.48
5:b2:16:ALA:O	5:b2:29:ARG:NH1	2.47	0.48
10:E2:31:PRO:HG3	10:E2:43:PRO:HG3	1.94	0.48
17:J2:59:LEU:HD22	17:J2:69:ARG:HA	1.96	0.48
23:P2:18:ARG:HB2	23:P2:36:LEU:HD13	1.94	0.48
26:S2:115:ARG:HA	26:S2:118:LYS:HE2	1.95	0.48
36:14:29:C:O3'	63:N5:172:ARG:NH2	2.46	0.48
36:14:70:A:H5'	39:a5:64:GLN:HE22	1.79	0.48
63:N5:159:ARG:NH2	63:N5:164:LEU:O	2.47	0.48
2:A2:90:ALA:HB2	2:A2:97:PRO:HD3	1.96	0.47
3:a2:5:ARG:HB2	3:a2:8:ASN:HA	1.96	0.47
3:a2:70:LYS:HD3	34:22:930:A:H5''	1.96	0.47
15:H2:48:GLU:OE2	15:H2:88:ARG:NH2	2.47	0.47
36:14:1940:G:OP1	74:R5:75:HIS:ND1	2.47	0.47
36:14:2987:A:H5''	72:K5:68:ARG:HH12	1.79	0.47
50:g5:90:ILE:HD13	71:Z5:81:LEU:HD11	1.95	0.47
68:S5:83:SER:OG	68:S5:86:GLY:O	2.29	0.47
4:B2:109:LYS:HG3	4:B2:113:MET:HE3	1.96	0.47
12:F2:124:LEU:HA	33:Z2:58:ARG:NE	2.25	0.47
13:G2:188:ARG:HD3	34:22:283:U:H5''	1.96	0.47
14:g2:18:GLY:HA3	14:g2:38:ARG:HB3	1.96	0.47
27:T2:102:ARG:NH1	34:22:1501:C:OP2	2.47	0.47
36:14:114:A:H4'	63:N5:49:ARG:HG2	1.96	0.47
36:14:2261:G:O2'	36:14:2263:C:N4	2.47	0.47
36:14:2351:U:H5''	66:P5:82:ARG:HG3	1.96	0.47
56:J5:10:ARG:NH1	56:J5:151:SER:O	2.48	0.47
80:A6:354:PHE:HE2	85:A6:701:GNP:H2'	1.79	0.47
1:A1:70:ILE:HD11	1:A1:86:VAL:HG23	1.95	0.47
10:E2:155:LYS:NZ	34:22:244:A:OP1	2.48	0.47
34:22:987:G:N2	34:22:1013:A:OP1	2.47	0.47
34:22:1163:A:N3	34:22:1613:U:O2'	2.44	0.47
36:14:2406:C:O2'	36:14:2619:G:N2	2.43	0.47
36:14:3027:A:H1'	80:A6:256:ARG:HH22	1.79	0.47
47:e5:100:ILE:O	47:e5:125:ARG:NH1	2.46	0.47
2:A2:198:MET:HG2	2:A2:200:ASP:H	1.79	0.47
6:C2:188:LEU:HD13	6:C2:196:VAL:HG11	1.96	0.47
15:H2:13:PRO:HA	15:H2:14:THR:HA	1.56	0.47
17:J2:17:ARG:NH1	34:22:4:C:O2'	2.38	0.47
32:Y2:60:PHE:H	32:Y2:71:GLY:HA2	1.79	0.47
36:14:1156:C:OP2	49:F5:94:LYS:NZ	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:31:VAL:HG12	2:A2:33:GLN:H	1.78	0.47
12:F2:192:GLU:OE1	33:Z2:63:SER:HB2	2.14	0.47
16:I2:64:ASN:ND2	34:22:257:A:N3	2.62	0.47
34:22:766:U:H5'	34:22:767:U:H5''	1.97	0.47
34:22:1537:C:O2'	34:22:1540:G:O6	2.33	0.47
36:14:3375:A:O2'	36:14:3378:C:OP2	2.32	0.47
43:c5:24:THR:HG23	43:c5:30:THR:HG22	1.95	0.47
70:V5:15:LEU:HD23	70:V5:53:SER:HB3	1.96	0.47
1:A1:176:LYS:HE3	80:A6:222:GLN:N	2.29	0.47
4:B2:87:ARG:NH1	4:B2:220:GLN:OE1	2.47	0.47
4:B2:144:ARG:NH2	4:B2:207:LEU:O	2.48	0.47
23:P2:126:VAL:HG21	34:22:1459:C:C4'	2.44	0.47
36:14:910:G:O6	40:A5:3:ARG:NH1	2.48	0.47
36:14:1595:U:O2'	36:14:1606:U:O2	2.33	0.47
2:A2:52:LYS:HE2	29:V2:82:VAL:HA	1.96	0.47
12:F2:127:GLN:HE22	12:F2:199:ILE:HG12	1.80	0.47
14:g2:38:ARG:HA	14:g2:67:ILE:HG23	1.97	0.47
17:J2:61:THR:HA	30:W2:97:ARG:HH22	1.80	0.47
23:P2:79:HIS:HD2	23:P2:102:PHE:HE1	1.61	0.47
34:22:632:U:O2'	34:22:1103:U:OP1	2.32	0.47
36:14:118:U:O4	36:14:148:G:N2	2.45	0.47
36:14:1694:U:H3	36:14:1752:A:H61	1.62	0.47
38:44:154:C:H5''	51:G5:181:LYS:HE2	1.95	0.47
44:C5:181:VAL:HG12	44:C5:182:LEU:HD12	1.96	0.47
44:C5:295:ILE:HD11	67:Q5:129:VAL:HA	1.96	0.47
47:e5:73:THR:OG1	47:e5:95:GLU:OE1	2.33	0.47
53:H5:19:SER:HB2	53:H5:26:LYS:HB3	1.95	0.47
53:H5:90:MET:HE2	53:H5:179:ILE:HG22	1.97	0.47
80:A6:332:LEU:HD22	80:A6:348:TRP:HH2	1.80	0.47
1:A1:67:ILE:HG22	1:A1:87:THR:HG22	1.97	0.47
16:I2:70:GLU:HG2	16:I2:112:TRP:HH2	1.79	0.47
36:14:1943:C:H5'	36:14:3346:U:H4'	1.96	0.47
36:14:2400:G:O6	36:14:2401:A:N6	2.48	0.47
36:14:3004:C:O2'	42:B5:99:LEU:O	2.31	0.47
53:H5:96:HIS:CE1	80:A6:280:THR:CG2	2.97	0.47
65:p5:51:ALA:HB3	65:p5:54:ILE:HD12	1.96	0.47
11:e2:10:ARG:NH1	34:22:566:C:O2'	2.48	0.47
16:I2:178:ARG:NH1	34:22:207:U:O2	2.42	0.47
34:22:1482:C:OP2	34:22:1521:G:N2	2.40	0.47
36:14:1419:A:H3'	44:C5:193:LYS:HZ2	1.79	0.47
36:14:1793:C:O2	40:A5:174:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:14:2163:C:H4'	40:A5:8:GLN:HA	1.97	0.47
36:14:3042:U:OP2	36:14:3092:C:N4	2.48	0.47
42:B5:71:GLU:OE2	79:W5:1:MET:N	2.48	0.47
44:C5:150:LEU:HD21	44:C5:172:VAL:HG11	1.96	0.47
49:F5:151:ARG:NH1	49:F5:206:LYS:O	2.48	0.47
71:Z5:95:VAL:HG21	71:Z5:113:VAL:HG11	1.97	0.47
9:d2:14:TYR:OH	34:22:1555:A:N6	2.47	0.47
12:F2:43:PHE:HB3	12:F2:46:TRP:HB2	1.97	0.47
17:J2:139:GLN:NE2	32:Y2:64:PHE:O	2.48	0.47
19:L2:113:PRO:O	19:L2:116:ARG:NH2	2.45	0.47
22:O2:16:VAL:HG12	22:O2:80:HIS:HB2	1.97	0.47
23:P2:98:ASN:ND2	23:P2:121:ILE:O	2.48	0.47
27:T2:63:ARG:NH2	34:22:1480:G:OP1	2.48	0.47
36:14:2510:U:H2'	36:14:2511:A:H8	1.80	0.47
36:14:3273:A:OP2	78:E5:77:ARG:NH2	2.48	0.47
78:E5:40:LEU:HD13	78:E5:84:VAL:HG11	1.96	0.47
8:D2:71:LEU:HD22	8:D2:75:LYS:HE3	1.97	0.46
34:22:610:G:HO2'	34:22:613:G:HO2'	1.63	0.46
39:a5:76:ASP:HB3	67:Q5:92:ARG:HG2	1.98	0.46
44:C5:35:VAL:HG11	44:C5:244:LEU:HD21	1.96	0.46
55:I5:46:PHE:HB2	55:I5:139:ARG:HH11	1.79	0.46
62:M5:113:THR:OG1	78:E5:176:PHE:O	2.33	0.46
6:C2:175:GLY:N	6:C2:195:ASP:OD2	2.47	0.46
10:E2:66:MET:SD	10:E2:78:THR:OG1	2.74	0.46
34:22:992:A:O2'	34:22:1785:U:O2	2.32	0.46
36:14:1455:U:O3'	46:d5:26:LYS:NZ	2.49	0.46
36:14:1863:G:N1	36:14:1866:C:OP2	2.44	0.46
36:14:2631:U:OP2	77:T5:4:SER:OG	2.30	0.46
36:14:2889:C:HO2'	36:14:2934:A:HO2'	1.62	0.46
38:44:126:A:O2'	38:44:129:C:N4	2.48	0.46
66:P5:177:ALA:HA	66:P5:180:LYS:HE3	1.96	0.46
80:A6:305:ILE:HD13	80:A6:588:ARG:HH12	1.80	0.46
10:E2:185:GLY:H	10:E2:189:LEU:HD13	1.79	0.46
31:X2:18:HIS:O	31:X2:22:ASN:ND2	2.49	0.46
34:22:40:A:H62	34:22:467:G:H21	1.62	0.46
34:22:1657:U:H5''	34:22:1658:G:H5''	1.96	0.46
36:14:2666:C:OP2	36:14:2687:G:N1	2.47	0.46
45:D5:15:ARG:HA	77:T5:20:ARG:HD3	1.98	0.46
24:Q2:90:VAL:HG11	24:Q2:117:LEU:HD21	1.98	0.46
25:R2:18:GLU:HA	25:R2:71:PHE:HA	1.97	0.46
33:Z2:74:SER:N	34:22:1534:G:C8	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:22:1191:U:C2	82:A3:34:OMG:C5'	2.98	0.46
36:14:591:G:O2'	78:E5:17:ALA:O	2.31	0.46
36:14:658:G:N2	44:C5:93:MET:O	2.42	0.46
36:14:1588:A:N3	59:I5:4:GLN:NE2	2.63	0.46
40:A5:136:ILE:HG13	40:A5:148:VAL:HG12	1.98	0.46
74:R5:31:GLU:HG3	74:R5:44:LEU:HD21	1.97	0.46
20:M2:46:ARG:HH22	34:22:1253:U:H3'	1.81	0.46
21:N2:86:GLU:OE2	34:22:961:U:O2'	2.30	0.46
25:R2:7:LYS:HE2	25:R2:11:ARG:HE	1.80	0.46
34:22:1533:C:N4	34:22:1534:G:O6	2.48	0.46
36:14:807:A:H61	36:14:934:G:H22	1.64	0.46
36:14:1863:G:H4'	74:R5:82:LYS:HD3	1.97	0.46
37:34:62:U:O4	37:34:63:A:N6	2.49	0.46
44:C5:207:VAL:HB	44:C5:227:THR:HG22	1.98	0.46
53:H5:94:TYR:OH	53:H5:141:LYS:NZ	2.49	0.46
63:N5:35:VAL:HA	63:N5:65:ARG:HD3	1.98	0.46
63:N5:84:PRO:HA	63:N5:87:GLN:HB2	1.97	0.46
80:A6:149:THR:OG1	80:A6:433:GLY:O	2.32	0.46
80:A6:175:HIS:O	80:A6:180:LYS:NZ	2.40	0.46
5:b2:52:THR:OG1	21:N2:56:ASP:OD2	2.28	0.46
19:L2:83:THR:HG21	34:22:325:G:H4'	1.97	0.46
36:14:896:A:H5'	40:A5:183:GLY:HA2	1.97	0.46
36:14:1493:G:OP2	36:14:1493:G:N2	2.47	0.46
36:14:1963:G:H1	36:14:2059:U:H3	1.62	0.46
56:J5:32:ARG:NH1	56:J5:120:ILE:O	2.42	0.46
72:K5:109:PRO:HG2	72:K5:112:TYR:HB2	1.98	0.46
26:S2:101:LEU:H	26:S2:104:ASN:HB3	1.81	0.46
30:W2:56:HIS:O	34:22:861:U:O2'	2.33	0.46
32:Y2:124:ARG:NH2	34:22:151:G:O6	2.49	0.46
36:14:693:A:OP1	44:C5:45:ASN:ND2	2.48	0.46
36:14:2901:G:O2'	36:14:3024:A:N1	2.47	0.46
36:14:2945:G:OP1	36:14:2945:G:N2	2.48	0.46
49:F5:135:ALA:HB2	49:F5:229:PHE:HA	1.98	0.46
55:I5:52:LEU:HB2	55:I5:152:LEU:HD23	1.97	0.46
70:V5:58:VAL:O	70:V5:76:ALA:N	2.49	0.46
80:A6:351:ILE:HD13	80:A6:377:LEU:HD22	1.98	0.46
1:A1:176:LYS:HE3	80:A6:222:GLN:C	2.41	0.46
5:b2:67:THR:OG1	5:b2:70:LYS:O	2.33	0.46
6:C2:116:LYS:HB2	6:C2:131:ILE:HD12	1.98	0.46
36:14:798:G:OP1	39:a5:33:GLY:N	2.47	0.46
36:14:952:A:N3	36:14:1114:U:O2'	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:14:974:G:OP1	67:Q5:16:ARG:NE	2.42	0.46
36:14:1899:G:O2'	36:14:2334:U:O4	2.29	0.46
36:14:3334:U:O2	36:14:3368:U:O2'	2.34	0.46
39:a5:81:LEU:HD11	39:a5:107:ALA:HB2	1.98	0.46
46:d5:20:LEU:HD11	46:d5:32:ALA:HB2	1.97	0.46
54:i5:74:LYS:HD3	54:i5:80:PHE:HD1	1.81	0.46
56:J5:55:ARG:CZ	82:A3:20:G:H22	2.27	0.46
12:F2:189:THR:OG1	33:Z2:98:GLN:NE2	2.49	0.46
15:H2:162:ILE:HG22	15:H2:165:LYS:HD2	1.98	0.46
16:I2:50:GLY:HA2	34:22:397:A:H4'	1.98	0.46
20:M2:52:LEU:HD11	20:M2:60:VAL:HG11	1.96	0.46
20:M2:97:LEU:HD22	20:M2:119:SER:H	1.81	0.46
36:14:590:G:H4'	44:C5:309:ARG:HH12	1.81	0.46
45:D5:60:ILE:HB	45:D5:80:SER:HB3	1.98	0.46
56:J5:55:ARG:CZ	82:A3:20:G:C2	2.99	0.46
66:P5:41:LEU:HD12	66:P5:150:VAL:HG11	1.98	0.46
78:E5:35:VAL:HG21	78:E5:90:LYS:HE2	1.98	0.46
4:B2:137:ILE:HD11	4:B2:172:LEU:HB3	1.97	0.46
6:C2:142:GLY:N	6:C2:153:SER:O	2.44	0.46
14:g2:149:ASP:OD2	25:R2:23:LYS:NZ	2.40	0.46
24:Q2:17:THR:OG1	24:Q2:70:THR:OG1	2.33	0.46
26:S2:82:PRO:HB2	26:S2:84:TRP:CD1	2.51	0.46
31:X2:73:ARG:HH21	31:X2:82:LYS:HB3	1.81	0.46
36:14:2483:G:N2	36:14:2486:A:OP2	2.40	0.46
36:14:3004:C:H4'	42:B5:99:LEU:HB2	1.97	0.46
48:f5:16:TYR:OH	48:f5:89:LEU:O	2.32	0.46
3:a2:4:LYS:HG3	3:a2:5:ARG:HG3	1.98	0.45
13:G2:175:ILE:HD13	34:22:78:A:H1'	1.98	0.45
20:M2:60:VAL:HG22	20:M2:122:VAL:HG22	1.98	0.45
26:S2:30:TYR:OH	34:22:1539:G:O4'	2.31	0.45
31:X2:69:ARG:HG3	31:X2:117:ILE:HG12	1.98	0.45
31:X2:143:PRO:HG3	80:A6:484:GLU:HB2	1.98	0.45
34:22:1352:G:N2	34:22:1373:C:O2	2.41	0.45
36:14:727:G:OP2	36:14:742:G:N2	2.47	0.45
42:B5:77:THR:HG21	42:B5:328:ILE:HG22	1.97	0.45
44:C5:23:PRO:HG2	44:C5:258:LEU:HD23	1.98	0.45
70:V5:18:PRO:HA	70:V5:51:ALA:HA	1.96	0.45
8:D2:23:GLU:HB3	18:K2:61:TRP:HE1	1.81	0.45
9:d2:34:TYR:OH	34:22:1487:A:OP1	2.34	0.45
31:X2:6:PRO:HG3	31:X2:14:LYS:HD3	1.97	0.45
31:X2:25:ALA:HB1	34:22:1108:G:H2'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:X2:69:ARG:HB3	31:X2:86:PHE:HE1	1.82	0.45
36:14:728:G:H5''	67:Q5:43:PRO:HB2	1.97	0.45
36:14:1778:G:O2'	36:14:1780:G:OP2	2.33	0.45
36:14:2843:U:H5''	36:14:2844:C:H5	1.81	0.45
38:44:111:A:H1'	57:j5:17:THR:HG21	1.98	0.45
62:M5:38:ILE:HG13	62:M5:44:VAL:HG12	1.98	0.45
30:W2:41:MET:HG2	30:W2:129:VAL:HG11	1.97	0.45
34:22:47:A:N7	34:22:98:U:O2'	2.47	0.45
35:f2:140:TYR:OH	35:f2:145:HIS:O	2.34	0.45
36:14:1055:A:N3	37:34:81:U:O2'	2.44	0.45
36:14:2389:C:H5''	66:P5:66:SER:HA	1.98	0.45
65:p5:7:LYS:O	65:p5:27:LYS:NZ	2.48	0.45
66:P5:61:ARG:HG2	66:P5:78:VAL:HG21	1.97	0.45
80:A6:447:VAL:HG21	80:A6:476:LEU:HD22	1.96	0.45
10:E2:85:GLY:N	10:E2:88:ASP:OD2	2.44	0.45
15:H2:51:VAL:HG23	15:H2:53:GLY:H	1.80	0.45
26:S2:116:LEU:HB3	26:S2:124:GLY:HA3	1.98	0.45
33:Z2:74:SER:CB	34:22:1534:G:OP2	2.63	0.45
36:14:499:G:OP1	48:f5:48:ARG:NH1	2.50	0.45
36:14:1962:G:H1'	36:14:2080:C:H42	1.80	0.45
36:14:2944:U:O2'	42:B5:251:CYS:SG	2.70	0.45
36:14:3129:A:N6	36:14:3131:U:O2	2.49	0.45
45:D5:99:TYR:HE2	45:D5:244:HIS:HE1	1.63	0.45
49:F5:186:HIS:O	49:F5:190:THR:OG1	2.29	0.45
50:g5:5:VAL:HG21	50:g5:31:ARG:HA	1.98	0.45
10:E2:45:ILE:HG13	10:E2:61:VAL:HG21	1.98	0.45
15:H2:64:VAL:HG22	15:H2:94:ALA:HB1	1.98	0.45
16:I2:159:GLN:HE22	16:I2:189:LEU:HD11	1.81	0.45
24:Q2:16:ALA:HB2	24:Q2:72:GLY:HA3	1.98	0.45
34:22:720:G:N2	34:22:720:G:OP2	2.49	0.45
36:14:129:U:H3	36:14:139:G:H1	1.65	0.45
52:h5:28:LEU:HB3	52:h5:32:LYS:HE2	1.98	0.45
15:H2:148:LYS:NZ	34:22:640:U:O2'	2.50	0.45
23:P2:108:ARG:HH21	26:S2:119:ILE:HA	1.81	0.45
31:X2:62:LYS:NZ	34:22:1136:U:OP1	2.45	0.45
33:Z2:73:GLY:HA3	34:22:1534:G:N9	2.31	0.45
34:22:895:G:H1	34:22:917:U:H3	1.63	0.45
36:14:337:G:H1	38:44:26:U:H3	1.65	0.45
36:14:371:G:N1	36:14:374:A:OP2	2.46	0.45
36:14:1846:C:OP1	36:14:1849:C:N4	2.44	0.45
36:14:3184:A:O2'	53:H5:23:ARG:NH1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:14:3212:C:OP2	62:M5:124:ARG:NH2	2.50	0.45
37:34:14:U:OP1	45:D5:24:ARG:NH1	2.50	0.45
42:B5:183:LEU:O	42:B5:191:LYS:NZ	2.45	0.45
53:H5:23:ARG:HD2	53:H5:39:LYS:HA	1.98	0.45
55:I5:30:LYS:HG3	55:I5:63:GLU:HG3	1.99	0.45
2:A2:50:VAL:H	25:R2:109:LEU:HD21	1.80	0.45
13:G2:102:VAL:HG13	13:G2:106:LEU:HD12	1.98	0.45
16:I2:78:ILE:HG12	16:I2:104:ILE:HG22	1.99	0.45
34:22:1208:A:O2'	34:22:1270:G:OP2	2.34	0.45
34:22:1445:G:N2	35:f2:89:LYS:O	2.49	0.45
36:14:1257:C:H42	36:14:1261:G:H22	1.64	0.45
36:14:2406:C:HO2'	36:14:2619:G:H21	1.63	0.45
36:14:2737:C:O2'	41:b5:36:ASP:OD1	2.32	0.45
36:14:2895:G:O2'	61:m5:100:TYR:O	2.33	0.45
37:34:17:A:OP1	45:D5:2:ALA:N	2.49	0.45
53:H5:90:MET:HG2	53:H5:181:VAL:HA	1.98	0.45
77:T5:92:ARG:HB3	77:T5:95:HIS:HD2	1.81	0.45
1:A1:33:GLN:NE2	1:A1:321:ASP:OD2	2.50	0.45
5:b2:20:LYS:NZ	34:22:959:U:OP2	2.50	0.45
12:F2:101:GLY:H	34:22:1166:A:H5''	1.82	0.45
13:G2:190:GLN:NE2	34:22:265:A:N7	2.64	0.45
14:g2:232:TYR:OH	14:g2:268:GLN:NE2	2.50	0.45
16:I2:4:SER:HB2	16:I2:24:LYS:HE2	1.98	0.45
31:X2:107:PHE:HE1	31:X2:123:LYS:HB3	1.81	0.45
36:14:1201:C:N4	36:14:2857:C:OP1	2.46	0.45
36:14:1235:U:H4'	36:14:1236:G:H5'	1.99	0.45
36:14:1705:U:O2	36:14:1786:G:O2'	2.34	0.45
36:14:3272:C:H5'	78:E5:78:ARG:HB2	1.99	0.45
75:X5:75:LYS:HB3	75:X5:81:ILE:HB	1.98	0.45
80:A6:258:PHE:HD1	80:A6:261:ASN:HD22	1.63	0.45
1:A1:68:LYS:N	1:A1:86:VAL:O	2.50	0.45
7:c2:65:ARG:NH2	81:X7:10:G:OP2	2.49	0.45
19:L2:102:LYS:O	31:X2:13:ARG:NH2	2.46	0.45
34:22:996:U:H3	34:22:1008:G:H1	1.65	0.45
36:14:1210:U:H5''	53:H5:62:ARG:HD3	1.99	0.45
36:14:2149:A:N6	36:14:2187:G:O2'	2.47	0.45
71:Z5:33:SER:HB2	71:Z5:40:HIS:HE1	1.82	0.45
7:c2:15:VAL:HG23	7:c2:28:VAL:HG22	1.99	0.45
10:E2:77:ARG:NH2	34:22:122:U:O3'	2.50	0.45
34:22:473:A:H5'	34:22:769:A:H1'	1.98	0.45
34:22:898:A:N6	34:22:914:G:O2'	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:14:696:C:OP2	44:C5:119:ARG:NH2	2.50	0.45
36:14:999:G:N3	36:14:1002:A:N6	2.65	0.45
36:14:1242:G:N2	36:14:1270:A:O2'	2.50	0.45
36:14:1553:U:H5''	36:14:1554:U:H5'	1.99	0.45
42:B5:47:LEU:HB3	42:B5:335:ILE:HD11	1.99	0.45
42:B5:57:VAL:HG22	42:B5:73:VAL:HG12	1.98	0.45
42:B5:232:ARG:NH1	42:B5:266:ARG:O	2.49	0.45
61:m5:97:ARG:HE	61:m5:122:ARG:HB3	1.82	0.45
68:S5:66:GLU:HB3	68:S5:69:PRO:HG3	1.98	0.45
78:E5:39:VAL:HG11	78:E5:158:TYR:HE2	1.83	0.45
3:a2:22:ARG:NH2	22:O2:131:GLY:O	2.50	0.44
10:E2:23:LEU:HD21	17:J2:6:ARG:HH12	1.81	0.44
10:E2:64:ILE:HD11	32:Y2:18:LEU:HD11	1.99	0.44
12:F2:182:ALA:O	12:F2:186:ASN:ND2	2.39	0.44
34:22:163:G:OP2	34:22:163:G:N2	2.47	0.44
36:14:733:G:N2	36:14:736:A:OP2	2.42	0.44
36:14:1048:A:H2'	55:I5:22:TYR:HE2	1.82	0.44
48:f5:67:MET:HE1	48:f5:90:PRO:HD3	1.98	0.44
53:H5:20:ILE:HG13	53:H5:25:VAL:HA	1.99	0.44
55:I5:29:SER:HB2	55:I5:125:LEU:HD12	1.98	0.44
14:g2:220:ILE:HB	14:g2:234:LEU:HB2	1.99	0.44
17:J2:78:ARG:NH1	34:22:763:G:OP1	2.50	0.44
34:22:1085:G:N2	34:22:1088:A:OP2	2.43	0.44
36:14:532:A:N6	36:14:555:U:O2	2.50	0.44
43:c5:25:LEU:O	43:c5:29:SER:OG	2.35	0.44
49:F5:96:PRO:HB2	49:F5:99:PRO:HD2	2.00	0.44
62:M5:20:VAL:HB	62:M5:70:PHE:HE1	1.83	0.44
75:X5:96:LYS:HG3	75:X5:107:VAL:HB	2.00	0.44
6:C2:97:ARG:NH2	34:22:1301:U:OP2	2.50	0.44
8:D2:54:ARG:CD	80:A6:23:ASP:OD2	2.65	0.44
12:F2:112:ARG:NH1	34:22:1529:C:OP1	2.49	0.44
20:M2:51:ALA:HB1	20:M2:57:ALA:HB2	2.00	0.44
25:R2:102:VAL:HG21	25:R2:119:LEU:HG	1.99	0.44
36:14:674:G:O6	67:Q5:56:LYS:NZ	2.49	0.44
36:14:2144:A:H1'	36:14:2281:A:H61	1.82	0.44
36:14:3116:G:OP1	36:14:3116:G:N2	2.41	0.44
36:14:3277:U:O4	66:P5:172:GLN:NE2	2.50	0.44
51:G5:171:LYS:NZ	51:G5:223:ALA:O	2.50	0.44
63:N5:120:TRP:HE1	63:N5:123:GLN:HB3	1.82	0.44
70:V5:93:LEU:HB3	79:W5:20:LEU:HB3	1.99	0.44
1:A1:146:VAL:HG23	1:A1:153:HIS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G2:74:LYS:HB3	13:G2:94:ARG:HG2	1.98	0.44
34:22:538:A:O2'	34:22:539:G:O4'	2.36	0.44
36:14:1184:A:H5''	62:M5:59:ASN:HD22	1.82	0.44
36:14:1419:A:OP1	38:44:20:U:O2'	2.32	0.44
36:14:1875:G:N7	74:R5:20:ARG:NH2	2.65	0.44
36:14:2631:U:OP1	36:14:2757:U:O2'	2.33	0.44
44:C5:283:THR:HB	44:C5:289:ILE:HD11	2.00	0.44
51:G5:133:LYS:HD2	51:G5:138:HIS:HE1	1.83	0.44
57:j5:19:CYS:O	59:l5:8:ARG:NH2	2.47	0.44
1:A1:264:LYS:HB3	1:A1:281:ILE:HG12	1.99	0.44
10:E2:22:LYS:NZ	34:22:758:U:OP1	2.50	0.44
19:L2:2:SER:HA	19:L2:113:PRO:HB3	1.98	0.44
22:O2:30:VAL:HG13	22:O2:39:ILE:HG13	2.00	0.44
34:22:1005:A:O2'	34:22:1784:C:O2'	2.34	0.44
36:14:2406:C:HO2'	36:14:2619:G:N2	2.14	0.44
44:C5:263:GLY:HA3	44:C5:269:SER:HA	1.98	0.44
48:f5:6:ARG:NH1	48:f5:8:TYR:O	2.51	0.44
51:G5:187:GLY:HA2	51:G5:190:VAL:HG12	2.00	0.44
52:h5:85:THR:HG23	52:h5:88:LEU:H	1.82	0.44
8:D2:24:PHE:HZ	8:D2:72:LEU:HD13	1.82	0.44
8:D2:160:SER:OG	34:22:1329:A:OP2	2.31	0.44
21:N2:66:ILE:HG23	21:N2:67:THR:HG23	2.00	0.44
23:P2:96:ILE:O	23:P2:102:PHE:HA	2.17	0.44
25:R2:24:LEU:HD21	25:R2:34:LEU:HD22	1.99	0.44
36:14:2898:G:N7	61:m5:125:LYS:NZ	2.66	0.44
42:B5:19:ARG:HB2	42:B5:232:ARG:HH21	1.81	0.44
10:E2:3:ARG:NH2	34:22:94:U:OP2	2.50	0.44
23:P2:22:LEU:HD23	23:P2:25:LEU:HD12	1.99	0.44
34:22:286:C:N4	34:22:287:G:O6	2.50	0.44
36:14:627:U:H4'	36:14:1399:A:H1'	1.99	0.44
36:14:2454:G:O6	36:14:2484:A:N6	2.41	0.44
46:d5:75:ILE:HG12	46:d5:93:VAL:HG22	2.00	0.44
50:g5:13:TYR:O	50:g5:18:ASN:ND2	2.51	0.44
1:A1:66:LYS:HB3	1:A1:96:ASN:HD21	1.83	0.44
1:A1:119:LYS:NZ	1:A1:126:MET:SD	2.90	0.44
15:H2:101:LYS:HD2	34:22:639:U:H5''	2.00	0.44
23:P2:123:TYR:O	23:P2:123:TYR:CD2	2.70	0.44
30:W2:2:THR:N	34:22:1034:C:O2'	2.44	0.44
34:22:417:A:O2'	34:22:418:G:OP2	2.32	0.44
34:22:1151:A:O3'	34:22:1766:A:N6	2.51	0.44
34:22:1793:G:H1'	34:22:1794:A:H2'	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:B5:80:ASP:OD2	42:B5:314:TYR:OH	2.35	0.44
52:h5:101:THR:HG23	52:h5:104:GLN:H	1.83	0.44
75:X5:77:GLU:HG2	75:X5:133:LEU:HD12	2.00	0.44
77:T5:30:TYR:OH	77:T5:94:GLU:OE2	2.30	0.44
78:E5:149:ILE:HG12	78:E5:155:LEU:HD12	2.00	0.44
80:A6:521:PRO:HG3	80:A6:541:LEU:HD13	2.00	0.44
1:A1:170:TYR:HB3	1:A1:187:LYS:HE2	1.99	0.44
36:14:147:U:O4	51:G5:183:LYS:NZ	2.45	0.44
36:14:1779:C:N4	74:R5:88:ARG:O	2.51	0.44
36:14:2196:C:O2'	36:14:2270:A:N3	2.44	0.44
36:14:2515:A:O3'	63:N5:31:ARG:NH2	2.51	0.44
45:D5:95:TRP:HD1	45:D5:158:ARG:HA	1.82	0.44
53:H5:20:ILE:HG22	53:H5:22:SER:H	1.82	0.44
75:X5:111:ASN:HB2	75:X5:123:TYR:HB2	2.00	0.44
78:E5:101:PHE:HZ	78:E5:137:ASP:HB3	1.83	0.44
12:F2:50:GLU:HA	12:F2:65:ARG:HH22	1.83	0.43
12:F2:93:LEU:HD23	12:F2:172:ILE:HG23	1.99	0.43
23:P2:126:VAL:HG21	34:22:1459:C:O4'	2.18	0.43
31:X2:126:LYS:HE2	31:X2:129:GLY:HA2	2.00	0.43
36:14:28:C:OP1	63:N5:192:LYS:NZ	2.38	0.43
36:14:1050:U:OP2	77:T5:13:TYR:OH	2.26	0.43
36:14:3241:G:OP2	42:B5:153:LYS:NZ	2.47	0.43
45:D5:107:ARG:HG3	45:D5:251:PRO:HG3	2.00	0.43
70:V5:15:LEU:HD13	70:V5:51:ALA:HB3	2.00	0.43
80:A6:174:GLY:HA2	80:A6:274:LEU:HD12	1.99	0.43
2:A2:69:ASN:OD1	6:C2:244:SER:OG	2.36	0.43
8:D2:54:ARG:HD2	80:A6:23:ASP:OD2	2.18	0.43
14:g2:42:LEU:HD11	14:g2:68:VAL:HG11	2.00	0.43
30:W2:11:LEU:HD23	30:W2:14:ILE:HD12	2.00	0.43
36:14:840:C:H5'	36:14:1724:U:H5	1.83	0.43
36:14:1001:G:O2'	36:14:1041:U:OP2	2.36	0.43
36:14:1388:U:O2'	47:e5:99:ASN:O	2.32	0.43
36:14:1447:G:N7	66:P5:25:SER:OG	2.50	0.43
36:14:3084:C:OP1	79:W5:38:SER:OG	2.32	0.43
56:J5:55:ARG:HH21	82:A3:20:G:H22	1.53	0.43
78:E5:154:LEU:HD23	78:E5:157:GLN:HE21	1.83	0.43
7:c2:18:ARG:NH2	34:22:1615:C:OP1	2.52	0.43
10:E2:37:LYS:HB2	10:E2:40:GLU:HG2	2.00	0.43
28:U2:70:THR:OG1	28:U2:72:ASN:OD1	2.36	0.43
34:22:1267:G:O2'	34:22:1448:G:O2'	2.35	0.43
42:B5:252:ILE:HG21	42:B5:260:VAL:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:I5:51:HIS:HB2	55:I5:166:ILE:HD11	1.99	0.43
56:J5:86:VAL:HG21	56:J5:111:ASP:HB3	2.00	0.43
80:A6:184:MET:HE2	80:A6:220:MET:HE3	2.00	0.43
8:D2:69:LEU:HD23	8:D2:72:LEU:HD12	1.99	0.43
31:X2:126:LYS:NZ	34:22:30:G:OP1	2.45	0.43
32:Y2:57:VAL:O	32:Y2:94:TYR:OH	2.36	0.43
34:22:56:U:O2'	34:22:57:G:O4'	2.33	0.43
34:22:1693:A:H61	34:22:1709:C:H42	1.67	0.43
36:14:2838:A:H4'	55:I5:74:LYS:HD2	2.00	0.43
40:A5:190:ARG:HG3	40:A5:191:LEU:HD12	1.99	0.43
62:M5:20:VAL:O	62:M5:66:THR:OG1	2.32	0.43
3:a2:51:ARG:NH2	7:c2:37:SER:O	2.51	0.43
14:g2:85:TRP:NE1	14:g2:111:MET:SD	2.91	0.43
34:22:460:A:H3'	34:22:461:G:H8	1.83	0.43
36:14:75:G:O3'	60:L5:70:ARG:NH2	2.49	0.43
36:14:1127:G:N2	36:14:1130:A:OP2	2.41	0.43
36:14:1868:G:N2	36:14:2118:C:O2	2.51	0.43
36:14:1959:G:H1	36:14:2082:U:H3	1.65	0.43
40:A5:45:VAL:HB	40:A5:61:VAL:HG22	2.01	0.43
68:S5:80:ARG:HE	77:T5:156:TYR:HB2	1.83	0.43
80:A6:255:HIS:HB2	80:A6:258:PHE:HD2	1.83	0.43
15:H2:107:ARG:NH1	34:22:741:C:O2	2.45	0.43
24:Q2:21:HIS:CE1	24:Q2:68:ARG:HH12	2.37	0.43
25:R2:44:LYS:HG3	25:R2:47:ARG:HH21	1.83	0.43
36:14:3368:U:H1'	36:14:3370:A:H1'	2.01	0.43
51:G5:99:PRO:HG2	51:G5:190:VAL:HG23	1.99	0.43
3:a2:80:HIS:CD2	81:X7:12:A:C2	3.07	0.43
34:22:1001:A:OP1	82:A3:38:A:O2'	2.36	0.43
34:22:1158:C:H1'	34:22:1161:C:H41	1.83	0.43
36:14:14:U:O2'	75:X5:42:ARG:NE	2.51	0.43
36:14:3086:A:O2'	42:B5:365:PHE:O	2.36	0.43
36:14:3386:G:OP1	46:d5:10:ARG:NH2	2.51	0.43
53:H5:89:LYS:HG2	53:H5:145:VAL:HG22	2.00	0.43
63:N5:62:TYR:HD2	63:N5:134:LEU:HD13	1.83	0.43
63:N5:104:GLU:HA	63:N5:160:GLU:HG3	2.01	0.43
76:Y5:119:ILE:HG22	76:Y5:124:GLY:HA3	2.00	0.43
2:A2:49:ASN:HD22	2:A2:52:LYS:HD2	1.83	0.43
14:g2:109:ASP:HB2	14:g2:127:ARG:HD2	2.01	0.43
15:H2:117:THR:OG1	34:22:638:U:O3'	2.35	0.43
22:O2:123:SER:HB2	34:22:885:G:H21	1.83	0.43
26:S2:2:SER:OG	26:S2:3:LEU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:22:1533:C:H4'	34:22:1539:G:C6	2.54	0.43
36:14:590:G:N1	36:14:611:A:OP2	2.51	0.43
36:14:805:G:N1	36:14:939:U:O4	2.51	0.43
36:14:2512:C:OP1	51:G5:249:ARG:NH1	2.46	0.43
36:14:3073:A:O2'	46:d5:62:ARG:NH2	2.52	0.43
52:h5:66:VAL:HG11	75:X5:50:ALA:HB1	2.00	0.43
14:g2:211:ILE:HB	14:g2:223:TRP:HB2	2.01	0.43
30:W2:26:LEU:HD21	30:W2:60:LYS:HD3	2.01	0.43
31:X2:103:LEU:N	31:X2:126:LYS:O	2.51	0.43
32:Y2:37:LYS:HG3	34:22:522:U:H5''	2.01	0.43
34:22:1542:G:N2	34:22:1568:C:O2'	2.47	0.43
36:14:938:C:O2	36:14:2813:A:O2'	2.37	0.43
36:14:938:C:H3'	39:a5:26:ARG:HH12	1.84	0.43
40:A5:134:VAL:HG12	40:A5:151:PRO:HD3	2.00	0.43
51:G5:165:PHE:HZ	63:N5:3:ALA:HB1	1.84	0.43
70:V5:38:ALA:HB3	70:V5:59:MET:HB2	2.00	0.43
36:14:3050:U:H4'	79:W5:17:ARG:HG3	2.01	0.43
42:B5:306:THR:HG21	42:B5:316:GLU:HG2	2.00	0.43
53:H5:10:ILE:HG12	53:H5:72:LYS:HG3	2.00	0.43
80:A6:419:ALA:HB3	80:A6:478:LEU:HB2	2.00	0.43
23:P2:42:ARG:NH2	34:22:1550:A:OP2	2.50	0.42
31:X2:106:GLY:H	34:22:599:A:H4'	1.84	0.42
32:Y2:9:THR:N	34:22:780:A:O2'	2.47	0.42
36:14:1796:G:H4'	40:A5:22:LEU:HD11	2.00	0.42
36:14:2948:C:H5''	42:B5:243:HIS:HB3	1.99	0.42
28:U2:50:LEU:HD21	28:U2:95:ALA:HB2	2.01	0.42
29:V2:78:LEU:HD12	29:V2:79:LEU:HD12	2.01	0.42
36:14:714:G:N7	39:a5:111:LYS:NZ	2.54	0.42
36:14:1152:G:OP2	36:14:1152:G:N2	2.49	0.42
36:14:2700:G:O2'	36:14:2705:A:N1	2.45	0.42
37:34:44:C:O2'	45:D5:152:ARG:NH1	2.52	0.42
1:A1:21:LEU:HD12	1:A1:22:PRO:HD2	2.01	0.42
34:22:23:G:O2'	34:22:368:U:OP1	2.37	0.42
34:22:1523:G:OP2	34:22:1523:G:N2	2.48	0.42
36:14:638:C:O2'	36:14:1434:G:N2	2.50	0.42
44:C5:22:LEU:HD23	44:C5:255:PHE:HZ	1.84	0.42
44:C5:126:ILE:HD11	44:C5:233:LEU:HD11	2.00	0.42
45:D5:294:ALA:HA	55:I5:217:PHE:HB3	2.02	0.42
80:A6:542:ILE:HB	80:A6:566:PHE:HB2	2.00	0.42
82:A3:58:1MA:O2'	82:A3:60:C:OP2	2.29	0.42
22:O2:24:ASN:ND2	34:22:902:G:N7	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:22:495:C:H3'	34:22:496:G:H4'	2.01	0.42
34:22:901:G:OP2	34:22:901:G:N2	2.43	0.42
36:14:421:G:O6	36:14:2383:C:O2'	2.30	0.42
36:14:585:A:H4'	48:f5:72:THR:HG22	2.01	0.42
36:14:2418:G:OP2	36:14:2606:G:N2	2.53	0.42
40:A5:101:VAL:HA	40:A5:165:VAL:HA	2.01	0.42
42:B5:223:GLY:HA2	42:B5:271:GLY:HA3	2.00	0.42
49:F5:178:ILE:HD11	49:F5:187:GLU:HG3	2.00	0.42
6:C2:139:ILE:HG12	6:C2:218:ILE:HB	2.01	0.42
10:E2:11:ARG:NH1	10:E2:21:ASP:OD1	2.53	0.42
33:Z2:61:SER:OG	33:Z2:62:VAL:N	2.52	0.42
36:14:2146:C:OP1	40:A5:200:ARG:NH1	2.50	0.42
42:B5:115:LYS:NZ	42:B5:129:ALA:O	2.51	0.42
42:B5:168:LYS:HB3	42:B5:319:ASN:HD21	1.84	0.42
44:C5:318:LEU:HD21	49:F5:145:ARG:HH12	1.83	0.42
6:C2:205:ARG:NH1	34:22:7:G:N7	2.67	0.42
15:H2:67:LEU:HD12	15:H2:70:PHE:HB2	2.02	0.42
20:M2:63:VAL:HG11	20:M2:94:ALA:HB2	2.02	0.42
26:S2:57:ARG:HH22	33:Z2:74:SER:HB2	1.83	0.42
26:S2:139:LYS:HD3	34:22:1177:C:H41	1.84	0.42
34:22:1191:U:O2	82:A3:34:OMG:C5'	2.66	0.42
36:14:408:A:N3	36:14:655:C:O2'	2.52	0.42
36:14:433:A:OP2	48:f5:57:LYS:NZ	2.41	0.42
36:14:520:U:O4	44:C5:349:THR:OG1	2.34	0.42
36:14:533:A:N6	36:14:535:G:N3	2.67	0.42
36:14:1307:G:O2'	36:14:1308:A:O5'	2.35	0.42
36:14:2525:G:N7	40:A5:67:TYR:OH	2.50	0.42
51:G5:229:VAL:HA	51:G5:232:HIS:HD2	1.85	0.42
53:H5:180:TYR:OH	61:m5:90:ASN:ND2	2.47	0.42
73:n5:2:ARG:HD3	73:n5:5:TRP:CD1	2.55	0.42
82:A3:18:G:O2'	82:A3:60:C:N4	2.52	0.42
1:A1:365:LEU:HD21	80:A6:521:PRO:HD2	2.01	0.42
1:A1:372:LEU:HD22	1:A1:376:LEU:HD12	2.00	0.42
2:A2:101:ARG:HG2	2:A2:103:THR:H	1.85	0.42
15:H2:49:ILE:HD11	15:H2:172:VAL:HG22	2.01	0.42
16:I2:22:ARG:HB3	34:22:385:A:H5''	2.01	0.42
34:22:628:G:H21	34:22:971:A:H62	1.66	0.42
36:14:589:A:N6	36:14:610:G:O2'	2.45	0.42
38:44:68:G:OP2	57:j5:85:LYS:NZ	2.53	0.42
40:A5:27:ALA:HB3	40:A5:128:ARG:HH21	1.85	0.42
42:B5:41:VAL:HA	42:B5:185:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:210:THR:HA	1:A1:245:MET:HB3	2.02	0.42
2:A2:140:ASN:ND2	29:V2:31:SER:O	2.42	0.42
9:d2:23:VAL:HG22	18:K2:61:TRP:HZ3	1.84	0.42
15:H2:139:ARG:HB2	15:H2:151:LYS:HB2	2.02	0.42
16:I2:184:LEU:HD23	16:I2:189:LEU:HA	2.02	0.42
21:N2:20:ARG:HH22	34:22:861:U:H4'	1.85	0.42
21:N2:97:SER:HA	21:N2:100:LYS:HE2	2.01	0.42
26:S2:81:ILE:HA	26:S2:82:PRO:HD3	1.89	0.42
30:W2:46:TYR:HB3	30:W2:69:LEU:HD13	2.01	0.42
34:22:593:U:H4'	34:22:595:G:H4'	2.00	0.42
36:14:623:U:H4'	48:f5:86:ARG:HH22	1.84	0.42
44:C5:326:ARG:HG3	44:C5:327:LEU:HD12	2.01	0.42
5:b2:56:CYS:SG	5:b2:57:GLU:N	2.93	0.42
7:c2:29:ARG:HA	7:c2:41:VAL:HA	2.02	0.42
10:E2:17:HIS:O	10:E2:51:ARG:NH2	2.52	0.42
13:G2:70:PRO:HA	13:G2:99:GLY:HA3	2.02	0.42
16:I2:110:ARG:HH22	36:14:3352:U:H3	1.68	0.42
19:L2:106:ASN:ND2	34:22:349:U:OP2	2.51	0.42
23:P2:130:ARG:H	23:P2:130:ARG:CD	2.11	0.42
26:S2:4:VAL:CG2	33:Z2:42:LEU:CD2	2.98	0.42
32:Y2:29:HIS:ND1	32:Y2:32:ARG:O	2.47	0.42
36:14:1463:U:H3	36:14:1467:A:H62	1.66	0.42
36:14:1920:U:O2'	36:14:1932:A:N7	2.46	0.42
80:A6:406:LEU:HD12	80:A6:423:GLY:HA2	2.02	0.42
80:A6:451:GLN:O	80:A6:475:THR:N	2.50	0.42
12:F2:187:ILE:HG22	33:Z2:63:SER:HA	2.02	0.42
22:O2:47:LYS:NZ	22:O2:62:LEU:O	2.53	0.42
30:W2:11:LEU:HD21	30:W2:37:PHE:HE2	1.85	0.42
30:W2:88:LYS:O	30:W2:92:ASN:ND2	2.53	0.42
34:22:1291:G:H1	34:22:1324:G:H22	1.66	0.42
36:14:691:A:N7	44:C5:48:GLN:NE2	2.67	0.42
36:14:3022:G:N7	80:A6:211:LYS:NZ	2.47	0.42
37:34:64:A:H5'	37:34:65:G:H5''	2.02	0.42
40:A5:147:ARG:HA	40:A5:157:VAL:HA	2.02	0.42
56:J5:55:ARG:CZ	82:A3:19:G:O2'	2.68	0.42
62:M5:28:SER:HB3	62:M5:31:LYS:HB2	2.01	0.42
66:P5:179:GLN:HA	66:P5:182:ILE:HD12	2.02	0.42
77:T5:92:ARG:HB3	77:T5:95:HIS:CD2	2.54	0.42
80:A6:405:VAL:HG13	80:A6:421:VAL:HG13	2.02	0.42
11:e2:11:ALA:O	31:X2:94:ASN:ND2	2.53	0.41
14:g2:255:ALA:HB2	14:g2:292:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:T2:60:SER:HB2	34:22:1479:A:H5''	2.02	0.41
36:14:824:C:H5''	40:A5:21:ARG:HG3	2.01	0.41
36:14:978:G:O2'	36:14:979:U:O2	2.38	0.41
36:14:2110:G:O2'	36:14:2112:U:OP2	2.37	0.41
38:44:142:C:OP1	63:N5:38:ARG:NH1	2.51	0.41
63:N5:35:VAL:HG12	63:N5:36:ILE:HG13	2.01	0.41
2:A2:121:VAL:HG23	2:A2:141:ILE:HG21	2.02	0.41
22:O2:61:MET:HG3	22:O2:100:ALA:HB1	2.02	0.41
34:22:646:C:H42	34:22:688:G:H1	1.68	0.41
36:14:2168:A:N6	36:14:2170:U:O2	2.53	0.41
36:14:2392:C:H1'	42:B5:266:ARG:HH21	1.84	0.41
36:14:2621:G:N2	82:A3:74:C:C4	2.88	0.41
38:44:83:C:O2'	38:44:85:G:N2	2.53	0.41
45:D5:34:LYS:HG2	77:T5:27:LEU:HD21	2.02	0.41
80:A6:594:LEU:HB2	80:A6:602:ALA:HB3	2.02	0.41
1:A1:148:GLN:HB2	1:A1:254:GLY:HA3	2.01	0.41
25:R2:27:ASP:O	25:R2:31:ASN:ND2	2.53	0.41
36:14:969:C:OP1	77:T5:82:ASN:ND2	2.53	0.41
36:14:1134:G:O2'	36:14:2642:A:N3	2.48	0.41
36:14:2592:G:H4'	36:14:2594:C:C2	2.55	0.41
51:G5:172:LYS:HD2	54:i5:39:PHE:HE1	1.86	0.41
71:Z5:27:LYS:HB3	71:Z5:42:LEU:HB2	2.01	0.41
74:R5:134:HIS:HE1	74:R5:136:ARG:HB3	1.85	0.41
80:A6:285:SER:HA	80:A6:289:LEU:HD12	2.01	0.41
1:A1:45:LYS:HD2	1:A1:107:PHE:HD1	1.85	0.41
1:A1:319:LEU:HB2	1:A1:351:VAL:HG22	2.01	0.41
13:G2:186:ARG:NH2	34:22:269:G:OP2	2.44	0.41
19:L2:57:LYS:NZ	34:22:326:G:OP1	2.49	0.41
34:22:1362:U:O2'	34:22:1363:U:O2	2.32	0.41
36:14:1751:G:OP1	58:k5:26:LYS:NZ	2.47	0.41
42:B5:161:LEU:HB3	42:B5:178:LEU:HD11	2.02	0.41
42:B5:216:ASP:HB2	42:B5:339:ARG:HB3	2.02	0.41
51:G5:178:ALA:HB2	51:G5:218:ILE:HD13	2.02	0.41
66:P5:122:ALA:HB3	66:P5:143:PRO:HG2	2.01	0.41
77:T5:66:ASN:O	77:T5:73:GLY:N	2.53	0.41
1:A1:210:THR:OG1	1:A1:245:MET:O	2.35	0.41
36:14:1750:A:O2'	36:14:1752:A:OP2	2.35	0.41
36:14:2150:G:O2'	36:14:2189:U:OP1	2.35	0.41
36:14:2178:A:H1'	36:14:2180:G:C6	2.56	0.41
36:14:3022:G:O5'	80:A6:213:SER:OG	2.33	0.41
38:44:97:A:O2'	52:h5:59:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:J5:13:LYS:HE3	56:J5:134:PRO:HG3	2.03	0.41
66:P5:67:ILE:HB	66:P5:80:LYS:HE2	2.02	0.41
14:g2:89:LEU:HD21	14:g2:110:VAL:HG11	2.03	0.41
14:g2:153:GLN:H	14:g2:172:ALA:HB3	1.86	0.41
21:N2:108:ASP:OD1	34:22:878:G:O2'	2.34	0.41
31:X2:57:LEU:HB3	31:X2:59:ILE:HG12	2.02	0.41
33:Z2:77:ARG:NH1	34:22:1533:C:C6	2.78	0.41
34:22:1502:G:N2	34:22:1505:A:OP2	2.50	0.41
36:14:209:A:N3	44:C5:221:ASN:ND2	2.69	0.41
36:14:426:G:H5'	47:e5:50:ILE:HG22	2.03	0.41
36:14:3009:G:O2'	42:B5:14:LEU:O	2.34	0.41
42:B5:215:ILE:HD11	42:B5:324:VAL:HG21	2.02	0.41
57:j5:34:CYS:SG	57:j5:35:SER:N	2.94	0.41
70:V5:104:ASN:OD1	70:V5:108:GLU:N	2.54	0.41
75:X5:105:VAL:HG21	75:X5:135:ILE:HD12	2.03	0.41
8:D2:7:LYS:HE2	28:U2:27:THR:HG21	2.03	0.41
12:F2:118:LEU:HD22	12:F2:129:PRO:HB2	2.01	0.41
14:g2:12:THR:HG22	14:g2:311:ARG:HG2	2.02	0.41
23:P2:29:SER:HB2	23:P2:32:ASP:HB2	2.02	0.41
28:U2:28:SER:HB2	28:U2:112:VAL:HG22	2.02	0.41
28:U2:41:ILE:HG23	28:U2:103:ILE:HD11	2.01	0.41
33:Z2:73:GLY:HA3	34:22:1534:G:C1'	2.51	0.41
34:22:1472:C:O2'	34:22:1534:G:N2	2.54	0.41
36:14:123:A:OP1	51:G5:105:LYS:NZ	2.40	0.41
36:14:1857:C:N4	36:14:1858:A:N1	2.69	0.41
36:14:3216:G:O2'	36:14:3219:G:O2'	2.25	0.41
44:C5:193:LYS:HA	44:C5:198:ARG:HA	2.03	0.41
51:G5:69:LEU:HD21	63:N5:24:ARG:HD2	2.03	0.41
51:G5:81:THR:HA	51:G5:222:PHE:HZ	1.85	0.41
4:B2:91:VAL:HA	4:B2:96:LEU:HA	2.03	0.41
5:b2:17:ARG:O	34:22:1070:C:O2'	2.38	0.41
12:F2:65:ARG:HA	12:F2:66:GLN:HA	1.86	0.41
12:F2:72:HIS:ND1	24:Q2:79:TYR:OH	2.39	0.41
13:G2:33:GLY:N	13:G2:52:ILE:O	2.53	0.41
15:H2:21:ALA:HA	15:H2:24:PHE:HD2	1.85	0.41
16:I2:159:GLN:O	16:I2:163:GLY:N	2.54	0.41
36:14:2186:U:O2'	36:14:2313:A:N3	2.47	0.41
36:14:2242:A:H5''	40:A5:244:GLY:HA3	2.02	0.41
44:C5:335:ALA:HA	44:C5:338:LYS:HA	2.02	0.41
55:I5:91:VAL:HG23	55:I5:135:ILE:HA	2.02	0.41
68:S5:124:LEU:HA	77:T5:153:PRO:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:164:ASN:HA	2:A2:170:ILE:HD11	2.03	0.41
4:B2:117:TRP:HE3	4:B2:153:HIS:HB3	1.85	0.41
8:D2:39:VAL:HG23	8:D2:48:VAL:HG22	2.02	0.41
8:D2:113:LEU:HD11	8:D2:117:ARG:HD2	2.03	0.41
10:E2:30:ARG:NH2	34:22:298:C:O2'	2.46	0.41
12:F2:70:VAL:HG23	12:F2:72:HIS:H	1.85	0.41
13:G2:13:GLN:NE2	34:22:151:G:N3	2.68	0.41
34:22:1297:G:N2	34:22:1300:A:OP2	2.41	0.41
36:14:1554:U:O2'	36:14:1555:U:O5'	2.36	0.41
36:14:1953:G:N1	36:14:2093:A:N7	2.68	0.41
36:14:2282:U:OP1	36:14:2973:G:O2'	2.38	0.41
36:14:3294:A:H5'	42:B5:128:LYS:HD3	2.03	0.41
37:34:79:A:H62	37:34:101:G:H21	1.67	0.41
38:44:104:A:OP1	57:j5:21:ARG:NH2	2.53	0.41
42:B5:92:TYR:HB2	42:B5:157:VAL:HG23	2.03	0.41
46:d5:13:THR:HG23	46:d5:72:ARG:HH11	1.85	0.41
55:I5:60:LEU:O	55:I5:127:ALA:N	2.52	0.41
56:J5:55:ARG:HD2	82:A3:20:G:C2	2.24	0.41
68:S5:80:ARG:HB3	68:S5:122:HIS:HB2	2.02	0.41
70:V5:79:VAL:HB	70:V5:118:VAL:HG22	2.03	0.41
74:R5:134:HIS:CE1	74:R5:136:ARG:HB3	2.56	0.41
76:Y5:68:GLY:HA2	76:Y5:84:LYS:HD2	2.03	0.41
80:A6:184:MET:HG2	80:A6:249:ILE:HD11	2.03	0.41
17:J2:143:ILE:HA	17:J2:144:PRO:HD3	1.89	0.41
24:Q2:13:LYS:HG3	24:Q2:14:LYS:H	1.85	0.41
26:S2:4:VAL:HG21	33:Z2:42:LEU:CD2	2.45	0.41
36:14:1970:U:H3	36:14:2052:G:H1	1.69	0.41
36:14:3068:U:OP2	74:R5:62:ARG:NH1	2.50	0.41
80:A6:263:ILE:HA	80:A6:266:ILE:HG12	2.01	0.41
1:A1:305:VAL:HG21	1:A1:368:ILE:HG22	2.02	0.40
5:b2:22:LYS:HG2	34:22:864:U:H3	1.86	0.40
34:22:648:G:H22	34:22:687:G:H1'	1.87	0.40
34:22:732:G:O2'	34:22:733:A:O4'	2.39	0.40
36:14:90:C:OP1	39:a5:59:ARG:NH1	2.47	0.40
36:14:1814:A:H4'	36:14:1815:U:H5'	2.03	0.40
52:h5:33:VAL:HG13	75:X5:141:TYR:HB3	2.03	0.40
56:J5:92:ARG:HH12	56:J5:94:ARG:HD2	1.85	0.40
62:M5:25:LYS:HE2	62:M5:62:GLN:HG2	2.03	0.40
80:A6:528:PHE:HB2	80:A6:593:VAL:HB	2.02	0.40
16:I2:36:THR:OG1	16:I2:59:ARG:N	2.54	0.40
17:J2:113:VAL:HG13	17:J2:118:LEU:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Y2:92:VAL:HG21	32:Y2:99:LYS:HD3	2.04	0.40
32:Y2:109:LYS:NZ	34:22:458:G:OP1	2.44	0.40
34:22:1561:U:H2'	34:22:1562:G:H8	1.85	0.40
36:14:627:U:H2'	36:14:628:A:C8	2.57	0.40
36:14:1474:A:O2'	46:d5:57:GLN:NE2	2.45	0.40
36:14:1486:G:H21	50:g5:6:THR:HG22	1.86	0.40
66:P5:114:VAL:HA	66:P5:150:VAL:HA	2.02	0.40
68:S5:8:GLN:HB3	68:S5:64:ILE:HD11	2.03	0.40
72:K5:77:SER:HB2	72:K5:104:VAL:HG12	2.02	0.40
15:H2:50:ASP:HA	15:H2:56:LYS:HA	2.03	0.40
27:T2:37:VAL:HG11	27:T2:100:ILE:HD11	2.03	0.40
36:14:53:G:OP2	57:j5:48:ASN:ND2	2.47	0.40
36:14:1284:C:O2'	36:14:1285:G:O4'	2.40	0.40
38:44:131:A:H2'	38:44:132:G:H8	1.87	0.40
40:A5:19:HIS:ND1	40:A5:190:ARG:O	2.42	0.40
47:e5:82:LEU:HD11	47:e5:112:ALA:HB2	2.03	0.40
51:G5:41:GLN:HB3	51:G5:44:ARG:HH12	1.86	0.40
56:J5:55:ARG:NH2	82:A3:20:G:H22	2.06	0.40
62:M5:23:ILE:HA	62:M5:63:VAL:HG23	2.03	0.40
66:P5:50:GLN:HB3	66:P5:55:GLN:HB3	2.03	0.40
80:A6:483:PRO:HA	80:A6:486:ILE:HD12	2.03	0.40
16:I2:8:ARG:HA	16:I2:18:ARG:HE	1.85	0.40
20:M2:97:LEU:HD13	20:M2:119:SER:HA	2.03	0.40
28:U2:103:ILE:HA	28:U2:106:ILE:HG22	2.03	0.40
34:22:29:U:H2'	34:22:30:G:H8	1.86	0.40
36:14:31:C:OP2	63:N5:187:ARG:NH2	2.47	0.40
36:14:153:U:H4'	36:14:158:G:H4'	2.03	0.40
36:14:2444:C:H42	36:14:2502:A:H61	1.69	0.40
45:D5:211:LEU:HB3	45:D5:219:PHE:HB2	2.03	0.40
51:G5:96:LYS:HB3	51:G5:204:ARG:HH12	1.86	0.40
60:L5:54:LEU:HD11	60:L5:119:TYR:CG	2.55	0.40
80:A6:144:LYS:HE2	80:A6:437:THR:HG21	2.03	0.40
1:A1:215:SER:HB2	1:A1:219:TYR:HB2	2.02	0.40
2:A2:71:GLU:HA	2:A2:95:ALA:H	1.87	0.40
4:B2:38:PHE:CG	4:B2:73:LEU:HD13	2.57	0.40
14:g2:3:SER:OG	14:g2:4:ASN:N	2.55	0.40
26:S2:11:PHE:CE1	33:Z2:41:ILE:HG13	2.56	0.40
36:14:23:A:OP1	57:j5:44:THR:N	2.51	0.40
36:14:1602:A:H5'	74:R5:37:SER:HA	2.04	0.40
63:N5:178:HIS:O	63:N5:181:ASN:ND2	2.55	0.40
80:A6:596:LYS:HG2	80:A6:601:ILE:HD13	2.02	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	
1	A1	379/381 (100%)	352 (93%)	27 (7%)	0	100	100
2	A2	205/207 (99%)	185 (90%)	19 (9%)	1 (0%)	24	55
3	a2	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
4	B2	212/214 (99%)	197 (93%)	15 (7%)	0	100	100
5	b2	79/81 (98%)	74 (94%)	5 (6%)	0	100	100
6	C2	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
7	c2	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
8	D2	221/223 (99%)	210 (95%)	11 (5%)	0	100	100
9	d2	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
10	E2	258/260 (99%)	233 (90%)	25 (10%)	0	100	100
11	e2	58/60 (97%)	55 (95%)	3 (5%)	0	100	100
12	F2	204/206 (99%)	182 (89%)	22 (11%)	0	100	100
13	G2	224/226 (99%)	204 (91%)	18 (8%)	2 (1%)	14	43
14	g2	316/318 (99%)	299 (95%)	17 (5%)	0	100	100
15	H2	182/184 (99%)	166 (91%)	16 (9%)	0	100	100
16	I2	184/199 (92%)	163 (89%)	21 (11%)	0	100	100
17	J2	183/185 (99%)	174 (95%)	9 (5%)	0	100	100
18	K2	94/96 (98%)	82 (87%)	12 (13%)	0	100	100
19	L2	153/155 (99%)	140 (92%)	13 (8%)	0	100	100
20	M2	122/124 (98%)	95 (78%)	27 (22%)	0	100	100
21	N2	148/150 (99%)	140 (95%)	8 (5%)	0	100	100
22	O2	125/127 (98%)	114 (91%)	11 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	P2	122/124 (98%)	113 (93%)	9 (7%)	0	100	100
24	Q2	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
25	R2	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
26	S2	143/145 (99%)	128 (90%)	14 (10%)	1 (1%)	18	49
27	T2	141/143 (99%)	135 (96%)	6 (4%)	0	100	100
28	U2	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
29	V2	85/87 (98%)	72 (85%)	13 (15%)	0	100	100
30	W2	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
31	X2	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
32	Y2	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
33	Z2	68/70 (97%)	68 (100%)	0	0	100	100
35	f2	69/71 (97%)	56 (81%)	13 (19%)	0	100	100
39	a5	146/148 (99%)	129 (88%)	16 (11%)	1 (1%)	18	49
40	A5	250/252 (99%)	235 (94%)	15 (6%)	0	100	100
41	b5	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
42	B5	384/386 (100%)	368 (96%)	16 (4%)	0	100	100
43	c5	95/97 (98%)	95 (100%)	0	0	100	100
44	C5	359/361 (99%)	330 (92%)	29 (8%)	0	100	100
45	D5	294/296 (99%)	281 (96%)	13 (4%)	0	100	100
46	d5	107/109 (98%)	99 (92%)	8 (8%)	0	100	100
47	e5	125/127 (98%)	118 (94%)	7 (6%)	0	100	100
48	f5	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
49	F5	220/222 (99%)	211 (96%)	7 (3%)	2 (1%)	14	43
50	g5	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
51	G5	231/233 (99%)	219 (95%)	12 (5%)	0	100	100
52	h5	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
53	H5	189/191 (99%)	173 (92%)	16 (8%)	0	100	100
54	i5	97/99 (98%)	89 (92%)	8 (8%)	0	100	100
55	I5	207/220 (94%)	201 (97%)	6 (3%)	0	100	100
56	J5	167/169 (99%)	155 (93%)	12 (7%)	0	100	100
57	j5	85/87 (98%)	81 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	k5	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
59	l5	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
60	L5	191/193 (99%)	174 (91%)	15 (8%)	2 (1%)	12	40
61	m5	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
62	M5	134/136 (98%)	123 (92%)	11 (8%)	0	100	100
63	N5	201/203 (99%)	187 (93%)	14 (7%)	0	100	100
64	o5	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
65	p5	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
66	P5	181/183 (99%)	175 (97%)	6 (3%)	0	100	100
67	Q5	183/185 (99%)	175 (96%)	8 (4%)	0	100	100
68	S5	170/172 (99%)	158 (93%)	12 (7%)	0	100	100
69	U5	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
70	V5	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
71	Z5	133/135 (98%)	123 (92%)	10 (8%)	0	100	100
72	K5	195/197 (99%)	191 (98%)	4 (2%)	0	100	100
73	n5	23/25 (92%)	23 (100%)	0	0	100	100
74	R5	186/188 (99%)	177 (95%)	9 (5%)	0	100	100
75	X5	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
76	Y5	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
77	T5	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
78	E5	153/175 (87%)	144 (94%)	9 (6%)	0	100	100
79	W5	96/98 (98%)	83 (86%)	13 (14%)	0	100	100
80	A6	535/611 (88%)	496 (93%)	39 (7%)	0	100	100
All	All	11887/12157 (98%)	11117 (94%)	761 (6%)	9 (0%)	49	75

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	S2	14	ILE
13	G2	149	LYS
60	L5	77	LEU
49	F5	234	GLU
39	a5	46	ASP
49	F5	157	ASN

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Mol	Chain	Res	Type
60	L5	63	VAL
13	G2	173	PRO
2	A2	4	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	344/344 (100%)	344 (100%)	0	100	100
2	A2	174/174 (100%)	173 (99%)	1 (1%)	78	81
3	a2	84/84 (100%)	84 (100%)	0	100	100
4	B2	191/191 (100%)	191 (100%)	0	100	100
5	b2	70/70 (100%)	70 (100%)	0	100	100
6	C2	176/176 (100%)	176 (100%)	0	100	100
7	c2	56/56 (100%)	56 (100%)	0	100	100
8	D2	182/182 (100%)	182 (100%)	0	100	100
9	d2	47/47 (100%)	47 (100%)	0	100	100
10	E2	221/221 (100%)	221 (100%)	0	100	100
11	e2	51/51 (100%)	51 (100%)	0	100	100
12	F2	173/173 (100%)	173 (100%)	0	100	100
13	G2	193/193 (100%)	193 (100%)	0	100	100
14	g2	261/261 (100%)	261 (100%)	0	100	100
15	H2	165/165 (100%)	165 (100%)	0	100	100
16	I2	150/160 (94%)	150 (100%)	0	100	100
17	J2	158/158 (100%)	158 (100%)	0	100	100
18	K2	89/89 (100%)	89 (100%)	0	100	100
19	L2	136/136 (100%)	136 (100%)	0	100	100
20	M2	100/100 (100%)	100 (100%)	0	100	100
21	N2	127/127 (100%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	O2	96/96 (100%)	96 (100%)	0	100	100
23	P2	104/104 (100%)	104 (100%)	0	100	100
24	Q2	117/117 (100%)	117 (100%)	0	100	100
25	R2	113/113 (100%)	113 (100%)	0	100	100
26	S2	128/128 (100%)	128 (100%)	0	100	100
27	T2	115/115 (100%)	115 (100%)	0	100	100
28	U2	100/100 (100%)	99 (99%)	1 (1%)	68	76
29	V2	74/74 (100%)	74 (100%)	0	100	100
30	W2	110/110 (100%)	110 (100%)	0	100	100
31	X2	119/119 (100%)	119 (100%)	0	100	100
32	Y2	112/112 (100%)	111 (99%)	1 (1%)	70	78
33	Z2	61/61 (100%)	61 (100%)	0	100	100
35	f2	43/62 (69%)	43 (100%)	0	100	100
39	a5	118/118 (100%)	118 (100%)	0	100	100
40	A5	194/194 (100%)	194 (100%)	0	100	100
41	b5	46/46 (100%)	46 (100%)	0	100	100
42	B5	322/322 (100%)	322 (100%)	0	100	100
43	c5	81/81 (100%)	81 (100%)	0	100	100
44	C5	288/288 (100%)	288 (100%)	0	100	100
45	D5	244/244 (100%)	244 (100%)	0	100	100
46	d5	96/96 (100%)	96 (100%)	0	100	100
47	e5	109/109 (100%)	109 (100%)	0	100	100
48	f5	90/90 (100%)	90 (100%)	0	100	100
49	F5	186/186 (100%)	186 (100%)	0	100	100
50	g5	95/95 (100%)	95 (100%)	0	100	100
51	G5	191/191 (100%)	191 (100%)	0	100	100
52	h5	104/104 (100%)	104 (100%)	0	100	100
53	H5	171/171 (100%)	170 (99%)	1 (1%)	78	81
54	i5	81/81 (100%)	81 (100%)	0	100	100
55	I5	180/186 (97%)	180 (100%)	0	100	100
56	J5	147/147 (100%)	146 (99%)	1 (1%)	76	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	j5	70/70 (100%)	70 (100%)	0	100	100
58	k5	68/68 (100%)	68 (100%)	0	100	100
59	l5	45/45 (100%)	45 (100%)	0	100	100
60	L5	154/154 (100%)	154 (100%)	0	100	100
61	m5	47/47 (100%)	47 (100%)	0	100	100
62	M5	107/107 (100%)	107 (100%)	0	100	100
63	N5	175/175 (100%)	175 (100%)	0	100	100
64	o5	90/90 (100%)	90 (100%)	0	100	100
65	p5	71/71 (100%)	71 (100%)	0	100	100
66	P5	145/145 (100%)	145 (100%)	0	100	100
67	Q5	150/150 (100%)	149 (99%)	1 (1%)	76	80
68	S5	156/156 (100%)	156 (100%)	0	100	100
69	U5	87/87 (100%)	87 (100%)	0	100	100
70	V5	104/104 (100%)	104 (100%)	0	100	100
71	Z5	115/115 (100%)	115 (100%)	0	100	100
72	K5	160/160 (100%)	160 (100%)	0	100	100
73	n5	23/23 (100%)	23 (100%)	0	100	100
74	R5	153/153 (100%)	153 (100%)	0	100	100
75	X5	105/105 (100%)	105 (100%)	0	100	100
76	Y5	109/109 (100%)	109 (100%)	0	100	100
77	T5	136/136 (100%)	136 (100%)	0	100	100
78	E5	135/152 (89%)	135 (100%)	0	100	100
79	W5	86/86 (100%)	86 (100%)	0	100	100
80	A6	478/538 (89%)	478 (100%)	0	100	100
All	All	10152/10264 (99%)	10146 (100%)	6 (0%)	87	90

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A2	133	ILE
28	U2	20	ILE
32	Y2	35	VAL
53	H5	48	VAL
56	J5	171	VAL

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Mol	Chain	Res	Type
67	Q5	98	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (159) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	12	ASN
1	A1	96	ASN
1	A1	153	HIS
1	A1	292	ASN
1	A1	345	ASN
2	A2	23	HIS
2	A2	109	ASN
3	a2	11	ASN
3	a2	72	HIS
4	B2	101	HIS
4	B2	118	GLN
4	B2	194	ASN
5	b2	9	HIS
6	C2	89	GLN
6	C2	94	GLN
7	c2	27	GLN
8	D2	56	GLN
8	D2	74	GLN
9	d2	5	ASN
9	d2	37	ASN
10	E2	98	ASN
10	E2	142	HIS
10	E2	259	GLN
11	e2	17	GLN
12	F2	44	ASN
12	F2	104	ASN
12	F2	127	GLN
12	F2	158	GLN
12	F2	224	ASN
13	G2	22	HIS
13	G2	65	GLN
13	G2	190	GLN
13	G2	201	GLN
14	g2	64	HIS
14	g2	147	HIS
14	g2	174	ASN
14	g2	198	ASN

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Mol	Chain	Res	Type
14	g2	268	GLN
14	g2	308	ASN
15	H2	5	GLN
15	H2	11	GLN
16	I2	32	GLN
16	I2	103	GLN
16	I2	159	GLN
17	J2	142	ASN
17	J2	155	HIS
18	K2	32	HIS
18	K2	58	GLN
20	M2	70	ASN
20	M2	111	ASN
23	P2	114	HIS
24	Q2	62	ASN
24	Q2	83	GLN
25	R2	48	ASN
25	R2	123	ASN
26	S2	71	GLN
26	S2	74	GLN
26	S2	89	GLN
27	T2	64	HIS
28	U2	87	HIS
29	V2	21	ASN
30	W2	15	ASN
30	W2	64	GLN
30	W2	80	ASN
30	W2	92	ASN
31	X2	18	HIS
31	X2	94	ASN
33	Z2	38	HIS
33	Z2	98	GLN
39	a5	14	HIS
39	a5	40	HIS
39	a5	41	HIS
39	a5	64	GLN
39	a5	74	ASN
40	A5	140	ASN
40	A5	194	ASN
40	A5	209	HIS
40	A5	211	HIS
40	A5	218	HIS

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Mol	Chain	Res	Type
41	b5	43	HIS
42	B5	109	HIS
42	B5	184	ASN
42	B5	319	ASN
44	C5	48	GLN
44	C5	114	ASN
44	C5	361	HIS
45	D5	45	ASN
45	D5	63	GLN
45	D5	81	HIS
45	D5	244	HIS
46	d5	43	HIS
47	e5	13	HIS
47	e5	21	HIS
47	e5	52	GLN
47	e5	71	HIS
47	e5	104	ASN
48	f5	42	GLN
49	F5	112	ASN
49	F5	166	ASN
50	g5	11	ASN
50	g5	14	ASN
50	g5	69	HIS
51	G5	61	GLN
51	G5	138	HIS
51	G5	232	HIS
51	G5	243	GLN
52	h5	16	GLN
52	h5	59	ASN
52	h5	99	GLN
53	H5	96	HIS
53	H5	149	ASN
56	J5	6	GLN
56	J5	43	GLN
56	J5	109	HIS
57	j5	57	HIS
59	l5	4	GLN
59	l5	43	ASN
61	m5	90	ASN
62	M5	41	GLN
62	M5	126	GLN
63	N5	37	HIS

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Mol	Chain	Res	Type
63	N5	156	HIS
63	N5	181	ASN
64	o5	23	HIS
66	P5	97	ASN
66	P5	116	HIS
66	P5	133	HIS
66	P5	145	HIS
67	Q5	15	HIS
68	S5	68	HIS
68	S5	154	HIS
68	S5	157	GLN
69	U5	87	ASN
69	U5	88	GLN
70	V5	98	ASN
70	V5	132	ASN
71	Z5	40	HIS
71	Z5	57	HIS
71	Z5	122	HIS
72	K5	65	ASN
74	R5	3	ASN
74	R5	134	HIS
74	R5	156	ASN
76	Y5	4	GLN
76	Y5	66	GLN
76	Y5	110	HIS
76	Y5	120	GLN
77	T5	5	HIS
77	T5	131	GLN
77	T5	134	GLN
78	E5	157	GLN
79	W5	58	HIS
79	W5	59	HIS
80	A6	140	GLN
80	A6	239	HIS
80	A6	261	ASN
80	A6	281	ASN
80	A6	373	ASN
80	A6	501	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	22	1779/1798 (98%)	367 (20%)	42 (2%)
36	14	3292/3396 (96%)	562 (17%)	74 (2%)
37	34	120/121 (99%)	10 (8%)	0
38	44	157/158 (99%)	34 (21%)	0
81	X7	11/20 (55%)	6 (54%)	0
82	A3	75/76 (98%)	24 (32%)	2 (2%)
All	All	5434/5569 (97%)	1003 (18%)	118 (2%)

All (1003) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	22	2	A
34	22	3	U
34	22	25	C
34	22	26	A
34	22	27	U
34	22	34	G
34	22	42	G
34	22	45	U
34	22	47	A
34	22	57	G
34	22	68	A
34	22	69	G
34	22	72	A
34	22	73	U
34	22	74	U
34	22	81	G
34	22	100	A
34	22	104	A
34	22	111	U
34	22	114	C
34	22	115	G
34	22	116	U
34	22	131	C
34	22	132	U
34	22	133	U
34	22	134	U
34	22	135	A
34	22	136	C
34	22	137	U
34	22	138	A
34	22	140	A
34	22	141	U

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Mol	Chain	Res	Type
34	22	144	U
34	22	145	A
34	22	153	G
34	22	158	U
34	22	166	C
34	22	178	U
34	22	185	U
34	22	192	U
34	22	193	U
34	22	195	G
34	22	197	A
34	22	200	A
34	22	217	A
34	22	219	A
34	22	232	U
34	22	233	C
34	22	242	U
34	22	250	C
34	22	261	U
34	22	265	A
34	22	272	U
34	22	278	U
34	22	279	G
34	22	280	U
34	22	281	G
34	22	288	A
34	22	290	G
34	22	299	A
34	22	302	U
34	22	313	U
34	22	316	A
34	22	321	C
34	22	322	G
34	22	323	A
34	22	337	G
34	22	338	C
34	22	352	A
34	22	359	A
34	22	360	A
34	22	361	C
34	22	399	A
34	22	400	A

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Mol	Chain	Res	Type
34	22	402	C
34	22	404	G
34	22	416	A
34	22	417	A
34	22	418	G
34	22	423	G
34	22	424	C
34	22	425	A
34	22	426	G
34	22	428	A
34	22	434	G
34	22	439	U
34	22	445	A
34	22	452	A
34	22	453	U
34	22	456	A
34	22	475	A
34	22	477	A
34	22	484	C
34	22	488	G
34	22	492	A
34	22	493	U
34	22	494	U
34	22	495	C
34	22	496	G
34	22	497	G
34	22	498	G
34	22	499	U
34	22	501	U
34	22	502	U
34	22	504	U
34	22	505	A
34	22	506	A
34	22	507	U
34	22	508	U
34	22	510	G
34	22	511	A
34	22	513	U
34	22	519	C
34	22	539	G
34	22	541	A
34	22	544	A

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Mol	Chain	Res	Type
34	22	555	A
34	22	556	A
34	22	557	G
34	22	558	U
34	22	559	C
34	22	565	C
34	22	568	G
34	22	578	U
34	22	579	A
34	22	581	U
34	22	582	U
34	22	594	A
34	22	595	G
34	22	611	U
34	22	619	A
34	22	620	A
34	22	623	A
34	22	624	G
34	22	629	U
34	22	639	U
34	22	650	U
34	22	654	C
34	22	655	G
34	22	656	G
34	22	658	C
34	22	677	G
34	22	684	A
34	22	686	C
34	22	687	G
34	22	689	G
34	22	694	U
34	22	696	C
34	22	698	U
34	22	700	C
34	22	705	U
34	22	706	A
34	22	708	C
34	22	709	C
34	22	710	U
34	22	712	G
34	22	717	C
34	22	718	U

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Mol	Chain	Res	Type
34	22	719	U
34	22	721	U
34	22	722	G
34	22	723	G
34	22	725	U
34	22	727	U
34	22	731	C
34	22	732	G
34	22	733	A
34	22	734	A
34	22	735	C
34	22	736	C
34	22	741	C
34	22	742	U
34	22	743	U
34	22	754	A
34	22	755	A
34	22	756	A
34	22	765	G
34	22	766	U
34	22	774	A
34	22	775	G
34	22	781	U
34	22	783	G
34	22	787	G
34	22	789	A
34	22	794	U
34	22	811	A
34	22	813	U
34	22	814	A
34	22	816	G
34	22	818	C
34	22	820	U
34	22	821	U
34	22	823	G
34	22	824	G
34	22	826	U
34	22	829	A
34	22	833	U
34	22	840	U
34	22	841	U
34	22	846	G

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Mol	Chain	Res	Type
34	22	849	C
34	22	850	A
34	22	857	U
34	22	860	U
34	22	863	A
34	22	876	G
34	22	898	A
34	22	912	U
34	22	913	G
34	22	914	G
34	22	915	A
34	22	925	G
34	22	933	A
34	22	934	C
34	22	935	U
34	22	942	G
34	22	944	A
34	22	951	A
34	22	960	U
34	22	966	A
34	22	988	A
34	22	992	A
34	22	993	A
34	22	1003	A
34	22	1004	U
34	22	1005	A
34	22	1012	U
34	22	1024	U
34	22	1026	A
34	22	1028	C
34	22	1039	A
34	22	1040	G
34	22	1051	G
34	22	1052	U
34	22	1053	G
34	22	1058	U
34	22	1061	A
34	22	1074	G
34	22	1076	A
34	22	1082	C
34	22	1091	A
34	22	1092	A

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Mol	Chain	Res	Type
34	22	1096	C
34	22	1097	U
34	22	1098	U
34	22	1099	U
34	22	1100	G
34	22	1113	A
34	22	1114	G
34	22	1138	A
34	22	1158	C
34	22	1160	A
34	22	1167	G
34	22	1185	U
34	22	1194	A
34	22	1196	A
34	22	1197	C
34	22	1199	G
34	22	1200	G
34	22	1207	C
34	22	1208	A
34	22	1217	A
34	22	1218	G
34	22	1227	A
34	22	1228	G
34	22	1229	G
34	22	1232	U
34	22	1243	G
34	22	1244	A
34	22	1245	G
34	22	1246	C
34	22	1251	U
34	22	1254	U
34	22	1258	U
34	22	1284	C
34	22	1285	U
34	22	1290	U
34	22	1314	U
34	22	1315	U
34	22	1316	G
34	22	1321	A
34	22	1327	C
34	22	1337	A
34	22	1339	C

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Mol	Chain	Res	Type
34	22	1340	U
34	22	1344	A
34	22	1345	A
34	22	1362	U
34	22	1363	U
34	22	1364	G
34	22	1370	U
34	22	1371	A
34	22	1372	U
34	22	1373	C
34	22	1389	C
34	22	1390	U
34	22	1399	C
34	22	1413	U
34	22	1415	U
34	22	1427	A
34	22	1428	G
34	22	1431	C
34	22	1432	U
34	22	1436	A
34	22	1445	G
34	22	1446	A
34	22	1448	G
34	22	1457	C
34	22	1459	C
34	22	1460	A
34	22	1471	A
34	22	1473	U
34	22	1474	G
34	22	1482	C
34	22	1486	G
34	22	1490	C
34	22	1492	A
34	22	1506	G
34	22	1516	A
34	22	1521	G
34	22	1523	G
34	22	1524	A
34	22	1535	U
34	22	1536	G
34	22	1537	C
34	22	1538	U

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Mol	Chain	Res	Type
34	22	1540	G
34	22	1542	G
34	22	1557	U
34	22	1559	A
34	22	1568	C
34	22	1569	A
34	22	1574	G
34	22	1584	G
34	22	1600	A
34	22	1601	G
34	22	1616	G
34	22	1626	U
34	22	1631	A
34	22	1634	C
34	22	1646	C
34	22	1657	U
34	22	1658	G
34	22	1680	G
34	22	1682	U
34	22	1684	U
34	22	1689	A
34	22	1696	G
34	22	1697	G
34	22	1700	C
34	22	1702	A
34	22	1704	U
34	22	1713	G
34	22	1756	A
34	22	1760	G
34	22	1762	A
34	22	1769	U
34	22	1770	U
34	22	1780	G
34	22	1782	A
34	22	1783	C
34	22	1792	G
34	22	1793	G
34	22	1794	A
34	22	1796	C
34	22	1797	A
34	22	1798	U
36	14	13	A

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Mol	Chain	Res	Type
36	14	14	U
36	14	15	C
36	14	21	G
36	14	26	A
36	14	40	A
36	14	43	A
36	14	49	A
36	14	59	G
36	14	60	A
36	14	65	A
36	14	66	A
36	14	86	G
36	14	92	G
36	14	93	C
36	14	110	G
36	14	113	C
36	14	115	A
36	14	121	A
36	14	122	A
36	14	133	U
36	14	134	U
36	14	136	G
36	14	148	G
36	14	156	G
36	14	157	A
36	14	182	U
36	14	187	A
36	14	189	G
36	14	190	U
36	14	191	U
36	14	200	C
36	14	206	G
36	14	210	U
36	14	211	A
36	14	218	G
36	14	219	A
36	14	234	G
36	14	240	U
36	14	249	U
36	14	252	U
36	14	269	G
36	14	283	G

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Mol	Chain	Res	Type
36	14	286	U
36	14	295	A
36	14	298	U
36	14	305	U
36	14	323	A
36	14	329	U
36	14	338	A
36	14	339	C
36	14	343	U
36	14	349	A
36	14	350	C
36	14	352	A
36	14	353	G
36	14	370	U
36	14	376	G
36	14	398	A
36	14	401	U
36	14	402	A
36	14	403	C
36	14	421	G
36	14	422	A
36	14	439	C
36	14	521	A
36	14	534	U
36	14	535	G
36	14	546	C
36	14	547	G
36	14	548	G
36	14	555	U
36	14	557	A
36	14	558	U
36	14	559	A
36	14	578	A
36	14	579	G
36	14	589	A
36	14	592	A
36	14	604	G
36	14	609	G
36	14	611	A
36	14	620	U
36	14	621	A
36	14	622	A

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Mol	Chain	Res	Type
36	14	637	C
36	14	642	U
36	14	649	A
36	14	677	A
36	14	681	U
36	14	690	A
36	14	691	A
36	14	705	A
36	14	712	G
36	14	715	A
36	14	764	U
36	14	765	C
36	14	766	U
36	14	767	U
36	14	776	U
36	14	777	U
36	14	781	G
36	14	785	G
36	14	786	A
36	14	787	G
36	14	806	A
36	14	817	A
36	14	830	A
36	14	835	G
36	14	849	C
36	14	861	C
36	14	874	U
36	14	879	U
36	14	880	G
36	14	896	A
36	14	908	G
36	14	914	A
36	14	916	G
36	14	917	A
36	14	922	U
36	14	925	A
36	14	937	G
36	14	938	C
36	14	940	G
36	14	944	C
36	14	959	C
36	14	960	U

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Mol	Chain	Res	Type
36	14	963	G
36	14	974	G
36	14	979	U
36	14	980	A
36	14	981	U
36	14	982	C
36	14	984	G
36	14	1001	G
36	14	1002	A
36	14	1006	A
36	14	1010	G
36	14	1015	U
36	14	1016	C
36	14	1017	C
36	14	1024	G
36	14	1025	A
36	14	1037	C
36	14	1041	U
36	14	1047	A
36	14	1049	C
36	14	1064	A
36	14	1065	A
36	14	1075	A
36	14	1076	C
36	14	1081	U
36	14	1093	A
36	14	1094	U
36	14	1095	U
36	14	1098	A
36	14	1103	A
36	14	1104	G
36	14	1117	G
36	14	1131	G
36	14	1144	U
36	14	1153	A
36	14	1159	A
36	14	1180	A
36	14	1181	U
36	14	1192	C
36	14	1196	C
36	14	1201	C
36	14	1205	A

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Mol	Chain	Res	Type
36	14	1206	G
36	14	1209	G
36	14	1222	G
36	14	1235	U
36	14	1236	G
36	14	1241	U
36	14	1242	G
36	14	1244	A
36	14	1246	G
36	14	1248	C
36	14	1253	U
36	14	1254	C
36	14	1258	U
36	14	1262	G
36	14	1263	A
36	14	1264	G
36	14	1269	U
36	14	1270	A
36	14	1271	A
36	14	1272	C
36	14	1273	A
36	14	1274	A
36	14	1278	A
36	14	1285	G
36	14	1287	A
36	14	1308	A
36	14	1309	U
36	14	1313	G
36	14	1316	C
36	14	1317	A
36	14	1323	G
36	14	1325	U
36	14	1330	A
36	14	1331	U
36	14	1348	U
36	14	1349	G
36	14	1351	U
36	14	1353	U
36	14	1355	A
36	14	1356	U
36	14	1357	G
36	14	1386	A

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Mol	Chain	Res	Type
36	14	1392	G
36	14	1399	A
36	14	1400	G
36	14	1419	A
36	14	1430	U
36	14	1434	G
36	14	1435	A
36	14	1437	C
36	14	1446	A
36	14	1447	G
36	14	1470	U
36	14	1480	G
36	14	1482	A
36	14	1483	G
36	14	1488	G
36	14	1493	G
36	14	1495	U
36	14	1496	C
36	14	1508	C
36	14	1523	U
36	14	1524	A
36	14	1554	U
36	14	1555	U
36	14	1556	C
36	14	1557	A
36	14	1560	G
36	14	1562	C
36	14	1563	C
36	14	1567	U
36	14	1568	U
36	14	1569	U
36	14	1570	U
36	14	1571	A
36	14	1572	U
36	14	1576	G
36	14	1578	C
36	14	1582	C
36	14	1583	A
36	14	1588	A
36	14	1589	A
36	14	1593	A
36	14	1596	C

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Mol	Chain	Res	Type
36	14	1605	A
36	14	1606	U
36	14	1607	U
36	14	1629	U
36	14	1630	U
36	14	1639	C
36	14	1642	A
36	14	1643	A
36	14	1645	U
36	14	1656	A
36	14	1657	C
36	14	1683	A
36	14	1714	A
36	14	1715	A
36	14	1716	U
36	14	1724	U
36	14	1725	C
36	14	1730	G
36	14	1736	G
36	14	1741	A
36	14	1742	U
36	14	1749	A
36	14	1751	G
36	14	1752	A
36	14	1760	A
36	14	1765	U
36	14	1766	G
36	14	1770	G
36	14	1775	G
36	14	1780	G
36	14	1796	G
36	14	1797	A
36	14	1808	G
36	14	1814	A
36	14	1816	A
36	14	1817	G
36	14	1820	U
36	14	1821	U
36	14	1835	A
36	14	1841	A
36	14	1847	A
36	14	1849	C

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Mol	Chain	Res	Type
36	14	1850	A
36	14	1866	C
36	14	1867	A
36	14	1878	G
36	14	1880	U
36	14	1893	A
36	14	1901	A
36	14	1906	G
36	14	1941	C
36	14	1944	U
36	14	1948	G
36	14	1949	G
36	14	1954	G
36	14	1955	U
36	14	1966	U
36	14	1967	U
36	14	1973	G
36	14	1974	A
36	14	1975	C
36	14	1976	G
36	14	2044	U
36	14	2047	A
36	14	2048	G
36	14	2060	A
36	14	2067	U
36	14	2068	U
36	14	2071	A
36	14	2072	G
36	14	2076	G
36	14	2077	U
36	14	2078	C
36	14	2079	G
36	14	2080	C
36	14	2081	U
36	14	2087	C
36	14	2088	A
36	14	2089	A
36	14	2090	U
36	14	2091	U
36	14	2092	A
36	14	2094	C
36	14	2095	G

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Mol	Chain	Res	Type
36	14	2099	A
36	14	2107	A
36	14	2112	U
36	14	2113	A
36	14	2114	C
36	14	2121	G
36	14	2122	G
36	14	2131	A
36	14	2140	U
36	14	2159	U
36	14	2160	G
36	14	2169	G
36	14	2174	G
36	14	2175	U
36	14	2176	U
36	14	2179	C
36	14	2205	U
36	14	2209	U
36	14	2210	G
36	14	2223	A
36	14	2225	U
36	14	2228	A
36	14	2244	A
36	14	2249	G
36	14	2257	C
36	14	2272	G
36	14	2273	G
36	14	2282	U
36	14	2286	U
36	14	2287	C
36	14	2288	G
36	14	2307	G
36	14	2308	C
36	14	2309	A
36	14	2310	U
36	14	2313	A
36	14	2314	U
36	14	2315	G
36	14	2334	U
36	14	2336	U
36	14	2339	C
36	14	2373	A

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Mol	Chain	Res	Type
36	14	2374	C
36	14	2375	G
36	14	2376	G
36	14	2378	C
36	14	2386	A
36	14	2394	G
36	14	2397	A
36	14	2401	A
36	14	2402	A
36	14	2403	G
36	14	2404	A
36	14	2411	U
36	14	2418	G
36	14	2435	G
36	14	2443	A
36	14	2444	C
36	14	2447	A
36	14	2448	G
36	14	2453	U
36	14	2454	G
36	14	2459	A
36	14	2462	A
36	14	2468	A
36	14	2469	G
36	14	2486	A
36	14	2487	U
36	14	2488	A
36	14	2506	U
36	14	2510	U
36	14	2511	A
36	14	2512	C
36	14	2514	U
36	14	2515	A
36	14	2522	G
36	14	2523	A
36	14	2526	C
36	14	2531	C
36	14	2532	U
36	14	2537	U
36	14	2538	U
36	14	2539	C
36	14	2541	U

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Mol	Chain	Res	Type
36	14	2542	U
36	14	2544	U
36	14	2547	A
36	14	2548	C
36	14	2552	C
36	14	2558	U
36	14	2561	A
36	14	2571	U
36	14	2572	C
36	14	2573	G
36	14	2580	A
36	14	2581	U
36	14	2585	G
36	14	2593	A
36	14	2594	C
36	14	2606	G
36	14	2607	G
36	14	2614	G
36	14	2652	U
36	14	2656	A
36	14	2672	G
36	14	2674	A
36	14	2677	G
36	14	2678	A
36	14	2681	U
36	14	2691	A
36	14	2694	A
36	14	2696	A
36	14	2703	A
36	14	2704	A
36	14	2705	A
36	14	2706	G
36	14	2715	A
36	14	2728	G
36	14	2729	U
36	14	2753	G
36	14	2755	C
36	14	2777	G
36	14	2778	G
36	14	2796	G
36	14	2800	G
36	14	2801	A

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Mol	Chain	Res	Type
36	14	2803	A
36	14	2804	A
36	14	2810	C
36	14	2814	G
36	14	2817	A
36	14	2818	U
36	14	2834	G
36	14	2842	U
36	14	2844	C
36	14	2845	A
36	14	2860	U
36	14	2867	C
36	14	2871	G
36	14	2872	A
36	14	2873	U
36	14	2874	G
36	14	2875	U
36	14	2887	A
36	14	2899	C
36	14	2918	G
36	14	2923	U
36	14	2935	U
36	14	2936	A
36	14	2938	G
36	14	2941	A
36	14	2942	C
36	14	2951	G
36	14	2957	G
36	14	2971	A
36	14	2972	G
36	14	2983	C
36	14	2996	U
36	14	2997	G
36	14	3011	A
36	14	3012	A
36	14	3030	G
36	14	3049	A
36	14	3078	U
36	14	3080	G
36	14	3086	A
36	14	3092	C
36	14	3098	G

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Mol	Chain	Res	Type
36	14	3121	U
36	14	3122	A
36	14	3130	A
36	14	3131	U
36	14	3142	A
36	14	3143	C
36	14	3153	U
36	14	3154	C
36	14	3155	U
36	14	3156	U
36	14	3157	U
36	14	3165	A
36	14	3170	A
36	14	3172	A
36	14	3173	G
36	14	3174	A
36	14	3176	G
36	14	3179	U
36	14	3181	C
36	14	3185	U
36	14	3186	A
36	14	3187	A
36	14	3199	G
36	14	3206	C
36	14	3207	U
36	14	3208	G
36	14	3209	A
36	14	3216	G
36	14	3217	C
36	14	3218	A
36	14	3219	G
36	14	3243	A
36	14	3244	A
36	14	3247	G
36	14	3270	U
36	14	3271	G
36	14	3276	G
36	14	3279	A
36	14	3294	A
36	14	3304	U
36	14	3313	U
36	14	3319	U

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Mol	Chain	Res	Type
36	14	3320	A
36	14	3341	U
36	14	3345	G
36	14	3352	U
36	14	3353	G
36	14	3354	U
36	14	3355	U
36	14	3356	G
36	14	3368	U
36	14	3369	G
36	14	3370	A
36	14	3375	A
36	14	3378	C
36	14	3390	G
36	14	3396	U
37	34	42	A
37	34	54	U
37	34	55	A
37	34	65	G
37	34	76	A
37	34	77	G
37	34	87	G
37	34	99	G
37	34	112	G
37	34	121	U
38	44	23	U
38	44	24	G
38	44	34	U
38	44	35	C
38	44	37	A
38	44	38	U
38	44	39	G
38	44	49	G
38	44	51	G
38	44	59	A
38	44	62	C
38	44	63	G
38	44	71	A
38	44	80	A
38	44	81	U
38	44	82	U
38	44	84	C

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Mol	Chain	Res	Type
38	44	85	G
38	44	86	U
38	44	87	G
38	44	90	U
38	44	91	C
38	44	95	G
38	44	104	A
38	44	106	C
38	44	107	G
38	44	113	U
38	44	118	C
38	44	125	U
38	44	126	A
38	44	138	A
38	44	151	C
38	44	152	G
38	44	155	A
81	X7	8	A
81	X7	10	G
81	X7	11	U
81	X7	12	A
81	X7	13	A
81	X7	17	U
82	A3	9	A
82	A3	11	C
82	A3	14	A
82	A3	15	G
82	A3	16	H2U
82	A3	17	H2U
82	A3	18	G
82	A3	20	G
82	A3	21	A
82	A3	22	G
82	A3	25	C
82	A3	26	M2G
82	A3	46	7MG
82	A3	47	U
82	A3	48	C
82	A3	49	5MC
82	A3	52	U
82	A3	54	5MU
82	A3	55	PSU

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Mol	Chain	Res	Type
82	A3	56	C
82	A3	57	G
82	A3	58	1MA
82	A3	59	U
82	A3	76	A

All (118) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	22	56	U
34	22	73	U
34	22	99	C
34	22	131	C
34	22	133	U
34	22	139	C
34	22	216	U
34	22	280	U
34	22	315	A
34	22	322	G
34	22	417	A
34	22	444	C
34	22	497	G
34	22	503	G
34	22	538	A
34	22	555	A
34	22	578	U
34	22	580	A
34	22	622	A
34	22	657	U
34	22	686	C
34	22	720	G
34	22	721	U
34	22	782	U
34	22	812	A
34	22	819	G
34	22	1113	A
34	22	1137	A
34	22	1157	A
34	22	1207	C
34	22	1250	U
34	22	1344	A
34	22	1388	A

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Mol	Chain	Res	Type
34	22	1447	C
34	22	1481	C
34	22	1491	U
34	22	1568	C
34	22	1573	A
34	22	1600	A
34	22	1696	G
34	22	1761	U
34	22	1769	U
36	14	13	A
36	14	199	A
36	14	210	U
36	14	239	G
36	14	282	G
36	14	337	G
36	14	338	A
36	14	352	A
36	14	533	A
36	14	547	G
36	14	763	G
36	14	764	U
36	14	786	A
36	14	916	G
36	14	979	U
36	14	1015	U
36	14	1064	A
36	14	1094	U
36	14	1097	G
36	14	1103	A
36	14	1116	G
36	14	1253	U
36	14	1307	G
36	14	1317	A
36	14	1355	A
36	14	1418	A
36	14	1493	G
36	14	1554	U
36	14	1559	A
36	14	1562	C
36	14	1570	U
36	14	1656	A
36	14	1715	A

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Mol	Chain	Res	Type
36	14	1729	A
36	14	1748	G
36	14	1750	A
36	14	1815	U
36	14	1816	A
36	14	1846	C
36	14	1848	G
36	14	1866	C
36	14	1900	A
36	14	1943	C
36	14	1965	C
36	14	2043	U
36	14	2046	U
36	14	2080	C
36	14	2086	A
36	14	2090	U
36	14	2093	A
36	14	2112	U
36	14	2209	U
36	14	2227	C
36	14	2286	U
36	14	2307	G
36	14	2309	A
36	14	2335	G
36	14	2447	A
36	14	2468	A
36	14	2487	U
36	14	2509	U
36	14	2513	U
36	14	2525	G
36	14	2537	U
36	14	2541	U
36	14	2570	U
36	14	2580	A
36	14	2593	A
36	14	2705	A
36	14	2950	G
36	14	2971	A
36	14	3011	A
36	14	3121	U
36	14	3198	U
82	A3	19	G

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Mol	Chain	Res	Type
82	A3	58	1MA

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

14 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
82	5MC	A3	49	82	19,22,23	0.97	1 (5%)	26,32,35	1.20	3 (11%)
82	5MU	A3	54	82	19,22,23	1.11	2 (10%)	27,32,35	1.39	4 (14%)
82	YYG	A3	37	82	38,42,43	1.63	10 (26%)	45,62,65	2.79	15 (33%)
82	PSU	A3	39	82	18,21,22	2.64	7 (38%)	21,30,33	1.75	5 (23%)
82	1MA	A3	58	82	21,25,26	1.19	3 (14%)	30,37,40	1.39	3 (10%)
82	7MG	A3	46	82	23,26,27	3.25	7 (30%)	27,39,42	2.23	8 (29%)
82	M2G	A3	26	84,82	24,27,28	1.28	2 (8%)	33,40,43	1.39	5 (15%)
82	H2U	A3	17	82	18,21,22	1.19	2 (11%)	19,30,33	1.20	3 (15%)
82	H2U	A3	16	82	18,21,22	1.22	2 (11%)	19,30,33	1.34	3 (15%)
82	5MC	A3	40	82	19,22,23	1.55	1 (5%)	26,32,35	1.21	4 (15%)
82	OMC	A3	32	82	19,22,23	1.57	3 (15%)	25,31,34	1.32	4 (16%)
82	OMG	A3	34	81,82	22,25,27	1.74	3 (13%)	32,37,41	1.78	7 (21%)
82	PSU	A3	55	82	18,21,22	2.71	7 (38%)	21,30,33	1.64	5 (23%)
82	2MG	A3	10	82	23,26,27	2.12	6 (26%)	33,38,41	2.06	8 (24%)

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
82	5MC	A3	49	82	-	2/7/25/26	0/2/2/2
82	5MU	A3	54	82	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	YYG	A3	37	82	-	7/24/42/43	0/4/4/4
82	PSU	A3	39	82	-	0/7/25/26	0/2/2/2
82	1MA	A3	58	82	-	2/7/25/26	0/3/3/3
82	7MG	A3	46	82	-	3/7/37/38	0/3/3/3
82	M2G	A3	26	84,82	-	2/11/29/30	0/3/3/3
82	H2U	A3	17	82	-	3/7/38/39	0/2/2/2
82	H2U	A3	16	82	-	5/7/38/39	0/2/2/2
82	5MC	A3	40	82	-	0/7/25/26	0/2/2/2
82	OMC	A3	32	82	-	0/9/27/28	0/2/2/2
82	OMG	A3	34	81,82	-	2/7/25/28	0/3/3/3
82	PSU	A3	55	82	-	4/7/25/26	0/2/2/2
82	2MG	A3	10	82	-	2/9/27/28	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	A3	46	7MG	C8-N9	9.18	1.51	1.45
82	A3	46	7MG	C5-N7	7.35	1.44	1.35
82	A3	10	2MG	C2-N2	6.43	1.46	1.33
82	A3	55	PSU	C1'-C5	6.10	1.64	1.50
82	A3	39	PSU	C1'-C5	5.91	1.63	1.50
82	A3	40	5MC	C5-C4	-5.71	1.39	1.44
82	A3	46	7MG	C4-N9	5.53	1.44	1.37
82	A3	34	OMG	C2-N2	5.00	1.45	1.34
82	A3	55	PSU	C6-N1	4.73	1.44	1.36
82	A3	39	PSU	C6-N1	4.72	1.44	1.36
82	A3	10	2MG	C6-N1	4.57	1.47	1.38
82	A3	26	M2G	C2-N2	4.53	1.43	1.35
82	A3	46	7MG	C2-N2	4.47	1.44	1.34
82	A3	55	PSU	C2-N1	4.39	1.42	1.36
82	A3	55	PSU	C4-N3	4.39	1.47	1.38
82	A3	37	YYG	O23-C21	4.33	1.41	1.34
82	A3	39	PSU	C4-N3	4.30	1.46	1.38
82	A3	39	PSU	C2-N1	4.08	1.42	1.36
82	A3	55	PSU	C2-N3	3.96	1.44	1.37
82	A3	39	PSU	C2-N3	3.95	1.44	1.37
82	A3	46	7MG	C4-N3	3.91	1.43	1.34
82	A3	32	OMC	C2-N1	3.89	1.48	1.40
82	A3	10	2MG	C4-N3	3.76	1.42	1.34
82	A3	46	7MG	C6-N1	3.75	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	A3	34	OMG	C6-N1	3.75	1.45	1.38
82	A3	37	YYG	C12-N1	3.61	1.48	1.40
82	A3	32	OMC	C4-N4	3.60	1.42	1.33
82	A3	32	OMC	C2-N3	3.57	1.43	1.36
82	A3	46	7MG	C2-N3	3.55	1.41	1.33
82	A3	16	H2U	C2-N1	3.50	1.40	1.35
82	A3	17	H2U	C2-N3	3.47	1.44	1.38
82	A3	16	H2U	C2-N3	3.38	1.43	1.38
82	A3	17	H2U	C2-N1	3.29	1.40	1.35
82	A3	37	YYG	C21-N20	3.13	1.42	1.34
82	A3	34	OMG	C4-N3	3.05	1.41	1.34
82	A3	26	M2G	C4-N3	2.90	1.40	1.34
82	A3	54	5MU	C4-N3	2.90	1.44	1.38
82	A3	37	YYG	C6-N1	2.85	1.48	1.42
82	A3	49	5MC	C5-C4	-2.84	1.42	1.44
82	A3	10	2MG	C2-N1	2.76	1.41	1.36
82	A3	37	YYG	C15-N20	2.67	1.51	1.45
82	A3	55	PSU	O4'-C1'	-2.60	1.40	1.43
82	A3	55	PSU	C4-C5	2.51	1.51	1.44
82	A3	39	PSU	C4-C5	2.48	1.51	1.44
82	A3	10	2MG	C4-N9	2.48	1.44	1.38
82	A3	54	5MU	C2-N1	2.43	1.42	1.38
82	A3	58	1MA	CM1-N1	2.40	1.51	1.46
82	A3	37	YYG	O18-C16	2.33	1.39	1.33
82	A3	37	YYG	C15-C16	2.32	1.58	1.52
82	A3	58	1MA	C4-N3	2.31	1.40	1.35
82	A3	37	YYG	C2-N3	2.30	1.42	1.38
82	A3	58	1MA	C2-N1	2.28	1.40	1.35
82	A3	39	PSU	O4'-C1'	-2.28	1.40	1.43
82	A3	10	2MG	C8-N9	2.27	1.42	1.37
82	A3	37	YYG	C14-C15	2.19	1.58	1.53
82	A3	37	YYG	C5-N7	2.03	1.43	1.39

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	A3	37	YYG	C1'-N9-C8	-7.48	105.47	126.73
82	A3	10	2MG	C2-N3-C4	7.35	121.20	112.00
82	A3	37	YYG	C10-C11-N2	-7.26	104.76	119.32
82	A3	37	YYG	O23-C21-N20	6.96	122.48	110.77
82	A3	37	YYG	C5-C4-N3	-6.87	118.41	123.99
82	A3	37	YYG	O23-C21-O22	-5.66	116.38	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	A3	46	7MG	C2-N3-C4	5.58	121.91	112.30
82	A3	46	7MG	C4-C5-N7	5.38	111.73	105.38
82	A3	34	OMG	C2-N3-C4	5.21	121.28	112.30
82	A3	58	1MA	C5-C4-N3	-4.75	120.28	127.27
82	A3	37	YYG	N9-C4-N3	4.60	136.89	129.45
82	A3	10	2MG	C2-N1-C6	-4.45	119.18	124.55
82	A3	34	OMG	C5-C4-N3	-4.19	121.73	128.39
82	A3	39	PSU	N1-C2-N3	4.08	119.47	115.17
82	A3	39	PSU	C4-N3-C2	-4.07	120.76	126.37
82	A3	46	7MG	C5-C6-N1	4.04	118.04	110.94
82	A3	55	PSU	C4-N3-C2	-3.99	120.87	126.37
82	A3	10	2MG	N9-C4-N3	3.95	133.85	125.95
82	A3	10	2MG	C5-C4-N3	-3.87	122.23	128.39
82	A3	34	OMG	N9-C4-N3	3.85	133.65	125.95
82	A3	37	YYG	O18-C16-C15	3.82	121.21	111.49
82	A3	55	PSU	N1-C2-N3	3.81	119.19	115.17
82	A3	37	YYG	O18-C16-O17	-3.64	116.77	123.85
82	A3	54	5MU	C4-N3-C2	-3.56	122.67	127.34
82	A3	46	7MG	C5-C4-N3	-3.51	121.55	128.13
82	A3	26	M2G	C5-C4-N3	-3.47	122.87	128.39
82	A3	37	YYG	O6-C6-N1	-3.31	115.14	119.87
82	A3	58	1MA	C2-N3-C4	3.26	118.92	112.53
82	A3	26	M2G	N9-C4-N3	3.16	132.26	125.95
82	A3	54	5MU	C6-N1-C2	-3.15	118.17	121.30
82	A3	37	YYG	C2-N1-C12	-3.14	104.29	109.94
82	A3	54	5MU	N3-C2-N1	3.09	118.91	114.89
82	A3	16	H2U	O2-C2-N1	3.05	126.77	123.10
82	A3	26	M2G	C1'-N9-C4	2.99	135.32	126.49
82	A3	46	7MG	N9-C4-N3	2.99	129.84	125.46
82	A3	46	7MG	N1-C2-N3	-2.97	117.88	123.32
82	A3	34	OMG	C2-N1-C6	-2.97	119.73	125.11
82	A3	16	H2U	C5-C4-N3	2.96	119.84	116.69
82	A3	10	2MG	O6-C6-N1	-2.89	114.68	120.11
82	A3	34	OMG	O6-C6-N1	-2.86	114.74	120.11
82	A3	32	OMC	C6-N1-C2	-2.81	115.71	120.46
82	A3	26	M2G	C1'-N9-C8	-2.81	118.74	126.73
82	A3	39	PSU	O2-C2-N1	-2.78	119.92	122.79
82	A3	16	H2U	O2-C2-N3	-2.77	116.38	121.49
82	A3	32	OMC	N4-C4-N3	2.75	122.82	117.91
82	A3	32	OMC	C1'-N1-C2	2.74	124.50	118.44
82	A3	37	YYG	C24-O23-C21	2.74	118.80	115.63
82	A3	17	H2U	O2-C2-N1	2.70	126.35	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	A3	37	YYG	C3-N3-C4	-2.69	117.90	123.11
82	A3	34	OMG	C1'-N9-C8	-2.64	119.22	126.73
82	A3	17	H2U	C5-C4-N3	2.64	119.49	116.69
82	A3	17	H2U	O2-C2-N3	-2.61	116.68	121.49
82	A3	49	5MC	C5-C4-N3	2.55	124.37	121.75
82	A3	37	YYG	C14-C13-C12	2.54	118.54	113.36
82	A3	40	5MC	O2-C2-N3	-2.50	118.39	122.33
82	A3	39	PSU	O4-C4-N3	-2.48	115.45	120.11
82	A3	58	1MA	N9-C4-N3	2.48	132.54	126.90
82	A3	54	5MU	C5-C6-N1	2.47	126.00	123.31
82	A3	46	7MG	C6-C5-C4	-2.47	118.05	122.40
82	A3	39	PSU	C6-N1-C2	-2.44	120.43	122.69
82	A3	55	PSU	O2-C2-N1	-2.43	120.28	122.79
82	A3	49	5MC	O2-C2-N3	-2.41	118.52	122.33
82	A3	32	OMC	C5-C4-N3	-2.40	117.27	121.32
82	A3	55	PSU	O4-C4-N3	-2.35	115.70	120.11
82	A3	10	2MG	N2-C2-N3	2.34	123.49	120.51
82	A3	46	7MG	O6-C6-N1	-2.32	115.76	120.11
82	A3	37	YYG	O22-C21-N20	-2.27	121.14	124.86
82	A3	26	M2G	C2-N3-C4	2.23	116.63	112.51
82	A3	34	OMG	C1'-N9-C4	2.20	132.98	126.49
82	A3	10	2MG	C5-C6-N1	2.20	118.84	113.25
82	A3	55	PSU	C6-N1-C2	-2.19	120.66	122.69
82	A3	10	2MG	N9-C8-N7	-2.16	109.39	113.40
82	A3	40	5MC	C1'-N1-C2	2.16	123.22	118.44
82	A3	40	5MC	C6-N1-C2	-2.10	118.16	120.95
82	A3	40	5MC	C5-C4-N3	2.08	123.88	121.75
82	A3	37	YYG	N3-C2-N2	-2.07	123.77	126.62
82	A3	49	5MC	N4-C4-N3	-2.03	114.83	118.51

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	A3	16	H2U	O4'-C4'-C5'-O5'
82	A3	16	H2U	C3'-C4'-C5'-O5'
82	A3	16	H2U	O4'-C1'-N1-C6
82	A3	17	H2U	O4'-C4'-C5'-O5'
82	A3	17	H2U	C3'-C4'-C5'-O5'
82	A3	26	M2G	C3'-C4'-C5'-O5'
82	A3	37	YYG	C15-C16-O18-C19
82	A3	37	YYG	N20-C21-O23-C24

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Mol	Chain	Res	Type	Atoms
82	A3	37	YYG	O22-C21-O23-C24
82	A3	49	5MC	O4'-C4'-C5'-O5'
82	A3	54	5MU	O4'-C4'-C5'-O5'
82	A3	37	YYG	O17-C16-O18-C19
82	A3	46	7MG	C3'-C4'-C5'-O5'
82	A3	54	5MU	C3'-C4'-C5'-O5'
82	A3	55	PSU	C3'-C4'-C5'-O5'
82	A3	55	PSU	O4'-C4'-C5'-O5'
82	A3	26	M2G	O4'-C4'-C5'-O5'
82	A3	58	1MA	C3'-C4'-C5'-O5'
82	A3	46	7MG	O4'-C4'-C5'-O5'
82	A3	49	5MC	C3'-C4'-C5'-O5'
82	A3	10	2MG	O4'-C4'-C5'-O5'
82	A3	58	1MA	O4'-C4'-C5'-O5'
82	A3	16	H2U	C4'-C5'-O5'-P
82	A3	16	H2U	O4'-C1'-N1-C2
82	A3	37	YYG	C12-C13-C14-C15
82	A3	46	7MG	C4'-C5'-O5'-P
82	A3	55	PSU	C4'-C5'-O5'-P
82	A3	55	PSU	O4'-C1'-C5-C4
82	A3	34	OMG	C3'-C4'-C5'-O5'
82	A3	10	2MG	C3'-C4'-C5'-O5'
82	A3	37	YYG	C14-C15-C16-O18
82	A3	37	YYG	C14-C15-C16-O17
82	A3	17	H2U	O4'-C1'-N1-C6
82	A3	34	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	A3	58	1MA	1	0
82	A3	34	OMG	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1068 ligands modelled in this entry, 1066 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
86	5CR	A3	101	82	13,14,15	0.62	0	16,17,19	1.09	2 (12%)
85	GNP	A6	701	84	34,34,34	1.81	5 (14%)	47,54,54	1.32	5 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	5CR	A3	101	82	-	0/9/10/12	0/1/1/1
85	GNP	A6	701	84	-	8/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	A6	701	GNP	PA-O3A	-6.40	1.52	1.59
85	A6	701	GNP	PB-O3A	-5.17	1.52	1.59
85	A6	701	GNP	PG-O1G	3.42	1.51	1.46
85	A6	701	GNP	PB-O2B	-3.21	1.48	1.56
85	A6	701	GNP	PG-O2G	-2.03	1.51	1.56

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	A6	701	GNP	O1G-PG-N3B	-4.37	105.34	111.77
85	A6	701	GNP	O2B-PB-O1B	4.07	118.59	109.87
85	A6	701	GNP	O1B-PB-N3B	-3.99	105.90	111.77
85	A6	701	GNP	O3G-PG-O1G	-3.34	105.08	113.45
85	A6	701	GNP	O2G-PG-O3G	2.95	115.51	107.59
86	A3	101	5CR	O-C-CA	-2.90	117.31	124.77
86	A3	101	5CR	CG-CB-CA	-2.16	110.43	113.51

There are no chirality outliers.

All (8) torsion outliers are listed below:

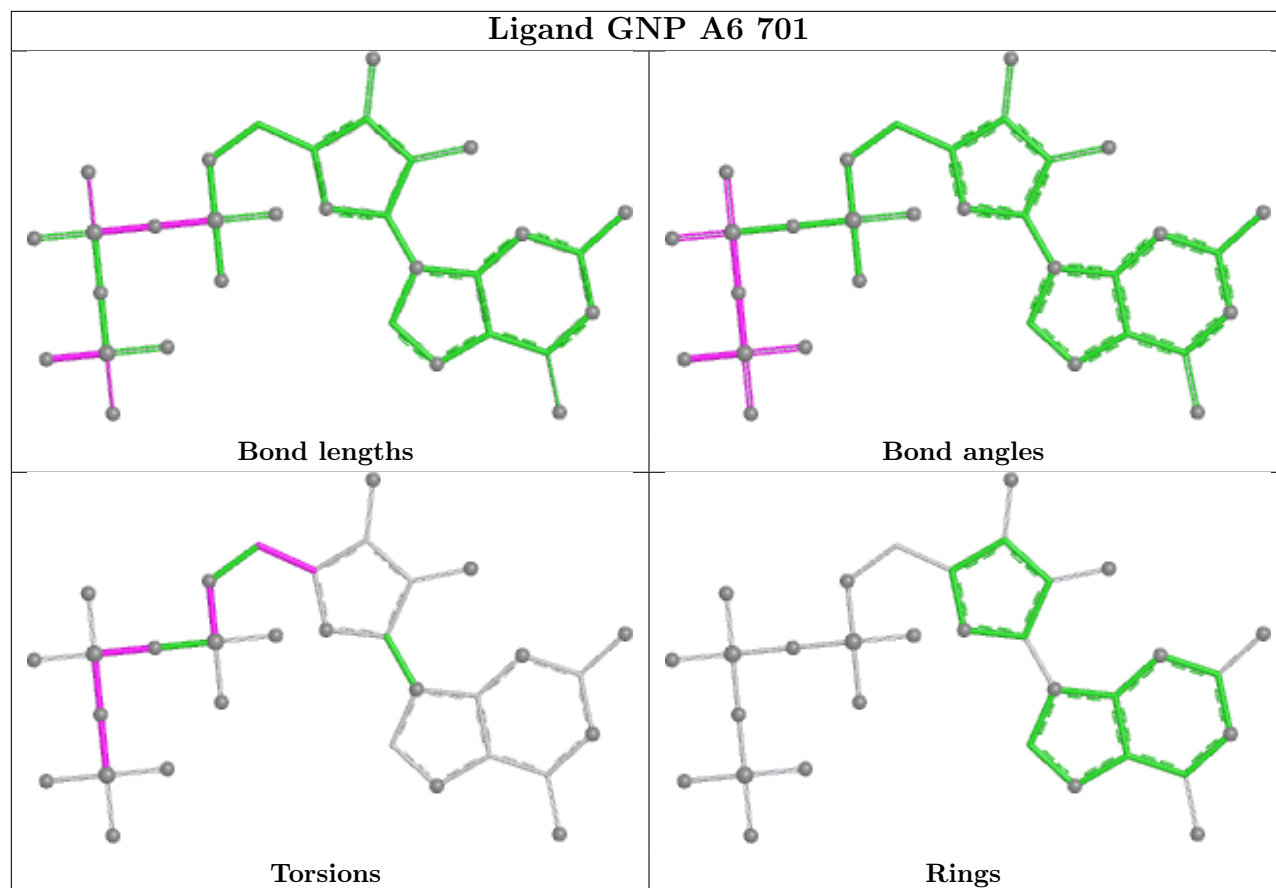
Mol	Chain	Res	Type	Atoms
85	A6	701	GNP	PB-N3B-PG-O1G
85	A6	701	GNP	PG-N3B-PB-O1B
85	A6	701	GNP	PG-N3B-PB-O3A
85	A6	701	GNP	PA-O3A-PB-O2B
85	A6	701	GNP	C5'-O5'-PA-O3A
85	A6	701	GNP	C5'-O5'-PA-O1A
85	A6	701	GNP	C3'-C4'-C5'-O5'
85	A6	701	GNP	PA-O3A-PB-O1B

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A3	101	5CR	3	0
85	A6	701	GNP	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

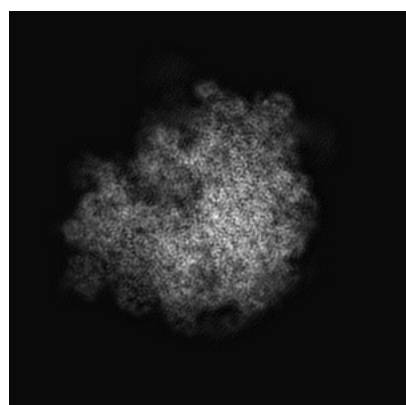
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4140. These allow visual inspection of the internal detail of the map and identification of artifacts.

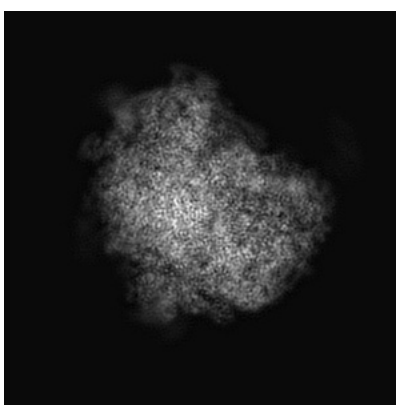
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

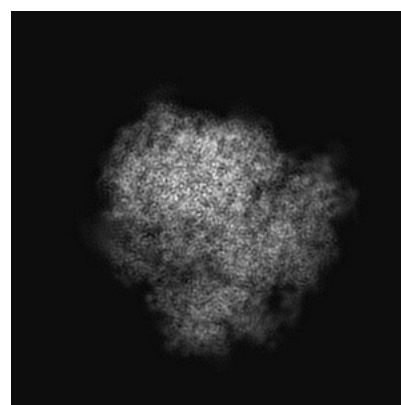
6.1.1 Primary map



X



Y

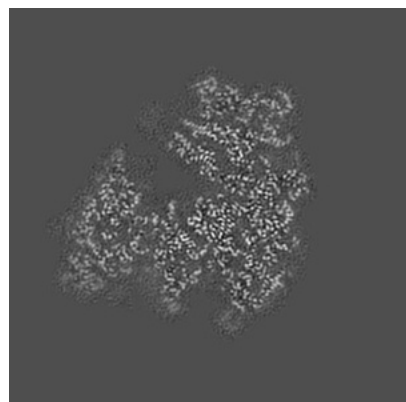


Z

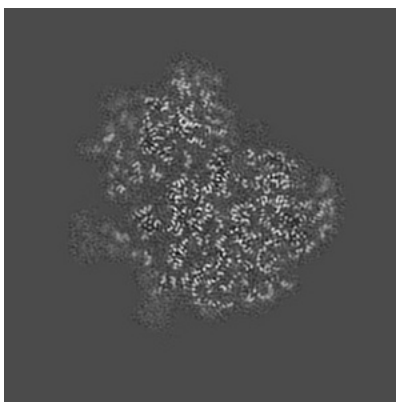
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

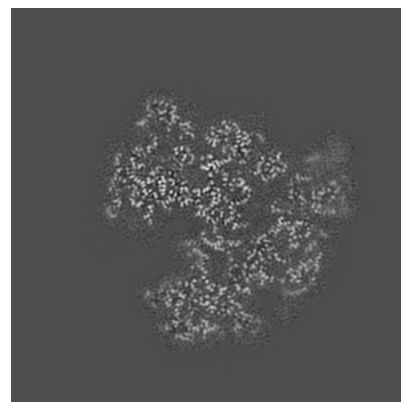
6.2.1 Primary map



X Index: 206



Y Index: 206

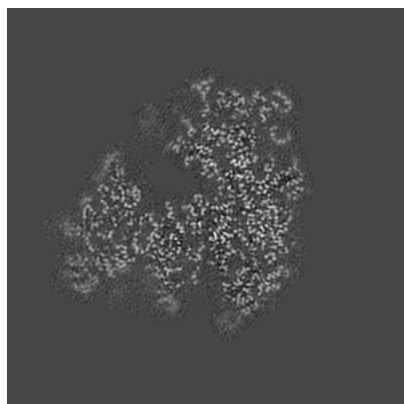


Z Index: 206

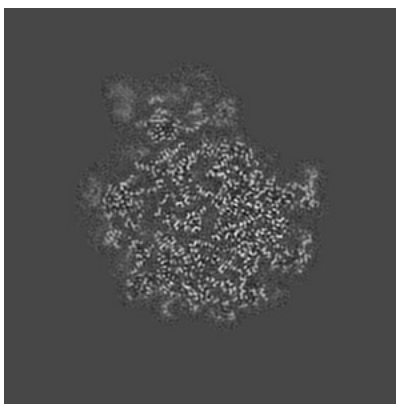
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

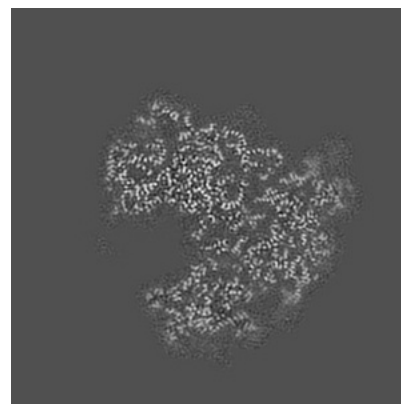
6.3.1 Primary map



X Index: 209



Y Index: 239

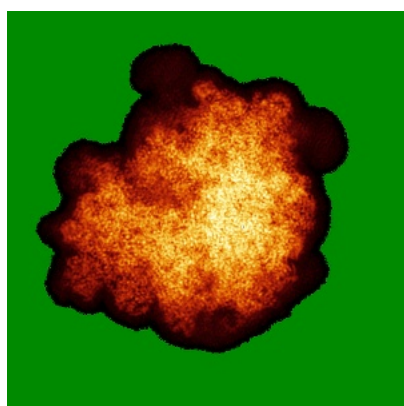


Z Index: 198

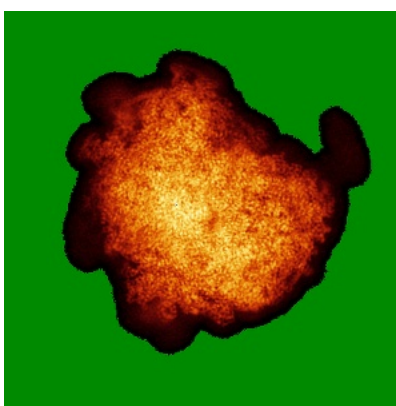
The images above show the largest variance slices of the map in three orthogonal directions.

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

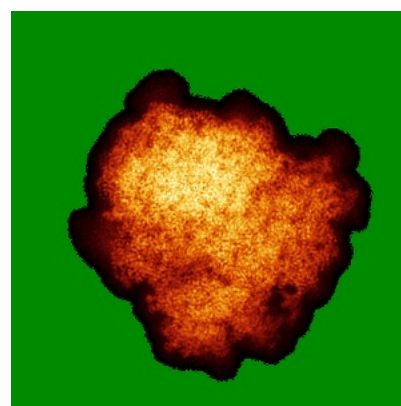
6.4.1 Primary map



X



Y

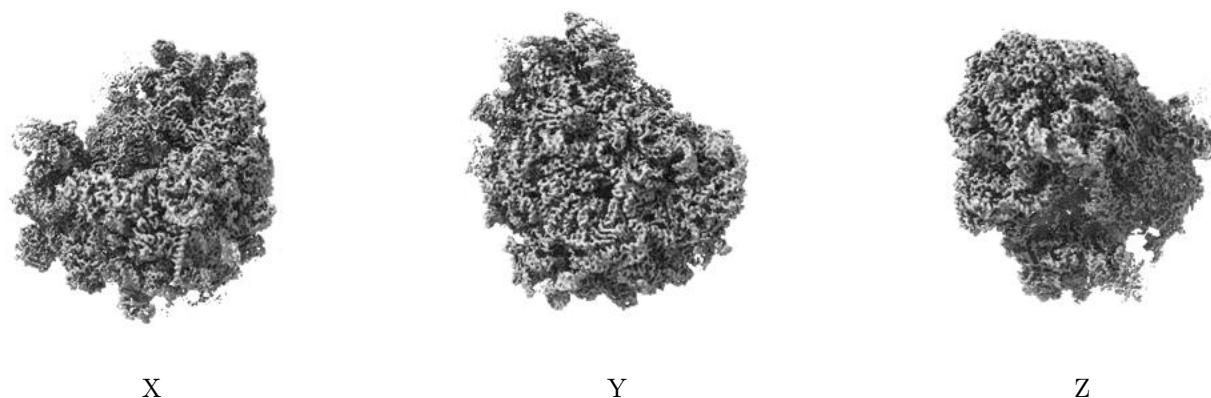


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

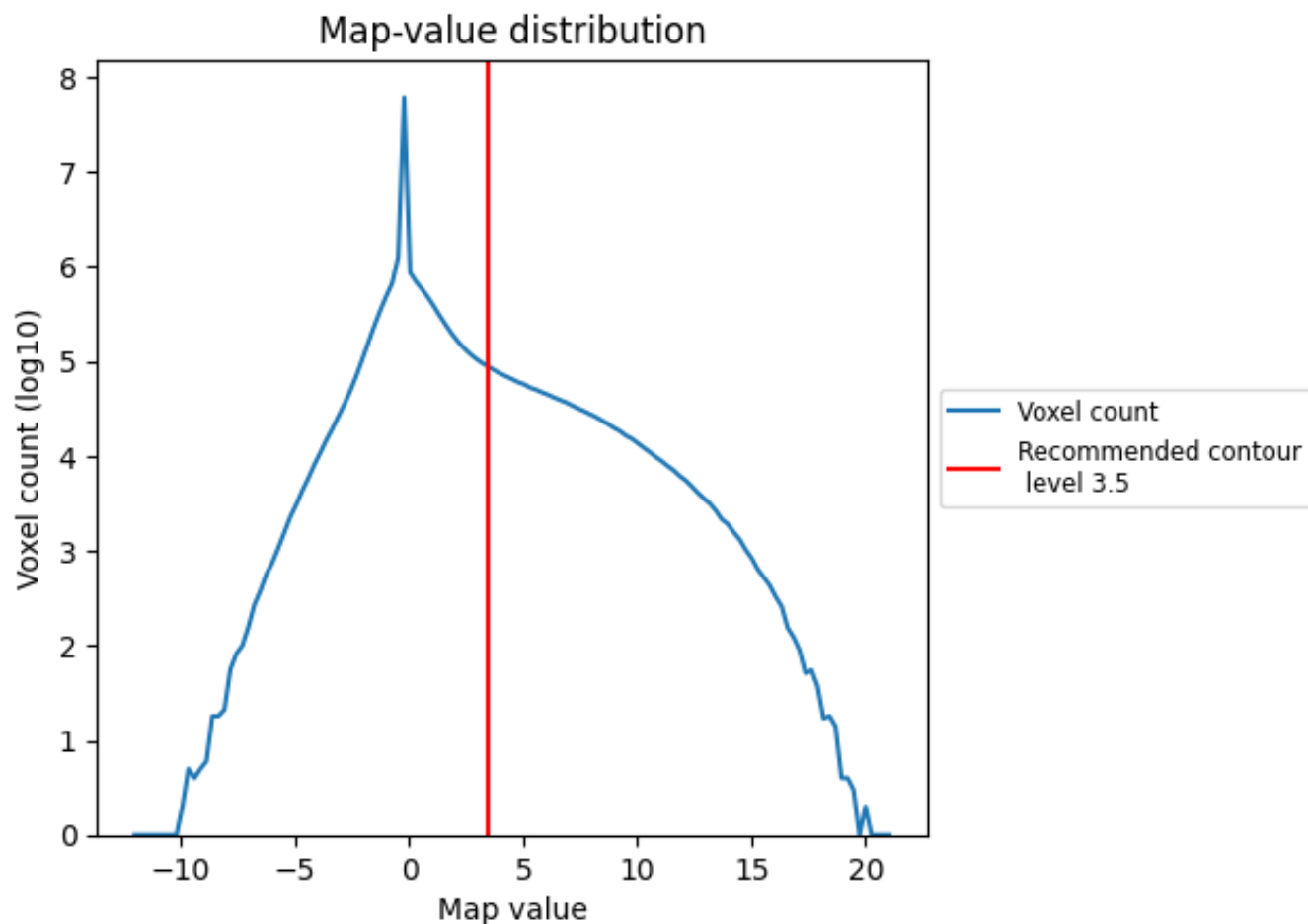
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

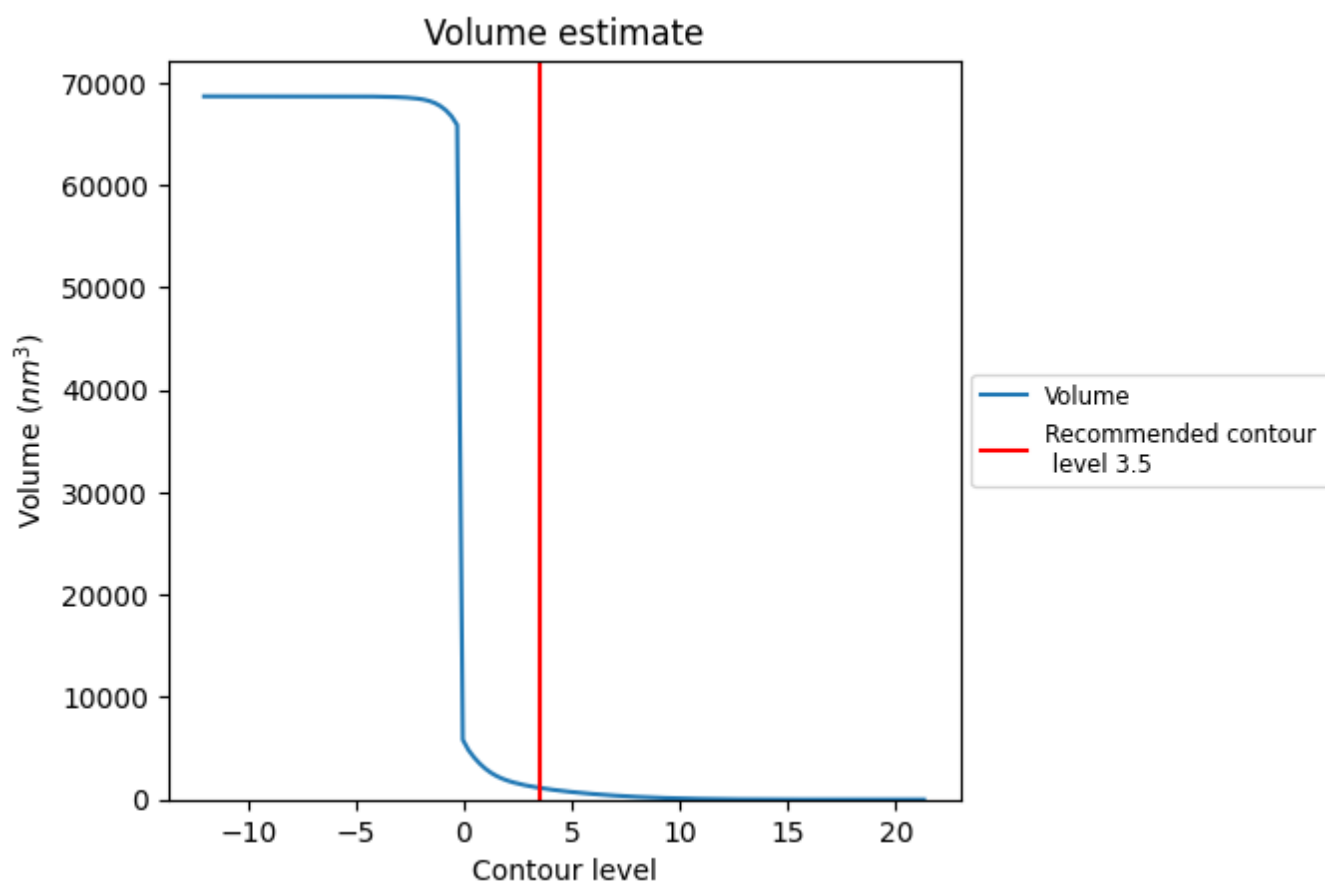
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

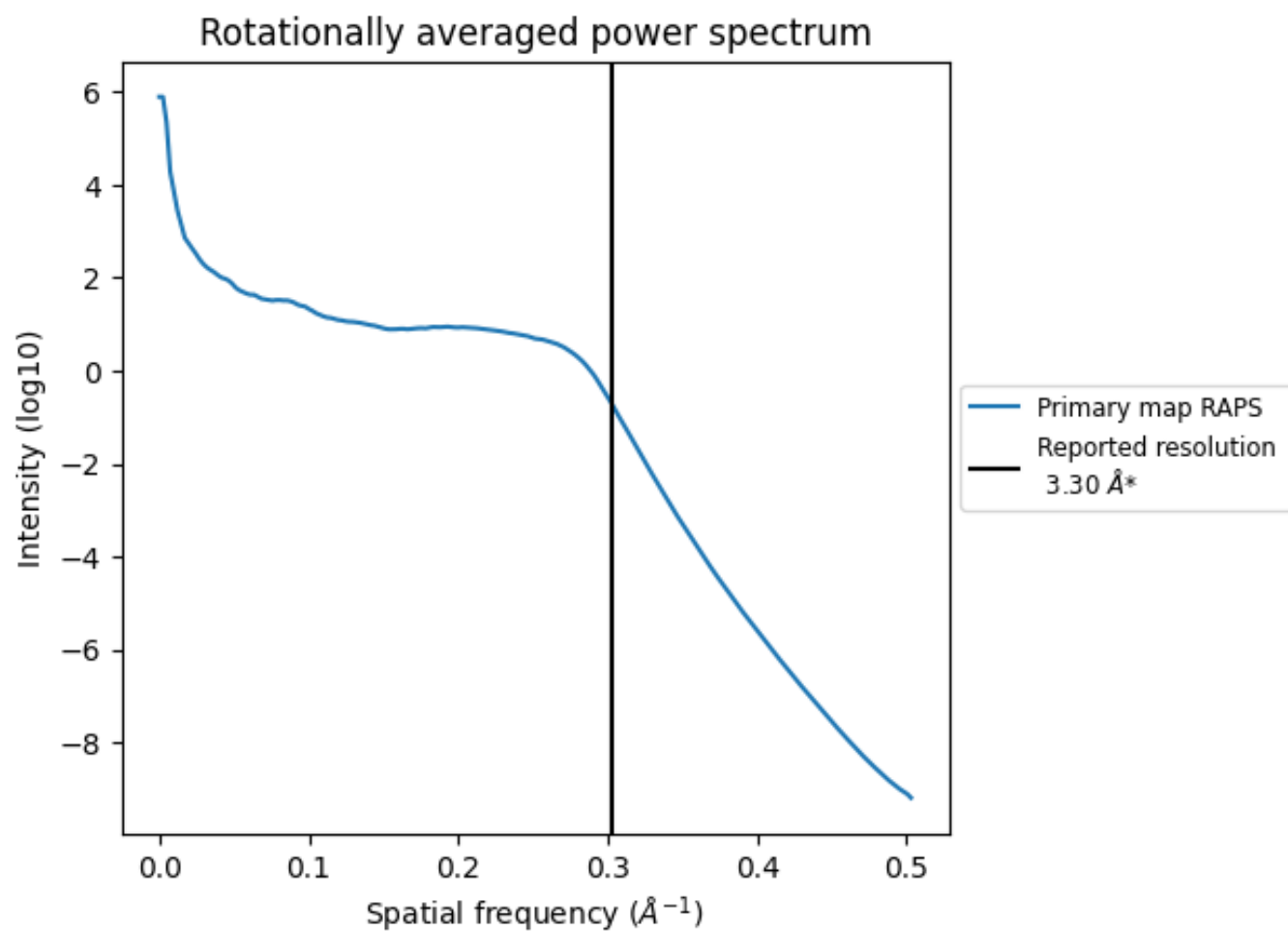
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1149 nm³; this corresponds to an approximate mass of 1038 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

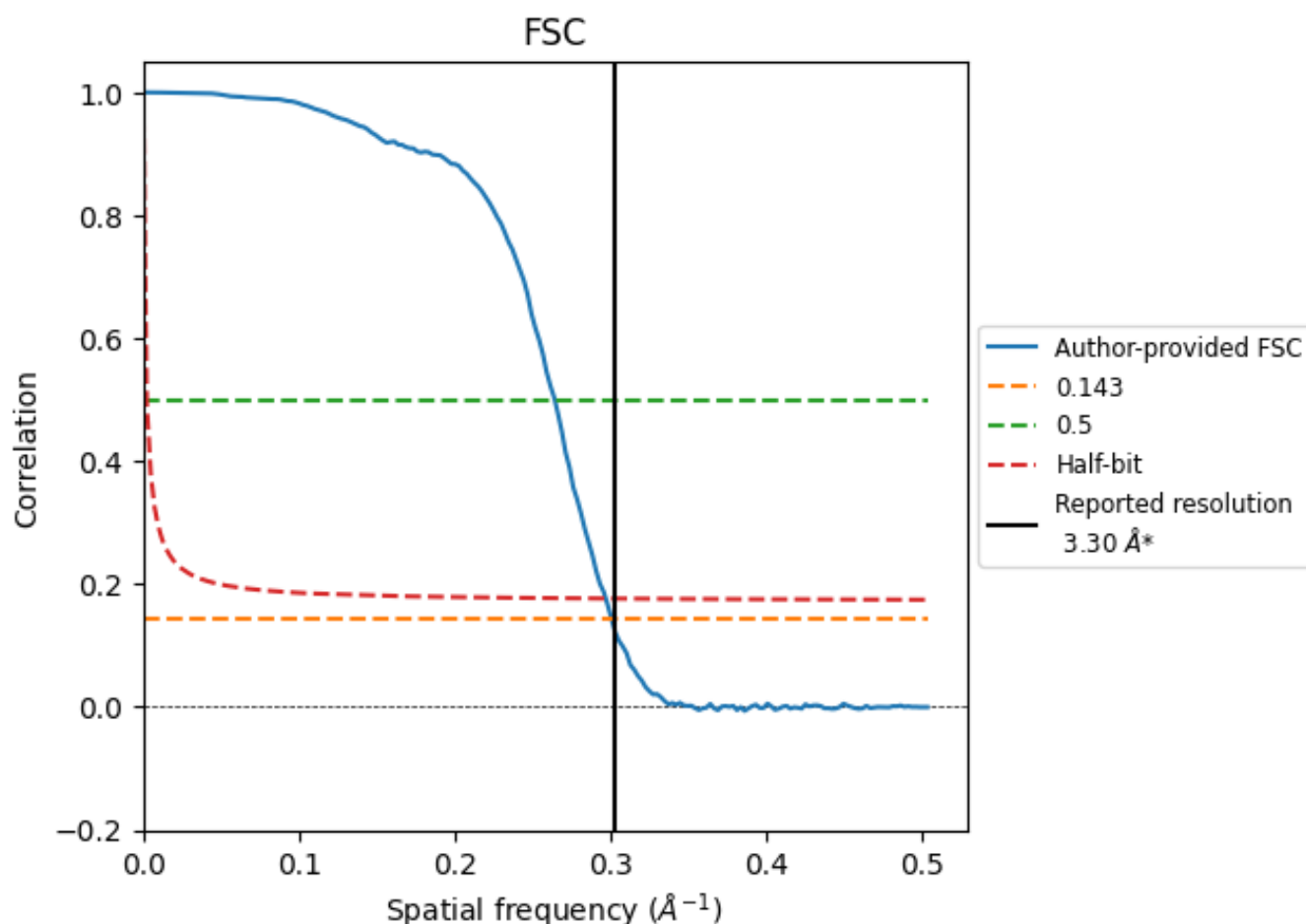


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

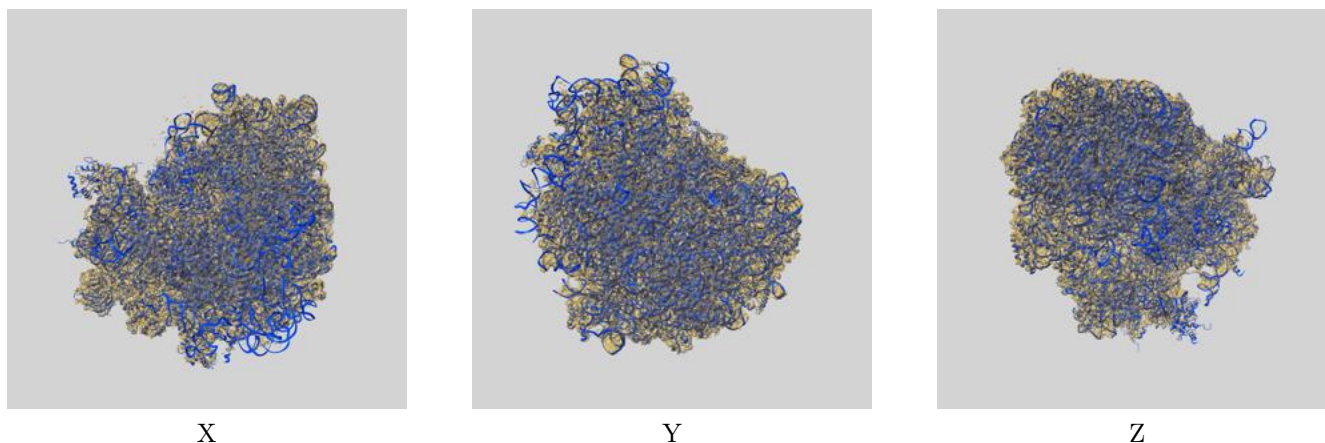
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.33	3.79	3.37
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

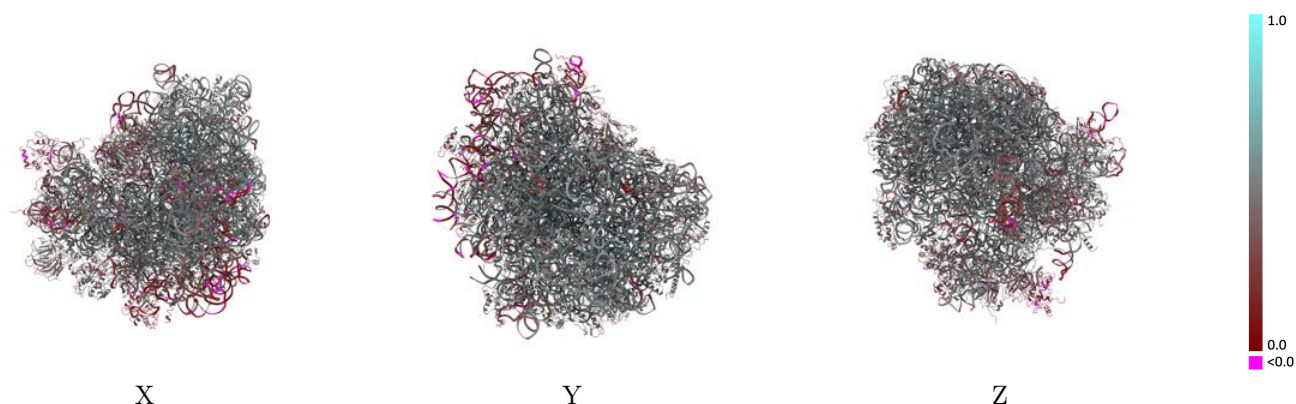
This section contains information regarding the fit between EMDB map EMD-4140 and PDB model 5M1J. Per-residue inclusion information can be found in section [3](#) on page [24](#).

9.1 Map-model overlay [i](#)



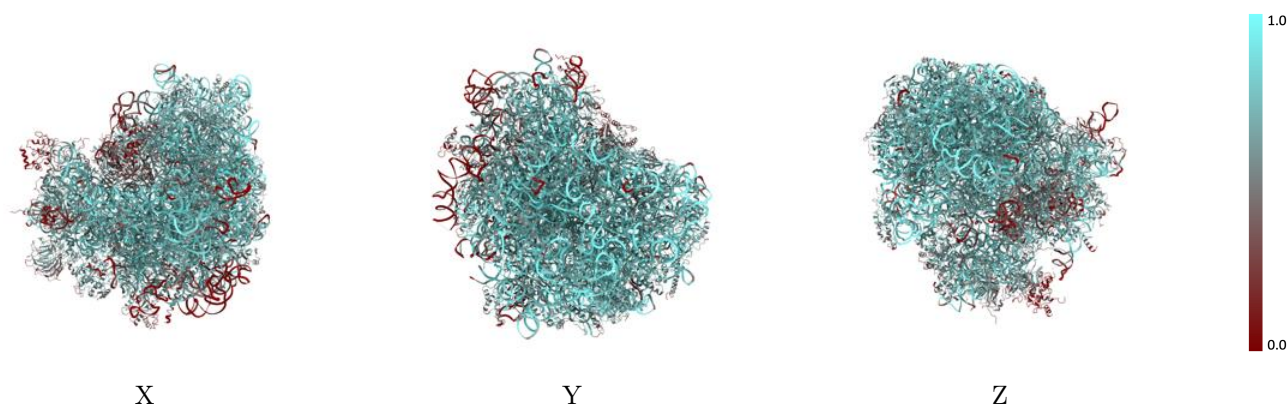
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



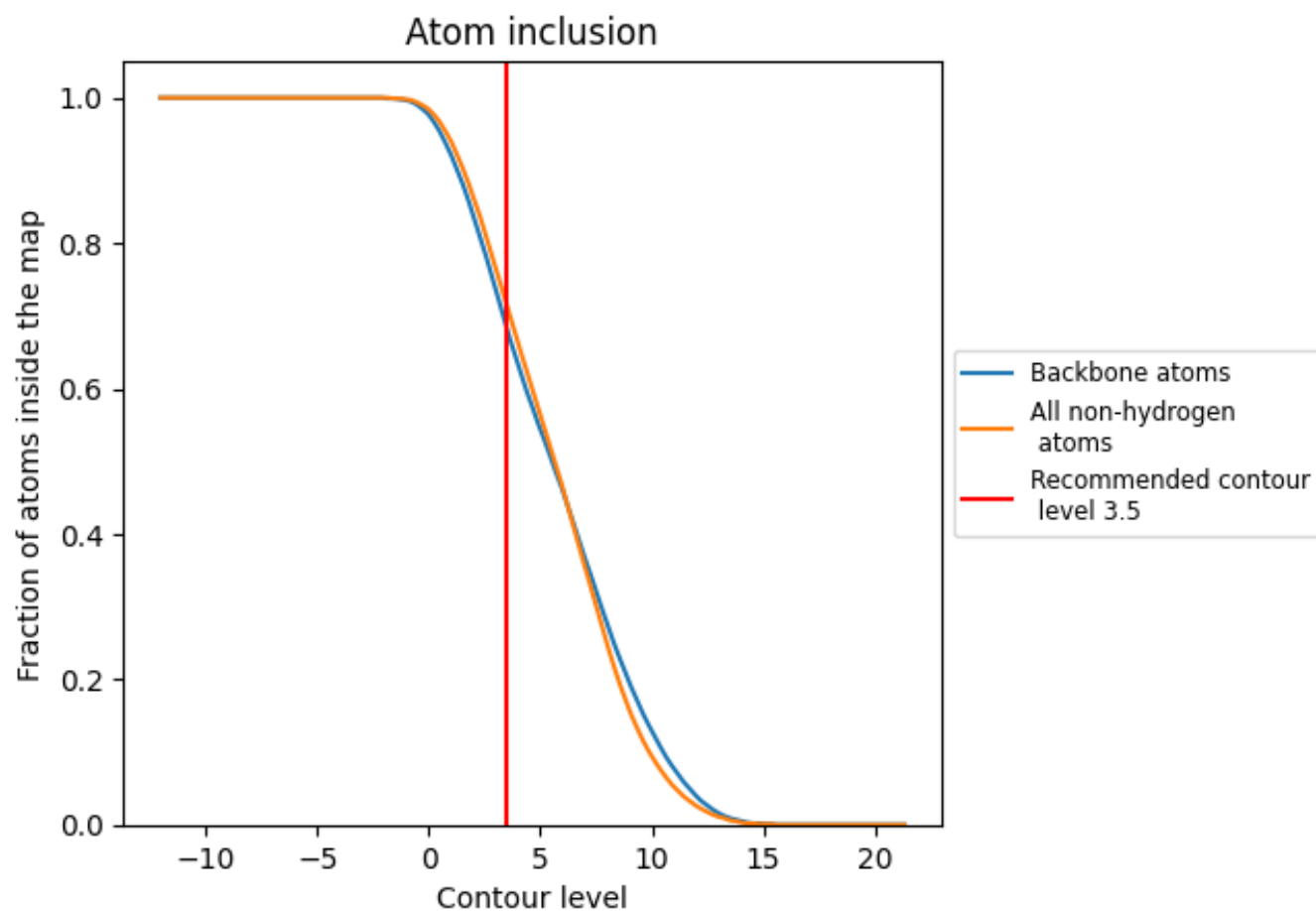
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 71% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7140	 0.4500
14	 0.8080	 0.4760
22	 0.7850	 0.4560
34	 0.8820	 0.5110
44	 0.8650	 0.5010
A1	 0.4290	 0.3930
A2	 0.6230	 0.4220
A3	 0.7560	 0.4830
A5	 0.7330	 0.4970
A6	 0.2620	 0.3170
B2	 0.6170	 0.4110
B5	 0.7060	 0.4680
C2	 0.6860	 0.4660
C5	 0.7070	 0.4570
D2	 0.5900	 0.4120
D5	 0.6310	 0.4150
E2	 0.6600	 0.4450
E5	 0.6230	 0.4440
F2	 0.5650	 0.3700
F5	 0.7110	 0.4720
G2	 0.5570	 0.3830
G5	 0.6170	 0.4160
H2	 0.4940	 0.3310
H5	 0.6450	 0.4520
I2	 0.6480	 0.4210
I5	 0.6570	 0.4460
J2	 0.6600	 0.4440
J5	 0.6080	 0.3880
K2	 0.5250	 0.3470
K5	 0.7200	 0.4870
L2	 0.6330	 0.4520
L5	 0.6820	 0.4510
M2	 0.0920	 0.1650
M5	 0.6520	 0.4380
N2	 0.6520	 0.4290



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Chain	Atom inclusion	Q-score
N5	 0.7620	 0.5020
O2	 0.6630	 0.4420
P2	 0.5150	 0.3600
P5	 0.6810	 0.4310
Q2	 0.6310	 0.4090
Q5	 0.7250	 0.4750
R2	 0.5770	 0.3890
R5	 0.6440	 0.4420
S2	 0.5540	 0.3540
S5	 0.6910	 0.4670
T2	 0.5810	 0.3910
T5	 0.7020	 0.4680
U2	 0.5100	 0.3610
U5	 0.5960	 0.4020
V2	 0.6040	 0.3960
V5	 0.6610	 0.4760
W2	 0.7090	 0.4780
W5	 0.4480	 0.3500
X2	 0.6680	 0.4740
X5	 0.6890	 0.4780
X7	 0.4980	 0.4460
Y2	 0.6000	 0.4010
Y5	 0.6760	 0.4690
Z2	 0.5890	 0.4250
Z5	 0.6390	 0.4170
a2	 0.6930	 0.4500
a5	 0.7020	 0.4470
b2	 0.6280	 0.4240
b5	 0.6620	 0.4330
c2	 0.6080	 0.4490
c5	 0.6520	 0.4460
d2	 0.7300	 0.4580
d5	 0.6650	 0.4500
e2	 0.5470	 0.4060
e5	 0.7140	 0.5000
f2	 0.2070	 0.2050
f5	 0.7460	 0.5180
g2	 0.5010	 0.3710
g5	 0.6840	 0.4650
h5	 0.6640	 0.4510
i5	 0.6040	 0.3940
j5	 0.7860	 0.5090

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Chain	Atom inclusion	Q-score
k5	 0.5940	 0.4010
l5	 0.7160	 0.4750
m5	 0.6780	 0.4670
n5	 0.7080	 0.4820
o5	 0.6510	 0.4710
p5	 0.6490	 0.4480