



Full wwPDB EM Validation Report ⓘ

Jul 8, 2026 – 04:43 PM JST

PDB ID : 23WI / pdb_000023wi
EMDB ID : EMD-67081
Title : Subtomogram average of 70S ribosome (11x11) using CRYO ARM 300II
Authors : Yanagisawa, H.; Makino, F.; Eisenstein, F.; Miyata, T.; Kinoshita, M.; Kikkawa, M.; Namba, K.
Deposited on : 2026-02-23
Resolution : 2.60 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

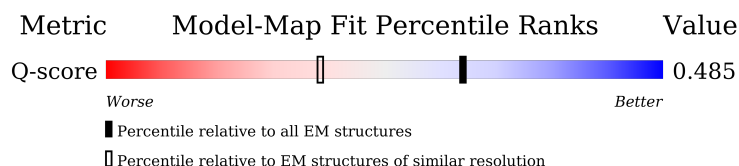
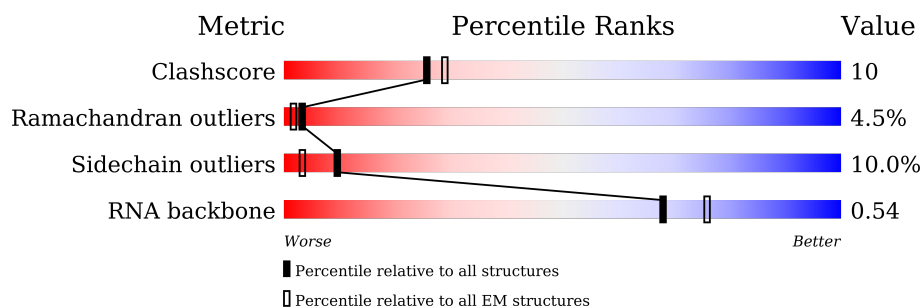
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	a	1539	79% 60% 32% 8%
2	b	218	100% 51% 41% 6%
3	c	206	98% 58% 36% 5%

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Mol	Chain	Length	Quality of chain
4	d	205	
5	e	157	
6	f	100	
7	g	151	
8	h	129	
9	i	127	
10	j	98	
11	k	116	
12	l	123	
13	m	114	
14	n	101	
15	o	88	
16	p	82	
17	q	80	
18	r	65	
19	s	79	
20	t	85	
21	u	65	
22	A	886	
23	B	120	
24	C	271	
25	D	209	
26	E	201	
27	F	177	
28	G	176	

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Mol	Chain	Length	Quality of chain
29	J	142	
30	K	122	
31	L	143	
32	M	136	
33	N	120	
34	O	116	
35	P	114	
36	Q	117	
37	R	103	
38	S	110	
39	T	93	
40	U	102	
41	V	94	
42	W	75	
43	X	77	
44	Y	63	
45	Z	58	
46	0	56	
47	1	50	
48	2	46	
49	3	64	
50	4	38	
51	6	66	
52	5	2014	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	5MU	5	1939	-	-	X	-

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 141435 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called RNA (1539-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1539	Total	C	N	O	P	0	0
			33029	14738	6052	10700	1539		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 6 is a protein called Small ribosomal subunit protein bS6, non-modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			794	495	164	132	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 22 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A	886	Total	C	N	O	P	0	0
			19047	8500	3532	6129	886		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	5MC	U	conflict	GB 2962093202

- Molecule 23 is a RNA chain called 30S ribosomal protein S.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

- Molecule 24 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 25 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 28 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 29 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 30 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 31 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 32 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 33 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 34 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	O	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 35 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 36 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Q	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 37 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 38 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 39 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 40 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	U	102	Total	C	N	O		
			779	492	146	141	0	0

- Molecule 41 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	V	94	Total	C	N	O	S	
			753	479	137	134	3	0

- Molecule 42 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	W	75	Total	C	N	O	S	
			575	356	116	102	1	0

- Molecule 43 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	X	77	Total	C	N	O	S	
			625	388	129	106	2	0

- Molecule 44 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	Y	63	Total	C	N	O	S	
			509	313	99	95	2	0

- Molecule 45 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	Z	58	Total	C	N	O	S	
			449	281	87	79	2	0

- Molecule 46 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	0	56	Total	C	N	O	S	
			444	269	94	80	1	0

- Molecule 47 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 48 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 49 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 50 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 51 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 52 is a RNA chain called RNA (2014-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
52	5	2014	Total	C	N	O	P	0	0
			43229	19288	7928	13999	2014		

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	a	82	Total	Mg	0
			82	82	
53	n	1	Total	Mg	0
			1	1	
53	A	63	Total	Mg	0
			63	63	

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Mol	Chain	Residues	Atoms		AltConf
53	B	7	Total 7	Mg 7	0
53	C	1	Total 1	Mg 1	0
53	D	1	Total 1	Mg 1	0
53	E	1	Total 1	Mg 1	0
53	N	1	Total 1	Mg 1	0
53	0	1	Total 1	Mg 1	0
53	5	170	Total 170	Mg 170	0

- Molecule 54 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
54	a	1	Total 1	Cl 1	0
54	5	1	Total 1	Cl 1	0

- Molecule 55 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
55	B	1	Total 1	Na 1	0
55	5	1	Total 1	Na 1	0

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	4	1	Total 1	Zn 1	0
56	6	1	Total 1	Zn 1	0

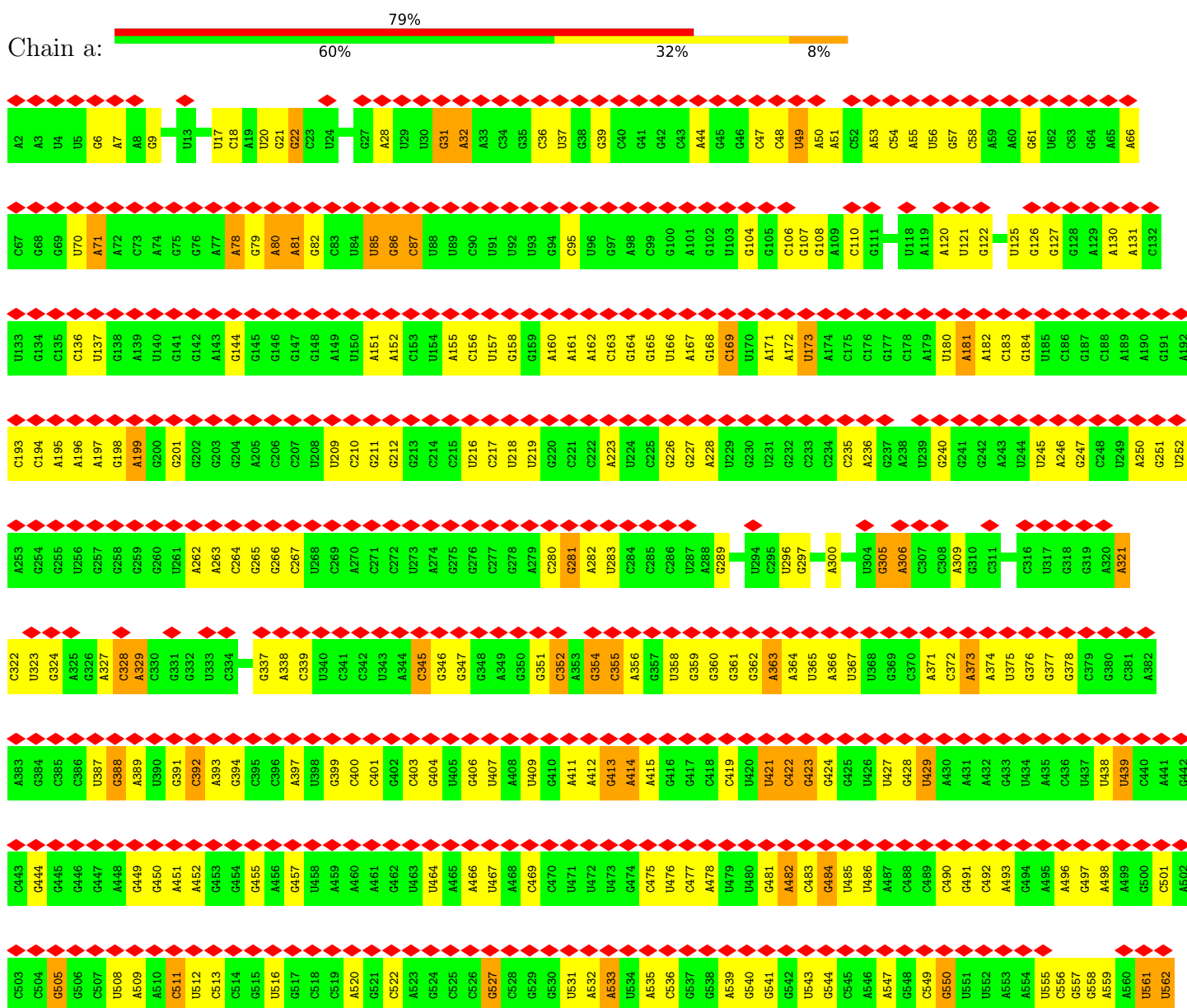
- Molecule 57 is water.

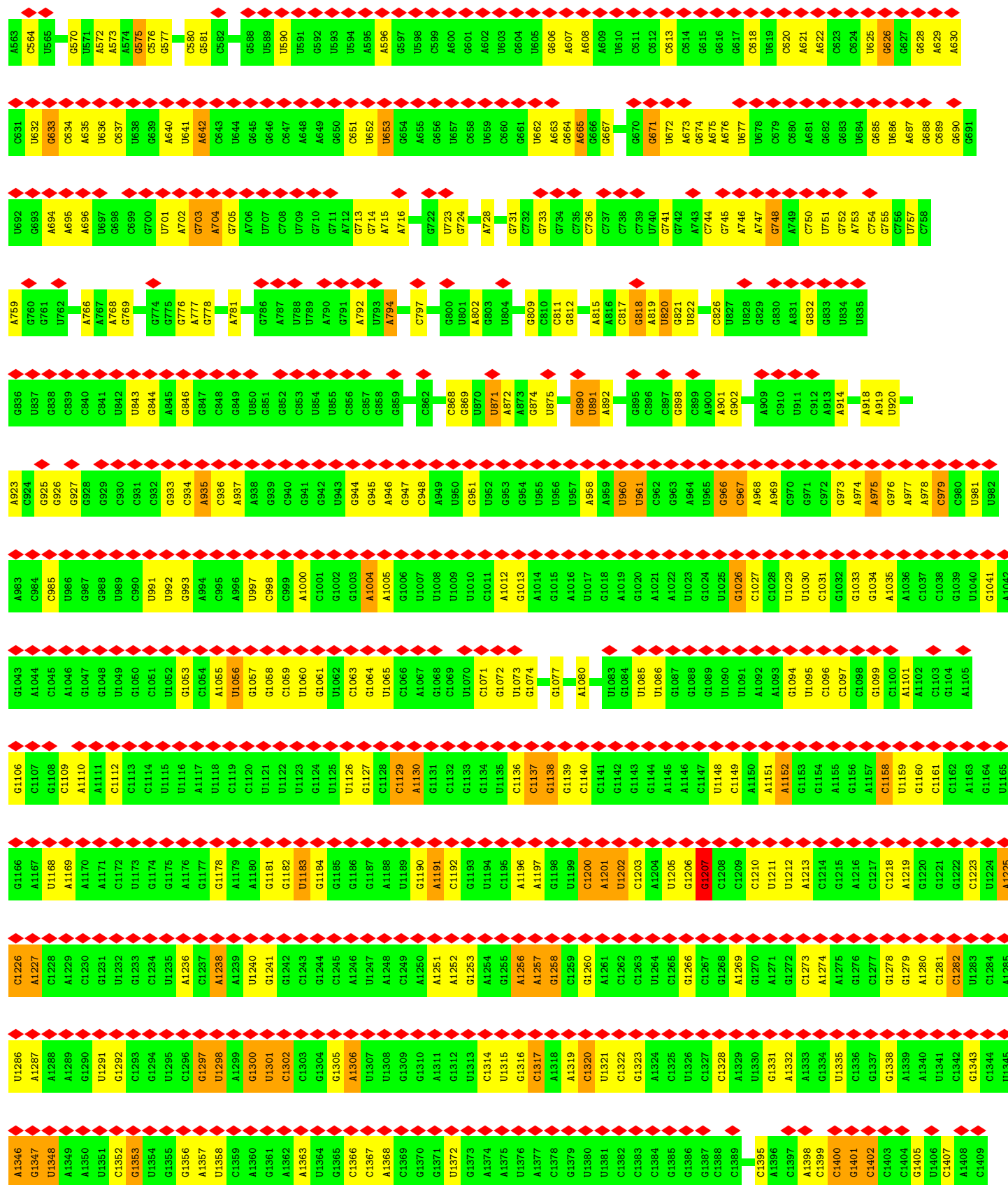
Mol	Chain	Residues	Atoms		AltConf
57	a	9	Total 9	O 9	0
57	A	2	Total 2	O 2	0
57	D	1	Total 1	O 1	0
57	K	1	Total 1	O 1	0
57	5	8	Total 8	O 8	0

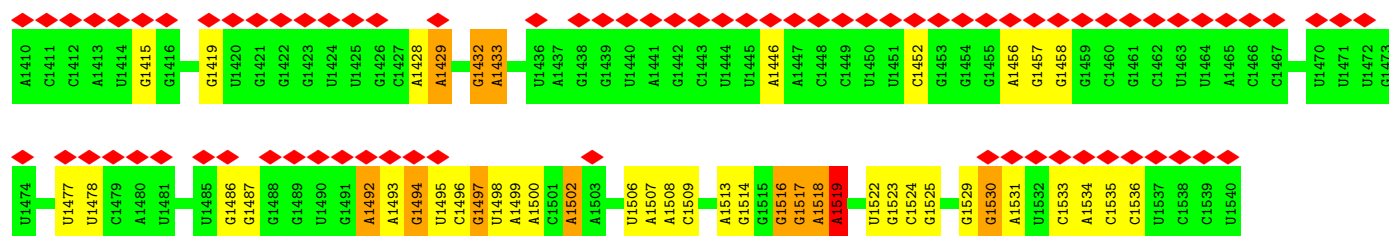
3 Residue-property plots

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.

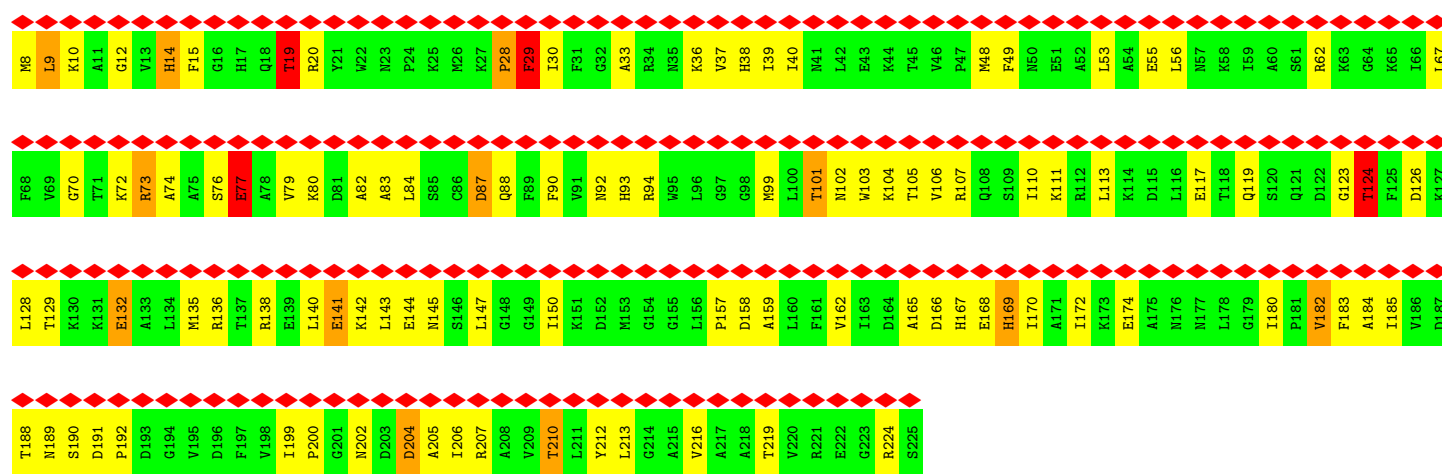
• Molecule 1: RNA (1539-MER)







• Molecule 2: Small ribosomal subunit protein uS2

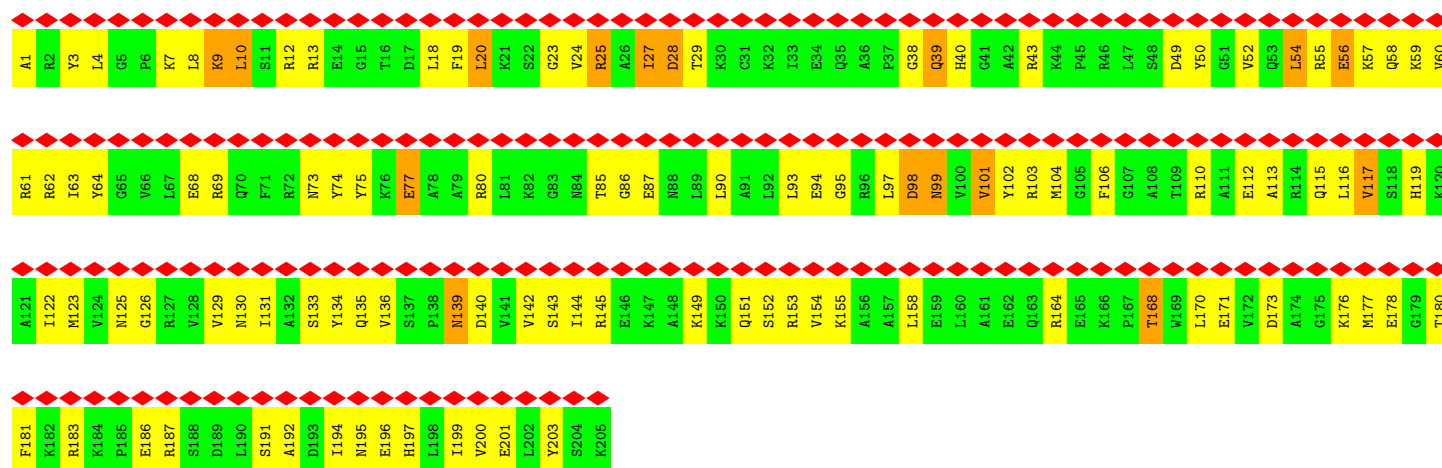


• Molecule 3: Small ribosomal subunit protein uS3

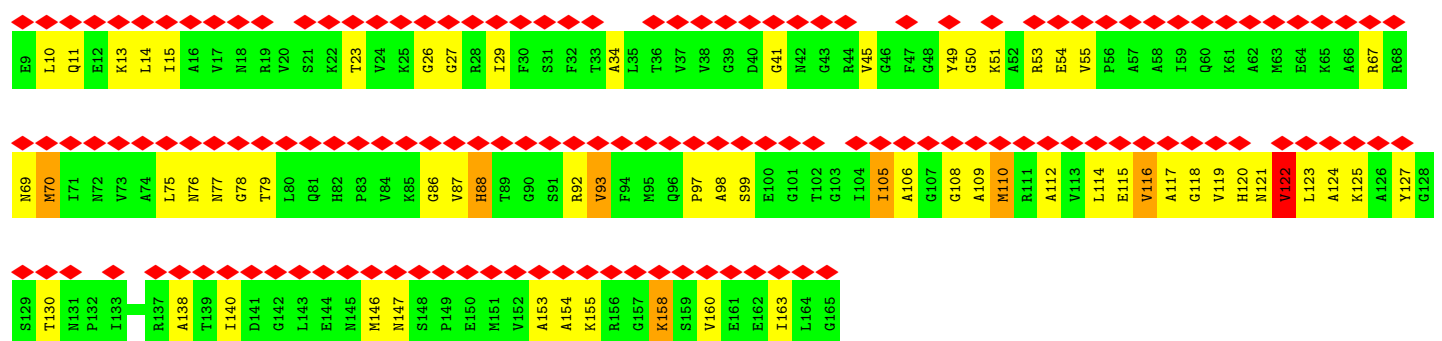
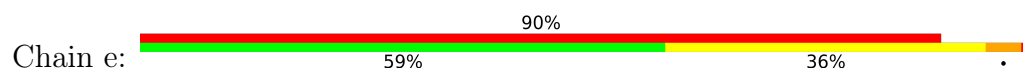


• Molecule 4: Small ribosomal subunit protein uS4

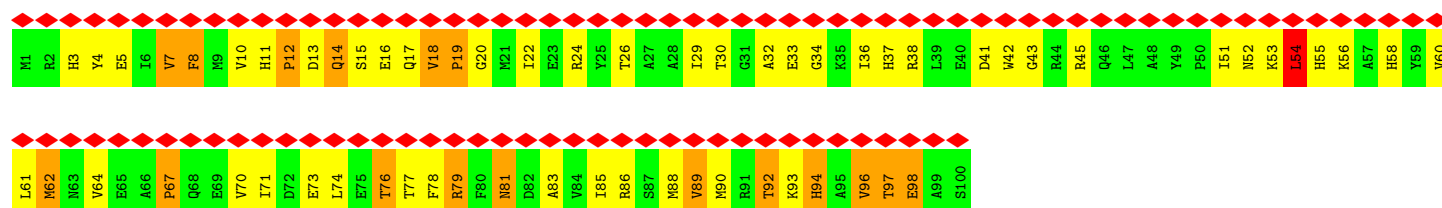




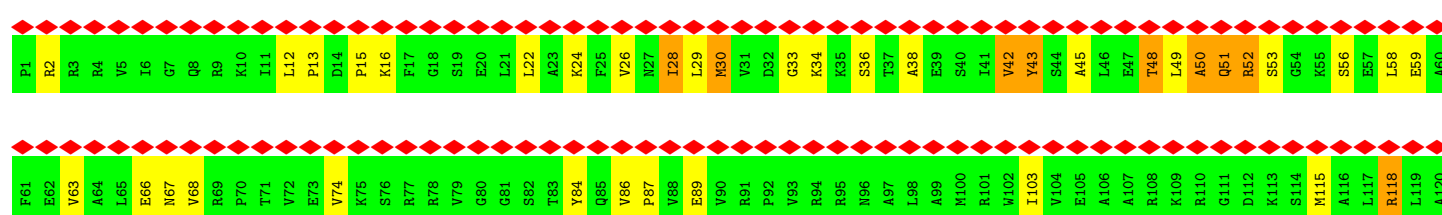
• Molecule 5: Small ribosomal subunit protein uS5

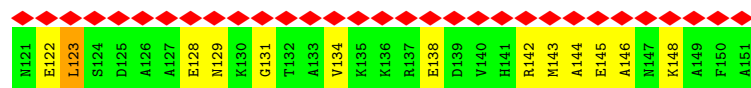


• Molecule 6: Small ribosomal subunit protein bS6, non-modified isoform



• Molecule 7: Small ribosomal subunit protein uS7





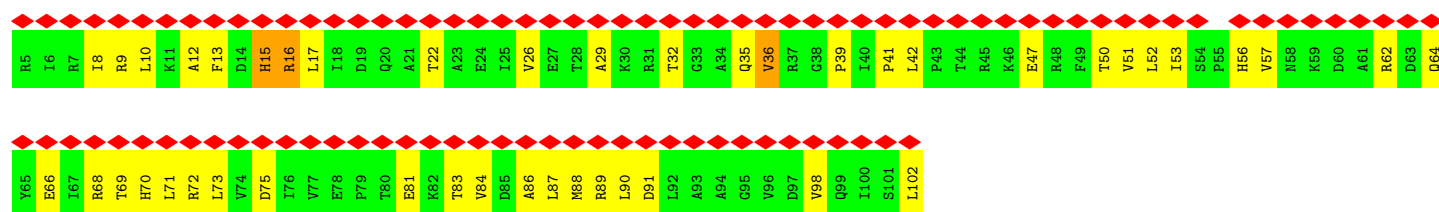
• Molecule 8: Small ribosomal subunit protein uS8



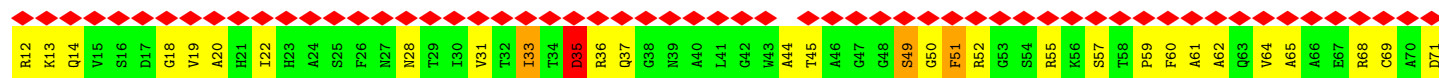
• Molecule 9: Small ribosomal subunit protein uS9

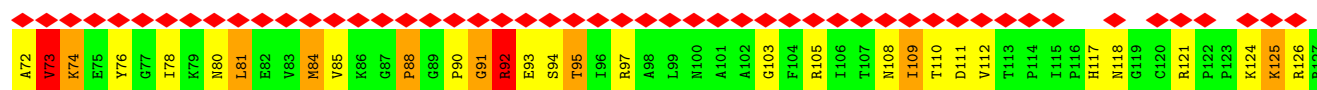


• Molecule 10: Small ribosomal subunit protein uS10



• Molecule 11: Small ribosomal subunit protein uS11





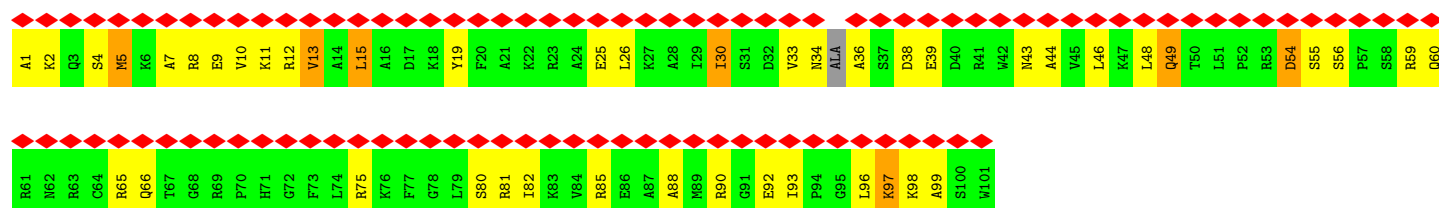
• Molecule 12: Small ribosomal subunit protein uS12



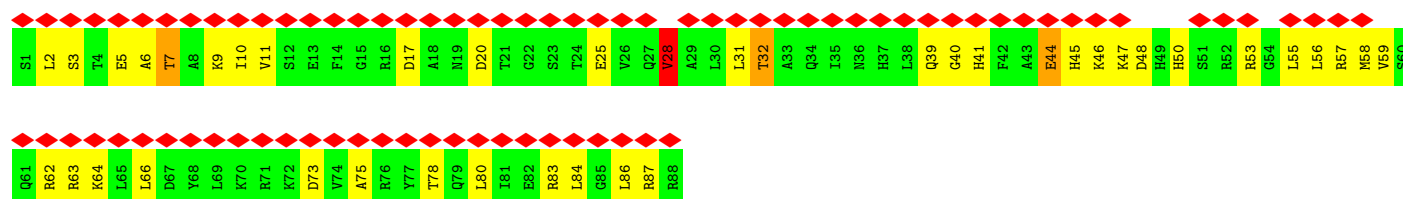
• Molecule 13: Small ribosomal subunit protein uS13



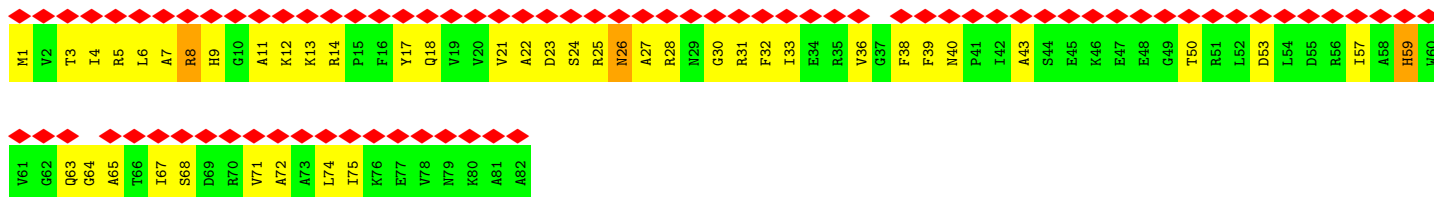
• Molecule 14: Small ribosomal subunit protein uS14



• Molecule 15: Small ribosomal subunit protein uS15



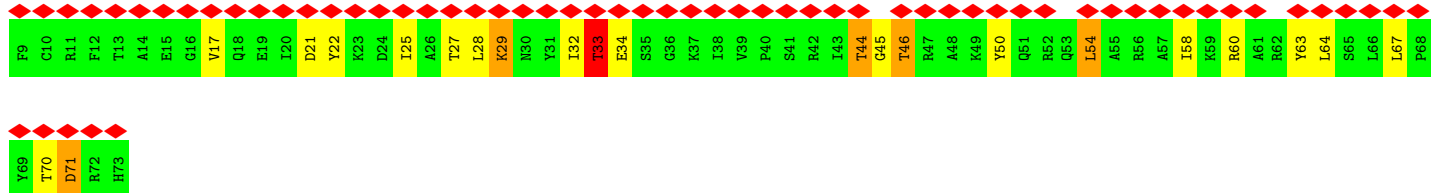
- Molecule 16: 30S ribosomal protein S16



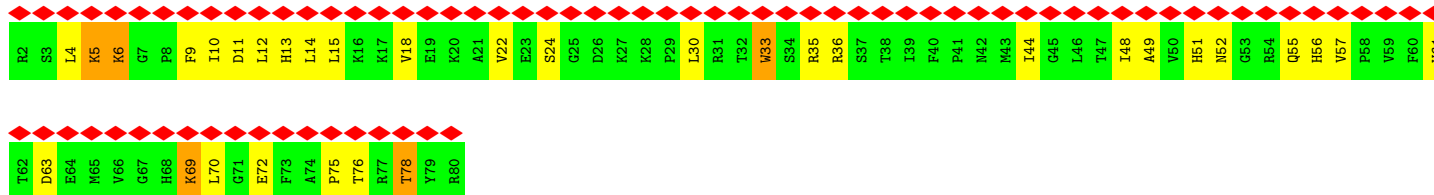
- Molecule 17: Small ribosomal subunit protein uS17



- Molecule 18: Small ribosomal subunit protein bS18



- Molecule 19: Small ribosomal subunit protein uS19

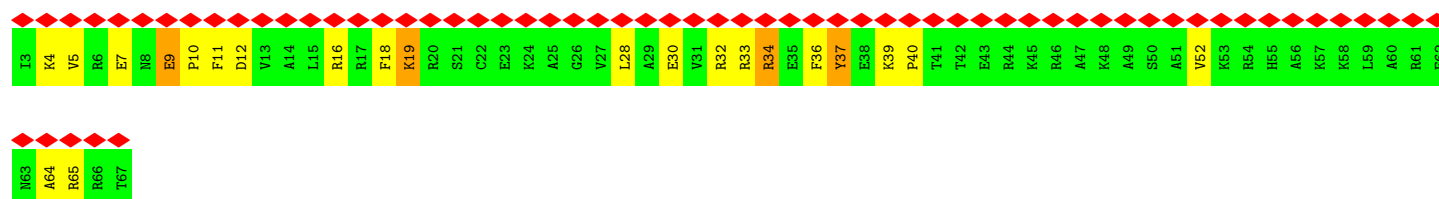


- Molecule 20: Small ribosomal subunit protein bS20

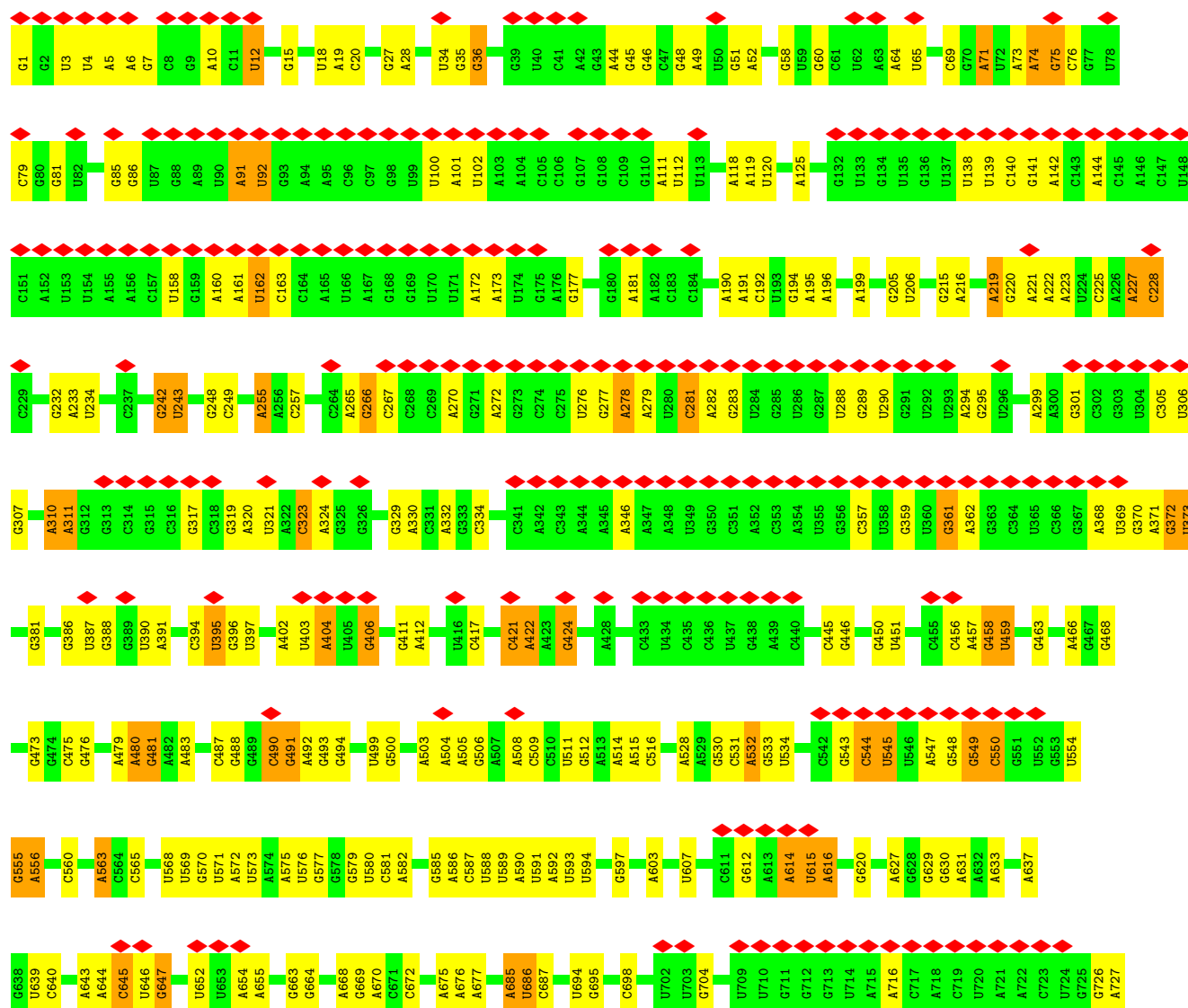


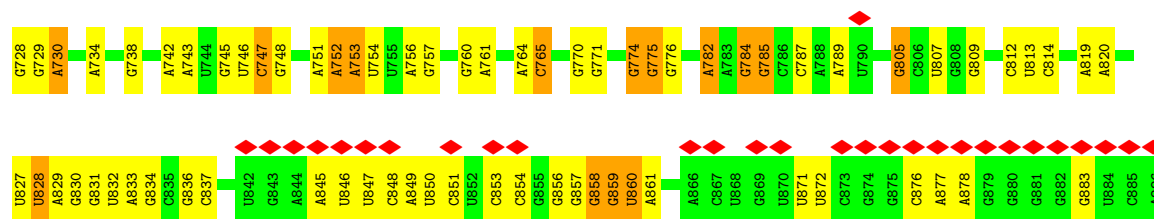


• Molecule 21: Small ribosomal subunit protein bS21

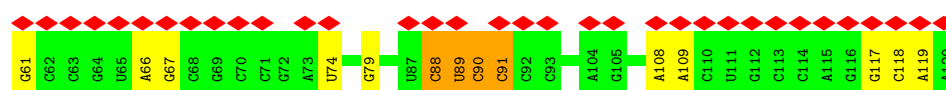
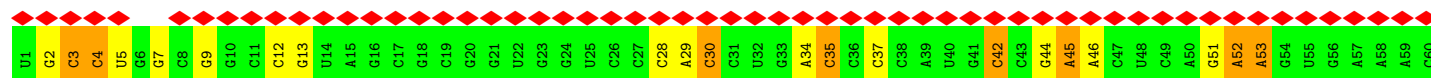
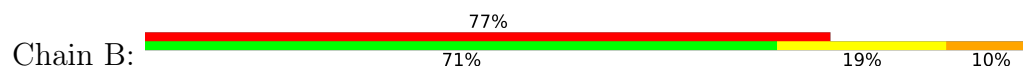


• Molecule 22: 16S rRNA

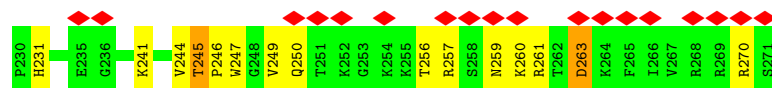
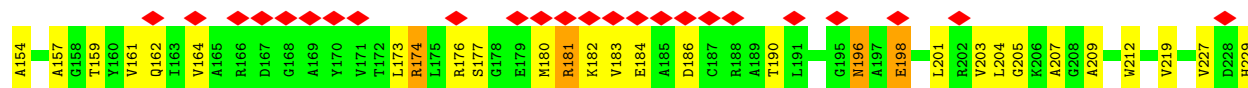
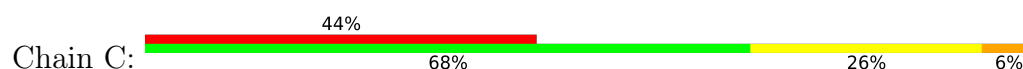




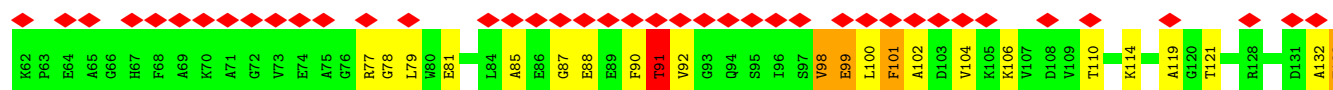
• Molecule 23: 30S ribosomal protein S

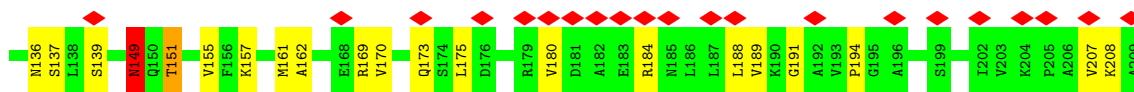


• Molecule 24: Large ribosomal subunit protein uL2

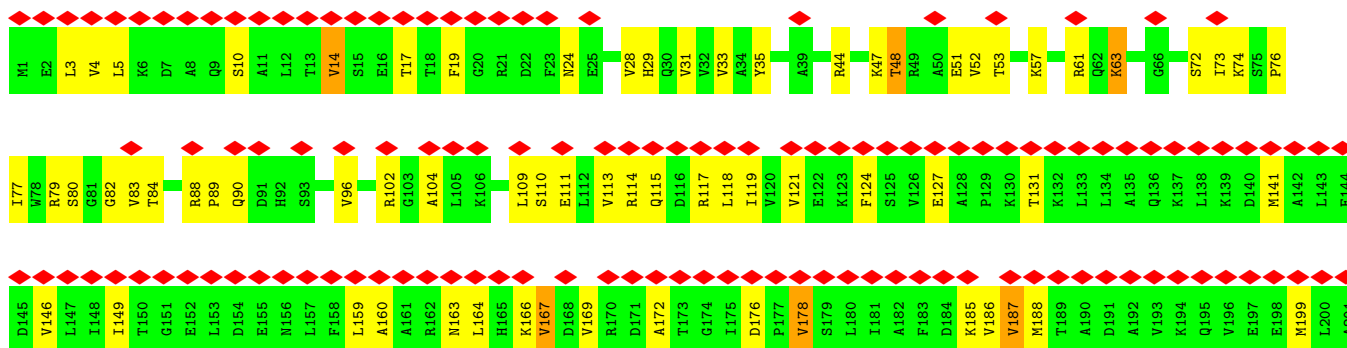


• Molecule 25: Large ribosomal subunit protein uL3

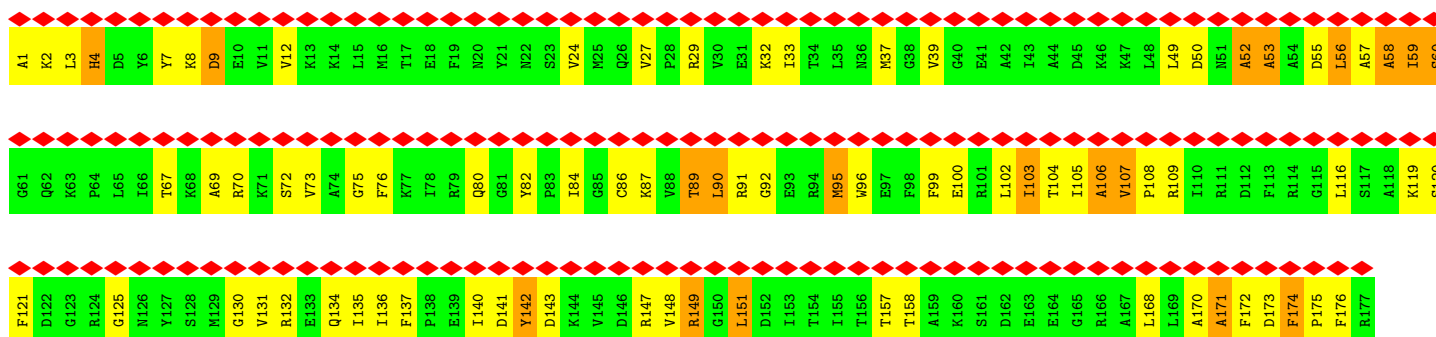




• Molecule 26: 50S ribosomal protein L4



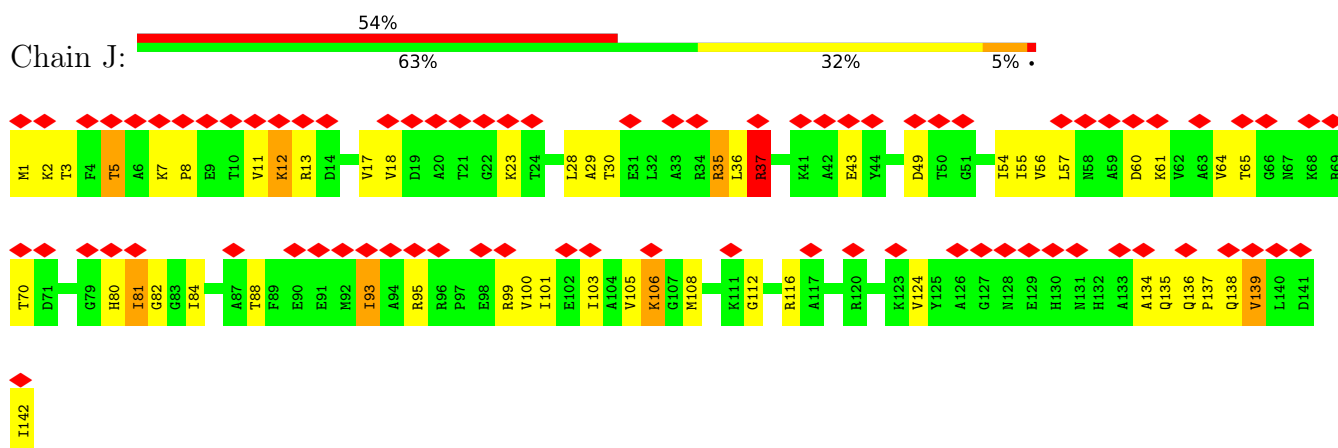
• Molecule 27: 50S ribosomal protein L5



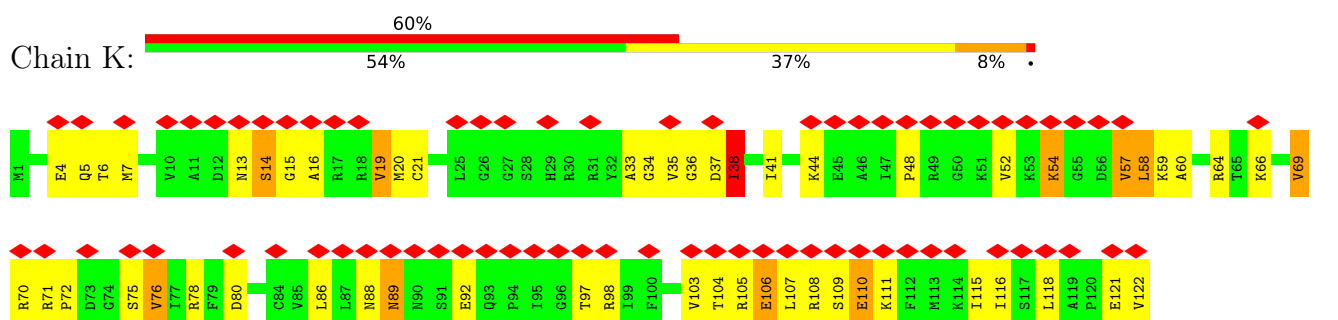
• Molecule 28: Large ribosomal subunit protein uL6



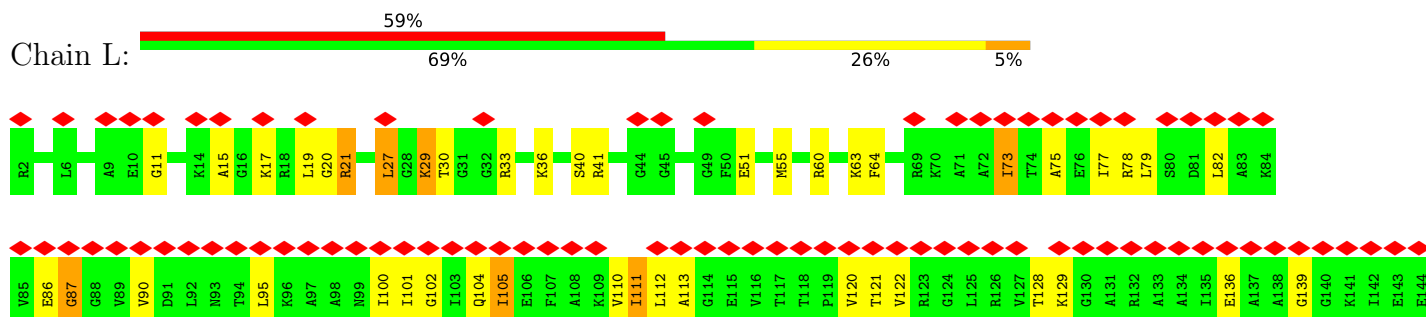
• Molecule 29: 50S ribosomal protein L13



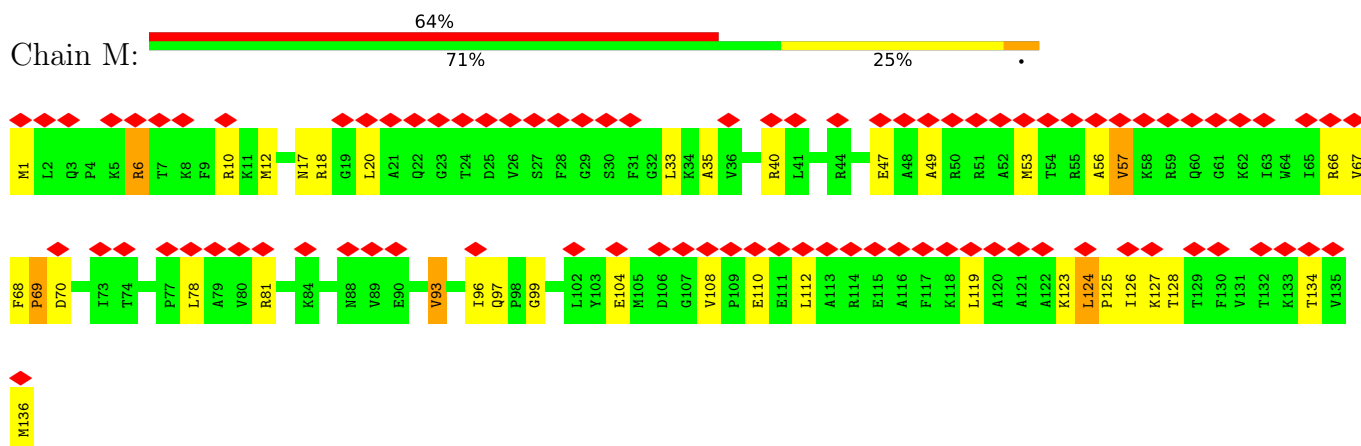
- Molecule 30: Large ribosomal subunit protein uL14



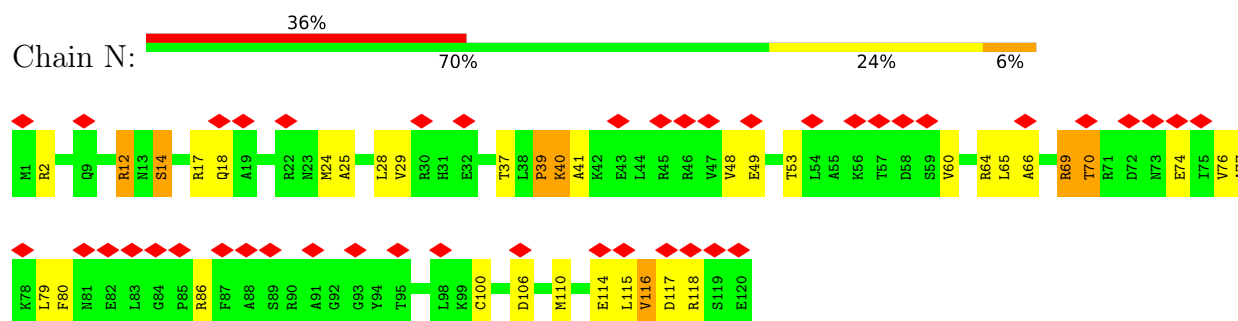
- Molecule 31: Large ribosomal subunit protein uL15



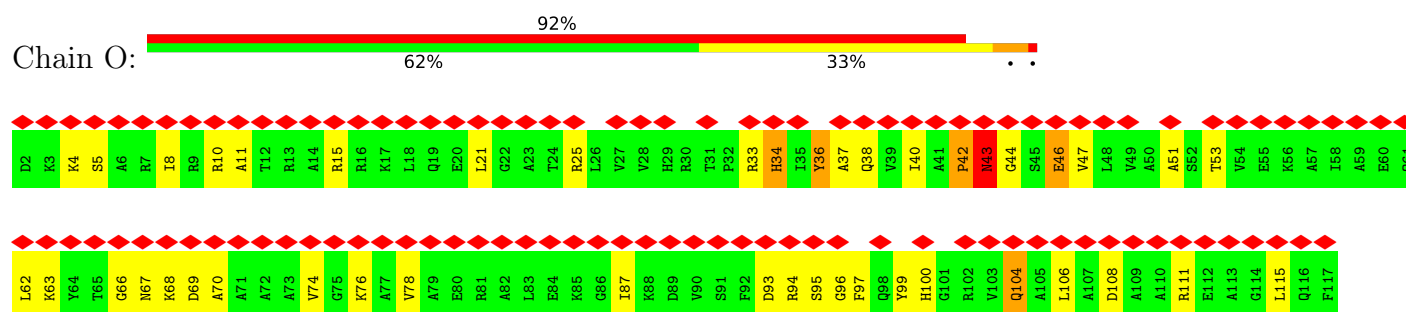
- Molecule 32: 50S ribosomal protein L16



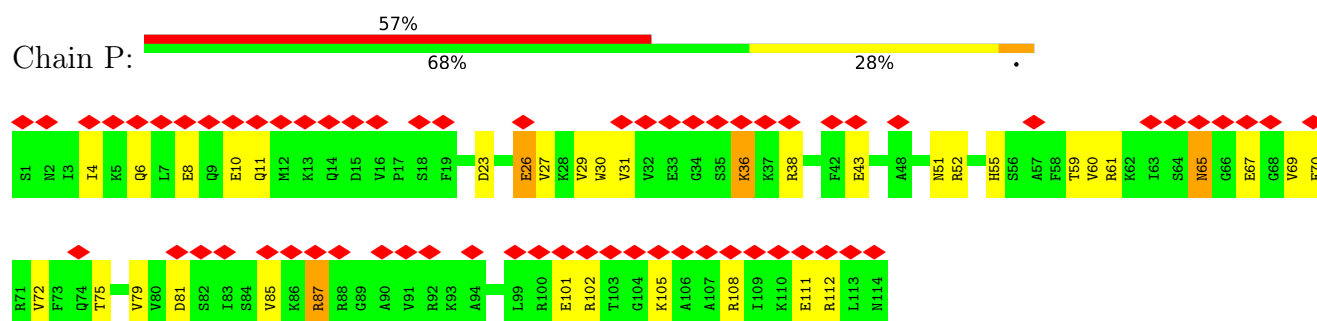
- Molecule 33: Large ribosomal subunit protein bL17



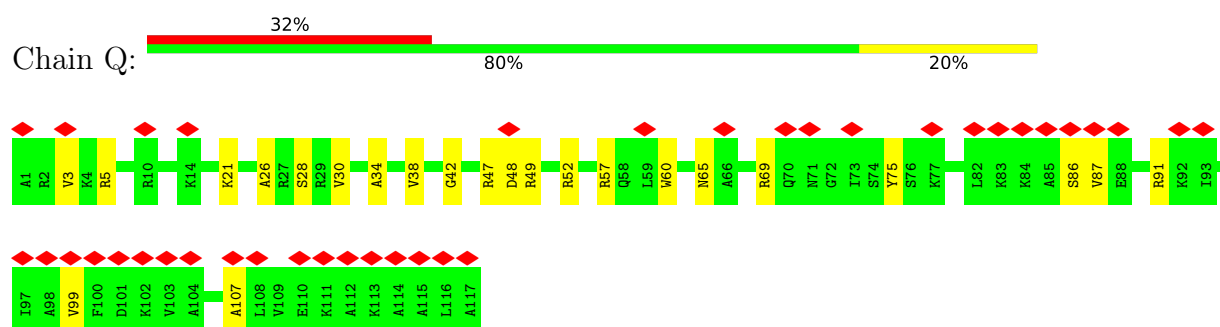
- Molecule 34: 50S ribosomal protein L18



- Molecule 35: 50S ribosomal protein L19

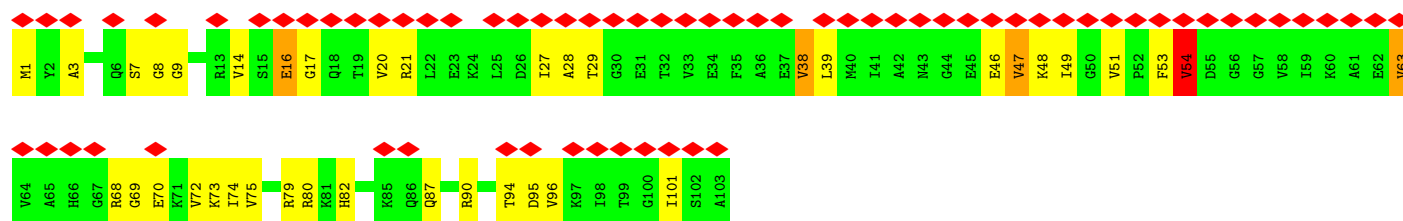


- Molecule 36: 50S ribosomal protein L20

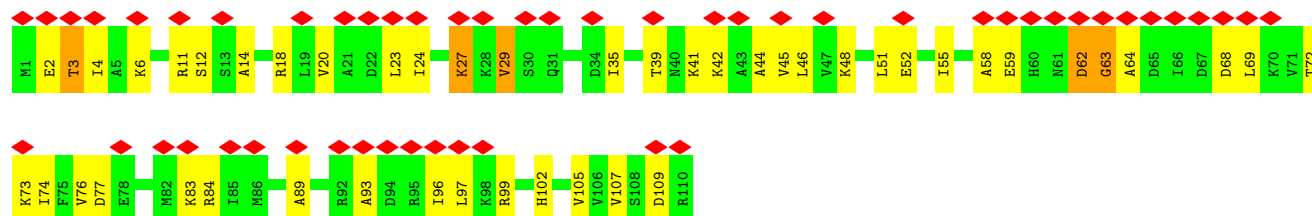


- Molecule 37: 50S ribosomal protein L21

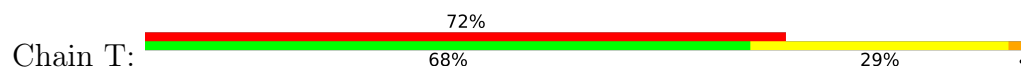




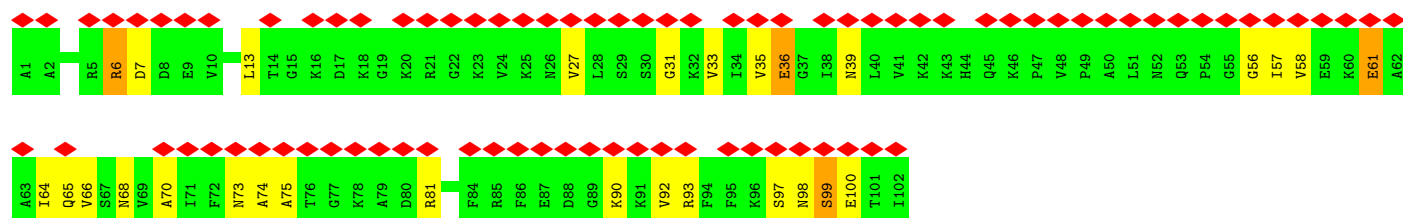
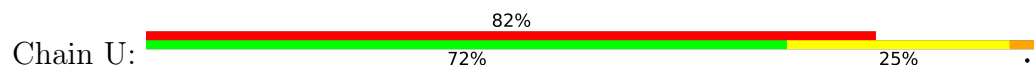
• Molecule 38: 50S ribosomal protein L22



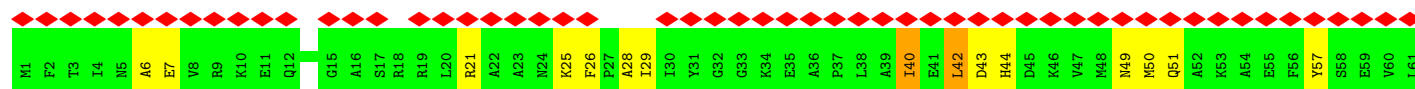
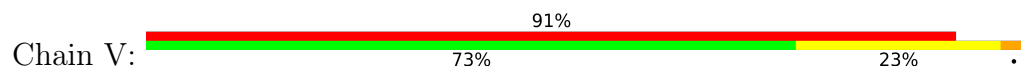
• Molecule 39: 50S ribosomal protein L23



• Molecule 40: Large ribosomal subunit protein uL24

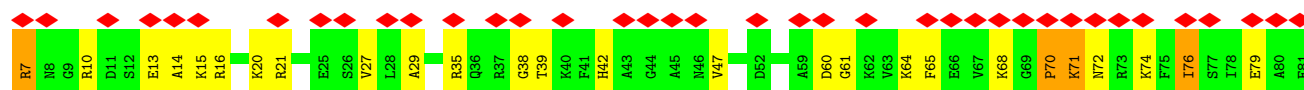


• Molecule 41: 50S ribosomal protein L25

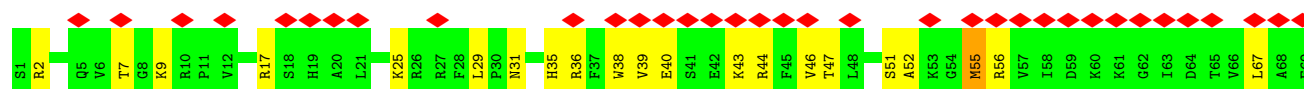




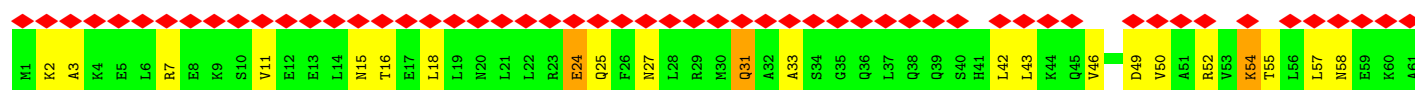
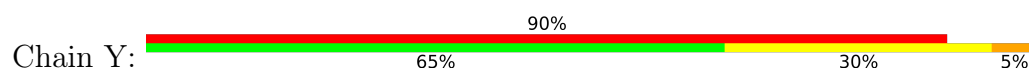
- Molecule 42: 50S ribosomal protein L27



- Molecule 43: 50S ribosomal protein L28



- Molecule 44: Large ribosomal subunit protein uL29



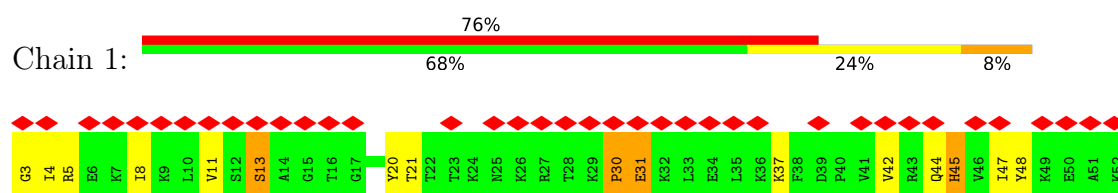
- Molecule 45: 50S ribosomal protein L30



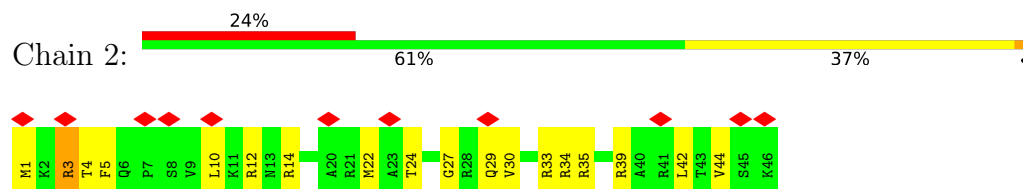
- Molecule 46: Large ribosomal subunit protein bL32



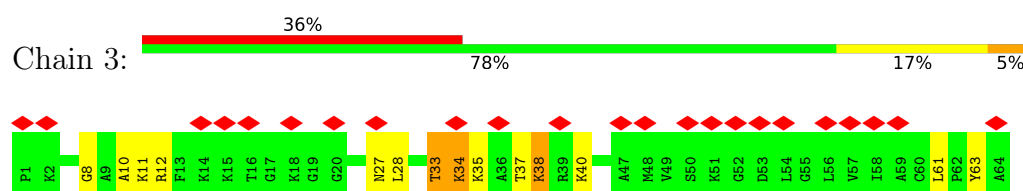
- Molecule 47: 50S ribosomal protein L33



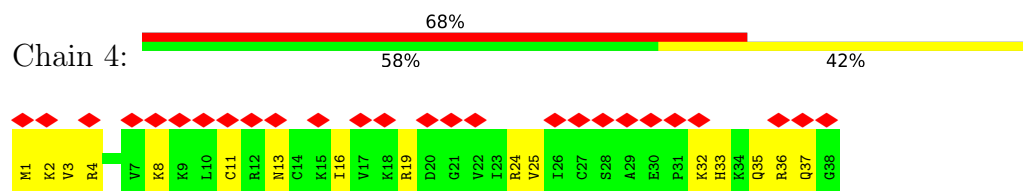
• Molecule 48: 50S ribosomal protein L34



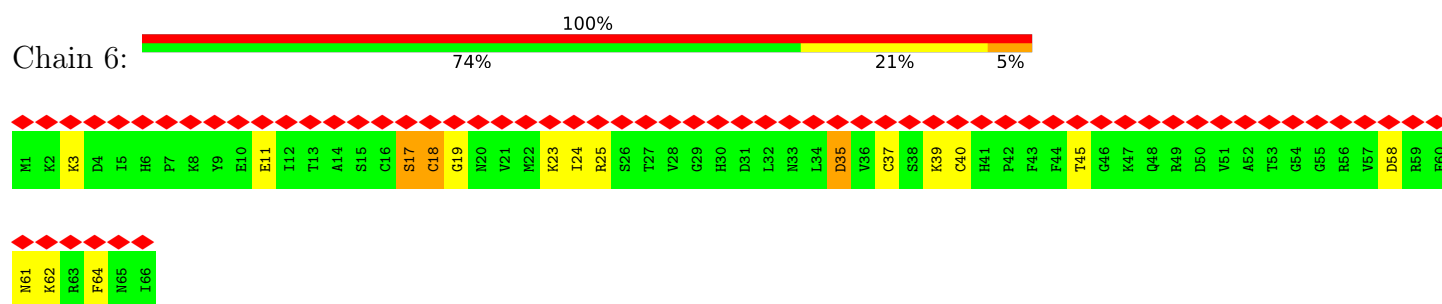
• Molecule 49: 50S ribosomal protein L35



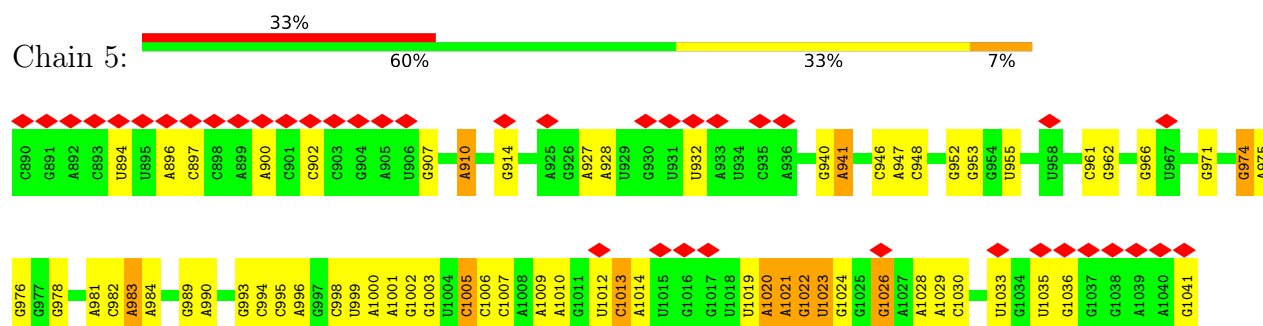
• Molecule 50: 50S ribosomal protein L36



• Molecule 51: Large ribosomal subunit protein bL31



• Molecule 52: RNA (2014-MER)



G2035	G2038	U2039	C2040	C2042	C2043	G2049	C2050	A2051	A2052	G2053	A2054	C2055	G2056	A2060	G2061	A2062	C2063	C2064	C2065	G2069	A2070	A2071	C2072	C2073	U2074	U2075	U2076	A2077	C2084	U2085	U2086	G2087	U2092	G2093	A2094	A2095	C2096	A2097	U2098	U2099	G2100	A2101	G2102	C2103	C2104	A2105	G2106	C2107	A2108	U2109	G2110	U2111							
C1941	C1942	U1943	U1946	C1947	G1954	U1955	U1956	A1960	C1961	C1962	U1963	G1964	C1965	A1966	C1967	A1970	U1971	G1972	G1980	A1981	U1982	C1990	U1991	G1992	U1993	C1997	A1998	C1999	G2010	U2011	C2012	A2013	U2016	U2017	G2018	A2019	C2020	C2021	U2022	C2023	G2024	C2025	U2026	G2027	A2030	A2031	C2032	A2033	U2034										
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C1102	A1103	C1104	U1105	U1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	C1114	G1115	G1116	C1117	C1118	U1119	G1120	G1125	A1126	A1129	U1130	G1131	U1132	A1133	A1134	C1135	U1141	A1142	C1146	A1147	U1148	G1149	C1150	C1153	G1154	A1155	U1159	G1168	A1169	C1170	G1171	C1172	U1173	U1174	A1175	U1176	G1177	C1178	G1179	U1180	U1181							
G1042	C1043	C1044	C1045	A1046	G1047	A1048	C1049	A1050	G1051	C1052	C1053	A1054	G1055	G1056	A1057	U1058	G1059	U1060	U1061	G1062	G1063	C1064	U1065	U1066	A1067	G1068	A1069	A1070	G1071	C1072	A1073	G1074	C1075	C1076	A1077	U1078	C1079	A1080	U1081	U1082	U1083	A1084	A1085	A1086	G1087	A1088	A1089	A1090	G1091	C1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101

A2820	A2821	A2822	A2823	C2824	U2832	U2833	U2834	U2835	U2836	A2837	G2838	G2839	U2847	G2848	U2849	A2850	G2854	G2855	A2856	G2857	G2858	G2859	A2860	U2861	C2862	G2863	G2864	A2865	C2866	C2867	G2868	G2869	A2870	C2878	A2879	A2882	C2883	U2884	U2887	G2888	U2889	U2890	U2898	C2899	A2700	U2701	G2709	G2710	A2711	C2712	U2713	G2714	G2715	U2716	G2717	G2718	G2719	U2720	A2721	C2722	C2723	U2724	A2725	A2726	A2727	U2728	G2731	A2813	A2814	C2815	G2816	U2817	U2818	G2819	A2820	A2821	A2822	A2823	A2824	A2825	A2826	A2827	A2828	A2829	A2830	A2831	A2832	A2833	A2834	A2835	A2836	A2837	A2838	A2839	A2840	A2841	A2842	A2843	A2844	A2845	A2846	A2847	A2848	A2849	A2850	A2851	A2852	A2853	A2854	A2855	A2856	A2857	A2858	A2859	A2860	A2861	A2862	A2863	A2864	A2865	A2866	A2867	A2868	A2869	A2870	A2871	A2872	A2873	A2874	A2875	A2876	A2877	A2878	A2879	A2880	A2881	A2882	A2883	A2884	A2885	A2886	A2887	A2888	A2889	A2890	A2891	A2892	A2893	A2894	A2895	A2896	A2897	A2898	A2899	A2900	C2901	C2902	U2903	U2904	U2905	U2906	U2907	U2908	U2909	U2910	U2911	U2912	U2913	U2914	U2915	U2916	U2917	U2918	U2919	U2920	U2921	U2922	U2923	U2924	U2925	U2926	U2927	U2928	U2929	U2930	U2931	U2932	U2933	U2934	U2935	U2936	U2937	U2938	U2939	U2940	U2941	U2942	U2943	U2944	U2945	U2946	U2947	U2948	U2949	U2950	U2951	U2952	U2953	U2954	U2955	U2956	U2957	U2958	U2959	U2960	U2961	U2962	U2963	U2964	U2965	U2966	U2967	U2968	U2969	U2970	U2971	U2972	U2973	U2974	U2975	U2976	U2977	U2978	U2979	U2980	U2981	U2982	U2983	U2984	U2985	U2986	U2987	U2988	U2989	U2990	U2991	U2992	U2993	U2994	U2995	U2996	U2997	U2998	U2999	U3000	U3001	U3002	U3003	U3004	U3005	U3006	U3007	U3008	U3009	U3010	U3011	U3012	U3013	U3014	U3015	U3016	U3017	U3018	U3019	U3020	U3021	U3022	U3023	U3024	U3025	U3026	U3027	U3028	U3029	U3030	U3031	U3032	U3033	U3034	U3035	U3036	U3037	U3038	U3039	U3040	U3041	U3042	U3043	U3044	U3045	U3046	U3047	U3048	U3049	U3050	U3051	U3052	U3053	U3054	U3055	U3056	U3057	U3058	U3059	U3060	U3061	U3062	U3063	U3064	U3065	U3066	U3067	U3068	U3069	U3070	U3071	U3072	U3073	U3074	U3075	U3076	U3077	U3078	U3079	U3080	U3081	U3082	U3083	U3084	U3085	U3086	U3087	U3088	U3089	U3090	U3091	U3092	U3093	U3094	U3095	U3096	U3097	U3098	U3099	U3100	U3101	U3102	U3103	U3104	U3105	U3106	U3107	U3108	U3109	U3110	U3111	U3112	U3113	U3114	U3115	U3116	U3117	U3118	U3119	U3120	U3121	U3122	U3123	U3124	U3125	U3126	U3127	U3128	U3129	U3130	U3131	U3132	U3133	U3134	U3135	U3136	U3137	U3138	U3139	U3140	U3141	U3142	U3143	U3144	U3145	U3146	U3147	U3148	U3149	U3150	U3151	U3152	U3153	U3154	U3155	U3156	U3157	U3158	U3159	U3160	U3161	U3162	U3163	U3164	U3165	U3166	U3167	U3168	U3169	U3170	U3171	U3172	U3173	U3174	U3175	U3176	U3177	U3178	U3179	U3180	U3181	U3182	U3183	U3184	U3185	U3186	U3187	U3188	U3189	U3190	U3191	U3192	U3193	U3194	U3195	U3196	U3197	U3198	U3199	U3200	U3201	U3202	U3203	U3204	U3205	U3206	U3207	U3208	U3209	U3210	U3211	U3212	U3213	U3214	U3215	U3216	U3217	U3218	U3219	U3220	U3221	U3222	U3223	U3224	U3225	U3226	U3227	U3228	U3229	U3230	U3231	U3232	U3233	U3234	U3235	U3236	U3237	U3238	U3239	U3240	U3241	U3242	U3243	U3244	U3245	U3246	U3247	U3248	U3249	U3250	U3251	U3252	U3253	U3254	U3255	U3256	U3257	U3258	U3259	U3260	U3261	U3262	U3263	U3264	U3265	U3266	U3267	U3268	U3269	U3270	U3271	U3272	U3273	U3274	U3275	U3276	U3277	U3278	U3279	U3280	U3281	U3282	U3283	U3284	U3285	U3286	U3287	U3288	U3289	U3290	U3291	U3292	U3293	U3294	U3295	U3296	U3297	U3298	U3299	U3300	U3301	U3302	U3303	U3304	U3305	U3306	U3307	U3308	U3309	U3310	U3311	U3312	U3313	U3314	U3315	U3316	U3317	U3318	U3319	U3320	U3321	U3322	U3323	U3324	U3325	U3326	U3327	U3328	U3329	U3330	U3331	U3332	U3333	U3334	U3335	U3336	U3337	U3338	U3339	U3340	U3341	U3342	U3343	U3344	U3345	U3346	U3347	U3348	U3349	U3350	U3351	U3352	U3353	U3354	U3355	U3356	U3357	U3358	U3359	U3360	U3361	U3362	U3363	U3364	U3365	U3366	U3367	U3368	U3369	U3370	U3371	U3372	U3373	U3374	U3375	U3376	U3377	U3378	U3379	U3380	U3381	U3382	U3383	U3384	U3385	U3386	U3387	U3388	U3389	U3390	U3391	U3392	U3393	U3394	U3395	U3396	U3397	U3398	U3399	U3400	U3401	U3402	U3403	U3404	U3405	U3406	U3407	U3408	U3409	U3410	U3411	U3412	U3413	U3414	U3415	U3416	U3417	U3418	U3419	U3420	U3421	U3422	U3423	U3424	U3425	U3426	U3427	U3428	U3429	U3430	U3431	U3432	U3433	U3434	U3435	U3436	U3437	U3438	U3439	U3440	U3441	U3442	U3443	U3444	U3445	U3446	U3447	U3448	U3449	U3450	U3451	U3452	U3453	U3454	U3455	U3456	U3457	U3458	U3459	U3460	U3461	U3462	U3463	U3464	U3465	U3466	U3467	U3468	U3469	U3470	U3471	U3472	U3473	U3474	U3475	U3476	U3477	U3478	U3479	U3480	U3481	U3482	U3483	U3484	U3485	U3486	U3487	U3488	U3489	U3490	U3491	U3492	U3493	U3494	U3495	U3496	U3497	U3498	U3499	U3500	U3501	U3502	U3503	U3504	U3505	U3506	U3507	U3508	U3509	U3510	U3511	U3512	U3513	U3514	U3515	U3516	U3517	U3518	U3519	U3520	U3521	U3522	U3523	U3524	U3525	U3526	U3527	U3528	U3529	U3530	U3531	U3532	U3533	U3534	U3535	U3536	U3537	U3538	U3539	U3540	U3541	U3542	U3543	U3544	U3545	U3546	U3547	U3548	U3549	U3550	U3551	U3552	U3553	U3554	U3555	U3556	U3557	U3558	U3559	U3560	U3561	U3562	U3563	U3564	U3565	U3566	U3567	U3568	U3569	U3570	U3571	U3572	U3573	U3574	U3575	U3576	U3577	U3578	U3579	U3580	U3581	U3582	U3583	U3584	U3585	U3586	U3587	U3588	U3589	U3590	U3591	U3592	U3593	U3594	U3595	U3596	U3597	U3598	U3599	U3600	U3601	U3602	U3603	U3604	U3605	U3606	U3607	U3608	U3609	U3610	U3611	U3612	U3613	U3614	U3615	U3616	U3617	U3618	U3619	U3620	U3621	U3622	U3623	U3624	U3625	U3626	U3627	U3628	U3629	U3630	U3631	U3632	U3633	U3634	U3635	U3636	U3637	U3638	U3639	U3640	U3641	U3642	U3643	U3644	U3645	U3646	U3647	U3648	U3649	U3650	U3651	U3652	U3653	U3654	U3655	U3656	U3657	U3658	U3659	U3660	U3661	U3662	U3663	U3664	U3665	U3666	U3667	U3668	U3669	U3670	U3671	U3672	U3673	U3674	U3675	U3676	U3677	U3678	U3679	U3680	U3681	U3682	U3683	U3684	U3685	U3686	U3687	U3688	U3689	U3690	U3691	U3692	U3693	U3694	U3695	U3696	U3697	U3698	U3699	U3700	U3701	U3702	U3703	U3704	U3705	U3706	U3707	U3708	U3709	U3710	U3711	U3712	U3713	U3714	U3715	U3716	U3717	U3718	U3719	U3720	U3721	U3722	U3723	U3724	U3725	U3726	U3727	U3728	U3729	U3730	U3731	U3732	U3733	U3734	U3735	U3736	U3737	U3738	U3739	U3740	U3741	U3742	U3743	U3744	U3745	U3746	U3747	U3748	U3749	U3750	U3751	U3752	U3753	U3754	U3755	U3756	U3757	U3758	U3759	U3760	U3761	U3762	U3763	U3764	U3765	U3766	U3767	U3768	U3769	U3770	U3771	U3772	U3773	U3774	U3775	U3776	U3777	U3778	U3779	U3780	U3781	U3782	U3783	U3784	U3785	U3786	U3787	U3788	U3789	U3790	U3791	U3792	U3793	U3794	U3795	U3796	U3797	U3798	U3799	U3800	U3801	U3802	U3803	U3804	U3805	U3806	U3807	U3808	U3809	U3810	U3811	U3812	U3813	U3814	U3815	U3816	U3817	U3818	U3819	U3820	U3821	U3822	U3823	U3824	U3825	U3826	U3827	U3828	U3829	U3830	U3831	U3832	U3833	U3834	U3835	U3836	U3837	U3838	U3839	U3840	U3841	U3842	U3843	U3844	U3845	U3846	U3847	U3848	U3849	U3850	U3851	U3852	U3853	U3854	U3855	U3856	U3857	U3858	U3859	U3860	U3861	U3862	U3863	U3864	U3865	U3866	U3867	U3868	U3869	U3870	U3871	U3872	U3873	U3874	U3875	U3876	U3877	U3878	U3879	U3880	U3881	U3882	U3883	U3884	U3885	U3886	U3887	U3888	U3889	U3890	U3891	U3892	U3893	U3894	U3895	U3896	U3897	U3898	U3899	U3900	U3901	U3902	U3903	U3904	U3905	U3906	U3907	U3908	U3909	U3910	U3911	U3912	U3913	U3914	U3915	U3916	U3917	U3918	U3919	U3920	U3921	U3922	U3923	U3924	U3925	U3926	U3927	U3928	U3929	U3930	U3931	U3932	U3933	U3934	U3935	U3936	U3937	U3938	U3939	U3940	U3941	U3942	U3943	U3944	U3945	U3946	U3947	U3948	U3949	U3950	U3951	U3952	U3953	U3954	U3955	U3956	U3957	U3958	U3959	U3960	U3961	U3962	U3963	U3964	U3965	U3966	U3967	U3968	U3969	U3970	U3971	U3972	U3973	U3974	U3975	U3976	U3977	U3978	U3979	U3980	U3981	U3982	U
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4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	16677	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	84	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.030	Depositor
Minimum map value	-0.016	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0077	Depositor
Map size (Å)	533.27997, 533.27997, 533.27997	wwPDB
Map dimensions	528, 528, 528	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMU, 7MG, ZN, PSU, MG, OMC, MA6, CL, 2MA, 6MZ, H2U, 3TD, 1MG, 5MC, UR3, 2MG, 4OC, NA, OMG

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	a	0.10	0/36701	0.27	0/57246
2	b	0.26	0/1735	0.55	0/2338
3	c	0.29	0/1651	0.56	0/2225
4	d	0.28	0/1665	0.60	0/2227
5	e	0.34	0/1154	0.52	0/1554
6	f	0.34	0/835	0.66	0/1128
7	g	0.22	0/1195	0.51	0/1602
8	h	0.33	0/989	0.58	0/1326
9	i	0.24	0/1034	0.55	0/1375
10	j	0.23	0/796	0.56	0/1077
11	k	0.31	0/885	0.57	0/1195
12	l	0.25	0/969	0.54	0/1300
13	m	0.23	0/892	0.54	0/1193
14	n	0.25	0/805	0.61	0/1071
15	o	0.34	0/722	0.63	0/964
16	p	0.27	0/659	0.63	0/884
17	q	0.25	0/657	0.59	1/881 (0.1%)
18	r	0.32	0/511	0.48	0/689
19	s	0.20	0/652	0.56	0/877
20	t	0.29	0/671	0.59	0/888
21	u	0.27	0/500	0.58	0/668
22	A	0.10	0/21270	0.28	0/33183
23	B	0.09	0/2876	0.26	0/4483
24	C	0.48	0/2121	0.56	0/2852
25	D	0.49	0/1586	0.58	0/2134
26	E	0.44	0/1571	0.58	0/2113
27	F	0.24	0/1434	0.58	0/1926
28	G	0.30	0/1343	0.61	1/1816 (0.1%)
29	J	0.44	0/1152	0.62	1/1551 (0.1%)
30	K	0.44	0/947	0.64	0/1268
31	L	0.46	0/1054	0.55	0/1403

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	M	0.44	0/1093	0.52	0/1460
33	N	0.47	0/973	0.68	2/1301 (0.2%)
34	O	0.37	0/902	0.54	0/1209
35	P	0.43	0/929	0.51	0/1242
36	Q	0.49	0/960	0.58	1/1278 (0.1%)
37	R	0.46	0/829	0.56	1/1107 (0.1%)
38	S	0.46	0/864	0.62	0/1156
39	T	0.39	0/744	0.55	0/994
40	U	0.36	0/787	0.51	0/1051
41	V	0.37	0/766	0.51	0/1025
42	W	0.48	0/582	0.60	0/769
43	X	0.43	0/635	0.46	0/848
44	Y	0.30	0/510	0.47	0/677
45	Z	0.44	0/453	0.52	0/605
46	0	0.44	0/450	0.50	0/599
47	1	0.38	0/416	0.58	0/554
48	2	0.51	0/380	0.50	0/498
49	3	0.48	0/513	0.52	0/676
50	4	0.44	0/303	0.51	0/397
51	6	0.21	0/531	0.48	0/709
52	5	0.10	0/47904	0.28	0/74727
All	All	0.21	0/152556	0.37	7/228319 (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
4	d	0	1
28	G	0	1
29	J	0	1
31	L	0	1
32	M	0	1
All	All	0	5

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	Q	21	LYS	CD-CE-NZ	7.57	136.11	111.90
33	N	14	SER	CA-C-N	6.32	131.38	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	N	14	SER	C-N-CA	6.32	131.38	120.58
29	J	37	ARG	CA-CB-CG	5.54	125.18	114.10
37	R	47	VAL	CG1-CB-CG2	-5.28	99.19	110.80
28	G	68	ARG	CA-CB-CG	5.11	124.32	114.10
17	q	29	LYS	CB-CG-CD	5.03	122.87	111.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	G	148	ARG	Sidechain
29	J	37	ARG	Sidechain
31	L	21	ARG	Sidechain
32	M	18	ARG	Sidechain
4	d	181	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	33029	0	16645	422	0
2	b	1704	0	1732	76	0
3	c	1624	0	1699	62	0
4	d	1643	0	1710	99	0
5	e	1141	0	1170	37	0
6	f	817	0	808	56	0
7	g	1181	0	1240	36	0
8	h	979	0	1034	35	0
9	i	1022	0	1070	35	0
10	j	786	0	828	39	0
11	k	869	0	878	48	0
12	l	955	0	1019	38	0
13	m	883	0	944	42	0
14	n	794	0	835	36	0
15	o	714	0	737	23	0
16	p	649	0	666	37	0
17	q	648	0	691	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	r	504	0	502	22	0
19	s	637	0	665	25	0
20	t	665	0	714	31	0
21	u	495	0	486	22	0
22	A	19047	0	9577	226	0
23	B	2572	0	1302	21	0
24	C	2082	0	2157	53	0
25	D	1565	0	1616	47	0
26	E	1552	0	1619	36	0
27	F	1410	0	1447	66	0
28	G	1323	0	1374	35	0
29	J	1129	0	1162	30	0
30	K	938	0	1012	38	0
31	L	1045	0	1117	29	0
32	M	1074	0	1157	22	0
33	N	960	0	1000	26	0
34	O	892	0	923	34	0
35	P	917	0	965	25	0
36	Q	947	0	1022	17	0
37	R	816	0	839	29	0
38	S	857	0	922	28	0
39	T	738	0	807	15	0
40	U	779	0	834	20	0
41	V	753	0	780	17	0
42	W	575	0	592	17	0
43	X	625	0	655	17	0
44	Y	509	0	543	12	0
45	Z	449	0	491	16	0
46	0	444	0	461	7	0
47	1	409	0	440	10	0
48	2	377	0	418	13	0
49	3	504	0	574	12	0
50	4	302	0	340	11	0
51	6	522	0	520	14	0
52	5	43229	0	21767	463	0
53	0	1	0	0	0	0
53	5	170	0	0	0	0
53	A	63	0	0	0	0
53	B	7	0	0	0	0
53	C	1	0	0	0	0
53	D	1	0	0	0	0
53	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	N	1	0	0	0	0
53	a	82	0	0	0	0
53	n	1	0	0	0	0
54	5	1	0	0	0	0
54	a	1	0	0	0	0
55	5	1	0	0	0	0
55	B	1	0	0	0	0
56	4	1	0	0	0	0
56	6	1	0	0	0	0
57	5	8	0	0	2	0
57	A	2	0	0	1	0
57	D	1	0	0	0	0
57	K	1	0	0	1	0
57	a	9	0	0	3	0
All	All	141435	0	94506	2382	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 10.

All (2382) 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)
52:5:1939:5MU:C4	52:5:1939:5MU:C5	1.83	1.63
52:5:1939:5MU:C6	52:5:1939:5MU:N1	1.68	1.57
11:k:124:LYS:O	21:u:34:ARG:NH1	1.86	1.09
22:A:858:G:O2'	52:5:2268:A:O2'	1.75	1.02
27:F:92:GLY:H	27:F:95:MET:HE2	1.27	0.99
48:2:12:ARG:HE	48:2:44:VAL:HG21	1.26	0.99
8:h:105:THR:OG1	8:h:108:GLY:O	1.81	0.98
4:d:28:ASP:O	4:d:29:THR:OG1	1.82	0.97
1:a:354:G:O2'	1:a:389:A:OP1	1.81	0.96
30:K:13:ASN:O	30:K:15:GLY:N	1.99	0.94
31:L:95:LEU:HD22	31:L:100:ILE:HD11	1.48	0.93
52:5:2832:U:O2'	52:5:2833:U:OP2	1.87	0.92
52:5:2326:C:O2'	52:5:2327:A:OP1	1.86	0.92
11:k:126:ARG:O	21:u:34:ARG:NH2	2.03	0.92
52:5:1939:5MU:C4	52:5:1939:5MU:C6	2.52	0.91
1:a:687:A:N6	1:a:703:G:O2'	2.04	0.91
22:A:481:G:O2'	22:A:506:G:N2	2.03	0.91
1:a:125:U:HO2'	1:a:634:C:HO2'	1.16	0.90
39:T:4:GLU:OE1	39:T:4:GLU:N	2.04	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:195:A:O2'	1:a:196:A:O4'	1.90	0.89
1:a:401:C:O2'	1:a:621:A:N3	2.06	0.88
30:K:109:SER:O	30:K:111:LYS:N	2.07	0.88
6:f:12:PRO:O	6:f:15:SER:OG	1.91	0.88
52:5:1068:G:N2	52:5:1095:A:O2'	2.07	0.88
17:q:17:GLU:N	17:q:17:GLU:OE1	2.07	0.87
38:S:2:GLU:O	38:S:3:THR:OG1	1.90	0.87
24:C:132:ARG:NH1	24:C:186:ASP:OD1	2.07	0.87
22:A:310:A:O2'	22:A:311:A:O5'	1.93	0.87
25:D:184:ARG:NH2	35:P:6:GLN:OE1	2.08	0.86
34:O:40:ILE:HD13	34:O:47:VAL:HG12	1.57	0.86
11:k:92:ARG:NH2	11:k:111:ASP:OD1	2.08	0.86
52:5:1962:5MC:O2'	52:5:1964:G:OP2	1.94	0.86
1:a:1492:A:O2'	1:a:1493:A:O4'	1.93	0.86
1:a:1137:C:O2'	1:a:1138:G:N2	2.08	0.86
52:5:2848:G:O2'	52:5:2868:A:N6	2.10	0.85
29:J:1:MET:SD	29:J:2:LYS:N	2.50	0.84
52:5:1845:G:N2	52:5:1895:C:O2	2.09	0.84
22:A:774:G:O2'	22:A:775:G:O5'	1.96	0.84
4:d:60:VAL:HG21	4:d:199:ILE:HD11	1.59	0.84
22:A:227:A:O2'	22:A:228:C:O5'	1.96	0.83
23:B:5:U:OP1	23:B:61:G:O2'	1.96	0.83
1:a:127:G:O2'	17:q:5:ARG:NH2	2.10	0.83
1:a:1058:G:N2	1:a:1202:U:O4	2.12	0.83
52:5:1939:5MU:C6	52:5:1939:5MU:C2	2.65	0.83
1:a:522:C:OP1	12:l:116:TYR:OH	1.97	0.83
29:J:80:HIS:O	29:J:82:GLY:N	2.11	0.83
23:B:45:A:O4'	27:F:91:ARG:NH1	2.10	0.82
38:S:62:ASP:O	38:S:64:ALA:N	2.13	0.82
48:2:12:ARG:NE	48:2:44:VAL:HG21	1.94	0.82
14:n:46:LEU:HG	19:s:12:LEU:HD21	1.59	0.82
1:a:421:U:O2'	1:a:422:C:OP1	1.96	0.82
52:5:1173:U:O2'	52:5:1177:G:N2	2.12	0.82
32:M:66:ARG:NH1	32:M:104:GLU:OE2	2.13	0.82
31:L:29:LYS:O	31:L:30:THR:OG1	1.96	0.82
29:J:23:LYS:NZ	29:J:142:ILE:OXT	2.13	0.81
7:g:26:VAL:HG22	7:g:42:VAL:HG21	1.63	0.81
52:5:1900:A:O2'	52:5:1901:A:OP2	1.97	0.81
2:b:92:ASN:OD1	2:b:93:HIS:ND1	2.13	0.81
22:A:597:G:O2'	31:L:11:GLY:O	1.98	0.81
4:d:125:ASN:ND2	4:d:140:ASP:OD1	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:N:69:ARG:O	33:N:70:THR:OG1	1.99	0.81
4:d:10:LEU:HD13	4:d:62:ARG:HD2	1.60	0.81
2:b:206:ILE:O	2:b:210:THR:OG1	1.99	0.80
1:a:1301:U:O2'	1:a:1302:C:OP1	1.98	0.80
1:a:392:C:OP2	16:p:13:LYS:N	2.13	0.80
1:a:1063:C:OP2	1:a:1064:G:O2'	2.00	0.80
22:A:71:A:OP2	22:A:112:U:O2'	1.98	0.80
3:c:69:THR:HG21	3:c:75:VAL:HG21	1.64	0.80
25:D:149:ASN:ND2	52:5:2053:G:OP1	2.15	0.79
28:G:83:THR:HG22	28:G:133:LYS:HG2	1.62	0.79
18:r:28:LEU:HD22	18:r:67:LEU:HD11	1.63	0.79
22:A:219:A:N3	22:A:234:U:O2'	2.15	0.79
52:5:2469:A:N6	52:5:2481:G:O2'	2.16	0.79
27:F:141:ASP:O	27:F:143:ASP:N	2.15	0.79
33:N:49:GLU:OE1	52:5:2839:G:O2'	2.01	0.79
16:p:27:ALA:O	16:p:30:GLY:N	2.15	0.78
52:5:1626:A:O2'	52:5:1627:G:OP2	1.99	0.78
1:a:31:G:O2'	1:a:32:A:O5'	2.00	0.78
27:F:1:ALA:O	27:F:4:HIS:N	2.16	0.78
49:3:33:THR:OG1	52:5:2420:C:OP1	2.01	0.78
4:d:113:ALA:O	4:d:117:VAL:HG23	1.83	0.78
4:d:123:MET:O	4:d:143:SER:N	2.16	0.78
27:F:119:LYS:O	27:F:121:PHE:N	2.16	0.78
22:A:807:U:OP2	31:L:41:ARG:NH2	2.15	0.77
25:D:88:GLU:N	25:D:88:GLU:OE1	2.17	0.77
3:c:27:GLU:N	3:c:27:GLU:OE1	2.17	0.77
20:t:20:ASN:HD21	20:t:65:LEU:HD13	1.48	0.77
40:U:61:GLU:OE1	40:U:61:GLU:N	2.18	0.77
1:a:345:C:OP1	35:P:38:ARG:NH1	2.18	0.77
18:r:71:ASP:N	18:r:71:ASP:OD1	2.18	0.77
52:5:1826:G:O2'	52:5:1971:U:OP2	2.02	0.77
1:a:362:G:N2	1:a:365:U:OP2	2.16	0.76
1:a:235:C:O2'	17:q:72:TRP:NE1	2.19	0.76
1:a:701:U:OP1	1:a:702:A:O2'	2.01	0.76
52:5:1417:C:O2'	52:5:1587:G:O2'	2.02	0.76
17:q:68:LYS:O	17:q:69:THR:OG1	2.02	0.76
24:C:135:PRO:O	24:C:138:SER:OG	2.02	0.76
1:a:339:C:OP2	30:K:98:ARG:NH1	2.18	0.76
1:a:404:G:O2'	1:a:498:A:N1	2.17	0.76
23:B:37:C:O2	34:O:100:HIS:NE2	2.19	0.76
26:E:24:ASN:O	26:E:28:VAL:HG23	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:L:51:GLU:OE1	31:L:60:ARG:NH2	2.19	0.76
22:A:270:A:N1	22:A:369:U:O2'	2.18	0.75
28:G:74:MET:O	28:G:78:VAL:HG22	1.86	0.75
1:a:1178:G:N2	1:a:1181:G:OP2	2.19	0.75
1:a:1266:G:N2	1:a:1269:A:OP2	2.19	0.75
22:A:572:A:OP2	37:R:80:ARG:NH2	2.19	0.75
2:b:92:ASN:OD1	2:b:93:HIS:N	2.20	0.75
1:a:533:A:O2'	1:a:535:A:OP2	2.05	0.75
4:d:154:VAL:HG12	4:d:177:MET:HE3	1.68	0.75
27:F:170:ALA:O	27:F:173:ASP:N	2.20	0.74
1:a:543:U:OP1	4:d:13:ARG:NE	2.20	0.74
52:5:1858:A:N6	52:5:1884:G:O2'	2.19	0.74
1:a:413:G:O2'	1:a:414:A:OP2	2.06	0.74
52:5:1779:U:OP2	52:5:1784:A:N6	2.21	0.74
1:a:309:A:O2'	1:a:607:A:N1	2.20	0.74
4:d:131:ILE:HG22	4:d:133:SER:H	1.53	0.74
27:F:102:LEU:HD12	27:F:106:ALA:HB3	1.69	0.74
1:a:427:U:OP1	4:d:12:ARG:NH2	2.21	0.74
3:c:61:LYS:NZ	3:c:96:VAL:O	2.20	0.74
5:e:146:MET:SD	5:e:147:ASN:N	2.61	0.74
22:A:837:C:N3	52:5:941:A:N6	2.34	0.74
52:5:1111:A:O2'	52:5:1112:G:OP1	2.06	0.74
37:R:7:SER:O	37:R:9:GLY:N	2.21	0.74
6:f:90:MET:SD	18:r:60:ARG:NH2	2.61	0.73
52:5:1359:A:OP1	57:5:3201:HOH:O	2.06	0.73
3:c:99:GLN:NE2	3:c:101:ASN:OD1	2.21	0.73
5:e:86:GLY:O	5:e:138:ALA:HB1	1.87	0.73
52:5:1071:G:N2	52:5:1089:A:O2'	2.21	0.73
1:a:618:C:O2'	16:p:14:ARG:NH1	2.21	0.73
16:p:7:ALA:O	16:p:9:HIS:ND1	2.21	0.73
52:5:1417:C:HO2'	52:5:1587:G:HO2'	1.35	0.73
1:a:297:G:N2	1:a:300:A:OP2	2.22	0.73
9:i:46:VAL:HG23	9:i:47:VAL:H	1.54	0.73
1:a:1126:U:O2'	1:a:1281:C:O4'	2.07	0.73
15:o:6:ALA:O	15:o:10:ILE:HD12	1.88	0.73
22:A:310:A:HO2'	22:A:311:A:P	2.12	0.73
27:F:59:ILE:HG23	27:F:60:SER:H	1.52	0.73
23:B:3:C:O2'	23:B:4:C:OP1	2.04	0.72
30:K:66:LYS:NZ	57:K:201:HOH:O	2.21	0.72
1:a:809:G:OP2	15:o:47:LYS:NZ	2.22	0.72
18:r:28:LEU:HD21	18:r:58:ILE:HD12	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:F:125:GLY:O	27:F:157:THR:OG1	2.08	0.72
34:O:46:GLU:OE1	34:O:46:GLU:N	2.23	0.72
12:l:20:VAL:HG23	12:l:20:VAL:O	1.90	0.72
22:A:568:U:H1'	52:5:2030:6MZ:H9C1	1.72	0.72
22:A:516:C:OP1	46:O:9:ARG:NH2	2.23	0.72
34:O:42:PRO:O	34:O:44:GLY:N	2.22	0.72
52:5:1125:G:OP2	52:5:1126:A:O2'	2.06	0.71
52:5:1939:5MU:C6	52:5:1939:5MU:C1'	2.73	0.71
4:d:97:LEU:O	4:d:101:VAL:HG23	1.90	0.71
52:5:2725:A:O2'	52:5:2726:A:O5'	2.04	0.71
36:Q:57:ARG:NH1	52:5:1154:G:OP2	2.23	0.71
5:e:155:LYS:O	5:e:158:LYS:NZ	2.21	0.71
4:d:77:GLU:OE1	4:d:77:GLU:N	2.24	0.71
34:O:40:ILE:CD1	34:O:47:VAL:HG12	2.21	0.71
47:1:31:GLU:N	47:1:31:GLU:OE1	2.24	0.71
1:a:392:C:HO2'	1:a:483:C:HO2'	1.22	0.71
52:5:1028:A:N3	52:5:2486:C:O2'	2.20	0.71
25:D:132:ALA:O	25:D:133:THR:HG23	1.90	0.70
1:a:1238:A:OP1	1:a:1335:U:O2'	2.06	0.70
28:G:25:ILE:HD12	28:G:74:MET:HE3	1.73	0.70
1:a:107:G:O6	20:t:9:ARG:NH1	2.25	0.70
52:5:2595:G:N2	52:5:2598:A:OP2	2.22	0.70
10:j:10:LEU:HD12	10:j:10:LEU:O	1.91	0.70
18:r:44:THR:O	18:r:46:THR:HG23	1.92	0.70
1:a:511:C:O2'	1:a:512:U:O5'	2.09	0.70
52:5:1360:G:OP2	57:5:3201:HOH:O	2.08	0.70
15:o:32:THR:OG1	15:o:62:ARG:NH1	2.23	0.70
24:C:256:THR:OG1	52:5:1797:G:O2'	2.08	0.70
26:E:111:GLU:OE1	26:E:114:ARG:NH2	2.23	0.70
1:a:1305:G:O2'	1:a:1306:A:O5'	2.10	0.70
27:F:130:GLY:O	27:F:132:ARG:NH1	2.24	0.70
1:a:757:U:OP1	1:a:822:U:O2'	2.10	0.70
7:g:66:GLU:N	7:g:66:GLU:OE1	2.25	0.70
22:A:534:U:O2'	36:Q:48:ASP:OD2	2.10	0.70
1:a:981:U:OP1	14:n:8:ARG:NH1	2.24	0.69
27:F:50:ASP:O	27:F:53:ALA:HB3	1.93	0.69
12:l:33:CYS:O	12:l:34:THR:HG23	1.92	0.69
32:M:123:LYS:NZ	52:5:2483:C:N3	2.38	0.69
42:W:65:PHE:CE2	42:W:76:ILE:HD11	2.26	0.69
49:3:27:ASN:O	49:3:35:LYS:NZ	2.25	0.69
6:f:8:PHE:CE1	6:f:62:MET:HE1	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:373:A:O2'	1:a:451:A:N7	2.26	0.69
17:q:45:VAL:HG23	17:q:72:TRP:O	1.94	0.68
2:b:166:ASP:OD2	2:b:189:ASN:ND2	2.26	0.68
10:j:13:PHE:O	10:j:70:HIS:NE2	2.26	0.68
17:q:45:VAL:HG23	17:q:72:TRP:C	2.18	0.68
29:J:81:ILE:HD11	52:5:2514:U:H5''	1.76	0.68
37:R:82:HIS:O	37:R:82:HIS:ND1	2.27	0.68
28:G:136:ASP:O	28:G:140:ILE:HG22	1.94	0.68
24:C:106:PRO:HG2	24:C:109:LEU:HD22	1.75	0.68
6:f:18:VAL:O	6:f:20:GLY:N	2.26	0.68
6:f:88:MET:SD	6:f:90:MET:HE2	2.34	0.67
22:A:381:G:OP1	43:X:17:ARG:NH1	2.27	0.67
15:o:31:LEU:HD22	15:o:58:MET:HB2	1.76	0.67
1:a:438:U:O2'	1:a:439:U:O5'	2.13	0.67
16:p:59:HIS:HD1	16:p:59:HIS:C	2.03	0.67
27:F:55:ASP:O	27:F:59:ILE:HG22	1.95	0.67
33:N:106:ASP:OD2	52:5:1649:G:O2'	2.05	0.67
33:N:114:GLU:OE1	33:N:114:GLU:N	2.28	0.67
1:a:898:G:N2	1:a:901:A:OP2	2.28	0.67
22:A:579:G:O2'	52:5:2019:A:OP1	2.12	0.67
9:i:47:VAL:HG12	9:i:78:ILE:HG21	1.77	0.67
27:F:49:LEU:O	27:F:52:ALA:HB3	1.95	0.67
1:a:419:C:OP1	1:a:513:C:O2'	2.13	0.66
1:a:490:C:OP1	4:d:145:ARG:NH2	2.28	0.66
52:5:971:G:OP1	52:5:974:G:O2'	2.12	0.66
1:a:1405:G:O2'	1:a:1518:MA6:O2'	2.10	0.66
24:C:256:THR:HG1	52:5:1797:G:HO2'	1.40	0.66
30:K:70:ARG:NH1	52:5:2684:U:O4'	2.28	0.66
52:5:1019:U:OP1	52:5:1035:U:O2'	2.10	0.66
52:5:1607:C:N4	52:5:1622:G:OP2	2.23	0.66
13:m:33:LEU:HD12	13:m:34:ALA:N	2.11	0.66
52:5:1067:A:O2'	52:5:1068:G:OP1	2.12	0.66
31:L:19:LEU:HD12	31:L:27:LEU:CD1	2.25	0.66
40:U:73:ASN:OD1	40:U:75:ALA:HB3	1.95	0.66
16:p:5:ARG:NH2	16:p:26:ASN:O	2.28	0.66
22:A:704:G:O2'	22:A:727:A:N6	2.27	0.66
33:N:25:ALA:O	33:N:29:VAL:HG23	1.94	0.66
1:a:407:U:O2'	4:d:112:GLU:OE1	2.09	0.66
16:p:36:VAL:HG13	16:p:36:VAL:O	1.96	0.66
22:A:279:A:H61	22:A:361:G:C2'	2.09	0.66
25:D:45:TYR:OH	52:5:2636:C:O2'	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:115:GLN:O	4:d:119:HIS:ND1	2.28	0.66
6:f:92:THR:OG1	6:f:93:LYS:N	2.29	0.66
1:a:31:G:OP2	1:a:306:A:N6	2.29	0.66
40:U:98:ASN:O	40:U:100:GLU:N	2.27	0.66
1:a:1405:G:HO2'	1:a:1518:MA6:HO2'	1.44	0.66
52:5:1447:C:O2'	52:5:1544:A:N3	2.28	0.66
1:a:549:C:OP1	4:d:69:ARG:NH2	2.29	0.66
2:b:72:LYS:O	2:b:74:ALA:N	2.29	0.66
11:k:109:ILE:N	11:k:109:ILE:HD12	2.10	0.66
22:A:192:C:OP1	57:A:3301:HOH:O	2.14	0.65
52:5:1026:G:OP2	52:5:1134:A:O2'	2.07	0.65
31:L:21:ARG:NH1	52:5:1250:G:OP2	2.29	0.65
4:d:60:VAL:HG21	4:d:199:ILE:CD1	2.26	0.65
27:F:92:GLY:N	27:F:95:MET:HE2	2.06	0.65
24:C:203:VAL:O	24:C:205:GLY:N	2.29	0.65
27:F:134:GLN:OE1	27:F:149:ARG:NE	2.27	0.65
22:A:27:G:O2'	22:A:28:A:OP2	2.14	0.65
2:b:56:LEU:HD13	2:b:216:VAL:HG13	1.79	0.65
2:b:14:HIS:ND1	2:b:212:TYR:OH	2.30	0.65
4:d:102:TYR:O	4:d:164:ARG:NH1	2.30	0.65
17:q:16:MET:N	17:q:16:MET:SD	2.70	0.65
1:a:673:A:H2'	1:a:674:G:C8	2.32	0.65
20:t:77:ASN:OD1	20:t:78:LEU:N	2.30	0.65
11:k:84:MET:SD	11:k:110:THR:OG1	2.55	0.65
1:a:1347:G:HO2'	1:a:1348:U:P	2.20	0.64
25:D:91:THR:OG1	25:D:92:VAL:N	2.29	0.64
26:E:79:ARG:O	26:E:80:SER:OG	2.14	0.64
35:P:87:ARG:NH2	35:P:111:GLU:OE1	2.30	0.64
4:d:94:GLU:OE2	4:d:99:ASN:ND2	2.31	0.64
25:D:161:MET:SD	52:5:2049:G:N2	2.70	0.64
45:Z:4:ILE:HD11	45:Z:56:VAL:CG2	2.27	0.64
1:a:131:A:O2'	1:a:262:A:N3	2.30	0.64
24:C:123:ILE:O	24:C:123:ILE:HG22	1.98	0.64
2:b:168:GLU:OE1	2:b:168:GLU:N	2.30	0.64
8:h:6:ILE:O	8:h:10:LEU:HD22	1.98	0.64
49:3:33:THR:O	49:3:35:LYS:N	2.30	0.64
52:5:2646:C:OP2	52:5:2732:G:O2'	2.16	0.64
25:D:81:GLU:OE2	52:5:2635:A:O2'	2.12	0.64
34:O:106:LEU:C	34:O:106:LEU:HD23	2.23	0.64
42:W:70:PRO:O	42:W:72:ASN:N	2.30	0.64
6:f:62:MET:HB3	6:f:64:VAL:HG13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:29:ALA:HB1	10:j:83:THR:HG23	1.80	0.64
36:Q:34:ALA:O	36:Q:38:VAL:HG23	1.98	0.64
13:m:3:ILE:HD11	13:m:21:ILE:HD11	1.78	0.64
35:P:105:LYS:O	35:P:108:ARG:NH1	2.31	0.64
1:a:967:5MC:OP2	1:a:968:A:O2'	2.07	0.63
22:A:686:U:O4	48:2:12:ARG:NH1	2.30	0.63
23:B:42:C:N3	27:F:89:THR:OG1	2.27	0.63
1:a:1169:A:O2'	2:b:138:ARG:NH2	2.31	0.63
28:G:80:GLU:OE1	28:G:80:GLU:N	2.32	0.63
1:a:1151:A:O2'	1:a:1152:A:OP1	2.15	0.63
1:a:652:U:O2'	1:a:653:U:O5'	2.13	0.63
6:f:90:MET:HE1	18:r:22:TYR:CE1	2.34	0.63
22:A:307:G:N1	22:A:310:A:OP2	2.30	0.63
22:A:500:G:N1	22:A:503:A:OP2	2.28	0.63
25:D:136:ASN:ND2	25:D:139:SER:O	2.32	0.63
25:D:180:VAL:HG23	25:D:180:VAL:O	1.96	0.63
32:M:108:VAL:CG1	32:M:112:LEU:HD23	2.28	0.63
1:a:1077:G:N2	1:a:1080:A:OP2	2.29	0.63
22:A:227:A:O2'	22:A:228:C:O4'	2.17	0.63
26:E:44:ARG:NH2	52:5:1248:G:OP1	2.31	0.63
42:W:13:GLU:O	42:W:15:LYS:NZ	2.31	0.63
1:a:690:G:OP2	11:k:28:ASN:ND2	2.23	0.63
1:a:1059:C:O3'	14:n:85:ARG:NH2	2.32	0.63
52:5:1094:U:N3	52:5:1097:U:OP2	2.32	0.63
4:d:123:MET:N	4:d:143:SER:O	2.31	0.63
25:D:99:GLU:HA	25:D:99:GLU:OE1	1.99	0.63
28:G:109:SER:OG	52:5:2667:C:N3	2.30	0.63
8:h:10:LEU:HD12	8:h:74:ILE:HD11	1.81	0.62
27:F:151:LEU:C	27:F:151:LEU:HD12	2.24	0.62
8:h:89:ASP:N	8:h:89:ASP:OD1	2.30	0.62
21:u:19:LYS:HD2	21:u:19:LYS:N	2.13	0.62
24:C:159:THR:HG23	24:C:176:ARG:HG3	1.82	0.62
52:5:1176:U:O2'	52:5:1177:G:O4'	2.16	0.62
45:Z:40:THR:HB	45:Z:41:PRO:HD2	1.81	0.62
52:5:2333:A:H4'	52:5:2334:U:O5'	1.99	0.62
8:h:21:LYS:O	8:h:64:TYR:OH	2.17	0.62
28:G:158:GLY:O	28:G:162:ARG:NH2	2.32	0.62
52:5:1266:G:O2'	52:5:2012:G:O6	2.16	0.62
52:5:1939:5MU:C4	52:5:1939:5MU:C5M	2.76	0.62
2:b:29:PHE:O	2:b:30:ILE:HG23	1.99	0.62
3:c:119:ILE:HD11	3:c:136:ALA:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:105:ILE:HD11	5:e:123:LEU:HD23	1.81	0.62
26:E:5:LEU:HD13	26:E:10:SER:O	1.99	0.62
43:X:38:TRP:NE1	43:X:40:GLU:OE1	2.30	0.62
1:a:464:U:O2'	1:a:466:A:N7	2.26	0.62
2:b:14:HIS:HD1	2:b:212:TYR:HH	1.48	0.62
3:c:150:VAL:HG12	3:c:199:VAL:HG12	1.82	0.62
17:q:20:ILE:O	17:q:45:VAL:HG12	2.00	0.62
52:5:981:A:OP2	52:5:982:C:N4	2.25	0.62
6:f:29:ILE:CD1	6:f:64:VAL:HG11	2.30	0.62
6:f:32:ALA:O	6:f:34:GLY:N	2.33	0.62
1:a:1106:G:O2'	3:c:168:ARG:NH1	2.32	0.62
5:e:76:ASN:O	5:e:78:GLY:N	2.32	0.62
13:m:15:VAL:HG23	13:m:16:ILE:HD12	1.81	0.61
29:J:135:GLN:OE1	29:J:135:GLN:N	2.33	0.61
31:L:29:LYS:C	31:L:30:THR:HG1	2.04	0.61
41:V:43:ASP:OD1	41:V:44:HIS:N	2.33	0.61
1:a:979:C:OP1	1:a:1223:C:N4	2.33	0.61
23:B:28:C:OP1	34:O:36:TYR:OH	2.19	0.61
2:b:124:THR:O	2:b:124:THR:OG1	2.17	0.61
3:c:35:ASP:OD1	3:c:56:ILE:HG21	2.00	0.61
3:c:91:ALA:HB2	3:c:98:ALA:HB3	1.82	0.61
27:F:9:ASP:OD1	27:F:9:ASP:N	2.33	0.61
29:J:81:ILE:HD11	52:5:2514:U:C5'	2.31	0.61
5:e:114:LEU:HD22	5:e:119:VAL:HG21	1.83	0.61
7:g:22:LEU:O	7:g:26:VAL:HG23	2.01	0.61
19:s:9:PHE:O	19:s:10:ILE:HG23	2.01	0.61
3:c:89:VAL:HG23	3:c:90:VAL:H	1.66	0.61
3:c:156:LEU:HD12	3:c:156:LEU:O	2.01	0.61
4:d:117:VAL:HG22	4:d:122:ILE:HG13	1.83	0.61
34:O:37:ALA:HB3	34:O:78:VAL:HG21	1.83	0.61
52:5:1668:A:O2'	52:5:1674:G:N7	2.25	0.61
1:a:1347:G:O6	9:i:11:ARG:NH2	2.34	0.61
9:i:66:VAL:HG22	9:i:74:GLN:OE1	2.01	0.61
36:Q:52:ARG:NH2	52:5:994:C:OP1	2.34	0.61
1:a:182:A:N1	1:a:223:A:O2'	2.32	0.61
3:c:30:ASP:OD1	14:n:65:ARG:NH1	2.32	0.61
24:C:75:ALA:HB1	24:C:93:VAL:HG12	1.83	0.61
46:O:30:ASP:O	46:O:34:GLY:HA2	2.01	0.61
1:a:1148:U:O2'	9:i:67:LYS:NZ	2.32	0.60
11:k:73:VAL:HG23	11:k:73:VAL:O	2.01	0.60
47:1:21:THR:HG21	52:5:2419:U:H4'	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:5:1527:G:N1	52:5:1544:A:OP2	2.34	0.60
2:b:53:LEU:HB3	2:b:219:THR:HG21	1.83	0.60
27:F:84:ILE:C	27:F:84:ILE:HD12	2.26	0.60
1:a:28:A:O2'	1:a:296:U:OP1	2.16	0.60
26:E:48:THR:O	26:E:52:VAL:HG23	2.01	0.60
29:J:65:THR:OG1	52:5:1141:U:OP2	2.18	0.60
1:a:392:C:O2'	1:a:483:C:O2'	1.99	0.60
3:c:22:PHE:HE1	10:j:69:THR:HG23	1.67	0.60
4:d:75:TYR:CE1	4:d:203:TYR:HB3	2.36	0.60
22:A:85:G:OP1	40:U:6:ARG:N	2.32	0.60
22:A:586:A:N1	22:A:809:G:O2'	2.31	0.60
22:A:615:U:H4'	22:A:616:A:OP2	2.01	0.60
17:q:66:LEU:HD23	17:q:66:LEU:C	2.26	0.60
51:6:11:GLU:HG3	51:6:25:ARG:HD2	1.82	0.60
3:c:91:ALA:HA	3:c:94:ALA:HB3	1.84	0.60
51:6:17:SER:O	51:6:19:GLY:N	2.35	0.60
52:5:2627:G:N2	52:5:2777:G:OP2	2.34	0.60
52:5:2867:G:O2'	52:5:2868:A:P	2.60	0.60
22:A:190:A:OP2	43:X:25:LYS:NZ	2.35	0.60
24:C:257:ARG:NH1	24:C:263:ASP:OD1	2.34	0.60
37:R:27:ILE:HG22	37:R:28:ALA:H	1.66	0.60
1:a:421:U:HO2'	1:a:422:C:P	2.24	0.59
1:a:618:C:O2	1:a:622:A:N6	2.35	0.59
1:a:1200:C:O2'	1:a:1205:U:O4	2.19	0.59
4:d:135:GLN:NE2	4:d:135:GLN:O	2.35	0.59
24:C:75:ALA:HB1	24:C:93:VAL:CG1	2.32	0.59
4:d:56:GLU:OE1	4:d:199:ILE:HD11	2.02	0.59
15:o:28:VAL:HG11	15:o:80:LEU:HD21	1.82	0.59
39:T:58:VAL:HG22	39:T:85:VAL:HG13	1.84	0.59
45:Z:11:SER:OG	52:5:989:G:OP2	2.17	0.59
1:a:1316:G:N1	1:a:1319:A:OP2	2.33	0.59
12:l:34:THR:OG1	12:l:53:ARG:O	2.15	0.59
16:p:7:ALA:O	16:p:9:HIS:N	2.36	0.59
50:4:2:LYS:NZ	52:5:2478:A:OP2	2.34	0.59
52:5:2629:U:O2'	52:5:2630:G:O5'	2.19	0.59
12:l:23:LEU:HD22	12:l:58:ASN:HD22	1.66	0.59
22:A:91:A:O2'	22:A:92:U:O4'	2.19	0.59
22:A:283:G:H1	22:A:357:C:H42	1.51	0.59
1:a:766:A:OP2	1:a:812:G:N2	2.33	0.59
7:g:144:ALA:O	7:g:146:ALA:N	2.36	0.59
19:s:51:HIS:ND1	19:s:55:GLN:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:5:2522:U:O2'	52:5:2647:U:OP1	2.11	0.59
1:a:1129:C:O2'	1:a:1130:A:N7	2.35	0.59
6:f:81:ASN:OD1	6:f:83:ALA:N	2.35	0.59
24:C:244:VAL:HG12	24:C:250:GLN:HA	1.84	0.59
52:5:2788:C:O2'	52:5:2809:A:N3	2.34	0.59
1:a:613:C:OP1	4:d:80:ARG:NH2	2.35	0.59
1:a:944:G:N1	1:a:1338:G:OP2	2.35	0.59
22:A:774:G:N2	22:A:787:C:O2'	2.33	0.59
11:k:62:ALA:HB1	11:k:95:THR:HB	1.83	0.59
24:C:106:PRO:CG	24:C:109:LEU:HD22	2.33	0.59
39:T:64:LYS:NZ	52:5:1601:G:OP1	2.26	0.59
16:p:67:ILE:CD1	16:p:72:ALA:HB2	2.33	0.58
18:r:54:LEU:O	18:r:58:ILE:HD13	2.02	0.58
26:E:113:VAL:HG22	26:E:118:LEU:HD23	1.84	0.58
29:J:17:VAL:HG23	29:J:137:PRO:HB2	1.85	0.58
1:a:403:C:H5'	4:d:131:ILE:HG23	1.83	0.58
22:A:18:U:O2'	22:A:554:U:OP1	2.21	0.58
24:C:270:ARG:NH2	52:5:1798:U:OP2	2.34	0.58
1:a:769:G:H4'	1:a:1513:A:H4'	1.85	0.58
2:b:14:HIS:CG	2:b:14:HIS:O	2.57	0.58
14:n:54:ASP:O	14:n:56:SER:N	2.37	0.58
27:F:140:ILE:H	27:F:140:ILE:HD12	1.68	0.58
52:5:2075:U:OP2	52:5:2238:G:O2'	2.21	0.58
3:c:171:ARG:HG2	3:c:173:PRO:HD3	1.85	0.58
26:E:124:PHE:CE2	26:E:141:MET:HE1	2.39	0.58
22:A:69:C:O2	22:A:73:A:O2'	2.20	0.58
40:U:33:VAL:HG13	40:U:66:VAL:HG22	1.85	0.58
2:b:113:LEU:HD11	2:b:144:GLU:OE1	2.03	0.58
3:c:112:ALA:HB1	3:c:199:VAL:HG23	1.86	0.58
22:A:858:G:O2'	22:A:859:G:OP1	2.22	0.58
27:F:70:ARG:NH1	52:5:2298:A:OP1	2.34	0.58
40:U:27:VAL:HG12	40:U:33:VAL:HG12	1.86	0.58
1:a:674:G:H21	11:k:117:HIS:HB2	1.69	0.58
7:g:30:MET:SD	7:g:33:GLY:N	2.74	0.58
24:C:128:THR:HG1	24:C:190:THR:HG1	1.52	0.58
39:T:6:ARG:NH2	39:T:42:GLU:OE1	2.37	0.58
49:3:38:LYS:NZ	52:5:2365:G:O6	2.35	0.58
1:a:826:C:O2	8:h:15:ASN:ND2	2.37	0.58
14:n:30:ILE:HG21	14:n:44:ALA:HB2	1.86	0.58
22:A:687:C:H1'	48:2:4:THR:HG22	1.86	0.58
32:M:53:MET:O	32:M:57:VAL:HG22	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1347:G:O2'	1:a:1348:U:P	2.61	0.57
3:c:120:THR:HG23	3:c:188:ALA:HB2	1.86	0.57
44:Y:24:GLU:HB3	44:Y:46:VAL:HG21	1.86	0.57
42:W:29:ALA:N	42:W:60:ASP:OD1	2.37	0.57
52:5:1416:G:O2'	52:5:1417:C:O5'	2.22	0.57
15:o:7:THR:O	15:o:11:VAL:HG23	2.04	0.57
27:F:72:SER:OG	27:F:80:GLN:N	2.38	0.57
30:K:41:ILE:HD11	30:K:58:LEU:CD1	2.34	0.57
35:P:59:THR:OG1	35:P:72:VAL:HG12	2.05	0.57
46:0:2:VAL:HG13	52:5:2016:U:H1'	1.86	0.57
6:f:96:VAL:O	6:f:97:THR:HG23	2.04	0.57
24:C:30:ALA:O	24:C:32:LEU:N	2.38	0.57
29:J:84:ILE:HG23	29:J:84:ILE:O	2.02	0.57
34:O:62:LEU:HD13	34:O:70:ALA:HB1	1.86	0.57
1:a:750:C:O2'	15:o:20:ASP:OD1	2.20	0.57
1:a:1190:G:O2'	3:c:2:GLN:O	2.17	0.57
22:A:332:A:O2'	22:A:334:C:OP2	2.22	0.57
22:A:549:G:O2'	22:A:550:C:OP1	2.22	0.57
1:a:321:A:N6	1:a:328:C:O2'	2.38	0.57
1:a:901:A:O2'	1:a:1513:A:OP1	2.11	0.57
7:g:49:LEU:HD22	7:g:123:LEU:HD12	1.84	0.57
17:q:47:ASP:N	17:q:47:ASP:OD1	2.38	0.57
43:X:35:HIS:CD2	43:X:55:MET:HE1	2.39	0.57
52:5:1070:A:O2'	52:5:1097:U:OP1	2.21	0.57
52:5:2682:A:H61	52:5:2728:U:H1'	1.70	0.57
1:a:677:U:H3	1:a:713:G:H22	1.53	0.57
7:g:74:VAL:HG21	7:g:143:MET:HE2	1.87	0.57
11:k:45:THR:O	11:k:49:SER:OG	2.21	0.57
7:g:48:THR:O	7:g:52:ARG:HG2	2.05	0.57
10:j:26:VAL:HG13	10:j:36:VAL:HG21	1.87	0.57
24:C:245:THR:HG23	24:C:249:VAL:O	2.04	0.57
1:a:1281:C:O2'	1:a:1282:C:OP1	2.14	0.57
4:d:103:ARG:HB3	4:d:170:LEU:HD21	1.85	0.57
12:l:100:ALA:O	12:l:101:LEU:HB2	2.05	0.57
30:K:34:GLY:O	30:K:36:GLY:N	2.37	0.57
52:5:2110:G:N1	52:5:2120:G:N7	2.53	0.57
1:a:620:C:C2	1:a:621:A:C8	2.92	0.57
1:a:979:C:O2	14:n:59:ARG:NH1	2.31	0.57
4:d:168:THR:O	4:d:183:ARG:NH2	2.37	0.57
29:J:81:ILE:HG23	29:J:81:ILE:O	2.04	0.57
1:a:1056:U:OP1	3:c:162:ALA:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1151:A:HO2'	1:a:1152:A:P	2.27	0.56
4:d:158:LEU:HB2	4:d:177:MET:HE1	1.86	0.56
52:5:2659:G:N2	52:5:2662:A:OP2	2.37	0.56
15:o:17:ASP:OD1	15:o:17:ASP:N	2.38	0.56
22:A:770:G:H5'	48:2:10:LEU:HD23	1.87	0.56
22:A:877:A:O2'	52:5:900:A:N6	2.37	0.56
1:a:1405:G:N2	1:a:1518:MA6:H8	2.19	0.56
4:d:197:HIS:NE2	4:d:201:GLU:OE2	2.38	0.56
7:g:38:ALA:O	7:g:42:VAL:HG23	2.05	0.56
8:h:29:SER:O	8:h:33:VAL:HG22	2.05	0.56
22:A:257:C:O2	31:L:104:GLN:NE2	2.38	0.56
35:P:8:GLU:OE2	35:P:55:HIS:NE2	2.36	0.56
1:a:106:C:H2'	1:a:107:G:O4'	2.05	0.56
22:A:730:A:OP1	52:5:1775:U:O2'	2.16	0.56
47:1:20:TYR:OH	52:5:2347:C:O2'	2.23	0.56
1:a:324:G:N1	1:a:327:A:OP2	2.39	0.56
3:c:120:THR:HG23	3:c:188:ALA:CB	2.36	0.56
12:l:109:ARG:HB2	12:l:118:VAL:HG21	1.87	0.56
15:o:3:SER:O	15:o:7:THR:HG23	2.05	0.56
1:a:1000:A:N6	1:a:1041:G:O6	2.39	0.56
20:t:19:HIS:O	20:t:23:ARG:HG2	2.06	0.56
22:A:585:G:N7	36:Q:5:ARG:NH2	2.53	0.56
32:M:108:VAL:HG13	32:M:112:LEU:HD23	1.87	0.56
6:f:11:HIS:HD2	6:f:54:LEU:HD22	1.71	0.56
6:f:36:ILE:HD12	6:f:37:HIS:N	2.21	0.56
22:A:555:G:HO2'	22:A:556:A:H8	1.54	0.56
32:M:35:ALA:HB1	32:M:126:ILE:HD12	1.88	0.56
38:S:99:ARG:NH2	52:5:1262:A:OP1	2.38	0.56
52:5:2800:A:H3'	52:5:2801:G:H5'	1.88	0.56
19:s:44:ILE:HD13	19:s:61:VAL:HG12	1.88	0.56
33:N:100:CYS:O	33:N:100:CYS:SG	2.63	0.56
1:a:483:C:OP2	1:a:484:G:O2'	2.18	0.55
1:a:811:C:O2'	1:a:901:A:N1	2.37	0.55
6:f:93:LYS:O	6:f:94:HIS:ND1	2.39	0.55
16:p:23:ASP:OD2	16:p:25:ARG:N	2.29	0.55
22:A:859:G:O2'	22:A:860:U:P	2.64	0.55
30:K:13:ASN:N	30:K:13:ASN:OD1	2.40	0.55
30:K:76:VAL:HG13	35:P:72:VAL:HG22	1.87	0.55
17:q:28:VAL:HG11	17:q:39:ARG:HG3	1.88	0.55
25:D:4:LEU:HD12	25:D:101:PHE:CE2	2.41	0.55
52:5:2629:U:HO2'	52:5:2630:G:P	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:156:C:H2'	1:a:157:U:O4'	2.06	0.55
4:d:24:VAL:HG23	4:d:25:ARG:N	2.21	0.55
7:g:68:VAL:HG21	7:g:103:ILE:HD11	1.88	0.55
9:i:50:PRO:HG2	9:i:82:ILE:HG21	1.89	0.55
20:t:53:MET:O	20:t:56:ILE:HG22	2.06	0.55
22:A:91:A:O2'	22:A:92:U:P	2.63	0.55
52:5:1129:A:HO2'	52:5:2515:C:HO2'	1.54	0.55
7:g:45:ALA:HA	7:g:48:THR:OG1	2.07	0.55
22:A:301:G:OP2	40:U:81:ARG:NH2	2.37	0.55
48:2:30:VAL:HG22	48:2:33:ARG:NH2	2.22	0.55
1:a:80:A:N6	1:a:81:A:N1	2.54	0.55
4:d:59:LYS:HE3	4:d:194:ILE:HG22	1.89	0.55
22:A:820:A:H4'	22:A:836:G:H22	1.70	0.55
25:D:114:LYS:NZ	52:5:2723:C:OP1	2.38	0.55
31:L:19:LEU:HD12	31:L:27:LEU:HD12	1.89	0.55
52:5:1474:U:O4	52:5:1475:G:N2	2.39	0.55
52:5:1171:G:H2'	52:5:1172:C:O4'	2.07	0.55
1:a:520:A:O2'	12:l:69:GLU:OE2	2.21	0.55
6:f:18:VAL:O	6:f:19:PRO:C	2.50	0.55
25:D:9:VAL:HG13	25:D:9:VAL:O	2.07	0.55
1:a:373:A:C2	1:a:374:A:C8	2.95	0.55
12:l:82:ARG:NH1	12:l:83:GLY:O	2.39	0.55
22:A:394:C:H2'	22:A:395:U:O4'	2.07	0.55
32:M:35:ALA:O	32:M:99:GLY:N	2.39	0.55
37:R:74:ILE:HD12	37:R:74:ILE:N	2.22	0.55
51:6:18:CYS:SG	51:6:19:GLY:N	2.80	0.55
1:a:1517:G:O6	1:a:1518:MA6:H92	2.07	0.55
2:b:33:ALA:HB3	2:b:37:VAL:O	2.06	0.55
4:d:55:ARG:C	4:d:55:ARG:HD3	2.31	0.55
22:A:58:G:O2'	22:A:73:A:N1	2.33	0.55
25:D:207:VAL:HG13	25:D:208:LYS:N	2.21	0.55
34:O:21:LEU:HD11	52:5:2379:G:H4'	1.89	0.55
4:d:112:GLU:OE2	4:d:153:ARG:NH1	2.39	0.55
12:l:88:ASP:OD1	12:l:88:ASP:N	2.39	0.55
21:u:33:ARG:HG2	21:u:34:ARG:HG2	1.88	0.55
34:O:104:GLN:NE2	34:O:108:ASP:OD2	2.40	0.55
39:T:57:VAL:HG12	39:T:86:THR:CG2	2.37	0.55
1:a:409:U:H5'	4:d:24:VAL:HG22	1.89	0.54
12:l:20:VAL:O	12:l:22:ALA:N	2.39	0.54
14:n:39:GLU:O	14:n:43:ASN:ND2	2.40	0.54
15:o:39:GLN:NE2	22:A:716:A:O4'	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:458:G:O2'	22:A:459:U:P	2.65	0.54
22:A:569:U:O2'	52:5:983:A:N1	2.36	0.54
32:M:17:ASN:OD1	32:M:97:GLN:NE2	2.40	0.54
44:Y:42:LEU:O	44:Y:46:VAL:HG23	2.07	0.54
50:4:1:MET:N	52:5:2526:G:N3	2.56	0.54
1:a:180:U:O2	1:a:195:A:N7	2.40	0.54
1:a:246:A:C2	1:a:282:A:C5	2.94	0.54
1:a:1057:G:H1'	3:c:194:VAL:HG11	1.87	0.54
2:b:132:GLU:HA	2:b:135:MET:HE2	1.88	0.54
26:E:109:LEU:O	26:E:113:VAL:HG23	2.07	0.54
27:F:95:MET:HG2	27:F:96:TRP:N	2.22	0.54
47:1:8:ILE:C	47:1:8:ILE:HD12	2.32	0.54
52:5:2391:G:O2'	52:5:2429:G:N2	2.40	0.54
52:5:2431:U:O2'	52:5:2433:A:N7	2.40	0.54
1:a:652:U:HO2'	1:a:653:U:P	2.30	0.54
9:i:101:GLY:O	9:i:103:VAL:N	2.36	0.54
19:s:5:LYS:HD3	19:s:5:LYS:C	2.32	0.54
22:A:616:A:O2'	26:E:199:MET:HE3	2.07	0.54
28:G:73:SER:HA	28:G:76:ILE:HD12	1.89	0.54
30:K:33:ALA:HB1	30:K:37:ASP:HB2	1.88	0.54
30:K:41:ILE:HD11	30:K:58:LEU:HD11	1.89	0.54
33:N:12:ARG:O	33:N:17:ARG:NH1	2.39	0.54
40:U:31:GLY:O	40:U:66:VAL:HG23	2.07	0.54
22:A:205:G:HO2'	22:A:206:U:P	2.31	0.54
22:A:851:C:O2'	45:Z:42:ALA:O	2.24	0.54
33:N:79:LEU:O	33:N:80:PHE:HB2	2.08	0.54
52:5:2808:G:H4'	52:5:2809:A:O5'	2.08	0.54
1:a:664:G:H22	1:a:741:G:H1	1.55	0.54
18:r:33:THR:OG1	18:r:34:GLU:N	2.41	0.54
22:A:75:G:H22	22:A:111:A:H2	1.55	0.54
52:5:2637:U:H2'	52:5:2638:G:O4'	2.07	0.54
9:i:56:MET:O	9:i:58:GLU:N	2.40	0.54
20:t:13:SER:O	20:t:14:GLU:C	2.51	0.54
37:R:27:ILE:HG22	37:R:28:ALA:N	2.22	0.54
1:a:337:G:H2'	1:a:338:A:C8	2.43	0.54
2:b:117:GLU:HA	2:b:140:LEU:HD11	1.90	0.54
4:d:19:PHE:O	4:d:110:ARG:NH1	2.40	0.54
4:d:60:VAL:CG2	4:d:199:ILE:HD11	2.35	0.54
13:m:6:ILE:C	13:m:8:ILE:HD12	2.33	0.54
22:A:784:G:H5'	22:A:785:G:OP1	2.07	0.54
52:5:2113:U:O4	52:5:2119:A:N6	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:85:U:H4'	1:a:86:G:O5'	2.08	0.54
4:d:149:LYS:NZ	4:d:176:LYS:O	2.31	0.54
10:j:47:GLU:OE1	10:j:47:GLU:N	2.41	0.54
28:G:10:VAL:O	28:G:10:VAL:HG22	2.08	0.54
31:L:110:VAL:O	31:L:111:ILE:O	2.26	0.54
37:R:49:ILE:HD12	37:R:51:VAL:O	2.08	0.54
1:a:561:U:O2'	1:a:562:U:OP2	2.17	0.54
19:s:11:ASP:HB3	19:s:13:HIS:CE1	2.43	0.54
52:5:974:G:O2'	52:5:989:G:N2	2.35	0.54
52:5:2712:C:O2'	52:5:2713:U:P	2.65	0.54
4:d:49:ASP:O	4:d:52:VAL:HG22	2.07	0.54
22:A:205:G:O2'	22:A:206:U:OP2	2.22	0.54
37:R:14:VAL:HG12	37:R:20:VAL:HG11	1.89	0.54
43:X:67:LEU:HD22	43:X:77:TYR:CG	2.42	0.54
52:5:2286:G:H4'	52:5:2287:A:O4'	2.08	0.54
1:a:201:G:O2'	1:a:469:C:O2'	2.26	0.53
1:a:492:C:H2'	1:a:493:A:C8	2.43	0.53
52:5:1965:C:OP1	52:5:1966:A:O2'	2.19	0.53
1:a:747:A:H2'	1:a:748:G:O4'	2.08	0.53
24:C:209:ALA:HA	24:C:212:TRP:CE2	2.42	0.53
37:R:29:THR:O	37:R:63:VAL:HG23	2.08	0.53
38:S:23:LEU:HD22	46:0:23:ALA:HB2	1.89	0.53
1:a:890:G:O2'	1:a:891:U:P	2.66	0.53
6:f:88:MET:HE3	18:r:63:TYR:HD2	1.73	0.53
7:g:49:LEU:HD13	7:g:123:LEU:HB2	1.91	0.53
10:j:10:LEU:HB3	10:j:98:VAL:HG12	1.90	0.53
14:n:12:ARG:O	14:n:13:VAL:C	2.51	0.53
52:5:2327:A:H2'	52:5:2328:A:C8	2.43	0.53
52:5:2564:A:OP1	52:5:2648:G:O2'	2.21	0.53
52:5:2884:U:O2'	52:5:2885:G:O5'	2.25	0.53
1:a:1492:A:N6	12:l:46:SER:OG	2.42	0.53
10:j:29:ALA:HB1	10:j:83:THR:CG2	2.39	0.53
19:s:33:TRP:CD1	19:s:51:HIS:HD2	2.27	0.53
20:t:61:ALA:HB1	20:t:68:LYS:HA	1.91	0.53
52:5:1022:G:N2	52:5:1023:U:O4	2.37	0.53
1:a:345:C:HO2'	1:a:346:G:N2	2.06	0.53
4:d:10:LEU:HD12	4:d:20:LEU:HD11	1.91	0.53
6:f:88:MET:SD	18:r:64:LEU:HD21	2.48	0.53
11:k:49:SER:HB3	11:k:68:ARG:HD3	1.91	0.53
20:t:4:LYS:HG3	20:t:6:ALA:H	1.73	0.53
29:J:93:ILE:HD13	29:J:93:ILE:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:K:121:GLU:HG2	30:K:122:VAL:HG23	1.91	0.53
52:5:1869:G:O2'	52:5:1872:A:N6	2.41	0.53
5:e:130:THR:HG22	5:e:130:THR:O	2.09	0.53
8:h:4:ASP:HB3	8:h:7:ALA:HB3	1.89	0.53
13:m:50:GLY:O	13:m:53:ASP:OD1	2.27	0.53
16:p:6:LEU:HD13	16:p:17:TYR:CG	2.44	0.53
22:A:514:A:N3	22:A:581:C:O2'	2.34	0.53
40:U:64:ILE:HG12	40:U:65:GLN:N	2.23	0.53
44:Y:3:ALA:O	44:Y:7:ARG:NH1	2.41	0.53
52:5:976:G:O2'	52:5:1155:A:O2'	2.26	0.53
52:5:1022:G:HI1'	52:5:1023:U:OP2	2.09	0.53
52:5:2627:G:O2'	52:5:2781:A:N1	2.31	0.53
2:b:49:PHE:CE1	2:b:53:LEU:HD21	2.43	0.53
9:i:43:ALA:O	9:i:46:VAL:HG22	2.09	0.53
11:k:72:ALA:O	11:k:73:VAL:HG12	2.08	0.53
15:o:44:GLU:O	15:o:46:LYS:N	2.42	0.53
37:R:1:MET:HE2	37:R:1:MET:HA	1.91	0.53
1:a:355:C:O2'	1:a:388:G:N3	2.38	0.53
1:a:457:G:N2	1:a:475:C:O2	2.31	0.53
1:a:973:G:OP2	1:a:974:A:O2'	2.26	0.53
1:a:1399:C:O2	1:a:1502:A:N6	2.41	0.53
14:n:4:SER:O	14:n:5:MET:C	2.52	0.53
14:n:88:ALA:HB2	14:n:96:LEU:HD23	1.90	0.53
17:q:16:MET:C	17:q:17:GLU:OE1	2.51	0.53
42:W:61:GLY:HA3	42:W:79:GLU:O	2.09	0.53
52:5:1275:A:N1	52:5:1295:C:O2'	2.34	0.53
52:5:1900:A:O2'	52:5:1901:A:P	2.66	0.53
52:5:1980:G:O2'	52:5:1982:U:OP2	2.24	0.53
1:a:328:C:H4'	1:a:329:A:H5'	1.91	0.53
20:t:10:ALA:O	20:t:14:GLU:HG2	2.09	0.53
38:S:35:ILE:O	38:S:39:THR:OG1	2.22	0.53
17:q:27:PHE:O	17:q:28:VAL:C	2.50	0.52
22:A:372:G:O2'	22:A:373:U:P	2.67	0.52
28:G:87:GLN:OE1	28:G:89:VAL:HG23	2.09	0.52
28:G:132:LEU:H	28:G:132:LEU:HD23	1.73	0.52
8:h:94:VAL:O	8:h:95:MET:HB2	2.08	0.52
22:A:644:A:H2'	22:A:645:C:O4'	2.10	0.52
25:D:151:THR:O	52:5:1130:U:O4	2.28	0.52
27:F:56:LEU:O	27:F:59:ILE:HG23	2.09	0.52
29:J:37:ARG:NH1	52:5:1007:C:OP1	2.42	0.52
51:6:39:LYS:O	51:6:40:CYS:SG	2.67	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:5:1372:U:O2'	52:5:2212:A:N3	2.36	0.52
1:a:1366:C:O2'	10:j:62:ARG:NH2	2.42	0.52
3:c:39:ARG:HB2	3:c:54:ILE:HD11	1.90	0.52
48:2:24:THR:HG23	48:2:27:GLY:H	1.73	0.52
52:5:2138:G:H2'	52:5:2139:U:O4'	2.10	0.52
7:g:58:LEU:HD23	7:g:58:LEU:H	1.74	0.52
11:k:57:SER:O	11:k:90:PRO:HG3	2.09	0.52
16:p:40:ASN:HB3	16:p:43:ALA:HB2	1.92	0.52
22:A:756:A:H2'	22:A:757:G:O4'	2.10	0.52
52:5:1296:G:OP1	52:5:2709:G:O2'	2.23	0.52
52:5:2328:A:H2'	52:5:2329:U:C6	2.44	0.52
1:a:1458:G:OP1	20:t:29:THR:OG1	2.27	0.52
4:d:155:LYS:HE2	4:d:155:LYS:HA	1.91	0.52
10:j:8:ILE:HD11	10:j:87:LEU:HD11	1.91	0.52
4:d:191:SER:OG	4:d:192:ALA:N	2.42	0.52
5:e:121:ASN:C	5:e:122:VAL:HG13	2.34	0.52
6:f:88:MET:HE3	18:r:63:TYR:CD2	2.45	0.52
9:i:16:ALA:C	9:i:17:ARG:HG3	2.34	0.52
11:k:108:ASN:C	11:k:109:ILE:HD12	2.35	0.52
17:q:60:ILE:CG2	17:q:72:TRP:HB3	2.39	0.52
44:Y:27:ASN:O	44:Y:31:GLN:NE2	2.43	0.52
14:n:33:VAL:O	14:n:33:VAL:HG13	2.09	0.52
19:s:70:LEU:HD22	19:s:70:LEU:H	1.73	0.52
22:A:228:C:N4	52:5:2407:A:N3	2.57	0.52
22:A:549:G:HO2'	22:A:550:C:P	2.32	0.52
34:O:33:ARG:O	34:O:34:HIS:HB2	2.08	0.52
52:5:1928:A:H2'	52:5:1929:G:O4'	2.10	0.52
3:c:91:ALA:HB2	3:c:98:ALA:CB	2.39	0.52
3:c:138:GLN:O	3:c:142:ARG:HG2	2.10	0.52
9:i:47:VAL:HG12	9:i:78:ILE:CG2	2.38	0.52
12:l:86:VAL:O	12:l:87:LYS:HB3	2.10	0.52
24:C:174:ARG:NH1	24:C:180:MET:SD	2.83	0.52
30:K:80:ASP:OD2	35:P:61:ARG:NH2	2.42	0.52
39:T:61:LEU:HD11	39:T:82:LYS:HD3	1.92	0.52
52:5:1171:G:H8	52:5:1171:G:O5'	1.93	0.52
1:a:751:U:H2'	1:a:752:G:O4'	2.10	0.52
7:g:50:ALA:O	7:g:51:GLN:C	2.53	0.52
10:j:50:THR:HG22	10:j:62:ARG:CD	2.40	0.52
19:s:36:ARG:O	19:s:69:LYS:NZ	2.41	0.52
22:A:771:G:OP1	48:2:14:ARG:NH1	2.43	0.52
22:A:856:G:H2'	22:A:857:G:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:7:G:O2'	34:O:38:GLN:NE2	2.43	0.52
24:C:70:LYS:O	24:C:117:SER:OG	2.26	0.52
27:F:170:ALA:O	27:F:172:PHE:N	2.43	0.52
48:2:30:VAL:O	48:2:34:ARG:HG2	2.10	0.52
1:a:404:G:O6	4:d:1:ALA:N	2.43	0.52
1:a:414:A:OP2	1:a:428:G:N2	2.39	0.52
4:d:104:MET:HE2	4:d:170:LEU:HB2	1.91	0.52
6:f:15:SER:HA	6:f:18:VAL:HG23	1.91	0.52
22:A:675:A:N3	52:5:2443:C:O2'	2.41	0.52
24:C:149:LYS:HD3	52:5:2204:G:H4'	1.92	0.52
25:D:102:ALA:HA	25:D:180:VAL:HG21	1.92	0.52
27:F:59:ILE:HG23	27:F:60:SER:N	2.23	0.52
28:G:41:GLU:OE1	28:G:42:VAL:N	2.42	0.52
30:K:19:VAL:CG1	30:K:41:ILE:HD13	2.39	0.52
37:R:94:THR:O	37:R:94:THR:HG23	2.10	0.52
49:3:33:THR:O	49:3:34:LYS:C	2.53	0.52
52:5:1939:5MU:C5	52:5:1939:5MU:C2	2.93	0.52
1:a:481:G:O2'	1:a:483:C:N4	2.41	0.51
1:a:1398:A:N6	5:e:26:GLY:O	2.42	0.51
13:m:3:ILE:CD1	13:m:21:ILE:HD11	2.40	0.51
16:p:21:VAL:O	16:p:32:PHE:HB2	2.10	0.51
30:K:13:ASN:O	30:K:14:SER:C	2.52	0.51
34:O:94:ARG:HB3	34:O:97:PHE:O	2.09	0.51
52:5:1626:A:O2'	52:5:1627:G:P	2.68	0.51
52:5:1857:G:O2'	52:5:1858:A:O5'	2.25	0.51
52:5:2286:G:H4'	52:5:2287:A:O5'	2.09	0.51
1:a:1297:G:H1'	1:a:1298:U:OP2	2.10	0.51
4:d:61:ARG:NH1	4:d:68:GLU:OE1	2.41	0.51
37:R:3:ALA:HB3	37:R:101:ILE:HD12	1.92	0.51
44:Y:50:VAL:O	44:Y:54:LYS:HG3	2.09	0.51
52:5:2291:U:OP1	52:5:2380:C:O2'	2.27	0.51
52:5:2867:G:HO2'	52:5:2868:A:P	2.33	0.51
1:a:520:A:H61	1:a:533:A:H61	1.57	0.51
1:a:1320:C:O2'	19:s:72:GLU:OE2	2.17	0.51
5:e:79:THR:OG1	5:e:97:PRO:O	2.28	0.51
11:k:35:ASP:OD1	11:k:35:ASP:N	2.32	0.51
13:m:9:PRO:HG2	13:m:44:ILE:HD13	1.91	0.51
20:t:20:ASN:HD21	20:t:65:LEU:CD1	2.21	0.51
20:t:25:SER:O	20:t:29:THR:OG1	2.21	0.51
27:F:106:ALA:O	27:F:109:ARG:N	2.38	0.51
51:6:11:GLU:OE2	51:6:23:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:5:1141:U:H4'	52:5:1142:A:O4'	2.10	0.51
52:5:2533:U:OP1	52:5:2665:A:O2'	2.28	0.51
1:a:322:C:H2'	1:a:323:U:C6	2.46	0.51
1:a:1151:A:H1'	10:j:41:PRO:HB3	1.93	0.51
3:c:71:ARG:HD3	3:c:74:ILE:HD12	1.92	0.51
4:d:106:PHE:CD2	4:d:144:ILE:HD11	2.45	0.51
5:e:108:GLY:O	5:e:109:ALA:HB3	2.11	0.51
11:k:20:ALA:HB2	11:k:81:LEU:HD12	1.92	0.51
22:A:571:U:C5	52:5:2030:6MZ:H9	2.46	0.51
29:J:93:ILE:CD1	29:J:100:VAL:HG21	2.40	0.51
37:R:49:ILE:HG22	37:R:54:VAL:HA	1.92	0.51
51:6:58:ASP:O	51:6:62:LYS:HG3	2.09	0.51
1:a:508:U:H4'	4:d:50:TYR:CD2	2.46	0.51
15:o:28:VAL:HG21	15:o:66:LEU:CD2	2.39	0.51
18:r:28:LEU:HD21	18:r:58:ILE:CD1	2.40	0.51
22:A:323:C:H2'	52:5:1205:A:N1	2.26	0.51
22:A:463:G:N2	22:A:466:A:OP2	2.36	0.51
24:C:60:ALA:O	24:C:62:ARG:NH1	2.39	0.51
37:R:39:LEU:HD23	37:R:49:ILE:HD11	1.92	0.51
42:W:15:LYS:NZ	52:5:2261:C:OP1	2.37	0.51
45:Z:36:GLU:O	45:Z:37:ARG:NH1	2.43	0.51
46:0:22:THR:HG23	46:0:22:THR:O	2.11	0.51
52:5:1130:U:O2'	52:5:1131:G:P	2.69	0.51
52:5:1433:A:H2'	52:5:1434:A:C8	2.45	0.51
8:h:74:ILE:HG23	8:h:74:ILE:O	2.11	0.51
22:A:728:G:H3'	22:A:729:G:H5'	1.92	0.51
22:A:833:A:H2'	22:A:834:G:C8	2.45	0.51
22:A:883:G:H21	52:5:894:U:H1'	1.76	0.51
52:5:1475:G:O2'	52:5:1476:U:P	2.68	0.51
2:b:202:ASN:OD1	2:b:205:ALA:HB2	2.11	0.51
9:i:115:VAL:HG21	10:j:62:ARG:HB2	1.93	0.51
22:A:421:C:O2'	22:A:422:A:P	2.69	0.51
25:D:25:THR:HG23	25:D:191:GLY:O	2.09	0.51
3:c:4:VAL:HG13	3:c:4:VAL:O	2.10	0.51
3:c:60:ALA:O	3:c:61:LYS:HB3	2.11	0.51
5:e:10:LEU:HD23	5:e:67:ARG:NH1	2.25	0.51
6:f:13:ASP:OD1	6:f:13:ASP:N	2.37	0.51
37:R:16:GLU:OE1	37:R:17:GLY:N	2.44	0.51
1:a:776:G:N2	1:a:802:A:OP2	2.42	0.51
2:b:76:SER:O	2:b:77:GLU:C	2.53	0.51
2:b:185:ILE:HD12	2:b:199:ILE:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:10:VAL:HG12	6:f:11:HIS:N	2.26	0.51
6:f:51:ILE:O	6:f:52:ASN:OD1	2.29	0.51
13:m:9:PRO:CG	13:m:17:ALA:HB1	2.40	0.51
17:q:66:LEU:HD23	17:q:66:LEU:O	2.11	0.51
27:F:58:ALA:O	27:F:59:ILE:C	2.54	0.51
32:M:40:ARG:HD3	32:M:93:VAL:HG21	1.92	0.51
35:P:29:VAL:CG2	35:P:79:VAL:HG12	2.40	0.51
38:S:3:THR:HG21	38:S:58:ALA:HB2	1.92	0.51
52:5:1111:A:O2'	52:5:1112:G:P	2.68	0.51
52:5:1111:A:HO2'	52:5:1112:G:P	2.33	0.51
52:5:2467:C:H2'	52:5:2468:A:O4'	2.11	0.51
1:a:427:U:O2'	1:a:541:G:OP1	2.28	0.51
1:a:635:A:H2'	1:a:636:U:C6	2.46	0.51
1:a:652:U:O4	1:a:752:G:O2'	2.20	0.51
1:a:933:G:N7	7:g:2:ARG:NH2	2.58	0.51
1:a:960:U:H4'	1:a:961:U:O5'	2.11	0.51
22:A:494:G:H4'	38:S:6:LYS:HG3	1.92	0.51
22:A:548:G:O2'	22:A:549:G:O4'	2.29	0.51
27:F:37:MET:SD	27:F:56:LEU:HD12	2.51	0.51
33:N:39:PRO:O	33:N:41:ALA:N	2.44	0.51
52:5:1322:A:C5	52:5:1323:C:C5	2.99	0.51
52:5:2867:G:O2'	52:5:2868:A:O5'	2.28	0.51
1:a:373:A:N3	1:a:482:A:N6	2.59	0.50
1:a:1182:G:H4'	1:a:1183:U:O5'	2.12	0.50
1:a:1218:C:H2'	1:a:1219:A:C8	2.46	0.50
4:d:64:TYR:CD2	4:d:93:LEU:HD13	2.46	0.50
8:h:100:ILE:C	8:h:100:ILE:HD12	2.35	0.50
14:n:12:ARG:O	14:n:15:LEU:HG	2.10	0.50
47:l:30:PRO:O	47:l:31:GLU:C	2.54	0.50
52:5:1020:A:H1'	52:5:1021:A:OP2	2.11	0.50
1:a:636:U:H2'	1:a:637:C:H6	1.76	0.50
1:a:671:G:O2'	6:f:79:ARG:NH2	2.44	0.50
5:e:153:ALA:HB2	5:e:163:ILE:CB	2.41	0.50
11:k:44:ALA:HB3	11:k:69:CYS:HB2	1.93	0.50
24:C:154:ALA:HB2	24:C:161:VAL:HG23	1.93	0.50
33:N:37:THR:HG22	33:N:110:MET:HE1	1.91	0.50
1:a:978:A:C4	1:a:1319:A:C2	2.99	0.50
2:b:99:MET:HA	2:b:106:VAL:HG11	1.93	0.50
34:O:67:ASN:ND2	34:O:69:ASP:OD1	2.44	0.50
35:P:65:ASN:OD1	35:P:65:ASN:N	2.45	0.50
1:a:359:G:C6	1:a:360:G:C5	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:376:G:H2'	1:a:377:G:O4'	2.11	0.50
2:b:92:ASN:OD1	2:b:92:ASN:C	2.55	0.50
16:p:22:ALA:HB2	16:p:32:PHE:HB3	1.93	0.50
24:C:161:VAL:HG12	24:C:162:GLN:N	2.27	0.50
25:D:114:LYS:HZ1	52:5:2723:C:P	2.34	0.50
30:K:13:ASN:C	30:K:15:GLY:N	2.69	0.50
30:K:19:VAL:HG11	30:K:41:ILE:HD13	1.93	0.50
52:5:2287:A:O2'	52:5:2288:A:O5'	2.25	0.50
1:a:797:C:OP1	11:k:126:ARG:NH2	2.44	0.50
1:a:1000:A:C6	1:a:1041:G:C6	2.99	0.50
2:b:128:LEU:HD12	2:b:132:GLU:HG2	1.94	0.50
37:R:38:VAL:O	37:R:54:VAL:HG23	2.11	0.50
52:5:2553:G:O4'	52:5:2582:G:O2'	2.23	0.50
1:a:323:U:H2'	1:a:324:G:O4'	2.12	0.50
1:a:409:U:C5'	4:d:24:VAL:HG22	2.41	0.50
33:N:115:LEU:O	33:N:117:ASP:N	2.45	0.50
52:5:2266:A:H4'	52:5:2267:A:N3	2.26	0.50
1:a:155:A:N6	1:a:167:A:N6	2.60	0.50
1:a:160:A:H2'	1:a:161:A:O4'	2.12	0.50
1:a:714:G:H2'	1:a:715:A:C8	2.47	0.50
2:b:15:PHE:HB2	2:b:39:ILE:HG23	1.93	0.50
6:f:26:THR:O	6:f:30:THR:OG1	2.28	0.50
12:l:86:VAL:HG23	12:l:88:ASP:H	1.76	0.50
16:p:11:ALA:O	16:p:14:ARG:N	2.41	0.50
24:C:90:ILE:HD12	24:C:102:TYR:CD1	2.47	0.50
31:L:30:THR:O	31:L:33:ARG:HG2	2.11	0.50
44:Y:49:ASP:OD1	44:Y:52:ARG:NH1	2.44	0.50
52:5:2258:C:O2'	52:5:2427:C:OP2	2.29	0.50
1:a:345:C:O2'	1:a:346:G:N2	2.45	0.50
1:a:511:C:O3'	4:d:43:ARG:NH2	2.45	0.50
1:a:575:G:O2'	1:a:821:G:OP2	2.27	0.50
1:a:1500:A:OP2	57:a:1704:HOH:O	2.19	0.50
6:f:13:ASP:O	6:f:16:GLU:N	2.45	0.50
17:q:66:LEU:HD22	17:q:70:LYS:HD3	1.93	0.50
25:D:11:MET:C	25:D:12:THR:HG23	2.37	0.50
27:F:32:LYS:O	27:F:33:ILE:HD13	2.11	0.50
33:N:24:MET:HE1	33:N:40:LYS:HB3	1.94	0.50
33:N:86:ARG:O	33:N:86:ARG:HG2	2.12	0.50
33:N:116:VAL:HG23	33:N:116:VAL:O	2.11	0.50
36:Q:107:ALA:HB3	37:R:46:GLU:OE1	2.11	0.50
42:W:70:PRO:C	42:W:72:ASN:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:t:46:ALA:O	20:t:49:ALA:N	2.45	0.50
21:u:9:GLU:HB2	21:u:10:PRO:CD	2.42	0.50
31:L:86:GLU:O	31:L:87:GLY:C	2.54	0.50
52:5:2506:U:O2	52:5:2506:U:H2'	2.11	0.50
1:a:422:C:O2'	1:a:423:G:N2	2.46	0.49
6:f:81:ASN:OD1	6:f:81:ASN:C	2.55	0.49
10:j:71:LEU:O	10:j:72:ARG:NE	2.45	0.49
22:A:549:G:O2'	22:A:550:C:P	2.70	0.49
30:K:57:VAL:O	30:K:58:LEU:HB3	2.10	0.49
52:5:2867:G:O2'	52:5:2868:A:H8	1.95	0.49
2:b:70:GLY:HA3	2:b:79:VAL:HG21	1.94	0.49
2:b:87:ASP:OD2	2:b:224:ARG:NH1	2.45	0.49
10:j:81:GLU:HA	10:j:84:VAL:HG12	1.94	0.49
16:p:6:LEU:HB3	16:p:17:TYR:HB3	1.94	0.49
22:A:871:U:H2'	22:A:872:U:C6	2.47	0.49
27:F:99:PHE:O	27:F:103:ILE:HG12	2.11	0.49
31:L:95:LEU:CD2	31:L:100:ILE:HD11	2.33	0.49
9:i:16:ALA:O	9:i:17:ARG:HG3	2.12	0.49
9:i:103:VAL:HG22	9:i:103:VAL:O	2.11	0.49
13:m:55:LEU:O	13:m:59:VAL:HG22	2.12	0.49
14:n:7:ALA:O	14:n:10:VAL:HG12	2.11	0.49
28:G:51:PHE:CE1	28:G:68:ARG:HA	2.47	0.49
36:Q:57:ARG:NH2	52:5:998:C:OP2	2.45	0.49
51:6:37:CYS:SG	51:6:39:LYS:O	2.69	0.49
52:5:948:C:O2	52:5:984:A:O2'	2.17	0.49
1:a:280:C:O2'	1:a:281:G:P	2.70	0.49
1:a:527:7MG:HM73	12:l:87:LYS:HZ1	1.77	0.49
1:a:1495:U:O2'	52:5:1919:A:N1	2.36	0.49
4:d:104:MET:HE1	4:d:171:GLU:O	2.11	0.49
6:f:32:ALA:HB2	6:f:70:VAL:HG11	1.94	0.49
12:l:98:ARG:NH2	12:l:104:SER:O	2.39	0.49
16:p:67:ILE:HD13	16:p:72:ALA:HB2	1.94	0.49
22:A:242:G:O2'	22:A:243:U:P	2.70	0.49
52:5:2140:G:N2	52:5:2152:G:N7	2.61	0.49
1:a:746:A:H2'	1:a:747:A:C8	2.47	0.49
1:a:1055:A:C2	1:a:1206:G:C4	3.00	0.49
2:b:165:ALA:HA	2:b:172:ILE:HD11	1.95	0.49
6:f:41:ASP:OD1	6:f:43:GLY:N	2.45	0.49
13:m:18:LEU:O	13:m:21:ILE:HG13	2.13	0.49
20:t:20:ASN:ND2	20:t:65:LEU:HD13	2.25	0.49
22:A:483:A:O2'	40:U:56:GLY:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:685:A:N1	22:A:787:C:H1'	2.28	0.49
48:2:1:MET:N	52:5:1619:G:O2'	2.46	0.49
52:5:1872:A:H2'	52:5:1873:G:O4'	2.13	0.49
9:i:12:LYS:O	9:i:13:SER:OG	2.27	0.49
12:l:28:GLN:HG3	12:l:81:ILE:O	2.11	0.49
22:A:44:A:H2'	22:A:45:G:O4'	2.12	0.49
22:A:528:A:C2	52:5:2043:C:H4'	2.48	0.49
22:A:554:U:H2'	22:A:555:G:O4'	2.13	0.49
25:D:20:VAL:HG12	25:D:21:SER:N	2.27	0.49
52:5:1360:G:N7	52:5:1361:G:C8	2.81	0.49
52:5:1847:G:H21	52:5:1848:A:H62	1.60	0.49
7:g:138:GLU:O	7:g:142:ARG:HG2	2.13	0.49
13:m:15:VAL:HG23	13:m:16:ILE:CD1	2.43	0.49
13:m:51:GLN:O	13:m:54:THR:OG1	2.30	0.49
16:p:31:ARG:CG	16:p:32:PHE:H	2.26	0.49
40:U:6:ARG:NH1	40:U:7:ASP:OD1	2.45	0.49
40:U:57:ILE:N	40:U:57:ILE:HD12	2.28	0.49
52:5:1130:U:O2'	52:5:1131:G:OP1	2.27	0.49
1:a:1071:C:OP1	5:e:53:ARG:NH2	2.45	0.49
8:h:104:SER:C	8:h:105:THR:HG23	2.38	0.49
10:j:12:ALA:O	10:j:70:HIS:CE1	2.66	0.49
11:k:85:VAL:O	11:k:112:VAL:HG22	2.12	0.49
17:q:68:LYS:C	17:q:69:THR:HG1	2.09	0.49
18:r:70:THR:OG1	18:r:71:ASP:N	2.45	0.49
31:L:79:LEU:HD12	31:L:112:LEU:HD12	1.95	0.49
33:N:60:VAL:HG13	52:5:1454:C:O2'	2.13	0.49
36:Q:65:ASN:HB2	36:Q:75:TYR:HB2	1.94	0.49
52:5:1288:G:OP2	52:5:1288:G:N2	2.35	0.49
52:5:2349:G:O6	52:5:2369:A:N6	2.46	0.49
52:5:2808:G:H5'	52:5:2809:A:OP1	2.13	0.49
2:b:55:GLU:HA	2:b:55:GLU:OE1	2.13	0.49
3:c:32:LEU:O	3:c:32:LEU:HD13	2.13	0.49
6:f:13:ASP:C	6:f:15:SER:N	2.70	0.49
52:5:2286:G:H5''	52:5:2287:A:OP1	2.12	0.49
1:a:713:G:H2'	1:a:714:G:C8	2.48	0.49
14:n:34:ASN:OD1	14:n:36:ALA:HB3	2.13	0.49
16:p:26:ASN:OD1	16:p:26:ASN:N	2.44	0.49
18:r:25:ILE:HA	18:r:28:LEU:HB3	1.95	0.49
21:u:9:GLU:HB2	21:u:10:PRO:HD3	1.95	0.49
52:5:1315:C:O2'	52:5:1392:A:N3	2.41	0.49
52:5:1966:A:N3	52:5:2592:G:O2'	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:5:2025:C:H2'	52:5:2026:U:C6	2.48	0.49
22:A:75:G:N3	22:A:75:G:H2'	2.28	0.48
23:B:2:G:O6	23:B:119:A:N6	2.46	0.48
24:C:231:HIS:CD2	24:C:231:HIS:N	2.81	0.48
50:4:19:ARG:NE	52:5:2756:U:OP2	2.42	0.48
1:a:161:A:H2'	1:a:162:A:O4'	2.13	0.48
1:a:1317:C:H4'	14:n:48:LEU:HD21	1.95	0.48
4:d:10:LEU:HD23	4:d:10:LEU:H	1.78	0.48
7:g:29:LEU:O	7:g:30:MET:C	2.55	0.48
11:k:61:ALA:O	11:k:64:VAL:HG12	2.12	0.48
11:k:80:ASN:HB3	11:k:105:ARG:HB3	1.95	0.48
20:t:14:GLU:HA	20:t:17:ARG:HG2	1.95	0.48
22:A:645:C:H2'	22:A:647:G:C8	2.48	0.48
22:A:743:A:O2'	52:5:1659:G:OP1	2.29	0.48
27:F:87:LYS:NZ	52:5:2314:A:OP1	2.46	0.48
28:G:51:PHE:HE2	28:G:71:LEU:HD12	1.76	0.48
52:5:962:G:H21	52:5:2250:G:H1	1.61	0.48
1:a:53:A:N1	1:a:359:G:C6	2.81	0.48
1:a:296:U:O2'	1:a:556:C:O2	2.30	0.48
1:a:376:G:O6	1:a:387:U:O2	2.32	0.48
1:a:1201:A:H1'	1:a:1202:U:OP2	2.13	0.48
3:c:167:TYR:OH	5:e:54:GLU:OE1	2.19	0.48
18:r:28:LEU:HD22	18:r:67:LEU:CD1	2.38	0.48
22:A:560:C:O2'	36:Q:47:ARG:NH1	2.46	0.48
30:K:64:ARG:NE	35:P:67:GLU:OE2	2.45	0.48
52:5:1452:G:O2'	52:5:1453:A:OP2	2.25	0.48
1:a:375:U:C2	1:a:376:G:C8	3.01	0.48
1:a:1300:G:O2'	1:a:1301:U:P	2.71	0.48
1:a:1399:C:H1'	1:a:1400:C:OP2	2.12	0.48
3:c:72:PRO:O	3:c:76:ILE:HG13	2.13	0.48
3:c:102:ILE:HD12	3:c:102:ILE:N	2.27	0.48
5:e:93:VAL:HG13	5:e:110:MET:HE3	1.94	0.48
8:h:38:VAL:HG11	8:h:102:VAL:HG22	1.94	0.48
52:5:1196:C:C2	52:5:1197:G:C8	3.02	0.48
52:5:1378:A:O2'	52:5:1380:G:OP2	2.31	0.48
52:5:1432:G:H2'	52:5:1433:A:C8	2.49	0.48
1:a:1182:G:H5'	1:a:1183:U:OP1	2.14	0.48
3:c:122:GLN:HB3	3:c:127:VAL:HG11	1.96	0.48
12:l:32:VAL:O	12:l:33:CYS:HB3	2.12	0.48
22:A:281:C:H42	22:A:359:G:H1	1.61	0.48
27:F:82:TYR:O	27:F:84:ILE:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:G:126:THR:O	28:G:128:THR:N	2.46	0.48
38:S:29:VAL:HG13	38:S:55:ILE:HD11	1.94	0.48
1:a:393:A:C2	1:a:394:G:N7	2.82	0.48
1:a:607:A:H3'	1:a:608:A:H8	1.79	0.48
2:b:110:ILE:HD11	2:b:150:ILE:HG23	1.95	0.48
3:c:52:SER:OG	3:c:68:HIS:O	2.12	0.48
4:d:9:LYS:HB2	4:d:12:ARG:HH21	1.77	0.48
4:d:10:LEU:HD23	4:d:10:LEU:N	2.28	0.48
4:d:56:GLU:OE2	4:d:195:ASN:N	2.46	0.48
10:j:50:THR:HG22	10:j:62:ARG:HD3	1.94	0.48
10:j:86:ALA:HA	10:j:90:LEU:HD12	1.95	0.48
13:m:101:THR:O	13:m:101:THR:HG22	2.12	0.48
22:A:676:A:C2	52:5:2070:A:O4'	2.67	0.48
27:F:29:ARG:O	27:F:158:THR:HG23	2.14	0.48
29:J:17:VAL:HG22	29:J:55:ILE:HB	1.94	0.48
52:5:2266:A:H4'	52:5:2267:A:O5'	2.14	0.48
2:b:49:PHE:O	2:b:53:LEU:HG	2.14	0.48
12:l:3:VAL:HG23	17:q:33:TYR:HB3	1.96	0.48
22:A:421:C:HO2'	22:A:422:A:P	2.36	0.48
31:L:33:ARG:HD3	31:L:40:SER:HA	1.96	0.48
38:S:48:LYS:O	38:S:52:GLU:HG3	2.13	0.48
52:5:2655:G:O2'	52:5:2656:U:P	2.71	0.48
13:m:15:VAL:O	13:m:19:THR:HG23	2.13	0.48
22:A:249:C:O2	49:3:11:LYS:NZ	2.38	0.48
22:A:475:C:O2	22:A:479:A:N6	2.38	0.48
22:A:639:U:H2'	22:A:640:C:C6	2.48	0.48
27:F:7:TYR:O	27:F:9:ASP:N	2.46	0.48
28:G:88:LEU:HD11	28:G:95:ALA:HB2	1.95	0.48
28:G:97:VAL:HG13	28:G:97:VAL:O	2.14	0.48
50:4:11:CYS:HB3	50:4:33:HIS:CE1	2.49	0.48
1:a:674:G:H2'	1:a:675:A:H8	1.78	0.48
1:a:1096:C:H2'	1:a:1097:C:H6	1.79	0.48
7:g:129:ASN:HA	7:g:134:VAL:HG11	1.96	0.48
10:j:102:LEU:N	10:j:102:LEU:HD12	2.29	0.48
11:k:61:ALA:O	11:k:64:VAL:CG1	2.61	0.48
22:A:321:U:C1'	26:E:159:LEU:HD22	2.44	0.48
24:C:128:THR:OG1	24:C:190:THR:OG1	2.27	0.48
51:6:17:SER:O	51:6:18:CYS:C	2.56	0.48
52:5:1326:U:HO2'	52:5:2010:G:HO2'	1.62	0.48
52:5:1338:G:O2'	52:5:1393:A:N1	2.39	0.48
4:d:196:GLU:O	4:d:200:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:47:VAL:HG23	9:i:48:ARG:N	2.29	0.48
30:K:16:ALA:CB	30:K:86:LEU:HD11	2.44	0.48
52:5:1209:U:O2'	52:5:1237:A:N1	2.46	0.48
1:a:54:C:H2'	1:a:352:C:H41	1.79	0.47
2:b:123:GLY:O	2:b:124:THR:C	2.57	0.47
4:d:87:GLU:HG2	4:d:187:ARG:HE	1.78	0.47
4:d:95:GLY:O	4:d:136:VAL:N	2.27	0.47
5:e:13:LYS:NZ	5:e:115:GLU:OE1	2.32	0.47
6:f:90:MET:HE1	18:r:22:TYR:CZ	2.49	0.47
9:i:15:ALA:HB3	9:i:67:LYS:HZ3	1.79	0.47
12:l:41:PRO:HG3	12:l:49:ARG:HG3	1.96	0.47
12:l:98:ARG:HB2	12:l:116:TYR:HA	1.95	0.47
18:r:28:LEU:HD23	18:r:28:LEU:O	2.13	0.47
23:B:3:C:C2'	23:B:4:C:OP1	2.61	0.47
23:B:29:A:H2'	23:B:30:C:O4'	2.14	0.47
23:B:74:U:O2	41:V:29:ILE:HD13	2.14	0.47
25:D:48:ILE:HD12	25:D:50:VAL:CG1	2.44	0.47
25:D:58:ASN:C	25:D:58:ASN:OD1	2.57	0.47
27:F:32:LYS:HD3	27:F:91:ARG:NH2	2.30	0.47
32:M:127:LYS:NZ	52:5:1030:C:OP2	2.45	0.47
52:5:1041:G:H1	52:5:1114:C:H42	1.62	0.47
1:a:580:C:H2'	1:a:581:G:O4'	2.14	0.47
1:a:1071:C:H2'	1:a:1072:G:H8	1.78	0.47
8:h:27:PRO:O	8:h:32:LYS:NZ	2.47	0.47
9:i:83:THR:HG21	9:i:102:PHE:HB3	1.94	0.47
10:j:66:GLU:HB3	14:n:99:ALA:HB2	1.96	0.47
25:D:170:VAL:HG13	25:D:194:PRO:HB3	1.96	0.47
32:M:49:ALA:HB2	32:M:124:LEU:HD13	1.96	0.47
39:T:13:ALA:HB1	44:Y:33:ALA:HB1	1.94	0.47
43:X:2:ARG:NH1	52:5:1365:A:OP1	2.42	0.47
52:5:966:G:C1'	52:5:2267:A:H62	2.28	0.47
52:5:1858:A:C2	52:5:1885:A:H1'	2.49	0.47
52:5:2291:U:O2'	52:5:2374:C:O2	2.32	0.47
1:a:667:G:O2'	15:o:48:ASP:OD1	2.13	0.47
52:5:978:G:O4'	52:5:1001:A:H2	1.97	0.47
1:a:555:U:H2'	1:a:556:C:C6	2.50	0.47
18:r:29:LYS:O	18:r:29:LYS:HD3	2.15	0.47
22:A:612:G:N2	22:A:614:A:O2'	2.47	0.47
22:A:753:A:H8	22:A:753:A:OP2	1.96	0.47
25:D:155:VAL:HG21	52:5:2618:G:H21	1.79	0.47
29:J:5:THR:O	29:J:7:LYS:NZ	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:J:99:ARG:O	29:J:103:ILE:HD12	2.14	0.47
34:O:51:ALA:HB3	34:O:78:VAL:CG2	2.44	0.47
52:5:2515:C:H2'	52:5:2516:A:H8	1.79	0.47
52:5:2832:U:C2'	52:5:2833:U:OP2	2.62	0.47
1:a:78:A:H2'	1:a:79:G:O4'	2.15	0.47
1:a:549:C:H2'	1:a:550:G:C1'	2.44	0.47
1:a:945:G:C2	1:a:946:A:C8	3.03	0.47
1:a:1356:G:H2'	1:a:1357:A:C8	2.49	0.47
3:c:89:VAL:HG23	3:c:90:VAL:N	2.30	0.47
6:f:17:GLN:O	6:f:18:VAL:C	2.57	0.47
16:p:27:ALA:O	16:p:28:ARG:C	2.56	0.47
33:N:60:VAL:HG22	52:5:1454:C:O2'	2.14	0.47
41:V:75:GLN:HA	41:V:75:GLN:OE1	2.14	0.47
48:2:35:ARG:HG2	48:2:42:LEU:HD11	1.96	0.47
52:5:1570:A:H2'	52:5:1571:A:C8	2.49	0.47
52:5:1918:A:O2'	52:5:1920:C:N4	2.48	0.47
1:a:672:U:H2'	1:a:673:A:C8	2.49	0.47
1:a:923:A:O2'	1:a:1399:C:OP2	2.24	0.47
6:f:8:PHE:HE1	6:f:62:MET:HE1	1.77	0.47
7:g:66:GLU:OE2	7:g:67:ASN:ND2	2.48	0.47
13:m:78:ARG:O	13:m:82:LEU:HD13	2.15	0.47
26:E:117:ARG:HA	26:E:185:LYS:HD3	1.95	0.47
28:G:101:VAL:HG22	28:G:115:GLN:OE1	2.14	0.47
40:U:39:ASN:OD1	40:U:64:ILE:HB	2.14	0.47
43:X:76:LYS:HA	43:X:76:LYS:HE3	1.97	0.47
52:5:1864:U:OP1	52:5:2410:G:O2'	2.27	0.47
52:5:2245:U:O2'	52:5:2436:G:OP2	2.27	0.47
52:5:2349:G:C6	52:5:2369:A:C6	3.02	0.47
1:a:391:G:O2'	1:a:392:C:OP1	2.29	0.47
1:a:640:A:H2'	1:a:641:U:O4'	2.15	0.47
2:b:204:ASP:OD1	2:b:204:ASP:N	2.42	0.47
11:k:19:VAL:HG11	11:k:84:MET:HE2	1.97	0.47
15:o:40:GLY:O	15:o:44:GLU:OE2	2.33	0.47
19:s:49:ALA:HB1	19:s:56:HIS:HB3	1.96	0.47
22:A:227:A:O2'	22:A:228:C:P	2.71	0.47
22:A:481:G:H4'	22:A:481:G:OP1	2.14	0.47
25:D:35:THR:OG1	25:D:49:GLN:O	2.22	0.47
27:F:170:ALA:O	27:F:171:ALA:C	2.57	0.47
28:G:132:LEU:HD23	28:G:132:LEU:N	2.28	0.47
30:K:16:ALA:HB2	30:K:86:LEU:HD11	1.95	0.47
33:N:60:VAL:O	33:N:64:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:N:69:ARG:O	33:N:70:THR:CB	2.62	0.47
34:O:51:ALA:HB3	34:O:78:VAL:HG22	1.95	0.47
34:O:53:THR:HG22	34:O:62:LEU:CD1	2.45	0.47
45:Z:43:ILE:O	45:Z:47:ILE:HG13	2.15	0.47
52:5:1009:A:N3	52:5:1153:C:O2'	2.43	0.47
52:5:2238:G:H2'	52:5:2238:G:N3	2.29	0.47
1:a:618:C:C2	1:a:622:A:N6	2.82	0.47
1:a:744:C:H2'	1:a:745:G:H8	1.80	0.47
1:a:1026:G:H2'	1:a:1027:C:C6	2.50	0.47
3:c:46:LEU:C	3:c:48:LYS:H	2.22	0.47
3:c:52:SER:HG	3:c:68:HIS:C	2.14	0.47
4:d:104:MET:HE1	4:d:180:THR:H	1.79	0.47
5:e:86:GLY:O	5:e:138:ALA:CB	2.61	0.47
8:h:50:VAL:O	8:h:50:VAL:HG13	2.14	0.47
14:n:7:ALA:O	14:n:8:ARG:C	2.57	0.47
22:A:490:C:H4'	22:A:491:G:OP2	2.14	0.47
34:O:62:LEU:HD13	34:O:70:ALA:CB	2.45	0.47
37:R:69:GLY:O	37:R:90:ARG:NE	2.42	0.47
52:5:1000:A:H2'	52:5:1001:A:C8	2.50	0.47
52:5:1321:A:C4	52:5:1322:A:C8	3.02	0.47
52:5:1506:U:H2'	52:5:1507:C:C6	2.50	0.47
52:5:2725:A:O2'	52:5:2726:A:C8	2.67	0.47
1:a:53:A:C6	1:a:359:G:C6	3.03	0.47
1:a:1004:A:N3	1:a:1026:G:C6	2.82	0.47
4:d:101:VAL:CG1	4:d:113:ALA:HB1	2.44	0.47
17:q:21:VAL:HA	17:q:43:LEU:O	2.15	0.47
19:s:10:ILE:CD1	19:s:15:LEU:HD22	2.45	0.47
21:u:33:ARG:HG2	21:u:34:ARG:CG	2.45	0.47
21:u:39:LYS:O	21:u:40:PRO:C	2.57	0.47
28:G:88:LEU:CD2	28:G:161:VAL:HG13	2.45	0.47
29:J:101:ILE:O	29:J:105:VAL:HG23	2.14	0.47
30:K:88:ASN:O	30:K:89:ASN:C	2.57	0.47
41:V:25:LYS:HG2	41:V:43:ASP:HA	1.96	0.47
42:W:42:HIS:N	42:W:74:LYS:O	2.44	0.47
47:1:3:GLY:O	47:1:5:ARG:N	2.46	0.47
52:5:1213:A:N6	52:5:1236:G:H1'	2.29	0.47
52:5:1360:G:C8	52:5:1361:G:C8	3.02	0.47
52:5:1799:G:H4'	52:5:1800:C:O5'	2.15	0.47
52:5:2333:A:H5''	52:5:2334:U:OP1	2.15	0.47
52:5:2346:A:H4'	52:5:2347:C:OP2	2.15	0.47
1:a:180:U:H2'	1:a:181:A:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1302:C:H42	13:m:13:HIS:CD2	2.33	0.47
2:b:167:HIS:C	2:b:167:HIS:HD1	2.23	0.47
5:e:88:HIS:HB3	5:e:138:ALA:HB2	1.96	0.47
9:i:50:PRO:O	9:i:51:LEU:HD23	2.14	0.47
26:E:164:LEU:HB3	26:E:167:VAL:HG23	1.97	0.47
27:F:106:ALA:O	27:F:107:VAL:C	2.57	0.47
30:K:70:ARG:NH2	52:5:2683:C:O2	2.48	0.47
39:T:6:ARG:O	39:T:10:VAL:HG23	2.15	0.47
40:U:99:SER:O	40:U:99:SER:OG	2.25	0.47
52:5:1048:A:OP2	52:5:1110:G:N2	2.48	0.47
52:5:1182:G:H2'	52:5:1183:U:O4'	2.14	0.47
52:5:1856:U:H2'	52:5:1857:G:O4'	2.14	0.47
1:a:17:U:H2'	1:a:18:C:C6	2.48	0.46
1:a:358:U:H2'	1:a:359:G:H8	1.79	0.46
3:c:74:ILE:O	3:c:75:VAL:C	2.56	0.46
4:d:7:LYS:HB3	4:d:20:LEU:HD13	1.95	0.46
22:A:81:G:HO2'	22:A:295:G:HO2'	1.59	0.46
22:A:782:A:N7	24:C:219:VAL:HG21	2.30	0.46
29:J:29:ALA:HB1	29:J:108:MET:SD	2.55	0.46
41:V:65:VAL:O	41:V:65:VAL:HG13	2.15	0.46
50:4:3:VAL:HG21	52:5:2539:C:H5'	1.96	0.46
52:5:2496:C:C2'	52:5:2497:A:O5'	2.63	0.46
52:5:2638:G:H1'	52:5:2778:A:H61	1.80	0.46
13:m:6:ILE:HG13	13:m:7:ASN:H	1.81	0.46
29:J:35:ARG:CB	29:J:54:ILE:HD11	2.46	0.46
33:N:66:ALA:O	33:N:69:ARG:O	2.33	0.46
41:V:7:GLU:OE1	41:V:7:GLU:N	2.48	0.46
42:W:38:GLY:HA2	52:5:2330:G:H21	1.80	0.46
50:4:4:ARG:NH2	52:5:2477:U:O2	2.48	0.46
52:5:1396:U:C5'	52:5:1397:U:OP2	2.63	0.46
4:d:98:ASP:OD1	4:d:98:ASP:N	2.32	0.46
4:d:104:MET:HE1	4:d:180:THR:N	2.29	0.46
10:j:52:LEU:HD23	10:j:62:ARG:HG2	1.97	0.46
14:n:97:LYS:HG3	14:n:98:LYS:N	2.30	0.46
22:A:591:U:C2	22:A:592:A:C8	3.04	0.46
27:F:168:LEU:O	27:F:171:ALA:HB3	2.14	0.46
47:1:13:SER:OG	47:1:47:ILE:O	2.32	0.46
1:a:606:G:N2	1:a:632:U:OP1	2.46	0.46
1:a:871:U:H5''	1:a:872:A:OP2	2.16	0.46
1:a:1321:U:OP2	1:a:1322:C:O2'	2.32	0.46
2:b:12:GLY:HA3	2:b:207:ARG:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:85:LYS:O	3:c:89:VAL:HG22	2.15	0.46
5:e:106:ALA:HB2	5:e:124:ALA:HB3	1.97	0.46
6:f:29:ILE:HA	6:f:32:ALA:HB3	1.96	0.46
20:t:34:VAL:O	20:t:35:TYR:C	2.59	0.46
21:u:7:GLU:HB3	21:u:11:PHE:HB3	1.97	0.46
24:C:66:PHE:O	24:C:150:GLY:O	2.34	0.46
38:S:14:ALA:O	38:S:18:ARG:HB2	2.15	0.46
52:5:2847:U:H2'	52:5:2848:G:O4'	2.15	0.46
52:5:2865:U:OP2	52:5:2866:U:O2'	2.24	0.46
5:e:92:ARG:HB3	5:e:127:TYR:HB2	1.97	0.46
19:s:52:ASN:O	19:s:76:THR:HG22	2.16	0.46
22:A:499:U:H2'	22:A:500:G:O4'	2.16	0.46
26:E:35:TYR:CD1	26:E:178:VAL:HG21	2.50	0.46
35:P:26:GLU:HG3	35:P:43:GLU:HG3	1.97	0.46
37:R:53:PHE:N	37:R:53:PHE:CD1	2.80	0.46
38:S:4:ILE:N	38:S:4:ILE:HD12	2.30	0.46
52:5:1021:A:N6	52:5:1142:A:H61	2.14	0.46
52:5:1130:U:O2'	52:5:1131:G:H8	1.99	0.46
52:5:2103:C:H2'	52:5:2104:C:C6	2.50	0.46
52:5:2286:G:C5'	52:5:2287:A:O4'	2.64	0.46
1:a:264:C:H2'	1:a:265:G:O4'	2.15	0.46
1:a:544:G:OP2	4:d:13:ARG:NH1	2.40	0.46
1:a:1256:A:O2'	1:a:1257:A:H5''	2.14	0.46
11:k:110:THR:HG22	21:u:4:LYS:HG3	1.97	0.46
15:o:55:LEU:O	15:o:58:MET:HG2	2.15	0.46
16:p:31:ARG:CG	16:p:32:PHE:N	2.78	0.46
20:t:34:VAL:O	20:t:37:ALA:N	2.48	0.46
25:D:110:THR:HG21	25:D:169:ARG:HE	1.79	0.46
52:5:2460:U:C2	52:5:2461:A:C8	3.03	0.46
52:5:2902:C:H2'	52:5:2903:U:O4'	2.16	0.46
1:a:642:A:C8	8:h:106:SER:HA	2.50	0.46
4:d:86:GLY:CA	4:d:196:GLU:OE1	2.64	0.46
20:t:13:SER:O	20:t:16:ALA:N	2.47	0.46
20:t:80:ALA:O	20:t:84:LYS:HB3	2.15	0.46
45:Z:6:ILE:CG2	45:Z:54:VAL:HG13	2.46	0.46
52:5:1049:C:C2	52:5:1050:A:C8	3.04	0.46
52:5:1930:G:O2'	52:5:1931:U:O5'	2.34	0.46
52:5:2346:A:H3'	52:5:2347:C:C5'	2.45	0.46
2:b:103:TRP:HA	2:b:106:VAL:HG22	1.97	0.46
6:f:11:HIS:CD2	6:f:54:LEU:HD22	2.50	0.46
7:g:68:VAL:HG12	7:g:134:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:10:LEU:CB	10:j:98:VAL:HG12	2.46	0.46
10:j:52:LEU:HB2	14:n:81:ARG:HD2	1.97	0.46
11:k:33:ILE:HG13	11:k:69:CYS:SG	2.56	0.46
13:m:66:GLY:O	13:m:70:ARG:HG2	2.15	0.46
14:n:81:ARG:HG3	14:n:82:ILE:N	2.31	0.46
21:u:64:ALA:O	21:u:65:ARG:CB	2.63	0.46
24:C:117:SER:HA	24:C:128:THR:O	2.16	0.46
32:M:12:MET:HA	52:5:910:A:H62	1.81	0.46
52:5:1434:A:H2'	52:5:1435:G:H8	1.80	0.46
52:5:1688:U:O2'	52:5:1700:A:N7	2.40	0.46
52:5:1712:U:OP2	52:5:1713:A:O2'	2.24	0.46
52:5:1720:U:H2'	52:5:1721:G:O4'	2.16	0.46
52:5:2446:G:N2	52:5:2449:H2U:O2	2.44	0.46
52:5:2712:C:HO2'	52:5:2713:U:P	2.38	0.46
1:a:70:U:H4'	1:a:71:A:O5'	2.16	0.46
1:a:590:U:OP1	8:h:30:LYS:HD2	2.16	0.46
1:a:792:A:H1'	1:a:794:A:N7	2.31	0.46
1:a:1256:A:C2'	1:a:1257:A:OP2	2.63	0.46
1:a:1343:G:H4'	9:i:123:ARG:HB3	1.97	0.46
1:a:1346:A:H2'	1:a:1346:A:N3	2.31	0.46
11:k:125:LYS:O	21:u:34:ARG:NH1	2.48	0.46
13:m:6:ILE:CG1	13:m:7:ASN:H	2.29	0.46
22:A:220:G:O2'	22:A:233:A:N3	2.40	0.46
22:A:548:G:C2'	22:A:549:G:O4'	2.64	0.46
27:F:69:ALA:O	27:F:80:GLN:NE2	2.49	0.46
31:L:77:ILE:N	31:L:77:ILE:HD12	2.31	0.46
38:S:77:ASP:OD1	38:S:102:HIS:HB2	2.16	0.46
1:a:628:G:H2'	1:a:629:A:O4'	2.16	0.46
1:a:715:A:H2'	1:a:716:A:C8	2.51	0.46
1:a:1086:U:H3	1:a:1099:G:H22	1.62	0.46
7:g:134:VAL:O	7:g:138:GLU:HG2	2.16	0.46
15:o:75:ALA:O	15:o:78:THR:OG1	2.31	0.46
20:t:46:ALA:O	20:t:47:GLN:C	2.59	0.46
22:A:581:C:H2'	22:A:582:A:H8	1.81	0.46
22:A:593:U:H2'	22:A:594:U:C6	2.50	0.46
26:E:47:LYS:HB2	26:E:51:GLU:HB2	1.98	0.46
28:G:68:ARG:C	28:G:68:ARG:HD3	2.41	0.46
41:V:6:ALA:CB	41:V:40:ILE:HD11	2.46	0.46
45:Z:12:ALA:O	45:Z:20:LYS:NZ	2.40	0.46
52:5:947:A:H2'	52:5:948:C:C6	2.51	0.46
52:5:1028:A:H2'	52:5:1029:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:5:2813:A:C4	52:5:2814:A:C8	3.04	0.46
1:a:1109:C:OP2	3:c:175:HIS:ND1	2.49	0.45
1:a:1158:C:C4	1:a:1160:G:C8	3.04	0.45
1:a:1428:A:H2'	1:a:1429:A:O4'	2.16	0.45
10:j:22:THR:O	10:j:26:VAL:HG23	2.16	0.45
10:j:29:ALA:CB	10:j:83:THR:HG23	2.44	0.45
17:q:45:VAL:HG21	17:q:60:ILE:HG12	1.98	0.45
22:A:445:C:H2'	22:A:446:G:O4'	2.16	0.45
22:A:629:G:N3	22:A:639:U:O2'	2.48	0.45
22:A:836:G:C5	22:A:837:C:C5	3.04	0.45
23:B:90:C:H2'	23:B:91:C:O4'	2.16	0.45
40:U:13:LEU:HD11	40:U:70:ALA:HB2	1.98	0.45
51:6:61:ASN:O	51:6:64:PHE:N	2.49	0.45
52:5:966:G:O4'	52:5:2267:A:N6	2.49	0.45
52:5:1003:G:O2'	52:5:1010:A:N1	2.42	0.45
52:5:1941:C:N4	52:5:1965:C:O4'	2.49	0.45
52:5:2576:G:O2'	52:5:2579:C:OP2	2.28	0.45
1:a:429:U:H5'	4:d:8:LEU:HD23	1.98	0.45
8:h:70:VAL:HG12	8:h:71:VAL:N	2.30	0.45
12:l:87:LYS:HG2	12:l:87:LYS:O	2.16	0.45
13:m:52:ILE:HG22	13:m:56:ARG:NH1	2.32	0.45
22:A:468:G:N7	48:2:39:ARG:NH2	2.63	0.45
26:E:3:LEU:HD23	26:E:14:VAL:CG2	2.46	0.45
27:F:55:ASP:O	27:F:58:ALA:HB3	2.15	0.45
52:5:1349:C:C2	52:5:1350:C:C5	3.04	0.45
52:5:2118:U:O2	52:5:2145:C:N4	2.49	0.45
52:5:2537:U:H2'	52:5:2538:C:C6	2.51	0.45
1:a:235:C:O2'	17:q:72:TRP:CE2	2.69	0.45
1:a:1160:G:C2	1:a:1161:C:C6	3.05	0.45
1:a:1315:U:H2'	1:a:1316:G:O4'	2.15	0.45
4:d:4:LEU:HG	4:d:4:LEU:O	2.17	0.45
8:h:30:LYS:O	8:h:33:VAL:HG23	2.16	0.45
11:k:59:PRO:O	11:k:62:ALA:HB3	2.16	0.45
20:t:73:ARG:O	20:t:77:ASN:ND2	2.50	0.45
22:A:607:U:C5	22:A:620:G:C4	3.04	0.45
25:D:12:THR:HG21	35:P:4:ILE:HG23	1.99	0.45
25:D:106:LYS:HA	25:D:175:LEU:O	2.17	0.45
26:E:77:ILE:O	26:E:77:ILE:HG22	2.15	0.45
52:5:1794:A:H2'	52:5:1795:C:C6	2.52	0.45
1:a:82:G:H22	1:a:87:C:H42	1.63	0.45
1:a:686:U:HO2'	1:a:687:A:C5'	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1004:A:H2'	1:a:1005:A:O4'	2.16	0.45
1:a:1358:U:OP1	14:n:75:ARG:HB3	2.16	0.45
7:g:56:SER:HB3	7:g:59:GLU:OE2	2.17	0.45
13:m:106:ARG:NH2	13:m:110:GLY:O	2.49	0.45
16:p:33:ILE:N	16:p:33:ILE:HD12	2.32	0.45
19:s:30:LEU:HB2	19:s:48:ILE:HG22	1.97	0.45
22:A:279:A:H61	22:A:361:G:H2'	1.80	0.45
22:A:544:C:O3'	22:A:545:U:O4'	2.34	0.45
27:F:151:LEU:HD12	27:F:151:LEU:O	2.17	0.45
28:G:40:VAL:CG1	28:G:64:ALA:HA	2.46	0.45
33:N:28:LEU:HD23	33:N:48:VAL:HG21	1.98	0.45
52:5:1900:A:HO2'	52:5:1901:A:P	2.31	0.45
52:5:2038:G:H2'	52:5:2039:U:O4'	2.16	0.45
52:5:2629:U:O2'	52:5:2630:G:P	2.75	0.45
52:5:2723:C:H2'	52:5:2724:U:O4'	2.16	0.45
1:a:511:C:O2'	4:d:40:HIS:CD2	2.69	0.45
1:a:1060:U:H4'	10:j:53:ILE:HG22	1.98	0.45
1:a:1112:C:H1'	3:c:178:ARG:HE	1.81	0.45
1:a:1530:G:H2'	1:a:1531:A:C8	2.51	0.45
5:e:14:LEU:HD13	5:e:14:LEU:C	2.41	0.45
7:g:15:PRO:HG2	7:g:43:TYR:OH	2.15	0.45
8:h:112:ASP:OD1	8:h:112:ASP:N	2.49	0.45
20:t:66:ILE:C	20:t:68:LYS:H	2.25	0.45
26:E:166:LYS:N	26:E:166:LYS:HD3	2.32	0.45
27:F:57:ALA:O	27:F:58:ALA:C	2.59	0.45
30:K:38:ILE:HA	30:K:60:ALA:O	2.17	0.45
42:W:21:ARG:HG3	42:W:27:VAL:CG1	2.46	0.45
49:3:40:LYS:NZ	52:5:2419:U:OP1	2.42	0.45
52:5:1275:A:OP2	52:5:1646:C:N4	2.42	0.45
52:5:1378:A:O2'	52:5:1380:G:N7	2.49	0.45
52:5:1802:A:H2'	52:5:1803:A:C8	2.52	0.45
52:5:2064:C:H2'	52:5:2065:C:C6	2.52	0.45
52:5:2086:U:H2'	52:5:2087:G:C8	2.51	0.45
2:b:62:ARG:CZ	2:b:62:ARG:HA	2.46	0.45
21:u:19:LYS:N	21:u:19:LYS:CD	2.80	0.45
22:A:36:G:N3	22:A:450:G:O2'	2.49	0.45
22:A:91:A:O2'	22:A:92:U:O5'	2.35	0.45
22:A:576:U:H2'	22:A:577:G:C8	2.52	0.45
24:C:196:ASN:C	24:C:198:GLU:H	2.25	0.45
25:D:9:VAL:O	35:P:4:ILE:HD11	2.17	0.45
27:F:134:GLN:NE2	27:F:147:ARG:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:L:77:ILE:O	31:L:110:VAL:O	2.35	0.45
52:5:1786:A:H1'	52:5:1938:A:N6	2.32	0.45
9:i:17:ARG:HB2	9:i:65:THR:OG1	2.17	0.45
11:k:12:ARG:O	11:k:13:LYS:HB3	2.17	0.45
14:n:46:LEU:CG	19:s:12:LEU:HD21	2.39	0.45
15:o:28:VAL:HG21	15:o:66:LEU:HD21	1.98	0.45
26:E:72:SER:C	26:E:74:LYS:N	2.74	0.45
45:Z:7:THR:HA	45:Z:33:HIS:O	2.17	0.45
52:5:1795:C:H2'	52:5:1796:U:O4'	2.16	0.45
1:a:694:A:H2'	1:a:695:A:O4'	2.16	0.45
2:b:166:ASP:OD1	2:b:166:ASP:N	2.49	0.45
4:d:58:GLN:O	4:d:62:ARG:HG2	2.16	0.45
10:j:22:THR:HG21	10:j:39:PRO:HB3	1.99	0.45
14:n:49:GLN:NE2	19:s:12:LEU:HG	2.32	0.45
16:p:7:ALA:O	16:p:8:ARG:C	2.60	0.45
21:u:33:ARG:CG	21:u:34:ARG:HG2	2.47	0.45
22:A:458:G:O2'	22:A:459:U:OP2	2.35	0.45
22:A:859:G:C2'	22:A:860:U:OP2	2.65	0.45
25:D:26:VAL:HG21	35:P:4:ILE:HD13	1.97	0.45
29:J:60:ASP:O	29:J:61:LYS:HD2	2.16	0.45
30:K:78:ARG:NH2	35:P:70:GLU:OE1	2.40	0.45
34:O:11:ALA:HB2	34:O:95:SER:C	2.42	0.45
41:V:28:ALA:HB1	41:V:89:ILE:O	2.17	0.45
42:W:39:THR:O	42:W:39:THR:HG22	2.16	0.45
49:3:10:ALA:HA	49:3:61:LEU:HD21	1.99	0.45
52:5:1874:C:H2'	52:5:1875:G:O4'	2.17	0.45
52:5:2077:A:OP1	52:5:2238:G:N2	2.43	0.45
52:5:2838:G:C4	52:5:2839:G:C8	3.05	0.45
1:a:366:A:O3'	1:a:394:G:N2	2.50	0.45
1:a:570:G:H1'	1:a:820:U:C4	2.51	0.45
1:a:1060:U:H5''	10:j:53:ILE:CG2	2.47	0.45
1:a:1256:A:H1'	1:a:1258:G:C5	2.52	0.45
1:a:1300:G:HO2'	1:a:1301:U:P	2.40	0.45
1:a:1499:A:OP2	57:a:1704:HOH:O	2.21	0.45
2:b:9:LEU:HD13	2:b:9:LEU:C	2.42	0.45
2:b:119:GLN:O	2:b:123:GLY:N	2.43	0.45
2:b:126:ASP:OD1	2:b:126:ASP:O	2.35	0.45
4:d:129:VAL:HG11	4:d:134:TYR:CG	2.52	0.45
11:k:94:SER:O	11:k:95:THR:C	2.58	0.45
29:J:81:ILE:CD1	52:5:2514:U:H5''	2.45	0.45
30:K:107:LEU:HD21	30:K:115:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Y:15:ASN:O	44:Y:18:LEU:N	2.50	0.45
52:5:1434:A:H2'	52:5:1435:G:C8	2.51	0.45
52:5:1746:A:H2'	52:5:1747:U:C6	2.52	0.45
1:a:20:U:H2'	1:a:21:G:O4'	2.17	0.45
1:a:151:A:C5	1:a:171:A:N6	2.84	0.45
1:a:401:C:O2	1:a:621:A:H2	1.99	0.45
1:a:651:C:N4	1:a:753:A:OP2	2.45	0.45
6:f:18:VAL:HG12	6:f:19:PRO:N	2.32	0.45
9:i:47:VAL:HG23	9:i:48:ARG:H	1.82	0.45
12:l:28:GLN:HG3	12:l:82:ARG:HA	1.98	0.45
22:A:306:U:H2'	22:A:307:G:O4'	2.16	0.45
23:B:45:A:C4	23:B:46:A:C8	3.05	0.45
24:C:30:ALA:O	24:C:31:PRO:C	2.60	0.45
27:F:168:LEU:C	27:F:168:LEU:HD13	2.42	0.45
41:V:49:ASN:OD1	41:V:50:MET:N	2.50	0.45
52:5:1796:U:H2'	52:5:1797:G:H8	1.80	0.45
52:5:2287:A:O2'	52:5:2288:A:H2'	2.17	0.45
1:a:36:C:H2'	1:a:37:U:O4'	2.17	0.44
1:a:438:U:O2'	1:a:439:U:P	2.75	0.44
1:a:1109:C:C2	1:a:1110:A:C8	3.05	0.44
9:i:18:VAL:HG13	9:i:64:ILE:HG12	1.99	0.44
9:i:46:VAL:O	9:i:47:VAL:C	2.61	0.44
9:i:64:ILE:HG22	9:i:65:THR:N	2.33	0.44
17:q:4:ILE:HD12	17:q:5:ARG:O	2.17	0.44
22:A:555:G:O2'	22:A:556:A:H8	1.99	0.44
22:A:832:U:H2'	22:A:833:A:H8	1.82	0.44
22:A:833:A:H2'	22:A:834:G:H8	1.82	0.44
27:F:106:ALA:C	27:F:108:PRO:HD2	2.42	0.44
32:M:125:PRO:HB3	52:5:2485:G:O3'	2.17	0.44
34:O:33:ARG:O	34:O:34:HIS:CB	2.66	0.44
34:O:87:ILE:H	34:O:87:ILE:HD12	1.82	0.44
52:5:1475:G:HO2'	52:5:1476:U:H6	1.63	0.44
1:a:413:G:C2'	1:a:414:A:OP2	2.64	0.44
1:a:781:A:O2'	1:a:1522:U:O2	2.34	0.44
1:a:975:A:N1	1:a:1366:C:O2'	2.41	0.44
1:a:1367:C:H4'	10:j:50:THR:HG21	2.00	0.44
17:q:44:HIS:O	17:q:70:LYS:HA	2.17	0.44
22:A:664:G:O2'	52:5:940:G:OP1	2.27	0.44
33:N:39:PRO:O	33:N:40:LYS:C	2.61	0.44
33:N:76:VAL:O	33:N:79:LEU:O	2.36	0.44
38:S:59:GLU:HA	38:S:64:ALA:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:X:70:LEU:O	43:X:73:ARG:N	2.51	0.44
44:Y:55:THR:O	44:Y:58:ASN:N	2.50	0.44
52:5:1386:C:H2'	52:5:1387:A:C8	2.52	0.44
52:5:1452:G:C2'	52:5:1453:A:OP2	2.65	0.44
52:5:1774:C:O2	52:5:1774:C:H2'	2.17	0.44
52:5:2331:G:O2'	52:5:2336:A:N1	2.41	0.44
1:a:70:U:H5''	1:a:71:A:OP1	2.17	0.44
1:a:505:G:P	1:a:535:A:H5'	2.57	0.44
1:a:818:G:C6	1:a:820:U:O2'	2.70	0.44
1:a:1477:U:H2'	1:a:1478:U:C6	2.52	0.44
4:d:98:ASP:O	4:d:101:VAL:HB	2.17	0.44
5:e:121:ASN:O	5:e:122:VAL:HG22	2.17	0.44
6:f:14:GLN:HA	6:f:17:GLN:HB2	1.99	0.44
22:A:672:C:H4'	26:E:84:THR:HG21	1.98	0.44
22:A:752:A:C1'	22:A:753:A:OP2	2.66	0.44
22:A:754:U:O2'	52:5:1272:A:N1	2.46	0.44
24:C:177:SER:OG	52:5:1799:G:N7	2.43	0.44
25:D:32:ASN:HD22	25:D:32:ASN:N	2.15	0.44
28:G:108:PHE:O	52:5:2666:C:N4	2.50	0.44
29:J:13:ARG:NH2	29:J:49:ASP:O	2.48	0.44
45:Z:6:ILE:HG23	45:Z:54:VAL:HG13	1.99	0.44
47:1:44:GLN:HA	47:1:44:GLN:OE1	2.17	0.44
52:5:1379:U:C6	52:5:1379:U:OP1	2.69	0.44
52:5:2020:A:C2	52:5:2022:U:O4'	2.71	0.44
52:5:2537:U:H2'	52:5:2538:C:H6	1.81	0.44
1:a:890:G:O2'	1:a:891:U:O5'	2.35	0.44
1:a:1226:C:H4'	1:a:1227:A:OP1	2.17	0.44
3:c:175:HIS:O	3:c:177:LEU:HD22	2.17	0.44
5:e:14:LEU:C	5:e:15:ILE:HD12	2.43	0.44
5:e:93:VAL:HG22	5:e:110:MET:HE3	1.98	0.44
7:g:34:LYS:HE2	7:g:34:LYS:HA	1.99	0.44
17:q:11:VAL:HG21	17:q:20:ILE:HD11	2.00	0.44
27:F:1:ALA:O	27:F:4:HIS:HB2	2.18	0.44
37:R:74:ILE:N	37:R:87:GLN:O	2.46	0.44
52:5:2291:U:H2'	52:5:2292:U:C6	2.53	0.44
52:5:2812:G:H2'	52:5:2813:A:O4'	2.18	0.44
52:5:2900:A:H2'	52:5:2901:C:O4'	2.18	0.44
2:b:180:ILE:O	2:b:182:VAL:HG13	2.18	0.44
4:d:75:TYR:CZ	4:d:203:TYR:HB3	2.52	0.44
4:d:186:GLU:OE2	4:d:187:ARG:NH2	2.51	0.44
12:l:20:VAL:O	12:l:20:VAL:CG2	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:4:LEU:HD22	19:s:9:PHE:HB2	2.00	0.44
20:t:22:SER:O	20:t:23:ARG:C	2.61	0.44
22:A:242:G:N2	22:A:255:A:OP2	2.38	0.44
22:A:372:G:C2'	22:A:373:U:OP2	2.65	0.44
22:A:577:G:O2'	52:5:1254:A:OP1	2.36	0.44
23:B:45:A:C1'	27:F:91:ARG:NH1	2.79	0.44
25:D:26:VAL:HA	25:D:188:LEU:HD23	2.00	0.44
25:D:100:LEU:O	25:D:102:ALA:N	2.50	0.44
25:D:119:ALA:O	25:D:162:ALA:HB1	2.18	0.44
26:E:149:ILE:HD11	26:E:172:ALA:HA	1.98	0.44
26:E:176:ASP:OD1	26:E:176:ASP:N	2.51	0.44
31:L:29:LYS:HD2	37:R:82:HIS:HD2	1.83	0.44
35:P:75:THR:O	35:P:75:THR:HG22	2.17	0.44
36:Q:42:GLY:HA3	37:R:75:VAL:HG21	2.00	0.44
38:S:96:ILE:O	38:S:97:LEU:HD23	2.18	0.44
42:W:16:ARG:HG3	52:5:2356:U:H4'	1.98	0.44
52:5:2687:U:H2'	52:5:2688:G:O4'	2.17	0.44
52:5:2756:U:C4	52:5:2759:G:O6	2.71	0.44
1:a:354:G:O2'	1:a:355:C:H5'	2.17	0.44
1:a:414:A:C2	1:a:415:A:C8	3.06	0.44
1:a:1192:C:OP2	3:c:3:LYS:NZ	2.44	0.44
1:a:1516:2MG:N2	1:a:1519:MA6:OP2	2.49	0.44
2:b:136:ARG:CZ	2:b:136:ARG:HA	2.48	0.44
14:n:26:LEU:HD22	14:n:26:LEU:H	1.83	0.44
24:C:87:SER:O	24:C:157:ALA:HB2	2.18	0.44
33:N:14:SER:OG	52:5:2690:U:OP1	2.33	0.44
33:N:37:THR:HG22	33:N:110:MET:CE	2.48	0.44
34:O:42:PRO:O	34:O:43:ASN:C	2.60	0.44
52:5:1069:A:N7	52:5:1073:A:N6	2.64	0.44
1:a:235:C:H2'	1:a:236:A:C8	2.53	0.44
1:a:1206:G:H2'	1:a:1207:2MG:O4'	2.17	0.44
1:a:1225:A:H5'	1:a:1226:C:OP2	2.18	0.44
2:b:55:GLU:OE1	2:b:55:GLU:CA	2.66	0.44
4:d:9:LYS:HA	4:d:12:ARG:HE	1.83	0.44
6:f:51:ILE:O	6:f:53:LYS:O	2.36	0.44
7:g:42:VAL:O	7:g:43:TYR:C	2.61	0.44
8:h:70:VAL:O	8:h:71:VAL:C	2.60	0.44
9:i:87:MET:SD	9:i:87:MET:N	2.89	0.44
10:j:9:ARG:O	10:j:9:ARG:HG3	2.18	0.44
11:k:81:LEU:N	11:k:81:LEU:HD23	2.33	0.44
13:m:9:PRO:HG3	13:m:17:ALA:HB1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:p:3:THR:HG23	16:p:3:THR:O	2.18	0.44
16:p:50:THR:HG21	16:p:74:LEU:HD22	2.00	0.44
20:t:50:PHE:O	20:t:53:MET:HG3	2.18	0.44
22:A:7:G:O4'	29:J:135:GLN:NE2	2.50	0.44
22:A:191:A:H2'	22:A:192:C:H6	1.83	0.44
22:A:813:U:H2'	22:A:814:C:C6	2.52	0.44
24:C:129:LEU:N	24:C:129:LEU:HD23	2.33	0.44
27:F:56:LEU:HA	27:F:59:ILE:CG2	2.47	0.44
34:O:99:TYR:OH	34:O:111:ARG:NH2	2.50	0.44
37:R:38:VAL:HG13	37:R:54:VAL:HG23	2.00	0.44
49:3:37:THR:HA	49:3:40:LYS:HD3	1.99	0.44
52:5:1378:A:C4'	52:5:1379:U:OP1	2.66	0.44
1:a:1347:G:O2'	1:a:1348:U:OP2	2.26	0.44
1:a:1494:G:C2	1:a:1495:U:C6	3.05	0.44
1:a:1496:C:H2'	1:a:1497:G:O4'	2.18	0.44
4:d:38:GLY:O	4:d:39:GLN:C	2.61	0.44
9:i:107:ALA:O	9:i:108:ARG:C	2.61	0.44
17:q:43:LEU:HD13	17:q:44:HIS:N	2.33	0.44
22:A:370:G:O2'	22:A:424:G:OP1	2.34	0.44
22:A:580:U:O3'	36:Q:30:VAL:HG13	2.17	0.44
30:K:4:GLU:HA	30:K:21:CYS:O	2.17	0.44
52:5:1177:G:H2'	52:5:1178:C:O4'	2.17	0.44
52:5:1357:C:H2'	52:5:1358:G:O4'	2.17	0.44
52:5:2557:G:H2'	52:5:2558:C:C6	2.53	0.44
1:a:359:G:C4	1:a:360:G:C8	3.06	0.44
1:a:936:C:C4	1:a:937:A:N7	2.86	0.44
3:c:107:LYS:HD3	3:c:110:LEU:HD12	2.00	0.44
11:k:78:ILE:C	11:k:78:ILE:HD12	2.43	0.44
20:t:4:LYS:O	20:t:7:LYS:HG2	2.16	0.44
21:u:28:LEU:HD23	21:u:28:LEU:C	2.42	0.44
22:A:615:U:C4'	22:A:616:A:OP2	2.66	0.44
22:A:805:G:N2	22:A:829:A:OP1	2.51	0.44
22:A:858:G:O3'	22:A:859:G:O4'	2.35	0.44
27:F:56:LEU:HD12	27:F:86:CYS:SG	2.58	0.44
29:J:135:GLN:O	29:J:136:GLN:C	2.60	0.44
31:L:101:ILE:HG13	31:L:102:GLY:H	1.82	0.44
34:O:67:ASN:O	34:O:70:ALA:N	2.51	0.44
35:P:30:TRP:NE1	35:P:81:ASP:HB2	2.33	0.44
38:S:69:LEU:HD11	38:S:107:VAL:HG12	1.99	0.44
42:W:65:PHE:HE2	42:W:76:ILE:HD11	1.78	0.44
46:O:24:VAL:HG13	46:O:25:THR:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:5:1563:U:H2'	52:5:1564:C:C6	2.53	0.44
52:5:2071:A:H2'	52:5:2072:C:C6	2.53	0.44
1:a:195:A:HO2'	1:a:196:A:C1'	2.21	0.43
1:a:875:U:O2'	8:h:14:ARG:HD2	2.17	0.43
1:a:1238:A:H2'	1:a:1238:A:N3	2.33	0.43
1:a:1314:C:H2'	1:a:1315:U:C6	2.53	0.43
2:b:67:LEU:HD12	2:b:157:PRO:CG	2.47	0.43
4:d:54:LEU:O	4:d:58:GLN:HG2	2.18	0.43
4:d:57:LYS:NZ	4:d:68:GLU:OE1	2.47	0.43
22:A:488:G:H22	22:A:491:G:H5''	1.83	0.43
24:C:245:THR:C	24:C:247:TRP:H	2.26	0.43
25:D:37:VAL:HG21	25:D:90:PHE:O	2.17	0.43
26:E:110:SER:OG	26:E:114:ARG:NH1	2.50	0.43
52:5:2011:U:H2'	52:5:2012:G:O4'	2.18	0.43
52:5:2514:U:H2'	52:5:2515:C:C6	2.53	0.43
52:5:2590:A:H2'	52:5:2591:C:H6	1.83	0.43
2:b:29:PHE:O	2:b:30:ILE:CG2	2.66	0.43
4:d:116:LEU:O	4:d:117:VAL:C	2.59	0.43
10:j:10:LEU:HD12	10:j:10:LEU:C	2.43	0.43
14:n:2:LYS:HG3	14:n:4:SER:OG	2.18	0.43
22:A:368:A:H2'	22:A:369:U:O4'	2.17	0.43
22:A:742:A:H2'	22:A:743:A:C8	2.52	0.43
25:D:173:GLN:HE21	52:5:2731:G:H4'	1.83	0.43
43:X:46:VAL:HG13	43:X:77:TYR:O	2.17	0.43
52:5:1565:C:O2'	52:5:1566:A:C8	2.72	0.43
52:5:1954:G:O2'	52:5:1956:U:O4	2.29	0.43
1:a:937:A:OP2	57:a:1705:HOH:O	2.21	0.43
2:b:8:MET:HE1	2:b:10:LYS:CG	2.48	0.43
4:d:151:GLN:O	4:d:153:ARG:N	2.52	0.43
5:e:154:ALA:HB1	8:h:65:PHE:CE2	2.54	0.43
8:h:63:LYS:NZ	8:h:63:LYS:HB3	2.34	0.43
10:j:15:HIS:CG	10:j:16:ARG:N	2.85	0.43
16:p:4:ILE:HG13	16:p:65:ALA:HB1	1.99	0.43
17:q:22:VAL:HG12	17:q:23:ALA:N	2.33	0.43
19:s:5:LYS:HG3	19:s:6:LYS:HE3	2.00	0.43
19:s:10:ILE:HD13	19:s:15:LEU:HD22	1.99	0.43
22:A:172:A:H2'	22:A:173:A:C8	2.53	0.43
22:A:487:C:H2'	22:A:488:G:O4'	2.18	0.43
28:G:23:ILE:HD11	28:G:42:VAL:HG11	2.01	0.43
30:K:105:ARG:O	30:K:108:ARG:HB3	2.19	0.43
32:M:35:ALA:HB1	32:M:126:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:W:7:ARG:N	42:W:7:ARG:CD	2.81	0.43
52:5:2326:C:HO2'	52:5:2327:A:P	2.31	0.43
52:5:2441:U:OP2	52:5:2586:U:O2'	2.35	0.43
52:5:2589:A:H2'	52:5:2590:A:H8	1.84	0.43
1:a:936:C:C2	1:a:937:A:C8	3.06	0.43
1:a:1281:C:HO2'	1:a:1282:C:P	2.35	0.43
1:a:1347:G:C2'	1:a:1348:U:OP2	2.67	0.43
3:c:70:ALA:HB2	3:c:105:VAL:CG2	2.48	0.43
9:i:122:ARG:NH1	9:i:123:ARG:O	2.52	0.43
11:k:50:GLY:O	11:k:51:PHE:C	2.62	0.43
16:p:36:VAL:O	16:p:36:VAL:CG1	2.65	0.43
22:A:493:G:H2'	22:A:494:G:O4'	2.18	0.43
22:A:588:U:H2'	22:A:589:U:C6	2.53	0.43
22:A:752:A:H1'	22:A:753:A:OP2	2.18	0.43
25:D:137:SER:OG	52:5:2580:PSU:OP1	2.21	0.43
33:N:77:ALA:O	33:N:79:LEU:O	2.36	0.43
41:V:28:ALA:HB3	41:V:40:ILE:HG23	2.01	0.43
52:5:1198:U:H2'	52:5:1199:U:C6	2.53	0.43
52:5:2655:G:C2'	52:5:2656:U:OP2	2.67	0.43
1:a:227:G:H2'	1:a:228:A:O4'	2.19	0.43
1:a:438:U:HO2'	1:a:439:U:H6	1.62	0.43
1:a:704:A:C4	1:a:705:G:C8	3.06	0.43
2:b:142:LYS:O	2:b:145:ASN:OD1	2.36	0.43
2:b:165:ALA:HB3	2:b:190:SER:HB3	2.01	0.43
5:e:158:LYS:N	5:e:158:LYS:HD3	2.33	0.43
7:g:86:VAL:HA	7:g:87:PRO:HD2	1.88	0.43
16:p:1:MET:HE3	16:p:24:SER:CB	2.49	0.43
17:q:46:HIS:CD2	17:q:66:LEU:CD1	3.01	0.43
21:u:36:PHE:O	21:u:37:TYR:CB	2.67	0.43
22:A:74:A:H4'	22:A:75:G:O5'	2.19	0.43
22:A:663:G:H5''	31:L:17:LYS:HD3	2.00	0.43
26:E:31:VAL:HG21	26:E:104:ALA:CB	2.49	0.43
27:F:135:ILE:C	27:F:135:ILE:HD12	2.44	0.43
35:P:23:ASP:OD1	35:P:112:ARG:NH2	2.51	0.43
52:5:1013:C:H2'	52:5:1014:A:H8	1.84	0.43
52:5:1441:G:H2'	52:5:1442:U:C6	2.54	0.43
52:5:1857:G:HO2'	52:5:1858:A:P	2.40	0.43
1:a:31:G:HO2'	1:a:32:A:C5'	2.20	0.43
1:a:235:C:H2'	1:a:236:A:H8	1.84	0.43
1:a:539:A:H2'	1:a:540:G:C8	2.54	0.43
1:a:672:U:H2'	1:a:673:A:H8	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:685:G:H2'	1:a:686:U:C6	2.53	0.43
1:a:778:G:O2'	11:k:121:ARG:O	2.36	0.43
1:a:1073:U:H2'	1:a:1074:G:O4'	2.19	0.43
7:g:36:SER:HA	9:i:42:THR:HG21	1.99	0.43
14:n:33:VAL:O	14:n:33:VAL:CG1	2.67	0.43
14:n:93:ILE:N	14:n:93:ILE:HD12	2.34	0.43
17:q:37:ILE:HG22	17:q:38:LYS:N	2.34	0.43
19:s:18:VAL:O	19:s:22:VAL:HG23	2.18	0.43
22:A:645:C:H2'	22:A:647:G:N7	2.34	0.43
25:D:100:LEU:C	25:D:102:ALA:H	2.25	0.43
28:G:32:LEU:HD12	28:G:32:LEU:N	2.34	0.43
52:5:1268:A:H1'	52:5:2013:A:N6	2.33	0.43
52:5:1829:A:C8	52:5:1830:C:C5	3.07	0.43
52:5:2834:G:H2'	52:5:2879:A:H61	1.83	0.43
1:a:444:G:C6	1:a:491:G:C6	3.06	0.43
1:a:451:A:O4'	1:a:452:A:C2	2.72	0.43
1:a:951:G:OP2	13:m:100:ARG:NH2	2.52	0.43
2:b:147:LEU:O	2:b:147:LEU:HG	2.19	0.43
6:f:55:HIS:C	6:f:56:LYS:HG3	2.43	0.43
11:k:108:ASN:N	11:k:108:ASN:OD1	2.52	0.43
13:m:9:PRO:HG2	13:m:17:ALA:HB1	2.00	0.43
15:o:5:GLU:O	15:o:9:LYS:HG2	2.19	0.43
16:p:59:HIS:C	16:p:59:HIS:ND1	2.65	0.43
26:E:127:GLU:OE1	26:E:127:GLU:N	2.49	0.43
29:J:12:LYS:CD	29:J:12:LYS:H	2.30	0.43
31:L:20:GLY:O	31:L:21:ARG:NE	2.51	0.43
38:S:42:LYS:O	38:S:45:VAL:HG22	2.18	0.43
38:S:63:GLY:O	38:S:64:ALA:HB3	2.18	0.43
50:4:2:LYS:HE2	50:4:32:LYS:O	2.17	0.43
52:5:1023:U:OP2	52:5:1024:G:N7	2.52	0.43
52:5:1295:C:C2	52:5:1296:G:C8	3.07	0.43
52:5:1678:A:C4	52:5:1679:A:C8	3.07	0.43
52:5:1946:U:H2'	52:5:1947:C:C6	2.54	0.43
52:5:2070:A:H2'	52:5:2071:A:O4'	2.18	0.43
52:5:2323:G:H2'	52:5:2324:U:O4'	2.18	0.43
1:a:1190:G:C4'	1:a:1191:A:OP2	2.67	0.43
1:a:1300:G:C2'	1:a:1301:U:OP2	2.67	0.43
1:a:1486:G:H2'	1:a:1487:G:O4'	2.19	0.43
2:b:67:LEU:HD12	2:b:157:PRO:HG2	2.00	0.43
4:d:143:SER:HB3	4:d:178:GLU:OE1	2.18	0.43
5:e:34:ALA:O	5:e:49:TYR:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:52:ASN:HD21	6:f:85:ILE:HD13	1.83	0.43
12:l:78:VAL:HG12	12:l:101:LEU:HD23	2.01	0.43
12:l:86:VAL:HG13	12:l:95:HIS:CE1	2.53	0.43
17:q:11:VAL:CG2	17:q:20:ILE:HD11	2.48	0.43
22:A:1:G:N1	52:5:2903:U:O2	2.52	0.43
22:A:242:G:H5''	49:3:63:TYR:CZ	2.53	0.43
22:A:479:A:H4'	22:A:480:A:OP1	2.19	0.43
22:A:511:U:O4	22:A:512:G:N1	2.51	0.43
22:A:851:C:O2'	45:Z:42:ALA:HA	2.18	0.43
22:A:876:C:H2'	22:A:877:A:O4'	2.19	0.43
23:B:12:C:O2	23:B:12:C:O4'	2.37	0.43
24:C:164:VAL:HG21	24:C:180:MET:HE1	2.00	0.43
27:F:3:LEU:HD12	27:F:100:GLU:HB2	1.99	0.43
27:F:173:ASP:O	27:F:174:PHE:CB	2.67	0.43
29:J:112:GLY:O	29:J:116:ARG:HG3	2.18	0.43
35:P:81:ASP:OD1	35:P:81:ASP:C	2.62	0.43
52:5:1416:G:H2'	52:5:1417:C:H6	1.83	0.43
52:5:1564:C:H2'	52:5:1565:C:O4'	2.19	0.43
52:5:2243:U:H2'	52:5:2244:U:C6	2.53	0.43
1:a:218:U:H2'	1:a:219:U:O4'	2.19	0.43
1:a:1073:U:O2	2:b:102:ASN:ND2	2.52	0.43
2:b:104:LYS:HA	2:b:107:ARG:HD2	2.01	0.43
2:b:138:ARG:O	2:b:141:GLU:HG3	2.18	0.43
4:d:131:ILE:H	4:d:131:ILE:HD12	1.83	0.43
8:h:4:ASP:CG	8:h:80:PRO:HD3	2.43	0.43
10:j:64:GLN:O	14:n:99:ALA:N	2.44	0.43
13:m:53:ASP:OD1	13:m:53:ASP:N	2.46	0.43
24:C:43:ASN:ND2	24:C:49:THR:HG21	2.34	0.43
25:D:85:ALA:C	25:D:87:GLY:H	2.27	0.43
27:F:9:ASP:O	27:F:12:VAL:HG12	2.18	0.43
30:K:116:ILE:C	30:K:116:ILE:HD12	2.43	0.43
41:V:80:HIS:CE1	41:V:83:LYS:HG3	2.53	0.43
52:5:1730:C:O2	52:5:1731:G:N1	2.52	0.43
52:5:1847:G:O2'	52:5:1848:A:H8	2.02	0.43
52:5:2497:A:N3	52:5:2498:OMC:N4	2.67	0.43
1:a:110:C:H4'	16:p:25:ARG:HD2	2.01	0.43
1:a:891:U:C2	1:a:892:A:C8	3.07	0.43
1:a:1130:A:O2'	9:i:4:GLN:NE2	2.52	0.43
3:c:158:GLY:HA3	3:c:192:TYR:CE2	2.54	0.43
5:e:45:VAL:CG2	5:e:117:ALA:HA	2.49	0.43
5:e:112:ALA:O	5:e:116:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:125:LYS:HD3	5:e:127:TYR:CE1	2.54	0.43
11:k:64:VAL:HG13	11:k:65:ALA:N	2.34	0.43
14:n:93:ILE:HD12	14:n:93:ILE:H	1.82	0.43
22:A:100:U:H4'	22:A:101:A:O4'	2.19	0.43
22:A:631:A:N3	52:5:2415:G:O2'	2.41	0.43
26:E:131:THR:HG22	26:E:160:ALA:O	2.19	0.43
28:G:83:THR:HG22	28:G:133:LYS:CG	2.41	0.43
30:K:69:VAL:HG21	30:K:106:GLU:OE1	2.19	0.43
31:L:73:ILE:HG13	31:L:73:ILE:O	2.18	0.43
36:Q:26:ALA:C	36:Q:28:SER:H	2.27	0.43
36:Q:91:ARG:NH2	52:5:1153:C:OP1	2.50	0.43
39:T:20:ALA:HA	39:T:31:VAL:HG21	2.01	0.43
39:T:52:GLU:N	39:T:52:GLU:OE1	2.51	0.43
52:5:2329:U:H2'	52:5:2330:G:C8	2.54	0.43
1:a:323:U:OP1	20:t:20:ASN:ND2	2.52	0.42
1:a:363:A:H2'	1:a:364:A:O4'	2.18	0.42
1:a:1096:C:H2'	1:a:1097:C:C6	2.54	0.42
1:a:1513:A:H2'	1:a:1514:G:C8	2.54	0.42
4:d:3:TYR:CZ	4:d:10:LEU:HD21	2.54	0.42
4:d:176:LYS:O	4:d:176:LYS:HD3	2.19	0.42
8:h:34:ALA:HB1	8:h:109:VAL:HG21	2.00	0.42
17:q:45:VAL:HG21	17:q:60:ILE:CG2	2.49	0.42
17:q:78:VAL:HG12	17:q:79:GLU:HG2	2.01	0.42
19:s:70:LEU:HD22	19:s:70:LEU:N	2.33	0.42
22:A:458:G:C2'	22:A:459:U:OP2	2.66	0.42
27:F:12:VAL:HG23	27:F:27:VAL:HG21	2.01	0.42
30:K:110:GLU:HG2	30:K:111:LYS:N	2.34	0.42
31:L:75:ALA:HB2	31:L:105:ILE:CD1	2.49	0.42
32:M:56:ALA:HB2	32:M:119:LEU:HD12	2.01	0.42
34:O:11:ALA:HB2	34:O:96:GLY:N	2.34	0.42
37:R:20:VAL:HG23	37:R:96:VAL:HG23	2.00	0.42
42:W:14:ALA:HB1	52:5:2271:G:OP1	2.18	0.42
42:W:47:VAL:HG21	42:W:76:ILE:HG22	2.01	0.42
45:Z:46:MET:O	45:Z:50:VAL:HG22	2.19	0.42
51:6:58:ASP:OD1	51:6:58:ASP:N	2.51	0.42
52:5:927:A:H2'	52:5:928:A:C8	2.54	0.42
52:5:2345:G:N3	52:5:2381:A:H2'	2.34	0.42
52:5:2812:G:H2'	52:5:2813:A:C8	2.54	0.42
52:5:2836:U:H2'	52:5:2837:A:C8	2.54	0.42
1:a:155:A:H2'	1:a:156:C:O4'	2.19	0.42
1:a:626:G:H4'	16:p:38:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1401:G:H2'	1:a:1402:4OC:O4'	2.19	0.42
3:c:18:ASN:O	3:c:55:VAL:HA	2.18	0.42
4:d:123:MET:HE3	4:d:126:GLY:HA2	2.01	0.42
13:m:58:GLU:O	13:m:59:VAL:C	2.62	0.42
13:m:95:PRO:C	13:m:96:VAL:HG23	2.43	0.42
22:A:242:G:C2'	22:A:243:U:OP2	2.66	0.42
31:L:78:ARG:HB3	31:L:113:ALA:CB	2.50	0.42
32:M:70:ASP:O	32:M:70:ASP:CG	2.62	0.42
38:S:20:VAL:HG11	38:S:44:ALA:HA	2.01	0.42
38:S:74:ILE:HD13	38:S:105:VAL:HG22	2.00	0.42
52:5:1469:A:H2'	52:5:1470:A:C8	2.54	0.42
52:5:2236:U:H2'	52:5:2237:G:O4'	2.19	0.42
1:a:58:C:H2'	1:a:58:C:O2	2.18	0.42
1:a:198:G:H2'	1:a:199:A:C8	2.54	0.42
1:a:662:U:H2'	1:a:663:A:C8	2.54	0.42
1:a:728:A:C8	15:o:53:ARG:CZ	3.02	0.42
1:a:1151:A:O2'	1:a:1152:A:P	2.76	0.42
3:c:161:ILE:C	3:c:161:ILE:HD12	2.43	0.42
10:j:13:PHE:HA	10:j:68:ARG:O	2.19	0.42
10:j:83:THR:O	10:j:87:LEU:HG	2.18	0.42
11:k:88:PRO:HD3	21:u:28:LEU:HD13	2.01	0.42
17:q:21:VAL:O	17:q:21:VAL:HG13	2.18	0.42
22:A:4:U:H2'	22:A:5:A:H8	1.83	0.42
22:A:388:G:N7	22:A:390:U:H2'	2.34	0.42
22:A:643:A:N1	52:5:2369:A:O2'	2.47	0.42
22:A:698:C:O2'	22:A:734:A:N6	2.52	0.42
34:O:15:ARG:NH2	34:O:95:SER:OG	2.48	0.42
49:3:27:ASN:ND2	52:5:2361:G:O3'	2.53	0.42
52:5:1418:G:N2	52:5:1579:A:C8	2.87	0.42
1:a:392:C:H2'	1:a:393:A:O4'	2.19	0.42
1:a:686:U:O2'	1:a:687:A:O4'	2.37	0.42
1:a:925:G:C2	1:a:927:G:C8	3.07	0.42
1:a:1328:C:OP1	13:m:27:THR:HG21	2.19	0.42
1:a:1432:G:C2'	1:a:1433:A:OP2	2.66	0.42
1:a:1456:A:H2'	1:a:1457:G:O4'	2.19	0.42
2:b:55:GLU:OE1	2:b:55:GLU:O	2.37	0.42
3:c:175:HIS:O	3:c:177:LEU:CD2	2.67	0.42
5:e:45:VAL:HG22	5:e:117:ALA:HA	2.00	0.42
6:f:52:ASN:OD1	6:f:52:ASN:O	2.37	0.42
6:f:77:THR:HG23	6:f:78:PHE:N	2.33	0.42
7:g:118:ARG:O	7:g:122:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:2:MET:HE2	8:h:2:MET:HA	2.01	0.42
10:j:91:ASP:OD1	10:j:91:ASP:N	2.51	0.42
13:m:3:ILE:HG22	13:m:56:ARG:CG	2.49	0.42
16:p:1:MET:O	16:p:23:ASP:OD1	2.38	0.42
18:r:45:GLY:O	18:r:46:THR:OG1	2.21	0.42
22:A:5:A:H2'	22:A:6:A:H8	1.85	0.42
22:A:310:A:O2'	22:A:311:A:H2'	2.19	0.42
22:A:569:U:H2'	22:A:570:G:O4'	2.19	0.42
22:A:764:A:O2'	22:A:765:C:H5'	2.20	0.42
31:L:90:VAL:HG13	31:L:95:LEU:HD21	2.02	0.42
34:O:93:ASP:OD1	34:O:93:ASP:N	2.52	0.42
51:6:17:SER:C	51:6:19:GLY:N	2.77	0.42
52:5:2287:A:C2'	52:5:2288:A:O5'	2.67	0.42
52:5:2609:U:H5'	52:5:2610:C:OP2	2.20	0.42
1:a:79:G:H2'	1:a:80:A:O4'	2.19	0.42
1:a:455:G:C2	1:a:478:A:C2	3.08	0.42
1:a:632:U:P	1:a:633:G:C8	3.12	0.42
1:a:1320:C:N4	19:s:36:ARG:HA	2.34	0.42
2:b:169:HIS:ND1	2:b:170:ILE:N	2.67	0.42
4:d:103:ARG:CB	4:d:170:LEU:HD21	2.49	0.42
5:e:69:ASN:O	5:e:70:MET:C	2.61	0.42
5:e:98:ALA:HB2	5:e:123:LEU:HG	2.00	0.42
6:f:32:ALA:C	6:f:34:GLY:H	2.27	0.42
7:g:24:LYS:O	7:g:28:ILE:HG13	2.20	0.42
17:q:22:VAL:HG12	17:q:23:ALA:O	2.19	0.42
22:A:12:U:O2	52:5:2626:C:H4'	2.18	0.42
22:A:91:A:O2'	22:A:92:U:OP2	2.37	0.42
22:A:402:A:H2'	22:A:403:U:O4'	2.20	0.42
22:A:565:C:OP2	37:R:80:ARG:N	2.49	0.42
22:A:630:G:N2	22:A:633:A:OP2	2.32	0.42
22:A:748:G:O6	22:A:751:A:H4'	2.20	0.42
24:C:119:VAL:HG23	24:C:120:ASP:N	2.35	0.42
28:G:126:THR:HG22	28:G:128:THR:H	1.84	0.42
28:G:137:LYS:HA	28:G:140:ILE:CG2	2.50	0.42
52:5:1265:A:O4'	52:5:1267:U:C6	2.73	0.42
52:5:2720:U:C2	52:5:2721:A:C8	3.08	0.42
1:a:1368:A:OP2	9:i:113:LYS:HD3	2.19	0.42
1:a:1507:A:H2'	1:a:1508:A:C8	2.55	0.42
2:b:132:GLU:OE2	2:b:136:ARG:CG	2.68	0.42
4:d:87:GLU:OE1	4:d:87:GLU:N	2.42	0.42
4:d:154:VAL:CG1	4:d:177:MET:HE3	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:45:VAL:HG21	5:e:117:ALA:HB2	2.00	0.42
8:h:64:TYR:CD1	8:h:64:TYR:N	2.86	0.42
8:h:107:LYS:HA	8:h:107:LYS:HE3	2.02	0.42
12:l:23:LEU:O	12:l:25:ALA:N	2.53	0.42
20:t:67:HIS:O	20:t:69:ASN:OD1	2.38	0.42
22:A:581:C:H2'	22:A:582:A:C8	2.55	0.42
22:A:828:U:H2'	22:A:829:A:C8	2.55	0.42
24:C:145:MET:HE3	24:C:153:LEU:HD21	2.02	0.42
25:D:37:VAL:HG23	25:D:92:VAL:CG2	2.48	0.42
26:E:113:VAL:HG22	26:E:118:LEU:CD2	2.49	0.42
30:K:76:VAL:HG13	35:P:72:VAL:CG2	2.49	0.42
36:Q:49:ARG:NE	52:5:993:G:OP1	2.50	0.42
52:5:1289:C:O2'	52:5:1330:C:H4'	2.20	0.42
52:5:1534:U:H1'	52:5:1538:G:N2	2.35	0.42
52:5:1609:A:H1'	52:5:1616:A:O4'	2.19	0.42
52:5:1697:G:OP2	52:5:1698:A:O2'	2.34	0.42
52:5:2505:G:O2'	52:5:2506:U:H5''	2.19	0.42
52:5:2815:C:C2	52:5:2816:G:C8	3.08	0.42
1:a:165:G:H2'	1:a:166:U:C6	2.55	0.42
1:a:375:U:O2'	1:a:376:G:H5'	2.19	0.42
1:a:695:A:H2'	1:a:696:A:C8	2.55	0.42
7:g:131:GLY:O	7:g:134:VAL:HG23	2.19	0.42
10:j:8:ILE:O	10:j:73:LEU:HD23	2.19	0.42
12:l:113:ARG:O	12:l:114:SER:C	2.63	0.42
22:A:79:C:O2'	22:A:346:A:N3	2.49	0.42
22:A:760:G:H2'	22:A:761:A:O4'	2.20	0.42
22:A:848:C:H2'	22:A:849:A:H8	1.83	0.42
26:E:29:HIS:NE2	52:5:1244:A:O2'	2.41	0.42
28:G:98:LYS:H	28:G:98:LYS:HD3	1.85	0.42
28:G:110:HIS:ND1	28:G:110:HIS:N	2.68	0.42
32:M:134:THR:OG1	41:V:79:ARG:NH2	2.53	0.42
38:S:59:GLU:HA	38:S:64:ALA:HB2	2.02	0.42
38:S:69:LEU:HD11	38:S:107:VAL:CG1	2.49	0.42
43:X:70:LEU:O	43:X:71:ARG:C	2.63	0.42
45:Z:4:ILE:HD11	45:Z:56:VAL:HG23	2.00	0.42
51:6:23:LYS:O	51:6:24:ILE:HG23	2.19	0.42
52:5:981:A:N1	52:5:2027:G:O2'	2.49	0.42
52:5:1001:A:H2'	52:5:1002:G:O4'	2.19	0.42
52:5:1036:G:C6	52:5:1120:G:C6	3.08	0.42
52:5:1118:C:H2'	52:5:1119:U:O4'	2.19	0.42
52:5:1538:G:H2'	52:5:1539:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:5:1737:G:O3'	52:5:1738:G:O4'	2.37	0.42
52:5:1746:A:H2'	52:5:1747:U:H6	1.85	0.42
52:5:1914:C:O2	52:5:1914:C:O4'	2.36	0.42
52:5:2547:A:H2'	52:5:2548:U:C6	2.54	0.42
1:a:481:G:H1'	1:a:483:C:N4	2.33	0.42
1:a:1513:A:H2'	1:a:1514:G:H8	1.85	0.42
2:b:101:THR:HG22	2:b:174:GLU:OE2	2.20	0.42
2:b:162:VAL:HB	2:b:184:ALA:HB1	2.01	0.42
12:l:53:ARG:HG2	12:l:63:THR:OG1	2.20	0.42
22:A:48:G:N1	22:A:177:G:OP2	2.50	0.42
22:A:161:A:H3'	22:A:162:U:H5''	2.01	0.42
23:B:117:G:H2'	23:B:118:C:O4'	2.20	0.42
26:E:119:ILE:O	26:E:187:VAL:HA	2.20	0.42
27:F:1:ALA:O	27:F:2:LYS:C	2.62	0.42
30:K:5:GLN:HA	30:K:20:MET:HE3	2.02	0.42
30:K:13:ASN:C	30:K:15:GLY:H	2.26	0.42
37:R:80:ARG:O	37:R:80:ARG:HG2	2.19	0.42
52:5:1055:G:O2'	52:5:1084:A:N6	2.53	0.42
52:5:1590:A:H2'	52:5:1591:A:H8	1.84	0.42
52:5:2040:G:H2'	52:5:2041:U:O4'	2.20	0.42
1:a:575:G:H2'	1:a:821:G:OP2	2.20	0.42
1:a:1291:U:H2'	1:a:1292:G:H8	1.84	0.42
1:a:1372:U:OP1	9:i:73:GLY:N	2.49	0.42
1:a:1415:G:C6	1:a:1486:G:C6	3.08	0.42
3:c:13:ILE:CD1	3:c:177:LEU:HB3	2.50	0.42
5:e:93:VAL:HG13	5:e:110:MET:CE	2.50	0.42
5:e:118:GLY:O	5:e:120:HIS:CE1	2.73	0.42
11:k:72:ALA:C	11:k:73:VAL:CG1	2.93	0.42
19:s:57:VAL:HG13	19:s:57:VAL:O	2.19	0.42
22:A:814:C:H1'	52:5:1225:G:N2	2.35	0.42
22:A:820:A:H4'	22:A:836:G:N2	2.34	0.42
27:F:131:VAL:HG13	27:F:136:ILE:HD13	2.01	0.42
52:5:1558:C:O4'	52:5:1560:G:C8	2.73	0.42
52:5:1999:C:H4'	52:5:2723:C:O2	2.19	0.42
52:5:2063:C:O2	52:5:2063:C:H2'	2.20	0.42
52:5:2070:A:H2'	52:5:2071:A:C8	2.55	0.42
52:5:2590:A:H2'	52:5:2591:C:C6	2.55	0.42
52:5:2822:G:O2'	52:5:2824:C:OP2	2.30	0.42
1:a:21:G:H2'	1:a:22:G:C8	2.55	0.42
1:a:355:C:C4	1:a:356:A:N7	2.88	0.42
1:a:374:A:C4	1:a:375:U:C5	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:399:G:C6	1:a:400:C:N4	2.88	0.42
1:a:675:A:H2'	1:a:676:A:O4'	2.20	0.42
1:a:868:C:H2'	1:a:869:G:O4'	2.20	0.42
1:a:1316:G:H22	1:a:1319:A:P	2.43	0.42
3:c:9:ILE:HD12	14:n:98:LYS:HD3	2.01	0.42
3:c:125:ARG:O	3:c:126:ARG:HB2	2.20	0.42
4:d:77:GLU:O	4:d:80:ARG:HG3	2.20	0.42
7:g:115:MET:HA	7:g:115:MET:HE3	2.00	0.42
9:i:27:ILE:N	9:i:27:ILE:HD12	2.35	0.42
15:o:50:HIS:ND1	15:o:50:HIS:N	2.68	0.42
27:F:89:THR:O	27:F:90:LEU:C	2.63	0.42
27:F:168:LEU:O	27:F:168:LEU:HD13	2.20	0.42
28:G:8:VAL:O	28:G:48:THR:HG22	2.20	0.42
29:J:13:ARG:NH1	29:J:49:ASP:O	2.49	0.42
32:M:33:LEU:HD11	32:M:128:THR:HB	2.00	0.42
32:M:69:PRO:O	32:M:70:ASP:OD1	2.37	0.42
38:S:93:ALA:HB2	52:5:1614:A:C2	2.55	0.42
40:U:64:ILE:HD11	40:U:68:ASN:CB	2.50	0.42
52:5:1067:A:HO2'	52:5:1068:G:P	2.39	0.42
52:5:1348:C:C5	52:5:1349:C:C5	3.07	0.42
52:5:1359:A:OP2	52:5:1371:G:N1	2.45	0.42
52:5:1638:C:O2	52:5:2698:U:O2'	2.37	0.42
52:5:1682:G:H2'	52:5:1683:U:C6	2.55	0.42
52:5:1694:C:H4'	52:5:1695:G:O5'	2.20	0.42
52:5:2241:A:H2'	52:5:2242:G:C8	2.55	0.42
52:5:2507:C:C2	52:5:2583:G:C2	3.08	0.42
1:a:193:C:H2'	1:a:194:C:O4'	2.20	0.41
1:a:246:A:C2	1:a:282:A:C6	3.08	0.41
1:a:1305:G:O2'	1:a:1306:A:H8	2.03	0.41
3:c:41:TYR:C	3:c:41:TYR:CD1	2.97	0.41
3:c:110:LEU:HD13	3:c:203:LYS:HE3	2.01	0.41
4:d:27:ILE:N	4:d:27:ILE:CD1	2.82	0.41
11:k:18:GLY:HA2	11:k:35:ASP:O	2.19	0.41
11:k:52:ARG:HE	11:k:52:ARG:HA	1.85	0.41
17:q:50:ASN:ND2	17:q:50:ASN:N	2.67	0.41
18:r:21:ASP:OD1	18:r:21:ASP:N	2.53	0.41
22:A:807:U:H1'	52:5:2445:2MG:OP1	2.20	0.41
24:C:259:ASN:O	24:C:260:LYS:HB2	2.20	0.41
26:E:88:ARG:O	26:E:90:GLN:N	2.53	0.41
28:G:43:LYS:O	28:G:50:THR:OG1	2.38	0.41
35:P:51:ASN:O	35:P:52:ARG:NE	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:V:92:VAL:HG13	41:V:92:VAL:O	2.20	0.41
42:W:68:LYS:HA	42:W:68:LYS:HE2	2.02	0.41
52:5:1005:C:C2	52:5:1006:C:C5	3.08	0.41
52:5:1053:C:H42	52:5:1106:G:H1	1.69	0.41
52:5:1724:G:O6	52:5:1737:G:C2	2.73	0.41
52:5:2229:U:H2'	52:5:2230:G:H8	1.85	0.41
52:5:2788:C:H2'	52:5:2789:C:C6	2.55	0.41
52:5:2793:C:H2'	52:5:2794:C:C6	2.54	0.41
1:a:476:U:H2'	1:a:477:C:C6	2.55	0.41
1:a:520:A:N6	1:a:533:A:H61	2.17	0.41
1:a:933:G:C2	1:a:935:A:O4'	2.73	0.41
1:a:958:A:H1'	1:a:985:C:O2'	2.20	0.41
2:b:82:ALA:HB3	2:b:213:LEU:HD21	2.00	0.41
4:d:142:VAL:O	4:d:178:GLU:OE1	2.38	0.41
7:g:12:LEU:HG	7:g:13:PRO:HD2	2.02	0.41
9:i:15:ALA:HB3	9:i:67:LYS:NZ	2.35	0.41
14:n:80:SER:O	14:n:81:ARG:C	2.63	0.41
17:q:6:THR:C	17:q:7:LEU:HD12	2.45	0.41
22:A:515:A:H1'	22:A:581:C:H1'	2.01	0.41
22:A:563:A:OP2	37:R:79:ARG:NH1	2.48	0.41
22:A:774:G:O2'	22:A:775:G:C5'	2.66	0.41
23:B:51:G:OP1	34:O:63:LYS:NZ	2.50	0.41
24:C:146:LYS:O	24:C:147:PRO:C	2.63	0.41
28:G:37:ASN:ND2	28:G:63:GLN:HE21	2.17	0.41
34:O:87:ILE:HD12	34:O:87:ILE:N	2.34	0.41
38:S:41:LYS:O	38:S:44:ALA:HB3	2.20	0.41
38:S:72:THR:C	38:S:73:LYS:HG3	2.45	0.41
47:1:37:LYS:HB2	47:1:48:TYR:CD1	2.54	0.41
52:5:1204:A:O4'	52:5:1206:G:C8	2.73	0.41
52:5:2185:U:H2'	52:5:2186:G:H8	1.85	0.41
52:5:2191:A:H2'	52:5:2192:U:O4'	2.20	0.41
1:a:216:U:H2'	1:a:217:C:C6	2.55	0.41
1:a:505:G:OP2	1:a:535:A:H5'	2.20	0.41
1:a:1148:U:H2'	1:a:1149:C:O4'	2.20	0.41
1:a:1273:C:H2'	1:a:1274:A:O4'	2.21	0.41
2:b:80:LYS:O	2:b:84:LEU:HG	2.20	0.41
11:k:62:ALA:O	11:k:65:ALA:N	2.53	0.41
12:l:79:ILE:HG22	12:l:103:CYS:HB2	2.02	0.41
12:l:86:VAL:CG1	12:l:95:HIS:CE1	3.03	0.41
13:m:84:CYS:O	13:m:85:TYR:C	2.62	0.41
17:q:25:GLU:OE2	17:q:40:THR:OG1	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:282:A:C6	22:A:359:G:C2	3.08	0.41
25:D:24:VAL:HA	25:D:189:VAL:O	2.20	0.41
25:D:59:ARG:O	25:D:60:VAL:C	2.63	0.41
25:D:133:THR:OG1	52:5:1993:U:H4'	2.20	0.41
40:U:73:ASN:C	40:U:75:ALA:H	2.28	0.41
50:4:11:CYS:SG	50:4:13:ASN:N	2.87	0.41
50:4:36:ARG:O	50:4:37:GLN:CB	2.69	0.41
52:5:1373:A:H5'	52:5:2212:A:H1'	2.01	0.41
52:5:1779:U:O2	52:5:1783:A:N6	2.54	0.41
52:5:1839:G:H2'	52:5:1839:G:N3	2.35	0.41
52:5:1904:G:O2'	52:5:1928:A:N1	2.48	0.41
52:5:1936:A:H3'	52:5:1937:A:H5'	2.02	0.41
52:5:2114:A:N6	52:5:2117:A:H62	2.19	0.41
1:a:108:G:O6	20:t:9:ARG:NH2	2.53	0.41
1:a:120:A:H1'	1:a:122:G:N7	2.36	0.41
1:a:158:G:N7	1:a:164:G:N1	2.68	0.41
1:a:321:A:H2'	1:a:322:C:C6	2.55	0.41
1:a:1060:U:H2'	1:a:1061:G:H8	1.84	0.41
1:a:1226:C:H2'	13:m:101:THR:HG22	2.02	0.41
3:c:28:PHE:CD1	3:c:28:PHE:C	2.98	0.41
6:f:3:HIS:HB2	6:f:92:THR:HA	2.01	0.41
6:f:8:PHE:N	6:f:8:PHE:CD1	2.89	0.41
10:j:15:HIS:HA	10:j:70:HIS:CE1	2.55	0.41
12:l:33:CYS:HA	12:l:54:VAL:HG22	2.03	0.41
12:l:72:ASN:ND2	12:l:102:ASP:O	2.37	0.41
16:p:53:ASP:O	16:p:57:ILE:HG13	2.20	0.41
17:q:43:LEU:HD11	17:q:72:TRP:CD1	2.55	0.41
17:q:58:VAL:HG12	17:q:59:GLU:N	2.36	0.41
22:A:5:A:H2'	22:A:6:A:C8	2.55	0.41
22:A:19:A:H2'	22:A:20:C:C6	2.55	0.41
22:A:172:A:H2'	22:A:173:A:H8	1.84	0.41
22:A:396:G:C6	22:A:397:U:C4	3.08	0.41
22:A:587:C:H4'	22:A:588:U:H6	1.85	0.41
24:C:1:ALA:O	24:C:2:VAL:C	2.63	0.41
24:C:174:ARG:HB2	24:C:180:MET:SD	2.59	0.41
26:E:61:ARG:NE	26:E:63:LYS:O	2.53	0.41
29:J:80:HIS:O	29:J:81:ILE:C	2.63	0.41
32:M:136:MET:HE3	41:V:57:TYR:CD1	2.55	0.41
37:R:68:ARG:NH1	52:5:1223:G:OP1	2.52	0.41
41:V:75:GLN:OE1	41:V:75:GLN:CA	2.68	0.41
43:X:31:ASN:O	43:X:51:SER:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:X:43:LYS:HA	43:X:43:LYS:HE3	2.02	0.41
43:X:52:ALA:O	43:X:56:ARG:HG3	2.20	0.41
43:X:67:LEU:HD22	43:X:77:TYR:CD1	2.55	0.41
45:Z:4:ILE:HD11	45:Z:56:VAL:HG21	2.00	0.41
52:5:1048:A:C2	52:5:1049:C:C6	3.09	0.41
52:5:1058:U:H2'	52:5:1059:G:O4'	2.20	0.41
52:5:1571:A:H2'	52:5:1572:A:C8	2.55	0.41
52:5:1796:U:H2'	52:5:1797:G:C8	2.55	0.41
52:5:1853:A:H2'	52:5:1854:A:C8	2.56	0.41
52:5:2591:C:H2'	52:5:2592:G:C8	2.56	0.41
52:5:2700:A:H2'	52:5:2701:U:H6	1.85	0.41
1:a:53:A:N6	1:a:359:G:O6	2.54	0.41
1:a:56:U:H2'	1:a:57:G:C8	2.56	0.41
1:a:82:G:H22	1:a:87:C:N4	2.19	0.41
1:a:263:A:OP1	20:t:73:ARG:NH1	2.54	0.41
1:a:411:A:C4	1:a:413:G:H1'	2.55	0.41
3:c:5:HIS:HA	3:c:6:PRO:HD2	1.95	0.41
4:d:28:ASP:C	4:d:29:THR:OG1	2.60	0.41
4:d:196:GLU:C	4:d:196:GLU:CD	2.89	0.41
14:n:54:ASP:O	14:n:56:SER:OG	2.26	0.41
16:p:39:PHE:CD1	16:p:40:ASN:N	2.89	0.41
21:u:36:PHE:HB3	21:u:40:PRO:HD3	2.02	0.41
26:E:76:PRO:HA	26:E:82:GLY:HA3	2.02	0.41
27:F:52:ALA:O	27:F:53:ALA:C	2.63	0.41
27:F:102:LEU:O	27:F:103:ILE:C	2.63	0.41
27:F:136:ILE:HG13	27:F:137:PHE:CD1	2.56	0.41
30:K:41:ILE:HD11	30:K:58:LEU:HD12	2.02	0.41
31:L:78:ARG:HB3	31:L:113:ALA:HB2	2.03	0.41
39:T:34:VAL:CG2	39:T:81:LYS:HG2	2.51	0.41
40:U:31:GLY:C	40:U:66:VAL:HG23	2.46	0.41
43:X:7:THR:OG1	43:X:9:LYS:HG3	2.20	0.41
52:5:2063:C:C2	52:5:2064:C:C6	3.09	0.41
52:5:2455:G:C4	52:5:2456:C:C5	3.08	0.41
52:5:2802:G:H2'	52:5:2803:G:O4'	2.20	0.41
1:a:55:A:C2	1:a:56:U:H1'	2.55	0.41
1:a:918:A:H2'	1:a:919:A:O4'	2.20	0.41
1:a:946:A:H2'	1:a:947:G:C8	2.55	0.41
1:a:1012:A:H2'	1:a:1013:G:O4'	2.20	0.41
2:b:143:LEU:O	2:b:147:LEU:HD23	2.21	0.41
3:c:54:ILE:O	3:c:54:ILE:CG1	2.69	0.41
6:f:42:TRP:CD1	6:f:42:TRP:N	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:67:PRO:HD2	6:f:70:VAL:HG22	2.03	0.41
7:g:50:ALA:O	7:g:53:SER:N	2.51	0.41
14:n:11:LYS:O	14:n:15:LEU:HG	2.20	0.41
15:o:25:GLU:O	15:o:28:VAL:HG12	2.21	0.41
21:u:28:LEU:O	21:u:32:ARG:HG2	2.20	0.41
22:A:144:A:C5'	39:T:2:ILE:HD11	2.51	0.41
22:A:194:G:H2'	22:A:195:A:O4'	2.21	0.41
22:A:591:U:N3	22:A:592:A:N7	2.68	0.41
28:G:148:ARG:HD3	28:G:163:TYR:CZ	2.55	0.41
32:M:96:ILE:HG21	32:M:126:ILE:HD13	2.02	0.41
36:Q:5:ARG:NH1	52:5:1251:C:OP2	2.45	0.41
48:2:3:ARG:HG3	48:2:5:PHE:H	1.86	0.41
50:4:8:LYS:O	50:4:35:GLN:NE2	2.54	0.41
52:5:1070:A:C4'	52:5:1071:G:OP2	2.68	0.41
52:5:2033:A:H1'	52:5:2035:G:OP2	2.19	0.41
1:a:66:A:H4'	1:a:173:U:C4	2.55	0.41
1:a:371:A:C2	1:a:391:G:C2	3.09	0.41
1:a:689:C:OP2	11:k:52:ARG:NH2	2.53	0.41
1:a:1227:A:OP2	13:m:109:LYS:HD2	2.21	0.41
2:b:38:HIS:CD2	2:b:38:HIS:N	2.88	0.41
2:b:102:ASN:O	2:b:105:THR:HG22	2.21	0.41
2:b:202:ASN:OD1	2:b:205:ALA:CB	2.69	0.41
3:c:81:GLU:HA	3:c:84:GLU:OE1	2.21	0.41
4:d:64:TYR:HD2	4:d:93:LEU:HD13	1.85	0.41
6:f:4:TYR:HB3	6:f:89:VAL:HG12	2.01	0.41
6:f:38:ARG:O	6:f:62:MET:O	2.38	0.41
8:h:28:SER:C	8:h:29:SER:HG	2.25	0.41
12:l:9:LYS:HG3	12:l:9:LYS:O	2.19	0.41
12:l:36:VAL:HG22	12:l:52:CYS:HB3	2.02	0.41
13:m:30:LYS:O	13:m:33:LEU:HG	2.21	0.41
13:m:91:ARG:HB3	13:m:92:ARG:NH1	2.36	0.41
15:o:40:GLY:O	15:o:41:HIS:C	2.61	0.41
22:A:243:U:O2	22:A:243:U:H2'	2.21	0.41
25:D:13:ARG:HH21	35:P:55:HIS:HA	1.86	0.41
26:E:72:SER:O	26:E:74:LYS:N	2.53	0.41
27:F:73:VAL:HG12	27:F:75:GLY:H	1.86	0.41
27:F:102:LEU:O	27:F:104:THR:N	2.53	0.41
36:Q:65:ASN:OD1	36:Q:69:ARG:NE	2.52	0.41
52:5:952:G:C6	52:5:966:G:C6	3.08	0.41
52:5:1883:U:H2'	52:5:1884:G:O4'	2.20	0.41
52:5:2051:A:H5'	52:5:2578:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:5:2121:G:H2'	52:5:2122:U:O4'	2.21	0.41
52:5:2146:C:O2'	52:5:2147:A:N7	2.53	0.41
1:a:250:A:O4'	1:a:252:U:C6	2.74	0.41
1:a:665:A:C1'	1:a:733:G:H1'	2.51	0.41
1:a:736:C:OP1	18:r:60:ARG:NH1	2.54	0.41
1:a:1126:U:C5	10:j:73:LEU:HD11	2.55	0.41
1:a:1352:C:H2'	1:a:1353:G:O4'	2.20	0.41
1:a:1405:G:H21	1:a:1518:MA6:H8	1.84	0.41
2:b:14:HIS:ND1	2:b:14:HIS:O	2.54	0.41
2:b:15:PHE:CD2	2:b:39:ILE:HG12	2.55	0.41
2:b:191:ASP:OD1	2:b:191:ASP:N	2.54	0.41
3:c:4:VAL:O	3:c:4:VAL:CG1	2.68	0.41
3:c:122:GLN:O	3:c:127:VAL:HG12	2.20	0.41
4:d:18:LEU:O	4:d:19:PHE:HB2	2.21	0.41
9:i:36:GLN:O	9:i:37:TYR:C	2.63	0.41
11:k:51:PHE:HB3	11:k:55:ARG:HB2	2.02	0.41
13:m:101:THR:O	13:m:101:THR:CG2	2.69	0.41
13:m:103:THR:C	13:m:104:ASN:HD22	2.29	0.41
16:p:11:ALA:O	16:p:12:LYS:C	2.63	0.41
21:u:11:PHE:O	21:u:12:ASP:HB2	2.21	0.41
22:A:3:U:H2'	22:A:4:U:C6	2.55	0.41
22:A:476:G:N1	22:A:479:A:OP2	2.48	0.41
22:A:774:G:O2'	22:A:775:G:P	2.79	0.41
24:C:129:LEU:HD21	24:C:134:ILE:HG12	2.02	0.41
31:L:55:MET:HA	31:L:55:MET:HE3	2.01	0.41
34:O:69:ASP:OD1	34:O:70:ALA:N	2.54	0.41
38:S:51:LEU:HD12	38:S:105:VAL:HG11	2.02	0.41
41:V:21:ARG:HA	41:V:25:LYS:O	2.20	0.41
46:O:4:GLN:O	52:5:2017:U:H4'	2.21	0.41
52:5:1800:C:C2	52:5:1818:U:O2	2.74	0.41
52:5:1990:C:H2'	52:5:1991:U:C1'	2.50	0.41
52:5:1999:C:OP1	52:5:2723:C:O2'	2.37	0.41
1:a:31:G:P	1:a:306:A:C6	3.14	0.41
1:a:86:G:H5''	1:a:87:C:OP1	2.21	0.41
1:a:136:C:H2'	1:a:137:U:O4'	2.21	0.41
1:a:168:G:C6	1:a:169:C:N4	2.89	0.41
1:a:477:C:H2'	1:a:478:A:C8	2.55	0.41
1:a:520:A:C2'	12:l:69:GLU:OE2	2.68	0.41
1:a:557:G:H2'	1:a:558:G:O4'	2.21	0.41
1:a:625:U:H2'	1:a:626:G:C8	2.56	0.41
1:a:872:A:C4	1:a:874:G:N7	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:948:C:C5	13:m:104:ASN:OD1	2.74	0.41
1:a:997:U:O2'	1:a:998:C:H5'	2.21	0.41
1:a:1181:G:H1'	1:a:1182:G:C4	2.56	0.41
1:a:1203:C:OP1	14:n:1:ALA:HA	2.21	0.41
1:a:1522:U:H2'	1:a:1523:G:H8	1.86	0.41
1:a:1524:C:H2'	1:a:1525:G:C8	2.56	0.41
4:d:19:PHE:HB2	4:d:110:ARG:CZ	2.51	0.41
6:f:5:GLU:HG3	6:f:61:LEU:HD11	2.02	0.41
6:f:7:VAL:HG22	6:f:61:LEU:HD13	2.03	0.41
6:f:41:ASP:CG	6:f:60:VAL:HG22	2.46	0.41
6:f:73:GLU:HA	6:f:76:THR:OG1	2.20	0.41
8:h:125:ILE:HG22	8:h:126:CYS:N	2.36	0.41
11:k:91:GLY:O	11:k:93:GLU:N	2.54	0.41
11:k:94:SER:O	11:k:97:ARG:HD2	2.21	0.41
14:n:9:GLU:O	14:n:13:VAL:HG23	2.21	0.41
16:p:67:ILE:HD12	16:p:68:SER:O	2.20	0.41
22:A:144:A:H5''	39:T:2:ILE:HD11	2.01	0.41
22:A:265:A:H4'	22:A:266:G:OP1	2.21	0.41
22:A:299:A:N3	22:A:319:G:O2'	2.44	0.41
22:A:301:G:C6	22:A:317:G:C6	3.08	0.41
22:A:320:A:N3	26:E:163:ASN:ND2	2.68	0.41
22:A:589:U:H2'	22:A:590:A:H8	1.85	0.41
22:A:704:G:H1'	22:A:727:A:H61	1.85	0.41
22:A:850:U:O2'	45:Z:22:THR:OG1	2.26	0.41
22:A:853:C:H2'	22:A:854:C:O4'	2.21	0.41
22:A:871:U:H4'	32:M:68:PHE:CD2	2.56	0.41
23:B:34:A:C2'	23:B:35:C:OP2	2.69	0.41
23:B:88:C:H4'	23:B:89:U:OP1	2.20	0.41
24:C:207:ALA:HB2	52:5:1790:C:O2'	2.21	0.41
27:F:136:ILE:HG13	27:F:137:PHE:N	2.36	0.41
30:K:44:LYS:O	30:K:54:LYS:HE3	2.20	0.41
34:O:67:ASN:O	34:O:68:LYS:C	2.64	0.41
37:R:21:ARG:HA	37:R:95:ASP:OD1	2.21	0.41
38:S:83:LYS:C	38:S:84:ARG:HG2	2.45	0.41
39:T:55:VAL:HG13	39:T:85:VAL:HG12	2.02	0.41
47:1:45:HIS:ND1	52:5:2372:U:O4'	2.54	0.41
50:4:16:ILE:HD13	50:4:25:VAL:HG22	2.02	0.41
52:5:974:G:O4'	52:5:990:A:N6	2.53	0.41
52:5:1223:G:C4	52:5:1225:G:OP2	2.74	0.41
52:5:1715:G:O2'	52:5:1716:U:H6	2.04	0.41
52:5:2061:G:N3	52:5:2063:C:C5	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:5:2678:C:H2'	52:5:2679:A:O4'	2.21	0.41
1:a:49:U:C2	1:a:361:G:N2	2.89	0.41
1:a:305:G:H5''	1:a:306:A:OP1	2.21	0.41
1:a:539:A:H2'	1:a:540:G:O4'	2.21	0.41
1:a:581:G:N1	1:a:759:A:OP2	2.40	0.41
1:a:768:A:H4'	1:a:1523:G:N2	2.36	0.41
1:a:1218:C:H2'	1:a:1219:A:H8	1.85	0.41
2:b:83:ALA:HB1	2:b:88:GLN:O	2.21	0.41
2:b:84:LEU:HD21	2:b:90:PHE:CE1	2.56	0.41
2:b:159:ALA:HB1	2:b:183:PHE:CZ	2.56	0.41
3:c:39:ARG:CB	3:c:54:ILE:HD11	2.51	0.41
3:c:190:THR:C	3:c:192:TYR:N	2.78	0.41
8:h:65:PHE:CD2	8:h:66:GLN:OE1	2.74	0.41
21:u:28:LEU:C	21:u:30:GLU:H	2.27	0.41
22:A:305:C:H2'	22:A:306:U:C6	2.56	0.41
22:A:532:A:H4'	22:A:533:G:C8	2.56	0.41
27:F:140:ILE:HG22	27:F:142:TYR:H	1.85	0.41
52:5:2074:U:H2'	52:5:2075:U:C6	2.56	0.41
52:5:2588:G:O6	52:5:2607:G:C6	2.74	0.41
52:5:2636:C:H2'	52:5:2637:U:C6	2.55	0.41
1:a:151:A:C2	1:a:152:A:H1'	2.56	0.40
1:a:891:U:O2	1:a:892:A:C8	2.74	0.40
1:a:946:A:H2'	1:a:947:G:H8	1.86	0.40
1:a:1432:G:O2'	1:a:1433:A:P	2.79	0.40
1:a:1494:G:C2	1:a:1495:U:C5	3.09	0.40
1:a:1508:A:H2'	1:a:1509:C:O4'	2.21	0.40
1:a:1519:MA6:H5''	1:a:1519:MA6:H8	2.03	0.40
2:b:28:PRO:O	2:b:30:ILE:N	2.54	0.40
4:d:129:VAL:HG12	4:d:130:ASN:N	2.36	0.40
6:f:10:VAL:CG1	6:f:11:HIS:N	2.84	0.40
7:g:128:GLU:OE1	7:g:128:GLU:N	2.41	0.40
8:h:30:LYS:O	8:h:33:VAL:CG2	2.68	0.40
11:k:71:ASP:HA	11:k:74:LYS:HD2	2.03	0.40
13:m:3:ILE:HG22	13:m:56:ARG:HG3	2.03	0.40
15:o:55:LEU:O	15:o:59:VAL:HG23	2.20	0.40
19:s:10:ILE:HD13	19:s:15:LEU:HB2	2.03	0.40
22:A:289:G:H2'	22:A:290:U:O4'	2.21	0.40
22:A:861:A:N3	23:B:79:G:O2'	2.51	0.40
24:C:153:LEU:HD23	52:5:1799:G:N2	2.36	0.40
26:E:29:HIS:O	26:E:33:VAL:HG23	2.22	0.40
29:J:138:GLN:O	29:J:139:VAL:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:N:65:LEU:O	33:N:69:ARG:HG3	2.21	0.40
35:P:36:LYS:HA	35:P:36:LYS:HE2	2.03	0.40
38:S:23:LEU:O	38:S:27:LYS:NZ	2.52	0.40
38:S:69:LEU:HA	38:S:109:ASP:HA	2.02	0.40
40:U:64:ILE:HD11	40:U:68:ASN:HB3	2.02	0.40
44:Y:58:ASN:OD1	44:Y:58:ASN:C	2.64	0.40
52:5:1775:U:O4	52:5:1789:A:H2	2.05	0.40
52:5:1791:A:C2	52:5:1829:A:O4'	2.74	0.40
52:5:2418:A:H2'	52:5:2419:U:O4'	2.21	0.40
52:5:2572:A:H5''	52:5:2574:G:H4'	2.03	0.40
1:a:125:U:O2'	1:a:634:C:O2'	2.00	0.40
1:a:171:A:H2'	1:a:172:A:C8	2.56	0.40
1:a:919:A:C2	1:a:920:U:C5	3.09	0.40
1:a:1251:A:H2'	1:a:1252:A:O4'	2.22	0.40
3:c:148:ILE:CG1	3:c:149:LYS:N	2.84	0.40
4:d:49:ASP:OD1	4:d:49:ASP:C	2.64	0.40
7:g:59:GLU:O	7:g:63:VAL:HG23	2.20	0.40
8:h:109:VAL:O	8:h:109:VAL:HG23	2.21	0.40
11:k:19:VAL:CG1	11:k:84:MET:HE2	2.51	0.40
11:k:59:PRO:O	11:k:60:PHE:C	2.65	0.40
12:l:56:LEU:CB	12:l:58:ASN:OD1	2.69	0.40
17:q:12:VAL:O	17:q:54:ILE:HG13	2.22	0.40
20:t:67:HIS:O	20:t:69:ASN:N	2.54	0.40
22:A:278:A:H2'	22:A:278:A:N3	2.35	0.40
22:A:492:A:H2'	22:A:493:G:O4'	2.22	0.40
22:A:831:G:H2'	22:A:832:U:O4'	2.21	0.40
29:J:106:LYS:HB2	29:J:106:LYS:HE2	1.94	0.40
35:P:6:GLN:OE1	35:P:6:GLN:C	2.63	0.40
45:Z:43:ILE:HD13	45:Z:46:MET:CE	2.52	0.40
52:5:1637:A:H4'	52:5:2711:A:O2'	2.21	0.40
1:a:511:C:O2'	4:d:40:HIS:NE2	2.52	0.40
6:f:53:LYS:O	6:f:54:LEU:O	2.40	0.40
11:k:72:ALA:O	11:k:73:VAL:CG1	2.68	0.40
13:m:56:ARG:NH2	51:6:35:ASP:OD1	2.54	0.40
17:q:15:LYS:O	17:q:15:LYS:HG3	2.20	0.40
22:A:288:U:C2	22:A:289:G:C8	3.09	0.40
22:A:404:A:H1'	22:A:406:G:C4	2.57	0.40
22:A:511:U:H4'	52:5:1235:G:H4'	2.02	0.40
24:C:123:ILE:O	24:C:123:ILE:CG2	2.67	0.40
25:D:11:MET:C	25:D:12:THR:CG2	2.95	0.40
30:K:35:VAL:HG22	30:K:69:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:L:64:PHE:CD2	31:L:64:PHE:C	2.99	0.40
36:Q:57:ARG:HA	36:Q:60:TRP:CE3	2.56	0.40
43:X:29:LEU:HD12	52:5:2230:G:H5''	2.03	0.40
49:3:8:GLY:O	49:3:12:ARG:NH1	2.44	0.40
52:5:1396:U:H5''	52:5:1397:U:OP2	2.21	0.40
1:a:31:G:OP2	1:a:306:A:C6	2.74	0.40
1:a:44:A:C6	1:a:399:G:C6	3.09	0.40
1:a:106:C:H2'	1:a:107:G:C8	2.56	0.40
1:a:107:G:O6	20:t:9:ARG:HD3	2.22	0.40
1:a:125:U:HO2'	1:a:126:G:H5'	1.87	0.40
1:a:450:G:C8	1:a:481:G:O6	2.74	0.40
1:a:509:A:C2	1:a:544:G:O4'	2.74	0.40
1:a:686:U:H2'	1:a:687:A:C8	2.57	0.40
1:a:875:U:O2'	8:h:14:ARG:NH1	2.44	0.40
1:a:935:A:H2'	1:a:936:C:O4'	2.21	0.40
1:a:1210:C:H2'	1:a:1211:U:O4'	2.21	0.40
2:b:19:THR:HG22	2:b:36:LYS:O	2.21	0.40
2:b:167:HIS:HB3	2:b:168:GLU:OE1	2.21	0.40
4:d:178:GLU:OE1	4:d:178:GLU:HA	2.22	0.40
6:f:3:HIS:CD2	6:f:94:HIS:HA	2.57	0.40
13:m:39:ALA:O	13:m:42:VAL:HG22	2.22	0.40
22:A:64:A:H2'	22:A:65:U:C6	2.57	0.40
22:A:754:U:H1'	52:5:1618:6MZ:H2	2.02	0.40
23:B:52:A:O2'	23:B:53:A:C8	2.75	0.40
24:C:83:ASP:OD2	24:C:90:ILE:HD13	2.22	0.40
24:C:241:LYS:O	52:5:1902:C:H4'	2.22	0.40
26:E:52:VAL:O	26:E:74:LYS:HE3	2.21	0.40
28:G:70:LEU:O	28:G:71:LEU:C	2.65	0.40
34:O:4:LYS:O	34:O:8:ILE:HG12	2.22	0.40
40:U:36:GLU:HG3	40:U:36:GLU:O	2.22	0.40
41:V:26:PHE:CE1	41:V:42:LEU:HD11	2.57	0.40
43:X:47:THR:O	43:X:47:THR:HG23	2.21	0.40
52:5:1058:U:H2'	52:5:1059:G:C8	2.56	0.40
52:5:1429:G:H2'	52:5:1430:G:H8	1.85	0.40
52:5:1493:C:H5''	52:5:1494:A:OP2	2.21	0.40
52:5:1715:G:HO2'	52:5:1716:U:P	2.43	0.40
52:5:1790:C:H2'	52:5:1791:A:C8	2.56	0.40
52:5:1932:A:H2'	52:5:1933:G:O4'	2.21	0.40
52:5:2092:U:H4'	52:5:2093:G:O5'	2.22	0.40
52:5:2107:G:C2	52:5:2183:A:C6	3.10	0.40
52:5:2233:U:H2'	52:5:2234:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:5:2454:G:C4	52:5:2455:G:C8	3.10	0.40
1:a:501:C:OP1	12:l:113:ARG:NH2	2.50	0.40
1:a:629:A:H2'	1:a:630:A:O4'	2.22	0.40
1:a:1238:A:H62	1:a:1301:U:H3	1.69	0.40
2:b:8:MET:HE1	2:b:10:LYS:HG2	2.03	0.40
7:g:89:GLU:C	7:g:89:GLU:CD	2.89	0.40
13:m:38:ILE:HD13	13:m:38:ILE:N	2.37	0.40
13:m:95:PRO:C	13:m:96:VAL:CG2	2.95	0.40
16:p:71:VAL:O	16:p:75:ILE:HG13	2.21	0.40
18:r:34:GLU:HB3	21:u:18:PHE:CZ	2.56	0.40
19:s:9:PHE:HE2	19:s:36:ARG:HG3	1.86	0.40
22:A:75:G:C2	22:A:76:C:C5	3.08	0.40
22:A:160:A:N3	52:5:2208:C:O2'	2.51	0.40
24:C:173:LEU:HD12	24:C:183:VAL:HG23	2.04	0.40
24:C:181:ARG:HG2	24:C:182:LYS:N	2.36	0.40
24:C:183:VAL:HG12	24:C:184:GLU:N	2.37	0.40
25:D:51:THR:HB	25:D:79:LEU:HD23	2.04	0.40
30:K:71:ARG:HB3	30:K:72:PRO:HD2	2.03	0.40
34:O:53:THR:HG23	34:O:74:VAL:HG21	2.04	0.40
39:T:51:PHE:O	39:T:52:GLU:C	2.65	0.40
44:Y:2:LYS:HB3	44:Y:52:ARG:HD3	2.04	0.40
44:Y:15:ASN:O	44:Y:16:THR:C	2.64	0.40
51:6:3:LYS:H	51:6:3:LYS:CD	2.34	0.40
52:5:1281:G:H2'	52:5:1282:U:C6	2.57	0.40
52:5:1406:U:C2	52:5:1407:G:C8	3.09	0.40
52:5:2832:U:HO2'	52:5:2833:U:P	2.28	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	216/218 (99%)	176 (82%)	29 (13%)	11 (5%)	1	2
3	c	204/206 (99%)	175 (86%)	22 (11%)	7 (3%)	3	4
4	d	203/205 (99%)	157 (77%)	35 (17%)	11 (5%)	1	1
5	e	155/157 (99%)	123 (79%)	19 (12%)	13 (8%)	0	0
6	f	98/100 (98%)	69 (70%)	17 (17%)	12 (12%)	0	0
7	g	149/151 (99%)	123 (83%)	18 (12%)	8 (5%)	1	1
8	h	127/129 (98%)	102 (80%)	16 (13%)	9 (7%)	1	1
9	i	125/127 (98%)	86 (69%)	32 (26%)	7 (6%)	1	1
10	j	96/98 (98%)	77 (80%)	11 (12%)	8 (8%)	0	0
11	k	114/116 (98%)	86 (75%)	17 (15%)	11 (10%)	0	0
12	l	121/123 (98%)	88 (73%)	28 (23%)	5 (4%)	2	3
13	m	112/114 (98%)	93 (83%)	16 (14%)	3 (3%)	4	7
14	n	96/101 (95%)	74 (77%)	17 (18%)	5 (5%)	1	2
15	o	86/88 (98%)	70 (81%)	12 (14%)	4 (5%)	2	2
16	p	80/82 (98%)	58 (72%)	20 (25%)	2 (2%)	4	8
17	q	78/80 (98%)	59 (76%)	14 (18%)	5 (6%)	1	1
18	r	63/65 (97%)	53 (84%)	6 (10%)	4 (6%)	1	1
19	s	77/79 (98%)	57 (74%)	16 (21%)	4 (5%)	1	2
20	t	83/85 (98%)	73 (88%)	5 (6%)	5 (6%)	1	1
21	u	63/65 (97%)	44 (70%)	16 (25%)	3 (5%)	2	2
24	C	269/271 (99%)	221 (82%)	38 (14%)	10 (4%)	2	3
25	D	207/209 (99%)	178 (86%)	21 (10%)	8 (4%)	2	3
26	E	199/201 (99%)	167 (84%)	28 (14%)	4 (2%)	6	12
27	F	175/177 (99%)	128 (73%)	30 (17%)	17 (10%)	0	0
28	G	174/176 (99%)	145 (83%)	22 (13%)	7 (4%)	2	3
29	J	140/142 (99%)	126 (90%)	8 (6%)	6 (4%)	2	2
30	K	120/122 (98%)	100 (83%)	14 (12%)	6 (5%)	1	2
31	L	141/143 (99%)	114 (81%)	17 (12%)	10 (7%)	1	1
32	M	134/136 (98%)	118 (88%)	14 (10%)	2 (2%)	8	18
33	N	118/120 (98%)	101 (86%)	12 (10%)	5 (4%)	2	3
34	O	114/116 (98%)	101 (89%)	8 (7%)	5 (4%)	2	2
35	P	112/114 (98%)	99 (88%)	12 (11%)	1 (1%)	14	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	Q	115/117 (98%)	111 (96%)	3 (3%)	1 (1%)	14	30
37	R	101/103 (98%)	81 (80%)	15 (15%)	5 (5%)	1	2
38	S	108/110 (98%)	93 (86%)	11 (10%)	4 (4%)	2	3
39	T	91/93 (98%)	80 (88%)	9 (10%)	2 (2%)	5	10
40	U	100/102 (98%)	86 (86%)	10 (10%)	4 (4%)	2	3
41	V	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
42	W	73/75 (97%)	68 (93%)	3 (4%)	2 (3%)	4	7
43	X	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
44	Y	61/63 (97%)	53 (87%)	6 (10%)	2 (3%)	3	5
45	Z	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
46	0	54/56 (96%)	48 (89%)	4 (7%)	2 (4%)	2	3
47	1	48/50 (96%)	40 (83%)	6 (12%)	2 (4%)	2	3
48	2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
49	3	62/64 (97%)	54 (87%)	6 (10%)	2 (3%)	3	5
50	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
51	6	64/66 (97%)	46 (72%)	17 (27%)	1 (2%)	7	16
All	All	5429/5528 (98%)	4480 (82%)	704 (13%)	245 (4%)	3	2

All (245) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	14	HIS
2	b	73	ARG
2	b	87	ASP
2	b	124	THR
4	d	74	TYR
5	e	70	MET
5	e	77	ASN
6	f	14	GLN
6	f	18	VAL
6	f	92	THR
8	h	70	VAL
8	h	71	VAL
8	h	95	MET
9	i	42	THR
10	j	57	VAL

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Mol	Chain	Res	Type
11	k	35	ASP
11	k	51	PHE
14	n	38	ASP
16	p	8	ARG
18	r	17	VAL
18	r	33	THR
19	s	78	THR
20	t	67	HIS
25	D	91	THR
25	D	101	PHE
27	F	52	ALA
27	F	53	ALA
27	F	58	ALA
27	F	59	ILE
27	F	107	VAL
27	F	120	SER
27	F	142	TYR
27	F	171	ALA
28	G	108	PHE
29	J	81	ILE
29	J	134	ALA
29	J	139	VAL
30	K	14	SER
30	K	89	ASN
30	K	110	GLU
31	L	111	ILE
34	O	43	ASN
37	R	8	GLY
38	S	12	SER
38	S	63	GLY
39	T	38	ALA
40	U	74	ALA
47	1	30	PRO
49	3	33	THR
51	6	18	CYS
2	b	19	THR
2	b	28	PRO
2	b	29	PHE
2	b	182	VAL
3	c	90	VAL
3	c	127	VAL
4	d	23	GLY

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Mol	Chain	Res	Type
4	d	28	ASP
4	d	85	THR
4	d	101	VAL
4	d	117	VAL
5	e	23	THR
5	e	122	VAL
6	f	54	LEU
6	f	94	HIS
7	g	30	MET
7	g	42	VAL
8	h	65	PHE
8	h	88	LYS
9	i	47	VAL
9	i	57	VAL
9	i	106	ASP
10	j	88	MET
11	k	14	GLN
11	k	91	GLY
11	k	103	GLY
12	l	101	LEU
13	m	11	HIS
14	n	13	VAL
14	n	54	ASP
17	q	49	ASN
18	r	50	TYR
20	t	34	VAL
20	t	68	LYS
21	u	37	TYR
24	C	204	LEU
24	C	227	VAL
25	D	16	THR
25	D	98	VAL
26	E	73	ILE
27	F	103	ILE
27	F	116	LEU
28	G	44	HIS
30	K	58	LEU
31	L	29	LYS
31	L	36	LYS
31	L	82	LEU
31	L	87	GLY
34	O	34	HIS

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Mol	Chain	Res	Type
35	P	65	ASN
36	Q	86	SER
38	S	3	THR
39	T	37	ASP
40	U	6	ARG
40	U	97	SER
42	W	71	LYS
44	Y	25	GLN
47	1	31	GLU
49	3	34	LYS
3	c	191	THR
4	d	39	GLN
4	d	152	SER
5	e	99	SER
6	f	19	PRO
6	f	33	GLU
6	f	67	PRO
6	f	86	ARG
7	g	16	LYS
7	g	43	TYR
7	g	50	ALA
7	g	145	GLU
8	h	47	ASP
8	h	67	GLY
9	i	37	TYR
9	i	95	SER
10	j	75	ASP
11	k	76	TYR
11	k	88	PRO
11	k	92	ARG
12	l	2	THR
12	l	27	PRO
12	l	77	SER
13	m	113	LYS
14	n	5	MET
14	n	55	SER
15	o	2	LEU
15	o	45	HIS
15	o	87	ARG
17	q	28	VAL
19	s	6	LYS
20	t	35	TYR

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Mol	Chain	Res	Type
24	C	2	VAL
27	F	8	LYS
27	F	90	LEU
27	F	176	PHE
28	G	45	ALA
28	G	58	ALA
28	G	70	LEU
28	G	153	PRO
30	K	75	SER
33	N	39	PRO
33	N	40	LYS
33	N	70	THR
33	N	116	VAL
33	N	118	ARG
34	O	42	PRO
37	R	48	LYS
38	S	89	ALA
40	U	99	SER
42	W	70	PRO
46	0	2	VAL
46	0	44	ALA
4	d	73	ASN
4	d	139	ASN
5	e	11	GLN
5	e	50	GLY
5	e	87	VAL
5	e	93	VAL
5	e	160	VAL
6	f	98	GLU
10	j	35	GLN
10	j	56	HIS
11	k	73	VAL
11	k	95	THR
12	l	41	PRO
17	q	17	GLU
17	q	79	GLU
18	r	46	THR
19	s	5	LYS
19	s	75	PRO
20	t	46	ALA
21	u	34	ARG
24	C	106	PRO

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Mol	Chain	Res	Type
24	C	147	PRO
27	F	174	PHE
29	J	28	LEU
31	L	128	THR
32	M	6	ARG
37	R	54	VAL
44	Y	24	GLU
2	b	77	GLU
3	c	2	GLN
3	c	75	VAL
4	d	20	LEU
5	e	88	HIS
6	f	12	PRO
6	f	96	VAL
7	g	84	TYR
10	j	36	VAL
10	j	89	ARG
11	k	125	LYS
24	C	120	ASP
24	C	229	HIS
25	D	149	ASN
26	E	83	VAL
26	E	89	PRO
27	F	106	ALA
28	G	127	GLN
29	J	35	ARG
3	c	60	ALA
5	e	27	GLY
7	g	51	GLN
8	h	33	VAL
8	h	38	VAL
27	F	60	SER
29	J	36	LEU
31	L	15	ALA
31	L	105	ILE
31	L	139	GLY
34	O	115	LEU
37	R	70	GLU
3	c	38	VAL
21	u	9	GLU
24	C	31	PRO
24	C	246	PRO

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Mol	Chain	Res	Type
27	F	175	PRO
37	R	38	VAL
2	b	192	PRO
15	o	28	VAL
16	p	64	GLY
25	D	60	VAL
25	D	78	GLY
25	D	104	VAL
26	E	186	VAL
30	K	38	ILE
2	b	200	PRO
32	M	69	PRO
5	e	41	GLY
17	q	20	ILE
24	C	112	GLY
34	O	66	GLY
9	i	66	VAL
10	j	42	LEU
13	m	96	VAL
31	L	73	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	180/180 (100%)	160 (89%)	20 (11%)	6	12
3	c	170/170 (100%)	157 (92%)	13 (8%)	12	27
4	d	172/172 (100%)	158 (92%)	14 (8%)	11	24
5	e	114/119 (96%)	104 (91%)	10 (9%)	9	21
6	f	87/87 (100%)	71 (82%)	16 (18%)	1	3
7	g	124/124 (100%)	118 (95%)	6 (5%)	23	47
8	h	104/104 (100%)	81 (78%)	23 (22%)	1	2
9	i	105/105 (100%)	98 (93%)	7 (7%)	15	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	j	86/86 (100%)	81 (94%)	5 (6%)	18	39
11	k	89/89 (100%)	75 (84%)	14 (16%)	2	4
12	l	103/103 (100%)	98 (95%)	5 (5%)	22	47
13	m	92/92 (100%)	79 (86%)	13 (14%)	3	6
14	n	79/83 (95%)	69 (87%)	10 (13%)	4	9
15	o	76/76 (100%)	64 (84%)	12 (16%)	2	4
16	p	65/65 (100%)	61 (94%)	4 (6%)	16	36
17	q	74/74 (100%)	68 (92%)	6 (8%)	11	24
18	r	48/56 (86%)	41 (85%)	7 (15%)	3	6
19	s	70/70 (100%)	63 (90%)	7 (10%)	7	16
20	t	65/65 (100%)	57 (88%)	8 (12%)	4	9
21	u	44/55 (80%)	40 (91%)	4 (9%)	9	19
24	C	216/216 (100%)	198 (92%)	18 (8%)	10	23
25	D	164/164 (100%)	147 (90%)	17 (10%)	7	14
26	E	165/165 (100%)	147 (89%)	18 (11%)	6	13
27	F	148/148 (100%)	135 (91%)	13 (9%)	9	21
28	G	137/137 (100%)	116 (85%)	21 (15%)	3	5
29	J	116/116 (100%)	99 (85%)	17 (15%)	3	6
30	K	103/103 (100%)	86 (84%)	17 (16%)	2	4
31	L	102/102 (100%)	95 (93%)	7 (7%)	14	32
32	M	109/109 (100%)	97 (89%)	12 (11%)	6	13
33	N	100/100 (100%)	94 (94%)	6 (6%)	17	37
34	O	86/86 (100%)	78 (91%)	8 (9%)	8	18
35	P	99/99 (100%)	87 (88%)	12 (12%)	5	10
36	Q	89/89 (100%)	86 (97%)	3 (3%)	32	60
37	R	84/84 (100%)	78 (93%)	6 (7%)	13	31
38	S	93/93 (100%)	85 (91%)	8 (9%)	10	22
39	T	80/80 (100%)	69 (86%)	11 (14%)	3	7
40	U	83/83 (100%)	76 (92%)	7 (8%)	10	23
41	V	78/78 (100%)	71 (91%)	7 (9%)	9	20
42	W	57/57 (100%)	50 (88%)	7 (12%)	4	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	X	67/67 (100%)	62 (92%)	5 (8%)	12	28
44	Y	55/55 (100%)	50 (91%)	5 (9%)	9	19
45	Z	48/48 (100%)	46 (96%)	2 (4%)	26	52
46	0	47/47 (100%)	44 (94%)	3 (6%)	16	35
47	1	45/45 (100%)	40 (89%)	5 (11%)	6	12
48	2	38/38 (100%)	35 (92%)	3 (8%)	11	26
49	3	51/51 (100%)	49 (96%)	2 (4%)	28	55
50	4	34/34 (100%)	33 (97%)	1 (3%)	37	65
51	6	59/59 (100%)	56 (95%)	3 (5%)	21	45
All	All	4500/4528 (99%)	4052 (90%)	448 (10%)	9	16

All (448) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	9	LEU
2	b	19	THR
2	b	20	ARG
2	b	29	PHE
2	b	40	ILE
2	b	48	MET
2	b	73	ARG
2	b	77	GLU
2	b	94	ARG
2	b	101	THR
2	b	111	LYS
2	b	124	THR
2	b	129	THR
2	b	132	GLU
2	b	141	GLU
2	b	158	ASP
2	b	169	HIS
2	b	188	THR
2	b	204	ASP
2	b	210	THR
3	c	15	LYS
3	c	27	GLU
3	c	42	LEU
3	c	46	LEU
3	c	54	ILE

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Mol	Chain	Res	Type
3	c	85	LYS
3	c	86	LEU
3	c	87	ARG
3	c	96	VAL
3	c	109	GLU
3	c	149	LYS
3	c	184	ASN
3	c	197	VAL
4	d	9	LYS
4	d	10	LEU
4	d	25	ARG
4	d	27	ILE
4	d	54	LEU
4	d	56	GLU
4	d	63	ILE
4	d	77	GLU
4	d	90	LEU
4	d	98	ASP
4	d	99	ASN
4	d	139	ASN
4	d	168	THR
4	d	173	ASP
5	e	29	ILE
5	e	51	LYS
5	e	55	VAL
5	e	75	LEU
5	e	105	ILE
5	e	110	MET
5	e	116	VAL
5	e	122	VAL
5	e	140	ILE
5	e	158	LYS
6	f	7	VAL
6	f	8	PHE
6	f	22	ILE
6	f	24	ARG
6	f	45	ARG
6	f	54	LEU
6	f	58	HIS
6	f	62	MET
6	f	71	ILE
6	f	74	LEU

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Mol	Chain	Res	Type
6	f	76	THR
6	f	79	ARG
6	f	81	ASN
6	f	89	VAL
6	f	97	THR
6	f	98	GLU
7	g	28	ILE
7	g	48	THR
7	g	52	ARG
7	g	118	ARG
7	g	123	LEU
7	g	148	LYS
8	h	4	ASP
8	h	10	LEU
8	h	11	THR
8	h	13	ILE
8	h	30	LYS
8	h	31	LEU
8	h	35	ILE
8	h	37	ASN
8	h	41	GLU
8	h	45	ILE
8	h	54	THR
8	h	55	LYS
8	h	58	LEU
8	h	64	TYR
8	h	65	PHE
8	h	66	GLN
8	h	68	LYS
8	h	82	LEU
8	h	84	ILE
8	h	89	ASP
8	h	94	VAL
8	h	113	ARG
8	h	124	ILE
9	i	17	ARG
9	i	40	ARG
9	i	64	ILE
9	i	66	VAL
9	i	83	THR
9	i	97	LEU
9	i	106	ASP

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Mol	Chain	Res	Type
10	j	15	HIS
10	j	16	ARG
10	j	17	LEU
10	j	32	THR
10	j	51	VAL
11	k	22	ILE
11	k	31	VAL
11	k	33	ILE
11	k	35	ASP
11	k	36	ARG
11	k	37	GLN
11	k	49	SER
11	k	73	VAL
11	k	74	LYS
11	k	81	LEU
11	k	84	MET
11	k	92	ARG
11	k	109	ILE
11	k	118	ASN
12	l	8	ARG
12	l	17	LYS
12	l	81	ILE
12	l	82	ARG
12	l	88	ASP
13	m	6	ILE
13	m	10	ASP
13	m	15	VAL
13	m	18	LEU
13	m	27	THR
13	m	57	ASP
13	m	64	VAL
13	m	69	ARG
13	m	76	ILE
13	m	80	MET
13	m	97	ARG
13	m	99	GLN
13	m	107	THR
14	n	15	LEU
14	n	19	TYR
14	n	25	GLU
14	n	30	ILE
14	n	49	GLN

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Mol	Chain	Res	Type
14	n	60	GLN
14	n	66	GLN
14	n	90	ARG
14	n	92	GLU
14	n	97	LYS
15	o	7	THR
15	o	28	VAL
15	o	32	THR
15	o	44	GLU
15	o	56	LEU
15	o	57	ARG
15	o	63	ARG
15	o	64	LYS
15	o	73	ASP
15	o	83	ARG
15	o	84	LEU
15	o	86	LEU
16	p	18	GLN
16	p	26	ASN
16	p	59	HIS
16	p	63	GLN
17	q	16	MET
17	q	32	ILE
17	q	43	LEU
17	q	48	GLU
17	q	50	ASN
17	q	61	ARG
18	r	27	THR
18	r	29	LYS
18	r	32	ILE
18	r	33	THR
18	r	44	THR
18	r	54	LEU
18	r	71	ASP
19	s	14	LEU
19	s	24	SER
19	s	33	TRP
19	s	35	ARG
19	s	63	ASP
19	s	69	LYS
19	s	78	THR
20	t	3	ILE

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Mol	Chain	Res	Type
20	t	29	THR
20	t	30	PHE
20	t	48	LYS
20	t	56	ILE
20	t	63	LYS
20	t	82	ILE
20	t	84	LYS
21	u	5	VAL
21	u	16	ARG
21	u	19	LYS
21	u	52	VAL
24	C	19	VAL
24	C	22	GLU
24	C	34	GLU
24	C	35	LYS
24	C	83	ASP
24	C	85	ASN
24	C	107	LYS
24	C	117	SER
24	C	129	LEU
24	C	138	SER
24	C	174	ARG
24	C	181	ARG
24	C	196	ASN
24	C	198	GLU
24	C	201	LEU
24	C	245	THR
24	C	261	ARG
24	C	263	ASP
25	D	2	ILE
25	D	11	MET
25	D	22	ILE
25	D	32	ASN
25	D	35	THR
25	D	48	ILE
25	D	50	VAL
25	D	52	THR
25	D	77	ARG
25	D	91	THR
25	D	98	VAL
25	D	99	GLU
25	D	121	THR

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Mol	Chain	Res	Type
25	D	133	THR
25	D	149	ASN
25	D	151	THR
25	D	157	LYS
26	E	4	VAL
26	E	14	VAL
26	E	17	THR
26	E	19	PHE
26	E	48	THR
26	E	53	THR
26	E	57	LYS
26	E	63	LYS
26	E	96	VAL
26	E	102	ARG
26	E	115	GLN
26	E	121	VAL
26	E	146	VAL
26	E	167	VAL
26	E	169	VAL
26	E	178	VAL
26	E	187	VAL
26	E	188	MET
27	F	4	HIS
27	F	9	ASP
27	F	24	VAL
27	F	39	VAL
27	F	56	LEU
27	F	67	THR
27	F	76	PHE
27	F	89	THR
27	F	95	MET
27	F	105	ILE
27	F	148	VAL
27	F	149	ARG
27	F	151	LEU
28	G	10	VAL
28	G	16	VAL
28	G	33	THR
28	G	40	VAL
28	G	41	GLU
28	G	48	THR
28	G	49	LEU

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Mol	Chain	Res	Type
28	G	50	THR
28	G	68	ARG
28	G	75	VAL
28	G	76	ILE
28	G	78	VAL
28	G	79	THR
28	G	86	LEU
28	G	91	VAL
28	G	112	VAL
28	G	131	VAL
28	G	138	GLN
28	G	140	ILE
28	G	153	PRO
28	G	168	VAL
29	J	3	THR
29	J	5	THR
29	J	8	PRO
29	J	11	VAL
29	J	12	LYS
29	J	18	VAL
29	J	30	THR
29	J	43	GLU
29	J	56	VAL
29	J	57	LEU
29	J	64	VAL
29	J	70	THR
29	J	88	THR
29	J	93	ILE
29	J	95	ARG
29	J	106	LYS
29	J	124	VAL
30	K	6	THR
30	K	7	MET
30	K	19	VAL
30	K	38	ILE
30	K	48	PRO
30	K	52	VAL
30	K	54	LYS
30	K	57	VAL
30	K	59	LYS
30	K	69	VAL
30	K	76	VAL

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Mol	Chain	Res	Type
30	K	92	GLU
30	K	97	THR
30	K	103	VAL
30	K	104	THR
30	K	106	GLU
30	K	118	LEU
31	L	27	LEU
31	L	63	LYS
31	L	120	VAL
31	L	121	THR
31	L	122	VAL
31	L	129	LYS
31	L	136	GLU
32	M	1	MET
32	M	6	ARG
32	M	10	ARG
32	M	20	LEU
32	M	47	GLU
32	M	57	VAL
32	M	67	VAL
32	M	78	LEU
32	M	81	ARG
32	M	93	VAL
32	M	110	GLU
32	M	124	LEU
33	N	2	ARG
33	N	12	ARG
33	N	18	GLN
33	N	53	THR
33	N	69	ARG
33	N	74	GLU
34	O	5	SER
34	O	10	ARG
34	O	25	ARG
34	O	36	TYR
34	O	43	ASN
34	O	46	GLU
34	O	76	LYS
34	O	104	GLN
35	P	10	GLU
35	P	11	GLN
35	P	26	GLU

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Mol	Chain	Res	Type
35	P	27	VAL
35	P	31	VAL
35	P	36	LYS
35	P	60	VAL
35	P	69	VAL
35	P	85	VAL
35	P	87	ARG
35	P	101	GLU
35	P	102	ARG
36	Q	3	VAL
36	Q	87	VAL
36	Q	99	VAL
37	R	16	GLU
37	R	47	VAL
37	R	54	VAL
37	R	63	VAL
37	R	72	VAL
37	R	73	LYS
38	S	11	ARG
38	S	24	ILE
38	S	27	LYS
38	S	29	VAL
38	S	46	LEU
38	S	62	ASP
38	S	68	ASP
38	S	76	VAL
39	T	6	ARG
39	T	12	ARG
39	T	32	LEU
39	T	33	LYS
39	T	48	GLN
39	T	49	LYS
39	T	63	VAL
39	T	74	ILE
39	T	85	VAL
39	T	86	THR
39	T	88	LYS
40	U	35	VAL
40	U	36	GLU
40	U	58	VAL
40	U	61	GLU
40	U	90	LYS

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Mol	Chain	Res	Type
40	U	92	VAL
40	U	93	ARG
41	V	40	ILE
41	V	42	LEU
41	V	51	GLN
41	V	71	LYS
41	V	73	LYS
41	V	83	LYS
41	V	85	LYS
42	W	7	ARG
42	W	10	ARG
42	W	20	LYS
42	W	35	ARG
42	W	64	LYS
42	W	71	LYS
42	W	76	ILE
43	X	36	ARG
43	X	39	VAL
43	X	44	ARG
43	X	55	MET
43	X	70	LEU
44	Y	11	VAL
44	Y	31	GLN
44	Y	43	LEU
44	Y	54	LYS
44	Y	57	LEU
45	Z	4	ILE
45	Z	54	VAL
46	0	28	SER
46	0	36	LYS
46	0	43	THR
47	1	4	ILE
47	1	11	VAL
47	1	13	SER
47	1	42	VAL
47	1	45	HIS
48	2	3	ARG
48	2	22	MET
48	2	29	GLN
49	3	28	LEU
49	3	38	LYS
50	4	24	ARG

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Mol	Chain	Res	Type
51	6	17	SER
51	6	35	ASP
51	6	45	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	17	HIS
2	b	35	ASN
2	b	38	HIS
2	b	108	GLN
3	c	7	ASN
3	c	18	ASN
3	c	68	HIS
3	c	99	GLN
3	c	101	ASN
4	d	39	GLN
4	d	70	GLN
4	d	99	ASN
4	d	115	GLN
4	d	151	GLN
5	e	18	ASN
5	e	88	HIS
5	e	121	ASN
7	g	67	ASN
8	h	3	GLN
9	i	4	GLN
11	k	23	HIS
11	k	27	ASN
11	k	37	GLN
11	k	118	ASN
12	l	95	HIS
13	m	7	ASN
13	m	11	HIS
13	m	13	HIS
13	m	104	ASN
14	n	66	GLN
15	o	36	ASN
15	o	49	HIS
16	p	18	GLN
16	p	40	ASN
17	q	8	GLN

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Mol	Chain	Res	Type
17	q	50	ASN
19	s	13	HIS
19	s	42	ASN
20	t	20	ASN
24	C	44	ASN
24	C	45	ASN
24	C	116	GLN
24	C	152	GLN
24	C	238	ASN
25	D	42	ASN
25	D	126	ASN
25	D	130	GLN
25	D	149	ASN
25	D	164	GLN
25	D	173	GLN
25	D	185	ASN
26	E	41	GLN
26	E	62	GLN
26	E	94	GLN
26	E	115	GLN
27	F	4	HIS
27	F	51	ASN
28	G	29	ASN
28	G	37	ASN
29	J	128	ASN
30	K	5	GLN
30	K	9	ASN
30	K	29	HIS
30	K	88	ASN
32	M	3	GLN
32	M	22	GLN
33	N	62	ASN
34	O	19	GLN
34	O	29	HIS
34	O	38	GLN
34	O	43	ASN
36	Q	36	GLN
36	Q	55	GLN
36	Q	70	GLN
36	Q	71	ASN
37	R	11	GLN
37	R	89	HIS

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Mol	Chain	Res	Type
38	S	9	HIS
38	S	31	GLN
38	S	60	HIS
38	S	61	ASN
39	T	15	HIS
39	T	48	GLN
40	U	45	GLN
40	U	65	GLN
40	U	68	ASN
43	X	35	HIS
51	6	33	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1538/1539 (99%)	241 (15%)	0
22	A	885/886 (99%)	145 (16%)	19 (2%)
23	B	119/120 (99%)	15 (12%)	4 (3%)
52	5	2013/2014 (99%)	326 (16%)	28 (1%)
All	All	4555/4559 (99%)	727 (15%)	51 (1%)

All (727) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	6	G
1	a	7	A
1	a	9	G
1	a	22	G
1	a	31	G
1	a	32	A
1	a	39	G
1	a	47	C
1	a	48	C
1	a	49	U
1	a	50	A
1	a	51	A
1	a	61	G
1	a	71	A
1	a	78	A
1	a	80	A
1	a	81	A

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Mol	Chain	Res	Type
1	a	85	U
1	a	86	G
1	a	87	C
1	a	95	C
1	a	104	G
1	a	121	U
1	a	130	A
1	a	144	G
1	a	163	C
1	a	169	C
1	a	173	U
1	a	181	A
1	a	183	C
1	a	184	G
1	a	197	A
1	a	199	A
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	226	G
1	a	240	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	266	G
1	a	267	C
1	a	281	G
1	a	283	U
1	a	289	G
1	a	305	G
1	a	306	A
1	a	321	A
1	a	328	C
1	a	329	A
1	a	345	C
1	a	347	G
1	a	351	G
1	a	352	C
1	a	354	G
1	a	355	C
1	a	363	A

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Mol	Chain	Res	Type
1	a	367	U
1	a	372	C
1	a	373	A
1	a	378	G
1	a	388	G
1	a	392	C
1	a	397	A
1	a	406	G
1	a	412	A
1	a	413	G
1	a	414	A
1	a	421	U
1	a	422	C
1	a	423	G
1	a	424	G
1	a	429	U
1	a	439	U
1	a	449	G
1	a	467	U
1	a	482	A
1	a	484	G
1	a	485	U
1	a	486	U
1	a	496	A
1	a	497	G
1	a	505	G
1	a	511	C
1	a	531	U
1	a	532	A
1	a	533	A
1	a	536	C
1	a	547	A
1	a	550	G
1	a	559	A
1	a	561	U
1	a	562	U
1	a	564	C
1	a	572	A
1	a	573	A
1	a	575	G
1	a	576	C
1	a	577	G

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Mol	Chain	Res	Type
1	a	596	A
1	a	626	G
1	a	633	G
1	a	642	A
1	a	653	U
1	a	665	A
1	a	671	G
1	a	688	G
1	a	703	G
1	a	704	A
1	a	723	U
1	a	724	G
1	a	731	G
1	a	748	G
1	a	754	C
1	a	755	G
1	a	777	A
1	a	794	A
1	a	815	A
1	a	817	C
1	a	818	G
1	a	819	A
1	a	820	U
1	a	832	G
1	a	843	U
1	a	844	G
1	a	846	G
1	a	871	U
1	a	890	G
1	a	891	U
1	a	902	G
1	a	914	A
1	a	926	G
1	a	934	C
1	a	935	A
1	a	960	U
1	a	961	U
1	a	966	2MG
1	a	969	A
1	a	975	A
1	a	976	G
1	a	977	A

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Mol	Chain	Res	Type
1	a	979	C
1	a	991	U
1	a	992	U
1	a	993	G
1	a	1004	A
1	a	1026	G
1	a	1029	U
1	a	1030	U
1	a	1031	C
1	a	1033	G
1	a	1034	G
1	a	1035	A
1	a	1053	G
1	a	1056	U
1	a	1065	U
1	a	1085	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1127	G
1	a	1129	C
1	a	1130	A
1	a	1136	C
1	a	1137	C
1	a	1138	G
1	a	1139	G
1	a	1140	C
1	a	1152	A
1	a	1158	C
1	a	1159	U
1	a	1168	U
1	a	1183	U
1	a	1184	G
1	a	1191	A
1	a	1196	A
1	a	1197	A
1	a	1200	C
1	a	1201	A
1	a	1202	U
1	a	1207	2MG
1	a	1212	U
1	a	1213	A

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Mol	Chain	Res	Type
1	a	1225	A
1	a	1226	C
1	a	1227	A
1	a	1236	A
1	a	1238	A
1	a	1240	U
1	a	1241	G
1	a	1253	G
1	a	1256	A
1	a	1257	A
1	a	1258	G
1	a	1260	G
1	a	1278	G
1	a	1279	G
1	a	1280	A
1	a	1282	C
1	a	1286	U
1	a	1287	A
1	a	1297	G
1	a	1298	U
1	a	1300	G
1	a	1301	U
1	a	1302	C
1	a	1306	A
1	a	1317	C
1	a	1320	C
1	a	1323	G
1	a	1331	G
1	a	1332	A
1	a	1346	A
1	a	1347	G
1	a	1348	U
1	a	1353	G
1	a	1363	A
1	a	1395	C
1	a	1400	C
1	a	1401	G
1	a	1419	G
1	a	1429	A
1	a	1432	G
1	a	1433	A
1	a	1446	A

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Mol	Chain	Res	Type
1	a	1452	C
1	a	1492	A
1	a	1494	G
1	a	1497	G
1	a	1502	A
1	a	1506	U
1	a	1517	G
1	a	1519	MA6
1	a	1529	G
1	a	1530	G
1	a	1533	C
1	a	1534	A
1	a	1535	C
1	a	1536	C
22	A	10	A
22	A	12	U
22	A	15	G
22	A	34	U
22	A	35	G
22	A	36	G
22	A	46	G
22	A	49	A
22	A	51	G
22	A	52	A
22	A	60	G
22	A	71	A
22	A	74	A
22	A	75	G
22	A	91	A
22	A	92	U
22	A	102	U
22	A	118	A
22	A	119	A
22	A	120	U
22	A	125	A
22	A	138	U
22	A	139	U
22	A	140	C
22	A	141	G
22	A	142	A
22	A	149	A
22	A	158	U

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Mol	Chain	Res	Type
22	A	162	U
22	A	163	C
22	A	181	A
22	A	196	A
22	A	199	A
22	A	215	G
22	A	216	A
22	A	219	A
22	A	221	A
22	A	222	A
22	A	223	A
22	A	225	C
22	A	228	C
22	A	232	G
22	A	242	G
22	A	243	U
22	A	248	G
22	A	255	A
22	A	266	G
22	A	267	C
22	A	272	A
22	A	276	U
22	A	277	G
22	A	278	A
22	A	281	C
22	A	294	A
22	A	311	A
22	A	323	C
22	A	324	A
22	A	329	G
22	A	330	A
22	A	361	G
22	A	362	A
22	A	371	A
22	A	372	G
22	A	373	U
22	A	386	G
22	A	387	U
22	A	391	A
22	A	395	U
22	A	404	A
22	A	406	G

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Mol	Chain	Res	Type
22	A	411	G
22	A	412	A
22	A	417	C
22	A	422	A
22	A	424	G
22	A	451	U
22	A	456	C
22	A	457	A
22	A	458	G
22	A	459	U
22	A	473	G
22	A	480	A
22	A	481	G
22	A	491	G
22	A	504	A
22	A	505	A
22	A	508	A
22	A	509	C
22	A	530	G
22	A	531	C
22	A	532	A
22	A	543	G
22	A	544	C
22	A	545	U
22	A	547	A
22	A	550	C
22	A	556	A
22	A	563	A
22	A	573	U
22	A	575	A
22	A	603	A
22	A	614	A
22	A	615	U
22	A	616	A
22	A	627	A
22	A	637	A
22	A	645	C
22	A	646	U
22	A	647	G
22	A	654	A
22	A	655	A
22	A	668	A

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Mol	Chain	Res	Type
22	A	669	G
22	A	670	A
22	A	677	A
22	A	685	A
22	A	686	U
22	A	694	U
22	A	695	G
22	A	726	G
22	A	730	A
22	A	738	G
22	A	747	5MC
22	A	752	A
22	A	753	A
22	A	765	C
22	A	775	G
22	A	776	G
22	A	782	A
22	A	784	G
22	A	785	G
22	A	789	A
22	A	805	G
22	A	812	C
22	A	819	A
22	A	827	U
22	A	828	U
22	A	830	G
22	A	845	A
22	A	846	U
22	A	847	U
22	A	858	G
22	A	859	G
22	A	860	U
22	A	878	A
23	B	4	C
23	B	9	G
23	B	13	G
23	B	30	C
23	B	35	C
23	B	42	C
23	B	44	G
23	B	45	A
23	B	53	A

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Mol	Chain	Res	Type
23	B	67	G
23	B	89	U
23	B	90	C
23	B	91	C
23	B	108	A
23	B	109	A
52	5	896	A
52	5	897	C
52	5	902	C
52	5	907	G
52	5	910	A
52	5	914	G
52	5	932	U
52	5	941	A
52	5	946	C
52	5	953	G
52	5	961	C
52	5	974	G
52	5	975	A
52	5	983	A
52	5	995	C
52	5	996	A
52	5	999	U
52	5	1005	C
52	5	1012	U
52	5	1013	C
52	5	1021	A
52	5	1023	U
52	5	1026	G
52	5	1033	U
52	5	1045	C
52	5	1046	A
52	5	1053	C
52	5	1054	A
52	5	1057	A
52	5	1059	G
52	5	1060	U
52	5	1061	U
52	5	1062	G
52	5	1064	C
52	5	1065	U
52	5	1066	U

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Mol	Chain	Res	Type
52	5	1068	G
52	5	1069	A
52	5	1070	A
52	5	1071	G
52	5	1075	C
52	5	1076	C
52	5	1079	C
52	5	1084	A
52	5	1088	A
52	5	1090	A
52	5	1104	C
52	5	1111	A
52	5	1112	G
52	5	1119	U
52	5	1130	U
52	5	1131	G
52	5	1132	U
52	5	1135	C
52	5	1174	U
52	5	1175	A
52	5	1176	U
52	5	1177	G
52	5	1179	G
52	5	1180	U
52	5	1204	A
52	5	1206	G
52	5	1211	C
52	5	1212	G
52	5	1227	G
52	5	1237	A
52	5	1248	G
52	5	1250	G
52	5	1253	A
52	5	1256	G
52	5	1271	G
52	5	1272	A
52	5	1273	U
52	5	1300	G
52	5	1301	A
52	5	1321	A
52	5	1329	U
52	5	1330	C

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Mol	Chain	Res	Type
52	5	1341	G
52	5	1345	C
52	5	1352	U
52	5	1365	A
52	5	1368	G
52	5	1378	A
52	5	1379	U
52	5	1383	A
52	5	1395	A
52	5	1396	U
52	5	1397	U
52	5	1416	G
52	5	1419	A
52	5	1420	A
52	5	1428	C
52	5	1453	A
52	5	1454	C
52	5	1456	G
52	5	1459	G
52	5	1461	C
52	5	1476	U
52	5	1482	G
52	5	1483	G
52	5	1490	A
52	5	1491	G
52	5	1504	A
52	5	1515	A
52	5	1524	G
52	5	1532	A
52	5	1533	C
52	5	1535	A
52	5	1536	C
52	5	1537	G
52	5	1555	G
52	5	1559	U
52	5	1560	G
52	5	1569	A
52	5	1578	U
52	5	1581	G
52	5	1584	U
52	5	1585	C
52	5	1608	A

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Mol	Chain	Res	Type
52	5	1627	G
52	5	1647	U
52	5	1648	U
52	5	1651	G
52	5	1670	C
52	5	1674	G
52	5	1677	A
52	5	1694	C
52	5	1695	G
52	5	1715	G
52	5	1716	U
52	5	1729	U
52	5	1730	C
52	5	1738	G
52	5	1756	G
52	5	1758	U
52	5	1764	C
52	5	1773	A
52	5	1776	G
52	5	1780	A
52	5	1782	U
52	5	1791	A
52	5	1800	C
52	5	1801	A
52	5	1808	A
52	5	1816	C
52	5	1818	U
52	5	1829	A
52	5	1833	C
52	5	1847	G
52	5	1858	A
52	5	1871	A
52	5	1896	G
52	5	1900	A
52	5	1901	A
52	5	1906	G
52	5	1907	G
52	5	1913	A
52	5	1914	C
52	5	1929	G
52	5	1930	G
52	5	1931	U

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Mol	Chain	Res	Type
52	5	1937	A
52	5	1938	A
52	5	1940	U
52	5	1941	C
52	5	1955	U
52	5	1960	A
52	5	1962	5MC
52	5	1965	C
52	5	1967	C
52	5	1970	A
52	5	1971	U
52	5	1972	G
52	5	1991	U
52	5	1992	G
52	5	1993	U
52	5	1997	C
52	5	2022	U
52	5	2023	C
52	5	2030	6MZ
52	5	2031	A
52	5	2032	G
52	5	2033	A
52	5	2043	C
52	5	2052	A
52	5	2055	C
52	5	2056	G
52	5	2060	A
52	5	2061	G
52	5	2062	A
52	5	2069	7MG
52	5	2072	C
52	5	2096	C
52	5	2100	G
52	5	2108	A
52	5	2110	G
52	5	2111	U
52	5	2112	G
52	5	2113	U
52	5	2116	G
52	5	2118	U
52	5	2119	A
52	5	2127	G

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Mol	Chain	Res	Type
52	5	2131	U
52	5	2132	U
52	5	2133	G
52	5	2145	C
52	5	2162	G
52	5	2164	C
52	5	2170	A
52	5	2172	U
52	5	2173	A
52	5	2189	U
52	5	2192	U
52	5	2198	A
52	5	2199	A
52	5	2204	G
52	5	2211	A
52	5	2213	U
52	5	2219	U
52	5	2225	A
52	5	2226	C
52	5	2238	G
52	5	2239	G
52	5	2250	G
52	5	2278	A
52	5	2283	C
52	5	2287	A
52	5	2288	A
52	5	2297	A
52	5	2305	U
52	5	2309	A
52	5	2311	A
52	5	2321	U
52	5	2322	A
52	5	2325	G
52	5	2327	A
52	5	2331	G
52	5	2334	U
52	5	2336	A
52	5	2345	G
52	5	2347	C
52	5	2350	C
52	5	2361	G
52	5	2382	G

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Mol	Chain	Res	Type
52	5	2383	G
52	5	2385	C
52	5	2392	A
52	5	2402	U
52	5	2406	A
52	5	2407	A
52	5	2423	U
52	5	2424	C
52	5	2425	A
52	5	2429	G
52	5	2430	A
52	5	2435	A
52	5	2441	U
52	5	2448	A
52	5	2475	C
52	5	2476	A
52	5	2494	G
52	5	2497	A
52	5	2502	G
52	5	2503	2MA
52	5	2505	G
52	5	2506	U
52	5	2518	A
52	5	2520	C
52	5	2529	G
52	5	2535	G
52	5	2547	A
52	5	2554	U
52	5	2567	G
52	5	2572	A
52	5	2573	C
52	5	2582	G
52	5	2585	U
52	5	2586	U
52	5	2602	A
52	5	2603	G
52	5	2609	U
52	5	2610	C
52	5	2613	U
52	5	2629	U
52	5	2630	G
52	5	2646	C

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Mol	Chain	Res	Type
52	5	2655	G
52	5	2656	U
52	5	2682	A
52	5	2689	U
52	5	2690	U
52	5	2713	U
52	5	2714	G
52	5	2716	C
52	5	2718	G
52	5	2722	G
52	5	2733	A
52	5	2744	G
52	5	2748	A
52	5	2764	A
52	5	2765	A
52	5	2769	U
52	5	2778	A
52	5	2779	U
52	5	2791	G
52	5	2794	C
52	5	2797	U
52	5	2799	A
52	5	2800	A
52	5	2809	A
52	5	2818	U
52	5	2820	A
52	5	2833	U
52	5	2835	A
52	5	2848	G
52	5	2850	A
52	5	2867	G
52	5	2868	A
52	5	2872	A
52	5	2873	A
52	5	2880	C
52	5	2883	A
52	5	2884	U
52	5	2894	G

All (51) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
22	A	51	G
22	A	86	G
22	A	91	A
22	A	227	A
22	A	242	G
22	A	310	A
22	A	372	G
22	A	421	C
22	A	458	G
22	A	490	C
22	A	549	G
22	A	555	G
22	A	615	U
22	A	652	U
22	A	752	A
22	A	774	G
22	A	784	G
22	A	858	G
22	A	859	G
23	B	3	C
23	B	52	A
23	B	66	A
23	B	88	C
52	5	1020	A
52	5	1022	G
52	5	1067	A
52	5	1070	A
52	5	1111	A
52	5	1130	U
52	5	1378	A
52	5	1458	U
52	5	1475	G
52	5	1626	A
52	5	1715	G
52	5	1857	G
52	5	1900	A
52	5	1930	G
52	5	1940	U
52	5	2286	G
52	5	2326	C
52	5	2333	A

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Mol	Chain	Res	Type
52	5	2391	G
52	5	2566	A
52	5	2629	U
52	5	2655	G
52	5	2712	C
52	5	2798	U
52	5	2808	G
52	5	2832	U
52	5	2867	G
52	5	2893	A

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

35 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$
52	OMG	5	2251	52	23,26,27	2.46	8 (34%)	33,38,41	2.47	10 (30%)
52	7MG	5	2069	52,22	22,26,27	4.43	10 (45%)	29,39,42	2.01	9 (31%)
1	2MG	a	1207	1	23,26,27	2.87	8 (34%)	32,38,41	2.65	11 (34%)
22	5MC	A	747	22	18,22,23	3.94	7 (38%)	26,32,35	1.04	2 (7%)
52	PSU	5	1917	52	18,21,22	1.11	1 (5%)	22,30,33	1.84	5 (22%)
52	H2U	5	2449	52	18,21,22	3.17	4 (22%)	21,30,33	2.06	5 (23%)
1	2MG	a	966	1	23,26,27	2.87	8 (34%)	32,38,41	2.72	11 (34%)
52	OMU	5	2552	52	19,22,23	3.55	8 (42%)	26,31,34	1.72	5 (19%)
52	5MC	5	1962	52	18,22,23	3.97	7 (38%)	26,32,35	1.05	2 (7%)
52	5MU	5	1939	52	19,22,23	8.24	7 (36%)	28,32,35	4.36	9 (32%)
52	PSU	5	2604	52	18,21,22	1.09	1 (5%)	22,30,33	1.93	5 (22%)
52	2MG	5	2445	52	23,26,27	2.76	9 (39%)	32,38,41	2.51	12 (37%)
52	6MZ	5	1618	52	22,25,26	2.20	4 (18%)	30,36,39	2.39	11 (36%)
52	6MZ	5	2030	52,22	22,25,26	2.17	4 (18%)	30,36,39	2.48	11 (36%)
52	PSU	5	2580	52	18,21,22	1.11	1 (5%)	22,30,33	1.95	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	a	967	1	18,22,23	3.96	7 (38%)	26,32,35	1.01	2 (7%)
52	PSU	5	955	52	18,21,22	1.10	1 (5%)	22,30,33	1.94	5 (22%)
52	2MA	5	2503	52,53	22,25,26	1.45	4 (18%)	33,37,40	4.16	11 (33%)
1	MA6	a	1519	1	23,26,27	1.15	3 (13%)	34,38,41	3.19	13 (38%)
52	2MG	5	1835	52	23,26,27	2.83	9 (39%)	32,38,41	2.61	12 (37%)
52	PSU	5	1911	52	18,21,22	1.09	1 (5%)	22,30,33	1.81	5 (22%)
1	4OC	a	1402	1	20,23,24	3.28	7 (35%)	26,32,35	0.86	1 (3%)
22	1MG	A	745	22	22,26,27	2.96	6 (27%)	33,39,42	1.66	6 (18%)
52	3TD	5	1915	52	18,22,23	4.27	7 (38%)	22,32,35	1.61	2 (9%)
1	2MG	a	1516	1	23,26,27	2.79	9 (39%)	32,38,41	2.64	13 (40%)
52	PSU	5	2504	52	18,21,22	1.11	1 (5%)	22,30,33	1.85	5 (22%)
52	PSU	5	2605	52	18,21,22	1.10	1 (5%)	22,30,33	1.90	5 (22%)
1	MA6	a	1518	1	23,26,27	1.13	2 (8%)	34,38,41	3.06	12 (35%)
1	UR3	a	1498	1	19,22,23	2.90	8 (42%)	26,32,35	1.33	3 (11%)
52	OMC	5	2498	52,53	19,22,23	2.83	7 (36%)	26,31,34	0.73	0
1	5MC	a	1407	1	18,22,23	3.96	7 (38%)	26,32,35	0.99	1 (3%)
1	PSU	a	516	1,53	18,21,22	1.12	1 (5%)	22,30,33	1.86	6 (27%)
22	PSU	A	746	22,53	18,21,22	1.16	1 (5%)	22,30,33	1.73	4 (18%)
1	7MG	a	527	1	22,26,27	4.43	9 (40%)	29,39,42	1.95	8 (27%)
52	PSU	5	2457	52	18,21,22	1.09	1 (5%)	22,30,33	1.96	6 (27%)

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
52	OMG	5	2251	52	-	0/9/27/28	0/3/3/3
52	7MG	5	2069	52,22	-	1/7/37/38	0/3/3/3
1	2MG	a	1207	1	-	2/9/27/28	0/3/3/3
22	5MC	A	747	22	-	1/7/25/26	0/2/2/2
52	PSU	5	1917	52	-	2/7/25/26	0/2/2/2
52	H2U	5	2449	52	-	0/7/38/39	0/2/2/2
1	2MG	a	966	1	-	1/9/27/28	0/3/3/3
52	OMU	5	2552	52	-	2/9/27/28	0/2/2/2
52	5MC	5	1962	52	-	1/7/25/26	0/2/2/2
52	5MU	5	1939	52	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PSU	5	2604	52	-	0/7/25/26	0/2/2/2
52	2MG	5	2445	52	-	2/9/27/28	0/3/3/3
52	6MZ	5	1618	52	-	0/9/27/28	0/3/3/3
52	6MZ	5	2030	52,22	-	2/9/27/28	0/3/3/3
52	PSU	5	2580	52	-	0/7/25/26	0/2/2/2
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
52	PSU	5	955	52	-	0/7/25/26	0/2/2/2
52	2MA	5	2503	52,53	-	2/7/25/26	0/3/3/3
1	MA6	a	1519	1	-	0/11/29/30	0/3/3/3
52	2MG	5	1835	52	-	0/9/27/28	0/3/3/3
52	PSU	5	1911	52	-	0/7/25/26	0/2/2/2
1	4OC	a	1402	1	-	2/9/29/30	0/2/2/2
22	1MG	A	745	22	-	0/7/25/26	0/3/3/3
52	3TD	5	1915	52	-	4/7/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/9/27/28	0/3/3/3
52	PSU	5	2504	52	-	0/7/25/26	0/2/2/2
52	PSU	5	2605	52	-	0/7/25/26	0/2/2/2
1	MA6	a	1518	1	-	2/11/29/30	0/3/3/3
1	UR3	a	1498	1	-	2/7/25/26	0/2/2/2
52	OMC	5	2498	52,53	-	0/9/27/28	0/2/2/2
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
1	PSU	a	516	1,53	-	0/7/25/26	0/2/2/2
22	PSU	A	746	22,53	-	1/7/25/26	0/2/2/2
1	7MG	a	527	1	-	0/7/37/38	0/3/3/3
52	PSU	5	2457	52	-	0/7/25/26	0/2/2/2

All (179) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	5	1939	5MU	C4-C5	23.58	1.83	1.44
52	5	1939	5MU	C6-N1	17.82	1.68	1.38
1	a	527	7MG	C8-N9	16.22	1.55	1.46
52	5	2069	7MG	C8-N9	16.13	1.55	1.46
52	5	1939	5MU	C4-N3	-14.78	1.11	1.38
52	5	1939	5MU	C6-C5	-12.84	1.13	1.34
52	5	1915	3TD	C6-C5	12.33	1.49	1.35
1	a	1407	5MC	C6-C5	10.02	1.51	1.34
1	a	967	5MC	C6-C5	9.95	1.50	1.34
52	5	1962	5MC	C6-C5	9.94	1.50	1.34
22	A	747	5MC	C6-C5	9.86	1.50	1.34
52	5	1915	3TD	C2-N1	9.73	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	5	2449	H2U	C2-N1	9.63	1.49	1.35
52	5	1618	6MZ	C6-N6	8.87	1.43	1.34
52	5	2030	6MZ	C6-N6	8.64	1.43	1.34
52	5	2552	OMU	C2-N1	8.25	1.51	1.38
52	5	2552	OMU	C2-N3	8.17	1.52	1.38
1	a	1402	4OC	C4-N3	8.07	1.46	1.32
22	A	745	1MG	C2-N2	8.03	1.48	1.34
1	a	1498	UR3	C2-N1	7.76	1.49	1.38
1	a	966	2MG	C2-N3	7.62	1.46	1.31
1	a	1207	2MG	C2-N3	7.60	1.46	1.31
52	5	2449	H2U	C2-N3	7.46	1.51	1.38
52	5	1835	2MG	C2-N3	7.37	1.46	1.31
1	a	1516	2MG	C2-N3	7.19	1.45	1.31
52	5	2445	2MG	C2-N3	6.99	1.45	1.31
22	A	745	1MG	C4-N3	6.84	1.50	1.34
52	5	1962	5MC	C2-N3	6.80	1.50	1.36
1	a	967	5MC	C2-N3	6.78	1.50	1.36
22	A	747	5MC	C2-N3	6.76	1.50	1.36
1	a	1407	5MC	C2-N3	6.73	1.50	1.36
22	A	745	1MG	C2-N3	6.70	1.46	1.34
52	5	2251	OMG	C4-N3	6.65	1.50	1.34
52	5	1962	5MC	C4-N3	6.64	1.45	1.34
1	a	967	5MC	C4-N3	6.63	1.45	1.34
22	A	747	5MC	C4-N3	6.60	1.45	1.34
1	a	1207	2MG	C4-N3	6.54	1.49	1.34
1	a	1407	5MC	C4-N3	6.52	1.45	1.34
1	a	966	2MG	C4-N3	6.52	1.49	1.34
1	a	527	7MG	C2-N3	6.50	1.48	1.33
52	5	2498	OMC	C2-N3	6.40	1.49	1.36
52	5	2069	7MG	C2-N3	6.37	1.48	1.33
52	5	1835	2MG	C4-N3	6.37	1.49	1.34
1	a	1407	5MC	C4-N4	6.35	1.50	1.34
52	5	2552	OMU	C6-C5	6.34	1.49	1.35
1	a	967	5MC	C4-N4	6.34	1.50	1.34
22	A	747	5MC	C4-N4	6.32	1.50	1.34
52	5	1962	5MC	C4-N4	6.32	1.50	1.34
1	a	1402	4OC	C6-C5	6.26	1.49	1.35
1	a	1498	UR3	C6-C5	6.17	1.49	1.35
1	a	1516	2MG	C4-N3	6.15	1.48	1.34
52	5	1915	3TD	C6-N1	6.08	1.46	1.36
52	5	2445	2MG	C4-N3	5.99	1.48	1.34
1	a	1402	4OC	C2-N3	5.99	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	5	2251	OMG	C2-N3	5.59	1.46	1.33
1	a	1207	2MG	C2-N2	5.59	1.45	1.33
52	5	2498	OMC	C6-C5	5.55	1.47	1.35
1	a	966	2MG	C2-N2	5.53	1.45	1.33
52	5	1835	2MG	C2-N2	5.43	1.45	1.33
1	a	1498	UR3	C2-N3	5.40	1.49	1.39
1	a	1516	2MG	C2-N2	5.29	1.45	1.33
52	5	2445	2MG	C2-N2	5.23	1.45	1.33
1	a	527	7MG	C4-N3	5.22	1.46	1.34
52	5	2069	7MG	C2-N1	5.16	1.50	1.37
52	5	2498	OMC	C4-N4	5.08	1.45	1.33
52	5	2069	7MG	C4-N3	5.07	1.46	1.34
1	a	527	7MG	C2-N1	5.05	1.50	1.37
52	5	2445	2MG	C2-N1	5.00	1.44	1.36
1	a	527	7MG	C2-N2	4.93	1.45	1.34
52	5	1835	2MG	C2-N1	4.91	1.44	1.36
1	a	966	2MG	C2-N1	4.90	1.44	1.36
1	a	1516	2MG	C2-N1	4.89	1.44	1.36
1	a	1207	2MG	C2-N1	4.89	1.44	1.36
52	5	2069	7MG	C2-N2	4.86	1.45	1.34
52	5	2552	OMU	C4-N3	4.83	1.47	1.38
52	5	2251	OMG	C2-N2	4.81	1.45	1.34
1	a	1407	5MC	C6-N1	4.80	1.46	1.38
52	5	1962	5MC	C6-N1	4.75	1.46	1.38
1	a	967	5MC	C6-N1	4.72	1.46	1.38
22	A	747	5MC	C6-N1	4.71	1.46	1.38
1	a	1402	4OC	C2-N1	4.60	1.50	1.40
52	5	1915	3TD	C2-N3	4.57	1.48	1.38
1	a	1402	4OC	C4-N4	4.55	1.45	1.35
1	a	967	5MC	C2-N1	4.52	1.49	1.40
52	5	1962	5MC	C2-N1	4.52	1.49	1.40
22	A	747	5MC	C2-N1	4.49	1.49	1.40
1	a	1407	5MC	C2-N1	4.43	1.49	1.40
52	5	1939	5MU	C2-N3	4.38	1.45	1.38
52	5	2069	7MG	C6-N1	4.33	1.46	1.38
52	5	2449	H2U	C4-N3	4.16	1.44	1.37
52	5	2498	OMC	C2-N1	4.07	1.48	1.40
1	a	527	7MG	C6-N1	4.05	1.46	1.38
52	5	2498	OMC	C4-N3	3.96	1.42	1.34
1	a	1402	4OC	C5-C4	3.95	1.49	1.40
22	A	746	PSU	C6-C5	3.94	1.39	1.35
52	5	2503	2MA	C6-N6	3.93	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	527	7MG	C5-C4	3.74	1.50	1.38
52	5	2069	7MG	C5-C4	3.70	1.50	1.38
1	a	516	PSU	C6-C5	3.68	1.39	1.35
52	5	2552	OMU	C6-N1	3.65	1.46	1.38
52	5	2504	PSU	C6-C5	3.62	1.39	1.35
52	5	1917	PSU	C6-C5	3.61	1.39	1.35
52	5	2605	PSU	C6-C5	3.61	1.39	1.35
1	a	1402	4OC	C6-N1	3.60	1.46	1.38
52	5	1911	PSU	C6-C5	3.60	1.39	1.35
52	5	955	PSU	C6-C5	3.58	1.39	1.35
22	A	745	1MG	C5-N7	-3.58	1.32	1.39
52	5	2604	PSU	C6-C5	3.56	1.39	1.35
52	5	2580	PSU	C6-C5	3.56	1.39	1.35
52	5	2457	PSU	C6-C5	3.50	1.39	1.35
52	5	2552	OMU	C5-C4	3.42	1.51	1.43
1	a	1498	UR3	C6-N1	3.31	1.46	1.38
22	A	745	1MG	C5-C6	3.27	1.53	1.45
52	5	2498	OMC	C6-N1	3.13	1.45	1.38
1	a	1207	2MG	C5-N7	-3.07	1.33	1.39
52	5	2251	OMG	C5-N7	-3.06	1.33	1.39
52	5	2449	H2U	O4-C4	-3.06	1.17	1.23
1	a	966	2MG	C5-N7	-3.03	1.33	1.39
52	5	2069	7MG	C5-C6	3.03	1.51	1.43
1	a	527	7MG	C5-C6	2.88	1.51	1.43
52	5	2498	OMC	C5-C4	2.82	1.49	1.42
52	5	2503	2MA	C5-N7	-2.81	1.33	1.39
52	5	1835	2MG	C5-N7	-2.79	1.33	1.39
1	a	1516	2MG	C5-N7	-2.79	1.33	1.39
52	5	2445	2MG	C6-N1	2.75	1.43	1.38
52	5	2445	2MG	C5-N7	-2.71	1.33	1.39
52	5	2552	OMU	O2-C2	-2.70	1.18	1.23
52	5	2251	OMG	C2-N1	2.69	1.44	1.37
1	a	1498	UR3	C5-C4	2.69	1.50	1.43
1	a	1516	2MG	C6-N1	2.69	1.43	1.38
52	5	2445	2MG	C5-C6	2.69	1.54	1.44
1	a	1516	2MG	C5-C6	2.68	1.54	1.44
52	5	2251	OMG	C5-C6	2.64	1.54	1.44
52	5	1835	2MG	C5-C6	2.63	1.54	1.44
52	5	1835	2MG	C6-N1	2.60	1.43	1.38
22	A	747	5MC	O2-C2	-2.57	1.18	1.23
1	a	967	5MC	O2-C2	-2.56	1.19	1.23
1	a	966	2MG	C5-C6	2.56	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1407	5MC	O2-C2	-2.55	1.19	1.23
52	5	1962	5MC	O2-C2	-2.55	1.19	1.23
52	5	1915	3TD	C4-N3	2.54	1.45	1.40
52	5	1939	5MU	O4-C4	-2.51	1.18	1.23
52	5	2445	2MG	C4-N9	-2.50	1.31	1.38
1	a	1207	2MG	C5-C6	2.50	1.53	1.44
52	5	2251	OMG	C6-N1	2.49	1.43	1.38
1	a	966	2MG	C6-N1	2.46	1.43	1.38
52	5	1835	2MG	O6-C6	-2.46	1.18	1.23
1	a	527	7MG	O6-C6	-2.44	1.18	1.23
52	5	2069	7MG	O6-C6	-2.43	1.19	1.23
1	a	966	2MG	O6-C6	-2.43	1.19	1.23
1	a	1516	2MG	O6-C6	-2.42	1.19	1.23
1	a	1207	2MG	O6-C6	-2.42	1.19	1.23
52	5	1915	3TD	O2-C2	-2.41	1.18	1.23
52	5	2445	2MG	O6-C6	-2.40	1.19	1.23
52	5	2251	OMG	O6-C6	-2.39	1.19	1.23
1	a	1518	MA6	C2-N1	2.38	1.38	1.33
52	5	1939	5MU	O2-C2	-2.37	1.18	1.23
1	a	1207	2MG	C6-N1	2.36	1.43	1.38
52	5	2030	6MZ	C8-N7	2.35	1.36	1.31
1	a	1519	MA6	C2-N1	2.34	1.38	1.33
52	5	2030	6MZ	C5-C4	-2.33	1.34	1.39
52	5	2069	7MG	C4-N9	-2.32	1.35	1.37
52	5	2503	2MA	C5-C4	-2.29	1.34	1.39
1	a	1519	MA6	C10-N6	2.29	1.50	1.45
52	5	2503	2MA	C8-N9	-2.29	1.33	1.37
1	a	1518	MA6	C10-N6	2.28	1.50	1.45
1	a	1516	2MG	C4-N9	-2.24	1.32	1.38
52	5	1618	6MZ	C8-N7	2.23	1.35	1.31
52	5	1618	6MZ	C5-C4	-2.22	1.34	1.39
52	5	2030	6MZ	C5-N7	-2.19	1.34	1.39
52	5	1618	6MZ	C5-N7	-2.15	1.35	1.39
22	A	745	1MG	C4-N9	-2.14	1.32	1.38
1	a	1519	MA6	C5-C4	-2.13	1.35	1.39
52	5	1835	2MG	C4-N9	-2.12	1.32	1.38
1	a	1498	UR3	C4-N3	2.12	1.45	1.40
1	a	1498	UR3	O2-C2	-2.10	1.18	1.22
52	5	1915	3TD	O4-C4	-2.07	1.18	1.23
52	5	2552	OMU	O2'-CM2	-2.04	1.35	1.42
1	a	1498	UR3	O4-C4	-2.01	1.19	1.23

All (234) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	5	1939	5MU	C5M-C5-C6	-13.72	104.52	122.85
52	5	1939	5MU	C5-C4-N3	12.67	126.13	115.31
52	5	2503	2MA	N6-C6-N1	-12.64	99.17	117.03
1	a	1519	MA6	N1-C6-N6	-10.31	105.81	117.08
1	a	1518	MA6	N1-C6-N6	-9.84	106.33	117.08
52	5	2503	2MA	C1'-N9-C8	9.78	149.21	127.14
52	5	2503	2MA	C4-N9-C1'	-9.48	104.02	126.59
52	5	2503	2MA	C5-C4-N3	-8.59	117.52	127.19
52	5	1939	5MU	C5M-C5-C4	-7.81	110.17	118.77
52	5	2503	2MA	C5-C6-N6	7.65	140.07	123.43
52	5	2449	H2U	C4-N3-C2	-7.23	119.80	125.79
1	a	966	2MG	C1'-N9-C8	-7.22	106.13	126.70
1	a	1207	2MG	C1'-N9-C8	-7.14	106.36	126.70
52	5	1835	2MG	C1'-N9-C8	-6.71	107.59	126.70
1	a	1516	2MG	C1'-N9-C8	-6.46	108.29	126.70
52	5	2251	OMG	C1'-N9-C8	6.46	145.08	126.70
1	a	966	2MG	C2-N3-C4	6.43	120.01	112.04
52	5	2251	OMG	C1'-N9-C4	-6.42	107.43	126.50
1	a	1516	2MG	C2-N3-C4	6.42	120.00	112.04
1	a	1207	2MG	C2-N3-C4	6.31	119.86	112.04
52	5	1835	2MG	C2-N3-C4	6.30	119.86	112.04
1	a	966	2MG	C1'-N9-C4	6.27	145.13	126.50
1	a	1207	2MG	C1'-N9-C4	6.23	145.01	126.50
52	5	2445	2MG	C2-N3-C4	6.14	119.66	112.04
52	5	2445	2MG	C1'-N9-C8	-6.11	109.30	126.70
1	a	1518	MA6	C5-C4-N3	-6.05	118.86	126.75
52	5	2030	6MZ	C9-N6-C6	-5.92	117.77	122.87
52	5	2251	OMG	C5-C4-N3	-5.89	118.91	128.46
52	5	2503	2MA	N3-C4-N9	5.86	135.11	126.99
1	a	1519	MA6	C4-N9-C1'	-5.71	112.99	126.59
52	5	2030	6MZ	N1-C2-N3	-5.67	119.73	128.60
1	a	1519	MA6	C5-C4-N3	-5.67	119.36	126.75
52	5	1835	2MG	C1'-N9-C4	5.64	143.26	126.50
52	5	1939	5MU	C4-N3-C2	-5.54	120.18	127.35
52	5	1618	6MZ	N1-C2-N3	-5.51	119.99	128.60
1	a	1516	2MG	C1'-N9-C4	5.50	142.85	126.50
1	a	1519	MA6	N1-C2-N3	-5.42	120.12	128.60
1	a	1519	MA6	C1'-N9-C8	5.29	139.07	127.14
22	A	745	1MG	C5-C4-N3	-5.17	120.07	128.46
1	a	966	2MG	C5-C4-N3	-5.14	120.12	128.46
52	5	2445	2MG	C1'-N9-C4	5.11	141.69	126.50
52	5	1618	6MZ	C5-C4-N3	-5.09	120.11	126.75
52	5	2552	OMU	C4-N3-C2	-5.08	119.88	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	5	2604	PSU	C4-N3-C2	-5.07	119.03	126.34
1	a	1207	2MG	C5-C4-N3	-5.04	120.29	128.46
1	a	1519	MA6	C5-C6-N6	5.01	134.03	125.30
52	5	1915	3TD	N1-C2-N3	5.00	120.08	116.14
52	5	2457	PSU	C4-N3-C2	-4.98	119.17	126.34
52	5	2457	PSU	N1-C2-N3	4.98	120.77	115.13
52	5	2605	PSU	C4-N3-C2	-4.97	119.18	126.34
52	5	2030	6MZ	C5-C4-N3	-4.95	120.29	126.75
52	5	2580	PSU	N1-C2-N3	4.95	120.74	115.13
1	a	1518	MA6	N1-C2-N3	-4.94	120.88	128.60
52	5	2069	7MG	C5-C6-N1	4.92	119.67	110.99
52	5	955	PSU	C4-N3-C2	-4.92	119.25	126.34
52	5	2580	PSU	C4-N3-C2	-4.89	119.29	126.34
52	5	955	PSU	N1-C2-N3	4.88	120.65	115.13
52	5	2604	PSU	N1-C2-N3	4.86	120.64	115.13
52	5	2251	OMG	C2-N3-C4	4.82	120.88	112.30
52	5	1917	PSU	C4-N3-C2	-4.79	119.43	126.34
1	a	1518	MA6	C5-C6-N6	4.79	133.64	125.30
52	5	2605	PSU	N1-C2-N3	4.77	120.53	115.13
52	5	2504	PSU	C4-N3-C2	-4.76	119.49	126.34
1	a	527	7MG	C5-C6-N1	4.75	119.36	110.99
52	5	2030	6MZ	N9-C8-N7	-4.69	107.49	113.91
52	5	2504	PSU	N1-C2-N3	4.68	120.43	115.13
1	a	1518	MA6	C4-N9-C1'	-4.67	115.46	126.59
1	a	516	PSU	N1-C2-N3	4.67	120.42	115.13
52	5	1917	PSU	N1-C2-N3	4.65	120.40	115.13
52	5	1911	PSU	C4-N3-C2	-4.64	119.65	126.34
1	a	516	PSU	C4-N3-C2	-4.64	119.65	126.34
52	5	1939	5MU	C5-C6-N1	-4.64	118.57	123.34
1	a	1516	2MG	C5-C4-N3	-4.63	120.94	128.46
52	5	1835	2MG	C5-C4-N3	-4.63	120.95	128.46
22	A	746	PSU	C4-N3-C2	-4.63	119.67	126.34
1	a	1498	UR3	C4-N3-C2	-4.63	120.21	124.56
22	A	746	PSU	N1-C2-N3	4.58	120.31	115.13
52	5	1618	6MZ	N9-C8-N7	-4.54	107.70	113.91
1	a	1518	MA6	C4-C5-C6	4.53	120.95	115.88
52	5	1911	PSU	N1-C2-N3	4.53	120.26	115.13
52	5	1939	5MU	C6-C5-C4	-4.51	114.26	118.03
52	5	1939	5MU	O4-C4-C5	-4.45	119.74	124.90
1	a	1516	2MG	C2-N1-C6	-4.41	119.40	124.48
1	a	1518	MA6	C1'-N9-C8	4.38	137.02	127.14
52	5	2069	7MG	C2-N3-C4	4.35	120.05	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	527	7MG	C2-N3-C4	4.29	119.95	112.30
52	5	2445	2MG	C2-N1-C6	-4.28	119.55	124.48
52	5	2445	2MG	C5-C4-N3	-4.19	121.67	128.46
1	a	966	2MG	C2-N1-C6	-4.16	119.69	124.48
1	a	1518	MA6	N3-C4-N9	4.14	133.90	127.08
52	5	1835	2MG	C2-N1-C6	-4.14	119.72	124.48
1	a	527	7MG	C5-C4-N3	-4.06	120.40	128.13
52	5	1915	3TD	C4-N3-C2	-3.99	120.28	124.61
1	a	1519	MA6	C4-C5-C6	3.95	120.30	115.88
52	5	1618	6MZ	C9-N6-C6	-3.90	119.51	122.87
1	a	1519	MA6	N9-C8-N7	-3.89	108.60	113.91
52	5	2069	7MG	C5-C4-N3	-3.88	120.73	128.13
1	a	1207	2MG	C2-N1-C6	-3.79	120.12	124.48
52	5	2251	OMG	N9-C4-N3	3.71	133.39	125.94
1	a	1519	MA6	N3-C4-N9	3.68	133.15	127.08
1	a	1519	MA6	C2-N3-C4	3.67	120.43	111.75
52	5	2445	2MG	N9-C8-N7	-3.66	106.49	113.39
52	5	2552	OMU	N3-C2-N1	3.62	119.69	114.89
52	5	1939	5MU	N3-C2-N1	3.61	119.68	114.89
52	5	1618	6MZ	C4-C5-C6	3.59	119.59	116.81
52	5	2030	6MZ	C2-N3-C4	3.58	120.22	111.75
22	A	747	5MC	C5-C6-N1	-3.58	119.65	123.34
52	5	1835	2MG	N9-C8-N7	-3.58	106.65	113.39
52	5	1962	5MC	C5-C6-N1	-3.57	119.67	123.34
22	A	745	1MG	C2-N3-C4	3.52	119.90	111.98
52	5	1618	6MZ	C2-N3-C4	3.51	120.05	111.75
1	a	1518	MA6	C2-N3-C4	3.50	120.03	111.75
1	a	1518	MA6	N9-C8-N7	-3.49	109.15	113.91
1	a	1516	2MG	N9-C8-N7	-3.49	106.83	113.39
52	5	2069	7MG	C4-C5-N7	3.48	110.36	105.53
1	a	1407	5MC	C5-C6-N1	-3.40	119.84	123.34
22	A	745	1MG	N9-C4-N3	3.36	132.69	125.94
1	a	1519	MA6	C2-N1-C6	3.34	119.64	111.75
52	5	2552	OMU	C5-C4-N3	3.33	119.82	114.84
1	a	966	2MG	N9-C8-N7	-3.33	107.13	113.39
52	5	2069	7MG	C5-C4-N9	3.32	110.66	106.35
52	5	2030	6MZ	C5-N7-C8	3.32	108.22	103.51
52	5	2449	H2U	N3-C2-N1	3.31	120.16	116.65
1	a	967	5MC	C5-C6-N1	-3.31	119.94	123.34
1	a	1207	2MG	N9-C8-N7	-3.25	107.28	113.39
52	5	1618	6MZ	C5-N7-C8	3.20	108.05	103.51
1	a	1518	MA6	C2-N1-C6	3.18	119.25	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	966	2MG	N9-C4-N3	3.17	132.31	125.94
52	5	2503	2MA	N9-C8-N7	-3.15	109.61	113.91
52	5	2030	6MZ	C4-C5-C6	3.15	119.25	116.81
1	a	1207	2MG	N9-C4-N3	3.14	132.24	125.94
52	5	1939	5MU	O4-C4-N3	-3.12	114.13	120.12
1	a	1516	2MG	CM2-N2-C2	-3.12	116.97	123.86
52	5	2251	OMG	C2-N1-C6	-3.11	119.44	125.10
52	5	1618	6MZ	N3-C4-N9	3.10	132.19	127.08
1	a	527	7MG	C4-C5-N7	3.10	109.83	105.53
52	5	2069	7MG	O6-C6-C5	-3.01	120.14	127.54
52	5	2580	PSU	O2-C2-N1	-2.98	119.52	122.79
22	A	745	1MG	N9-C8-N7	-2.96	107.81	113.39
52	5	2552	OMU	O4-C4-C5	-2.94	120.00	125.16
52	5	2503	2MA	N3-C2-N1	-2.93	120.32	125.72
1	a	527	7MG	C5-C4-N9	2.93	110.15	106.35
52	5	2457	PSU	O2-C2-N1	-2.92	119.57	122.79
1	a	527	7MG	O6-C6-C5	-2.91	120.39	127.54
52	5	2449	H2U	C5-C4-N3	2.90	119.90	116.65
52	5	955	PSU	O2-C2-N1	-2.85	119.65	122.79
52	5	1618	6MZ	C1'-N9-C8	-2.85	120.71	127.14
1	a	1519	MA6	C5-N7-C8	2.84	107.55	103.51
52	5	2503	2MA	C5-N7-C8	2.79	107.47	103.51
52	5	2503	2MA	C6-C5-C4	2.78	120.92	117.18
52	5	2030	6MZ	N3-C4-N9	2.76	131.62	127.08
52	5	2445	2MG	CM2-N2-C2	-2.75	117.79	123.86
52	5	2604	PSU	O2-C2-N1	-2.75	119.77	122.79
52	5	955	PSU	C6-C5-C4	2.74	120.11	118.20
52	5	2251	OMG	C5-C6-N1	2.72	120.08	113.19
52	5	2504	PSU	O2-C2-N1	-2.71	119.80	122.79
52	5	1917	PSU	O2-C2-N1	-2.70	119.81	122.79
1	a	516	PSU	O2-C2-N1	-2.69	119.83	122.79
52	5	2069	7MG	C2-N1-C6	-2.69	120.19	125.10
52	5	2503	2MA	CM2-C2-N1	2.68	121.34	117.15
52	5	1835	2MG	C5-C6-N1	2.68	119.99	113.19
1	a	1518	MA6	C5-N7-C8	2.68	107.31	103.51
1	a	1516	2MG	C5-C6-N1	2.68	119.99	113.19
1	a	527	7MG	N9-C4-N3	2.66	129.45	125.47
52	5	2605	PSU	O2-C2-N1	-2.65	119.87	122.79
1	a	966	2MG	C5-C6-N1	2.64	119.90	113.19
52	5	1911	PSU	O2-C2-N1	-2.63	119.89	122.79
52	5	1835	2MG	N9-C4-N3	2.62	131.20	125.94
52	5	2457	PSU	C6-C5-C4	2.60	120.02	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	5	2445	2MG	C5-C6-N1	2.60	119.79	113.19
22	A	746	PSU	O2-C2-N1	-2.58	119.95	122.79
1	a	1207	2MG	N1-C2-N3	-2.58	119.97	123.95
1	a	1498	UR3	C1'-N1-C2	2.57	121.33	116.99
1	a	1207	2MG	C5-C6-N1	2.54	119.65	113.19
22	A	745	1MG	C5-C6-N1	2.52	119.78	114.91
52	5	1618	6MZ	C4-N9-C8	2.52	108.46	105.73
52	5	2251	OMG	O6-C6-C5	-2.48	120.01	126.60
1	a	966	2MG	O6-C6-C5	-2.48	120.03	126.60
52	5	2580	PSU	C6-N1-C2	-2.48	120.15	122.68
52	5	2251	OMG	N9-C8-N7	-2.48	108.73	113.39
52	5	1835	2MG	N1-C2-N3	-2.47	120.13	123.95
52	5	2445	2MG	C8-N7-C5	2.47	108.70	104.24
52	5	1835	2MG	C8-N7-C5	2.46	108.70	104.24
52	5	2604	PSU	C6-C5-C4	2.45	119.91	118.20
52	5	2449	H2U	O2-C2-N1	-2.45	120.03	123.11
52	5	2030	6MZ	C4-N9-C8	2.44	108.38	105.73
1	a	966	2MG	N1-C2-N3	-2.44	120.18	123.95
52	5	2605	PSU	C6-C5-C4	2.43	119.90	118.20
1	a	1516	2MG	C8-N7-C5	2.43	108.64	104.24
52	5	2552	OMU	C1'-N1-C2	2.43	121.97	117.57
52	5	2449	H2U	C5-C6-N1	2.43	119.61	111.61
1	a	516	PSU	C6-C5-C4	2.42	119.89	118.20
1	a	1207	2MG	O6-C6-C5	-2.42	120.18	126.60
1	a	527	7MG	C2-N1-C6	-2.41	120.70	125.10
1	a	966	2MG	C8-N7-C5	2.41	108.59	104.24
1	a	1516	2MG	O6-C6-C5	-2.40	120.22	126.60
52	5	1835	2MG	O6-C6-C5	-2.39	120.26	126.60
1	a	1402	4OC	C6-C5-C4	2.36	119.85	116.96
1	a	1516	2MG	N9-C4-N3	2.36	130.67	125.94
52	5	2445	2MG	O6-C6-C5	-2.34	120.38	126.60
1	a	1516	2MG	N1-C2-N3	-2.34	120.34	123.95
52	5	2445	2MG	N1-C2-N3	-2.31	120.38	123.95
1	a	1207	2MG	C8-N7-C5	2.31	108.42	104.24
52	5	2504	PSU	C6-C5-C4	2.30	119.81	118.20
52	5	2030	6MZ	C4-C5-N7	-2.30	107.82	110.62
1	a	516	PSU	C6-N1-C2	-2.29	120.34	122.68
52	5	2457	PSU	C6-N1-C2	-2.28	120.35	122.68
52	5	2580	PSU	C6-C5-C4	2.26	119.78	118.20
52	5	1911	PSU	C6-C5-C4	2.26	119.78	118.20
52	5	2445	2MG	C4-C5-N7	-2.25	107.16	110.72
52	5	2580	PSU	O4'-C1'-C2'	2.25	108.32	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	967	5MC	CM5-C5-C6	-2.18	119.93	122.85
22	A	746	PSU	C6-N1-C2	-2.18	120.46	122.68
52	5	2504	PSU	C6-N1-C2	-2.17	120.46	122.68
52	5	1917	PSU	C6-C5-C4	2.16	119.71	118.20
52	5	955	PSU	C6-N1-C2	-2.15	120.48	122.68
1	a	1516	2MG	C4-C5-N7	-2.15	107.32	110.72
52	5	1835	2MG	CM2-N2-C2	-2.12	119.19	123.86
52	5	2069	7MG	N9-C4-N3	2.10	128.61	125.47
52	5	2030	6MZ	C5-C6-N1	2.10	120.44	118.20
52	5	1911	PSU	C6-N1-C2	-2.09	120.55	122.68
52	5	1917	PSU	C6-N1-C2	-2.09	120.55	122.68
1	a	1498	UR3	C6-N1-C2	-2.08	119.92	121.79
22	A	747	5MC	CM5-C5-C6	-2.07	120.08	122.85
52	5	1618	6MZ	C4-C5-N7	-2.07	108.10	110.62
52	5	1962	5MC	CM5-C5-C6	-2.06	120.09	122.85
52	5	2457	PSU	O4'-C1'-C2'	2.06	108.05	105.14
1	a	1519	MA6	C4-N9-C8	2.04	107.94	105.73
1	a	516	PSU	O4'-C1'-C2'	2.03	108.01	105.14
22	A	745	1MG	C8-N7-C5	2.03	107.91	104.24
52	5	2251	OMG	C8-N7-C5	2.03	107.91	104.24
52	5	2069	7MG	N2-C2-N1	2.02	121.02	116.71
52	5	2604	PSU	C6-N1-C2	-2.01	120.63	122.68
52	5	2605	PSU	C6-N1-C2	-2.00	120.63	122.68

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1207	2MG	O4'-C4'-C5'-O5'
1	a	1207	2MG	C3'-C4'-C5'-O5'
1	a	1498	UR3	O4'-C1'-N1-C2
52	5	1915	3TD	C2'-C1'-C5-C4
52	5	1915	3TD	O4'-C1'-C5-C4
52	5	1915	3TD	C2'-C1'-C5-C6
52	5	1915	3TD	O4'-C1'-C5-C6
52	5	2503	2MA	O4'-C4'-C5'-O5'
52	5	2552	OMU	O4'-C1'-N1-C2
52	5	2552	OMU	O4'-C1'-N1-C6
52	5	2030	6MZ	O4'-C4'-C5'-O5'
52	5	2030	6MZ	C3'-C4'-C5'-O5'
1	a	1402	4OC	O4'-C4'-C5'-O5'
1	a	1498	UR3	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
52	5	2445	2MG	C3'-C4'-C5'-O5'
1	a	1402	4OC	C3'-C4'-C5'-O5'
52	5	2445	2MG	O4'-C4'-C5'-O5'
52	5	1917	PSU	O4'-C4'-C5'-O5'
1	a	1518	MA6	O4'-C1'-N9-C4
52	5	2503	2MA	C3'-C4'-C5'-O5'
1	a	1518	MA6	O4'-C1'-N9-C8
52	5	1962	5MC	C4'-C5'-O5'-P
1	a	966	2MG	C3'-C4'-C5'-O5'
52	5	1917	PSU	C3'-C4'-C5'-O5'
22	A	747	5MC	C2'-C1'-N1-C2
22	A	746	PSU	O4'-C1'-C5-C6
52	5	2069	7MG	O4'-C4'-C5'-O5'

There are no ring outliers.

15 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	a	1207	2MG	1	0
52	5	2449	H2U	1	0
52	5	1962	5MC	1	0
52	5	1939	5MU	7	0
52	5	2445	2MG	1	0
52	5	1618	6MZ	1	0
52	5	2030	6MZ	2	0
52	5	2580	PSU	1	0
1	a	967	5MC	1	0
1	a	1519	MA6	2	0
1	a	1402	4OC	1	0
1	a	1516	2MG	1	0
1	a	1518	MA6	5	0
52	5	2498	OMC	1	0
1	a	527	7MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 334 ligands modelled in this entry, 334 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

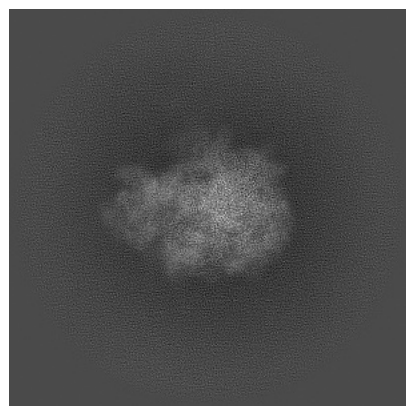
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67081. These allow visual inspection of the internal detail of the map and identification of artifacts.

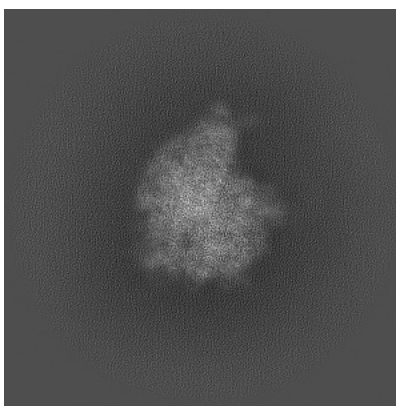
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

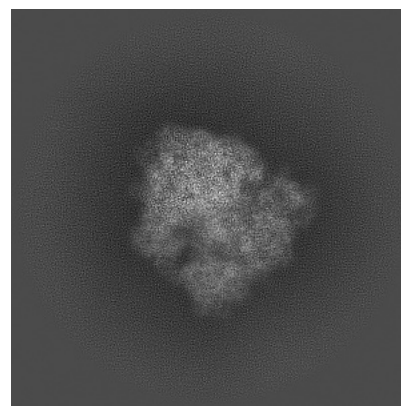
6.1.1 Primary map



X

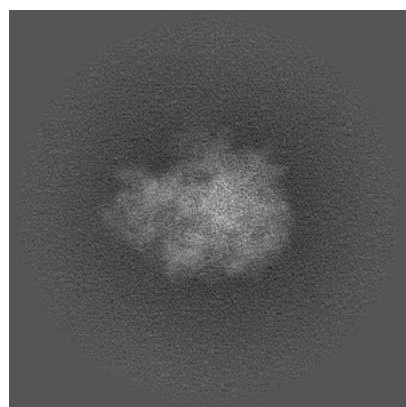


Y

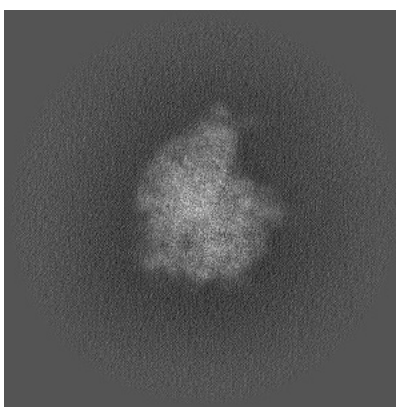


Z

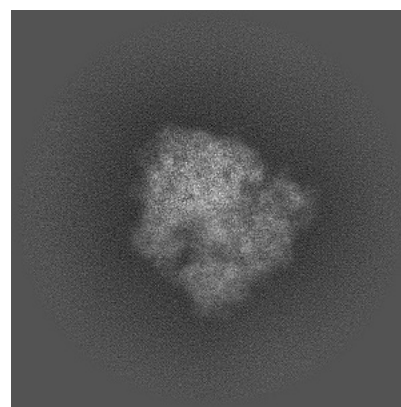
6.1.2 Raw map



X



Y

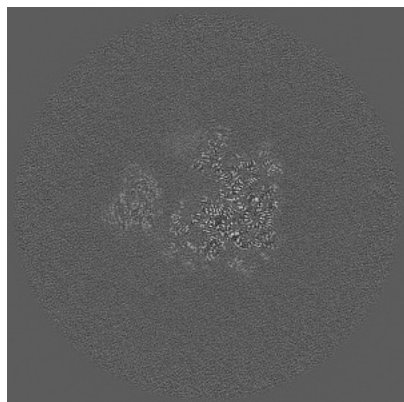


Z

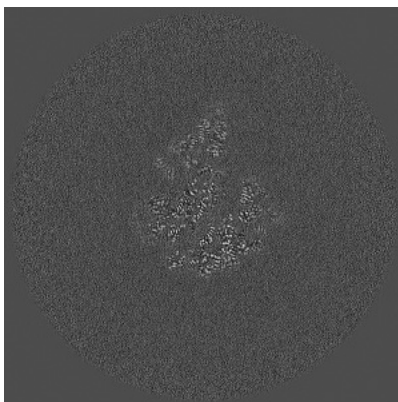
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

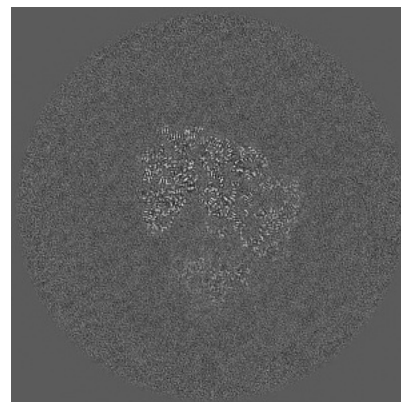
6.2.1 Primary map



X Index: 264

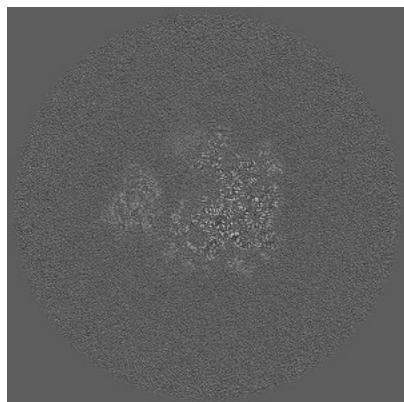


Y Index: 264

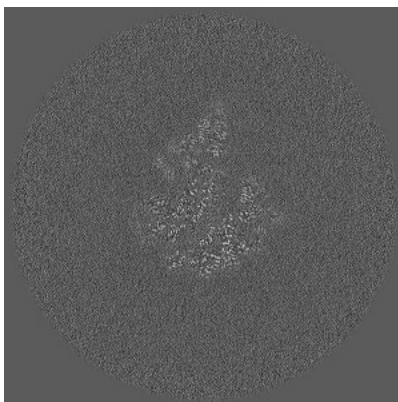


Z Index: 264

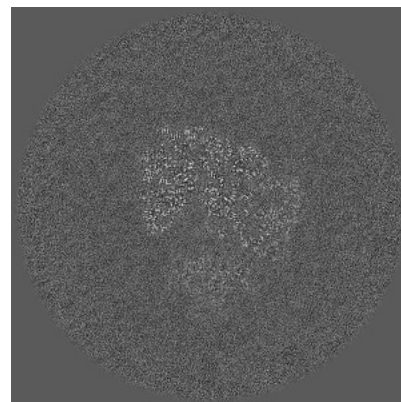
6.2.2 Raw map



X Index: 264



Y Index: 264

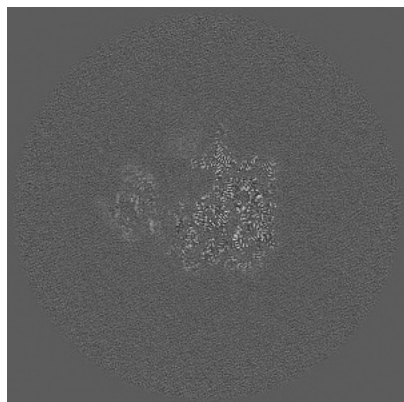


Z Index: 264

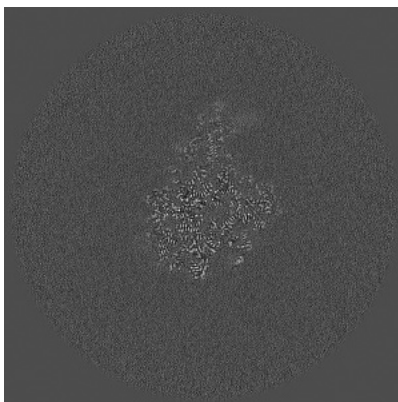
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

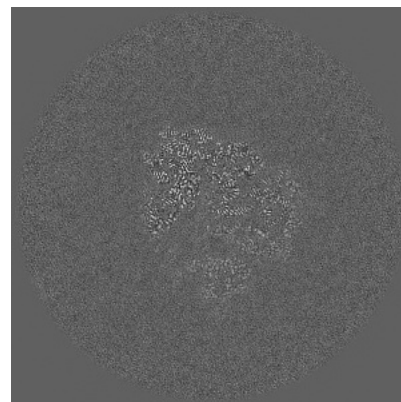
6.3.1 Primary map



X Index: 270

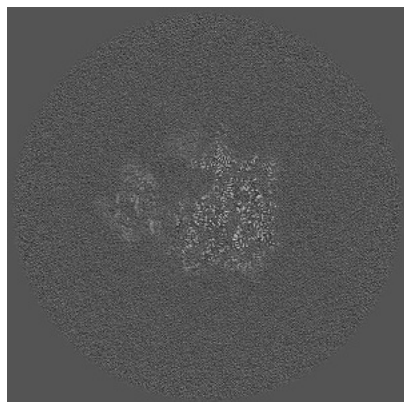


Y Index: 276

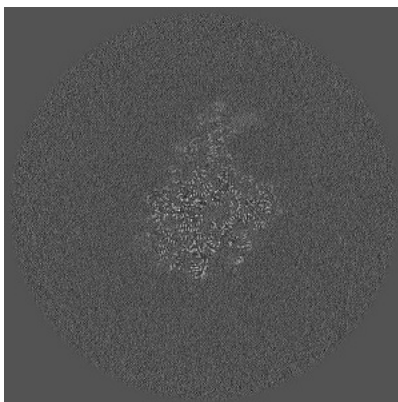


Z Index: 270

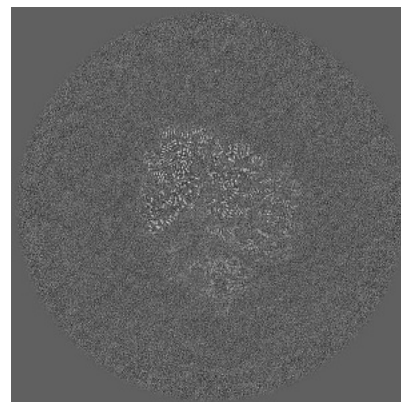
6.3.2 Raw map



X Index: 270



Y Index: 276

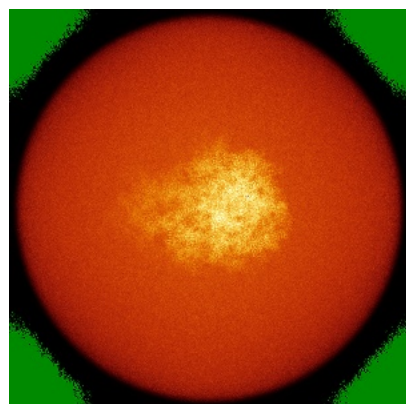


Z Index: 269

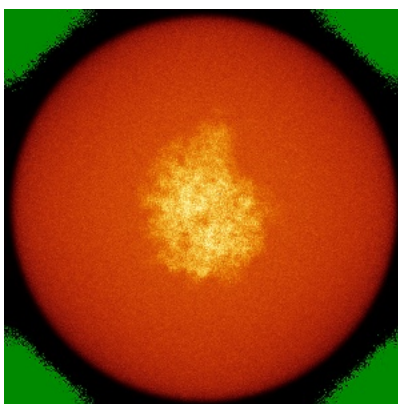
The images above show the largest variance slices of the map in three orthogonal directions.

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

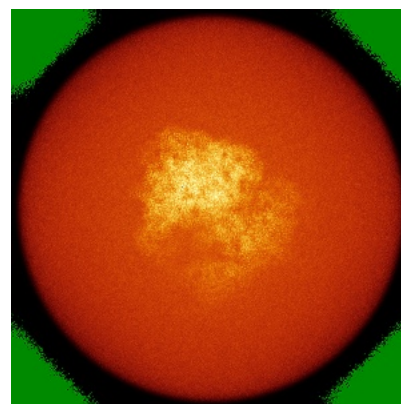
6.4.1 Primary map



X

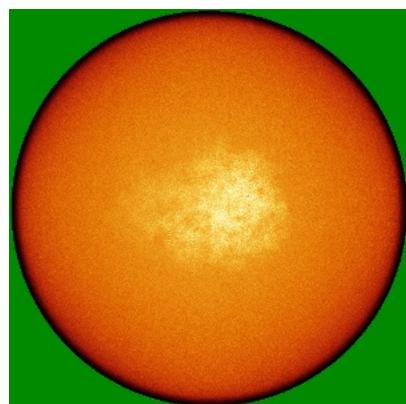


Y

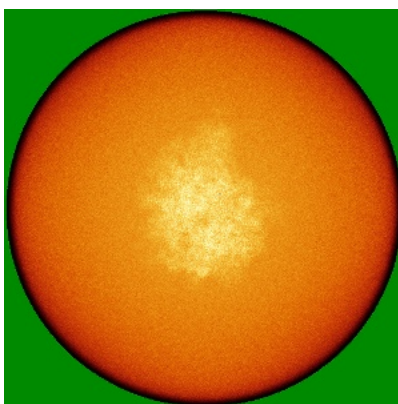


Z

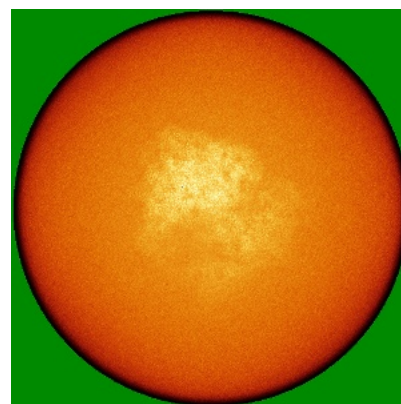
6.4.2 Raw map



X



Y

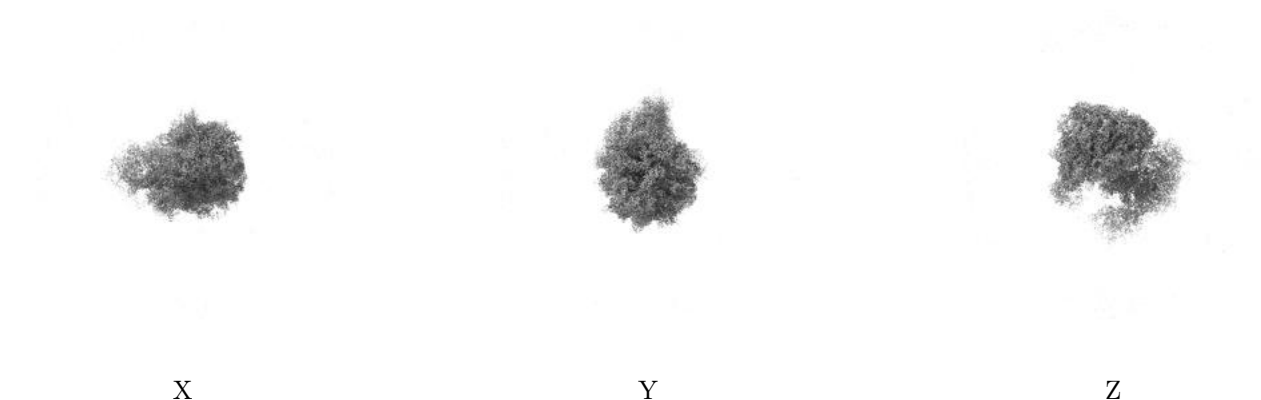


Z

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

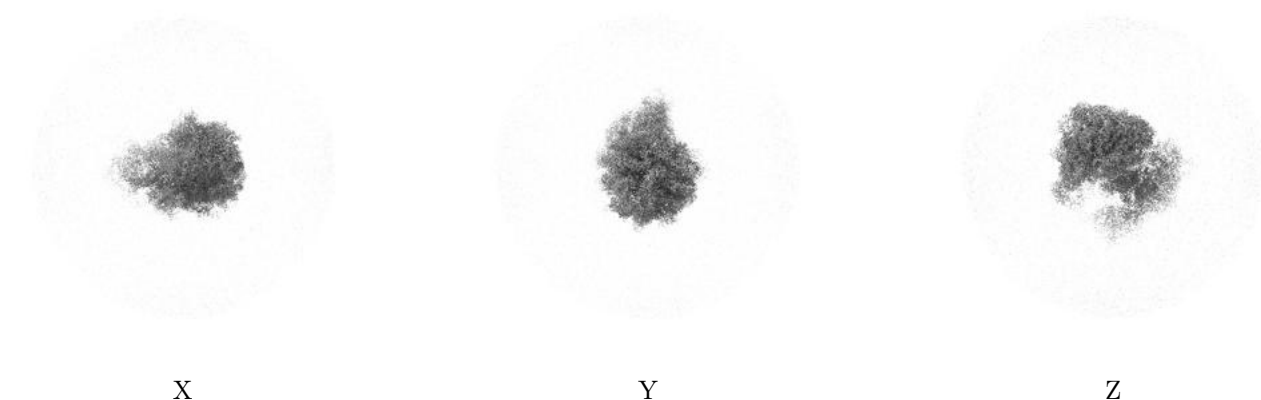
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0077. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

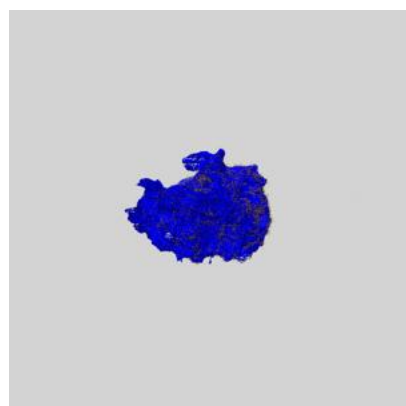
6.6 Mask visualisation [i](#)

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

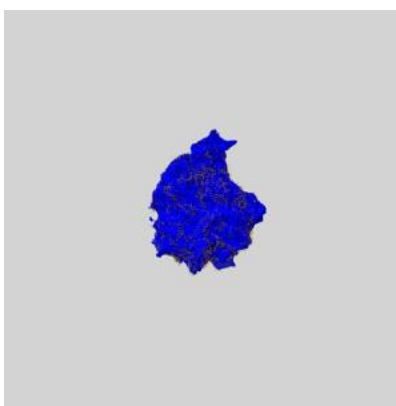
A mask typically either:

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

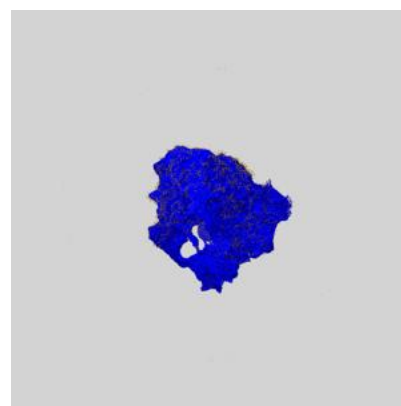
6.6.1 emd_67081_msk_1.map [i](#)



X



Y

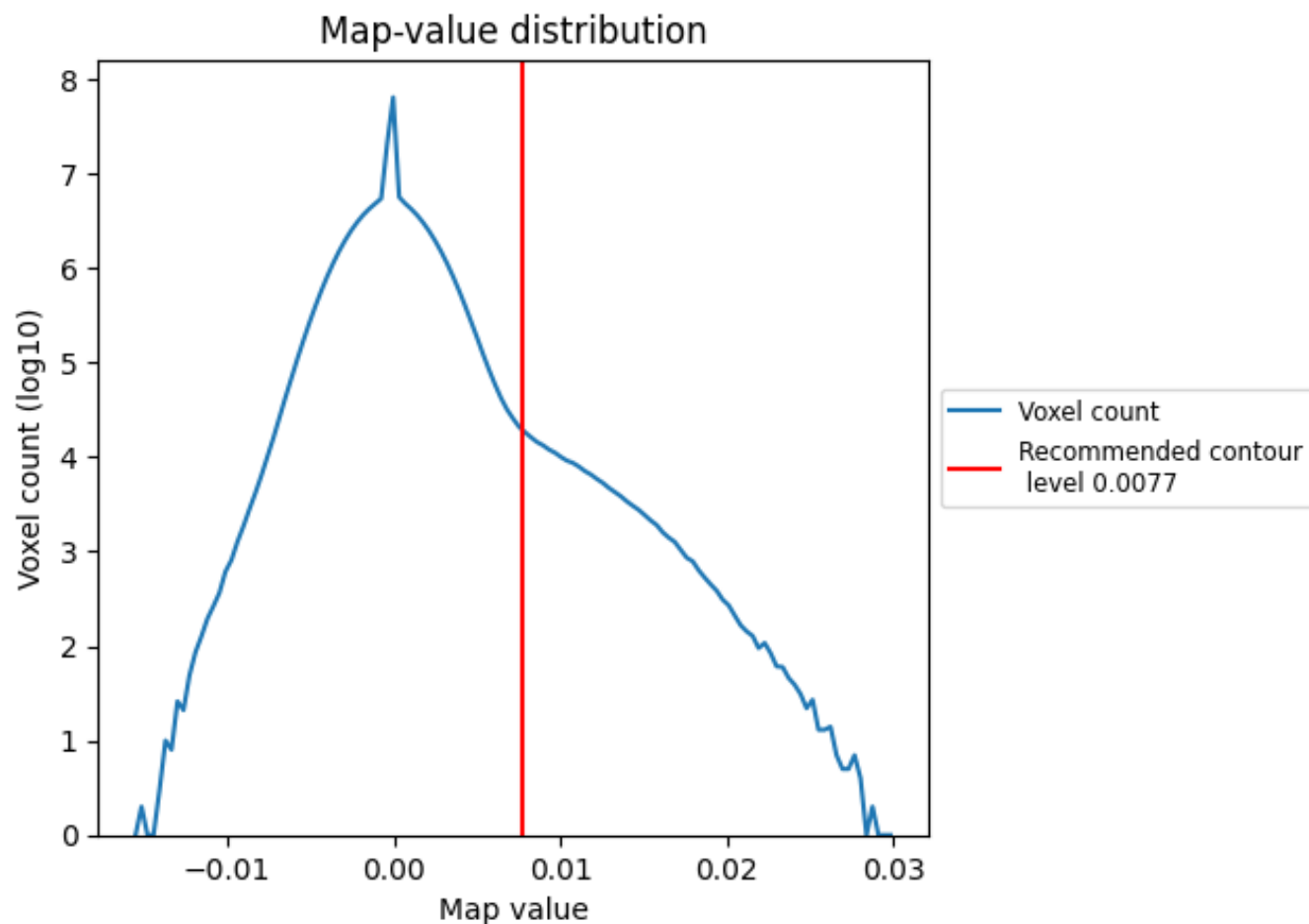


Z

7 Map analysis [i](#)

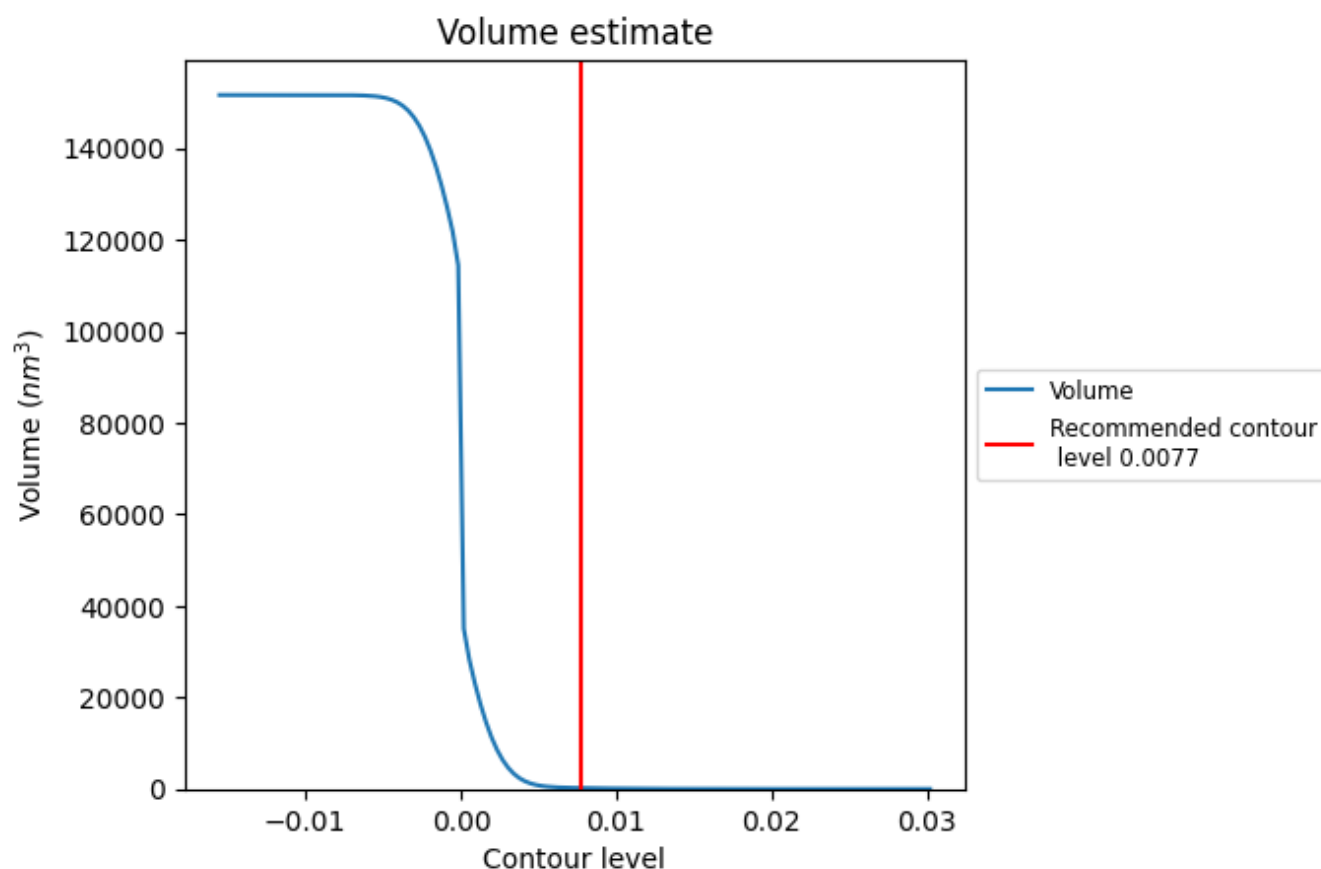
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

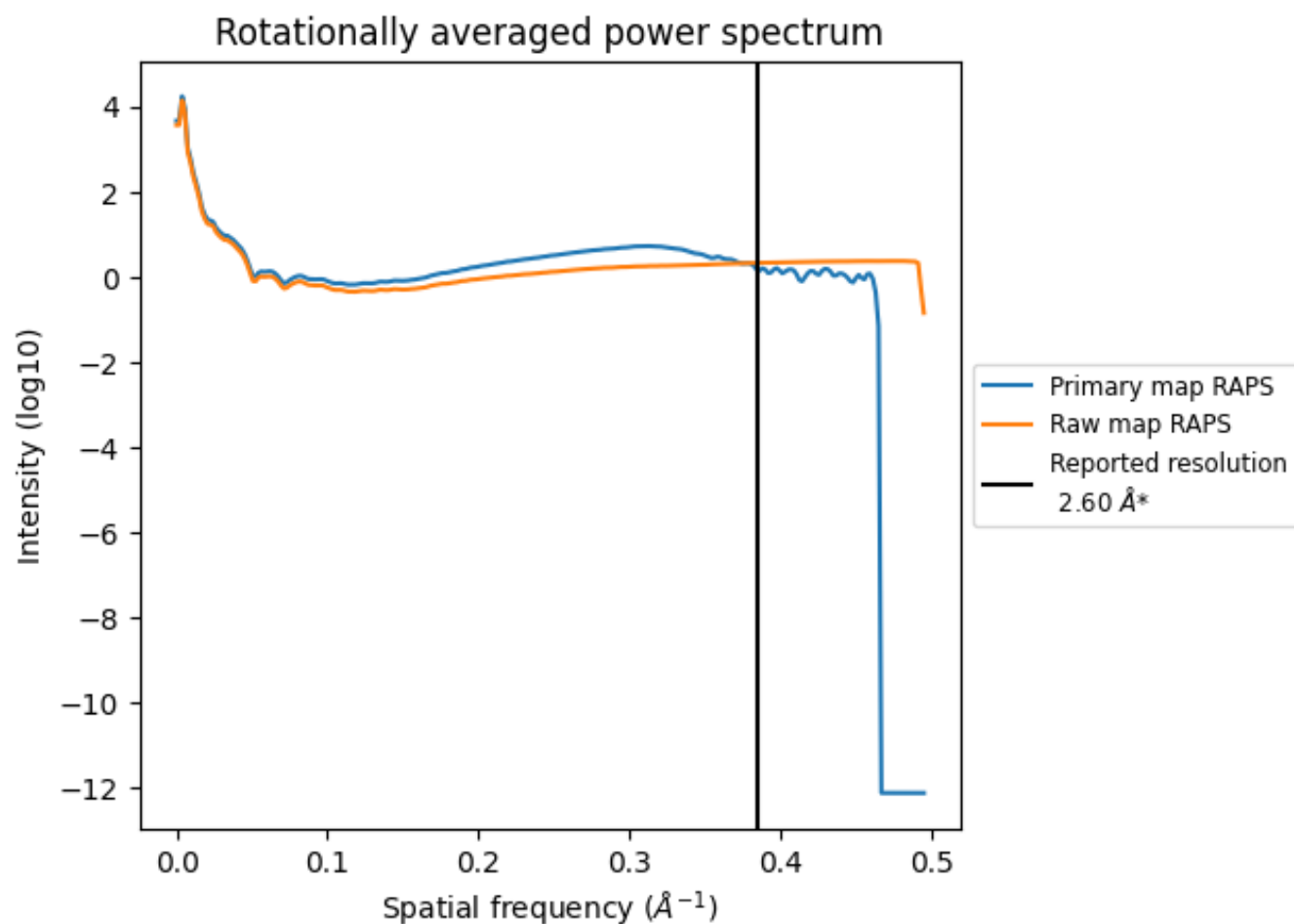
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 202 nm³; this corresponds to an approximate mass of 182 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 ⓘ

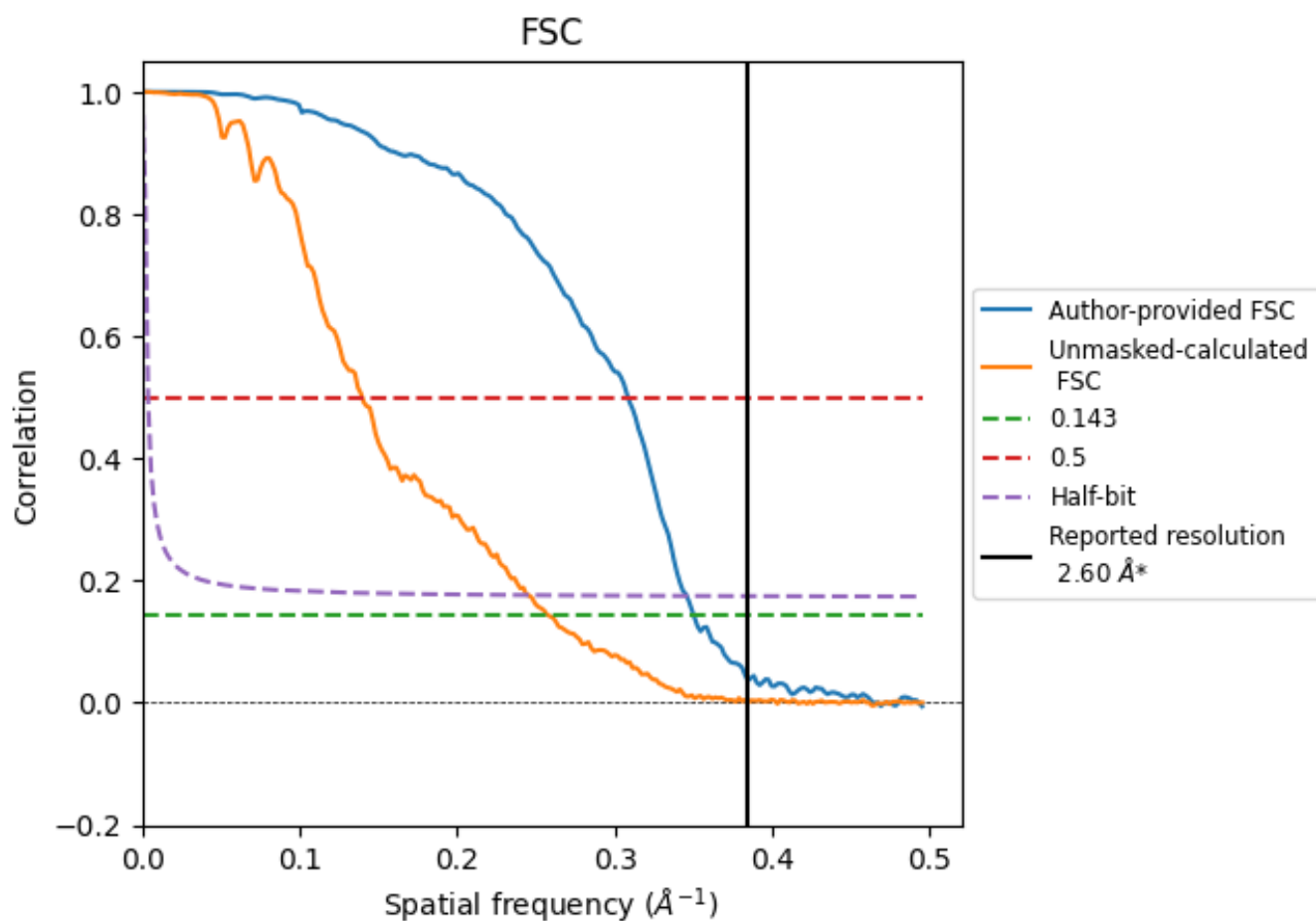


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

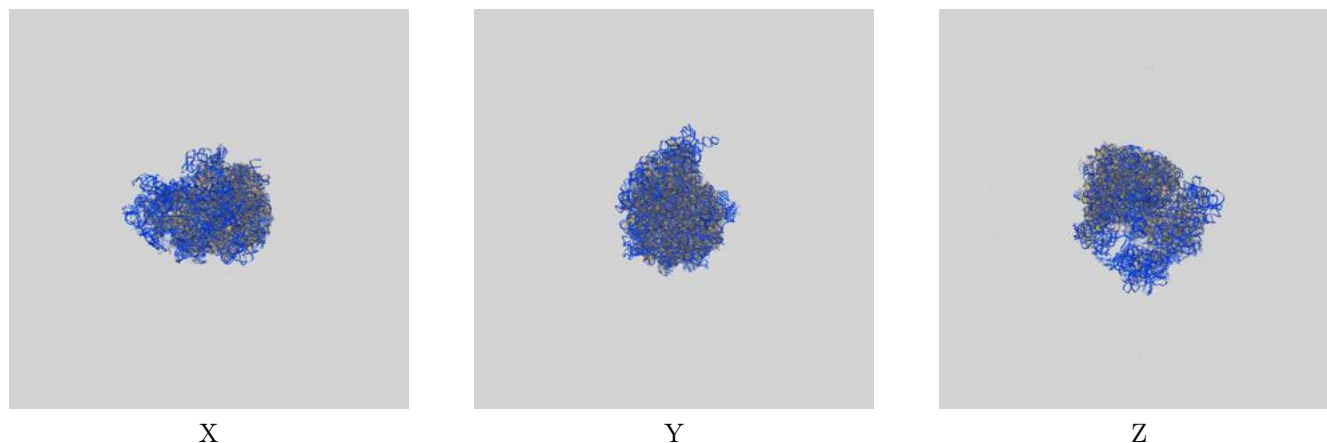
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.86	3.24	2.89
Unmasked-calculated*	3.88	7.16	4.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.88 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

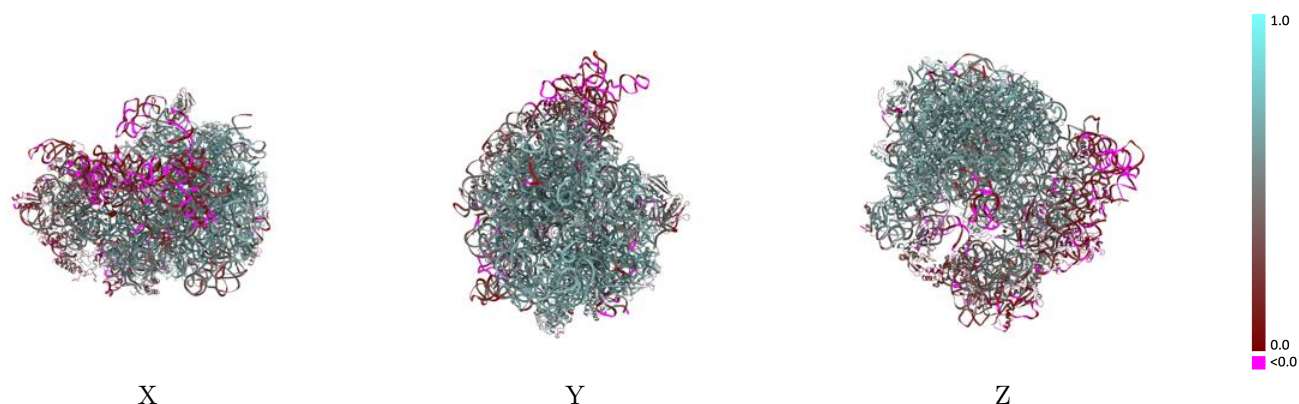
This section contains information regarding the fit between EMDB map EMD-67081 and PDB model 23WI. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



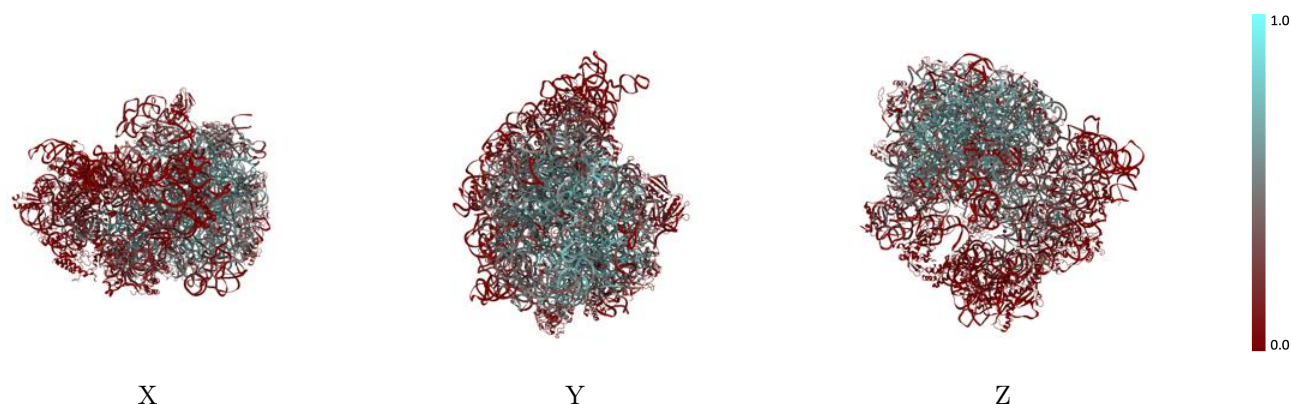
The images above show the 3D surface view of the map at the recommended contour level 0.0077 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



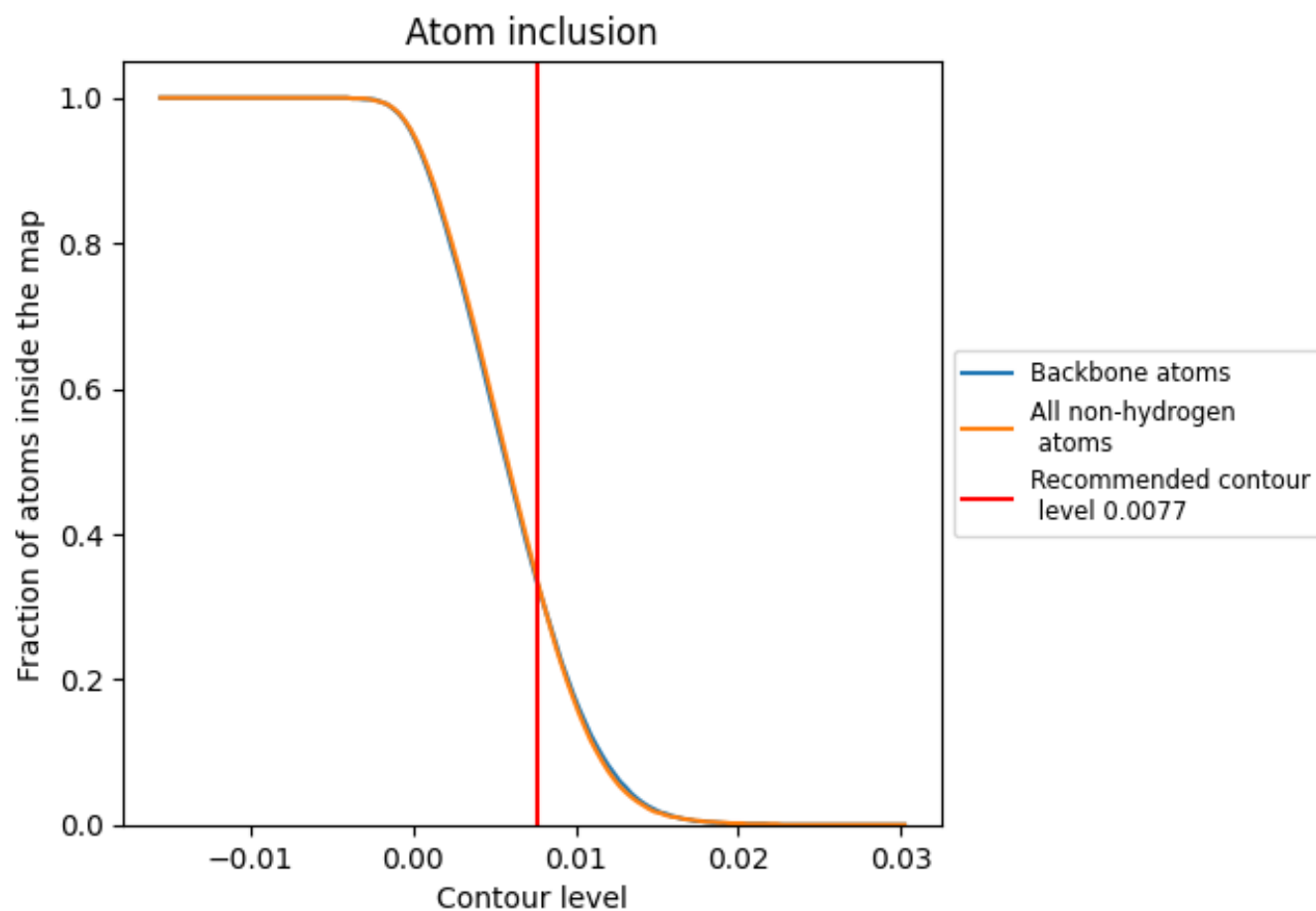
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0077).

9.4 Atom inclusion [i](#)



At the recommended contour level, 33% of all backbone atoms, 33% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0077) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3300	 0.4850
0	 0.4710	 0.5850
1	 0.2540	 0.5180
2	 0.5750	 0.6330
3	 0.5250	 0.6210
4	 0.3210	 0.5770
5	 0.4770	 0.5510
6	 0.0000	 0.1630
A	 0.5130	 0.5860
B	 0.2410	 0.5220
C	 0.4480	 0.6090
D	 0.4300	 0.6010
E	 0.3110	 0.5450
F	 0.0110	 0.3070
G	 0.0560	 0.4260
J	 0.3980	 0.5980
K	 0.3430	 0.5800
L	 0.3610	 0.5750
M	 0.3390	 0.5830
N	 0.4850	 0.6150
O	 0.1630	 0.5170
P	 0.3370	 0.5570
Q	 0.5380	 0.6380
R	 0.3340	 0.5320
S	 0.4010	 0.5730
T	 0.2850	 0.5190
U	 0.1980	 0.5080
V	 0.1900	 0.5290
W	 0.4100	 0.6060
X	 0.3790	 0.5740
Y	 0.1310	 0.4430
Z	 0.3570	 0.5860
a	 0.2070	 0.3990
b	 0.0110	 0.3020
c	 0.0550	 0.3980



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Chain	Atom inclusion	Q-score
d	 0.0190	 0.0900
e	 0.1570	 0.4970
f	 0.0540	 0.3960
g	 0.0010	 0.1740
h	 0.1600	 0.5120
i	 0.0110	 0.2470
j	 0.0250	 0.2690
k	 0.0820	 0.4290
l	 0.0510	 0.1700
m	 0.0040	 0.2730
n	 0.0250	 0.3640
o	 0.1460	 0.4570
p	 0.0480	 0.0790
q	 0.0410	 0.2800
r	 0.1420	 0.4810
s	 0.0020	 0.2630
t	 0.0370	 0.1700
u	 0.0150	 0.2100