Full wwPDB EM Validation Report ⓘ

Sep 16, 2026 – 07:33 AM EDT

PDB ID	:	6OSK / pdb_00006osk
EMDB ID	:	EMD-20184
Title	:	RF1 accommodated 70S complex at 60 ms
Authors	:	Fu, Z.; Indrisiunaite, G.; Kaledhonkar, S.; Shah, B.; Sun, M.; Chen, B.; Grassucci, R.A.; Ehrenberg, M.; Frank, J.
Deposited on	:	2019-05-01
Resolution	:	3.60 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:

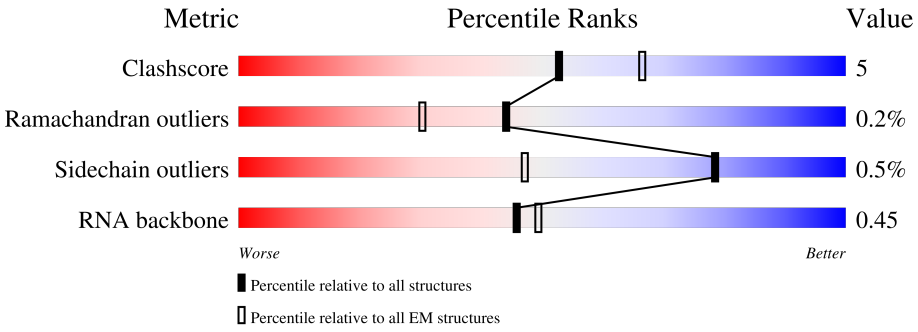
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

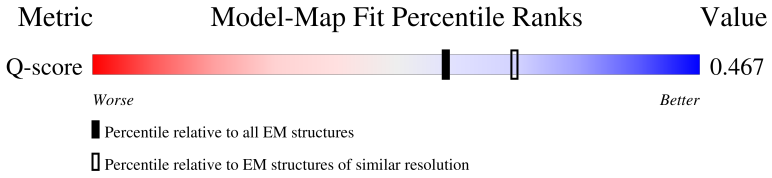
1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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 <=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	1	2903	7% 66% 29% 5%
2	2	1534	5% 66% 28% 6%
3	3	120	64% 29% 7%

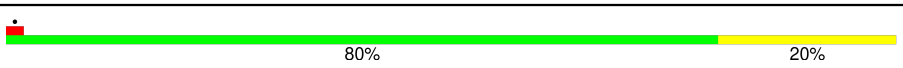
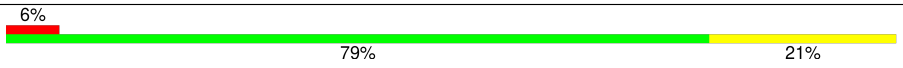
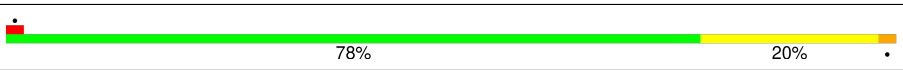
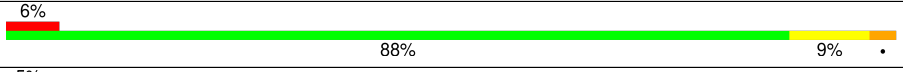
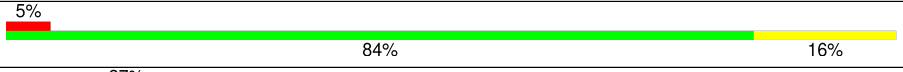
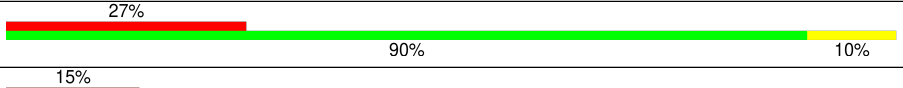
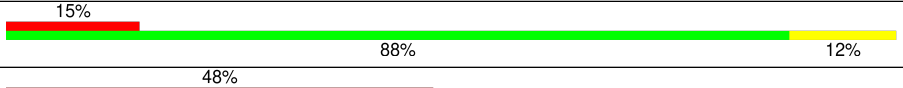
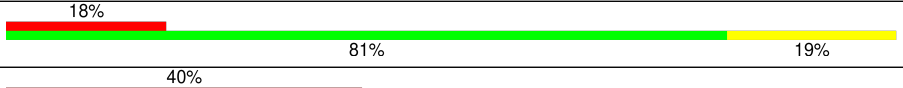
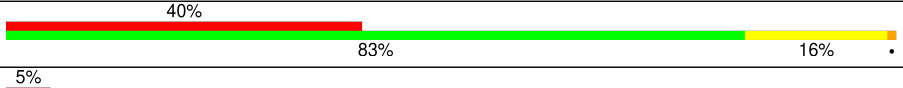
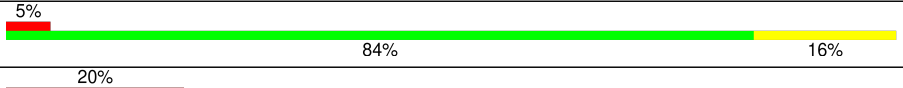
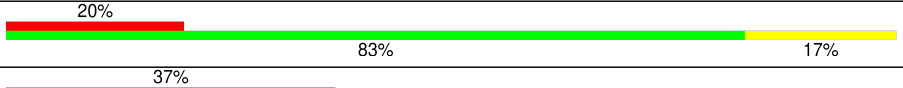
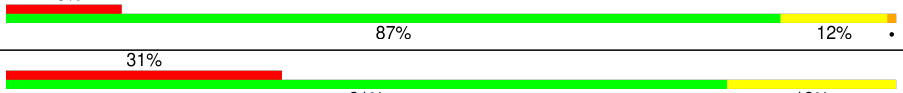
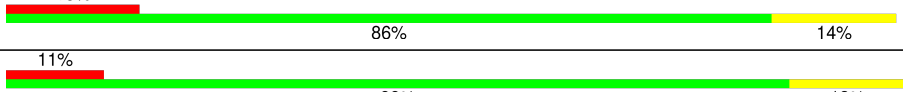
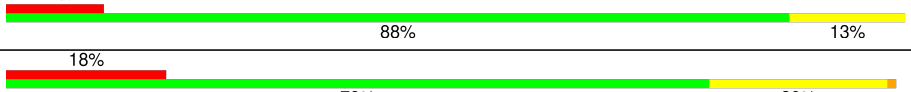
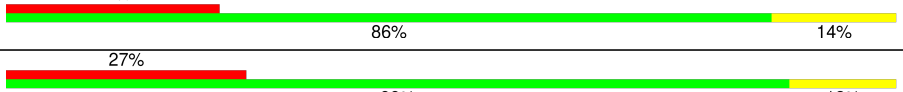
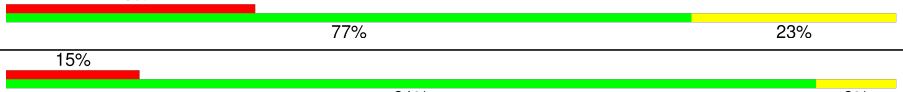
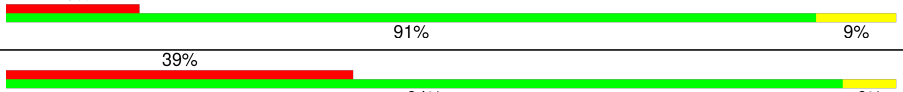
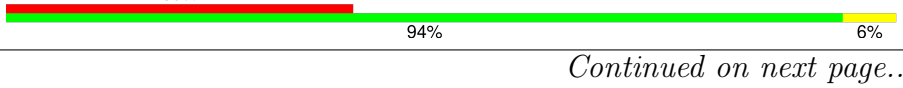
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Mol	Chain	Length	Quality of chain
4	4	9	67% 22% 11%
5	B	271	79% 21%
6	C	209	84% 15%
7	D	201	6% 87% 12%
8	E	177	35% 83% 16%
9	F	175	16% 89% 11%
10	G	149	74% 79% 21%
11	J	142	85% 15%
12	K	123	7% 87% 13%
13	L	144	83% 17%
14	M	136	83% 17%
15	N	119	86% 14%
16	O	116	16% 91% 9%
17	P	114	8% 84% 16%
18	Q	117	85% 15%
19	R	103	5% 83% 14%
20	S	110	87% 13%
21	T	94	11% 88% 12%
22	U	103	12% 86% 14%
23	V	94	18% 86% 14%
24	W	76	80% 20%
25	X	77	8% 87% 13%
26	Y	62	10% 87% 13%
27	Z	58	5% 83% 17%
28	a	66	100% 85% 15%

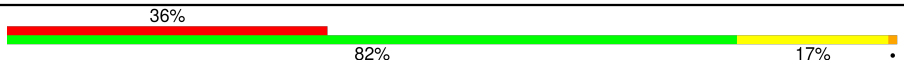
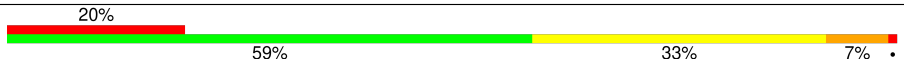
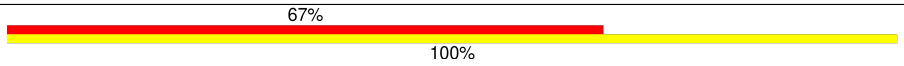
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Mol	Chain	Length	Quality of chain
29	b	56	
30	c	52	
31	d	46	
32	e	64	
33	f	38	
34	g	225	
35	h	208	
36	i	205	
37	j	156	
38	k	104	
39	l	151	
40	m	129	
41	n	127	
42	o	99	
43	p	117	
44	q	123	
45	r	116	
46	s	100	
47	t	88	
48	u	82	
49	v	80	
50	w	66	
51	x	83	
52	y	86	
53	z	70	

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Mol	Chain	Length	Quality of chain
54	A	259	
55	5	76	
56	6	3	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 146659 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	2903	62336	27816	11470	20147	2903	0	0

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	1534	32929	14693	6041	10661	1534	0	0

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	3	120	2569	1144	468	837	120	0	0

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	4	9	184	83	26	66	9	0	0

- Molecule 5 is a protein called 50S ribosomal protein L2.

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

- Molecule 6 is a protein called 50S ribosomal protein L3.

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

- Molecule 7 is a protein called 50S ribosomal protein L4.

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

- Molecule 8 is a protein called 50S ribosomal protein L5.

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

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 11 is a protein called 50S ribosomal protein L13.

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

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 14 is a protein called 50S ribosomal protein L16.

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

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 16 is a protein called 50S ribosomal protein L18.

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

- Molecule 17 is a protein called 50S ribosomal protein L19.

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

- Molecule 18 is a protein called 50S ribosomal protein L20.

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

- Molecule 19 is a protein called 50S ribosomal protein L21.

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

- Molecule 20 is a protein called 50S ribosomal protein L22.

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

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	U	103	Total	C	N	O	0	0
			788	498	148	142		

- Molecule 23 is a protein called 50S ribosomal protein L25.

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

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 25 is a protein called 50S ribosomal protein L28.

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

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 28 is a protein called 50S ribosomal protein L31.

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

- Molecule 29 is a protein called 50S ribosomal protein L32.

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

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	c	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 31 is a protein called 50S ribosomal protein L34.

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

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

- Molecule 36 is a protein called 30S ribosomal protein S4.

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

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 39 is a protein called 30S ribosomal protein S7.

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

- Molecule 40 is a protein called 30S ribosomal protein S8.

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

- Molecule 41 is a protein called 30S ribosomal protein S9.

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

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o	99	Total 790	C 495	N 151	O 143	S 1	0	0

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	p	117	Total 877	C 540	N 174	O 160	S 3	0	0

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	123	Total 957	C 591	N 196	O 165	S 5	0	0

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	116	Total 900	C 558	N 181	O 158	S 3	0	0

- Molecule 46 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	100	Total 805	C 499	N 164	O 139	S 3	0	0

- Molecule 47 is a protein called 30S ribosomal protein S15.

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

- Molecule 48 is a protein called 30S ribosomal protein S16.

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

- Molecule 49 is a protein called 30S ribosomal protein S17.

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

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	w	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	y	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

- Molecule 53 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	z	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 54 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	A	259	Total	C	N	O	S	0	0
			2014	1235	382	389	8		

- Molecule 55 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	5	76	Total	C	N	O	P	S	0	0
			1627	727	296	527	76	1		

- Molecule 56 is a protein called FME-PHE-PHE.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	6	3	Total	C	N	O	S	0	0
			32	24	3	4	1		

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	1	292	Total	Mg	0
			292	292	
57	2	1	Total	Mg	0
			1	1	
57	3	8	Total	Mg	0
			8	8	
57	C	1	Total	Mg	0
			1	1	
57	b	1	Total	Mg	0
			1	1	
57	f	1	Total	Mg	0
			1	1	
57	i	1	Total	Mg	0
			1	1	
57	5	2	Total	Mg	0
			2	2	

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	a	1	Total	Zn	0
			1	1	
58	f	1	Total	Zn	0
			1	1	

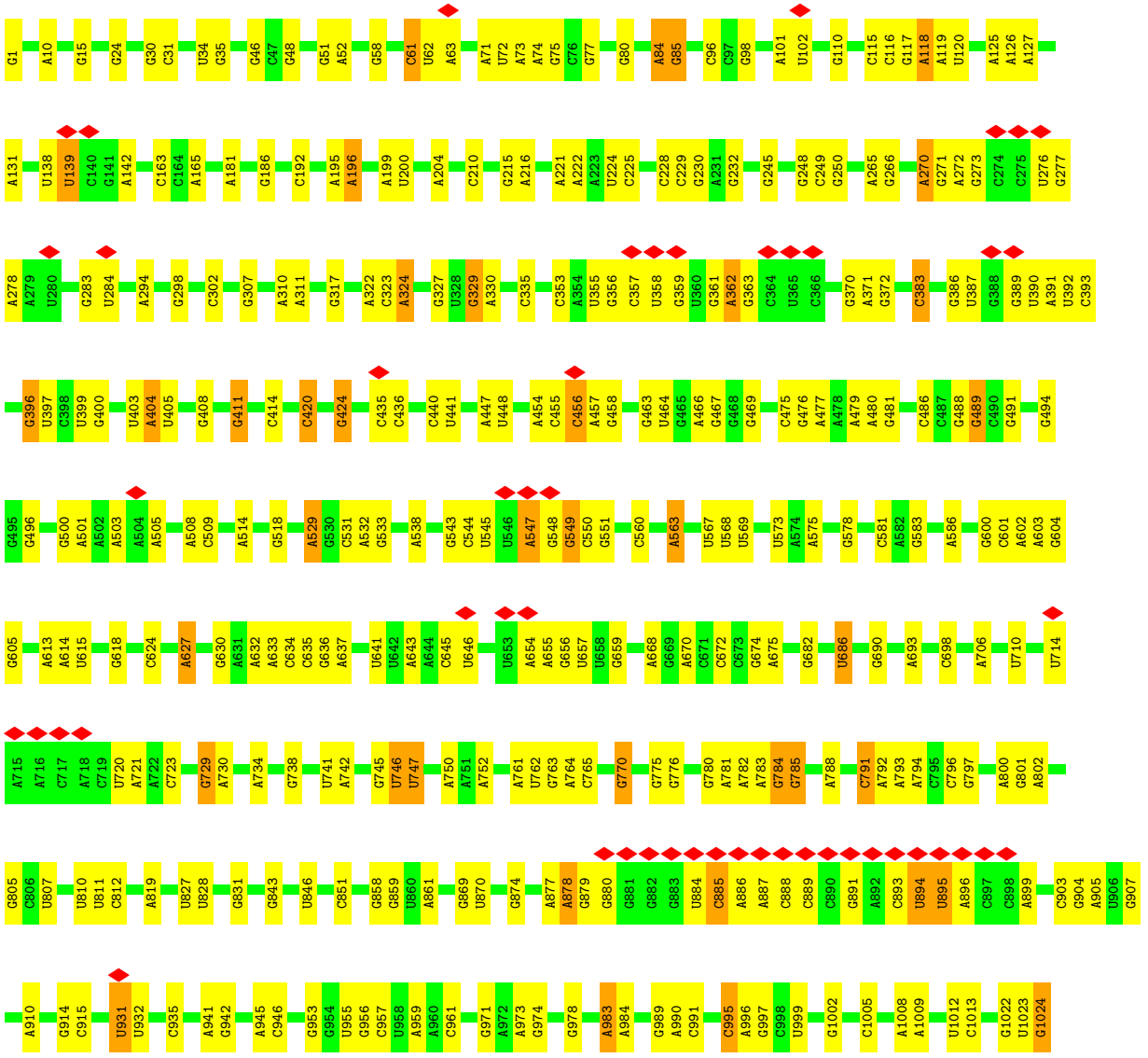
3 Residue-property plots (i)

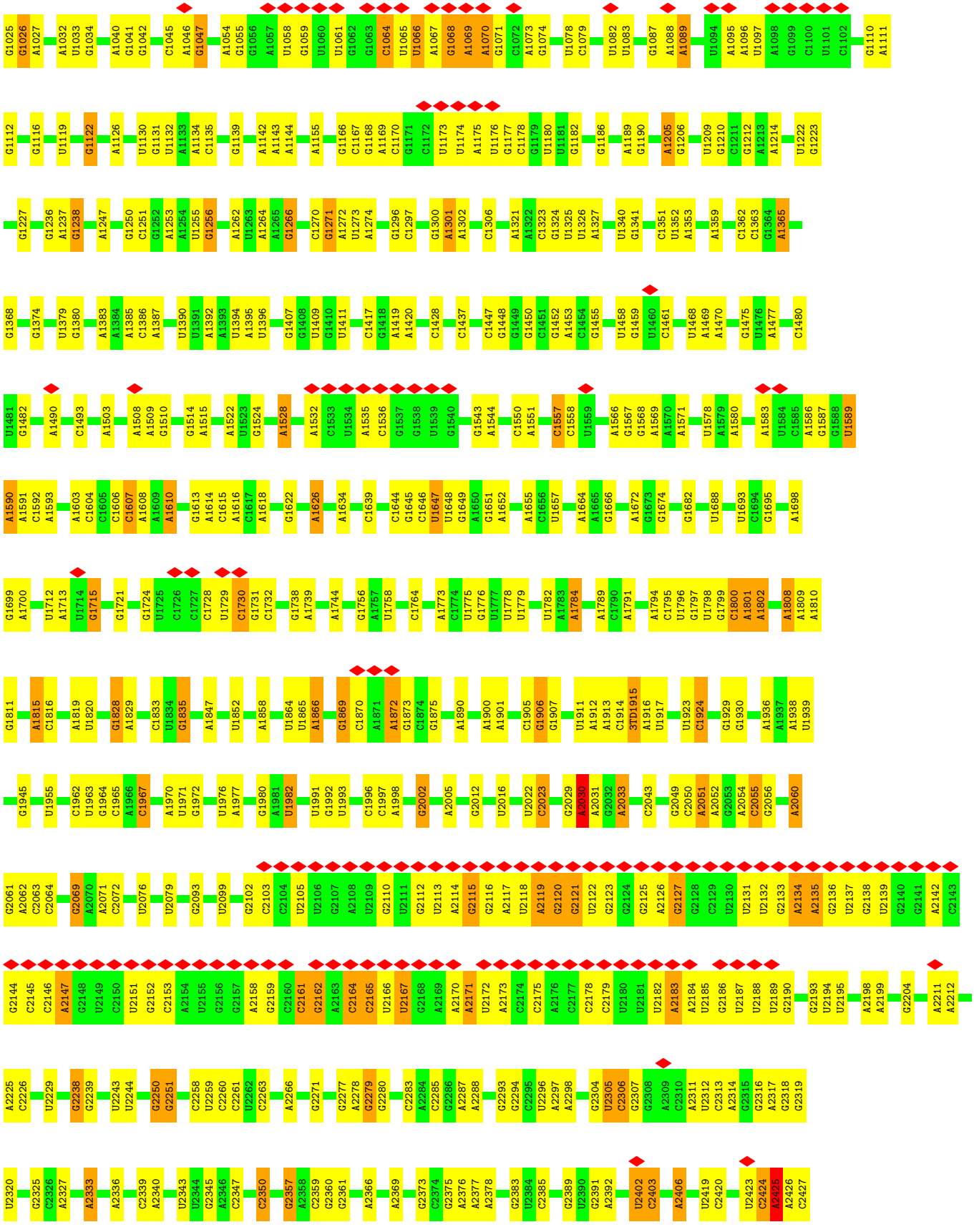
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

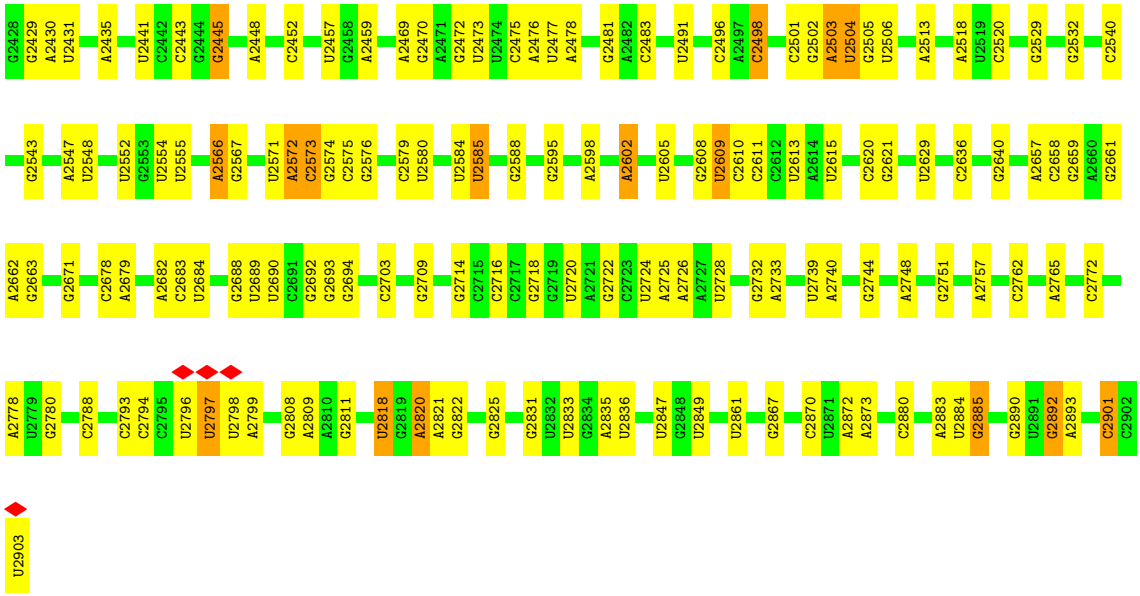
- Molecule 1: 23S ribosomal RNA

Chain 1:





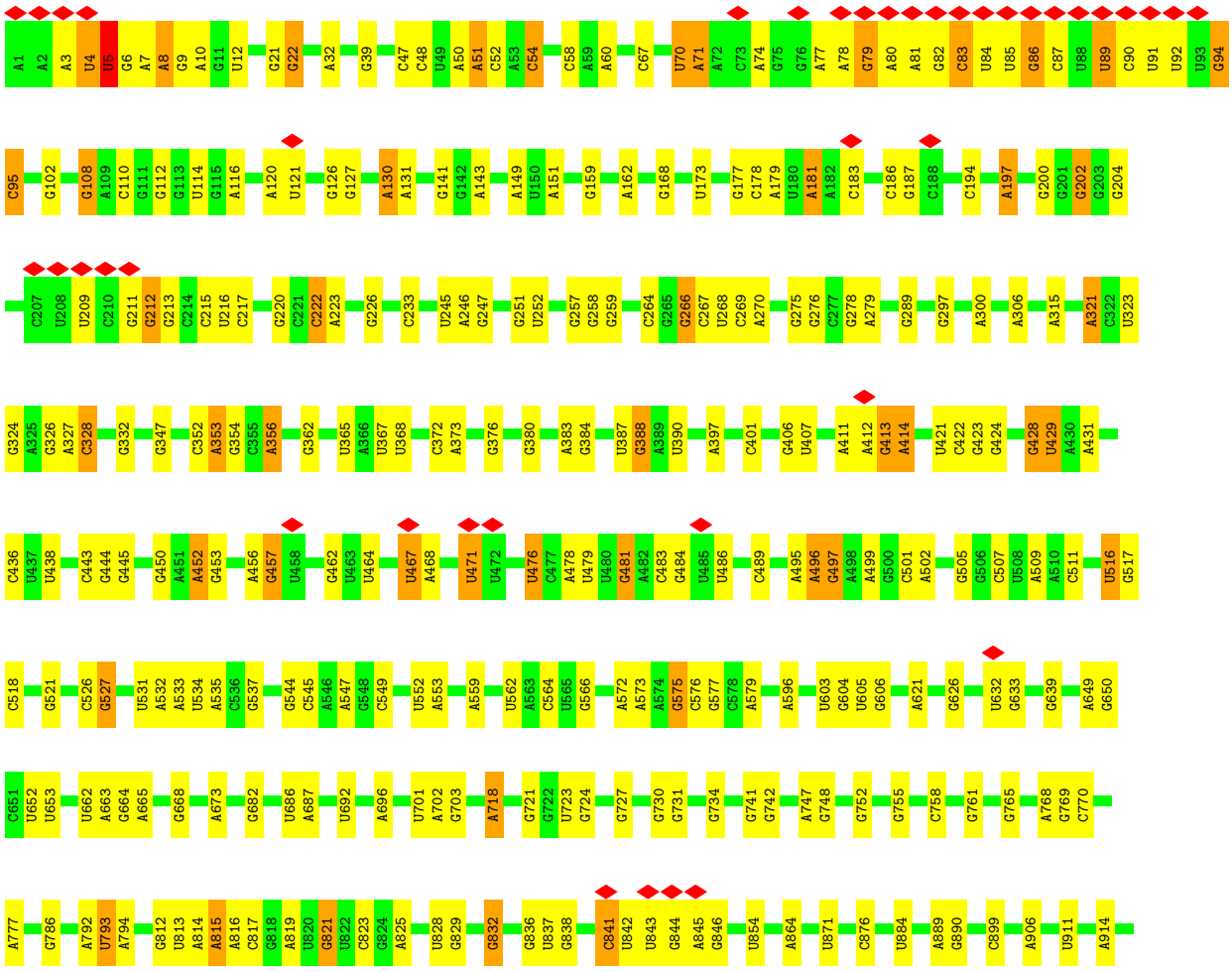

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G1112 G1116 U1119 G1122 A1126 U1130 G1131 U1132 A1133 A1134 C1135 G1139 A1142 A1143 A1144 A1155 G1166 C1167 G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 G1186 A1189 G1190 A1205 G1206 U1209 G1210 C1211 G1212 A1213 A1214 U1222 G1223
G1227 G1236 A1237 G1238 A1247 G1250 C1251 G1252 A1253 A1254 U1255 G1256 A1262 U1263 A1264 A1265 G1266 C1270 G1271 A1272 U1273 A1274 G1296 C1297 G1300 A1301 A1302 C1306 A1321 A1322 C1323 G1324 U1325 U1326 A1327 U1340 G1341 C1351 U1352 A1353 A1359 C1362 C1363 G1364 A1365
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G2061 A2062 C2063 C2064 G2069 G2148 A2070 A2071 C2072 U2076 U2079 G2093 U2099 G2102 C2103 C2104 U2105 U2106 G2107 A2108 U2109 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 G2128 C2129 U2130 U2131 U2132 G2133 A2134 A2135 G2136 U2137 G2138 U2139 G2140 G2141 A2142 C2143
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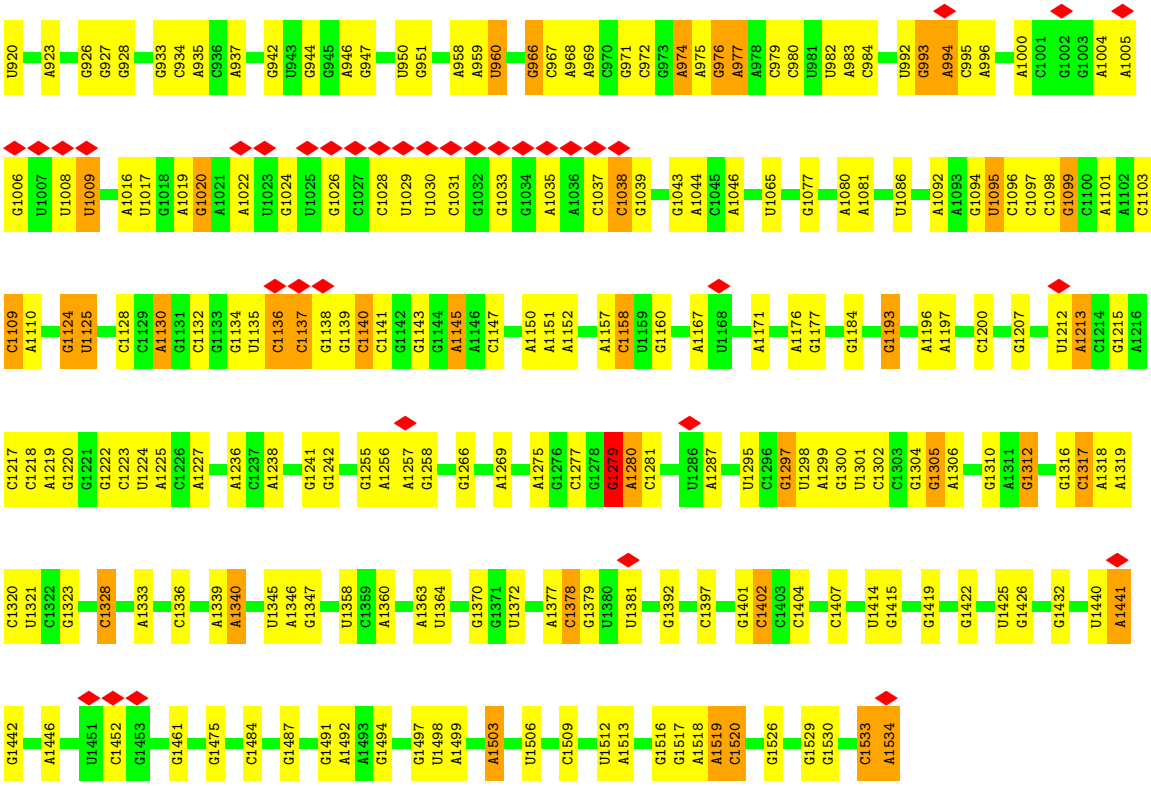


• Molecule 2: 16S ribosomal RNA

Chain 2:



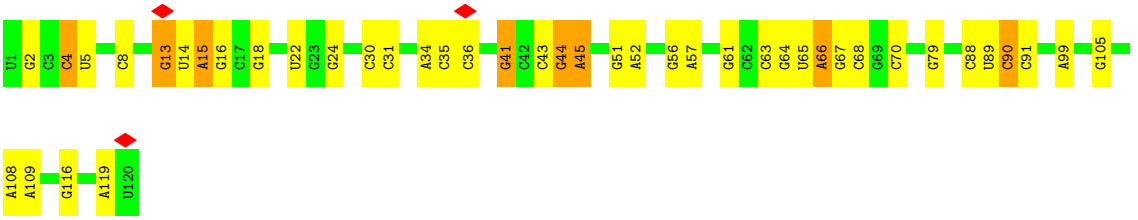




• Molecule 3: 5S ribosomal RNA

Chain 3:





• Molecule 4: mRNA

Chain 4:

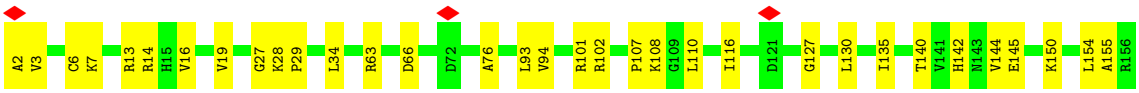


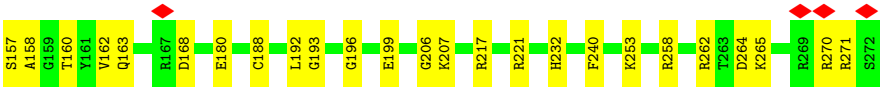


• Molecule 5: 50S ribosomal protein L2

Chain B:



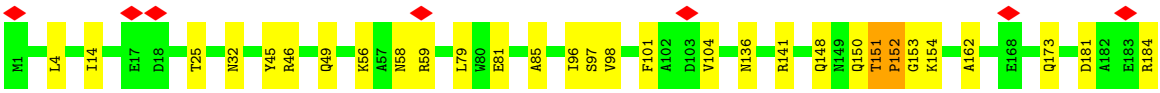


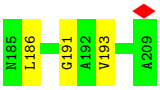


• Molecule 6: 50S ribosomal protein L3

Chain C:



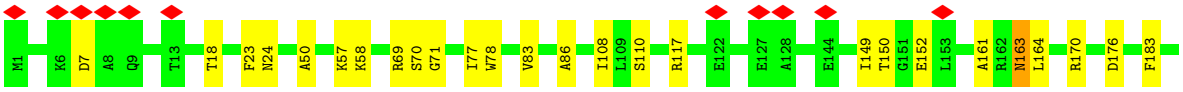




• Molecule 7: 50S ribosomal protein L4

Chain D:



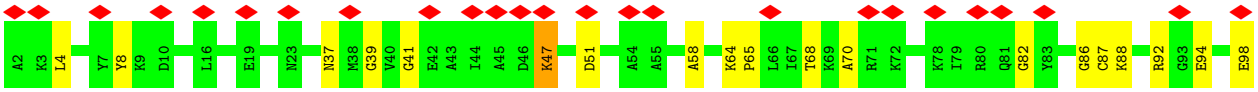


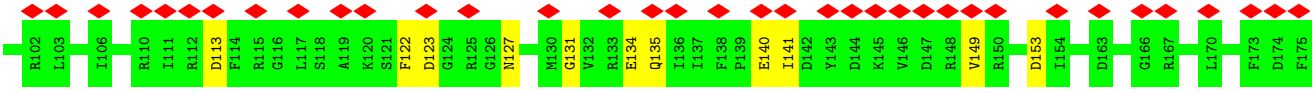


• Molecule 8: 50S ribosomal protein L5

Chain E:





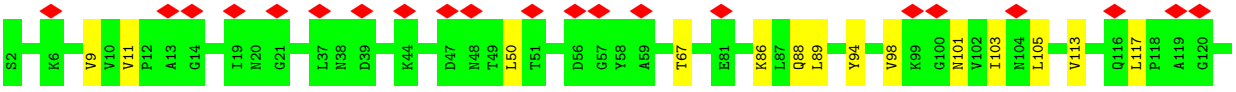


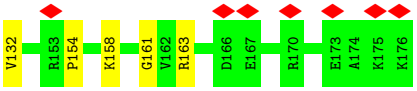


• Molecule 9: 50S ribosomal protein L6

Chain F:





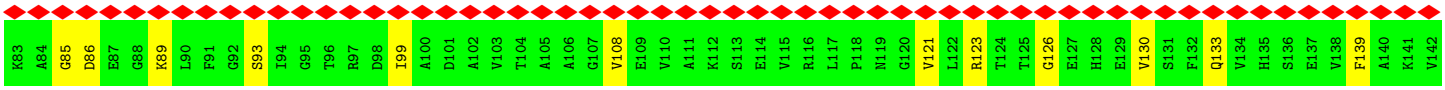


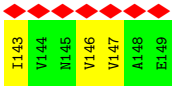
• Molecule 10: 50S ribosomal protein L9

Chain G:





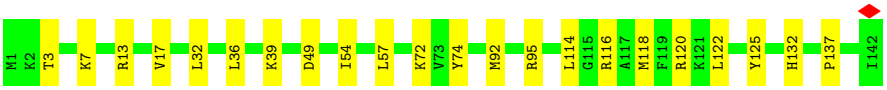




• Molecule 11: 50S ribosomal protein L13

Chain J:

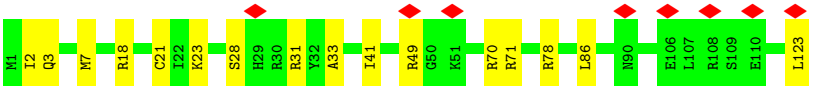




• Molecule 12: 50S ribosomal protein L14

Chain K:

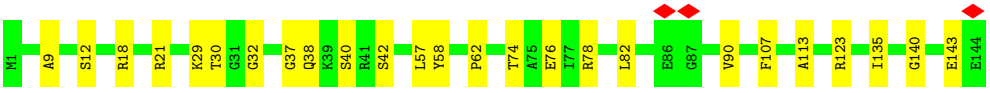




• Molecule 13: 50S ribosomal protein L15

Chain L:

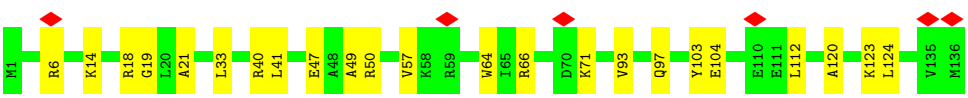




• Molecule 14: 50S ribosomal protein L16

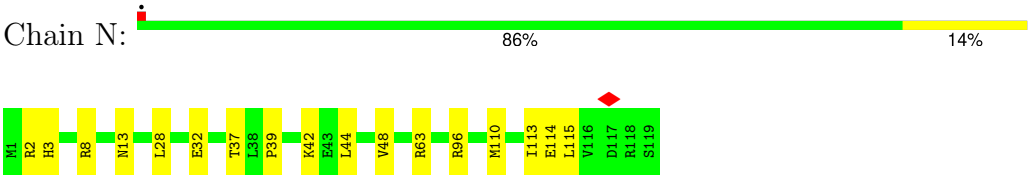
Chain M:





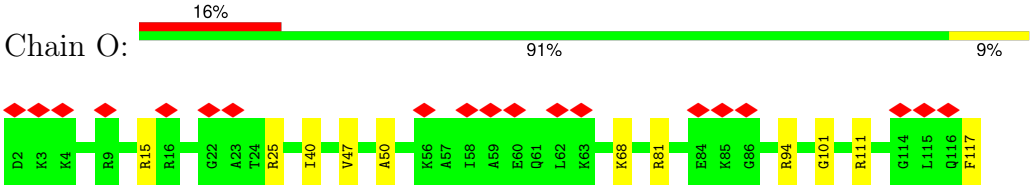
• Molecule 15: 50S ribosomal protein L17

Chain N:



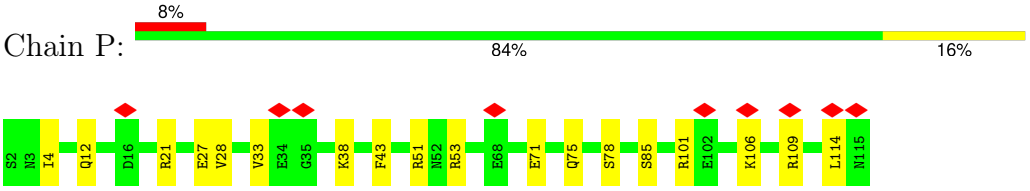
• Molecule 16: 50S ribosomal protein L18

Chain O:



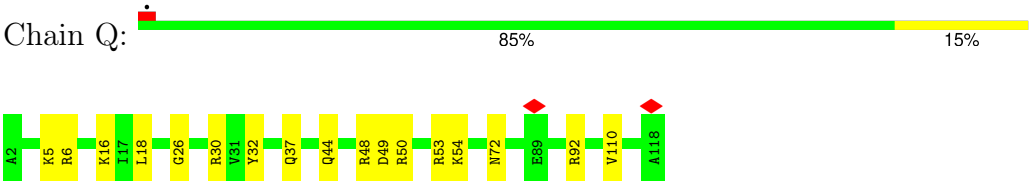
• Molecule 17: 50S ribosomal protein L19

Chain P:



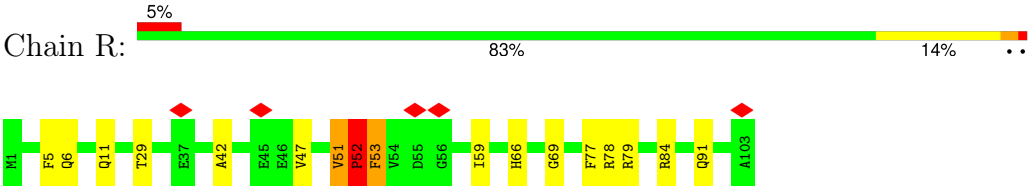
• Molecule 18: 50S ribosomal protein L20

Chain Q:



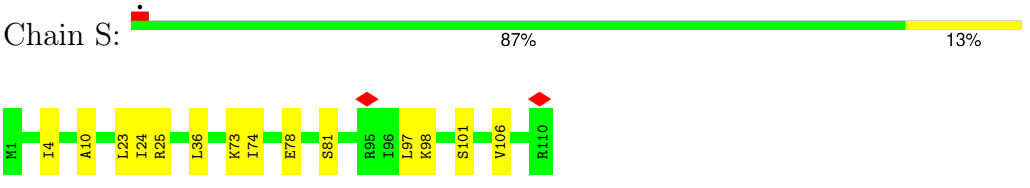
• Molecule 19: 50S ribosomal protein L21

Chain R:



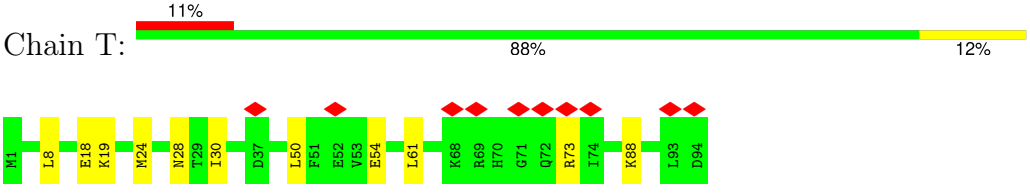
• Molecule 20: 50S ribosomal protein L22

Chain S:



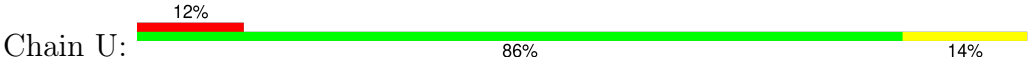
• Molecule 21: 50S ribosomal protein L23

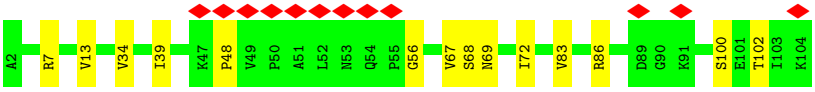
Chain T:



• Molecule 22: 50S ribosomal protein L24

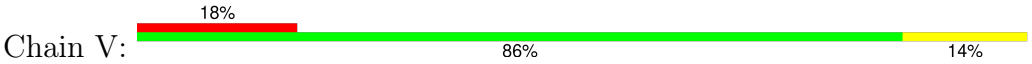
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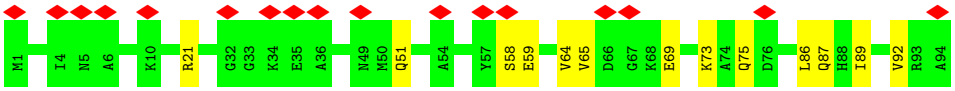




• Molecule 23: 50S ribosomal protein L25

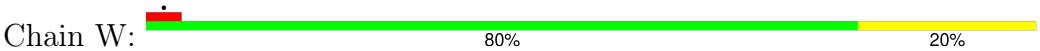
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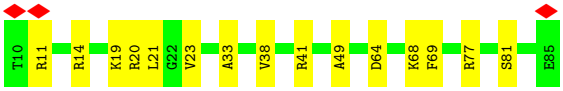




• Molecule 24: 50S ribosomal protein L27

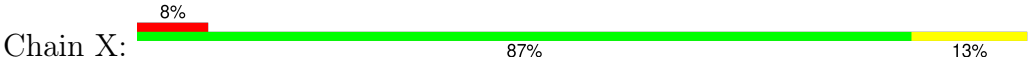
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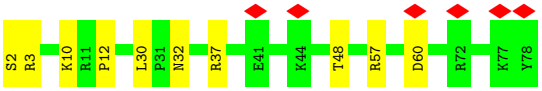




• Molecule 25: 50S ribosomal protein L28

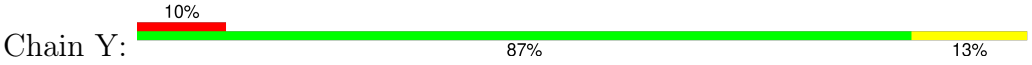
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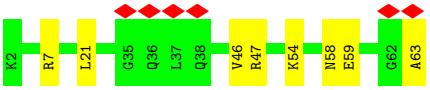




• Molecule 26: 50S ribosomal protein L29

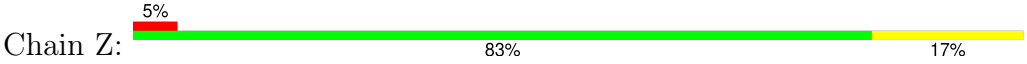
Chain Y:

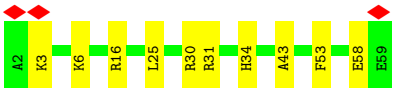




• Molecule 27: 50S ribosomal protein L30

Chain Z:





• Molecule 28: 50S ribosomal protein L31

Chain a:

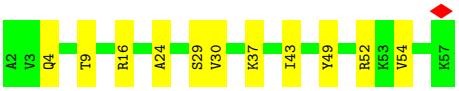




• Molecule 29: 50S ribosomal protein L32

Chain b:





• Molecule 30: 50S ribosomal protein L33

Chain c:

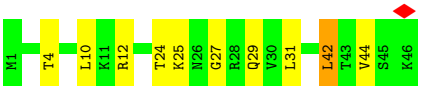




• Molecule 31: 50S ribosomal protein L34

Chain d:

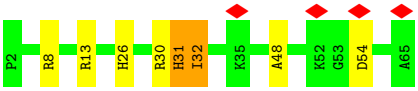




• Molecule 32: 50S ribosomal protein L35

Chain e:

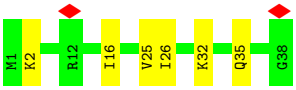




• Molecule 33: 50S ribosomal protein L36

Chain f:

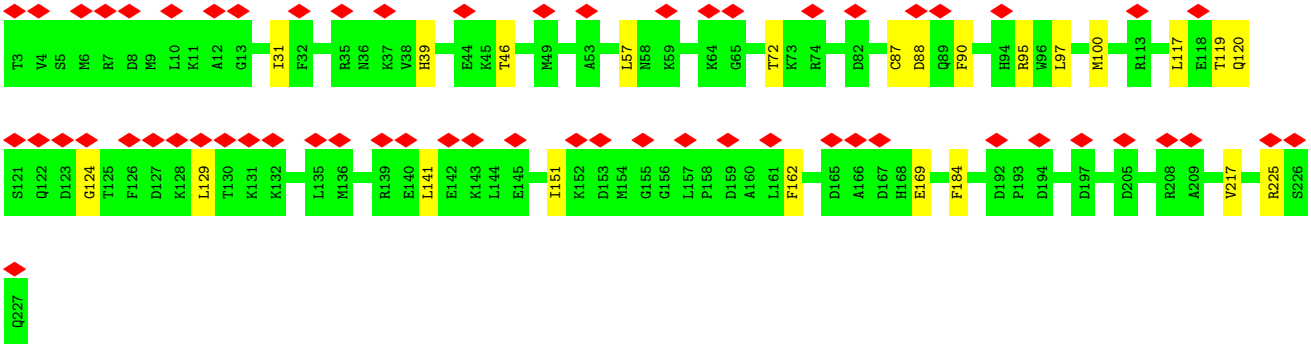




• Molecule 34: 30S ribosomal protein S2

Chain g:

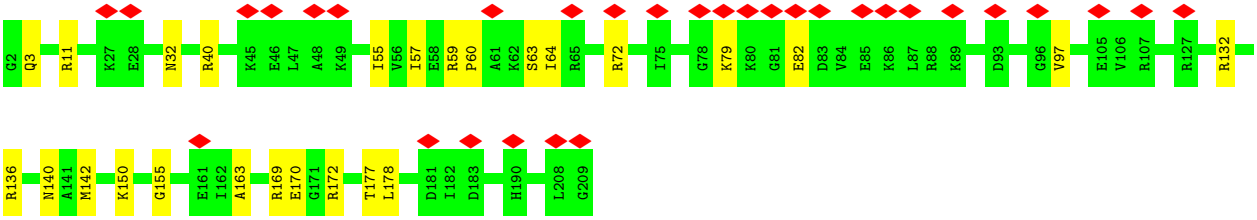




• Molecule 35: 30S ribosomal protein S3

Chain h:

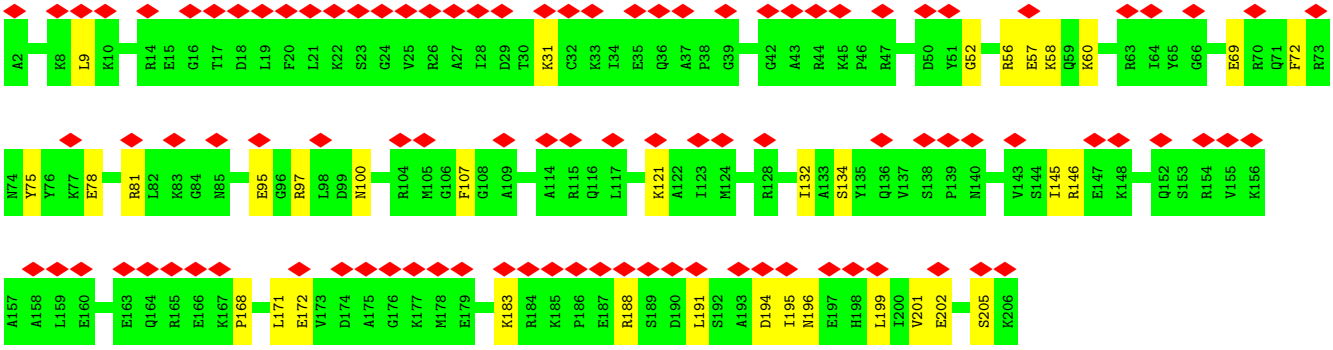




• Molecule 36: 30S ribosomal protein S4

Chain i:





• Molecule 37: 30S ribosomal protein S5

Chain j:

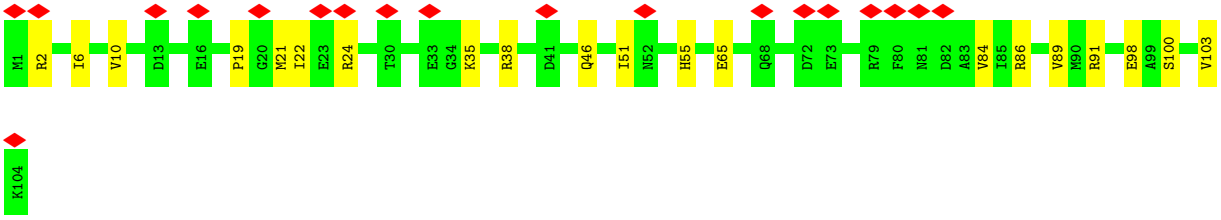




• Molecule 38: 30S ribosomal protein S6

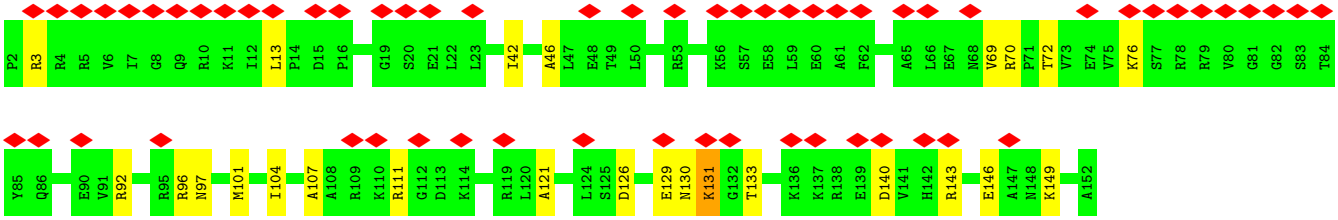
Chain k:



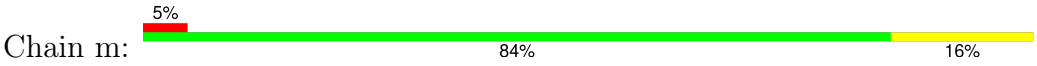


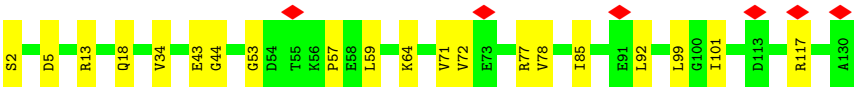
• Molecule 39: 30S ribosomal protein S7





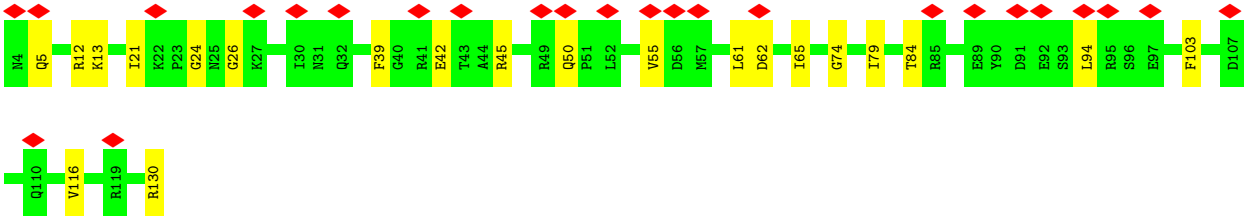
• Molecule 40: 30S ribosomal protein S8





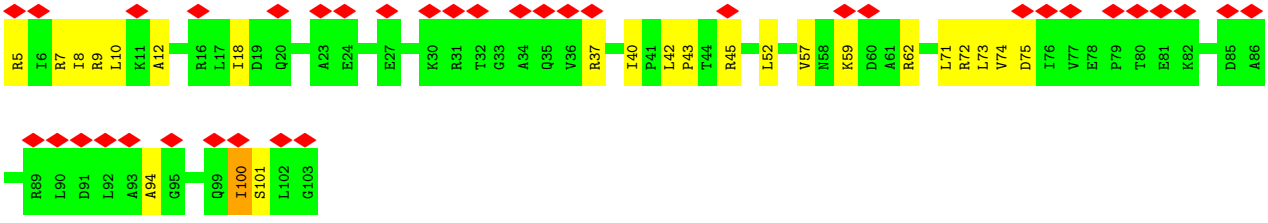
• Molecule 41: 30S ribosomal protein S9





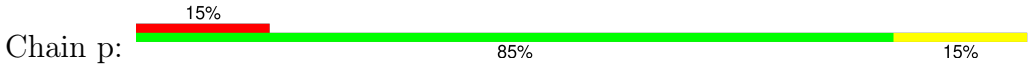
• Molecule 42: 30S ribosomal protein S10

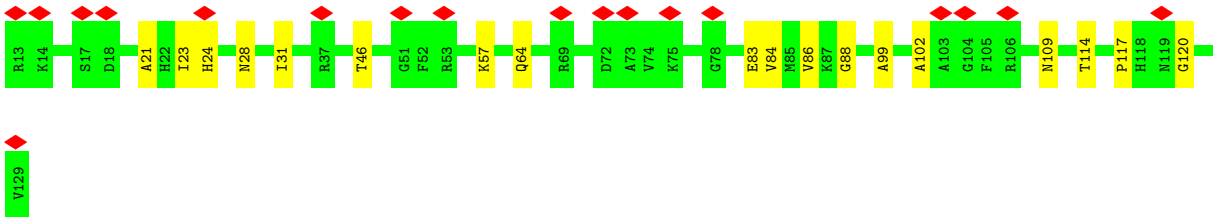




• Molecule 43: 30S ribosomal protein S11

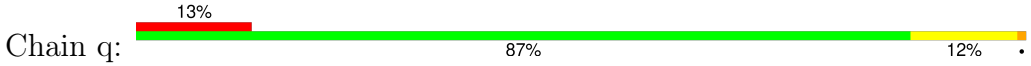
Chain p:





• Molecule 44: 30S ribosomal protein S12

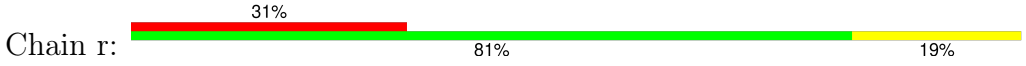
Chain q:

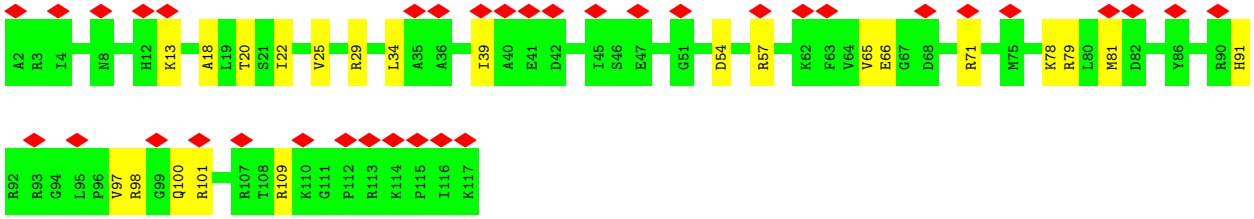




• Molecule 45: 30S ribosomal protein S13

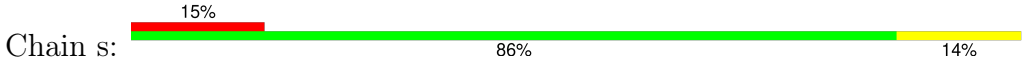
Chain r:

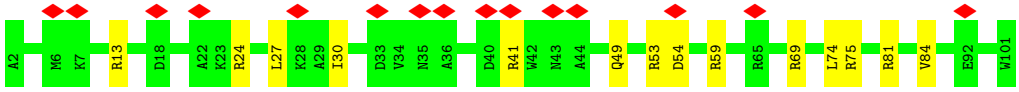




• Molecule 46: 30S ribosomal protein S14

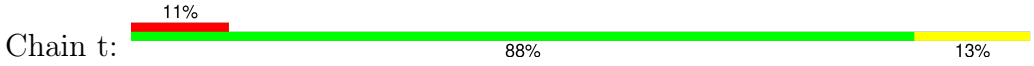
Chain s:

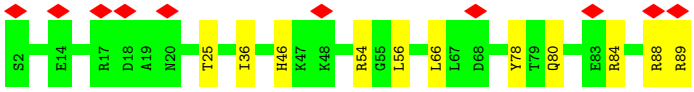




• Molecule 47: 30S ribosomal protein S15

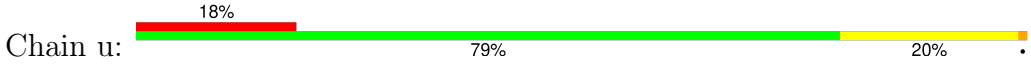
Chain t:

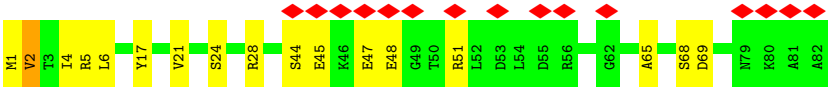




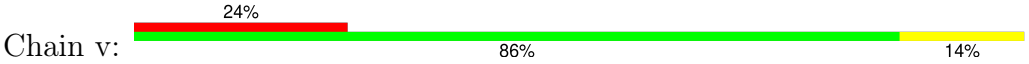
• Molecule 48: 30S ribosomal protein S16

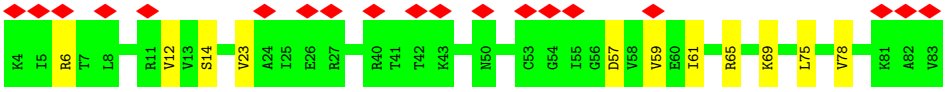
Chain u:



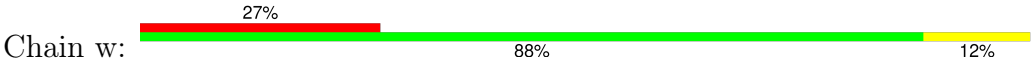


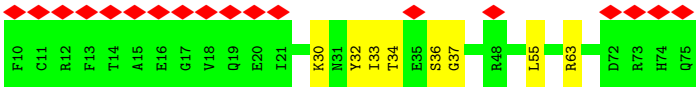
• Molecule 49: 30S ribosomal protein S17



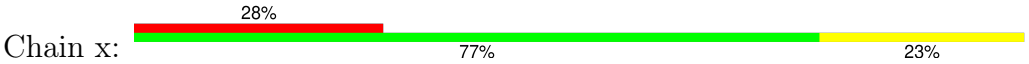


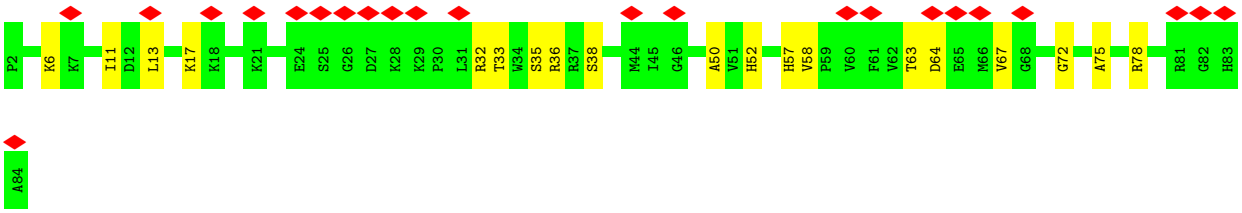
• Molecule 50: 30S ribosomal protein S18



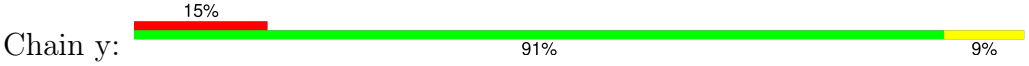


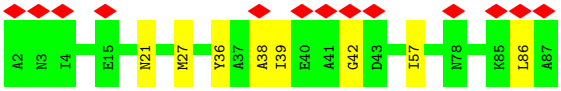
• Molecule 51: 30S ribosomal protein S19



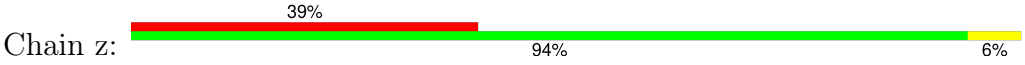


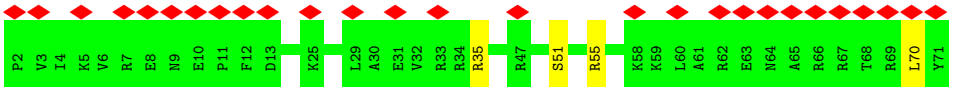
• Molecule 52: 30S ribosomal protein S20



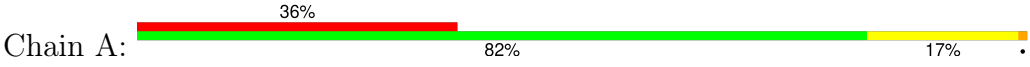


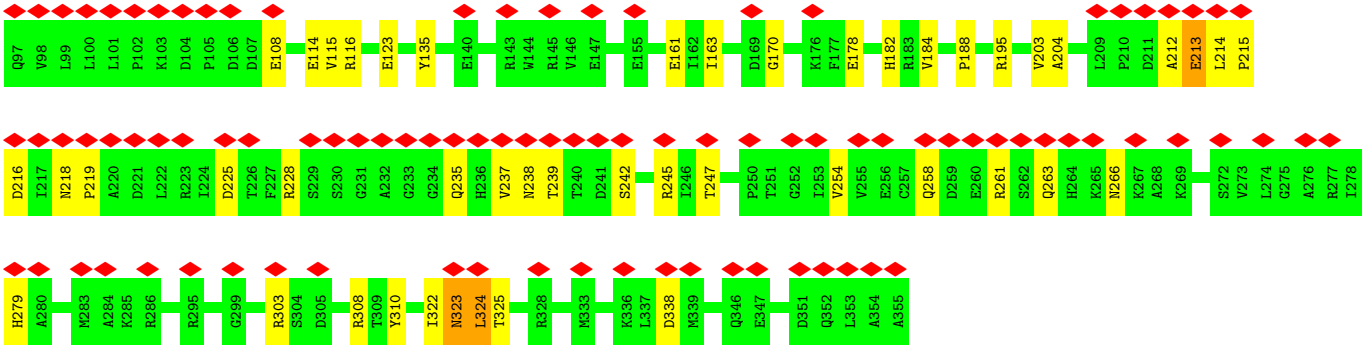
• Molecule 53: 30S ribosomal protein S21





• Molecule 54: Peptide chain release factor 1

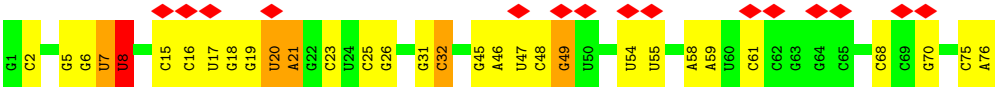




• Molecule 55: P-tRNA

Chain 5:





• Molecule 56: FME-PHE-PHE

Chain 6:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	202103	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	41.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.421	Depositor
Minimum map value	-0.221	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	421.12, 421.12, 421.12	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.645, 1.645, 1.645	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, H2U, 6MZ, OMU, G7M, ZN, 1MG, PSU, OMG, FME, 2MA, 5MU, MG, 0TD, OMC, UR3, MA6, 3TD, 5MC, 4OC, 4SU

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	1	0.44	0/69286	0.41	5/108087 (0.0%)
2	2	0.33	0/36590	0.36	2/57074 (0.0%)
3	3	0.29	0/2872	0.34	0/4478
4	4	0.45	0/203	0.42	0/312
5	B	0.52	0/2121	0.66	0/2852
6	C	0.49	0/1586	0.64	0/2134
7	D	0.44	0/1571	0.61	0/2113
8	E	0.29	0/1434	0.58	0/1926
9	F	0.28	0/1333	0.52	0/1805
10	G	0.33	1/1122 (0.1%)	0.63	2/1515 (0.1%)
11	J	0.46	0/1152	0.58	0/1551
12	K	0.46	0/955	0.62	0/1279
13	L	0.44	0/1062	0.61	0/1413
14	M	0.41	0/1093	0.57	0/1460
15	N	0.49	0/964	0.69	0/1289
16	O	0.28	0/902	0.60	0/1209
17	P	0.42	0/929	0.57	0/1242
18	Q	0.56	0/960	0.67	0/1278
19	R	0.46	0/829	0.67	1/1107 (0.1%)
20	S	0.51	0/864	0.58	0/1156
21	T	0.37	0/752	0.60	0/1005
22	U	0.37	0/796	0.60	0/1062
23	V	0.31	0/766	0.55	0/1025
24	W	0.45	0/589	0.60	0/779
25	X	0.42	0/635	0.55	0/848
26	Y	0.33	0/502	0.51	0/667
27	Z	0.45	0/452	0.61	0/605
28	a	0.24	0/531	0.50	0/709
29	b	0.47	0/450	0.68	0/599
30	c	0.34	0/433	0.58	0/576
31	d	0.57	0/380	0.72	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	e	0.50	0/513	0.68	0/676
33	f	0.42	0/303	0.62	0/397
34	g	0.31	0/1791	0.65	2/2413 (0.1%)
35	h	0.33	0/1663	0.57	0/2241
36	i	0.26	0/1665	0.56	0/2227
37	j	0.39	0/1165	0.67	4/1568 (0.3%)
38	k	0.31	0/867	0.62	0/1171
39	l	0.27	0/1195	0.57	0/1602
40	m	0.35	0/989	0.57	0/1326
41	n	0.29	0/1034	0.63	0/1375
42	o	0.30	0/800	0.57	0/1082
43	p	0.31	0/893	0.51	0/1205
44	q	0.38	0/960	0.65	0/1286
45	r	0.27	0/909	0.62	0/1215
46	s	0.29	0/817	0.55	0/1088
47	t	0.33	0/722	0.59	0/964
48	u	0.31	0/659	0.62	0/884
49	v	0.26	0/657	0.58	0/881
50	w	0.30	0/553	0.55	0/743
51	x	0.26	0/680	0.49	0/915
52	y	0.28	0/675	0.56	0/895
53	z	0.29	0/597	0.64	0/792
54	A	0.38	0/2046	0.65	0/2759
55	5	0.29	0/1704	0.36	0/2654
56	6	0.56	0/23	0.92	0/29
All	All	0.40	1/157994 (0.0%)	0.46	16/236041 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	77	THR	CA-CB	7.35	1.66	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	404	A	C4'-C3'-O3'	8.79	122.58	109.40
1	1	2820	A	C4'-C3'-O3'	-6.85	102.72	113.00
10	G	30	LEU	CA-C-N	6.49	124.33	120.24
10	G	30	LEU	C-N-CA	6.49	124.33	120.24
1	1	2425	A	C4'-C3'-O3'	6.36	118.94	109.40
2	2	1279	G	C4'-C3'-O3'	-6.30	103.56	113.00
34	g	46	THR	CA-C-N	5.62	124.83	120.33

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	g	46	THR	C-N-CA	5.62	124.83	120.33
2	2	5	U	C4'-C3'-O3'	5.38	117.46	109.40
37	j	55	GLU	CA-C-N	5.37	124.63	120.33
37	j	55	GLU	C-N-CA	5.37	124.63	120.33
1	1	729	G	C2'-C3'-O3'	-5.16	105.96	113.70
1	1	729	G	C3'-C2'-O2'	5.11	118.37	110.70
37	j	69	ARG	CA-C-N	5.04	129.56	122.46
37	j	69	ARG	C-N-CA	5.04	129.56	122.46
19	R	52	PRO	N-CA-C	-5.02	102.12	112.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	62336	0	31367	360	0
2	2	32929	0	16587	202	0
3	3	2569	0	1301	21	0
4	4	184	0	95	1	0
5	B	2082	0	2154	41	0
6	C	1565	0	1616	36	0
7	D	1552	0	1619	18	0
8	E	1410	0	1444	22	0
9	F	1313	0	1358	10	0
10	G	1111	0	1148	18	0
11	J	1129	0	1162	14	0
12	K	946	0	1023	12	0
13	L	1053	0	1129	19	0
14	M	1074	0	1157	15	0
15	N	951	0	994	11	0
16	O	892	0	923	7	0
17	P	917	0	962	12	0
18	Q	947	0	1019	12	0
19	R	816	0	839	23	0
20	S	857	0	922	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	T	746	0	811	7	0
22	U	788	0	843	10	0
23	V	753	0	780	7	0
24	W	582	0	599	10	0
25	X	625	0	652	9	0
26	Y	501	0	531	7	0
27	Z	448	0	488	6	0
28	a	522	0	521	10	0
29	b	444	0	458	8	0
30	c	426	0	464	8	0
31	d	377	0	418	7	0
32	e	504	0	572	9	0
33	f	302	0	340	4	0
34	g	1760	0	1787	12	0
35	h	1636	0	1710	16	0
36	i	1643	0	1707	20	0
37	j	1152	0	1196	13	0
38	k	848	0	846	12	0
39	l	1181	0	1238	17	0
40	m	979	0	1031	14	0
41	n	1022	0	1070	15	0
42	o	790	0	831	20	0
43	p	877	0	887	11	0
44	q	957	0	1017	12	0
45	r	900	0	965	18	0
46	s	805	0	844	12	0
47	t	714	0	734	8	0
48	u	649	0	666	11	0
49	v	648	0	691	9	0
50	w	544	0	560	4	0
51	x	663	0	688	14	0
52	y	669	0	719	5	0
53	z	589	0	629	3	0
54	A	2014	0	1981	35	0
55	5	1627	0	833	9	0
56	6	32	0	28	4	0
57	1	292	0	0	0	0
57	2	1	0	0	0	0
57	3	8	0	0	0	0
57	5	2	0	0	0	0
57	C	1	0	0	0	0
57	b	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	f	1	0	0	0	0
57	i	1	0	0	0	0
58	a	1	0	0	0	0
58	f	1	0	0	0	0
All	All	146659	0	98954	1039	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1039) 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)
6:C:151:THR:HG22	6:C:152:PRO:CD	1.23	1.68
6:C:151:THR:CG2	6:C:152:PRO:HD3	1.21	1.58
19:R:51:VAL:CG1	19:R:52:PRO:HD3	1.54	1.36
19:R:51:VAL:HG13	19:R:52:PRO:CD	1.53	1.34
19:R:52:PRO:O	19:R:53:PHE:CD2	1.84	1.29
1:1:783:A:H2'	1:1:784:G:H5'	1.26	1.16
19:R:52:PRO:O	19:R:53:PHE:CG	2.00	1.13
1:1:783:A:C2'	1:1:784:G:H5'	1.85	1.05
1:1:2571:U:O2'	6:C:151:THR:HG21	1.63	0.97
1:1:2571:U:HO2'	6:C:151:THR:HG21	1.38	0.87
2:2:823:C:HO2'	40:m:2:SER:N	1.78	0.81
6:C:151:THR:CG2	6:C:152:PRO:CD	2.07	0.79
1:1:2425:A:H5"	1:1:2427:C:O4'	1.83	0.78
1:1:2571:U:O2'	6:C:151:THR:CG2	2.31	0.78
34:g:87:CYS:O	34:g:88:ASP:OD1	2.02	0.78
2:2:1534:A:N3	2:2:1534:A:H2'	1.99	0.77
5:B:130:LEU:HD21	5:B:192:LEU:HD23	1.69	0.75
1:1:894:U:H4'	1:1:895:U:OP1	1.85	0.74
19:R:51:VAL:CB	19:R:52:PRO:HD3	2.18	0.73
54:A:123:GLU:HG3	54:A:188:PRO:HB3	1.71	0.73
1:1:1779:U:OP2	1:1:1784:A:N6	2.21	0.72
1:1:885:C:H2'	1:1:886:A:H8	1.54	0.69
54:A:225:ASP:HB2	54:A:245:ARG:HB3	1.74	0.69
54:A:258:GLN:HA	54:A:266:ASN:HD21	1.58	0.69
7:D:149:ILE:HG22	7:D:170:ARG:HB2	1.75	0.68
2:2:1106:G:H5"	35:h:172:ARG:HB3	1.75	0.67
1:1:400:G:N7	25:X:57:ARG:NH1	2.43	0.67
50:w:34:THR:HG23	50:w:36:SER:H	1.60	0.67
1:1:2127:G:H1	1:1:2161:C:H42	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:l:72:THR:HA	39:l:96:ARG:HH12	1.59	0.67
2:2:376:G:H1	2:2:387:U:H3	1.43	0.67
1:1:1607:C:N4	1:1:1622:G:OP2	2.28	0.67
35:h:132:ARG:HD3	35:h:136:ARG:HH21	1.59	0.66
17:P:106:LYS:HD3	17:P:109:ARG:HH22	1.61	0.66
2:2:993:G:H2'	2:2:995:C:H41	1.61	0.66
19:R:51:VAL:HG13	19:R:52:PRO:HD3	0.71	0.66
1:1:1362:C:HO2'	1:1:1810:A:HO2'	1.41	0.66
2:2:5:U:H4'	2:2:6:G:O4'	1.96	0.66
45:r:25:VAL:HG12	45:r:29:ARG:HD2	1.78	0.65
2:2:950:U:H3'	45:r:101:ARG:HH22	1.62	0.65
40:m:43:GLU:HG2	40:m:101:ILE:HG12	1.79	0.65
1:1:563:A:N3	18:Q:37:GLN:NE2	2.45	0.64
1:1:2261:C:OP1	24:W:19:LYS:NZ	2.29	0.64
9:F:98:VAL:HG22	9:F:103:ILE:HG12	1.79	0.64
6:C:151:THR:CG2	6:C:152:PRO:N	2.55	0.64
39:l:146:GLU:HG3	39:l:149:LYS:HD2	1.78	0.64
2:2:1347:G:O6	41:n:12:ARG:NH2	2.31	0.64
25:X:37:ARG:HG2	25:X:48:THR:HG22	1.79	0.64
13:L:74:THR:HG22	13:L:107:PHE:HB2	1.78	0.64
1:1:2392:A:OP2	32:e:31:HIS:CE1	2.50	0.63
41:n:84:THR:HG21	41:n:103:PHE:HB3	1.79	0.63
54:A:212:ALA:O	54:A:213:GLU:HB2	1.98	0.63
18:Q:44:GLN:HE21	19:R:77:PHE:HB3	1.63	0.63
2:2:673:A:H4'	38:k:86:ARG:HH12	1.64	0.63
20:S:10:ALA:HB3	20:S:101:SER:HB2	1.81	0.63
1:1:383:C:N3	1:1:391:A:N6	2.47	0.63
1:1:1066:U:H2'	1:1:1067:A:H2'	1.81	0.63
1:1:2064:C:O2'	1:1:2251:OMG:N2	2.31	0.63
54:A:116:ARG:HG2	54:A:161:GLU:HG2	1.80	0.63
2:2:1422:G:O2'	12:K:49:ARG:NH2	2.32	0.62
21:T:24:MET:HE2	21:T:30:ILE:HG22	1.81	0.62
55:5:8:4SU:HN3	55:5:23:C:H41	1.46	0.62
33:f:2:LYS:HB2	33:f:35:GLN:HG2	1.82	0.62
11:J:92:MET:SD	11:J:95:ARG:NH1	2.73	0.62
6:C:14:ILE:HG23	17:P:12:GLN:HE22	1.65	0.61
54:A:235:GLN:O	54:A:238:ASN:N	2.33	0.61
2:2:78:A:H61	2:2:91:U:H3	1.48	0.61
1:1:729:G:N3	1:1:729:G:H2'	2.13	0.61
43:p:88:GLY:H	43:p:114:THR:HG22	1.65	0.61
1:1:568:U:H1'	1:1:2030:6MZ:H9C1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:d:24:THR:HG23	31:d:27:GLY:H	1.66	0.61
37:j:55:GLU:HG3	37:j:57:PRO:HD2	1.81	0.61
1:1:630:G:N2	1:1:633:A:OP2	2.33	0.61
30:c:35:GLU:HG2	30:c:50:LYS:HG2	1.83	0.61
1:1:2114:A:N6	1:1:2167:U:O2'	2.34	0.61
1:1:2306:C:N4	8:E:39:GLY:O	2.33	0.61
2:2:1150:A:H4'	42:o:43:PRO:HG3	1.81	0.61
35:h:11:ARG:NH2	35:h:177:THR:O	2.33	0.61
2:2:1440:U:H3	2:2:1461:G:H1	1.48	0.60
46:s:41:ARG:NH2	51:x:6:LYS:O	2.34	0.60
2:2:1081:A:N7	37:j:52:LYS:NZ	2.49	0.60
2:2:1137:C:O2	2:2:1138:G:N2	2.34	0.60
1:1:2831:G:OP2	6:C:59:ARG:NH1	2.34	0.60
3:3:4:C:H42	3:3:116:G:H1	1.48	0.60
1:1:1026:G:H2'	1:1:1027:A:H8	1.66	0.60
2:2:501:C:OP1	44:q:114:ARG:NH2	2.35	0.60
1:1:1614:A:H8	1:1:1614:A:P	2.25	0.60
2:2:933:G:O6	39:l:3:ARG:NH2	2.32	0.60
36:i:75:TYR:OH	36:i:97:ARG:NH1	2.35	0.60
2:2:126:G:OP1	2:2:605:U:O2'	2.20	0.59
54:A:114:GLU:HB2	54:A:204:ALA:HB3	1.84	0.59
1:1:893:C:C2'	1:1:894:U:O5'	2.51	0.59
3:3:90:C:H5'	14:M:18:ARG:HB3	1.84	0.59
15:N:44:LEU:HD23	15:N:113:ILE:HD13	1.83	0.59
24:W:11:ARG:O	24:W:14:ARG:NH1	2.35	0.59
1:1:783:A:H2'	1:1:784:G:C5'	2.17	0.59
1:1:2575:C:H6	1:1:2575:C:O5'	1.85	0.59
2:2:4:U:H2'	2:2:5:U:H2'	1.83	0.59
54:A:261:ARG:NH2	55:5:75:C:OP2	2.35	0.59
15:N:28:LEU:HD23	15:N:48:VAL:HG21	1.84	0.59
22:U:72:ILE:HD12	22:U:83:VAL:HG21	1.85	0.59
45:r:34:LEU:HD22	45:r:39:ILE:HB	1.84	0.59
1:1:843:G:H1	1:1:935:C:H42	1.51	0.59
1:1:1274:A:N1	1:1:1644:C:O2'	2.33	0.59
35:h:150:LYS:HD3	35:h:169:ARG:HE	1.66	0.59
1:1:1688:U:O2'	1:1:1700:A:N7	2.34	0.59
1:1:2271:G:H5'	24:W:20:ARG:HG2	1.85	0.59
2:2:664:G:H22	2:2:741:G:H1	1.51	0.59
1:1:1327:A:N6	1:1:1647:U:O2	2.36	0.59
1:1:1604:C:O2'	1:1:1610:A:N1	2.36	0.59
54:A:115:VAL:HG22	54:A:203:VAL:HG22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:815:A:N7	2:2:1509:C:O2'	2.36	0.58
17:P:33:VAL:HG22	17:P:38:LYS:HG2	1.84	0.58
2:2:1321:U:O2	51:x:36:ARG:NH1	2.35	0.58
5:B:258:ARG:NH1	5:B:264:ASP:OD1	2.37	0.58
8:E:65:PRO:HB2	8:E:87:CYS:HB2	1.85	0.58
38:k:100:SER:HB2	38:k:103:VAL:HG23	1.85	0.58
1:1:1:G:O6	1:1:2901:C:N4	2.36	0.58
1:1:270:A:H5'	1:1:271:G:H5"	1.85	0.58
1:1:788:A:OP1	1:1:791:C:N4	2.33	0.58
19:R:6:GLN:HG2	19:R:11:GLN:HG2	1.84	0.58
1:1:2134:A:H1'	1:1:2159:G:H1'	1.84	0.58
6:C:4:LEU:HD23	6:C:32:ASN:HD22	1.68	0.58
41:n:24:GLY:H	41:n:61:LEU:HA	1.68	0.58
6:C:152:PRO:O	6:C:154:LYS:N	2.34	0.58
11:J:72:LYS:HE3	11:J:74:TYR:HE1	1.69	0.58
13:L:57:LEU:HD22	32:e:54:ASP:HB3	1.84	0.58
2:2:1130:A:O2'	41:n:5:GLN:NE2	2.36	0.58
1:1:538:A:H5"	11:J:7:LYS:HE2	1.85	0.58
1:1:2285:C:OP2	30:c:6:ARG:NH1	2.37	0.58
23:V:51:GLN:HG2	23:V:86:LEU:HD11	1.84	0.58
51:x:11:ILE:HG13	51:x:38:SER:HB3	1.85	0.58
2:2:544:G:OP1	36:i:56:ARG:NH2	2.37	0.58
6:C:49:GLN:HE21	6:C:79:LEU:HB3	1.68	0.58
19:R:52:PRO:HD2	19:R:53:PHE:N	2.19	0.58
2:2:8:A:N6	36:i:202:GLU:O	2.37	0.57
1:1:396:G:OP2	25:X:10:LYS:NZ	2.36	0.57
2:2:927:G:O2'	2:2:1503:A:N7	2.36	0.57
1:1:2532:G:O2'	1:1:2657:A:N1	2.37	0.57
1:1:2540:C:O2'	1:1:2740:A:N3	2.37	0.57
2:2:832:G:H1	2:2:854:U:H3	1.53	0.57
13:L:29:LYS:HG3	13:L:30:THR:HG23	1.87	0.57
34:g:90:PHE:HB3	34:g:151:ILE:HG22	1.85	0.57
45:r:54:ASP:OD1	45:r:57:ARG:NH1	2.37	0.57
1:1:1998:A:HO2'	1:1:2724:U:HO2'	1.51	0.57
33:f:2:LYS:NZ	33:f:32:LYS:O	2.37	0.57
51:x:33:THR:HG22	51:x:35:SER:H	1.68	0.57
51:x:36:ARG:NH2	51:x:72:GLY:O	2.38	0.57
3:3:34:A:N6	3:3:44:G:O2'	2.37	0.57
19:R:52:PRO:C	19:R:53:PHE:CG	2.81	0.57
1:1:1901:A:OP2	5:B:253:LYS:NZ	2.36	0.57
2:2:993:G:O2'	2:2:994:A:N7	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1086:U:H3	2:2:1099:G:H22	1.52	0.57
2:2:1157:A:H4'	2:2:1158:C:OP1	2.04	0.57
54:A:212:ALA:O	54:A:213:GLU:CB	2.53	0.57
2:2:1377:A:OP1	39:l:92:ARG:NH1	2.38	0.57
5:B:155:ALA:HB2	5:B:162:VAL:HG23	1.87	0.57
45:r:13:LYS:HB2	45:r:18:ALA:HB2	1.86	0.57
1:1:232:G:H22	1:1:420:C:H5'	1.68	0.57
8:E:123:ASP:OD2	8:E:127:ASN:HB2	2.05	0.57
14:M:66:ARG:NH1	14:M:104:GLU:OE2	2.38	0.57
37:j:157:ARG:NH2	40:m:99:LEU:O	2.37	0.57
48:u:4:ILE:HG12	48:u:21:VAL:HG22	1.85	0.57
2:2:159:G:N2	2:2:162:A:OP2	2.38	0.57
37:j:13:GLU:OE2	37:j:68:ARG:NH1	2.38	0.57
39:l:146:GLU:HA	39:l:149:LYS:HB2	1.87	0.57
1:1:323:C:H2'	7:D:163:ASN:ND2	2.20	0.56
2:2:944:G:O2'	2:2:1339:A:N6	2.37	0.56
10:G:27:ARG:NH1	25:X:60:ASP:OD2	2.38	0.56
35:h:155:GLY:HA2	35:h:163:ALA:HB1	1.86	0.56
1:1:1614:A:H8	1:1:1614:A:O5'	1.88	0.56
1:1:1852:U:O2	1:1:1890:A:N6	2.38	0.56
2:2:362:G:N2	2:2:365:U:OP2	2.38	0.56
5:B:130:LEU:HD21	5:B:192:LEU:CD2	2.36	0.56
1:1:1998:A:OP2	6:C:141:ARG:NH1	2.38	0.56
2:2:1077:G:N2	2:2:1080:A:OP2	2.37	0.56
3:3:18:G:H1	3:3:65:U:H3	1.52	0.56
2:2:202:G:N2	2:2:216:U:O2	2.37	0.56
2:2:401:C:O2'	2:2:621:A:N3	2.38	0.56
2:2:890:G:O2'	2:2:906:A:N6	2.38	0.56
2:2:1016:A:HO2'	2:2:1217:C:HO2'	1.54	0.56
3:3:22:U:H3	3:3:61:G:H1	1.54	0.56
1:1:1450:G:N2	1:1:1452:G:O6	2.35	0.56
20:S:23:LEU:HD22	29:b:24:ALA:HB2	1.88	0.56
1:1:2293:G:OP1	16:O:94:ARG:NH1	2.39	0.56
1:1:2885:G:O6	29:b:29:SER:OG	2.23	0.56
2:2:1096:C:H2'	2:2:1097:C:H6	1.71	0.56
20:S:24:ILE:HD13	20:S:36:LEU:HD11	1.86	0.56
2:2:662:U:O2'	2:2:836:G:OP1	2.23	0.56
5:B:144:VAL:HB	5:B:154:LEU:HB2	1.86	0.56
40:m:5:ASP:OD2	40:m:77:ARG:NH1	2.39	0.56
13:L:58:TYR:O	32:e:13:ARG:NH2	2.39	0.56
1:1:2258:C:O2'	1:1:2427:C:OP2	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:86:ARG:NH2	22:U:102:THR:OG1	2.39	0.55
1:1:643:A:N1	1:1:2369:A:O2'	2.36	0.55
1:1:752:A:H62	1:1:2609:U:H3	1.55	0.55
1:1:783:A:H2'	1:1:783:A:N3	2.22	0.55
1:1:1256:G:O2'	7:D:77:ILE:HD12	2.06	0.55
5:B:6:CYS:SG	5:B:13:ARG:NH2	2.79	0.55
23:V:64:VAL:HG22	23:V:69:GLU:HG3	1.89	0.55
1:1:370:G:O2'	1:1:424:G:OP1	2.24	0.55
1:1:2684:U:O4'	12:K:70:ARG:NH1	2.39	0.55
1:1:1363:C:O2'	1:1:1809:A:N3	2.35	0.55
1:1:1715:G:N2	1:1:1744:A:OP2	2.39	0.55
22:U:13:VAL:HG21	22:U:39:ILE:HG21	1.88	0.55
1:1:714:U:OP2	47:t:88:ARG:NH1	2.39	0.55
1:1:978:G:HO2'	1:1:1002:G:HO2'	1.52	0.55
1:1:1666:G:N3	12:K:3:GLN:NE2	2.55	0.55
39:l:97:ASN:HB3	39:l:101:MET:HE2	1.89	0.55
28:a:16:CYS:SG	28:a:17:SER:N	2.80	0.55
46:s:54:ASP:HA	46:s:59:ARG:HG2	1.89	0.55
1:1:1652:A:OP1	15:N:8:ARG:NH2	2.40	0.55
6:C:46:ARG:NH1	6:C:85:ALA:O	2.39	0.55
10:G:126:GLY:H	10:G:146:VAL:HB	1.71	0.55
19:R:52:PRO:CD	19:R:53:PHE:N	2.66	0.55
38:k:46:GLN:HE22	38:k:55:HIS:HB3	1.71	0.55
1:1:500:G:N1	1:1:503:A:OP2	2.39	0.55
2:2:1360:A:OP2	46:s:75:ARG:NH2	2.40	0.55
35:h:11:ARG:HE	35:h:178:LEU:HA	1.71	0.55
1:1:62:U:O2	1:1:63:A:N6	2.40	0.55
1:1:783:A:H4'	1:1:2588:G:H4'	1.88	0.55
1:1:1385:A:O2'	1:1:1396:U:O2	2.25	0.55
2:2:380:G:N2	2:2:383:A:OP2	2.39	0.55
6:C:151:THR:HG23	6:C:152:PRO:CD	2.29	0.55
9:F:88:GLN:HE21	9:F:163:ARG:HD2	1.72	0.55
1:1:210:C:OP1	31:d:29:GLN:NE2	2.40	0.54
1:1:447:A:OP1	18:Q:5:LYS:NZ	2.38	0.54
1:1:931:U:O4	1:1:1166:G:N2	2.40	0.54
1:1:2314:A:OP1	8:E:88:LYS:NZ	2.40	0.54
2:2:1328:C:O2'	45:r:29:ARG:NH1	2.40	0.54
1:1:956:G:O6	14:M:14:LYS:NZ	2.41	0.54
1:1:1945:G:N2	1:1:1963:U:O4	2.40	0.54
5:B:262:ARG:O	5:B:265:LYS:NZ	2.41	0.54
39:l:140:ASP:OD1	39:l:143:ARG:NH1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:i:9:LEU:HD11	36:i:31:LYS:HE3	1.88	0.54
36:i:188:ARG:HD2	36:i:191:LEU:HD12	1.88	0.54
1:1:682:G:O6	1:1:794:A:N6	2.40	0.54
1:1:750:A:OP1	1:1:1615:C:N4	2.40	0.54
1:1:1779:U:H5	1:1:1784:A:N7	2.06	0.54
1:1:1906:G:H1	1:1:1924:C:H42	1.54	0.54
1:1:2833:U:O2	6:C:58:ASN:ND2	2.40	0.54
2:2:462:G:N2	2:2:471:U:O2	2.41	0.54
8:E:98:GLU:OE2	28:a:25:ARG:NH1	2.40	0.54
40:m:44:GLY:O	40:m:64:LYS:NZ	2.40	0.54
54:A:322:ILE:HD12	54:A:324:LEU:HD11	1.88	0.54
1:1:1964:G:O2'	1:1:1967:C:OP2	2.26	0.54
28:a:35:ASP:OD1	45:r:57:ARG:NH2	2.40	0.54
1:1:1977:A:H2	5:B:14:ARG:HH22	1.55	0.54
8:E:113:ASP:OD1	45:r:71:ARG:NH2	2.41	0.54
27:Z:31:ARG:HD2	27:Z:34:HIS:HB2	1.90	0.54
1:1:138:U:O2'	1:1:139:U:H5"	2.08	0.54
1:1:874:G:N2	1:1:903:C:O2	2.35	0.54
1:1:2720:U:OP1	17:P:53:ARG:NH2	2.41	0.54
1:1:2788:C:O2'	1:1:2809:A:N3	2.38	0.54
7:D:117:ARG:NH2	7:D:183:PHE:O	2.35	0.54
36:i:57:GLU:OE2	36:i:196:ASN:N	2.39	0.54
1:1:2555:U:O2	54:A:228:ARG:NH1	2.41	0.54
2:2:58:C:O2'	2:2:388:G:N7	2.37	0.54
2:2:1280:A:OP1	42:o:9:ARG:NH1	2.40	0.54
10:G:85:GLY:N	10:G:89:LYS:O	2.40	0.54
30:c:8:LYS:HA	30:c:24:THR:HA	1.89	0.54
44:q:72:HIS:HB2	44:q:74:LEU:HD23	1.90	0.54
1:1:1869:G:N2	1:1:1872:A:OP2	2.39	0.54
2:2:1128:C:O2'	2:2:1147:C:N3	2.37	0.54
7:D:77:ILE:HG13	7:D:78:TRP:HD1	1.73	0.54
1:1:878:A:N6	1:1:899:A:O2'	2.42	0.53
2:2:1103:C:OP1	34:g:95:ARG:NH2	2.40	0.53
2:2:1242:G:H1	2:2:1295:U:H3	1.56	0.53
46:s:53:ARG:HD3	46:s:59:ARG:HH12	1.73	0.53
1:1:1264:A:OP1	29:b:16:ARG:NH1	2.36	0.53
2:2:923:A:N6	2:2:1392:G:O6	2.41	0.53
5:B:66:ASP:OD2	5:B:102:ARG:NH1	2.40	0.53
16:O:40:ILE:HG12	16:O:47:VAL:HG12	1.88	0.53
42:o:8:ILE:HB	42:o:74:VAL:HB	1.91	0.53
1:1:887:A:H4'	1:1:889:C:H41	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:376:G:H5”	48:u:5:ARG:HB2	1.90	0.53
3:3:43:C:O2	8:E:92:ARG:NH2	2.41	0.53
20:S:4:ILE:HG12	20:S:106:VAL:HG22	1.90	0.53
23:V:21:ARG:NH2	23:V:87:GLN:O	2.41	0.53
42:o:52:LEU:HB2	46:s:81:ARG:HD2	1.90	0.53
1:1:335:C:O2	22:U:68:SER:OG	2.26	0.53
54:A:218:ASN:HD22	54:A:219:PRO:HD2	1.73	0.53
1:1:1227:G:OP2	18:Q:16:LYS:NZ	2.39	0.53
2:2:668:G:O2’	47:t:46:HIS:ND1	2.40	0.53
4:4:21:A:H3’	54:A:195:ARG:HD2	1.89	0.53
36:i:60:LYS:NZ	36:i:194:ASP:O	2.42	0.53
2:2:181:A:O2’	2:2:194:C:N4	2.42	0.53
2:2:816:A:OP1	2:2:1526:G:O2’	2.26	0.53
36:i:172:GLU:HB2	36:i:183:LYS:HD2	1.89	0.53
54:A:235:GLN:HE22	56:6:79:PHE:N	2.07	0.53
54:A:247:THR:HA	54:A:254:VAL:HG12	1.90	0.53
1:1:1693:U:O2	5:B:14:ARG:NH1	2.41	0.53
1:1:2402:U:O2’	1:1:2403:C:H5”	2.08	0.53
2:2:1006:G:O6	2:2:1024:G:N2	2.41	0.53
1:1:390:U:H4’	1:1:391:A:H5’	1.89	0.53
1:1:1024:G:HO2’	1:1:1144:A:HO2’	1.55	0.53
1:1:2279:G:N7	24:W:14:ARG:NH2	2.56	0.53
1:1:2016:U:O2	29:b:4:GLN:NE2	2.39	0.53
1:1:2659:G:N2	1:1:2662:A:OP2	2.42	0.53
22:U:86:ARG:NH1	22:U:100:SER:OG	2.42	0.53
38:k:2:ARG:HB3	38:k:91:ARG:HH12	1.74	0.53
43:p:21:ALA:HB3	43:p:84:VAL:HG22	1.90	0.53
19:R:51:VAL:HG13	19:R:52:PRO:HD2	1.76	0.52
44:q:68:GLY:O	44:q:99:ARG:NH1	2.42	0.52
1:1:672:C:OP2	13:L:42:SER:OG	2.24	0.52
1:1:693:A:O2’	1:1:1353:A:N3	2.42	0.52
5:B:140:THR:HG22	5:B:163:GLN:HG2	1.91	0.52
7:D:150:THR:HG22	7:D:152:GLU:H	1.74	0.52
42:o:10:LEU:HB3	42:o:18:ILE:HD11	1.90	0.52
2:2:768:A:N3	2:2:1512:U:O2’	2.42	0.52
2:2:974:A:OP1	46:s:69:ARG:NH1	2.39	0.52
2:2:1441:A:H62	2:2:1461:G:H21	1.58	0.52
2:2:79:G:N2	2:2:90:C:O2	2.38	0.52
8:E:131:GLY:HA2	8:E:153:ASP:HA	1.91	0.52
1:1:997:G:OP1	18:Q:92:ARG:HD2	2.10	0.52
5:B:180:GLU:OE2	5:B:270:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:14:LYS:O	14:M:71:LYS:NZ	2.36	0.52
1:1:245:G:N7	32:e:8:ARG:NH2	2.42	0.52
1:1:1789:A:OP2	5:B:221:ARG:NH1	2.42	0.52
1:1:1996:C:OP2	12:K:31:ARG:NH2	2.42	0.52
2:2:222:C:H2'	2:2:223:A:C8	2.44	0.52
3:3:14:U:OP2	3:3:70:C:O2'	2.28	0.52
33:f:16:ILE:HG12	33:f:25:VAL:HG22	1.91	0.52
55:5:8:4SU:H6	55:5:45:G:H2'	1.90	0.52
2:2:770:C:O2'	2:2:899:C:N3	2.38	0.52
13:L:123:ARG:NE	13:L:143:GLU:OE2	2.41	0.52
24:W:21:LEU:HD21	24:W:41:ARG:HH21	1.75	0.52
1:1:85:G:C6	1:1:98:G:C2	2.97	0.52
1:1:2333:A:OP1	24:W:77:ARG:NH2	2.38	0.52
40:m:78:VAL:HG12	40:m:85:ILE:HG13	1.92	0.52
42:o:40:ILE:HD12	42:o:73:LEU:HD12	1.90	0.52
48:u:48:GLU:OE2	48:u:51:ARG:NH2	2.43	0.52
49:v:12:VAL:HG22	49:v:23:VAL:HG22	1.90	0.52
1:1:283:G:H1	1:1:357:C:H42	1.55	0.52
1:1:783:A:C2'	1:1:783:A:N3	2.73	0.52
1:1:2123:G:H22	1:1:2175:C:H42	1.58	0.52
2:2:1279:G:H2'	2:2:1279:G:N3	2.25	0.52
53:z:51:SER:OG	53:z:55:ARG:NH2	2.43	0.52
5:B:107:PRO:HD2	5:B:110:LEU:HD22	1.91	0.52
2:2:937:A:N6	2:2:1345:U:O4	2.38	0.51
2:2:1096:C:H2'	2:2:1097:C:C6	2.45	0.51
2:2:1297:G:N2	2:2:1298:U:O4	2.42	0.51
3:3:13:G:O2'	3:3:15:A:OP2	2.28	0.51
10:G:12:LEU:HB2	10:G:19:VAL:HG11	1.92	0.51
1:1:72:U:OP2	26:Y:54:LYS:NZ	2.43	0.51
2:2:553:A:H5"	44:q:21:VAL:HG21	1.91	0.51
7:D:18:THR:O	7:D:110:SER:OG	2.28	0.51
8:E:68:THR:N	8:E:86:GLY:O	2.40	0.51
16:O:68:LYS:HE2	16:O:101:GLY:HA2	1.92	0.51
1:1:1721:G:O2'	1:1:1739:A:N6	2.44	0.51
1:1:2115:G:O2'	1:1:2165:C:N4	2.42	0.51
2:2:202:G:O6	2:2:215:C:N4	2.43	0.51
1:1:1064:C:N4	1:1:1070:A:OP2	2.35	0.51
1:1:2052:A:O2'	6:C:148:GLN:O	2.26	0.51
2:2:1310:G:OP1	45:r:79:ARG:NH2	2.43	0.51
22:U:34:VAL:HG13	22:U:67:VAL:HG22	1.93	0.51
27:Z:16:ARG:HE	27:Z:53:PHE:HE2	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:r:22:ILE:HB	45:r:25:VAL:HG22	1.92	0.51
56:6:77:FME:SD	56:6:77:FME:N	2.83	0.51
1:1:2469:A:N6	1:1:2481:G:O2'	2.43	0.51
2:2:12:U:H4'	2:2:526:C:H4'	1.92	0.51
2:2:467:U:H2'	2:2:467:U:O2	2.11	0.51
2:2:1378:C:O2	39:l:76:LYS:NZ	2.42	0.51
1:1:746:PSU:O2'	1:1:2611:C:O2'	2.25	0.51
1:1:793:A:OP2	1:1:2071:A:O2'	2.27	0.51
2:2:390:U:O2'	48:u:28:ARG:NH2	2.39	0.51
2:2:727:G:N2	2:2:730:G:OP2	2.42	0.51
23:V:86:LEU:HD13	23:V:89:ILE:HD11	1.91	0.51
42:o:8:ILE:HG12	42:o:100:ILE:HG22	1.93	0.51
1:1:1251:C:OP2	18:Q:6:ARG:NH2	2.43	0.51
1:1:2164:C:H5"	1:1:2171:A:H62	1.75	0.51
19:R:77:PHE:HD1	19:R:84:ARG:HB3	1.75	0.51
40:m:92:LEU:O	40:m:117:ARG:NH2	2.44	0.51
1:1:2602:A:C5	54:A:237:VAL:HG22	2.45	0.51
5:B:29:PRO:HG2	5:B:34:LEU:HD11	1.93	0.51
39:l:69:VAL:HG21	39:l:104:ILE:HD11	1.93	0.51
1:1:329:G:OP2	22:U:69:ASN:ND2	2.42	0.51
1:1:411:G:OP2	1:1:2406:A:O2'	2.28	0.51
21:T:8:LEU:HD23	21:T:50:LEU:HD21	1.93	0.51
37:j:157:ARG:HH11	40:m:43:GLU:HG3	1.76	0.51
46:s:49:GLN:NE2	51:x:11:ILE:O	2.38	0.51
1:1:2892:G:H5"	1:1:2893:A:H5'	1.92	0.50
2:2:501:C:OP2	44:q:121:ARG:NH1	2.44	0.50
23:V:58:SER:O	23:V:73:LYS:NZ	2.43	0.50
1:1:476:G:N1	1:1:479:A:OP2	2.43	0.50
1:1:893:C:O2'	1:1:894:U:O5'	2.29	0.50
1:1:1798:U:OP2	5:B:271:ARG:NH2	2.44	0.50
1:1:2595:G:N2	1:1:2598:A:OP2	2.39	0.50
2:2:1193:G:O6	35:h:3:GLN:NE2	2.44	0.50
3:3:13:G:H4'	3:3:15:A:H2'	1.93	0.50
35:h:32:ASN:OD1	35:h:59:ARG:NH1	2.44	0.50
1:1:1009:A:OP1	11:J:39:LYS:NZ	2.41	0.50
26:Y:21:LEU:HD12	26:Y:46:VAL:HG13	1.91	0.50
1:1:397:U:H5"	25:X:32:ASN:HB2	1.94	0.50
1:1:796:C:OP1	7:D:57:LYS:NZ	2.45	0.50
2:2:321:A:N7	2:2:328:C:O2'	2.41	0.50
36:i:57:GLU:HG2	36:i:199:LEU:HB2	1.92	0.50
54:A:114:GLU:HG2	54:A:163:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:769:G:H4'	2:2:1513:A:H4'	1.93	0.50
38:k:38:ARG:NH1	38:k:98:GLU:O	2.45	0.50
1:1:392:U:H2'	1:1:393:C:H5'	1.93	0.50
1:1:486:C:H42	1:1:494:G:H1	1.59	0.50
5:B:157:SER:OG	5:B:158:ALA:N	2.43	0.50
10:G:86:ASP:OD1	10:G:86:ASP:N	2.41	0.50
15:N:32:GLU:HG2	15:N:115:LEU:HD12	1.93	0.50
36:i:121:LYS:O	36:i:146:ARG:NH1	2.40	0.50
39:l:111:ARG:NH1	39:l:126:ASP:OD2	2.44	0.50
1:1:560:C:O2	18:Q:48:ARG:NH1	2.44	0.50
1:1:1651:G:H4'	15:N:39:PRO:HG2	1.93	0.50
1:1:2483:C:N3	14:M:123:LYS:NZ	2.59	0.50
2:2:70:U:O2	2:2:71:A:N6	2.43	0.50
52:y:27:MET:HE3	52:y:57:ILE:HD11	1.93	0.50
1:1:1801:A:OP2	5:B:150:LYS:NZ	2.41	0.50
2:2:1134:G:H1	2:2:1140:C:H42	1.60	0.50
47:t:25:THR:HG23	47:t:66:LEU:HD12	1.93	0.50
1:1:210:C:OP1	31:d:25:LYS:NZ	2.43	0.50
1:1:602:A:HO2'	1:1:604:G:HO2'	1.54	0.50
1:1:1776:G:C8	1:1:1776:G:H5"	2.46	0.50
54:A:323:ASN:O	54:A:325:THR:CG2	2.60	0.50
1:1:115:C:HO2'	1:1:127:A:HO2'	1.59	0.49
2:2:127:G:O2'	49:v:6:ARG:NH1	2.45	0.49
2:2:1222:G:H5"	51:x:78:ARG:HD2	1.94	0.49
8:E:70:ALA:HB3	8:E:82:GLY:H	1.76	0.49
9:F:9:VAL:HB	9:F:50:LEU:HB2	1.93	0.49
11:J:36:LEU:HD11	11:J:122:LEU:HB2	1.94	0.49
12:K:2:ILE:HB	12:K:33:ALA:HB3	1.94	0.49
17:P:71:GLU:OE2	17:P:101:ARG:NE	2.45	0.49
1:1:1351:C:O2'	1:1:1571:A:N3	2.41	0.49
34:g:31:ILE:HG21	34:g:39:HIS:HD2	1.77	0.49
41:n:42:GLU:OE2	41:n:45:ARG:NH1	2.46	0.49
42:o:5:ARG:HH11	42:o:7:ARG:HH21	1.60	0.49
1:1:72:U:O4	26:Y:58:ASN:ND2	2.45	0.49
1:1:569:U:O2'	1:1:983:A:N1	2.39	0.49
1:1:885:C:H2'	1:1:886:A:C8	2.41	0.49
2:2:972:C:O2'	42:o:57:VAL:HG23	2.12	0.49
13:L:78:ARG:HG3	13:L:113:ALA:HB3	1.94	0.49
5:B:142:HIS:ND1	5:B:193:GLY:O	2.37	0.49
1:1:85:G:C5	1:1:98:G:N2	2.81	0.49
1:1:674:G:H1'	7:D:69:ARG:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2063:C:H1'	56:6:79:PHE:HB2	1.95	0.49
2:2:842:U:O2'	2:2:845:A:OP2	2.26	0.49
10:G:51:ARG:HB3	10:G:55:GLU:HG2	1.95	0.49
35:h:136:ARG:O	35:h:140:ASN:ND2	2.45	0.49
47:t:80:GLN:HE21	47:t:84:ARG:HH22	1.60	0.49
5:B:3:VAL:HG12	5:B:19:VAL:HG22	1.95	0.49
36:i:95:GLU:HA	36:i:100:ASN:HD22	1.77	0.49
1:1:990:A:N1	19:R:78:ARG:NH1	2.60	0.49
1:1:2023:C:H5"	1:1:2023:C:H6	1.78	0.49
45:r:97:VAL:HG23	45:r:109:ARG:HH22	1.75	0.49
1:1:1693:U:O4	1:1:1976:U:O2'	2.27	0.49
12:K:71:ARG:NH2	12:K:123:LEU:O	2.43	0.49
15:N:96:ARG:NH2	15:N:114:GLU:OE2	2.39	0.49
34:g:97:LEU:H	34:g:100:MET:HE3	1.78	0.49
37:j:12:GLN:HE21	37:j:117:VAL:HA	1.76	0.49
43:p:23:ILE:HD12	43:p:86:VAL:HG22	1.93	0.49
45:r:98:ARG:HB2	45:r:100:GLN:HE22	1.78	0.49
54:A:215:PRO:HG3	54:A:279:HIS:HB2	1.95	0.49
1:1:1866:A:N6	1:1:1875:G:O2'	2.46	0.49
1:1:1980:G:O2'	1:1:1982:U:OP2	2.24	0.49
11:J:125:TYR:OH	11:J:132:HIS:NE2	2.41	0.49
19:R:51:VAL:CG1	19:R:52:PRO:CD	2.42	0.49
33:f:25:VAL:HB	33:f:35:GLN:HB2	1.94	0.49
50:w:37:GLY:O	50:w:63:ARG:NH2	2.46	0.49
1:1:783:A:O2'	1:1:784:G:H5'	2.12	0.49
1:1:1306:C:H41	1:1:1606:C:H2'	1.77	0.49
1:1:1365:A:OP1	25:X:3:ARG:NH2	2.40	0.49
1:1:2572:A:N6	6:C:150:GLN:OE1	2.45	0.49
2:2:1534:A:N3	2:2:1534:A:C2'	2.74	0.49
5:B:93:LEU:HD11	5:B:101:ARG:HB3	1.95	0.49
23:V:59:GLU:O	23:V:73:LYS:NZ	2.45	0.49
1:1:224:U:OP2	1:1:408:G:N2	2.40	0.48
1:1:807:U:O2'	1:1:2060:A:N1	2.45	0.48
1:1:1528:A:N6	1:1:1543:G:O2'	2.46	0.48
1:1:2313:C:O4'	8:E:37:ASN:ND2	2.45	0.48
32:e:26:HIS:CE1	32:e:48:ALA:HB2	2.47	0.48
2:2:323:U:H5"	52:y:21:ASN:HD22	1.78	0.48
2:2:457:G:N2	2:2:476:U:O2	2.46	0.48
5:B:130:LEU:HD11	5:B:135:ILE:HG12	1.95	0.48
55:5:21:A:O2'	55:5:46:A:N6	2.46	0.48
1:1:84:A:N1	1:1:98:G:O2'	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1453:A:O2'	15:N:63:ARG:NH1	2.47	0.48
2:2:197:A:N1	2:2:220:G:O2'	2.40	0.48
2:2:959:A:O2'	2:2:984:C:O2'	2.26	0.48
7:D:58:LYS:NZ	7:D:70:SER:O	2.38	0.48
36:i:72:PHE:HA	36:i:75:TYR:HD2	1.78	0.48
43:p:117:PRO:HB2	43:p:120:GLY:H	1.77	0.48
50:w:30:LYS:HA	50:w:33:ILE:HG12	1.95	0.48
1:1:2339:C:O3'	3:3:41:G:N2	2.46	0.48
1:1:2420:C:H5"	30:c:8:LYS:HE3	1.96	0.48
2:2:212:G:H2'	2:2:213:G:H8	1.79	0.48
16:O:111:ARG:NH2	16:O:117:PHE:OXT	2.47	0.48
18:Q:26:GLY:O	18:Q:30:ARG:NH1	2.45	0.48
24:W:33:ALA:N	24:W:64:ASP:OD1	2.46	0.48
1:1:2119:A:N6	1:1:2167:U:O2'	2.47	0.48
1:1:2162:G:OP2	1:1:2164:C:N4	2.46	0.48
2:2:178:C:H2'	2:2:179:A:H8	1.78	0.48
2:2:1095:U:OP1	2:2:1108:G:N1	2.39	0.48
26:Y:59:GLU:HA	26:Y:63:ALA:HB3	1.96	0.48
34:g:162:PHE:HA	34:g:184:PHE:HB2	1.95	0.48
44:q:56:ARG:NE	44:q:62:GLU:OE1	2.35	0.48
1:1:1297:C:O2'	1:1:1302:A:N1	2.41	0.48
1:1:2692:G:H5"	1:1:2870:C:O2'	2.13	0.48
1:1:2822:G:O5'	1:1:2822:G:H8	1.95	0.48
1:1:1664:A:H61	1:1:1996:C:H42	1.62	0.48
2:2:21:G:H2'	2:2:22:G:C8	2.49	0.48
27:Z:6:LYS:HB2	27:Z:58:GLU:HB3	1.95	0.48
43:p:64:GLN:HB2	43:p:99:ALA:HB3	1.95	0.48
1:1:1190:G:H5"	13:L:32:GLY:HA2	1.96	0.48
2:2:246:A:N1	2:2:278:G:O2'	2.42	0.48
2:2:505:G:H5'	2:2:534:U:H2'	1.96	0.48
2:2:692:U:OP2	43:p:28:ASN:ND2	2.44	0.48
5:B:76:ALA:HB3	5:B:116:ILE:HG13	1.96	0.48
28:a:2:LYS:HB2	28:a:5:ILE:HG12	1.96	0.48
41:n:55:VAL:HG11	41:n:94:LEU:HD22	1.95	0.48
1:1:781:A:OP1	5:B:217:ARG:NH2	2.35	0.48
1:1:2722:G:O2'	15:N:3:HIS:O	2.29	0.48
24:W:68:LYS:NZ	24:W:69:PHE:O	2.45	0.48
54:A:338:ASP:OD1	54:A:338:ASP:N	2.46	0.48
1:1:1270:C:H5"	1:1:1271:G:H5'	1.96	0.47
1:1:2316:G:H2'	1:1:2317:A:H8	1.79	0.47
2:2:933:G:N7	39:l:3:ARG:NE	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:979:C:OP1	2:2:1223:C:N4	2.47	0.47
17:P:75:GLN:HB2	17:P:78:SER:HB2	1.95	0.47
1:1:195:A:H3'	1:1:196:A:H4'	1.96	0.47
1:1:307:G:N1	1:1:310:A:OP2	2.45	0.47
1:1:811:U:H2'	13:L:21:ARG:HA	1.95	0.47
1:1:2029:G:N1	1:1:2033:A:OP2	2.31	0.47
1:1:2576:G:O2'	1:1:2579:C:OP2	2.28	0.47
1:1:2818:U:OP2	15:N:42:LYS:NZ	2.47	0.47
2:2:94:G:H4'	2:2:95:C:H5'	1.95	0.47
2:2:718:A:O2'	53:z:35:ARG:NH2	2.41	0.47
6:C:56:LYS:HB2	6:C:59:ARG:HB3	1.96	0.47
9:F:101:ASN:HB2	9:F:117:LEU:HB2	1.97	0.47
36:i:132:ILE:HG22	36:i:134:SER:H	1.79	0.47
54:A:235:GLN:NE2	56:6:79:PHE:O	2.47	0.47
54:A:303:ARG:H	54:A:303:ARG:HD3	1.80	0.47
1:1:2076:U:OP2	1:1:2238:G:N2	2.43	0.47
7:D:176:ASP:OD1	7:D:176:ASP:N	2.45	0.47
16:O:15:ARG:HG2	16:O:25:ARG:HH22	1.79	0.47
49:v:61:ILE:HA	49:v:75:LEU:HA	1.96	0.47
51:x:36:ARG:NH2	51:x:75:ALA:O	2.47	0.47
1:1:138:U:H3'	1:1:138:U:O2	2.13	0.47
1:1:641:U:O2'	1:1:2350:C:OP1	2.31	0.47
2:2:496:A:N3	2:2:496:A:H2'	2.29	0.47
5:B:2:ALA:N	5:B:199:GLU:OE2	2.47	0.47
5:B:168:ASP:OD1	5:B:168:ASP:N	2.46	0.47
8:E:4:LEU:O	8:E:8:TYR:N	2.46	0.47
8:E:122:PHE:O	8:E:123:ASP:OD1	2.33	0.47
9:F:105:LEU:HB2	9:F:113:VAL:HB	1.97	0.47
30:c:8:LYS:HB3	30:c:24:THR:HG22	1.97	0.47
38:k:51:ILE:HD13	38:k:86:ARG:HE	1.79	0.47
48:u:2:VAL:HG13	48:u:65:ALA:HA	1.96	0.47
1:1:563:A:OP2	19:R:79:ARG:NH2	2.40	0.47
1:1:1071:G:O2'	1:1:1089:A:OP2	2.32	0.47
1:1:2120:G:N2	1:1:2179:C:O2	2.47	0.47
1:1:2571:U:HO2'	6:C:151:THR:CG2	2.16	0.47
2:2:911:U:OP2	44:q:94:ARG:NH2	2.42	0.47
5:B:107:PRO:HG2	5:B:127:GLY:HA2	1.97	0.47
7:D:58:LYS:HG2	7:D:71:GLY:HA2	1.96	0.47
41:n:12:ARG:HG3	41:n:13:LYS:H	1.80	0.47
1:1:514:A:N3	1:1:581:C:O2'	2.39	0.47
1:1:1613:G:H3'	1:1:1614:A:C5'	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:27:GLU:N	17:P:85:SER:O	2.46	0.47
54:A:242:SER:HA	54:A:263:GLN:HB3	1.96	0.47
1:1:729:G:H2'	1:1:1775:U:H1'	1.96	0.47
1:1:783:A:H8	1:1:1778:U:O2'	1.96	0.47
1:1:861:A:N3	3:3:79:G:O2'	2.48	0.47
1:1:1045:C:O2	1:1:1047:G:N1	2.48	0.47
1:1:1324:G:O2'	1:1:1326:U:OP2	2.27	0.47
1:1:1590:A:H2'	1:1:1591:A:C8	2.50	0.47
1:1:2343:U:O2'	1:1:2373:G:O2'	2.31	0.47
1:1:2883:A:OP1	29:b:49:TYR:OH	2.32	0.47
2:2:977:A:N6	2:2:1224:U:O4'	2.47	0.47
2:2:1255:G:OP2	42:o:45:ARG:NH1	2.47	0.47
2:2:1317:C:OP1	46:s:24:ARG:NH2	2.40	0.47
7:D:23:PHE:HE1	7:D:108:ILE:HG22	1.80	0.47
39:l:13:LEU:HD23	41:n:50:GLN:HE22	1.79	0.47
1:1:995:C:O2	11:J:3:THR:OG1	2.28	0.47
1:1:2808:G:O2'	1:1:2890:G:O6	2.29	0.47
20:S:25:ARG:NH1	20:S:74:ILE:O	2.44	0.47
39:l:42:ILE:O	39:l:46:ALA:N	2.46	0.47
1:1:690:G:O2'	1:1:780:G:OP1	2.32	0.47
1:1:2566:A:N1	12:K:28:SER:OG	2.42	0.47
2:2:575:G:O2'	2:2:821:G:OP2	2.32	0.47
22:U:86:ARG:NH1	22:U:100:SER:HG	2.12	0.47
40:m:18:GLN:HG3	40:m:72:VAL:HB	1.97	0.47
1:1:1477:A:N6	1:1:1514:G:O2'	2.48	0.47
1:1:1791:A:N6	1:1:1828:G:O2'	2.36	0.47
2:2:792:A:H4'	2:2:793:U:H5"	1.97	0.47
10:G:86:ASP:OD2	38:k:24:ARG:NH1	2.37	0.47
10:G:89:LYS:HD3	10:G:123:ARG:HH22	1.80	0.47
13:L:82:LEU:HD22	13:L:90:VAL:HG21	1.97	0.47
1:1:116:C:O2'	1:1:126:A:N3	2.45	0.46
1:1:2126:A:H4'	1:1:2127:G:H4'	1.97	0.46
2:2:112:G:H1	2:2:315:A:H61	1.62	0.46
2:2:1005:A:HO2'	2:2:1037:C:HO2'	1.61	0.46
46:s:74:LEU:HD12	46:s:84:VAL:HG21	1.97	0.46
2:2:186:C:N4	2:2:187:G:O6	2.48	0.46
2:2:258:G:H1	2:2:268:U:H3	1.62	0.46
3:3:66:A:N6	3:3:108:A:O5'	2.48	0.46
10:G:40:THR:HG22	10:G:42:LYS:H	1.80	0.46
10:G:51:ARG:HG3	10:G:54:LEU:HB3	1.97	0.46
10:G:93:SER:OG	10:G:121:VAL:O	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:g:57:LEU:HD13	34:g:217:VAL:HG13	1.96	0.46
36:i:58:LYS:NZ	36:i:69:GLU:OE1	2.43	0.46
1:1:1589:U:H1'	1:1:1590:A:H5'	1.97	0.46
1:1:1592:C:H2'	1:1:1593:A:C8	2.50	0.46
1:1:2658:C:OP1	9:F:158:LYS:NZ	2.39	0.46
6:C:186:LEU:HD21	17:P:4:ILE:HG21	1.97	0.46
1:1:1032:A:H2	1:1:1122:G:H22	1.61	0.46
2:2:81:A:N6	2:2:89:U:O2	2.49	0.46
2:2:837:U:H2'	2:2:838:G:H8	1.80	0.46
54:A:178:GLU:OE2	54:A:308:ARG:NH2	2.48	0.46
1:1:1791:A:H61	1:1:1828:G:HO2'	1.56	0.46
1:1:1796:U:H2'	1:1:1797:G:C8	2.51	0.46
1:1:2103:C:N4	1:1:2185:U:O4	2.48	0.46
2:2:823:C:O2'	40:m:2:SER:N	2.46	0.46
2:2:1109:C:C3'	2:2:1109:C:C6	2.99	0.46
14:M:64:TRP:HB2	14:M:104:GLU:HB2	1.98	0.46
29:b:52:ARG:HH21	29:b:54:VAL:HG12	1.80	0.46
1:1:2452:C:H4'	54:A:239:THR:HG21	1.97	0.46
1:1:2780:G:OP2	11:J:120:ARG:NE	2.40	0.46
6:C:101:PHE:HD1	6:C:104:VAL:HG21	1.81	0.46
1:1:2391:G:O2'	1:1:2424:C:N4	2.41	0.46
10:G:76:GLU:HG3	10:G:143:ILE:H	1.80	0.46
41:n:65:ILE:HD13	41:n:79:ILE:HG23	1.97	0.46
49:v:59:VAL:HG23	49:v:78:VAL:HG22	1.97	0.46
1:1:627:A:OP1	13:L:78:ARG:NH1	2.41	0.46
1:1:2683:C:OP1	17:P:51:ARG:NH2	2.48	0.46
2:2:765:G:N1	2:2:812:G:O2'	2.37	0.46
2:2:951:G:OP2	45:r:101:ARG:NH2	2.49	0.46
2:2:976:G:OP2	2:2:1358:U:O2'	2.34	0.46
10:G:79:THR:HG23	10:G:147:VAL:HG21	1.98	0.46
28:a:11:GLU:HA	28:a:25:ARG:HA	1.98	0.46
40:m:34:VAL:HG22	40:m:59:LEU:HD13	1.97	0.46
42:o:10:LEU:HB2	42:o:72:ARG:HB2	1.98	0.46
1:1:1008:A:H2	1:1:1009:A:H62	1.64	0.46
1:1:1054:A:H2'	1:1:1055:G:H8	1.80	0.46
1:1:1209:U:O2'	1:1:1237:A:N1	2.38	0.46
1:1:2472:G:O2'	1:1:2478:A:N6	2.48	0.46
1:1:2692:G:H1'	1:1:2847:U:H1'	1.98	0.46
2:2:429:U:H3	2:2:431:A:H62	1.64	0.46
3:3:13:G:H21	3:3:16:G:H1'	1.81	0.46
34:g:72:THR:OG1	34:g:169:GLU:OE2	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:j:13:GLU:HG2	37:j:39:VAL:HG12	1.98	0.46
2:2:696:A:N3	2:2:786:G:O2'	2.39	0.46
11:J:17:VAL:HG23	11:J:137:PRO:HB2	1.98	0.46
20:S:81:SER:HB3	20:S:97:LEU:HD12	1.98	0.46
31:d:12:ARG:HG3	31:d:44:VAL:HG11	1.98	0.46
44:q:27:CYS:HB2	44:q:30:LYS:HD3	1.98	0.46
45:r:78:LYS:HA	45:r:81:MET:HB2	1.98	0.46
1:1:624:C:O2'	1:1:657:U:OP1	2.30	0.45
1:1:971:G:O2'	1:1:983:A:N3	2.48	0.45
2:2:652:U:O4	2:2:752:G:O2'	2.33	0.45
3:3:5:U:OP1	3:3:61:G:O2'	2.32	0.45
1:1:456:C:H2'	21:T:73:ARG:HH21	1.80	0.45
1:1:1266:G:O2'	1:1:2012:G:O6	2.24	0.45
2:2:54:C:N4	2:2:353:A:OP2	2.47	0.45
2:2:297:G:N2	2:2:300:A:OP2	2.49	0.45
6:C:151:THR:HG23	6:C:152:PRO:N	2.30	0.45
5:B:145:GLU:HB2	5:B:188:CYS:HB3	1.98	0.45
10:G:133:GLN:HG3	10:G:139:PHE:HE1	1.80	0.45
45:r:91:HIS:HA	45:r:109:ARG:HH12	1.81	0.45
1:1:458:G:O2'	1:1:469:G:O6	2.24	0.45
1:1:578:G:OP1	1:1:1255:U:O2'	2.32	0.45
1:1:600:G:OP1	7:D:24:ASN:ND2	2.49	0.45
1:1:1645:G:H5"	1:1:1646:C:H5'	1.99	0.45
1:1:1819:A:H5"	5:B:160:THR:HG21	1.97	0.45
3:3:63:C:H2'	3:3:64:G:H8	1.81	0.45
35:h:40:ARG:NH1	35:h:55:ILE:O	2.50	0.45
1:1:2199:A:OP1	25:X:37:ARG:NH1	2.50	0.45
1:1:2584:U:H2'	1:1:2585:U:H2'	1.99	0.45
2:2:266:G:H3'	49:v:69:LYS:HB2	1.98	0.45
7:D:83:VAL:HB	7:D:86:ALA:HB2	1.98	0.45
8:E:64:LYS:HD3	28:a:5:ILE:HB	1.98	0.45
1:1:1730:C:H4'	1:1:1731:G:C4	2.51	0.45
1:1:2002:G:H5'	15:N:13:ASN:HA	1.98	0.45
2:2:545:C:O2'	2:2:549:C:H5"	2.17	0.45
2:2:1218:C:H2'	2:2:1219:A:C8	2.52	0.45
42:o:42:LEU:HB2	42:o:71:LEU:HB3	1.98	0.45
43:p:24:HIS:HB3	43:p:31:ILE:HB	1.99	0.45
1:1:358:U:H2'	1:1:359:G:H8	1.81	0.45
1:1:1392:A:N6	21:T:18:GLU:OE1	2.50	0.45
10:G:99:ILE:HG21	10:G:130:VAL:HG11	1.99	0.45
31:d:31:LEU:HD22	31:d:42:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:g:117:LEU:HB3	34:g:141:LEU:HD13	1.99	0.45
1:1:2757:A:N1	9:F:67:THR:OG1	2.43	0.45
2:2:60:A:N6	2:2:110:C:N3	2.65	0.45
2:2:143:A:H2	2:2:220:G:H22	1.65	0.45
3:3:66:A:H2	3:3:68:C:H41	1.64	0.45
6:C:181:ASP:OD2	6:C:184:ARG:NH2	2.50	0.45
14:M:40:ARG:HD3	14:M:93:VAL:HG11	1.99	0.45
3:3:43:C:N4	3:3:45:A:N1	2.64	0.45
1:1:2135:A:H62	1:1:2136:G:H21	1.65	0.45
1:1:2392:A:OP2	32:e:31:HIS:HE1	1.98	0.45
1:1:2772:C:H5'	6:C:173:GLN:HE21	1.82	0.45
7:D:161:ALA:HA	7:D:164:LEU:HD12	1.98	0.45
29:b:30:VAL:HG22	29:b:37:LYS:HG2	1.98	0.45
37:j:133:PRO:HA	37:j:136:VAL:HG12	1.99	0.45
12:K:78:ARG:NH2	17:P:71:GLU:OE1	2.49	0.44
13:L:135:ILE:HG22	13:L:140:GLY:HA3	2.00	0.44
54:A:323:ASN:O	54:A:325:THR:HG23	2.17	0.44
1:1:362:A:H3'	1:1:363:G:H8	1.82	0.44
1:1:1386:C:H2'	1:1:1387:A:C8	2.52	0.44
1:1:2688:G:N1	1:1:2720:U:OP2	2.34	0.44
2:2:496:A:O2'	2:2:497:G:H8	2.00	0.44
11:J:13:ARG:NH1	11:J:49:ASP:O	2.46	0.44
54:A:135:TYR:OH	54:A:178:GLU:OE1	2.32	0.44
54:A:214:LEU:O	54:A:214:LEU:HD12	2.18	0.44
1:1:636:G:N1	13:L:76:GLU:OE1	2.44	0.44
1:1:1394:U:H4'	1:1:1603:A:H4'	2.00	0.44
19:R:52:PRO:O	19:R:53:PHE:CE2	2.59	0.44
36:i:52:GLY:O	36:i:56:ARG:N	2.44	0.44
41:n:116:VAL:HG21	42:o:62:ARG:HB2	2.00	0.44
54:A:182:HIS:HB3	54:A:310:TYR:HE2	1.82	0.44
1:1:52:A:OP2	1:1:117:G:N1	2.41	0.44
2:2:1213:A:O2'	2:2:1215:G:N7	2.49	0.44
13:L:62:PRO:HB2	32:e:30:ARG:HH11	1.82	0.44
18:Q:72:ASN:HD22	18:Q:110:VAL:HG21	1.82	0.44
36:i:107:PHE:HB3	36:i:145:ILE:HD11	2.00	0.44
39:l:129:GLU:OE1	39:l:131:LYS:HB3	2.17	0.44
42:o:7:ARG:HB2	42:o:101:SER:HB2	1.99	0.44
1:1:58:G:O2'	1:1:73:A:N1	2.46	0.44
2:2:79:G:H2'	2:2:80:A:H8	1.82	0.44
2:2:252:U:O2	2:2:275:G:N2	2.50	0.44
43:p:28:ASN:O	43:p:57:LYS:NZ	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:720:U:H2'	1:1:721:A:H8	1.82	0.44
2:2:496:A:O2'	2:2:497:G:C8	2.65	0.44
6:C:45:TYR:OH	6:C:81:GLU:OE2	2.36	0.44
36:i:201:VAL:O	36:i:205:SER:OG	2.30	0.44
1:1:675:A:N3	1:1:2443:C:O2'	2.46	0.44
2:2:1009:U:H3	2:2:1020:G:H1	1.64	0.44
2:2:1135:U:O2'	2:2:1136:C:O2	2.29	0.44
9:F:86:LYS:HG2	9:F:132:VAL:HG22	1.99	0.44
34:g:88:ASP:OD2	34:g:225:ARG:CZ	2.66	0.44
36:i:168:PRO:HG2	36:i:171:LEU:HB2	1.98	0.44
43:p:83:GLU:HB2	43:p:109:ASN:HB2	2.00	0.44
1:1:720:U:H2'	1:1:721:A:C8	2.53	0.44
2:2:259:G:OP1	52:y:36:TYR:OH	2.32	0.44
5:B:16:VAL:HG22	5:B:206:GLY:HA3	2.00	0.44
9:F:89:LEU:HD23	9:F:94:TYR:HB3	2.00	0.44
30:c:10:LYS:HA	30:c:22:THR:HA	2.00	0.44
34:g:119:THR:O	34:g:124:GLY:N	2.37	0.44
1:1:1340:U:OP1	21:T:19:LYS:NZ	2.46	0.44
1:1:1365:A:OP2	25:X:2:SER:OG	2.28	0.44
1:1:1802:A:OP2	1:1:1815:A:N6	2.47	0.44
2:2:200:G:H1	2:2:217:C:H42	1.66	0.44
2:2:960:U:H2'	2:2:1225:A:H62	1.83	0.44
6:C:152:PRO:C	6:C:154:LYS:H	2.25	0.44
24:W:23:VAL:HG22	24:W:38:VAL:HG22	1.99	0.44
51:x:32:ARG:HA	51:x:50:ALA:HB3	2.00	0.44
1:1:601:C:O2'	1:1:605:G:H5"	2.18	0.43
1:1:831:G:O2'	13:L:38:GLN:OE1	2.36	0.43
1:1:893:C:H2'	1:1:894:U:O5'	2.18	0.43
2:2:928:G:O2'	2:2:1533:C:OP1	2.35	0.43
2:2:1038:C:N4	2:2:1039:G:O6	2.51	0.43
2:2:1520:C:H5"	2:2:1520:C:H6	1.83	0.43
48:u:68:SER:OG	48:u:69:ASP:N	2.50	0.43
54:A:108:GLU:HA	54:A:170:GLY:HA2	1.99	0.43
1:1:942:G:O2'	1:1:1189:A:N3	2.50	0.43
1:1:2144:G:O2'	1:1:2147:A:N6	2.51	0.43
1:1:2571:U:O2'	6:C:151:THR:CB	2.65	0.43
15:N:37:THR:HA	15:N:110:MET:HA	2.00	0.43
19:R:51:VAL:CB	19:R:52:PRO:CD	2.92	0.43
1:1:538:A:H4'	11:J:7:LYS:HG2	1.99	0.43
1:1:2054:A:OP1	1:1:2055:C:O2'	2.29	0.43
2:2:603:U:H2'	2:2:604:G:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:25:THR:OG1	6:C:191:GLY:O	2.33	0.43
10:G:8:LYS:HA	10:G:14:SER:HA	2.00	0.43
18:Q:49:ASP:O	18:Q:53:ARG:N	2.50	0.43
2:2:445:G:H1	2:2:489:C:H42	1.67	0.43
22:U:48:PRO:HG3	22:U:56:GLY:HA3	2.00	0.43
36:i:60:LYS:HE3	36:i:195:ILE:HG12	1.99	0.43
1:1:2573:C:N3	54:A:228:ARG:NH2	2.55	0.43
2:2:841:C:H2'	2:2:843:U:H5'	2.00	0.43
13:L:9:ALA:HB3	13:L:12:SER:HB2	2.00	0.43
19:R:29:THR:HG22	19:R:66:HIS:HD2	1.82	0.43
34:g:120:GLN:HA	34:g:124:GLY:HA3	1.99	0.43
41:n:130:ARG:HH11	55:5:32:4OC:P	2.42	0.43
1:1:1296:G:OP1	1:1:2709:G:O2'	2.30	0.43
1:1:1657:U:OP1	6:C:141:ARG:N	2.49	0.43
1:1:2123:G:N2	1:1:2175:C:N3	2.67	0.43
14:M:33:LEU:HD23	14:M:103:TYR:HD2	1.83	0.43
37:j:96:MET:HB3	37:j:111:MET:HE1	2.01	0.43
1:1:85:G:OP2	22:U:7:ARG:HB2	2.19	0.43
1:1:232:G:N1	1:1:420:C:OP1	2.45	0.43
1:1:686:U:O2'	31:d:4:THR:O	2.32	0.43
1:1:729:G:N3	1:1:729:G:C2'	2.80	0.43
1:1:1475:G:O2'	1:1:1514:G:O6	2.32	0.43
1:1:1477:A:N1	1:1:1557:C:O2'	2.48	0.43
2:2:920:U:O2'	2:2:1081:A:O2'	2.34	0.43
11:J:32:LEU:HD22	11:J:54:ILE:HG21	2.00	0.43
12:K:7:MET:HB3	12:K:18:ARG:HD2	2.01	0.43
12:K:41:ILE:HD11	12:K:86:LEU:HD22	2.00	0.43
20:S:73:LYS:HB2	20:S:106:VAL:HB	2.01	0.43
28:a:57:VAL:HG22	51:x:67:VAL:HG21	2.00	0.43
35:h:64:ILE:HG22	35:h:97:VAL:HG23	2.01	0.43
41:n:21:ILE:HG23	41:n:61:LEU:HD13	2.01	0.43
47:t:80:GLN:HE21	47:t:84:ARG:NH2	2.16	0.43
1:1:547:A:N6	1:1:549:G:OP2	2.52	0.43
14:M:47:GLU:OE2	14:M:50:ARG:NH1	2.50	0.43
37:j:15:LEU:HA	37:j:37:THR:HA	2.01	0.43
38:k:10:VAL:HA	38:k:84:VAL:HA	2.01	0.43
39:l:107:ALA:HB1	39:l:133:THR:HB	2.01	0.43
1:1:1655:A:N6	1:1:2005:A:O2'	2.51	0.43
6:C:152:PRO:C	6:C:154:LYS:N	2.77	0.43
7:D:7:ASP:OD1	7:D:7:ASP:N	2.52	0.43
25:X:12:PRO:HB3	25:X:30:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:3:LYS:HD2	27:Z:3:LYS:HA	1.87	0.43
29:b:43:ILE:HG22	29:b:49:TYR:HB2	2.00	0.43
1:1:440:C:H2'	1:1:441:U:H6	1.83	0.43
1:1:870:U:OP1	14:M:6:ARG:NH1	2.49	0.43
1:1:2250:G:C8	1:1:2496:C:H5"	2.54	0.43
1:1:2579:C:O2'	6:C:136:ASN:ND2	2.52	0.43
1:1:2620:C:O2'	6:C:162:ALA:O	2.33	0.43
2:2:257:G:H2'	2:2:258:G:C8	2.54	0.43
2:2:481:G:O2'	2:2:483:C:N4	2.52	0.43
2:2:1236:A:H4'	2:2:1304:G:H4'	2.01	0.43
2:2:1372:U:OP1	41:n:74:GLY:N	2.51	0.43
8:E:94:GLU:OE2	28:a:25:ARG:NH1	2.47	0.43
16:O:50:ALA:O	16:O:81:ARG:NH2	2.51	0.43
37:j:111:MET:HG3	37:j:140:THR:HG21	2.01	0.43
1:1:529:A:OP2	11:J:116:ARG:NH2	2.37	0.42
1:1:2340:A:H5'	3:3:41:G:H21	1.83	0.42
2:2:946:A:O2'	2:2:1333:A:N3	2.47	0.42
54:A:322:ILE:HB	54:A:324:LEU:HG	2.00	0.42
1:1:463:G:N2	1:1:466:A:OP2	2.45	0.42
1:1:729:G:C5	5:B:207:LYS:HB2	2.54	0.42
1:1:1568:G:N7	5:B:28:LYS:NZ	2.67	0.42
1:1:2472:G:N2	1:1:2477:U:OP1	2.40	0.42
2:2:979:C:O2	46:s:59:ARG:NH1	2.51	0.42
8:E:135:GLN:HG2	8:E:141:ILE:HG21	2.01	0.42
19:R:52:PRO:O	19:R:53:PHE:CB	2.62	0.42
43:p:99:ALA:HA	43:p:102:ALA:HB3	2.01	0.42
48:u:44:SER:N	48:u:47:GLU:OE2	2.42	0.42
52:y:38:ALA:O	52:y:42:GLY:N	2.52	0.42
1:1:783:A:N3	1:1:783:A:H3'	2.35	0.42
1:1:2050:C:N4	1:1:2051:A:N1	2.66	0.42
1:1:2304:G:H22	1:1:2312:U:H3	1.67	0.42
2:2:1316:G:N1	2:2:1319:A:OP2	2.52	0.42
30:c:9:ILE:HD13	30:c:25:LYS:HD2	2.02	0.42
36:i:78:GLU:OE2	36:i:81:ARG:NH1	2.51	0.42
42:o:37:ARG:HB3	42:o:75:ASP:HB3	2.00	0.42
44:q:46:ASN:ND2	44:q:89:0TD:SB	2.89	0.42
1:1:355:U:H2'	1:1:356:G:C8	2.53	0.42
1:1:1782:U:H1'	1:1:2609:U:H5"	2.01	0.42
1:1:1799:G:OP1	5:B:258:ARG:NE	2.47	0.42
1:1:2298:A:H61	1:1:2318:G:H1'	1.84	0.42
1:1:2359:C:O2'	32:e:54:ASP:OD2	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:67:C:H42	2:2:102:G:H1	1.66	0.42
2:2:130:A:N1	2:2:233:C:O2'	2.42	0.42
2:2:414:A:OP2	2:2:428:G:N2	2.50	0.42
5:B:232:HIS:CG	5:B:240:PHE:HE1	2.37	0.42
6:C:4:LEU:HD21	6:C:96:ILE:HG22	2.01	0.42
47:t:36:ILE:HG23	47:t:56:LEU:HD11	2.00	0.42
1:1:77:G:O3'	26:Y:7:ARG:NH2	2.52	0.42
1:1:1800:C:OP1	5:B:258:ARG:NH2	2.53	0.42
2:2:356:A:N3	2:2:368:U:O2'	2.46	0.42
2:2:533:A:O2'	2:2:535:A:OP2	2.34	0.42
2:2:1312:G:OP2	28:a:63:ARG:NH2	2.51	0.42
19:R:5:PHE:HB3	19:R:59:ILE:HD12	2.02	0.42
35:h:60:PRO:HB3	42:o:94:ALA:HA	2.01	0.42
38:k:35:LYS:HB2	38:k:65:GLU:HB3	2.01	0.42
1:1:567:U:OP2	13:L:29:LYS:NZ	2.50	0.42
2:2:264:C:O3'	49:v:65:ARG:NH2	2.53	0.42
2:2:269:C:H2'	2:2:270:A:C8	2.54	0.42
2:2:1158:C:H2'	2:2:1158:C:O2	2.18	0.42
5:B:94:VAL:HG11	5:B:116:ILE:HD11	2.02	0.42
8:E:134:GLU:HG3	8:E:149:VAL:HG13	2.01	0.42
19:R:42:ALA:HA	19:R:47:VAL:HA	2.02	0.42
42:o:12:ALA:HB3	42:o:18:ILE:HB	2.01	0.42
1:1:115:C:O2'	1:1:127:A:O2'	2.31	0.42
1:1:1550:C:H2'	1:1:1551:A:C8	2.54	0.42
1:1:2305:U:H5"	8:E:131:GLY:HA3	2.00	0.42
1:1:2357:G:N2	1:1:2360:G:OP2	2.41	0.42
2:2:10:A:HO2'	2:2:507:C:HO2'	1.61	0.42
2:2:1125:U:H4'	42:o:7:ARG:HH22	1.85	0.42
12:K:21:CYS:HA	12:K:41:ILE:HG22	2.01	0.42
38:k:21:MET:HA	38:k:24:ARG:HH21	1.85	0.42
48:u:44:SER:OG	48:u:45:GLU:N	2.53	0.42
49:v:12:VAL:HB	49:v:57:ASP:HB3	2.01	0.42
1:1:30:G:O2'	1:1:1214:A:N3	2.48	0.42
1:1:1447:C:O2'	1:1:1544:A:N3	2.53	0.42
1:1:1712:U:OP2	1:1:1713:A:O2'	2.35	0.42
1:1:2548:U:O2	12:K:23:LYS:NZ	2.51	0.42
2:2:972:C:OP2	42:o:59:LYS:NZ	2.41	0.42
6:C:97:SER:OG	6:C:98:VAL:N	2.53	0.42
8:E:58:ALA:HB2	8:E:65:PRO:HD3	2.02	0.42
10:G:73:ASN:HD21	10:G:108:VAL:HG23	1.84	0.42
18:Q:18:LEU:HD21	18:Q:32:TYR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:24:G:O2'	20:S:78:GLU:O	2.33	0.42
2:2:443:C:H2'	2:2:444:G:H8	1.85	0.42
2:2:662:U:H2'	2:2:663:A:C8	2.54	0.42
2:2:1414:U:H2'	2:2:1415:G:H8	1.85	0.42
21:T:28:ASN:ND2	21:T:88:LYS:O	2.52	0.42
27:Z:30:ARG:HB2	27:Z:31:ARG:HE	1.84	0.42
55:5:7:U:H5'	55:5:49:G:H5'	2.00	0.42
1:1:324:A:OP2	1:1:1205:A:N6	2.53	0.42
1:1:851:C:O2'	27:Z:43:ALA:O	2.38	0.42
2:2:946:A:H2'	2:2:947:G:C8	2.55	0.42
2:2:1441:A:H3'	2:2:1442:G:H8	1.85	0.42
3:3:30:C:H2'	3:3:31:C:O4'	2.20	0.42
8:E:140:GLU:OE2	28:a:26:SER:OG	2.29	0.42
14:M:41:LEU:HD22	14:M:124:LEU:HD22	2.02	0.42
26:Y:7:ARG:NH1	26:Y:59:GLU:OE1	2.53	0.42
1:1:1323:C:N4	1:1:1324:G:O6	2.53	0.41
1:1:2121:G:H1	1:1:2175:C:H41	1.68	0.41
1:1:2796:U:H1'	1:1:2797:U:H2'	2.02	0.41
37:j:72:ILE:HD12	37:j:72:ILE:HA	1.96	0.41
51:x:50:ALA:HB1	51:x:57:HIS:HB3	2.02	0.41
54:A:216:ASP:OD1	54:A:216:ASP:N	2.48	0.41
1:1:192:C:O2'	1:1:802:A:N3	2.52	0.41
1:1:1341:G:OP2	1:1:1394:U:O2'	2.35	0.41
2:2:1109:C:N4	2:2:1110:A:C5	2.88	0.41
2:2:1124:G:O2'	2:2:1145:A:N6	2.53	0.41
3:3:8:C:OP1	16:O:15:ARG:NH2	2.45	0.41
6:C:25:THR:HG21	6:C:193:VAL:HG22	2.01	0.41
14:M:57:VAL:HA	14:M:112:LEU:HD21	2.02	0.41
35:h:60:PRO:O	35:h:63:SER:OG	2.30	0.41
1:1:1568:G:OP2	5:B:63:ARG:NH1	2.48	0.41
1:1:2375:G:N2	1:1:2378:A:OP2	2.37	0.41
1:1:2678:C:H2'	1:1:2679:A:O4'	2.21	0.41
1:1:2849:U:O4	17:P:21:ARG:NH2	2.53	0.41
2:2:51:A:N7	2:2:114:U:O2'	2.51	0.41
13:L:37:GLY:N	13:L:40:SER:OG	2.43	0.41
41:n:26:GLY:N	41:n:62:ASP:OD1	2.52	0.41
1:1:298:G:O2'	1:1:322:A:N1	2.47	0.41
1:1:878:A:H3'	1:1:879:G:H8	1.85	0.41
1:1:1567:G:N2	5:B:27:GLY:O	2.54	0.41
2:2:324:G:N1	2:2:327:A:OP2	2.53	0.41
2:2:980:C:O2'	46:s:13:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1277:C:O2'	2:2:1279:G:H8	2.03	0.41
2:2:1425:U:H2'	2:2:1426:G:H8	1.85	0.41
38:k:6:ILE:HG12	38:k:89:VAL:HG22	2.01	0.41
48:u:6:LEU:HD23	48:u:17:TYR:CG	2.55	0.41
1:1:85:G:C6	1:1:98:G:N2	2.87	0.41
1:1:770:G:H5'	31:d:10:LEU:HD23	2.02	0.41
1:1:1682:G:OP2	1:1:1699:G:N2	2.50	0.41
1:1:2260:C:H42	1:1:2280:G:H1	1.66	0.41
2:2:501:C:H2'	2:2:502:A:C8	2.56	0.41
2:2:537:G:H5"	44:q:110:ARG:HH12	1.85	0.41
2:2:920:U:HO2'	2:2:1081:A:HO2'	1.67	0.41
2:2:1414:U:O2	2:2:1487:G:N2	2.53	0.41
17:P:28:VAL:O	17:P:43:PHE:N	2.54	0.41
37:j:156:LYS:HG2	40:m:71:VAL:HG13	2.02	0.41
45:r:20:THR:HA	45:r:25:VAL:HG23	2.03	0.41
45:r:98:ARG:HB2	45:r:100:GLN:NE2	2.35	0.41
52:y:39:ILE:HA	52:y:86:LEU:HD11	2.02	0.41
1:1:61:C:OP1	26:Y:47:ARG:NH1	2.47	0.41
1:1:783:A:O2'	1:1:785:G:OP1	2.31	0.41
1:1:783:A:H1'	1:1:1779:U:H1'	2.03	0.41
18:Q:50:ARG:O	18:Q:54:LYS:NZ	2.51	0.41
40:m:53:GLY:HA3	40:m:57:PRO:HA	2.03	0.41
1:1:48:G:O2'	1:1:118:A:N1	2.47	0.41
1:1:1915:3TD:H2'	1:1:1916:A:O4'	2.20	0.41
1:1:2183:A:H2'	1:1:2184:A:C8	2.56	0.41
2:2:452:A:H2'	2:2:453:G:O4'	2.21	0.41
2:2:825:A:O2'	40:m:13:ARG:NH2	2.51	0.41
2:2:1220:G:H1'	51:x:52:HIS:HD2	1.85	0.41
19:R:69:GLY:N	19:R:91:GLN:O	2.46	0.41
42:o:100:ILE:H	42:o:100:ILE:HG13	1.69	0.41
45:r:65:VAL:HB	45:r:66:GLU:H	1.72	0.41
1:1:2250:G:N3	1:1:2250:G:H5'	2.35	0.41
2:2:108:G:P	2:2:326:G:H22	2.44	0.41
2:2:606:G:N2	2:2:632:U:OP1	2.32	0.41
2:2:837:U:H2'	2:2:838:G:C8	2.56	0.41
2:2:1316:G:N2	2:2:1318:A:H3'	2.36	0.41
46:s:27:LEU:HD23	46:s:30:ILE:HD12	2.03	0.41
55:5:25:C:H2'	55:5:26:G:O4'	2.21	0.41
1:1:634:C:H2'	1:1:635:C:C6	2.56	0.41
1:1:741:U:H2'	1:1:742:A:C8	2.56	0.41
1:1:796:C:H2'	1:1:797:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:801:G:C8	7:D:50:ALA:HB2	2.56	0.41
1:1:1222:U:H2'	1:1:1223:G:C8	2.56	0.41
1:1:1301:A:H2	1:1:1626:A:H2	1.69	0.41
1:1:1447:C:H2'	1:1:1448:G:C8	2.56	0.41
1:1:1469:A:H2'	1:1:1470:A:C8	2.55	0.41
1:1:1794:A:H2'	1:1:1795:C:C6	2.55	0.41
1:1:2186:G:H2'	1:1:2187:U:C2	2.56	0.41
1:1:2693:G:H2'	1:1:2694:G:H8	1.86	0.41
2:2:83:C:O2	2:2:86:G:N1	2.53	0.41
2:2:552:U:O2'	44:q:83:ARG:O	2.30	0.41
2:2:1266:G:N2	2:2:1269:A:OP2	2.51	0.41
14:M:21:ALA:HB2	14:M:97:GLN:HB2	2.02	0.41
14:M:49:ALA:HB1	14:M:120:ALA:HB1	2.03	0.41
41:n:39:PHE:O	41:n:45:ARG:NE	2.43	0.41
50:w:32:TYR:CG	50:w:55:LEU:HD21	2.55	0.41
51:x:63:THR:HG22	51:x:64:ASP:H	1.86	0.41
1:1:2263:C:H42	1:1:2277:G:H1	1.68	0.41
2:2:443:C:H2'	2:2:444:G:C8	2.56	0.41
2:2:537:G:H5"	44:q:110:ARG:NH1	2.36	0.41
13:L:18:ARG:HH11	13:L:18:ARG:HD3	1.74	0.41
21:T:54:GLU:HB3	21:T:88:LYS:HD2	2.02	0.41
30:c:17:THR:HG21	30:c:42:VAL:HG21	2.03	0.41
32:e:31:HIS:ND1	32:e:31:HIS:C	2.79	0.41
1:1:1808:A:H3'	1:1:1809:A:C8	2.56	0.40
2:2:276:G:OP1	49:v:14:SER:OG	2.34	0.40
1:1:414:C:O2	1:1:1864:U:O2'	2.33	0.40
1:1:706:A:OP1	5:B:7:LYS:NZ	2.37	0.40
1:1:2151:U:H2'	1:1:2152:G:C8	2.57	0.40
1:1:2311:A:C6	8:E:41:GLY:HA3	2.56	0.40
2:2:663:A:H61	2:2:742:G:H1	1.68	0.40
2:2:1340:A:O2'	55:5:31:G:O2'	2.26	0.40
9:F:154:PRO:HA	9:F:161:GLY:HA3	2.03	0.40
23:V:75:GLN:HB2	23:V:92:VAL:HG23	2.02	0.40
24:W:49:ALA:HB3	24:W:81:SER:HB2	2.04	0.40
35:h:79:LYS:HB2	35:h:82:GLU:HB2	2.03	0.40
39:l:70:ARG:NH2	39:l:97:ASN:OD1	2.54	0.40
43:p:31:ILE:HG23	43:p:46:THR:HG22	2.03	0.40
47:t:78:TYR:OH	47:t:89:ARG:O	2.28	0.40
51:x:13:LEU:O	51:x:17:LYS:N	2.49	0.40
55:5:5:G:H2'	55:5:6:G:C8	2.56	0.40
1:1:488:G:H2'	1:1:489:G:H2'	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:904:G:H2'	1:1:905:A:C8	2.57	0.40
1:1:1068:G:H8	1:1:1069:A:H5'	1.86	0.40
1:1:2377:A:H2'	1:1:2378:A:C8	2.57	0.40
2:2:579:A:O2'	47:t:54:ARG:NH1	2.38	0.40
2:2:626:G:O3'	48:u:51:ARG:NH1	2.54	0.40
11:J:114:LEU:HG	11:J:118:MET:HE3	2.03	0.40
35:h:40:ARG:HG3	35:h:57:ILE:HD11	2.04	0.40
38:k:19:PRO:HA	38:k:22:ILE:HD12	2.03	0.40
49:v:12:VAL:N	49:v:57:ASP:O	2.51	0.40
54:A:214:LEU:O	54:A:214:LEU:HG	2.22	0.40
1:1:31:C:O2'	1:1:1238:G:OP1	2.39	0.40
1:1:632:A:N3	1:1:2403:C:O2'	2.43	0.40
2:2:450:G:N1	2:2:484:G:O6	2.54	0.40
2:2:977:A:O2'	2:2:979:C:OP2	2.32	0.40
2:2:1305:G:O2'	2:2:1306:A:O4'	2.39	0.40
5:B:108:LYS:HA	5:B:196:GLY:HA2	2.02	0.40
8:E:47:LYS:O	8:E:51:ASP:N	2.48	0.40
39:l:46:ALA:HB1	39:l:121:ALA:HB2	2.04	0.40
53:z:70:LEU:HD12	53:z:70:LEU:N	2.37	0.40
1:1:698:C:O2'	1:1:734:A:N6	2.54	0.40
2:2:413:G:N2	2:2:428:G:O3'	2.46	0.40
2:2:983:A:N1	2:2:1222:G:N2	2.69	0.40
3:3:91:C:OP1	14:M:19:GLY:N	2.45	0.40
10:G:14:SER:OG	10:G:15:LEU:N	2.54	0.40
35:h:142:MET:HE2	35:h:170:GLU:HG2	2.04	0.40
48:u:1:MET:O	48:u:24:SER:N	2.54	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	
5	B	269/271 (99%)	254 (94%)	15 (6%)	0	100	100
6	C	207/209 (99%)	195 (94%)	10 (5%)	2 (1%)	12	45
7	D	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
8	E	175/177 (99%)	163 (93%)	12 (7%)	0	100	100
9	F	173/175 (99%)	163 (94%)	10 (6%)	0	100	100
10	G	147/149 (99%)	135 (92%)	12 (8%)	0	100	100
11	J	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
12	K	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
13	L	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	M	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
15	N	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
16	O	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
17	P	112/114 (98%)	104 (93%)	8 (7%)	0	100	100
18	Q	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
19	R	101/103 (98%)	90 (89%)	9 (9%)	2 (2%)	6	32
20	S	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
21	T	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
22	U	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
23	V	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
24	W	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
25	X	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
26	Y	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
27	Z	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
28	a	64/66 (97%)	60 (94%)	4 (6%)	0	100	100
29	b	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
30	c	50/52 (96%)	50 (100%)	0	0	100	100
31	d	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
32	e	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	7	36
33	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
34	g	223/225 (99%)	211 (95%)	12 (5%)	0	100	100
35	h	206/208 (99%)	193 (94%)	13 (6%)	0	100	100
36	i	203/205 (99%)	194 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	j	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
38	k	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
39	l	149/151 (99%)	143 (96%)	6 (4%)	0	100	100
40	m	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
41	n	125/127 (98%)	115 (92%)	10 (8%)	0	100	100
42	o	97/99 (98%)	88 (91%)	9 (9%)	0	100	100
43	p	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
44	q	120/123 (98%)	108 (90%)	12 (10%)	0	100	100
45	r	114/116 (98%)	106 (93%)	8 (7%)	0	100	100
46	s	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
47	t	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
48	u	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
49	v	78/80 (98%)	71 (91%)	7 (9%)	0	100	100
50	w	64/66 (97%)	60 (94%)	4 (6%)	0	100	100
51	x	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
52	y	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
53	z	68/70 (97%)	68 (100%)	0	0	100	100
54	A	257/259 (99%)	236 (92%)	18 (7%)	3 (1%)	10	41
56	6	1/3 (33%)	0	0	1 (100%)	0	0
All	All	5866/5969 (98%)	5551 (95%)	306 (5%)	9 (0%)	44	72

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	R	53	PHE
54	A	213	GLU
54	A	323	ASN
54	A	324	LEU
19	R	52	PRO
56	6	78	PHE
6	C	153	GLY
32	e	32	ILE
6	C	152	PRO

5.3.2 Protein sidechains (i)

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	
5	B	216/216 (100%)	216 (100%)	0	100	100
6	C	164/164 (100%)	163 (99%)	1 (1%)	78	79
7	D	165/165 (100%)	164 (99%)	1 (1%)	78	79
8	E	148/148 (100%)	147 (99%)	1 (1%)	76	78
9	F	136/136 (100%)	135 (99%)	1 (1%)	76	78
10	G	114/114 (100%)	114 (100%)	0	100	100
11	J	116/116 (100%)	115 (99%)	1 (1%)	70	76
12	K	104/104 (100%)	104 (100%)	0	100	100
13	L	103/103 (100%)	103 (100%)	0	100	100
14	M	109/109 (100%)	109 (100%)	0	100	100
15	N	99/99 (100%)	98 (99%)	1 (1%)	68	75
16	O	86/86 (100%)	86 (100%)	0	100	100
17	P	99/99 (100%)	98 (99%)	1 (1%)	68	75
18	Q	89/89 (100%)	89 (100%)	0	100	100
19	R	84/84 (100%)	83 (99%)	1 (1%)	63	73
20	S	93/93 (100%)	92 (99%)	1 (1%)	65	74
21	T	81/81 (100%)	80 (99%)	1 (1%)	63	73
22	U	84/84 (100%)	84 (100%)	0	100	100
23	V	78/78 (100%)	77 (99%)	1 (1%)	61	72
24	W	58/58 (100%)	58 (100%)	0	100	100
25	X	67/67 (100%)	67 (100%)	0	100	100
26	Y	54/54 (100%)	54 (100%)	0	100	100
27	Z	48/48 (100%)	47 (98%)	1 (2%)	47	65
28	a	59/59 (100%)	59 (100%)	0	100	100
29	b	47/47 (100%)	46 (98%)	1 (2%)	47	65
30	c	47/47 (100%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	d	38/38 (100%)	37 (97%)	1 (3%)	40	62
32	e	51/51 (100%)	49 (96%)	2 (4%)	28	54
33	f	34/34 (100%)	33 (97%)	1 (3%)	37	60
34	g	187/187 (100%)	186 (100%)	1 (0%)	81	80
35	h	171/171 (100%)	170 (99%)	1 (1%)	78	79
36	i	172/172 (100%)	172 (100%)	0	100	100
37	j	119/119 (100%)	119 (100%)	0	100	100
38	k	91/91 (100%)	91 (100%)	0	100	100
39	l	124/124 (100%)	122 (98%)	2 (2%)	55	69
40	m	104/104 (100%)	104 (100%)	0	100	100
41	n	105/105 (100%)	105 (100%)	0	100	100
42	o	86/86 (100%)	85 (99%)	1 (1%)	63	73
43	p	90/90 (100%)	90 (100%)	0	100	100
44	q	102/102 (100%)	102 (100%)	0	100	100
45	r	94/94 (100%)	94 (100%)	0	100	100
46	s	83/83 (100%)	83 (100%)	0	100	100
47	t	76/76 (100%)	76 (100%)	0	100	100
48	u	65/65 (100%)	64 (98%)	1 (2%)	57	70
49	v	74/74 (100%)	74 (100%)	0	100	100
50	w	57/57 (100%)	57 (100%)	0	100	100
51	x	72/72 (100%)	71 (99%)	1 (1%)	59	71
52	y	65/65 (100%)	65 (100%)	0	100	100
53	z	60/60 (100%)	60 (100%)	0	100	100
54	A	210/210 (100%)	209 (100%)	1 (0%)	81	80
56	6	2/2 (100%)	2 (100%)	0	100	100
All	All	4880/4880 (100%)	4855 (100%)	25 (0%)	78	80

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	C	151	THR
7	D	163	ASN
8	E	47	LYS

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Mol	Chain	Res	Type
9	F	11	VAL
11	J	57	LEU
15	N	2	ARG
17	P	114	LEU
19	R	51	VAL
20	S	98	LYS
21	T	61	LEU
23	V	65	VAL
27	Z	25	LEU
29	b	9	THR
31	d	42	LEU
32	e	31	HIS
32	e	32	ILE
33	f	26	ILE
34	g	129	LEU
35	h	72	ARG
39	l	130	ASN
39	l	131	LYS
42	o	100	ILE
48	u	2	VAL
51	x	58	VAL
54	A	184	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
5	B	58	HIS
5	B	86	ASN
5	B	128	ASN
5	B	260	ASN
6	C	32	ASN
6	C	49	GLN
6	C	136	ASN
7	D	92	HIS
7	D	115	GLN
7	D	163	ASN
7	D	195	GLN
9	F	88	GLN
10	G	11	ASN
10	G	73	ASN
12	K	29	HIS
13	L	35	HIS

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Mol	Chain	Res	Type
14	M	60	GLN
15	N	31	HIS
16	O	38	GLN
16	O	98	GLN
16	O	100	HIS
17	P	12	GLN
17	P	52	ASN
17	P	56	HIS
18	Q	44	GLN
18	Q	72	ASN
19	R	6	GLN
20	S	61	ASN
21	T	28	ASN
22	U	74	ASN
23	V	87	GLN
24	W	46	HIS
28	a	20	ASN
30	c	26	ASN
34	g	39	HIS
34	g	178	ASN
35	h	190	HIS
36	i	41	HIS
37	j	12	GLN
37	j	89	HIS
37	j	97	GLN
37	j	132	ASN
38	k	3	HIS
38	k	17	GLN
38	k	46	GLN
38	k	63	ASN
38	k	68	GLN
39	l	130	ASN
40	m	4	GLN
41	n	50	GLN
41	n	110	GLN
41	n	126	GLN
43	p	22	HIS
43	p	119	ASN
45	r	14	HIS
45	r	105	ASN
46	s	71	HIS
47	t	20	ASN

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Mol	Chain	Res	Type
47	t	80	GLN
50	w	54	GLN
51	x	52	HIS
51	x	57	HIS
52	y	3	ASN
52	y	21	ASN
52	y	61	GLN
54	A	218	ASN
54	A	235	GLN
54	A	279	HIS
54	A	296	ASN
54	A	307	ASN
54	A	311	ASN
54	A	348	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2902/2903 (99%)	598 (20%)	9 (0%)
2	2	1532/1534 (99%)	295 (19%)	4 (0%)
3	3	119/120 (99%)	23 (19%)	0
4	4	8/9 (88%)	3 (37%)	0
55	5	75/76 (98%)	19 (25%)	2 (2%)
All	All	4636/4642 (99%)	938 (20%)	15 (0%)

All (938) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	15	G
1	1	34	U
1	1	35	G
1	1	46	G
1	1	51	G
1	1	61	C
1	1	71	A
1	1	74	A
1	1	75	G
1	1	80	G
1	1	84	A
1	1	85	G

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Mol	Chain	Res	Type
1	1	96	C
1	1	101	A
1	1	102	U
1	1	110	G
1	1	118	A
1	1	119	A
1	1	120	U
1	1	125	A
1	1	131	A
1	1	139	U
1	1	142	A
1	1	163	C
1	1	165	A
1	1	181	A
1	1	186	G
1	1	196	A
1	1	199	A
1	1	200	U
1	1	204	A
1	1	215	G
1	1	216	A
1	1	221	A
1	1	222	A
1	1	225	C
1	1	228	C
1	1	229	C
1	1	230	G
1	1	248	G
1	1	249	C
1	1	250	G
1	1	265	A
1	1	266	G
1	1	270	A
1	1	272	A
1	1	273	G
1	1	276	U
1	1	277	G
1	1	278	A
1	1	284	U
1	1	294	A
1	1	302	C
1	1	311	A

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Mol	Chain	Res	Type
1	1	317	G
1	1	324	A
1	1	327	G
1	1	329	G
1	1	330	A
1	1	353	C
1	1	361	G
1	1	362	A
1	1	371	A
1	1	372	G
1	1	383	C
1	1	386	G
1	1	387	U
1	1	389	G
1	1	396	G
1	1	399	U
1	1	403	U
1	1	404	A
1	1	405	U
1	1	411	G
1	1	420	C
1	1	424	G
1	1	435	C
1	1	436	C
1	1	448	U
1	1	454	A
1	1	455	C
1	1	456	C
1	1	457	A
1	1	464	U
1	1	467	G
1	1	475	C
1	1	477	A
1	1	480	A
1	1	481	G
1	1	489	G
1	1	491	G
1	1	496	G
1	1	501	A
1	1	505	A
1	1	508	A
1	1	509	C

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Mol	Chain	Res	Type
1	1	518	G
1	1	529	A
1	1	531	C
1	1	532	A
1	1	533	G
1	1	543	G
1	1	544	C
1	1	545	U
1	1	547	A
1	1	548	G
1	1	549	G
1	1	550	C
1	1	551	G
1	1	563	A
1	1	573	U
1	1	575	A
1	1	583	G
1	1	586	A
1	1	603	A
1	1	613	A
1	1	614	A
1	1	615	U
1	1	618	G
1	1	627	A
1	1	637	A
1	1	645	C
1	1	646	U
1	1	654	A
1	1	655	A
1	1	656	G
1	1	659	G
1	1	668	A
1	1	670	A
1	1	686	U
1	1	710	U
1	1	723	C
1	1	730	A
1	1	738	G
1	1	747	5MU
1	1	761	A
1	1	762	U
1	1	763	G

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Mol	Chain	Res	Type
1	1	764	A
1	1	765	C
1	1	770	G
1	1	775	G
1	1	776	G
1	1	782	A
1	1	784	G
1	1	785	G
1	1	791	C
1	1	792	A
1	1	800	A
1	1	805	G
1	1	810	U
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	846	U
1	1	858	G
1	1	859	G
1	1	869	G
1	1	877	A
1	1	878	A
1	1	880	G
1	1	884	U
1	1	885	C
1	1	888	C
1	1	891	G
1	1	894	U
1	1	895	U
1	1	896	A
1	1	907	G
1	1	910	A
1	1	914	G
1	1	915	C
1	1	931	U
1	1	932	U
1	1	941	A
1	1	945	A
1	1	946	C
1	1	953	G
1	1	957	C

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Mol	Chain	Res	Type
1	1	959	A
1	1	961	C
1	1	973	A
1	1	974	G
1	1	983	A
1	1	984	A
1	1	989	G
1	1	991	C
1	1	995	C
1	1	996	A
1	1	999	U
1	1	1005	C
1	1	1012	U
1	1	1013	C
1	1	1022	G
1	1	1023	U
1	1	1024	G
1	1	1025	G
1	1	1026	G
1	1	1033	U
1	1	1034	G
1	1	1040	A
1	1	1041	G
1	1	1042	G
1	1	1046	A
1	1	1047	G
1	1	1058	U
1	1	1059	G
1	1	1061	U
1	1	1064	C
1	1	1065	U
1	1	1066	U
1	1	1068	G
1	1	1069	A
1	1	1070	A
1	1	1073	A
1	1	1074	G
1	1	1078	U
1	1	1079	C
1	1	1082	U
1	1	1083	U
1	1	1087	G

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Mol	Chain	Res	Type
1	1	1088	A
1	1	1089	A
1	1	1095	A
1	1	1096	A
1	1	1097	U
1	1	1110	G
1	1	1111	A
1	1	1112	G
1	1	1116	G
1	1	1119	U
1	1	1122	G
1	1	1126	A
1	1	1130	U
1	1	1131	G
1	1	1132	U
1	1	1134	A
1	1	1135	C
1	1	1139	G
1	1	1142	A
1	1	1143	A
1	1	1155	A
1	1	1167	C
1	1	1168	G
1	1	1169	A
1	1	1170	C
1	1	1173	U
1	1	1174	U
1	1	1175	A
1	1	1176	U
1	1	1177	G
1	1	1178	C
1	1	1180	U
1	1	1182	G
1	1	1186	G
1	1	1205	A
1	1	1206	G
1	1	1210	G
1	1	1212	G
1	1	1236	G
1	1	1238	G
1	1	1247	A
1	1	1250	G

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Mol	Chain	Res	Type
1	1	1253	A
1	1	1256	G
1	1	1262	A
1	1	1266	G
1	1	1271	G
1	1	1272	A
1	1	1273	U
1	1	1300	G
1	1	1301	A
1	1	1321	A
1	1	1325	U
1	1	1352	U
1	1	1359	A
1	1	1365	A
1	1	1368	G
1	1	1374	G
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1390	U
1	1	1395	A
1	1	1407	G
1	1	1409	U
1	1	1411	U
1	1	1417	C
1	1	1419	A
1	1	1420	A
1	1	1428	C
1	1	1437	C
1	1	1455	G
1	1	1458	U
1	1	1459	G
1	1	1461	C
1	1	1468	U
1	1	1480	C
1	1	1482	G
1	1	1490	A
1	1	1493	C
1	1	1503	A
1	1	1508	A
1	1	1509	A
1	1	1510	G

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Mol	Chain	Res	Type
1	1	1515	A
1	1	1522	A
1	1	1524	G
1	1	1528	A
1	1	1532	A
1	1	1535	A
1	1	1536	C
1	1	1557	C
1	1	1558	C
1	1	1566	A
1	1	1569	A
1	1	1578	U
1	1	1580	A
1	1	1583	A
1	1	1586	A
1	1	1587	G
1	1	1589	U
1	1	1590	A
1	1	1607	C
1	1	1608	A
1	1	1610	A
1	1	1616	A
1	1	1626	A
1	1	1634	A
1	1	1639	C
1	1	1647	U
1	1	1648	U
1	1	1649	G
1	1	1672	A
1	1	1674	G
1	1	1695	G
1	1	1698	A
1	1	1715	G
1	1	1724	G
1	1	1728	C
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1738	G
1	1	1756	G
1	1	1758	U
1	1	1764	C

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Mol	Chain	Res	Type
1	1	1773	A
1	1	1784	A
1	1	1800	C
1	1	1801	A
1	1	1802	A
1	1	1808	A
1	1	1811	G
1	1	1815	A
1	1	1816	C
1	1	1820	U
1	1	1828	G
1	1	1829	A
1	1	1833	C
1	1	1835	2MG
1	1	1847	A
1	1	1858	A
1	1	1865	U
1	1	1866	A
1	1	1869	G
1	1	1870	C
1	1	1872	A
1	1	1873	G
1	1	1900	A
1	1	1905	C
1	1	1906	G
1	1	1907	G
1	1	1912	A
1	1	1913	A
1	1	1914	C
1	1	1923	U
1	1	1924	C
1	1	1929	G
1	1	1930	G
1	1	1936	A
1	1	1938	A
1	1	1955	U
1	1	1965	C
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1982	U

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Mol	Chain	Res	Type
1	1	1991	U
1	1	1992	G
1	1	1993	U
1	1	1997	C
1	1	2002	G
1	1	2022	U
1	1	2023	C
1	1	2030	6MZ
1	1	2031	A
1	1	2033	A
1	1	2043	C
1	1	2049	G
1	1	2051	A
1	1	2055	C
1	1	2056	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2069	G7M
1	1	2072	C
1	1	2079	U
1	1	2093	G
1	1	2099	U
1	1	2102	G
1	1	2105	U
1	1	2110	G
1	1	2112	G
1	1	2113	U
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2119	A
1	1	2120	G
1	1	2121	G
1	1	2122	U
1	1	2125	G
1	1	2127	G
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2134	A

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Mol	Chain	Res	Type
1	1	2135	A
1	1	2137	U
1	1	2138	G
1	1	2139	U
1	1	2142	A
1	1	2145	C
1	1	2146	C
1	1	2147	A
1	1	2153	C
1	1	2158	A
1	1	2161	C
1	1	2162	G
1	1	2164	C
1	1	2165	C
1	1	2166	U
1	1	2167	U
1	1	2170	A
1	1	2171	A
1	1	2172	U
1	1	2173	A
1	1	2178	C
1	1	2182	U
1	1	2183	A
1	1	2188	U
1	1	2189	U
1	1	2190	G
1	1	2193	G
1	1	2194	U
1	1	2195	U
1	1	2198	A
1	1	2204	G
1	1	2211	A
1	1	2212	A
1	1	2225	A
1	1	2226	C
1	1	2229	U
1	1	2238	G
1	1	2239	G
1	1	2243	U
1	1	2244	U
1	1	2250	G
1	1	2259	U

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Mol	Chain	Res	Type
1	1	2266	A
1	1	2278	A
1	1	2279	G
1	1	2283	C
1	1	2287	A
1	1	2288	A
1	1	2294	G
1	1	2296	U
1	1	2297	A
1	1	2305	U
1	1	2306	C
1	1	2307	G
1	1	2319	G
1	1	2320	U
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2336	A
1	1	2345	G
1	1	2347	C
1	1	2350	C
1	1	2357	G
1	1	2361	G
1	1	2366	A
1	1	2376	A
1	1	2383	G
1	1	2385	C
1	1	2389	G
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2419	U
1	1	2423	U
1	1	2424	C
1	1	2425	A
1	1	2426	A
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2435	A
1	1	2441	U
1	1	2445	2MG

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Mol	Chain	Res	Type
1	1	2448	A
1	1	2459	A
1	1	2470	G
1	1	2473	U
1	1	2475	C
1	1	2476	A
1	1	2491	U
1	1	2498	OMC
1	1	2501	C
1	1	2502	G
1	1	2503	2MA
1	1	2504	PSU
1	1	2505	G
1	1	2506	U
1	1	2513	A
1	1	2518	A
1	1	2520	C
1	1	2529	G
1	1	2543	G
1	1	2547	A
1	1	2554	U
1	1	2566	A
1	1	2567	G
1	1	2572	A
1	1	2573	C
1	1	2574	G
1	1	2585	U
1	1	2602	A
1	1	2608	G
1	1	2609	U
1	1	2610	C
1	1	2613	U
1	1	2615	U
1	1	2621	G
1	1	2629	U
1	1	2636	C
1	1	2640	G
1	1	2661	G
1	1	2663	G
1	1	2671	G
1	1	2682	A
1	1	2689	U

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Mol	Chain	Res	Type
1	1	2690	U
1	1	2703	C
1	1	2714	G
1	1	2716	C
1	1	2718	G
1	1	2725	A
1	1	2726	A
1	1	2728	U
1	1	2732	G
1	1	2733	A
1	1	2739	U
1	1	2744	G
1	1	2748	A
1	1	2751	G
1	1	2762	C
1	1	2765	A
1	1	2778	A
1	1	2793	C
1	1	2794	C
1	1	2797	U
1	1	2798	U
1	1	2799	A
1	1	2811	G
1	1	2818	U
1	1	2820	A
1	1	2821	A
1	1	2825	G
1	1	2835	A
1	1	2836	U
1	1	2861	U
1	1	2867	G
1	1	2872	A
1	1	2873	A
1	1	2880	C
1	1	2884	U
1	1	2885	G
1	1	2892	G
1	1	2901	C
1	1	2903	U
2	2	3	A
2	2	4	U
2	2	5	U

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Mol	Chain	Res	Type
2	2	7	A
2	2	8	A
2	2	9	G
2	2	22	G
2	2	32	A
2	2	39	G
2	2	47	C
2	2	48	C
2	2	50	A
2	2	51	A
2	2	52	C
2	2	54	C
2	2	70	U
2	2	71	A
2	2	74	A
2	2	77	A
2	2	79	G
2	2	82	G
2	2	83	C
2	2	84	U
2	2	85	U
2	2	86	G
2	2	87	C
2	2	89	U
2	2	92	U
2	2	94	G
2	2	95	C
2	2	108	G
2	2	116	A
2	2	120	A
2	2	121	U
2	2	130	A
2	2	131	A
2	2	141	G
2	2	149	A
2	2	151	A
2	2	168	G
2	2	173	U
2	2	177	G
2	2	181	A
2	2	183	C
2	2	197	A

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Mol	Chain	Res	Type
2	2	202	G
2	2	204	G
2	2	209	U
2	2	211	G
2	2	212	G
2	2	222	C
2	2	226	G
2	2	245	U
2	2	247	G
2	2	251	G
2	2	266	G
2	2	267	C
2	2	279	A
2	2	289	G
2	2	306	A
2	2	321	A
2	2	328	C
2	2	332	G
2	2	347	G
2	2	352	C
2	2	353	A
2	2	354	G
2	2	356	A
2	2	367	U
2	2	372	C
2	2	373	A
2	2	384	G
2	2	388	G
2	2	397	A
2	2	406	G
2	2	407	U
2	2	411	A
2	2	412	A
2	2	413	G
2	2	414	A
2	2	421	U
2	2	422	C
2	2	423	G
2	2	424	G
2	2	428	G
2	2	429	U
2	2	436	C

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Mol	Chain	Res	Type
2	2	438	U
2	2	452	A
2	2	456	A
2	2	457	G
2	2	464	U
2	2	467	U
2	2	468	A
2	2	471	U
2	2	476	U
2	2	478	A
2	2	479	U
2	2	481	G
2	2	486	U
2	2	495	A
2	2	496	A
2	2	497	G
2	2	499	A
2	2	509	A
2	2	511	C
2	2	517	G
2	2	518	C
2	2	521	G
2	2	527	G7M
2	2	531	U
2	2	532	A
2	2	547	A
2	2	559	A
2	2	562	U
2	2	564	C
2	2	566	G
2	2	572	A
2	2	573	A
2	2	575	G
2	2	576	C
2	2	577	G
2	2	596	A
2	2	633	G
2	2	639	G
2	2	649	A
2	2	650	G
2	2	653	U
2	2	665	A

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Mol	Chain	Res	Type
2	2	682	G
2	2	686	U
2	2	687	A
2	2	701	U
2	2	702	A
2	2	703	G
2	2	718	A
2	2	721	G
2	2	723	U
2	2	724	G
2	2	731	G
2	2	734	G
2	2	747	A
2	2	748	G
2	2	755	G
2	2	758	C
2	2	761	G
2	2	777	A
2	2	793	U
2	2	794	A
2	2	813	U
2	2	814	A
2	2	815	A
2	2	817	C
2	2	819	A
2	2	821	G
2	2	828	U
2	2	829	G
2	2	832	G
2	2	841	C
2	2	844	G
2	2	846	G
2	2	864	A
2	2	871	U
2	2	876	C
2	2	884	U
2	2	889	A
2	2	914	A
2	2	926	G
2	2	934	C
2	2	935	A
2	2	942	G

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Mol	Chain	Res	Type
2	2	958	A
2	2	960	U
2	2	966	2MG
2	2	968	A
2	2	969	A
2	2	971	G
2	2	974	A
2	2	975	A
2	2	976	G
2	2	977	A
2	2	982	U
2	2	992	U
2	2	993	G
2	2	994	A
2	2	996	A
2	2	1000	A
2	2	1004	A
2	2	1008	U
2	2	1009	U
2	2	1017	U
2	2	1019	A
2	2	1020	G
2	2	1022	A
2	2	1026	G
2	2	1028	C
2	2	1029	U
2	2	1030	U
2	2	1031	C
2	2	1033	G
2	2	1035	A
2	2	1038	C
2	2	1043	G
2	2	1044	A
2	2	1046	A
2	2	1065	U
2	2	1092	A
2	2	1094	G
2	2	1095	U
2	2	1098	C
2	2	1099	G
2	2	1101	A
2	2	1108	G

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Mol	Chain	Res	Type
2	2	1124	G
2	2	1125	U
2	2	1130	A
2	2	1132	C
2	2	1136	C
2	2	1137	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1143	G
2	2	1145	A
2	2	1151	A
2	2	1152	A
2	2	1158	C
2	2	1160	G
2	2	1167	A
2	2	1171	A
2	2	1176	A
2	2	1177	G
2	2	1184	G
2	2	1193	G
2	2	1196	A
2	2	1197	A
2	2	1200	C
2	2	1212	U
2	2	1213	A
2	2	1227	A
2	2	1238	A
2	2	1241	G
2	2	1256	A
2	2	1257	A
2	2	1258	G
2	2	1275	A
2	2	1279	G
2	2	1280	A
2	2	1281	C
2	2	1287	A
2	2	1297	G
2	2	1299	A
2	2	1300	G
2	2	1301	U
2	2	1302	C

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Mol	Chain	Res	Type
2	2	1305	G
2	2	1312	G
2	2	1317	C
2	2	1320	C
2	2	1323	G
2	2	1328	C
2	2	1336	C
2	2	1340	A
2	2	1346	A
2	2	1363	A
2	2	1364	U
2	2	1370	G
2	2	1378	C
2	2	1379	G
2	2	1381	U
2	2	1397	C
2	2	1401	G
2	2	1402	4OC
2	2	1404	C
2	2	1419	G
2	2	1432	G
2	2	1441	A
2	2	1446	A
2	2	1452	C
2	2	1475	G
2	2	1484	C
2	2	1491	G
2	2	1492	A
2	2	1494	G
2	2	1497	G
2	2	1499	A
2	2	1503	A
2	2	1506	U
2	2	1517	G
2	2	1519	MA6
2	2	1520	C
2	2	1529	G
2	2	1530	G
2	2	1533	C
2	2	1534	A
3	3	2	G
3	3	4	C

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Mol	Chain	Res	Type
3	3	13	G
3	3	15	A
3	3	24	G
3	3	35	C
3	3	36	C
3	3	41	G
3	3	44	G
3	3	45	A
3	3	51	G
3	3	52	A
3	3	56	G
3	3	57	A
3	3	66	A
3	3	67	G
3	3	88	C
3	3	89	U
3	3	90	C
3	3	99	A
3	3	105	G
3	3	109	A
3	3	119	A
4	4	19	U
4	4	20	A
4	4	21	A
55	5	2	C
55	5	7	U
55	5	8	4SU
55	5	15	C
55	5	16	C
55	5	17	U
55	5	18	G
55	5	19	G
55	5	20	H2U
55	5	21	A
55	5	47	U
55	5	48	C
55	5	49	G
55	5	58	A
55	5	59	A
55	5	61	C
55	5	68	C
55	5	70	G

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Mol	Chain	Res	Type
55	5	76	A

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	404	A
1	1	613	A
1	1	784	G
1	1	894	U
1	1	984	A
1	1	1379	U
1	1	2146	C
1	1	2193	G
1	1	2425	A
2	2	328	C
2	2	496	A
2	2	516	PSU
2	2	1109	C
55	5	8	4SU
55	5	17	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	1	2605	1	18,21,22	1.11	2 (11%)	21,30,33	2.06	4 (19%)
1	PSU	1	955	1	18,21,22	1.18	2 (11%)	21,30,33	2.07	4 (19%)
1	2MA	1	2503	57,1	22,25,26	3.54	9 (40%)	32,37,40	2.23	7 (21%)
1	5MU	1	1939	1	19,22,23	4.65	7 (36%)	27,32,35	3.92	9 (33%)
2	MA6	2	1518	2	23,26,27	1.60	4 (17%)	33,38,41	2.85	11 (33%)
2	2MG	2	1207	2	23,26,27	2.90	9 (39%)	33,38,41	2.38	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
56	FME	6	77	56	8,9,10	0.99	0	8,9,11	0.71	0
1	OMU	1	2552	57,1	19,22,23	2.81	7 (36%)	25,31,34	1.97	5 (20%)
1	PSU	1	2504	57,1	18,21,22	1.16	2 (11%)	21,30,33	2.30	4 (19%)
44	0TD	q	89	44	8,9,10	1.70	1 (12%)	6,11,13	2.34	2 (33%)
1	PSU	1	1917	1	18,21,22	1.11	2 (11%)	21,30,33	1.94	4 (19%)
2	PSU	2	516	2	18,21,22	1.41	3 (16%)	21,30,33	2.07	6 (28%)
1	1MG	1	745	1	23,26,27	2.67	7 (30%)	33,39,42	2.23	11 (33%)
1	5MC	1	1962	1	19,22,23	3.66	8 (42%)	26,32,35	1.16	2 (7%)
55	4SU	5	8	55	18,21,22	3.71	7 (38%)	25,30,33	2.29	5 (20%)
1	6MZ	1	2030	1	22,25,26	2.95	6 (27%)	29,36,39	4.78	14 (48%)
1	PSU	1	1911	1	18,21,22	1.17	2 (11%)	21,30,33	1.93	4 (19%)
2	5MC	2	967	2	19,22,23	3.80	8 (42%)	26,32,35	0.89	1 (3%)
1	PSU	1	746	57,1	18,21,22	1.13	3 (16%)	21,30,33	2.04	5 (23%)
2	G7M	2	527	2	23,26,27	3.54	11 (47%)	34,39,42	1.68	7 (20%)
55	4OC	5	32	55	20,23,24	2.95	8 (40%)	25,32,35	0.92	1 (4%)
2	2MG	2	966	2	23,26,27	2.94	7 (30%)	33,38,41	2.41	8 (24%)
1	6MZ	1	1618	1	22,25,26	2.87	5 (22%)	29,36,39	4.39	13 (44%)
1	G7M	1	2069	1	23,26,27	2.55	8 (34%)	34,39,42	2.36	10 (29%)
2	2MG	2	1516	2	23,26,27	2.83	8 (34%)	33,38,41	2.40	12 (36%)
55	H2U	5	20	55	18,21,22	3.20	5 (27%)	19,30,33	1.50	4 (21%)
1	PSU	1	2457	1	18,21,22	1.11	3 (16%)	21,30,33	2.58	6 (28%)
1	OMC	1	2498	57,1	19,22,23	2.66	7 (36%)	25,31,34	1.16	2 (8%)
1	3TD	1	1915	57,1	19,22,23	4.31	5 (26%)	23,32,35	2.01	4 (17%)
1	2MG	1	1835	1	23,26,27	2.86	7 (30%)	33,38,41	2.56	10 (30%)
1	OMG	1	2251	55,1	23,26,27	2.36	8 (34%)	32,38,41	1.96	7 (21%)
1	2MG	1	2445	1	23,26,27	2.81	8 (34%)	33,38,41	2.64	13 (39%)
1	PSU	1	2580	1	18,21,22	1.15	3 (16%)	21,30,33	2.07	4 (19%)
2	5MC	2	1407	2	19,22,23	3.77	8 (42%)	26,32,35	1.09	1 (3%)
2	MA6	2	1519	2	23,26,27	1.56	4 (17%)	33,38,41	2.77	12 (36%)
1	5MU	1	747	1	19,22,23	4.49	7 (36%)	27,32,35	3.98	12 (44%)
55	5MU	5	54	55	19,22,23	4.83	7 (36%)	27,32,35	3.78	9 (33%)
55	PSU	5	55	55	18,21,22	1.15	1 (5%)	21,30,33	1.90	4 (19%)
2	4OC	2	1402	2	20,23,24	2.84	8 (40%)	25,32,35	1.18	3 (12%)
2	UR3	2	1498	2	19,22,23	2.59	6 (31%)	26,32,35	1.64	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
1	2MA	1	2503	57,1	-	0/7/25/26	0/3/3/3
1	5MU	1	1939	1	-	0/7/25/26	0/2/2/2
2	MA6	2	1518	2	-	0/11/29/30	0/3/3/3
2	2MG	2	1207	2	-	0/9/27/28	0/3/3/3
56	FME	6	77	56	-	5/7/9/11	-
1	OMU	1	2552	57,1	-	0/9/27/28	0/2/2/2
1	PSU	1	2504	57,1	-	1/7/25/26	0/2/2/2
44	0TD	q	89	44	-	1/7/12/14	-
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
2	PSU	2	516	2	-	3/7/25/26	0/2/2/2
1	1MG	1	745	1	-	0/7/25/26	0/3/3/3
1	5MC	1	1962	1	-	0/7/25/26	0/2/2/2
55	4SU	5	8	55	-	2/7/25/26	0/2/2/2
1	6MZ	1	2030	1	-	2/9/27/28	0/3/3/3
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
2	5MC	2	967	2	-	0/7/25/26	0/2/2/2
1	PSU	1	746	57,1	-	3/7/25/26	0/2/2/2
2	G7M	2	527	2	-	3/7/25/26	0/3/3/3
55	4OC	5	32	55	-	0/9/29/30	0/2/2/2
2	2MG	2	966	2	-	2/9/27/28	0/3/3/3
1	6MZ	1	1618	1	-	2/9/27/28	0/3/3/3
1	G7M	1	2069	1	-	1/7/25/26	0/3/3/3
2	2MG	2	1516	2	-	0/9/27/28	0/3/3/3
55	H2U	5	20	55	-	4/7/38/39	0/2/2/2
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
1	OMC	1	2498	57,1	-	1/9/27/28	0/2/2/2
1	3TD	1	1915	57,1	-	2/7/25/26	0/2/2/2
1	2MG	1	1835	1	-	2/9/27/28	0/3/3/3
1	OMG	1	2251	55,1	-	0/9/27/28	0/3/3/3
1	2MG	1	2445	1	-	2/9/27/28	0/3/3/3
1	PSU	1	2580	1	-	0/7/25/26	0/2/2/2
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
2	MA6	2	1519	2	-	4/11/29/30	0/3/3/3
1	5MU	1	747	1	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MU	5	54	55	-	0/7/25/26	0/2/2/2
55	PSU	5	55	55	-	0/7/25/26	0/2/2/2
2	4OC	2	1402	2	-	2/9/29/30	0/2/2/2
2	UR3	2	1498	2	-	0/7/25/26	0/2/2/2

All (223) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1915	3TD	C6-C5	13.58	1.50	1.35
55	5	54	5MU	C2-N1	11.43	1.56	1.38
1	1	1618	6MZ	C6-N6	11.19	1.47	1.34
1	1	2030	6MZ	C6-N6	10.97	1.46	1.34
1	1	2503	2MA	C4-N3	10.73	1.48	1.34
2	2	527	G7M	C8-N7	10.46	1.50	1.33
55	5	54	5MU	C6-N1	10.41	1.55	1.38
55	5	20	H2U	C2-N1	10.05	1.49	1.35
1	1	1939	5MU	C6-N1	10.02	1.55	1.38
1	1	747	5MU	C2-N1	9.97	1.54	1.38
55	5	54	5MU	C4-C5	9.84	1.60	1.44
1	1	1915	3TD	C2-N1	9.71	1.49	1.37
1	1	1939	5MU	C2-N1	9.58	1.53	1.38
1	1	1939	5MU	C4-C5	9.47	1.60	1.44
1	1	747	5MU	C4-C5	9.45	1.60	1.44
2	2	1407	5MC	C6-C5	9.35	1.49	1.34
1	1	747	5MU	C6-N1	9.24	1.53	1.38
2	2	967	5MC	C6-C5	9.13	1.49	1.34
1	1	1962	5MC	C6-C5	8.70	1.48	1.34
1	1	1939	5MU	C4-N3	-8.66	1.22	1.38
1	1	747	5MU	C4-N3	-8.35	1.23	1.38
55	5	8	4SU	C4-N3	8.08	1.46	1.37
55	5	8	4SU	C2-N1	7.93	1.50	1.38
55	5	54	5MU	C4-N3	-7.68	1.24	1.38
2	2	966	2MG	C2-N3	7.30	1.45	1.32
2	2	967	5MC	C4-N3	7.24	1.45	1.34
1	1	1962	5MC	C4-N3	7.17	1.45	1.34
1	1	745	1MG	C2-N2	7.08	1.46	1.34
2	2	1207	2MG	C2-N3	7.04	1.45	1.32
55	5	32	4OC	C4-N3	7.02	1.44	1.32
1	1	1835	2MG	C2-N3	6.87	1.45	1.32
1	1	2445	2MG	C2-N3	6.80	1.45	1.32
2	2	966	2MG	C4-N3	6.79	1.49	1.34
2	2	1516	2MG	C2-N3	6.78	1.44	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1407	5MC	C4-N3	6.62	1.44	1.34
1	1	1835	2MG	C4-N3	6.61	1.49	1.34
2	2	1498	UR3	C2-N1	6.55	1.47	1.38
55	5	20	H2U	C2-N3	6.55	1.49	1.38
2	2	966	2MG	C2-N2	6.51	1.47	1.33
1	1	2503	2MA	C2-N3	6.49	1.45	1.34
2	2	1207	2MG	C2-N2	6.45	1.46	1.33
1	1	2069	G7M	C4-N3	6.35	1.48	1.34
1	1	2251	OMG	C4-N3	6.30	1.48	1.34
1	1	2552	OMU	C2-N1	6.29	1.48	1.38
2	2	1207	2MG	C4-N3	6.27	1.48	1.34
2	2	1402	4OC	C4-N3	6.23	1.43	1.32
1	1	2552	OMU	C2-N3	6.23	1.48	1.38
2	2	1516	2MG	C2-N2	6.20	1.46	1.33
2	2	967	5MC	C2-N3	6.20	1.48	1.36
1	1	1835	2MG	C2-N2	6.19	1.46	1.33
2	2	1516	2MG	C4-N3	6.12	1.48	1.34
1	1	745	1MG	C2-N3	6.12	1.43	1.33
2	2	1407	5MC	C2-N3	6.08	1.48	1.36
1	1	1962	5MC	C2-N3	6.07	1.48	1.36
2	2	1498	UR3	C6-C5	6.01	1.49	1.35
1	1	745	1MG	C4-N3	6.00	1.48	1.34
1	1	2445	2MG	C2-N2	5.97	1.45	1.33
1	1	2445	2MG	C4-N3	5.96	1.47	1.34
2	2	1402	4OC	C6-C5	5.95	1.48	1.35
55	5	32	4OC	C2-N3	5.88	1.48	1.36
55	5	8	4SU	C6-C5	5.83	1.48	1.35
2	2	527	G7M	C2-N3	5.81	1.47	1.33
1	1	2498	OMC	C2-N3	5.78	1.47	1.36
55	5	54	5MU	C6-C5	5.74	1.44	1.34
55	5	8	4SU	C2-N3	5.73	1.47	1.38
55	5	8	4SU	C4-S4	-5.72	1.58	1.68
1	1	2069	G7M	C5-N7	-5.64	1.32	1.39
1	1	1939	5MU	C6-C5	5.63	1.43	1.34
55	5	32	4OC	C6-C5	5.63	1.48	1.35
1	1	1915	3TD	C6-N1	5.61	1.45	1.36
1	1	2498	OMC	C6-C5	5.57	1.48	1.35
2	2	1407	5MC	C5-C4	5.56	1.48	1.44
2	2	527	G7M	C4-N3	5.50	1.46	1.34
2	2	967	5MC	C5-C4	5.44	1.48	1.44
1	1	2552	OMU	C6-C5	5.43	1.47	1.35
2	2	527	G7M	C8-N9	5.32	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2503	2MA	C6-N1	5.29	1.42	1.35
2	2	1402	4OC	C2-N3	5.25	1.46	1.36
1	1	2503	2MA	C2-N1	5.13	1.42	1.34
1	1	2498	OMC	C4-N3	5.05	1.44	1.34
1	1	2251	OMG	C2-N3	5.03	1.45	1.33
55	5	20	H2U	C4-N3	5.03	1.46	1.37
1	1	2069	G7M	C2-N3	4.93	1.45	1.33
1	1	1962	5MC	C5-C4	4.90	1.47	1.44
1	1	1915	3TD	C2-N3	4.90	1.48	1.38
2	2	967	5MC	C4-N4	4.83	1.46	1.34
2	2	1407	5MC	C4-N4	4.74	1.46	1.34
2	2	527	G7M	C2-N2	4.74	1.45	1.34
1	1	1962	5MC	C4-N4	4.72	1.46	1.34
1	1	747	5MU	C6-C5	4.65	1.42	1.34
2	2	1498	UR3	C2-N3	4.52	1.47	1.39
2	2	1207	2MG	C2-N1	4.51	1.43	1.36
2	2	1407	5MC	C6-N1	4.45	1.45	1.38
1	1	2251	OMG	C2-N2	4.42	1.44	1.34
1	1	2030	6MZ	C5-C4	-4.40	1.31	1.39
2	2	967	5MC	C6-N1	4.30	1.45	1.38
2	2	1516	2MG	C2-N1	4.25	1.43	1.36
1	1	2503	2MA	C5-C6	4.21	1.52	1.41
2	2	527	G7M	C5-N7	4.14	1.44	1.39
55	5	32	4OC	C4-N4	4.04	1.44	1.36
1	1	1835	2MG	C2-N1	4.00	1.43	1.36
1	1	2069	G7M	C2-N2	3.99	1.43	1.34
2	2	966	2MG	C2-N1	3.98	1.43	1.36
1	1	2445	2MG	C5-N7	-3.96	1.31	1.39
2	2	1402	4OC	C2-N1	3.95	1.48	1.40
1	1	1962	5MC	C6-N1	3.92	1.44	1.38
2	2	967	5MC	C2-N1	3.90	1.48	1.40
1	1	1618	6MZ	C5-C4	-3.81	1.32	1.39
1	1	2445	2MG	C2-N1	3.81	1.42	1.36
55	5	32	4OC	C2-N1	3.79	1.48	1.40
2	2	1407	5MC	C2-N1	3.78	1.48	1.40
55	5	55	PSU	C6-C5	3.77	1.39	1.35
2	2	1402	4OC	C4-N4	3.75	1.43	1.36
1	1	2030	6MZ	C8-N9	-3.73	1.31	1.37
2	2	516	PSU	C6-C5	3.71	1.39	1.35
1	1	1835	2MG	C5-N7	-3.70	1.31	1.39
1	1	2030	6MZ	C4-N9	-3.70	1.30	1.37
1	1	1962	5MC	C2-N1	3.70	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	966	2MG	C5-N7	-3.61	1.31	1.39
1	1	1911	PSU	C6-C5	3.59	1.39	1.35
2	2	1518	MA6	C6-N6	3.58	1.46	1.36
1	1	2503	2MA	C6-N6	-3.57	1.25	1.34
2	2	1519	MA6	C6-N6	3.56	1.46	1.36
1	1	2552	OMU	C4-N3	3.55	1.44	1.38
1	1	1618	6MZ	C8-N9	-3.55	1.31	1.37
1	1	2251	OMG	C5-N7	-3.54	1.32	1.39
2	2	1519	MA6	C8-N9	-3.54	1.31	1.37
1	1	2503	2MA	C5-N7	-3.54	1.32	1.39
1	1	2445	2MG	O6-C6	-3.54	1.16	1.23
1	1	1835	2MG	O6-C6	-3.51	1.16	1.23
1	1	2498	OMC	C4-N4	3.48	1.42	1.33
2	2	966	2MG	O6-C6	-3.48	1.17	1.23
1	1	2069	G7M	C5-C6	3.48	1.53	1.43
2	2	1518	MA6	C8-N9	-3.47	1.31	1.37
1	1	1962	5MC	O2-C2	-3.46	1.17	1.23
2	2	1516	2MG	O6-C6	-3.42	1.17	1.23
2	2	1207	2MG	C5-N7	-3.40	1.32	1.39
2	2	1407	5MC	O2-C2	-3.37	1.17	1.23
2	2	527	G7M	C2-N1	3.34	1.45	1.37
2	2	1516	2MG	C5-N7	-3.33	1.32	1.39
2	2	1519	MA6	C5-N7	-3.32	1.33	1.39
1	1	2498	OMC	O2-C2	-3.30	1.17	1.23
2	2	1402	4OC	C5-C4	3.30	1.48	1.41
2	2	1207	2MG	O6-C6	-3.28	1.17	1.23
2	2	967	5MC	O2-C2	-3.27	1.17	1.23
1	1	2605	PSU	C6-C5	3.26	1.38	1.35
1	1	2498	OMC	C2-N1	3.25	1.46	1.40
2	2	1518	MA6	C5-N7	-3.23	1.33	1.39
55	5	32	4OC	C5-C4	3.23	1.48	1.41
1	1	745	1MG	C5-N7	-3.22	1.32	1.39
2	2	527	G7M	C5-C6	3.22	1.52	1.43
2	2	1518	MA6	C5-C4	-3.22	1.33	1.39
1	1	2552	OMU	O4-C4	-3.17	1.18	1.24
1	1	955	PSU	C6-C5	3.15	1.38	1.35
1	1	1939	5MU	O4-C4	-3.14	1.17	1.23
55	5	8	4SU	C5-C4	3.14	1.46	1.42
2	2	1402	4OC	O2-C2	-3.08	1.18	1.23
1	1	1939	5MU	O2-C2	-3.07	1.17	1.23
1	1	1917	PSU	C6-C5	3.07	1.38	1.35
1	1	1618	6MZ	C4-N9	-3.03	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2580	PSU	C6-C5	3.00	1.38	1.35
1	1	2504	PSU	C6-C5	2.97	1.38	1.35
1	1	747	5MU	O2-C2	-2.97	1.17	1.23
1	1	746	PSU	C6-C5	2.95	1.38	1.35
1	1	2498	OMC	C6-N1	2.95	1.45	1.38
1	1	2069	G7M	O6-C6	-2.90	1.18	1.23
2	2	1519	MA6	C5-C4	-2.88	1.33	1.39
55	5	32	4OC	O2-C2	-2.88	1.18	1.23
1	1	2552	OMU	O2-C2	-2.88	1.18	1.23
1	1	2030	6MZ	C6-N1	-2.81	1.30	1.35
2	2	1402	4OC	C6-N1	2.81	1.44	1.38
55	5	54	5MU	O4-C4	-2.77	1.18	1.23
2	2	527	G7M	O6-C6	-2.77	1.18	1.23
1	1	2503	2MA	C4-N9	-2.74	1.32	1.37
1	1	1915	3TD	C4-N3	2.74	1.46	1.40
1	1	747	5MU	O4-C4	-2.72	1.18	1.23
1	1	2251	OMG	O6-C6	-2.66	1.18	1.23
2	2	527	G7M	C6-N1	2.64	1.43	1.38
55	5	20	H2U	O2-C2	-2.61	1.18	1.23
2	2	1498	UR3	O4-C4	-2.61	1.18	1.23
1	1	745	1MG	C2-N1	2.60	1.42	1.37
55	5	32	4OC	C6-N1	2.55	1.44	1.38
1	1	745	1MG	C4-N9	-2.53	1.31	1.38
1	1	1618	6MZ	C6-N1	-2.51	1.31	1.35
55	5	8	4SU	O2-C2	-2.49	1.18	1.23
55	5	54	5MU	O2-C2	-2.47	1.18	1.23
2	2	1516	2MG	C4-N9	-2.43	1.31	1.38
1	1	2030	6MZ	C5-C6	-2.41	1.36	1.41
2	2	516	PSU	C4-N3	-2.41	1.34	1.38
2	2	1498	UR3	C6-N1	2.38	1.43	1.38
1	1	2457	PSU	C6-C5	2.37	1.37	1.35
1	1	2457	PSU	O4'-C1'	-2.37	1.40	1.43
1	1	1911	PSU	C4-C5	-2.32	1.37	1.44
1	1	2457	PSU	C4-C5	-2.31	1.37	1.44
1	1	2552	OMU	C6-N1	2.30	1.43	1.38
1	1	2504	PSU	C4-C5	-2.30	1.38	1.44
44	q	89	0TD	CB-CA	-2.30	1.54	1.54
1	1	955	PSU	C4-C5	-2.30	1.38	1.44
2	2	1498	UR3	O2-C2	-2.27	1.18	1.22
2	2	1207	2MG	C5-C6	2.26	1.52	1.44
1	1	2251	OMG	C2-N1	2.25	1.43	1.37
1	1	745	1MG	C5-C6	2.25	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	5	20	H2U	O4-C4	-2.25	1.18	1.23
2	2	1207	2MG	C6-N1	2.25	1.43	1.38
1	1	2580	PSU	O4'-C1'	-2.24	1.40	1.43
1	1	2580	PSU	C4-C5	-2.23	1.38	1.44
2	2	966	2MG	C5-C6	2.22	1.52	1.44
2	2	1516	2MG	C5-C6	2.21	1.52	1.44
2	2	527	G7M	C4-N9	2.21	1.43	1.38
1	1	2251	OMG	C4-N9	-2.20	1.32	1.38
1	1	746	PSU	C4-C5	-2.19	1.38	1.44
1	1	2445	2MG	C4-N9	-2.17	1.32	1.38
1	1	1835	2MG	C5-C6	2.13	1.52	1.44
1	1	2251	OMG	C5-C6	2.13	1.52	1.44
1	1	2069	G7M	C2-N1	2.12	1.42	1.37
1	1	2503	2MA	C5-C4	-2.11	1.35	1.39
1	1	746	PSU	O4'-C1'	-2.10	1.40	1.43
2	2	516	PSU	C4-C5	2.09	1.50	1.44
1	1	2605	PSU	C4-C5	-2.07	1.38	1.44
2	2	1207	2MG	C4-N9	-2.06	1.32	1.38
1	1	2445	2MG	C5-C6	2.05	1.52	1.44
1	1	1917	PSU	C4-C5	-2.05	1.38	1.44
1	1	2069	G7M	C6-N1	2.01	1.42	1.38

All (255) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2030	6MZ	C4-N9-C8	15.42	121.93	105.74
1	1	1618	6MZ	C4-N9-C8	13.29	119.69	105.74
1	1	1939	5MU	C5-C4-N3	12.70	126.36	115.32
55	5	54	5MU	C5-C4-N3	12.60	126.27	115.32
1	1	2030	6MZ	N9-C8-N7	-11.48	97.65	113.94
1	1	747	5MU	C5-C4-N3	11.08	124.96	115.32
1	1	747	5MU	C5-C6-N1	-10.42	111.99	123.31
1	1	1939	5MU	C5-C6-N1	-10.38	112.03	123.31
1	1	1618	6MZ	N9-C8-N7	-9.86	99.95	113.94
55	5	54	5MU	C5-C6-N1	-9.81	112.65	123.31
2	2	1518	MA6	N1-C6-N6	-8.99	105.90	116.86
1	1	2030	6MZ	C5-C6-N1	8.74	127.53	118.15
1	1	1618	6MZ	C5-C6-N1	8.68	127.47	118.15
2	2	1519	MA6	N1-C6-N6	-8.24	106.82	116.86
1	1	1835	2MG	C2-N3-C4	7.46	121.33	112.00
55	5	8	4SU	C4-N3-C2	-7.29	120.33	127.31
2	2	966	2MG	C2-N3-C4	7.27	121.09	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2503	2MA	C5-C4-N3	-6.83	119.98	127.18
1	1	2445	2MG	C2-N3-C4	6.81	120.52	112.00
2	2	966	2MG	C5-C4-N3	-6.59	117.91	128.39
1	1	1835	2MG	C5-C4-N3	-6.55	117.97	128.39
1	1	747	5MU	C5M-C5-C6	-6.49	114.07	122.85
1	1	1618	6MZ	N3-C4-N9	6.41	138.06	127.17
2	2	1207	2MG	C2-N3-C4	6.34	119.94	112.00
1	1	2457	PSU	N1-C2-N3	6.31	121.83	115.17
55	5	54	5MU	O4-C4-C5	-6.29	117.72	124.92
1	1	2069	G7M	CN7-N7-C5	6.24	134.58	126.80
2	2	1518	MA6	N1-C2-N3	-6.14	119.29	128.58
1	1	2445	2MG	C5-C4-N3	-6.11	118.66	128.39
1	1	2030	6MZ	N1-C2-N3	-6.11	119.34	128.58
2	2	1516	2MG	C2-N3-C4	6.07	119.59	112.00
1	1	2552	OMU	C4-N3-C2	-6.03	119.12	126.61
1	1	1915	3TD	N1-C2-N3	6.03	120.52	116.13
1	1	1618	6MZ	C9-N6-C6	-5.99	117.29	122.85
1	1	2457	PSU	C4-N3-C2	-5.98	118.14	126.37
2	2	1519	MA6	N1-C2-N3	-5.97	119.55	128.58
2	2	1518	MA6	C5-C6-N6	5.92	134.70	125.33
1	1	747	5MU	C5M-C5-C4	5.85	125.03	118.78
1	1	2030	6MZ	N3-C4-N9	5.62	136.73	127.17
1	1	1939	5MU	O4-C4-C5	-5.61	118.50	124.92
2	2	1498	UR3	C4-N3-C2	-5.60	120.07	124.58
1	1	1939	5MU	C4-N3-C2	-5.59	120.01	127.34
1	1	745	1MG	C1'-N9-C4	-5.58	110.00	126.49
1	1	2504	PSU	N1-C2-N3	5.58	121.05	115.17
1	1	2445	2MG	C2-N1-C6	-5.49	117.91	124.55
1	1	2580	PSU	N1-C2-N3	5.49	120.95	115.17
1	1	2251	OMG	C5-C4-N3	-5.45	119.71	128.39
2	2	1519	MA6	C5-C6-N6	5.45	133.96	125.33
2	2	516	PSU	N1-C2-N3	5.40	120.86	115.17
1	1	2030	6MZ	C5-C4-N9	-5.38	99.95	105.81
1	1	747	5MU	C4-N3-C2	-5.37	120.29	127.34
1	1	746	PSU	C4-N3-C2	-5.37	118.98	126.37
1	1	1618	6MZ	N1-C2-N3	-5.36	120.47	128.58
1	1	2445	2MG	N1-C2-N2	5.30	121.97	116.56
2	2	1207	2MG	C5-C4-N3	-5.26	120.02	128.39
1	1	1939	5MU	N3-C2-N1	5.26	121.74	114.89
55	5	54	5MU	C4-N3-C2	-5.23	120.48	127.34
1	1	2030	6MZ	C9-N6-C6	-5.23	118.00	122.85
1	1	2605	PSU	N1-C2-N3	5.18	120.63	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	745	1MG	C5-C4-N3	-5.15	120.20	128.39
1	1	2504	PSU	C6-N1-C2	-5.14	117.92	122.69
1	1	2605	PSU	C4-N3-C2	-5.14	119.29	126.37
1	1	1917	PSU	N1-C2-N3	5.13	120.58	115.17
2	2	966	2MG	C2-N1-C6	-5.11	118.37	124.55
55	5	8	4SU	C5-C4-N3	5.10	119.50	114.75
1	1	747	5MU	O4-C4-C5	-5.08	119.10	124.92
1	1	1835	2MG	C2-N1-C6	-5.07	118.42	124.55
1	1	1618	6MZ	C5-C4-N9	-5.04	100.32	105.81
1	1	2503	2MA	N9-C8-N7	-5.02	106.81	113.94
1	1	745	1MG	C1'-N9-C8	5.02	141.00	126.73
1	1	747	5MU	N3-C2-N1	5.01	121.41	114.89
1	1	746	PSU	N1-C2-N3	5.00	120.44	115.17
1	1	955	PSU	N1-C2-N3	4.98	120.42	115.17
55	5	55	PSU	C4-N3-C2	-4.96	119.54	126.37
1	1	2069	G7M	C2-N3-C4	4.95	120.83	112.30
2	2	1519	MA6	C5-C4-N3	-4.92	119.94	126.72
1	1	1911	PSU	C4-N3-C2	-4.92	119.59	126.37
1	1	1917	PSU	C4-N3-C2	-4.86	119.68	126.37
1	1	2503	2MA	N3-C4-N9	4.85	133.14	126.99
1	1	1911	PSU	N1-C2-N3	4.83	120.26	115.17
1	1	2580	PSU	C4-N3-C2	-4.82	119.73	126.37
2	2	1516	2MG	C5-C4-N3	-4.82	120.73	128.39
2	2	1516	2MG	N1-C2-N2	4.79	121.45	116.56
1	1	2504	PSU	O2-C2-N1	-4.75	117.89	122.79
2	2	966	2MG	N9-C4-N3	4.74	135.43	125.95
55	5	55	PSU	N1-C2-N3	4.74	120.17	115.17
1	1	2457	PSU	O2-C2-N1	-4.72	117.92	122.79
2	2	1207	2MG	C2-N1-C6	-4.71	118.86	124.55
2	2	1207	2MG	N1-C2-N2	4.69	121.35	116.56
1	1	1618	6MZ	C1'-N9-C8	-4.68	116.71	127.09
1	1	2251	OMG	C2-N3-C4	4.65	120.30	112.30
1	1	2069	G7M	CN7-N7-C8	-4.63	117.78	124.79
1	1	1915	3TD	C1'-C5-C4	4.59	124.57	117.61
1	1	2069	G7M	C5-C4-N3	-4.59	119.48	128.15
2	2	1516	2MG	C2-N1-C6	-4.59	119.01	124.55
2	2	527	G7M	C2-N3-C4	4.57	120.17	112.30
1	1	955	PSU	C4-N3-C2	-4.52	120.14	126.37
1	1	2552	OMU	N3-C2-N1	4.52	120.77	114.89
2	2	1518	MA6	C5-C4-N3	-4.51	120.51	126.72
1	1	2030	6MZ	C5-N7-C8	4.48	110.48	103.45
44	q	89	0TD	OD2-CG-CB	4.47	122.81	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1835	2MG	N1-C2-N2	4.44	121.10	116.56
1	1	1835	2MG	N9-C4-N3	4.42	134.79	125.95
1	1	2504	PSU	C4-N3-C2	-4.39	120.33	126.37
55	5	54	5MU	N3-C2-N1	4.34	120.54	114.89
2	2	527	G7M	C5-C4-N3	-4.19	120.22	128.15
2	2	1518	MA6	N9-C8-N7	-4.19	107.99	113.94
2	2	1519	MA6	C4-C5-C6	4.17	120.22	115.91
1	1	2069	G7M	C5-C6-N1	4.12	120.36	111.84
2	2	527	G7M	C5-C6-N1	4.05	120.21	111.84
55	5	8	4SU	C5-C4-S4	-3.95	119.80	124.31
1	1	1939	5MU	O2-C2-N1	-3.95	117.66	122.80
55	5	20	H2U	N3-C2-N1	3.94	120.61	116.65
1	1	1915	3TD	C4-N3-C2	-3.94	120.44	124.61
1	1	2457	PSU	C6-C5-C4	3.90	120.81	118.17
1	1	1962	5MC	C5-C6-N1	-3.88	119.09	123.31
1	1	2030	6MZ	C4-C5-C6	-3.86	113.57	116.78
1	1	955	PSU	C6-N1-C2	-3.81	119.16	122.69
1	1	955	PSU	O2-C2-N1	-3.80	118.87	122.79
1	1	1618	6MZ	C5-N7-C8	3.77	109.38	103.45
2	2	1519	MA6	N9-C8-N7	-3.75	108.61	113.94
1	1	2503	2MA	C4-N9-C8	3.75	109.68	105.74
1	1	2445	2MG	CM2-N2-C2	-3.74	115.62	123.65
2	2	1518	MA6	C2-N1-C6	3.74	120.96	111.83
1	1	1618	6MZ	C5-C4-N3	-3.72	121.60	126.72
1	1	2030	6MZ	C1'-N9-C8	-3.70	118.87	127.09
1	1	745	1MG	C2-N3-C4	3.70	120.30	111.98
1	1	2030	6MZ	C6-C5-N7	3.67	136.43	132.43
55	5	8	4SU	N3-C2-N1	3.67	119.67	114.89
1	1	2552	OMU	C5-C4-N3	3.66	119.93	114.80
2	2	1519	MA6	C2-N1-C6	3.66	120.77	111.83
2	2	1498	UR3	C5-C4-N3	3.62	119.81	115.04
1	1	745	1MG	N9-C8-N7	-3.62	106.69	113.40
2	2	1516	2MG	C1'-N9-C4	-3.62	115.80	126.49
1	1	2445	2MG	N9-C4-N3	3.60	133.15	125.95
2	2	1407	5MC	C5-C6-N1	-3.59	119.41	123.31
1	1	2069	G7M	C1'-N9-C4	-3.59	115.88	126.49
1	1	1618	6MZ	C2-N3-C4	3.59	120.59	111.83
2	2	1518	MA6	C2-N3-C4	3.54	120.49	111.83
55	5	54	5MU	C5M-C5-C6	-3.53	118.07	122.85
1	1	747	5MU	C6-C5-C4	3.49	120.90	118.02
2	2	1519	MA6	C2-N3-C4	3.48	120.33	111.83
1	1	2251	OMG	N9-C4-N3	3.46	132.87	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2069	G7M	N9-C4-N3	3.42	132.79	125.95
1	1	2251	OMG	C2-N1-C6	-3.42	118.92	125.11
1	1	1939	5MU	C5M-C5-C6	-3.41	118.23	122.85
1	1	2503	2MA	N3-C2-N1	-3.41	119.76	125.77
1	1	2580	PSU	C6-N1-C2	-3.39	119.55	122.69
2	2	516	PSU	C4-N3-C2	-3.35	121.76	126.37
1	1	2030	6MZ	C2-N3-C4	3.34	120.00	111.83
55	5	54	5MU	C5M-C5-C4	3.34	122.34	118.78
2	2	1518	MA6	C4-C5-C6	3.33	119.36	115.91
1	1	2069	G7M	O6-C6-C5	-3.33	120.58	128.01
2	2	1516	2MG	CM2-N2-C2	-3.29	116.57	123.65
1	1	1939	5MU	C5M-C5-C4	3.28	122.29	118.78
2	2	516	PSU	C6-C5-C4	-3.28	115.96	118.17
2	2	1516	2MG	C1'-N9-C8	3.27	136.03	126.73
1	1	2605	PSU	O2-C2-N1	-3.22	119.47	122.79
1	1	747	5MU	O2-C2-N1	-3.20	118.64	122.80
1	1	2030	6MZ	C4-N9-C1'	-3.18	119.20	126.63
1	1	2069	G7M	C2-N1-C6	-3.14	119.42	125.11
55	5	8	4SU	C1'-N1-C2	3.13	123.22	117.59
2	2	1518	MA6	C4-C5-N7	-3.13	107.01	110.58
1	1	2552	OMU	O4-C4-C5	-3.12	119.78	125.16
2	2	1518	MA6	C5-N7-C8	3.10	108.32	103.45
1	1	2498	OMC	O2-C2-N3	-3.09	117.46	122.33
1	1	2457	PSU	C6-N1-C2	-3.08	119.84	122.69
2	2	966	2MG	C5-C6-N1	3.03	120.97	113.25
2	2	1207	2MG	C1'-N9-C4	-3.03	117.54	126.49
2	2	1402	4OC	O2-C2-N3	-3.02	117.57	122.33
1	1	2251	OMG	N9-C8-N7	-2.97	107.89	113.40
2	2	1518	MA6	C5-C4-N9	2.96	109.03	105.81
55	5	20	H2U	C5-C6-N1	2.96	120.46	111.52
1	1	745	1MG	CM1-N1-C6	2.94	122.19	117.64
2	2	1516	2MG	N9-C8-N7	-2.93	107.97	113.40
2	2	1207	2MG	N9-C4-N3	2.93	131.81	125.95
1	1	1835	2MG	C5-C6-N1	2.93	120.71	113.25
2	2	527	G7M	C2-N1-C6	-2.92	119.81	125.11
1	1	2445	2MG	O6-C6-C5	-2.91	118.85	126.53
2	2	1519	MA6	C5-N7-C8	2.89	107.99	103.45
1	1	2503	2MA	C5-N7-C8	2.89	107.98	103.45
1	1	2251	OMG	C5-C6-N1	2.87	120.56	113.25
1	1	1835	2MG	CM2-N2-C2	-2.85	117.53	123.65
1	1	1917	PSU	C6-N1-C2	-2.84	120.06	122.69
1	1	2445	2MG	C5-C6-N1	2.84	120.47	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2069	G7M	C1'-N9-C8	2.83	136.28	126.74
1	1	2445	2MG	N2-C2-N3	-2.83	116.91	120.51
55	5	20	H2U	C5-C4-N3	2.82	119.69	116.69
1	1	2580	PSU	O2-C2-N1	-2.82	119.89	122.79
2	2	1207	2MG	N9-C8-N7	-2.81	108.19	113.40
1	1	2445	2MG	N9-C8-N7	-2.80	108.21	113.40
1	1	745	1MG	N9-C4-N3	2.79	131.54	125.95
1	1	1835	2MG	O6-C6-C5	-2.79	119.17	126.53
2	2	516	PSU	O2-C2-N1	-2.78	119.92	122.79
2	2	1519	MA6	N3-C4-N9	2.78	131.90	127.17
1	1	745	1MG	C5-C6-N1	2.78	120.15	115.02
55	5	55	PSU	O2-C2-N1	-2.78	119.93	122.79
2	2	1207	2MG	C1'-N9-C8	2.77	134.61	126.73
1	1	746	PSU	O2-C2-N1	-2.76	119.94	122.79
1	1	2251	OMG	O6-C6-C5	-2.76	119.26	126.53
2	2	516	PSU	O3'-C3'-C4'	2.75	118.97	111.08
2	2	966	2MG	N9-C8-N7	-2.74	108.32	113.40
2	2	966	2MG	O6-C6-C5	-2.73	119.31	126.53
1	1	2605	PSU	C6-N1-C2	-2.73	120.16	122.69
2	2	1516	2MG	C5-C6-N1	2.71	120.16	113.25
2	2	1207	2MG	CM2-N2-C2	-2.71	117.83	123.65
1	1	1911	PSU	O2-C2-N1	-2.71	120.00	122.79
1	1	1835	2MG	N9-C8-N7	-2.70	108.39	113.40
2	2	1207	2MG	O6-C6-C5	-2.67	119.47	126.53
2	2	1207	2MG	C5-C6-N1	2.66	120.03	113.25
1	1	1939	5MU	O4-C4-N3	-2.65	115.14	120.11
1	1	1911	PSU	C6-N1-C2	-2.64	120.24	122.69
2	2	1402	4OC	CM4-N4-C4	-2.64	117.30	122.45
44	q	89	0TD	OD1-CG-CB	-2.62	116.95	122.44
2	2	1516	2MG	O6-C6-C5	-2.60	119.66	126.53
2	2	1498	UR3	C1'-N1-C2	2.59	121.28	117.04
2	2	1516	2MG	N9-C4-N3	2.58	131.11	125.95
2	2	1519	MA6	C4-C5-N7	-2.58	107.63	110.58
2	2	967	5MC	C5-C6-N1	-2.56	120.53	123.31
55	5	54	5MU	O2-C2-N1	-2.56	119.47	122.80
1	1	2445	2MG	C1'-N9-C4	-2.54	118.98	126.49
2	2	527	G7M	O6-C6-C5	-2.52	122.39	128.01
2	2	516	PSU	O3'-C3'-C2'	2.49	119.79	111.82
2	2	527	G7M	N9-C8-N7	-2.47	106.50	112.48
1	1	2030	6MZ	C5-C4-N3	-2.47	123.32	126.72
1	1	1618	6MZ	C4-C5-C6	-2.46	114.74	116.78
1	1	746	PSU	C6-C5-C4	2.43	119.81	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2445	2MG	C1'-N9-C8	2.38	133.50	126.73
55	5	32	4OC	C6-C5-C4	2.35	119.84	117.00
1	1	2552	OMU	O2-C2-N1	-2.35	119.74	122.80
1	1	747	5MU	C1'-N1-C2	2.33	121.79	117.59
1	1	2503	2MA	CM2-C2-N1	2.33	120.62	117.13
55	5	55	PSU	C6-N1-C2	-2.31	120.54	122.69
1	1	747	5MU	O4-C4-N3	-2.22	115.94	120.11
1	1	745	1MG	C8-N7-C5	2.20	108.19	104.26
55	5	54	5MU	O4-C4-N3	-2.19	116.00	120.11
2	2	966	2MG	N1-C2-N2	2.18	118.78	116.56
2	2	1519	MA6	C5-C4-N9	2.16	108.17	105.81
55	5	20	H2U	O2-C2-N1	-2.15	120.52	123.10
1	1	2498	OMC	C1'-N1-C2	2.13	123.14	118.44
2	2	527	G7M	C5-C4-N9	2.13	110.42	105.88
1	1	1917	PSU	O2-C2-N1	-2.11	120.61	122.79
1	1	2457	PSU	O4'-C1'-C2'	2.10	108.06	105.15
2	2	1516	2MG	N2-C2-N3	-2.10	117.84	120.51
1	1	745	1MG	CM1-N1-C2	-2.09	118.54	120.70
2	2	1402	4OC	C6-C5-C4	2.08	119.51	117.00
1	1	747	5MU	C1'-N1-C6	-2.06	117.76	121.15
1	1	745	1MG	C2-N1-C6	-2.06	119.27	120.99
1	1	746	PSU	C6-N1-C2	-2.06	120.78	122.69
1	1	1962	5MC	CM5-C5-C6	-2.05	120.08	122.85
1	1	2445	2MG	C8-N7-C5	2.04	107.90	104.26
2	2	1207	2MG	N2-C2-N3	-2.03	117.92	120.51
1	1	1618	6MZ	C6-C5-N7	2.03	134.64	132.43
1	1	1835	2MG	C8-N7-C5	2.02	107.87	104.26
1	1	1915	3TD	O4'-C1'-C2'	2.01	107.93	105.15

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	746	PSU	C2'-C1'-C5-C4
1	1	1618	6MZ	C5-C6-N6-C9
1	1	1618	6MZ	N1-C6-N6-C9
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C6
2	2	516	PSU	O4'-C1'-C5-C4
2	2	516	PSU	O4'-C1'-C5-C6
2	2	1402	4OC	O4'-C4'-C5'-O5'
2	2	1519	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
55	5	20	H2U	O4'-C1'-N1-C6
56	6	77	FME	O1-CN-N-CA
1	1	2445	2MG	C3'-C4'-C5'-O5'
2	2	966	2MG	O4'-C4'-C5'-O5'
2	2	966	2MG	C3'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
1	1	2030	6MZ	O4'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
2	2	527	G7M	C3'-C4'-C5'-O5'
55	5	20	H2U	O4'-C4'-C5'-O5'
55	5	20	H2U	C3'-C4'-C5'-O5'
56	6	77	FME	N-CA-CB-CG
1	1	1835	2MG	C3'-C4'-C5'-O5'
2	2	1402	4OC	C3'-C4'-C5'-O5'
1	1	2030	6MZ	C3'-C4'-C5'-O5'
1	1	1835	2MG	O4'-C4'-C5'-O5'
2	2	527	G7M	O4'-C4'-C5'-O5'
2	2	1519	MA6	C5-C6-N6-C10
56	6	77	FME	C-CA-CB-CG
55	5	8	4SU	O4'-C1'-N1-C6
55	5	8	4SU	O4'-C1'-N1-C2
55	5	20	H2U	O4'-C1'-N1-C2
44	q	89	0TD	CG-CB-SB-CSB
2	2	516	PSU	C3'-C4'-C5'-O5'
2	2	527	G7M	C4'-C5'-O5'-P
1	1	2504	PSU	O4'-C4'-C5'-O5'
1	1	747	5MU	C4'-C5'-O5'-P
2	2	1519	MA6	C4'-C5'-O5'-P
56	6	77	FME	CA-CB-CG-SD
1	1	746	PSU	O4'-C1'-C5-C6
1	1	2498	OMC	O4'-C4'-C5'-O5'
56	6	77	FME	CB-CA-N-CN
1	1	746	PSU	C2'-C1'-C5-C6
1	1	2069	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	6	77	FME	1	0
44	q	89	0TD	1	0
55	5	8	4SU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	2030	6MZ	1	0
1	1	746	PSU	1	0
55	5	32	4OC	1	0
1	1	1915	3TD	1	0
1	1	2251	OMG	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 309 ligands modelled in this entry, 309 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.

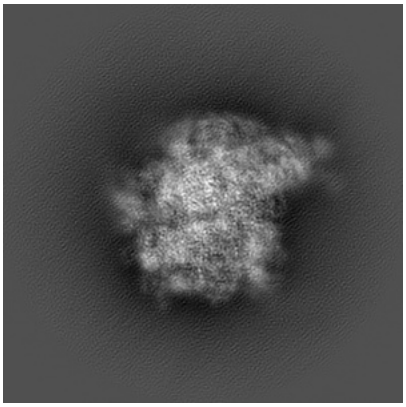
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20184. These allow visual inspection of the internal detail of the map and identification of artifacts.

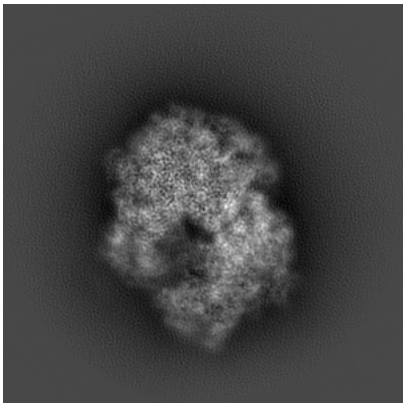
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

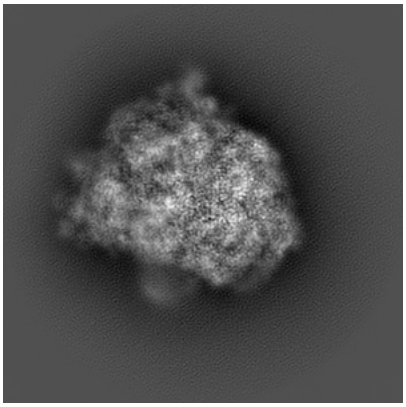
6.1.1 Primary map



X



Y

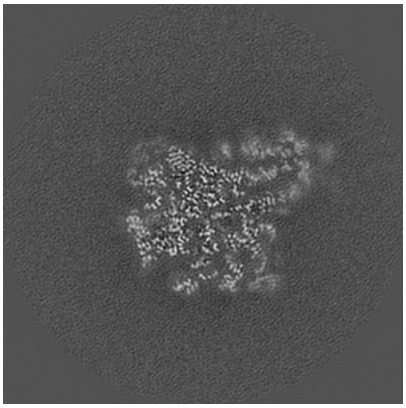


Z

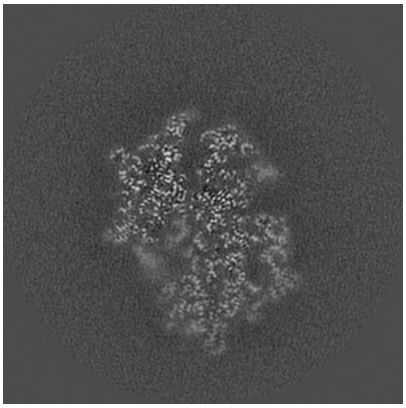
The images above show the map projected in three orthogonal directions.

6.2 Central slices

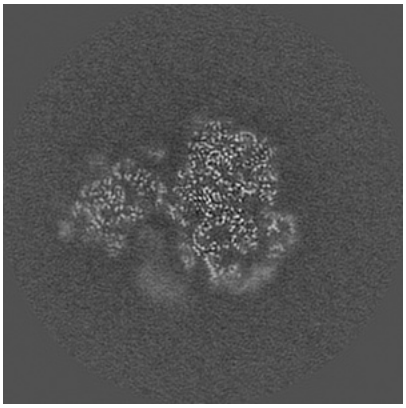
6.2.1 Primary map



X Index: 128



Y Index: 128

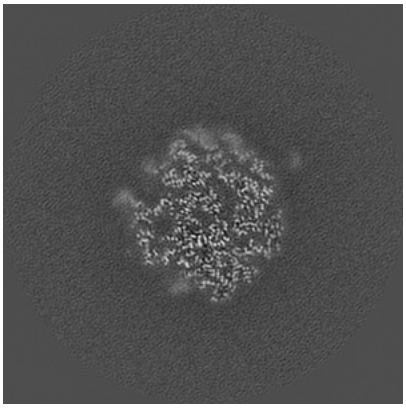


Z Index: 128

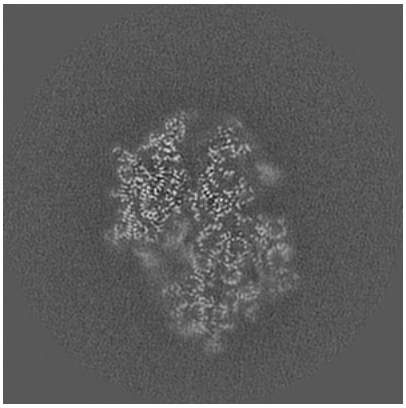
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

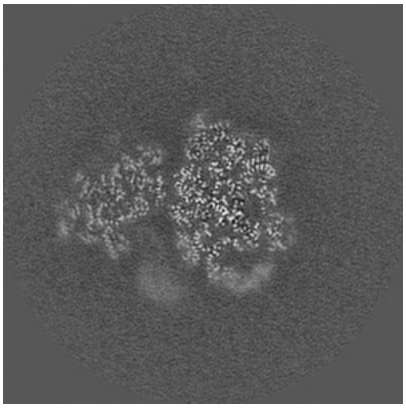
6.3.1 Primary map



X Index: 148



Y Index: 126

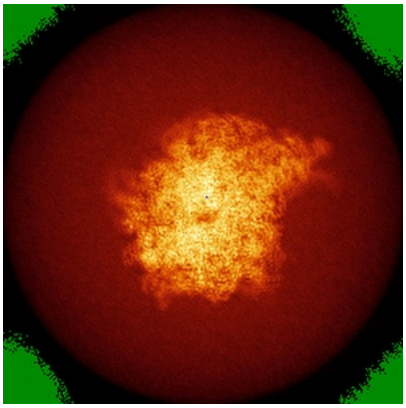


Z Index: 130

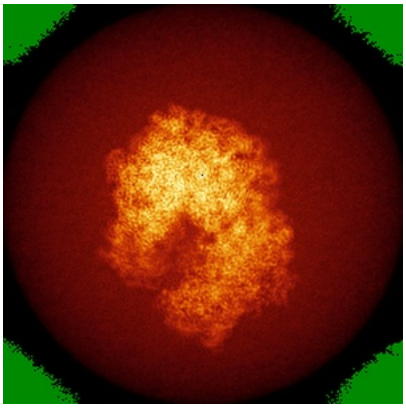
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

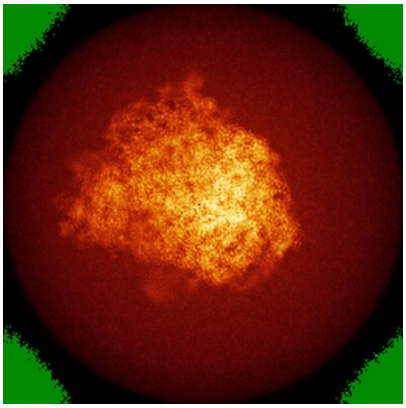
6.4.1 Primary map



X



Y

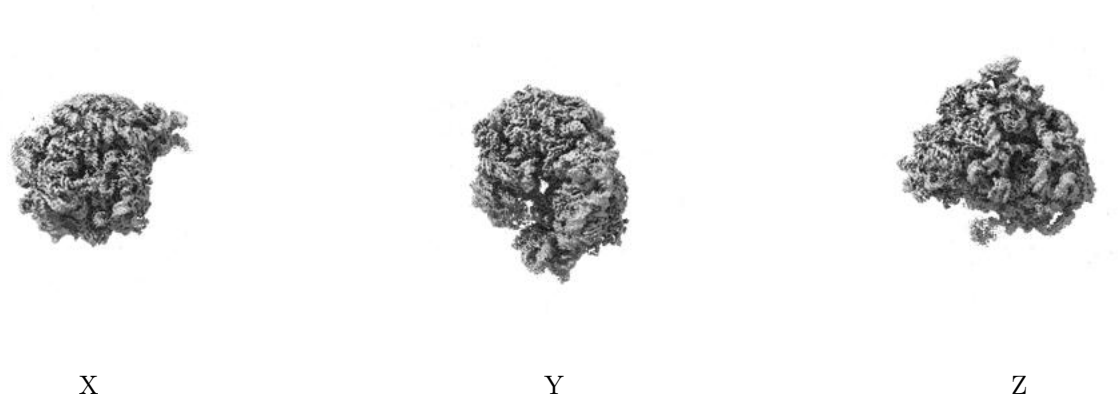


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

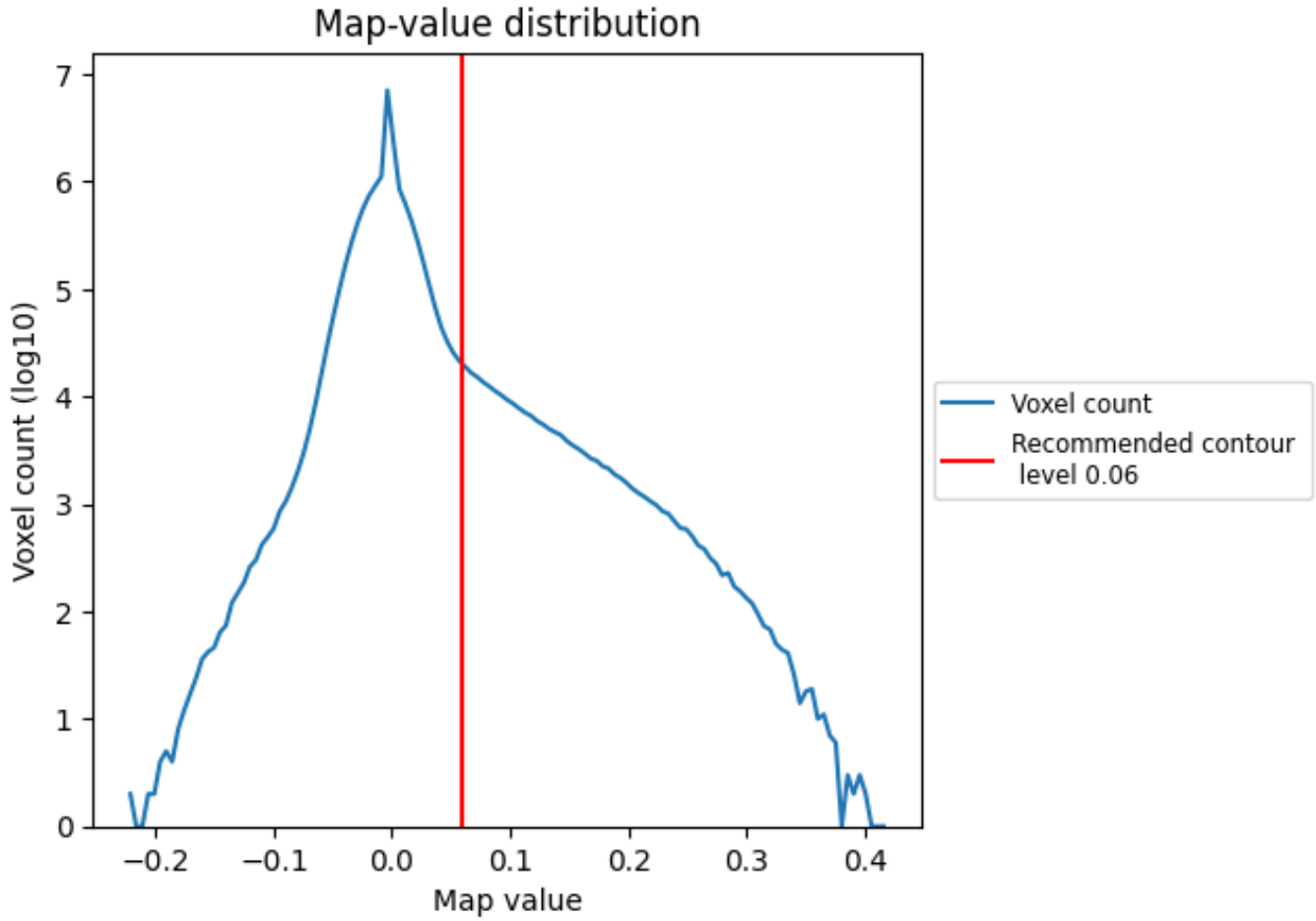
6.6 Mask visualisation (i)

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

7 Map analysis

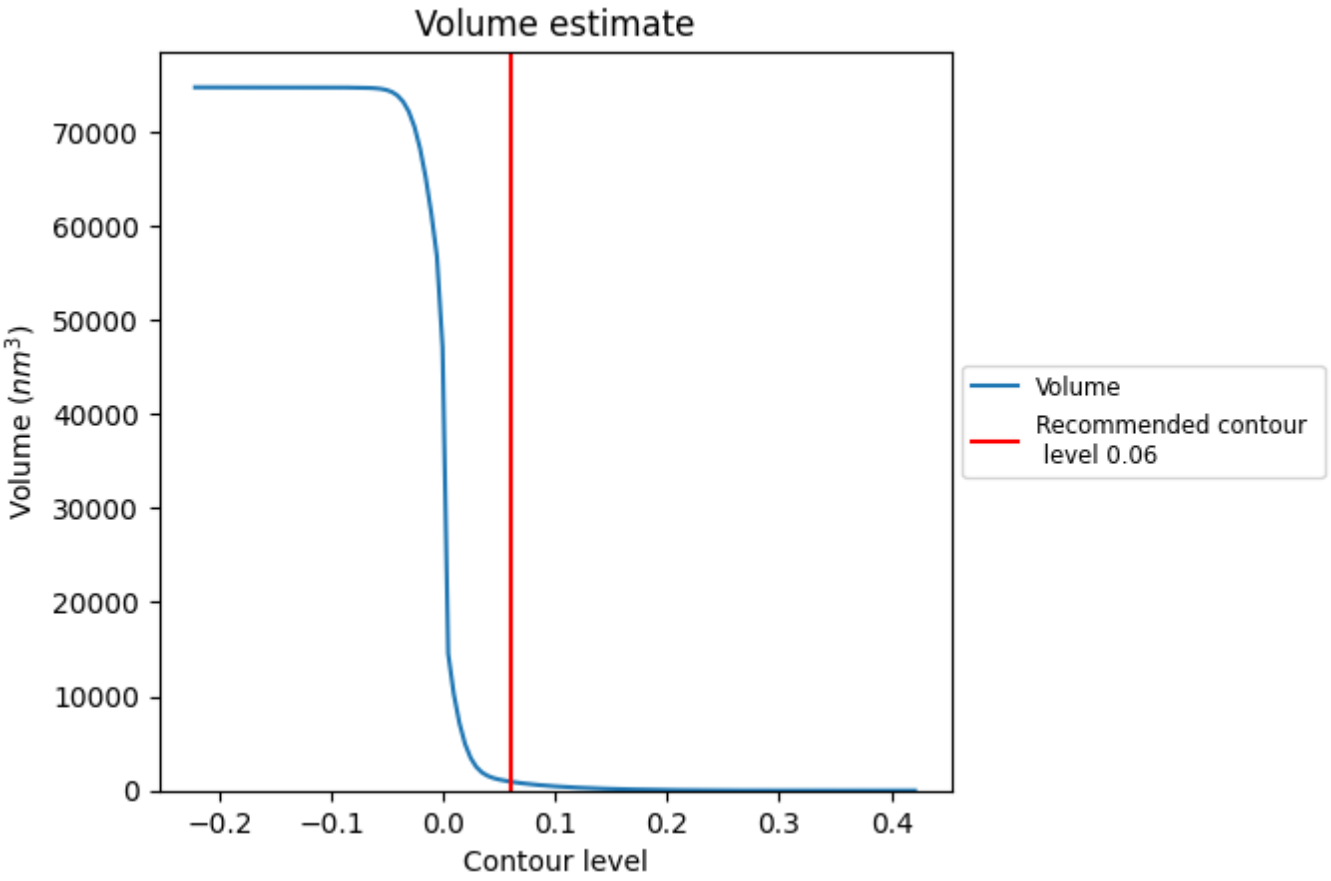
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

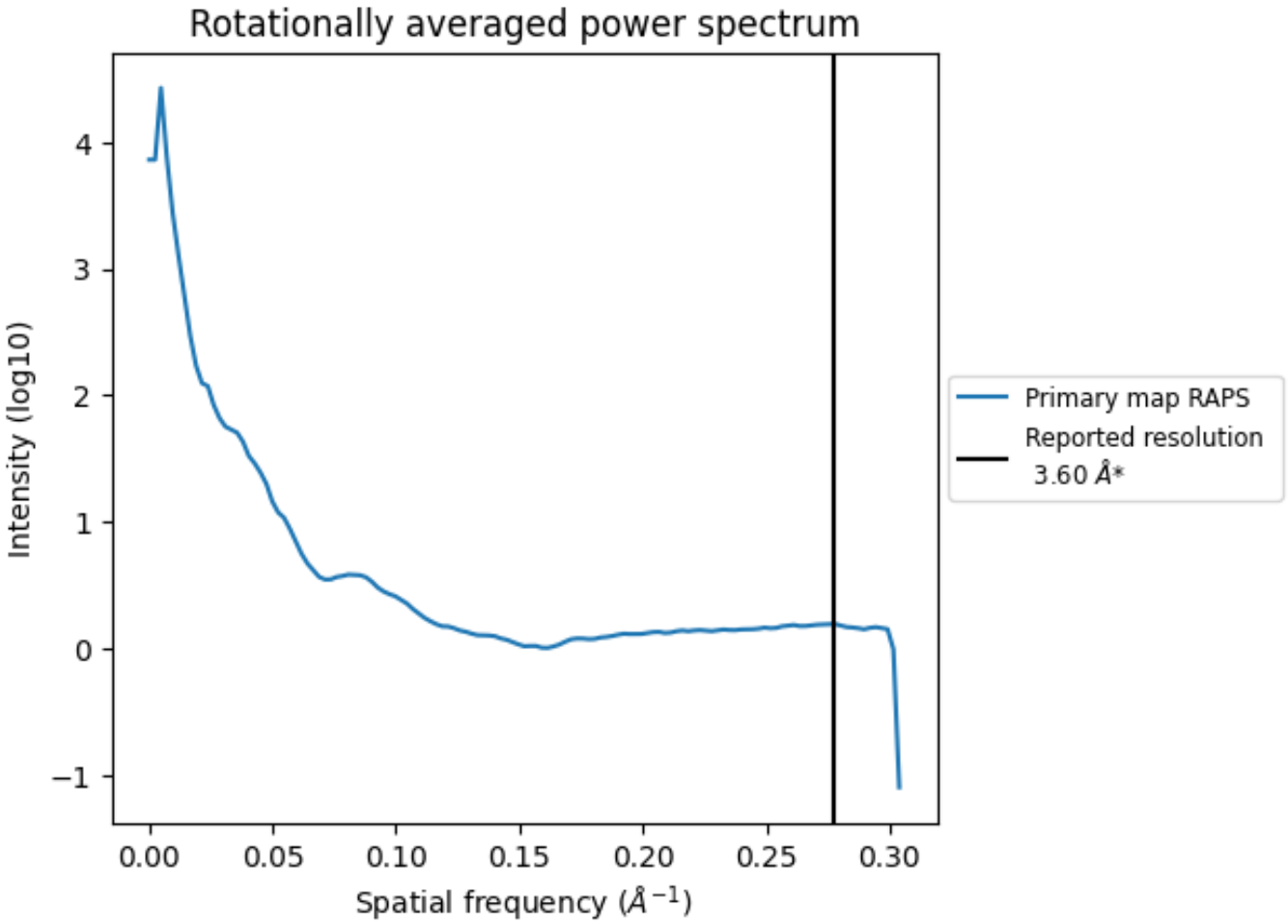
7.2 Volume estimate



The volume at the recommended contour level is 945 nm^3; this corresponds to an approximate mass of 854 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

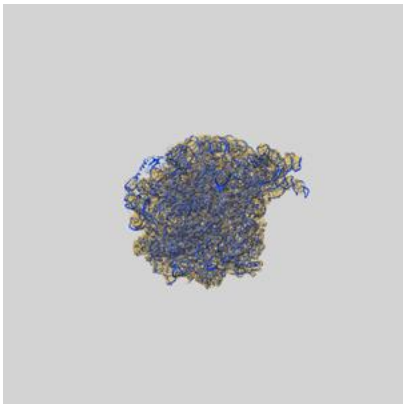
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

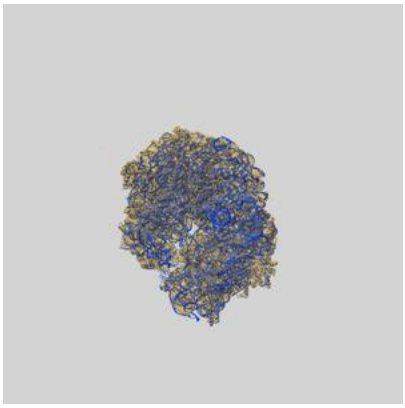
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20184 and PDB model 6OSK. Per-residue inclusion information can be found in section 3 on page 15.

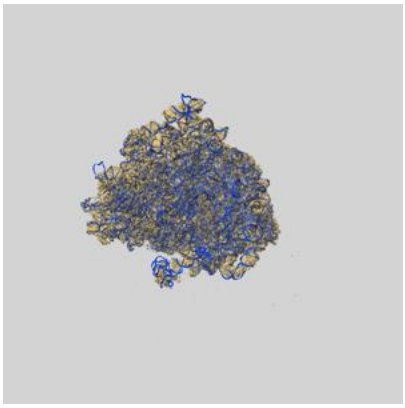
9.1 Map-model overlay



X



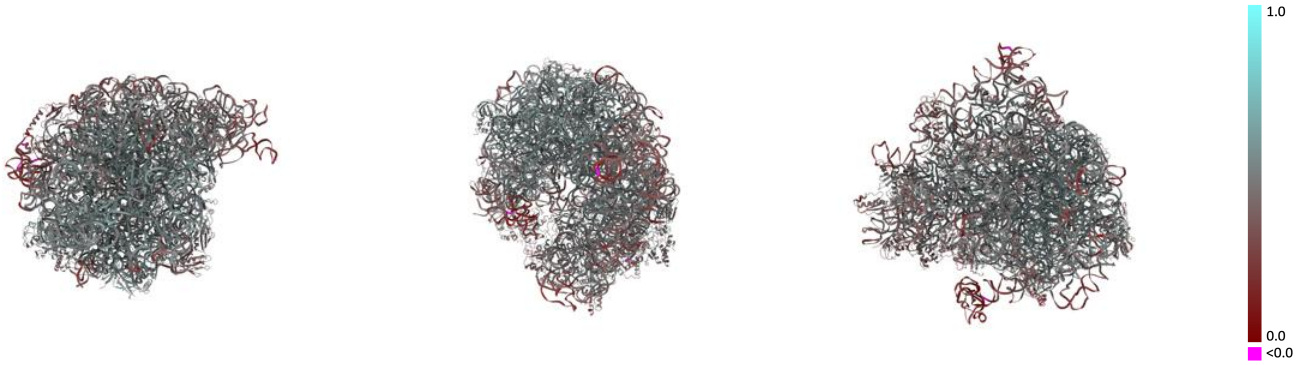
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

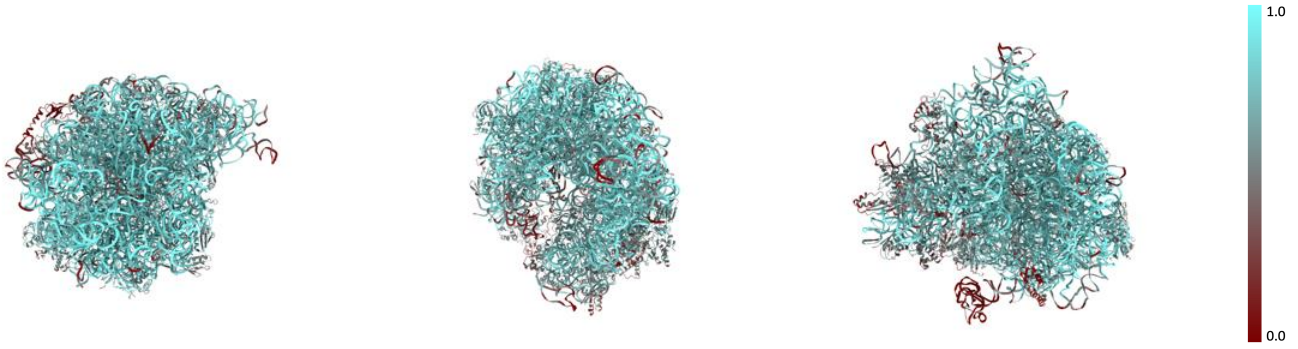
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

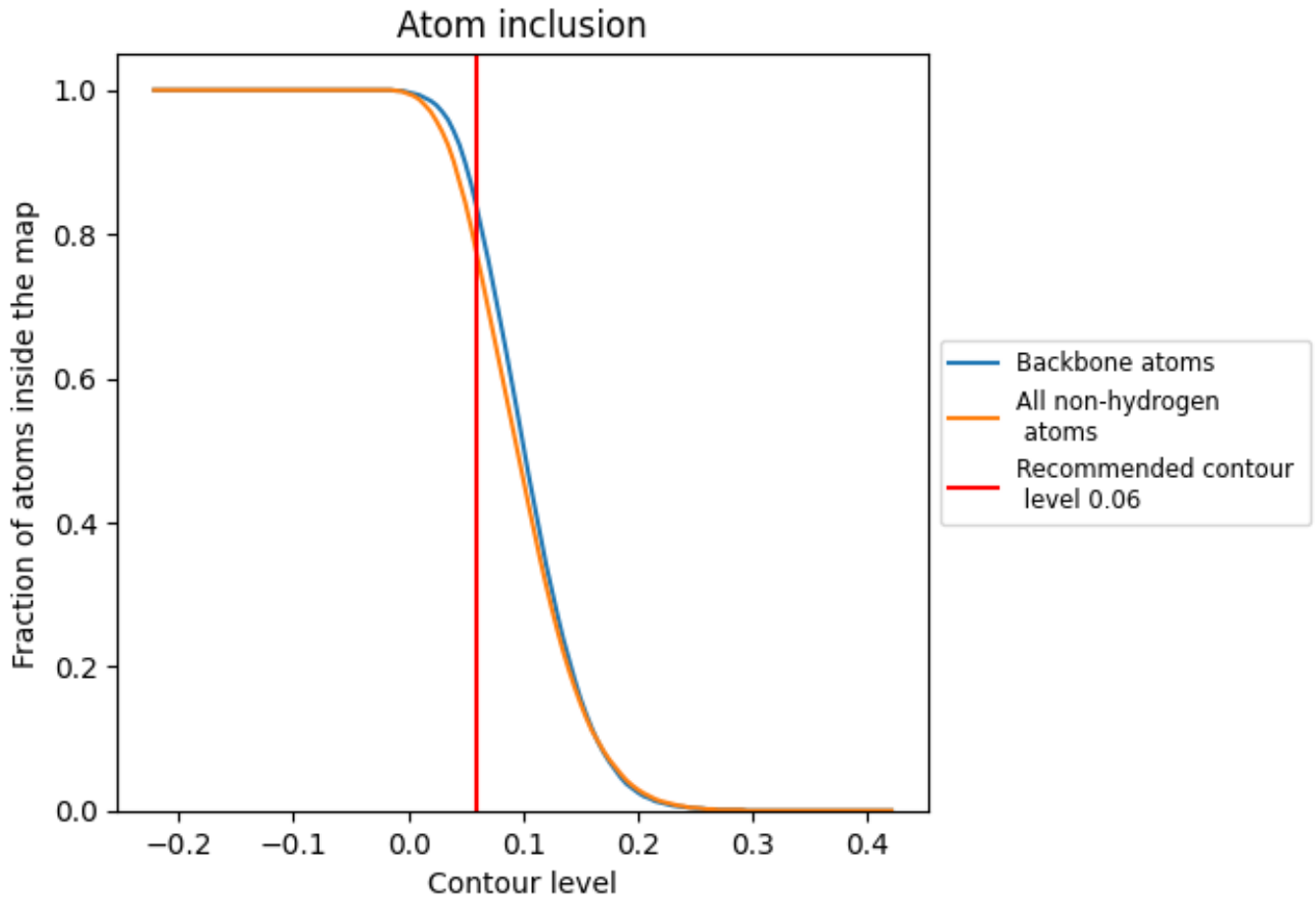
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 77% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7710	0.4670
1	0.8550	0.4830
2	0.8330	0.4470
3	0.8300	0.4240
4	0.7770	0.5030
5	0.6320	0.3710
6	0.4380	0.4210
A	0.4730	0.4330
B	0.7560	0.5360
C	0.7670	0.5280
D	0.7140	0.5080
E	0.4600	0.3880
F	0.5860	0.4280
G	0.1960	0.3400
J	0.7750	0.5330
K	0.6840	0.5190
L	0.7280	0.5180
M	0.6900	0.5080
N	0.8160	0.5370
O	0.6140	0.4280
P	0.6960	0.5160
Q	0.7900	0.5270
R	0.7620	0.5270
S	0.7430	0.5330
T	0.6660	0.4940
U	0.6300	0.4720
V	0.6060	0.4440
W	0.7330	0.5200
X	0.7210	0.5010
Y	0.6690	0.4600
Z	0.7500	0.5200
a	0.0000	0.1790
b	0.7670	0.5140
c	0.6700	0.5070
d	0.7910	0.5390



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Chain	Atom inclusion	Q-score
e	0.7370	0.5360
f	0.7140	0.5170
g	0.5410	0.4240
h	0.5820	0.4570
i	0.4150	0.3750
j	0.6840	0.4930
k	0.6110	0.4380
l	0.4510	0.4100
m	0.6570	0.4760
n	0.5480	0.4110
o	0.4720	0.4160
p	0.6250	0.4500
q	0.6280	0.4920
r	0.5200	0.4180
s	0.6030	0.4560
t	0.6350	0.4650
u	0.6050	0.4620
v	0.5440	0.4340
w	0.5330	0.4300
x	0.5160	0.4090
y	0.5570	0.4350
z	0.4620	0.3950