



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 02:50 pm GMT

PDB ID : 6XZA  
EMDB ID : EMD-10656  
Title : E. coli 70S ribosome in complex with dirithromycin, and deacylated tRNA(iMet) (focused classification).  
Authors : Pichkur, E.B.; Polikanov, Y.S.; Myasnikov, A.G.; Konevega, A.L.  
Deposited on : 2020-02-03  
Resolution : 2.66 Å(reported)  
Based on initial model : 4YBB

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

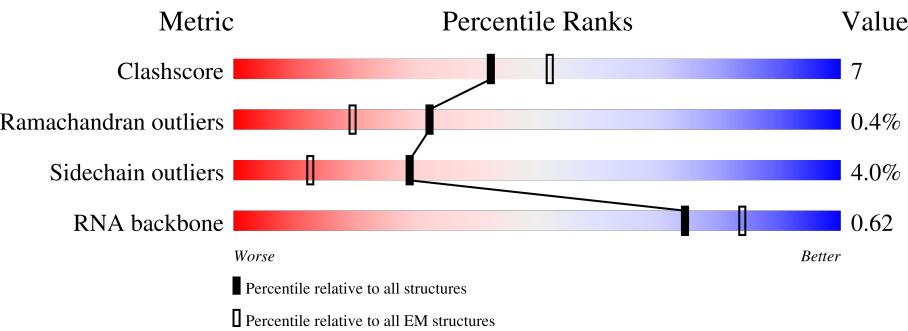
EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.66 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A1	1534	
2	B1	224	
3	C1	206	
4	D1	205	
5	E1	155	
6	F1	106	
7	G1	151	



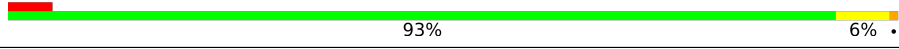


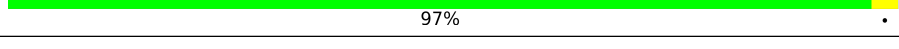
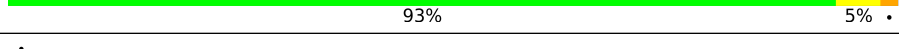
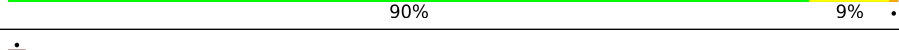
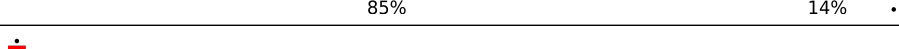
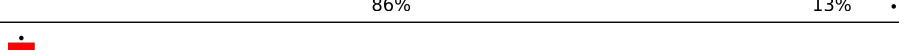

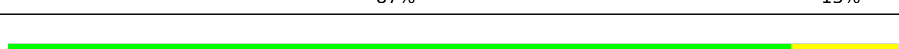


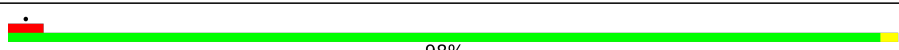
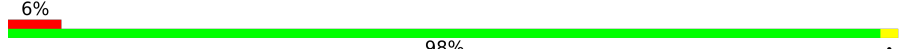

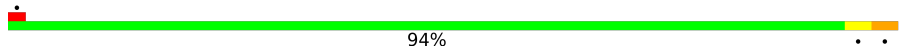
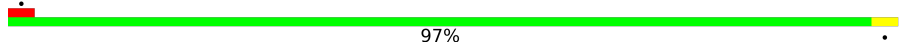


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Mol	Chain	Length	Quality of chain
8	H1	129	
9	I1	127	
10	J1	99	
11	K1	117	
12	L1	123	
13	M1	114	
14	N1	100	
15	O1	88	
16	P1	82	
17	Q1	80	
18	R1	55	
19	S1	79	
20	T1	86	
21	U1	56	
22	A2	2897	
23	B2	120	
24	C2	271	
25	D2	209	
26	E2	201	
27	F2	177	
28	G2	176	
29	H2	135	
30	I2	134	
31	J2	142	
32	K2	123	

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Mol	Chain	Length	Quality of chain
33	L2	144	 87% 13%
34	M2	136	 88% 11% .
35	N2	125	 5% 93% 6% .
36	O2	117	 80% 19% .
37	P2	114	 82% 17% .
38	Q2	117	 97% .
39	R2	103	 93% 5% .
40	S2	110	 90% 9% .
41	T2	93	 85% 14% .
42	U2	102	 86% 13% .
43	V2	94	 81% 18% .
44	W2	76	 87% 13%
45	X2	77	 88% 12%
46	Y2	62	 89% 11%
47	Z2	58	 90% 9% .
48	a2	56	 98% .
49	b2	51	 6% 98% .
50	c2	46	 96% .
51	d2	64	 94% . .
52	e2	38	 97% .
53	f2	76	 37% 39% 24%

## 2 Entry composition [i](#)

There are 54 unique types of molecules in this entry. The entry contains 143983 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	1523	Total	C	N	O	P	0	0
			32681	14576	5998	10584	1523		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C1	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D1	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E1	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F1	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G1	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H1	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I1	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J1	99	Total	C	N	O	S	0	0
			796	498	152	145	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K1	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L1	122	Total	C	N	O	S	0	0
			947	586	195	162	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M1	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N1	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O1	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P1	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q1	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R1	55	Total	C	N	O	0	0
			456	288	86	82		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S1	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T1	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U1	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A2	2897	Total	C	N	O	P	3	0
			62252	27778	11454	20121	2899		

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B2	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	C2	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	D2	209	Total	C	N	O	S	1	0
			1566	980	288	294	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	E2	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	F2	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 28 is a protein called 50S ribosomal protein L6.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	G2	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 29 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	H2	135	Total	C	N	O	S	0	0
			1023	649	179	192	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H2	85	VAL	SER	conflict	UNP P0A7J3
H2	86	THR	MET	conflict	UNP P0A7J3

- Molecule 30 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	I2	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	J2	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	K2	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L2	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	M2	136	Total	C	N	O	S	1	0
			1075	686	205	178	6		

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	N2	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	O2	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	P2	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Q2	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	R2	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	S2	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	T2	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	U2	102	Total	C	N	O		0	0
			780	492	146	142			

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	V2	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	W2	76	Total	C	N	O	S	1	0
			580	359	117	103	1		

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	X2	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Y2	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Z2	58	Total	C	N	O	S	2	0
			449	281	87	79	2		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	a2	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	b2	51	Total	C	N	O		0	0
			414	266	76	72			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	c2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	d2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

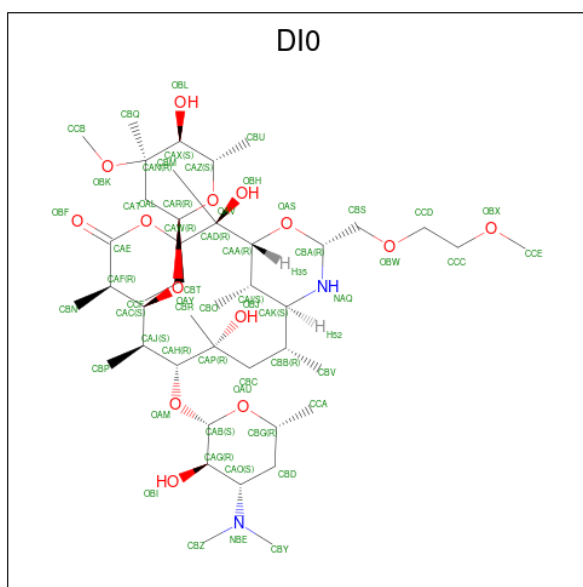
- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	e2	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 53 is a RNA chain called Deacylated tRNA<sup>i</sup>(Met).

Mol	Chain	Residues	Atoms						AltConf	Trace
53	f2	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 54 is Dirithromycin (three-letter code: DI0) (formula: C<sub>42</sub>H<sub>78</sub>N<sub>2</sub>O<sub>14</sub>).

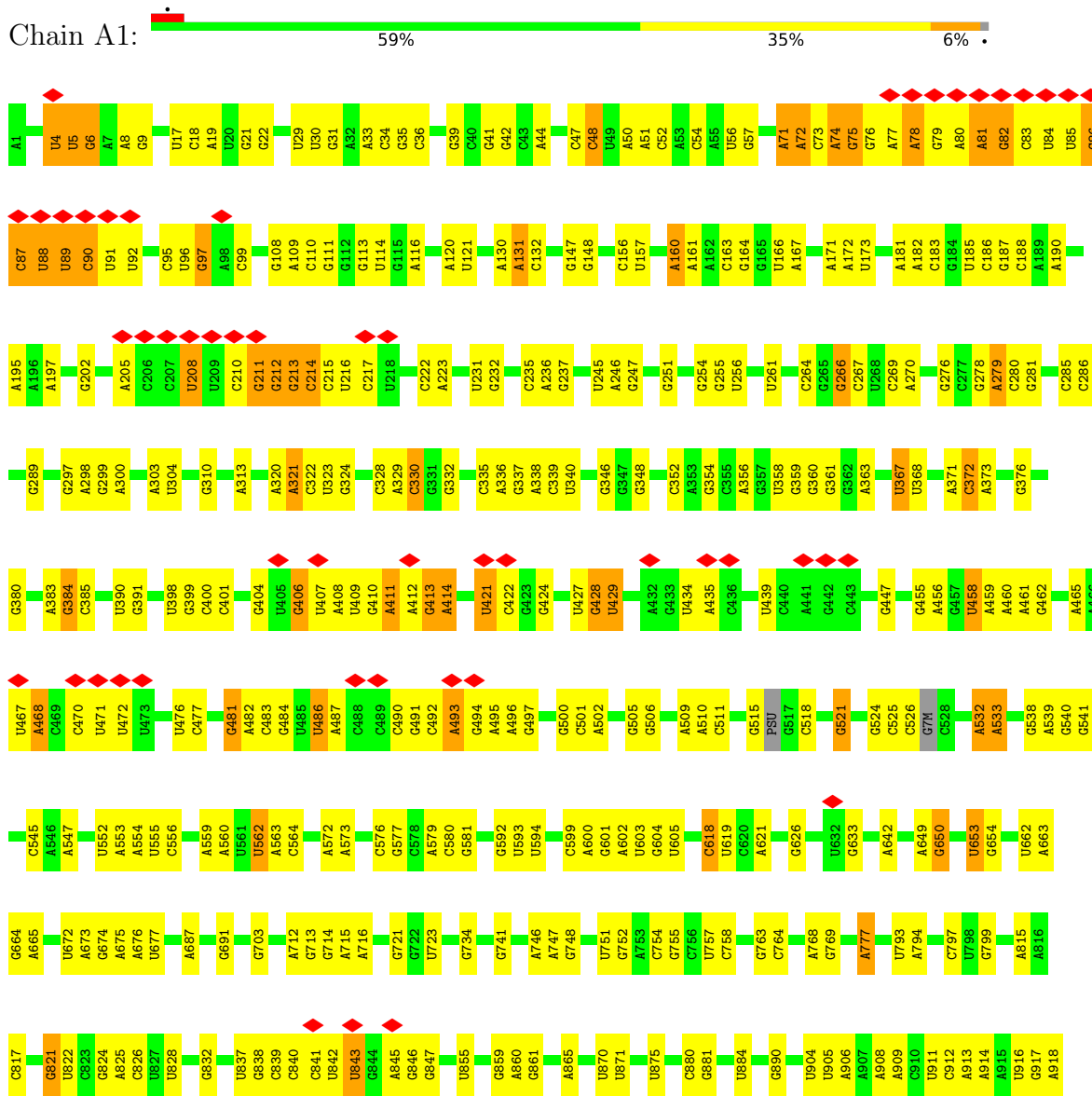


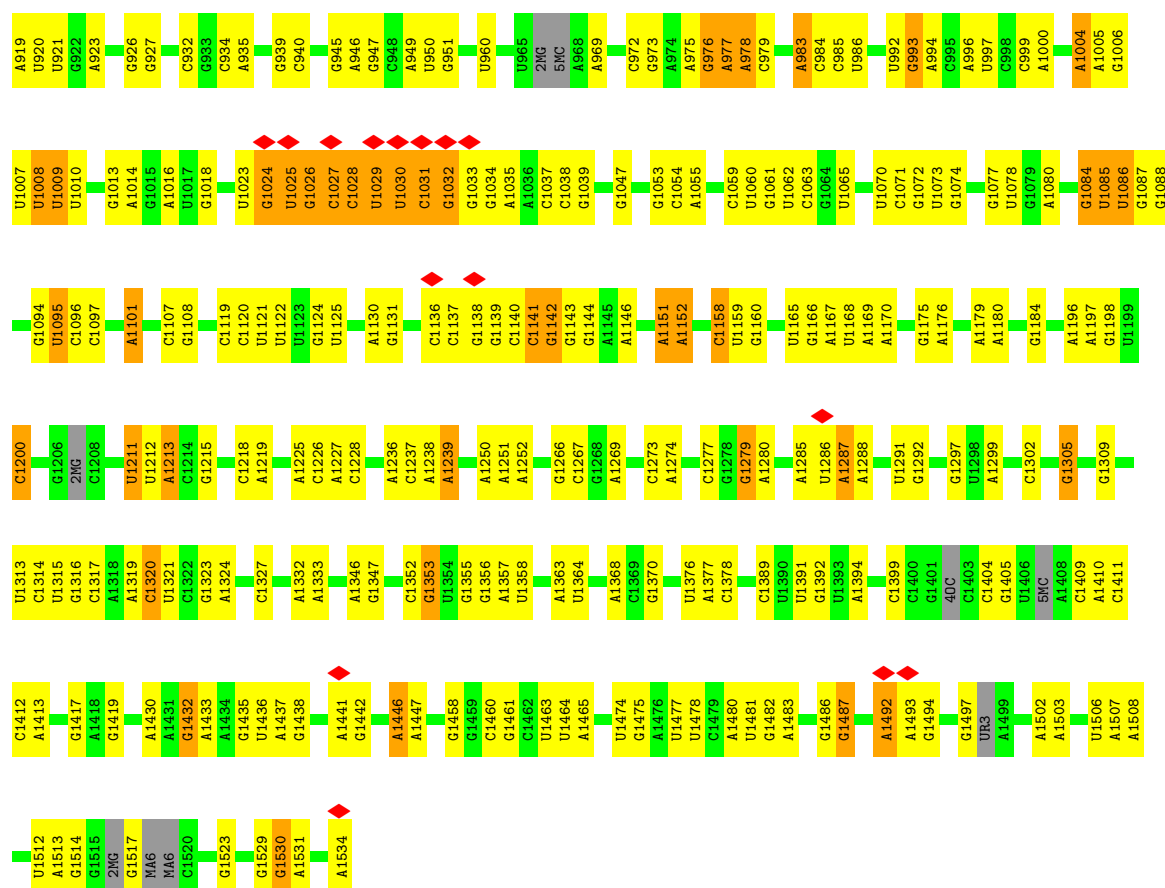
Mol	Chain	Residues	Atoms				AltConf
54	A2	1	Total	C	N	O	0
			58	42	2	14	

### 3 Residue-property plots

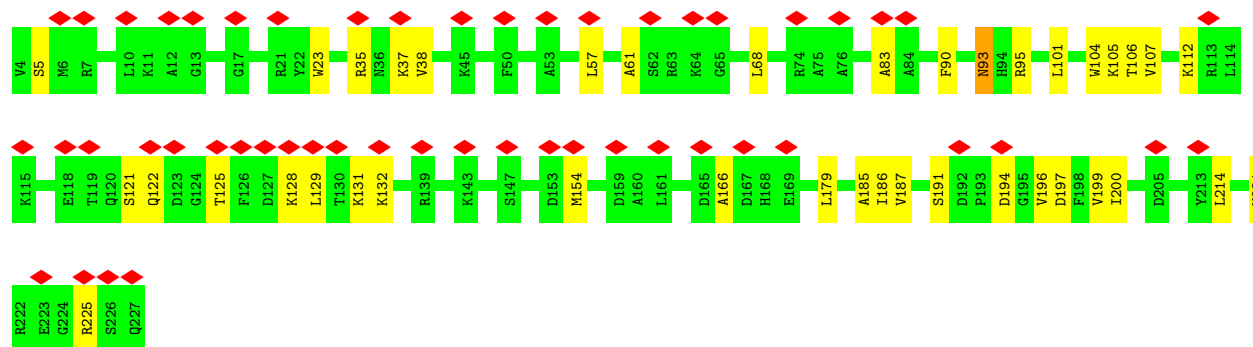
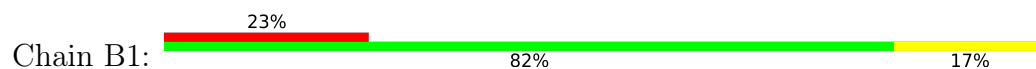
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: 16S rRNA

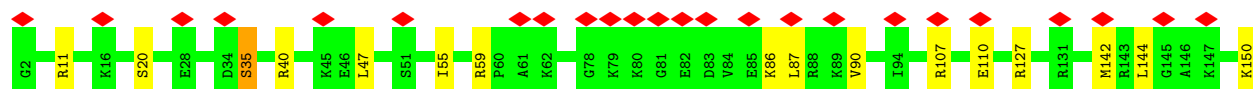
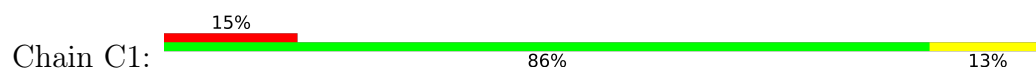


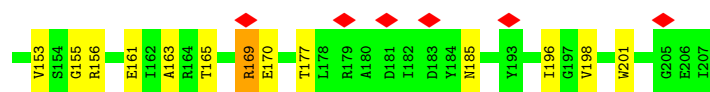


• Molecule 2: 30S ribosomal protein S2

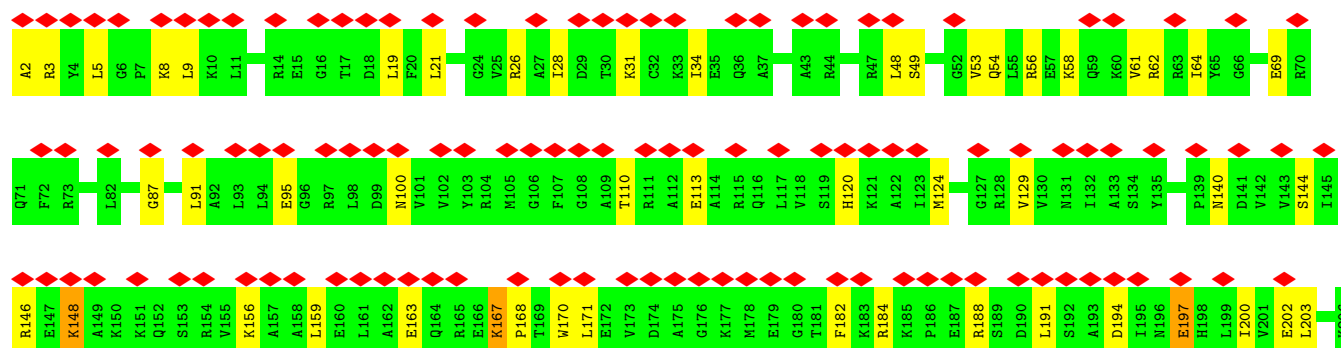
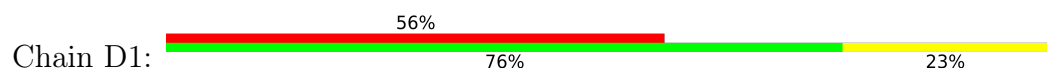


• Molecule 3: 30S ribosomal protein S3

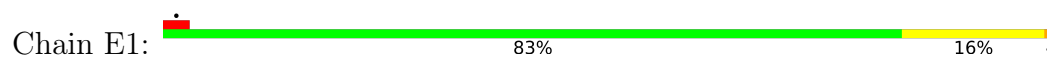




• Molecule 4: 30S ribosomal protein S4



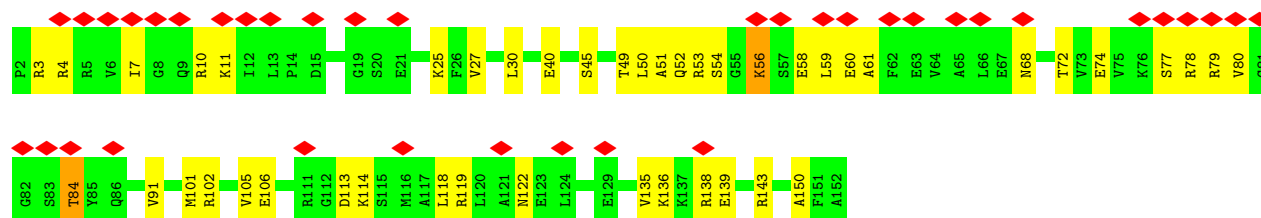
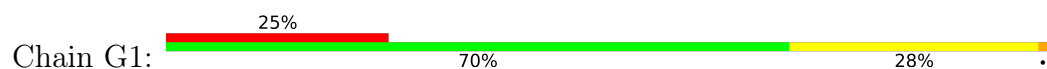
• Molecule 5: 30S ribosomal protein S5



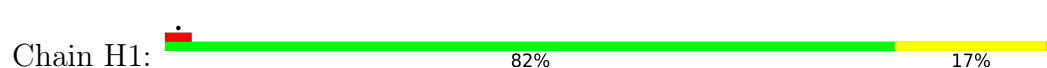
• Molecule 6: 30S ribosomal protein S6



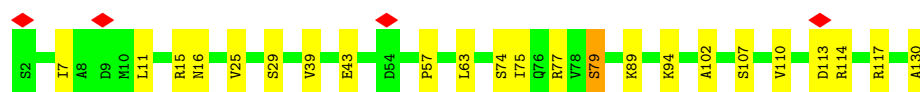
• Molecule 7: 30S ribosomal protein S7



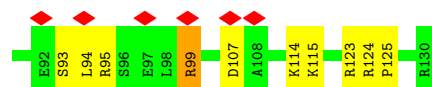
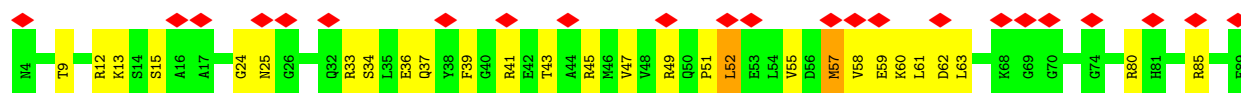
• Molecule 8: 30S ribosomal protein S8



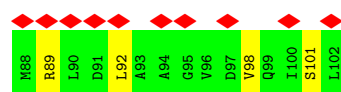
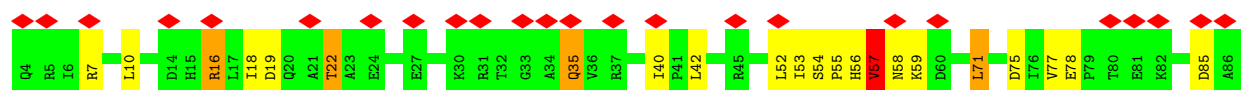
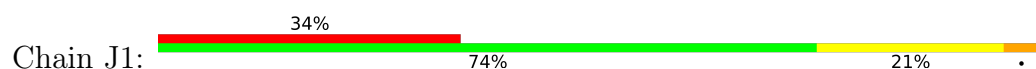




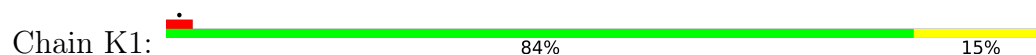
- Molecule 9: 30S ribosomal protein S9



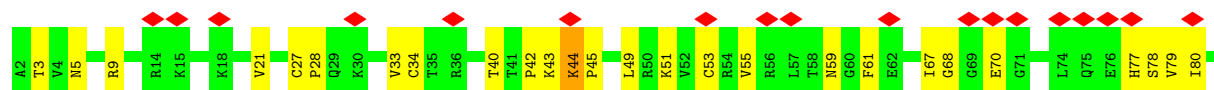
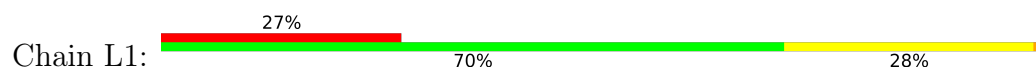
- Molecule 10: 30S ribosomal protein S10



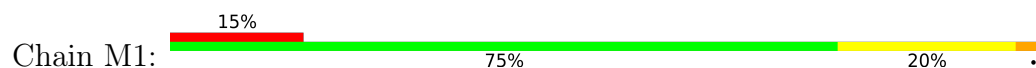
- Molecule 11: 30S ribosomal protein S11

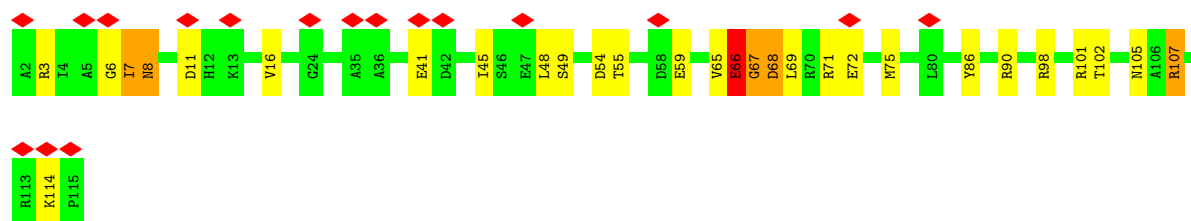


- Molecule 12: 30S ribosomal protein S12

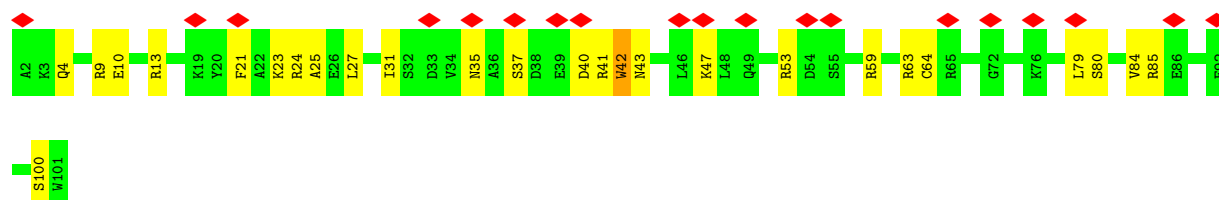
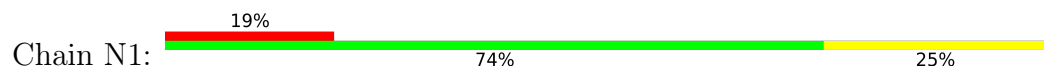


- Molecule 13: 30S ribosomal protein S13

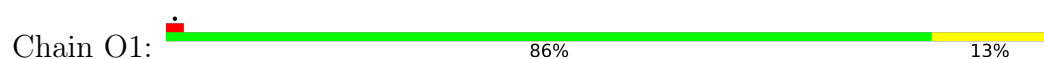




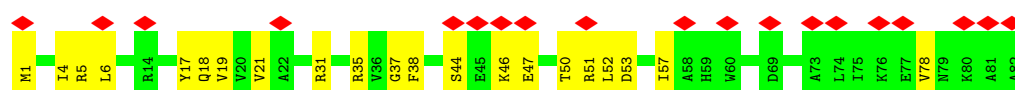
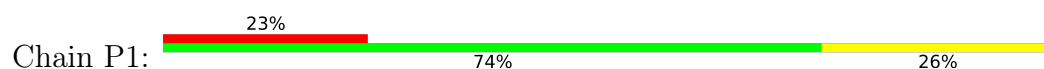
- Molecule 14: 30S ribosomal protein S14



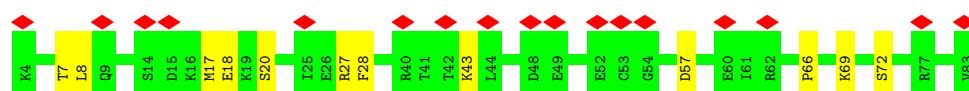
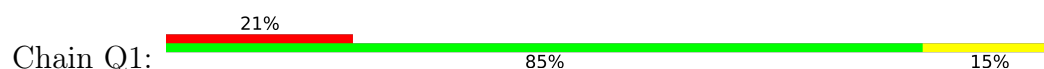
- Molecule 15: 30S ribosomal protein S15



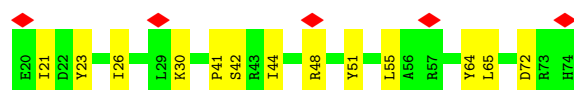
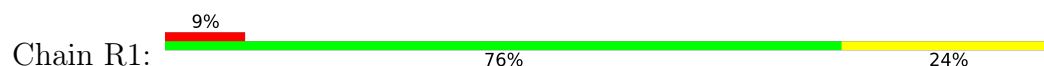
- Molecule 16: 30S ribosomal protein S16



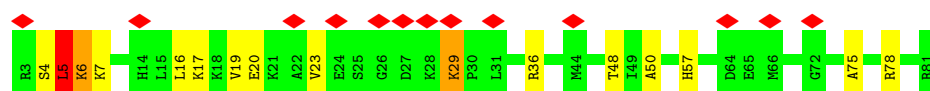
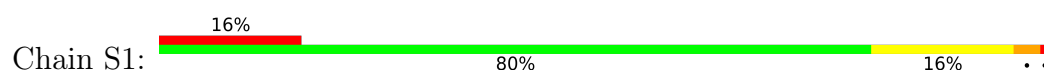
- Molecule 17: 30S ribosomal protein S17



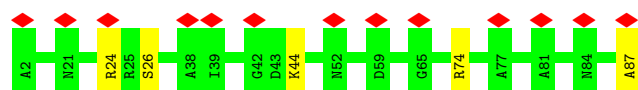
- Molecule 18: 30S ribosomal protein S18



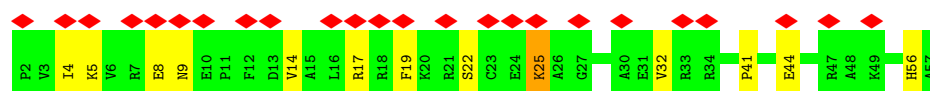
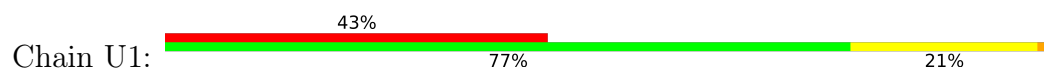
- Molecule 19: 30S ribosomal protein S19



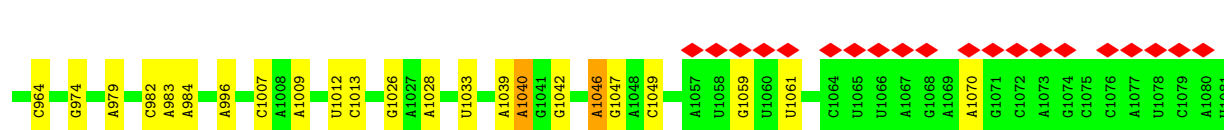
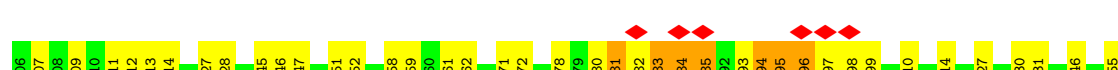
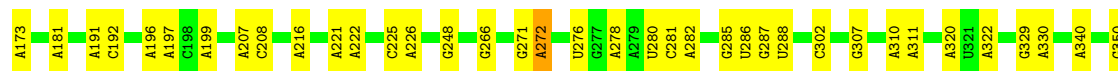
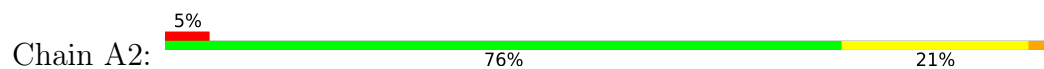
- Molecule 20: 30S ribosomal protein S20

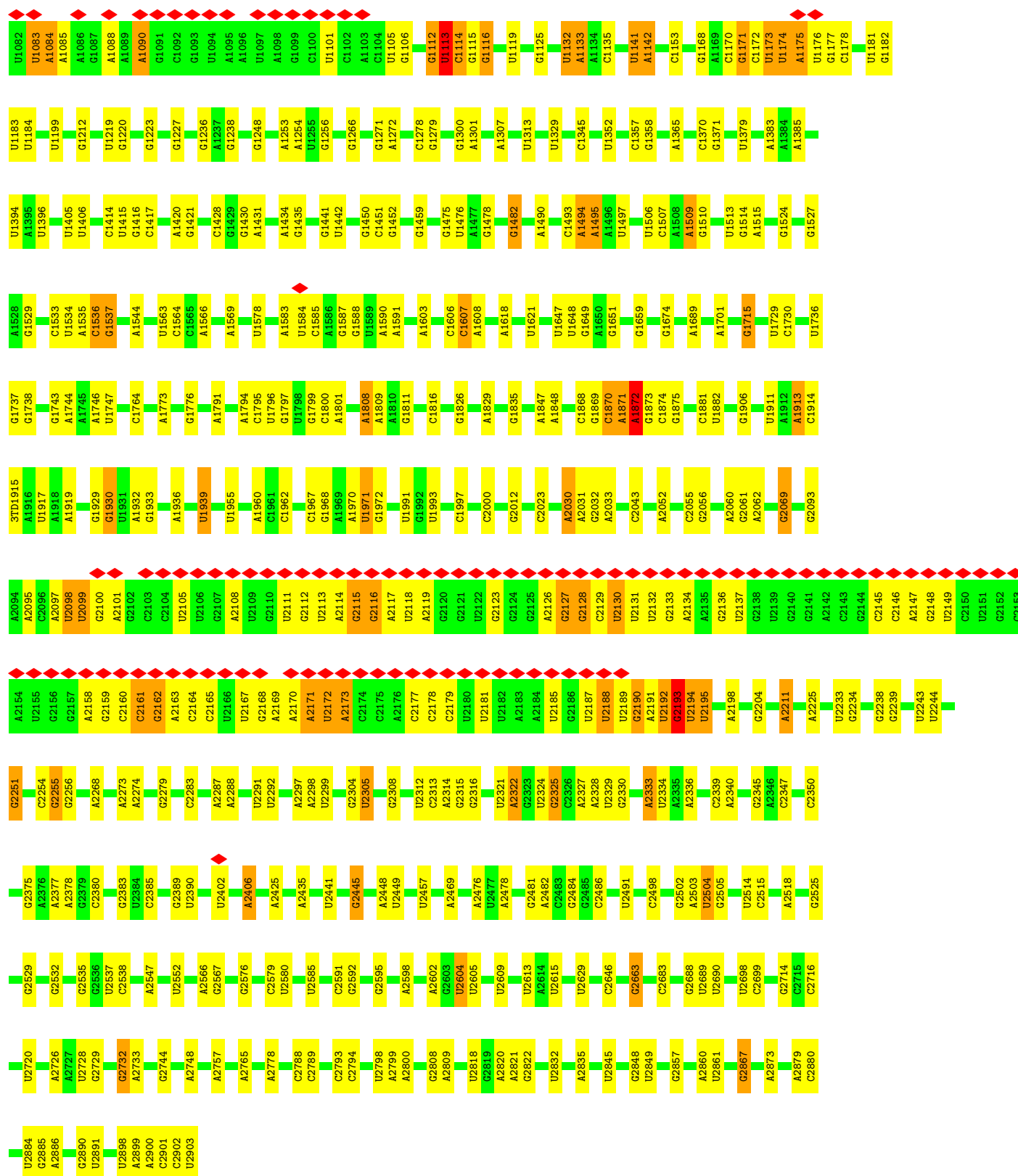


- Molecule 21: 30S ribosomal protein S21



- Molecule 22: 23S rRNA





• Molecule 23: 5S rRNA

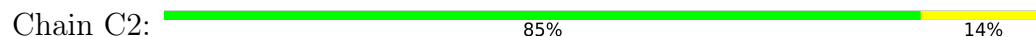
Chain B2:

80%

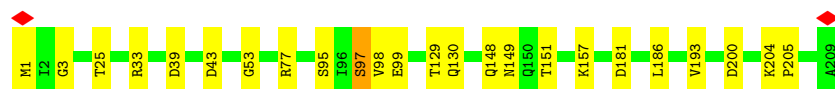
18%



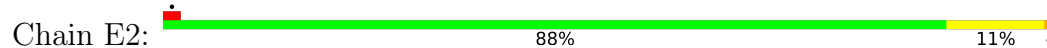
- Molecule 24: 50S ribosomal protein L2



- Molecule 25: 50S ribosomal protein L3



- Molecule 26: 50S ribosomal protein L4

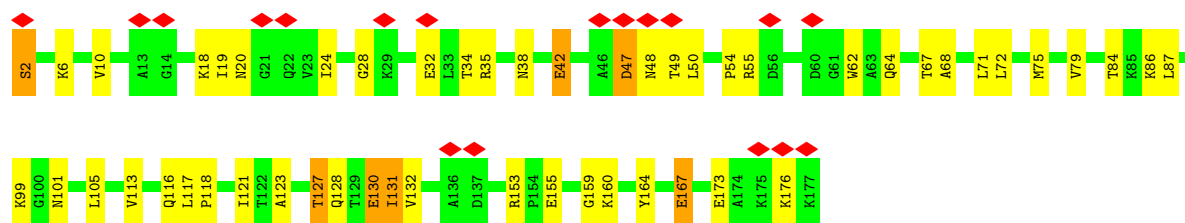


- Molecule 27: 50S ribosomal protein L5

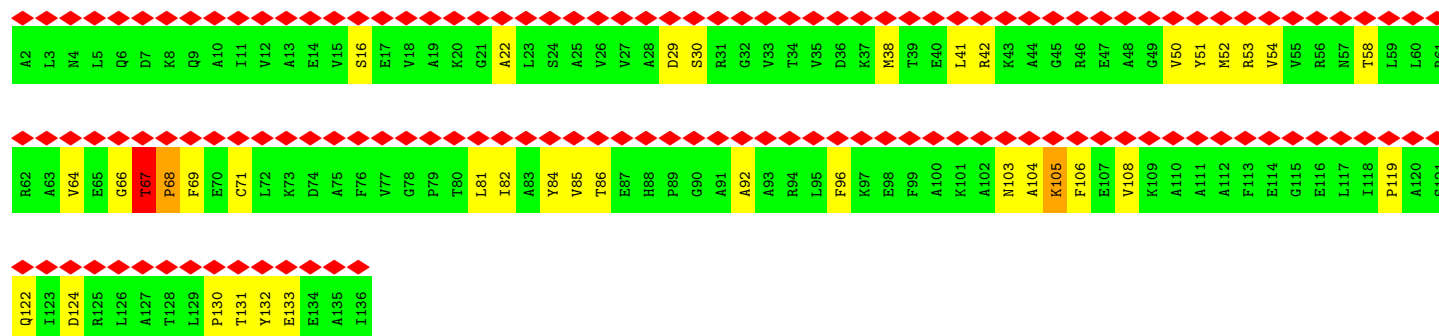
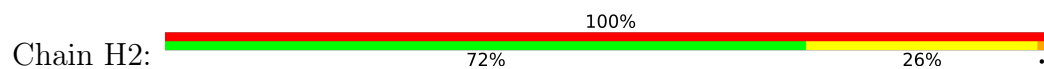


- Molecule 28: 50S ribosomal protein L6

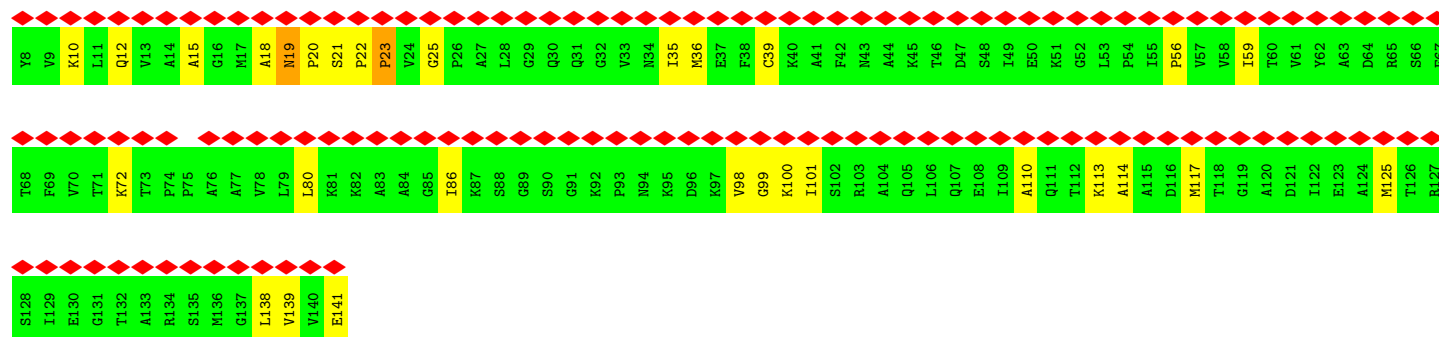
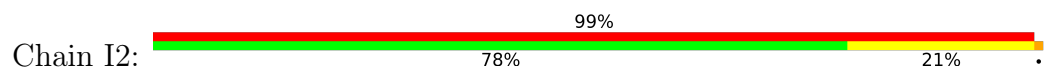




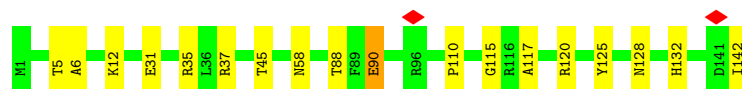
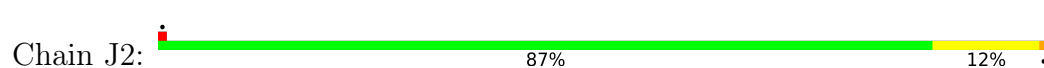
• Molecule 29: 50S ribosomal protein L10



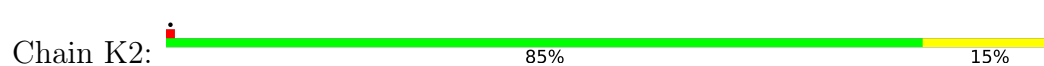
• Molecule 30: 50S ribosomal protein L11



• Molecule 31: 50S ribosomal protein L13

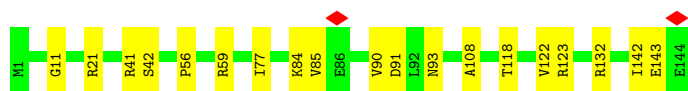


• Molecule 32: 50S ribosomal protein L14

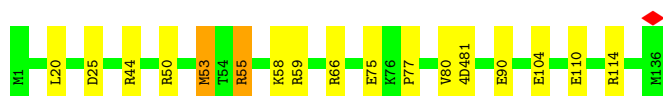




- Molecule 33: 50S ribosomal protein L15



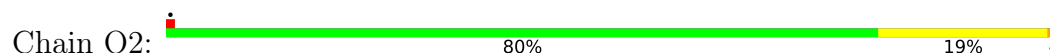
- Molecule 34: 50S ribosomal protein L16



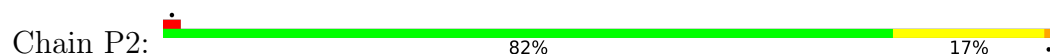
- Molecule 35: 50S ribosomal protein L17



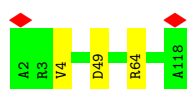
- Molecule 36: 50S ribosomal protein L18



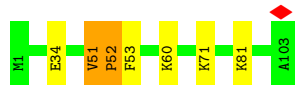
- Molecule 37: 50S ribosomal protein L19



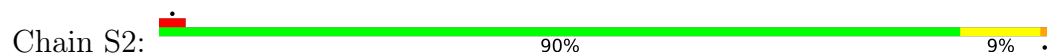
- Molecule 38: 50S ribosomal protein L20



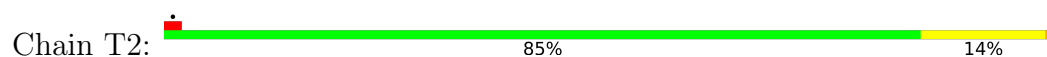
- Molecule 39: 50S ribosomal protein L21



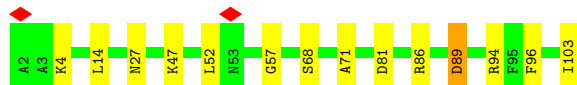
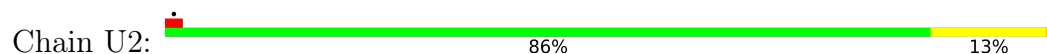
- Molecule 40: 50S ribosomal protein L22



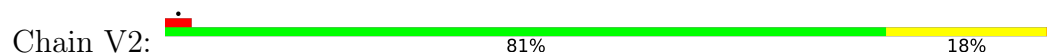
- Molecule 41: 50S ribosomal protein L23



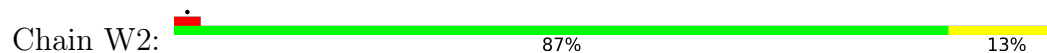
- Molecule 42: 50S ribosomal protein L24



- Molecule 43: 50S ribosomal protein L25



- Molecule 44: 50S ribosomal protein L27

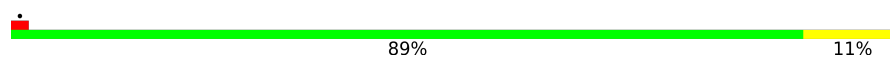


- Molecule 45: 50S ribosomal protein L28



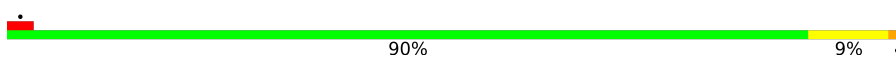


- Molecule 46: 50S ribosomal protein L29

Chain Y2:  89% 11%



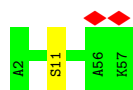
- Molecule 47: 50S ribosomal protein L30

Chain Z2:  90% 9%



- Molecule 48: 50S ribosomal protein L32

Chain a2:  98%



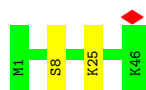
- Molecule 49: 50S ribosomal protein L33

Chain b2:  6% 98%



- Molecule 50: 50S ribosomal protein L34

Chain c2:  96%



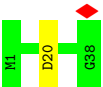
- Molecule 51: 50S ribosomal protein L35

Chain d2:  94%

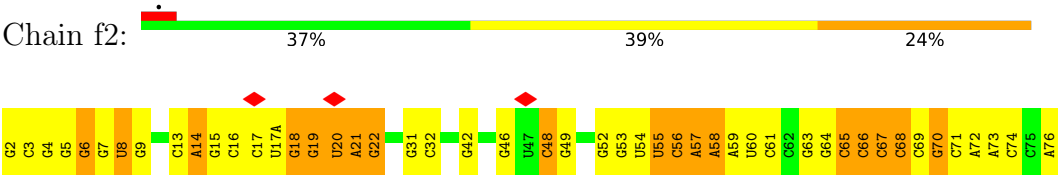


- Molecule 52: 50S ribosomal protein L36

Chain e2:  97%



• Molecule 53: Deacylated tRNAi(Met)



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66269	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	21.147	Depositor
Minimum map value	-12.937	Depositor
Average map value	-0.015	Depositor
Map value standard deviation	0.734	Depositor
Recommended contour level	2	Depositor
Map size (Å)	440.32, 440.32, 440.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, OMG, 6MZ, OMU, 2MG, DI0, 5MU, H2U, 4SU, 4D4, 2MA, G7M, OMC, 3TD, MEQ, 1MG, 5MC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A1	0.35	0/36586	0.78	1/57053 (0.0%)
2	B1	0.24	0/1784	0.41	0/2403
3	C1	0.28	0/1652	0.43	0/2225
4	D1	0.25	0/1665	0.41	0/2227
5	E1	0.27	0/1157	0.44	0/1557
6	F1	0.25	0/881	0.42	0/1189
7	G1	0.26	0/1196	0.37	0/1602
8	H1	0.26	0/989	0.43	0/1326
9	I1	0.30	0/1034	0.45	0/1375
10	J1	0.26	0/806	0.46	0/1089
11	K1	0.26	0/893	0.44	0/1205
12	L1	0.26	0/960	0.50	1/1286 (0.1%)
13	M1	0.27	0/893	0.44	0/1193
14	N1	0.27	0/817	0.40	0/1088
15	O1	0.24	0/722	0.38	0/964
16	P1	0.25	0/659	0.42	0/884
17	Q1	0.25	0/658	0.44	0/881
18	R1	0.25	0/463	0.40	0/621
19	S1	0.28	0/653	0.42	0/877
20	T1	0.25	0/676	0.38	0/895
21	U1	0.24	0/472	0.38	0/627
22	A2	0.73	5/69172 (0.0%)	0.75	11/107908 (0.0%)
23	B2	0.56	0/2872	0.71	0/4478
24	C2	0.37	0/2122	0.46	0/2852
25	D2	0.36	0/1576	0.46	0/2119
26	E2	0.34	0/1571	0.44	0/2113
27	F2	0.35	0/1435	0.51	0/1926
28	G2	0.30	0/1343	0.46	0/1816
29	H2	0.42	0/1037	0.60	0/1402
30	I2	0.48	0/993	0.66	0/1341
31	J2	0.37	0/1152	0.43	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	K2	0.36	0/955	0.47	0/1279
33	L2	0.34	0/1062	0.47	0/1413
34	M2	0.36	0/1081	0.45	0/1443
35	N2	0.35	0/1006	0.44	0/1345
36	O2	0.31	0/910	0.44	0/1219
37	P2	0.36	0/929	0.45	0/1242
38	Q2	0.40	0/960	0.38	0/1278
39	R2	0.37	0/829	0.48	0/1107
40	S2	0.32	0/864	0.44	0/1156
41	T2	0.32	0/745	0.42	0/994
42	U2	0.33	0/788	0.48	1/1051 (0.1%)
43	V2	0.33	0/766	0.42	0/1025
44	W2	0.37	0/587	0.44	0/776
45	X2	0.37	0/635	0.46	0/848
46	Y2	0.27	0/502	0.37	0/667
47	Z2	0.31	0/453	0.44	0/605
48	a2	0.35	0/450	0.45	0/599
49	b2	0.32	0/421	0.44	0/561
50	c2	0.34	0/380	0.43	0/498
51	d2	0.34	0/513	0.47	0/676
52	e2	0.35	0/303	0.44	0/397
53	f2	1.20	13/1725 (0.8%)	1.84	76/2689 (2.8%)
All	All	0.56	18/155753 (0.0%)	0.71	90/232941 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
29	H2	0	1
30	I2	0	1
39	R2	0	1
51	d2	0	1
53	f2	1	0
All	All	1	4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	f2	18	G	O3'-P	-10.45	1.48	1.61
53	f2	64	G	O3'-P	9.45	1.72	1.61

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A2	2254	C	O3'-P	-9.40	1.49	1.61
53	f2	2	G	O3'-P	-8.78	1.50	1.61
22	A2	2255	G	O3'-P	-8.57	1.50	1.61
53	f2	68	C	O3'-P	-8.26	1.51	1.61
22	A2	2255	G	P-OP2	-8.03	1.35	1.49
22	A2	401	A	O3'-P	-7.84	1.51	1.61
53	f2	73	A	O3'-P	-7.32	1.52	1.61
53	f2	6	G	O3'-P	-7.13	1.52	1.61
53	f2	57	A	O3'-P	6.71	1.69	1.61
22	A2	2255	G	P-OP1	-6.36	1.38	1.49
53	f2	60	U	O3'-P	6.29	1.68	1.61
53	f2	74	C	O3'-P	-6.18	1.53	1.61
53	f2	74	C	P-OP1	-5.47	1.39	1.49
53	f2	16	C	O3'-P	-5.29	1.54	1.61
53	f2	20	U	O3'-P	5.12	1.67	1.61
53	f2	72	A	O3'-P	-5.08	1.55	1.61

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	f2	72	A	N9-C1'-C2'	-14.35	95.34	114.00
53	f2	61	C	N1-C1'-C2'	-13.60	96.32	114.00
53	f2	5	G	C1'-C2'-O2'	-11.41	76.38	110.60
53	f2	6	G	N9-C1'-C2'	-11.19	99.46	114.00
22	A2	2255	G	C1'-C2'-O2'	-10.76	78.33	110.60
53	f2	73	A	C1'-C2'-O2'	-10.29	79.72	110.60
53	f2	57	A	C1'-C2'-O2'	-10.16	80.13	110.60
53	f2	73	A	N9-C1'-C2'	-10.07	100.91	114.00
53	f2	71	C	N1-C1'-C2'	-9.86	101.16	112.00
53	f2	64	G	P-O3'-C3'	-9.71	108.04	119.70
53	f2	74	C	C1'-C2'-O2'	-9.72	81.45	110.60
53	f2	74	C	O5'-P-OP1	-9.61	97.05	105.70
53	f2	53	G	N9-C1'-C2'	-9.25	101.82	112.00
22	A2	2255	G	N9-C1'-C2'	-9.21	101.87	112.00
53	f2	65	C	C1'-C2'-O2'	-9.09	83.34	110.60
53	f2	19	G	N9-C1'-C2'	9.01	125.71	114.00
53	f2	46	G	C6-N1-C2	-8.93	119.75	125.10
53	f2	4	G	C4'-C3'-O3'	8.89	130.78	113.00
53	f2	5	G	O5'-P-OP2	-8.86	97.73	105.70
53	f2	14	A	N9-C1'-C2'	-8.80	102.32	112.00
53	f2	14	A	C1'-C2'-O2'	-8.66	84.61	110.60
53	f2	3	C	C1'-C2'-O2'	-8.56	84.91	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	f2	56	C	C1'-C2'-O2'	-8.51	85.07	110.60
53	f2	13	C	C1'-C2'-O2'	-8.45	85.24	110.60
53	f2	71	C	C1'-C2'-O2'	-8.20	85.99	110.60
53	f2	2	G	C4'-C3'-O3'	8.14	129.28	113.00
53	f2	3	C	C4'-C3'-O3'	8.11	129.22	113.00
53	f2	71	C	C4'-C3'-O3'	8.10	129.20	113.00
53	f2	53	G	C4'-C3'-O3'	7.97	128.94	113.00
53	f2	48	C	P-O3'-C3'	7.96	129.25	119.70
53	f2	15	G	N9-C1'-C2'	-7.72	103.51	112.00
53	f2	22	G	C4'-C3'-O3'	7.55	128.11	113.00
53	f2	5	G	C4'-C3'-O3'	7.54	128.09	113.00
53	f2	65	C	C4'-C3'-O3'	7.52	128.03	113.00
53	f2	67	C	N1-C1'-C2'	-7.47	103.78	112.00
53	f2	13	C	C4'-C3'-O3'	7.36	127.71	113.00
53	f2	70	G	N9-C1'-C2'	-7.31	103.96	112.00
53	f2	68	C	N1-C1'-C2'	-7.16	104.13	112.00
53	f2	22	G	C1'-C2'-O2'	-7.06	89.42	110.60
53	f2	49	G	C1'-C2'-O2'	-7.03	89.52	110.60
53	f2	73	A	C4'-C3'-O3'	7.01	127.02	113.00
53	f2	19	G	P-O3'-C3'	7.00	128.10	119.70
53	f2	13	C	N1-C1'-C2'	-6.86	104.46	112.00
53	f2	70	G	C1'-C2'-O2'	-6.69	90.53	110.60
53	f2	57	A	N9-C1'-C2'	-6.68	104.65	112.00
53	f2	5	G	N9-C1'-C2'	-6.67	104.66	112.00
53	f2	58	A	C1'-C2'-O2'	6.65	130.54	110.60
22	A2	2255	G	C4'-C3'-O3'	6.62	126.24	113.00
53	f2	6	G	C4'-C3'-O3'	6.55	126.10	113.00
22	A2	2193	G	C2'-C3'-O3'	6.53	124.14	113.70
53	f2	4	G	C1'-C2'-O2'	-6.52	91.04	110.60
22	A2	1113	U	C2'-C3'-O3'	6.50	124.10	113.70
53	f2	4	G	N9-C1'-C2'	-6.49	104.86	112.00
53	f2	72	A	C4'-C3'-O3'	6.46	125.92	113.00
53	f2	3	C	O5'-P-OP1	-6.45	99.90	105.70
53	f2	52	G	P-O3'-C3'	6.44	127.43	119.70
53	f2	68	C	C1'-C2'-O2'	-6.37	91.50	110.60
53	f2	74	C	C3'-C2'-O2'	-6.29	95.06	113.30
53	f2	56	C	C3'-C2'-O2'	-6.24	95.20	113.30
53	f2	21	A	C1'-C2'-O2'	-6.22	91.94	110.60
53	f2	5	G	O5'-P-OP1	6.18	118.12	110.70
53	f2	73	A	O5'-P-OP1	6.17	118.10	110.70
12	L1	102	LEU	CA-CB-CG	6.10	129.32	115.30
53	f2	66	C	N1-C1'-C2'	-6.02	105.38	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	f2	58	A	P-O3'-C3'	6.01	126.92	119.70
53	f2	65	C	C3'-C2'-C1'	5.98	106.29	101.50
22	A2	1313	U	C2-N1-C1'	5.98	124.87	117.70
53	f2	46	G	C5-C6-N1	5.93	114.46	111.50
53	f2	69	C	N1-C1'-C2'	-5.88	105.53	112.00
53	f2	74	C	C4'-C3'-O3'	5.71	124.42	113.00
53	f2	61	C	C1'-C2'-O2'	-5.62	93.74	110.60
53	f2	2	G	O5'-P-OP2	5.60	117.42	110.70
22	A2	512	G	O4'-C1'-N9	5.58	112.66	108.20
53	f2	58	A	N9-C1'-C2'	5.54	121.20	114.00
53	f2	14	A	O5'-P-OP1	-5.46	100.78	105.70
53	f2	61	C	C3'-C2'-C1'	5.46	105.87	101.50
53	f2	69	C	O5'-C5'-C4'	-5.46	101.33	111.70
22	A2	2255	G	C3'-C2'-C1'	5.45	105.86	101.50
53	f2	68	C	O5'-P-OP2	-5.44	100.81	105.70
53	f2	14	A	C4'-C3'-O3'	5.42	123.83	113.00
53	f2	69	C	C5'-C4'-O4'	-5.35	102.67	109.10
22	A2	404	A	O4'-C1'-C2'	-5.26	100.54	105.80
53	f2	74	C	C3'-C2'-C1'	5.25	105.70	101.50
53	f2	14	A	C3'-C2'-O2'	-5.24	98.09	113.30
53	f2	56	C	C5'-C4'-O4'	-5.14	102.94	109.10
22	A2	12	U	N3-C2-O2	-5.04	118.67	122.20
42	U2	52	LEU	CA-CB-CG	5.02	126.85	115.30
1	A1	754	C	C2-N1-C1'	5.02	124.32	118.80
53	f2	56	C	C4'-C3'-O3'	5.01	123.03	113.00
22	A2	1872	A	O4'-C1'-N9	5.00	112.20	108.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	f2	58	A	C2'

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	H2	67	THR	Peptide
30	I2	98	VAL	Peptide
39	R2	51	VAL	Peptide
51	d2	31	HIS	Peptide



## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	32681	0	16454	408	0
2	B1	1753	0	1780	27	0
3	C1	1625	0	1696	20	0
4	D1	1643	0	1707	35	0
5	E1	1144	0	1182	25	0
6	F1	862	0	864	25	0
7	G1	1182	0	1238	22	0
8	H1	979	0	1031	15	0
9	I1	1022	0	1066	21	0
10	J1	796	0	836	18	0
11	K1	877	0	887	14	0
12	L1	947	0	1011	31	0
13	M1	884	0	941	52	0
14	N1	805	0	844	16	0
15	O1	714	0	733	20	0
16	P1	649	0	666	27	0
17	Q1	649	0	691	9	0
18	R1	456	0	478	9	0
19	S1	638	0	665	10	0
20	T1	670	0	719	3	0
21	U1	465	0	491	8	0
22	A2	62252	0	31324	377	0
23	B2	2569	0	1301	13	0
24	C2	2083	0	2154	21	0
25	D2	1566	0	1617	14	0
26	E2	1552	0	1619	13	0
27	F2	1411	0	1444	131	0
28	G2	1323	0	1371	30	0
29	H2	1023	0	1052	21	0
30	I2	979	0	1028	26	0
31	J2	1129	0	1162	10	0
32	K2	946	0	1021	10	0
33	L2	1053	0	1129	12	0
34	M2	1075	0	1155	10	0
35	N2	993	0	1034	6	0
36	O2	900	0	935	18	0
37	P2	917	0	962	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Q2	947	0	1019	3	0
39	R2	816	0	839	4	0
40	S2	857	0	922	6	0
41	T2	739	0	807	14	0
42	U2	780	0	831	7	0
43	V2	753	0	780	11	0
44	W2	580	0	593	5	0
45	X2	625	0	652	4	0
46	Y2	501	0	531	3	0
47	Z2	449	0	487	3	0
48	a2	444	0	458	0	0
49	b2	414	0	442	0	0
50	c2	377	0	418	0	0
51	d2	504	0	572	0	0
52	e2	302	0	343	0	0
53	f2	1625	0	828	0	0
54	A2	58	0	0	1	0
All	All	143983	0	96810	1431	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 7.

All (1431) 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:F1:14:GLN:OE1	6:F1:83:ALA:CB	1.66	1.41
22:A2:883:G:N2	22:A2:894:U:O2	1.56	1.37
22:A2:1:G:N2	22:A2:2902:C:O2	1.64	1.30
13:M1:3:ARG:NH2	27:F2:110:ARG:NH2	1.76	1.30
12:L1:44:LYS:HB3	12:L1:45:PRO:CD	1.61	1.29
16:P1:19:VAL:HG21	16:P1:52:LEU:CD2	1.66	1.26
13:M1:66:GLU:O	13:M1:68:ASP:N	1.70	1.23
16:P1:38:PHE:O	16:P1:52:LEU:HD11	1.41	1.21
27:F2:80:ARG:CG	27:F2:83:TYR:OH	1.89	1.20
5:E1:154:ALA:CB	5:E1:161:VAL:HG12	1.73	1.19
27:F2:80:ARG:CG	27:F2:83:TYR:CZ	2.25	1.18
27:F2:80:ARG:HG3	27:F2:83:TYR:CZ	1.79	1.18
22:A2:1:G:N1	22:A2:2902:C:N3	1.92	1.17
6:F1:14:GLN:OE1	6:F1:83:ALA:HB1	1.23	1.16
2:B1:196:VAL:CG2	2:B1:199:VAL:HG22	1.75	1.16
27:F2:108:VAL:CG1	27:F2:109:PRO:HD3	1.76	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M1:7:ILE:HD12	27:F2:112:ARG:HB3	1.20	1.15
27:F2:108:VAL:HG13	27:F2:109:PRO:CD	1.78	1.14
27:F2:80:ARG:HG3	27:F2:83:TYR:OH	0.97	1.14
27:F2:103:LEU:HB2	27:F2:107:ALA:CB	1.79	1.12
13:M1:7:ILE:HG21	27:F2:112:ARG:HA	1.24	1.10
12:L1:44:LYS:HB3	12:L1:45:PRO:HD2	1.19	1.09
2:B1:196:VAL:CG2	2:B1:199:VAL:CG2	2.31	1.09
16:P1:19:VAL:HG21	16:P1:52:LEU:HD21	1.35	1.09
2:B1:196:VAL:HG21	2:B1:199:VAL:HG22	1.10	1.08
1:A1:1158:C:O2'	2:B1:132:LYS:NZ	1.86	1.08
27:F2:80:ARG:HB2	27:F2:83:TYR:CZ	1.89	1.08
22:A2:884:U:O4	22:A2:893:C:C4	2.07	1.08
1:A1:1087:G:OP1	1:A1:1389:C:H4'	1.55	1.05
27:F2:80:ARG:CG	27:F2:83:TYR:CE2	2.40	1.04
22:A2:2898:U:H2'	22:A2:2899:A:C8	1.92	1.03
22:A2:882:G:N1	22:A2:895:U:O2	1.90	1.03
27:F2:80:ARG:HG2	27:F2:83:TYR:CE2	1.94	1.02
27:F2:80:ARG:CB	27:F2:83:TYR:CZ	2.42	1.02
22:A2:2097:A:N1	22:A2:2192:U:N3	2.08	1.01
13:M1:7:ILE:HD12	27:F2:112:ARG:CB	1.90	1.01
22:A2:2898:U:H2'	22:A2:2899:A:H8	1.24	1.00
27:F2:103:LEU:HB2	27:F2:107:ALA:HB3	1.38	1.00
15:O1:89:ARG:NH2	22:A2:715:A:H5''	1.78	0.99
22:A2:884:U:O4	22:A2:893:C:N3	1.96	0.99
13:M1:7:ILE:CD1	27:F2:112:ARG:HB3	1.93	0.98
1:A1:1494:G:C8	22:A2:1913:A:C2	2.52	0.98
13:M1:3:ARG:NH2	27:F2:110:ARG:HH21	1.46	0.96
22:A2:894:U:O2'	22:A2:895:U:OP1	1.82	0.95
22:A2:1:G:N1	22:A2:2902:C:C2	2.34	0.95
6:F1:14:GLN:OE1	6:F1:83:ALA:HB2	1.66	0.94
13:M1:3:ARG:HH22	27:F2:110:ARG:NH2	1.49	0.94
27:F2:110:ARG:HB3	27:F2:137:ILE:HG23	1.48	0.94
22:A2:884:U:C4	22:A2:893:C:N3	2.35	0.93
15:O1:89:ARG:CZ	22:A2:715:A:H5''	1.98	0.93
2:B1:196:VAL:HG21	2:B1:199:VAL:CG2	1.96	0.93
27:F2:80:ARG:HG3	27:F2:83:TYR:HH	1.34	0.93
13:M1:3:ARG:HH12	27:F2:110:ARG:HD3	1.35	0.92
27:F2:103:LEU:CB	27:F2:107:ALA:HB3	1.98	0.92
22:A2:2469:A:H4'	34:M2:55:ARG:HD2	1.51	0.92
22:A2:1:G:C2	22:A2:2902:C:O2	2.24	0.90
13:M1:3:ARG:HH22	27:F2:110:ARG:CZ	1.84	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A2:1847:A:HO2'	22:A2:1848:A:H8	0.98	0.90
12:L1:44:LYS:CB	12:L1:45:PRO:CD	2.45	0.90
27:F2:103:LEU:CB	27:F2:107:ALA:CB	2.50	0.89
16:P1:19:VAL:HG21	16:P1:52:LEU:HD23	1.54	0.89
22:A2:883:G:H1	22:A2:894:U:H3	0.89	0.89
22:A2:2116:G:O6	22:A2:2171:A:N6	2.06	0.89
5:E1:154:ALA:HB2	5:E1:161:VAL:HG12	1.52	0.88
16:P1:38:PHE:O	16:P1:52:LEU:CD1	2.21	0.88
1:A1:1494:G:O4'	22:A2:1913:A:N3	2.05	0.88
27:F2:103:LEU:CA	27:F2:107:ALA:HB3	2.03	0.88
27:F2:150:ARG:HG2	27:F2:150:ARG:HH11	1.38	0.88
27:F2:80:ARG:HB2	27:F2:83:TYR:CE2	2.08	0.87
22:A2:134:G:C6	22:A2:135:U:C4	2.62	0.87
22:A2:884:U:O4	22:A2:893:C:N4	2.08	0.86
27:F2:103:LEU:HA	27:F2:107:ALA:CB	2.06	0.86
16:P1:47:GLU:N	16:P1:47:GLU:OE2	2.08	0.86
27:F2:103:LEU:CA	27:F2:107:ALA:CB	2.54	0.85
22:A2:1:G:C6	22:A2:2902:C:N3	2.45	0.85
27:F2:80:ARG:CB	27:F2:83:TYR:CE2	2.60	0.85
2:B1:196:VAL:HG23	2:B1:199:VAL:HG23	1.59	0.84
13:M1:3:ARG:NH1	27:F2:110:ARG:HD3	1.92	0.84
12:L1:44:LYS:HB3	12:L1:45:PRO:HD3	1.59	0.84
22:A2:1049:C:H1'	22:A2:1113:U:O2'	1.77	0.83
6:F1:2:ARG:HD3	6:F1:91:ARG:CZ	2.07	0.83
15:O1:88:ARG:HA	15:O1:88:ARG:NE	1.93	0.83
28:G2:118:PRO:HG2	28:G2:121:ILE:HD13	1.60	0.82
1:A1:1086:U:H2'	1:A1:1086:U:OP2	1.79	0.82
22:A2:2099:U:N3	22:A2:2190:G:O6	2.10	0.81
5:E1:11:LEU:HD12	5:E1:11:LEU:O	1.80	0.81
27:F2:80:ARG:HG2	27:F2:83:TYR:HE2	1.43	0.80
27:F2:136:ILE:HG22	27:F2:136:ILE:O	1.81	0.80
2:B1:196:VAL:HG23	2:B1:199:VAL:CG2	2.12	0.80
22:A2:884:U:H3'	22:A2:885:C:H4'	1.64	0.80
22:A2:894:U:H2'	22:A2:895:U:H6	1.47	0.79
27:F2:135:GLN:O	27:F2:141:ILE:HG21	1.80	0.79
5:E1:154:ALA:CB	5:E1:161:VAL:CG1	2.59	0.79
13:M1:7:ILE:HB	27:F2:112:ARG:HG2	1.64	0.78
22:A2:2099:U:H2'	22:A2:2100:G:H8	1.47	0.78
22:A2:1:G:O6	22:A2:2902:C:N4	2.17	0.78
22:A2:883:G:C2	22:A2:894:U:O2	2.36	0.78
15:O1:89:ARG:HD2	22:A2:714:U:C5	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:F2:104:ILE:O	27:F2:108:VAL:HG11	1.84	0.78
1:A1:79:G:H1	1:A1:90:C:H42	1.32	0.77
22:A2:894:U:H2'	22:A2:895:U:C6	2.19	0.77
27:F2:103:LEU:HA	27:F2:107:ALA:HB2	1.63	0.77
27:F2:111:ILE:O	27:F2:111:ILE:HG13	1.83	0.77
13:M1:71:ARG:HH12	27:F2:115:ARG:HD2	1.50	0.77
22:A2:1:G:N1	22:A2:2902:C:O2	2.18	0.76
11:K1:109:ASN:OD1	21:U1:5:LYS:HG2	1.85	0.76
27:F2:135:GLN:NE2	27:F2:148:ARG:O	2.18	0.76
13:M1:3:ARG:HH21	27:F2:110:ARG:NH2	1.81	0.76
1:A1:1026:G:O6	1:A1:1034:G:N1	2.13	0.76
22:A2:882:G:C6	22:A2:883:G:N7	2.54	0.75
1:A1:71:A:N6	1:A1:99:C:O2	2.20	0.75
7:G1:139:GLU:O	7:G1:143:ARG:HG3	1.86	0.74
26:E2:7:ASP:N	26:E2:7:ASP:OD1	2.19	0.74
16:P1:50:THR:HG21	16:P1:78:VAL:CG2	2.18	0.74
23:B2:31:C:O2	23:B2:53:A:N6	2.20	0.74
27:F2:134:GLU:OE2	27:F2:149:VAL:HG13	1.87	0.74
27:F2:111:ILE:HD11	27:F2:114:PHE:HA	1.69	0.74
1:A1:1026:G:H1	1:A1:1034:G:H22	1.34	0.74
22:A2:142:A:C2	22:A2:143:C:C2	2.75	0.74
12:L1:44:LYS:CB	12:L1:45:PRO:HD2	2.06	0.74
13:M1:3:ARG:HH12	27:F2:110:ARG:CD	2.00	0.74
22:A2:63:A:H2	41:T2:70:HIS:CE1	2.05	0.74
27:F2:134:GLU:CD	27:F2:149:VAL:HG13	2.08	0.73
22:A2:2098:U:O2	22:A2:2191:A:H2	1.69	0.73
22:A2:611:C:C4	22:A2:612:G:C5	2.77	0.73
16:P1:19:VAL:CG2	16:P1:52:LEU:HD21	2.14	0.73
1:A1:261:U:OP2	20:T1:74:ARG:NH2	2.21	0.73
22:A2:2683:C:O2	32:K2:70:ARG:NH2	2.22	0.73
1:A1:865:A:H5'	1:A1:1078:U:O4	1.88	0.72
27:F2:149:VAL:HG12	27:F2:149:VAL:O	1.88	0.72
4:D1:95:GLU:HG3	4:D1:191:LEU:HD21	1.70	0.72
1:A1:8:A:N6	4:D1:202:GLU:O	2.22	0.72
16:P1:38:PHE:CE2	16:P1:51:ARG:HB3	2.24	0.72
22:A2:611:C:N4	22:A2:612:G:C6	2.58	0.72
24:C2:133:ARG:HB3	24:C2:186:ALA:HB1	1.71	0.72
27:F2:102:ARG:O	27:F2:106:ILE:HB	1.90	0.72
13:M1:71:ARG:NH1	27:F2:115:ARG:HD2	2.04	0.72
22:A2:883:G:N2	22:A2:894:U:C2	2.56	0.72
1:A1:673:A:H2'	1:A1:674:G:C8	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F1:14:GLN:OE1	6:F1:83:ALA:CA	2.37	0.71
1:A1:826:C:O2	8:H1:16:ASN:ND2	2.24	0.71
30:I2:113:LYS:O	30:I2:117:MET:N	2.23	0.71
31:J2:6:ALA:H	31:J2:45:THR:HG21	1.55	0.71
1:A1:1086:U:HO2'	1:A1:1087:G:H8	1.34	0.71
22:A2:611:C:C4	22:A2:612:G:C6	2.77	0.71
22:A2:884:U:H4'	22:A2:884:U:OP1	1.91	0.71
22:A2:1307:A:N6	22:A2:1606:C:O2	2.19	0.71
13:M1:7:ILE:HD13	27:F2:113:ASP:H	1.54	0.70
22:A2:1049:C:O2'	22:A2:1114:C:OP1	2.08	0.70
15:O1:36:ILE:O	15:O1:40:GLN:HG2	1.90	0.70
15:O1:47:LYS:O	15:O1:53:ARG:NH2	2.25	0.69
27:F2:80:ARG:HB2	27:F2:83:TYR:CE1	2.27	0.69
27:F2:108:VAL:HG13	27:F2:109:PRO:HD3	0.84	0.69
22:A2:1869:G:H21	22:A2:1872:A:H2	1.38	0.69
22:A2:1478:G:H1	22:A2:1513:U:H3	1.39	0.69
22:A2:2099:U:H2'	22:A2:2100:G:C8	2.27	0.69
19:S1:36:ARG:NH2	19:S1:75:ALA:O	2.25	0.69
22:A2:881:G:H2'	22:A2:882:G:C8	2.27	0.69
1:A1:401:C:O2'	1:A1:621:A:N3	2.26	0.69
8:H1:113:ASP:OD2	8:H1:117:ARG:NH2	2.26	0.69
1:A1:1086:U:O2'	1:A1:1087:G:H8	1.75	0.69
1:A1:1356:G:H2'	1:A1:1357:A:C8	2.28	0.69
15:O1:88:ARG:HA	15:O1:88:ARG:HE	1.56	0.68
1:A1:746:A:H2'	1:A1:747:A:C8	2.29	0.68
2:B1:221:VAL:O	2:B1:225:ARG:HG2	1.93	0.68
1:A1:664:G:H22	1:A1:741:G:H1	1.42	0.68
4:D1:148:LYS:H	4:D1:148:LYS:HD2	1.58	0.68
13:M1:7:ILE:HD13	27:F2:113:ASP:N	2.09	0.68
22:A2:2098:U:O2	22:A2:2191:A:C2	2.47	0.68
24:C2:2:ALA:N	24:C2:20:VAL:O	2.27	0.68
22:A2:1040:A:N1	22:A2:1115:G:N2	2.39	0.68
22:A2:141:G:H3'	22:A2:141:G:N3	2.09	0.68
27:F2:111:ILE:HA	27:F2:137:ILE:CD1	2.23	0.68
5:E1:153:VAL:O	5:E1:157:ARG:HG3	1.93	0.67
13:M1:66:GLU:O	13:M1:67:GLY:C	2.32	0.67
27:F2:103:LEU:O	27:F2:107:ALA:N	2.26	0.67
33:L2:85:VAL:HG11	33:L2:90:VAL:HG12	1.77	0.67
9:I1:123:ARG:NH1	9:I1:124:ARG:O	2.27	0.67
33:L2:56:PRO:HG2	33:L2:59:ARG:HG3	1.76	0.67
1:A1:875:U:O2'	8:H1:15:ARG:NH1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O1:39:LEU:HD22	15:O1:39:LEU:N	2.10	0.67
22:A2:139:U:C6	41:T2:1:MET:SD	2.88	0.67
1:A1:662:U:H2'	1:A1:663:A:C8	2.30	0.67
16:P1:52:LEU:N	16:P1:52:LEU:HD12	2.10	0.67
1:A1:840:C:N3	1:A1:842:U:O2'	2.27	0.66
10:J1:42:LEU:HB2	10:J1:71:LEU:HB3	1.77	0.66
1:A1:278:G:OP2	17:Q1:43:LYS:NZ	2.29	0.66
22:A2:136:G:C6	22:A2:137:U:C5	2.83	0.66
22:A2:894:U:C4	22:A2:895:U:C4	2.83	0.66
22:A2:1039:A:H2	22:A2:1116:G:H22	1.42	0.66
22:A2:611:C:C5	22:A2:612:G:C5	2.83	0.66
23:B2:43:C:O2	27:F2:92:ARG:NH2	2.29	0.66
1:A1:1517:G:N3	22:A2:1919:A:O2'	2.24	0.66
12:L1:68:GLY:O	12:L1:99:ARG:NH1	2.28	0.66
1:A1:310:G:H5''	16:P1:31:ARG:HB2	1.78	0.66
6:F1:14:GLN:CD	6:F1:83:ALA:HB2	2.15	0.66
16:P1:37:GLY:HA3	16:P1:52:LEU:HA	1.78	0.66
22:A2:2127:G:O2'	22:A2:2128:G:O4'	2.13	0.66
6:F1:14:GLN:CD	6:F1:83:ALA:CB	2.61	0.65
13:M1:7:ILE:CG2	27:F2:112:ARG:HA	2.15	0.65
17:Q1:17:MET:HE3	17:Q1:20:SER:OG	1.96	0.65
31:J2:88:THR:OG1	31:J2:90:GLU:OE2	2.14	0.65
1:A1:1031:C:O2'	1:A1:1032:G:OP2	2.15	0.65
22:A2:611:C:C5	22:A2:612:G:C6	2.84	0.65
9:I1:12:ARG:NH2	9:I1:107:ASP:OD2	2.30	0.65
7:G1:68:ASN:O	7:G1:138:ARG:NH1	2.29	0.65
18:R1:41:PRO:HG2	18:R1:44:ILE:HD13	1.77	0.65
4:D1:188:ARG:O	4:D1:188:ARG:NH1	2.30	0.65
27:F2:134:GLU:OE1	27:F2:149:VAL:CG1	2.45	0.64
22:A2:1482:G:H1'	22:A2:1509:A:H61	1.62	0.64
39:R2:51:VAL:O	39:R2:53:PHE:N	2.30	0.64
3:C1:40:ARG:NH1	3:C1:55:ILE:O	2.31	0.64
22:A2:2127:G:O2'	22:A2:2128:G:O5'	2.15	0.64
46:Y2:11:VAL:O	46:Y2:15:ASN:ND2	2.29	0.64
1:A1:1004:A:H5''	1:A1:1024:G:H22	1.61	0.64
30:I2:100:LYS:CB	30:I2:141:GLU:HB2	2.27	0.64
1:A1:674:G:H2'	1:A1:675:A:H8	1.62	0.64
1:A1:1305:G:H21	1:A1:1332:A:H2	1.45	0.64
3:C1:47:LEU:HD21	3:C1:87:LEU:HD11	1.79	0.64
27:F2:150:ARG:HG2	27:F2:150:ARG:NH1	2.10	0.64
22:A2:1871:A:O2'	22:A2:1872:A:N3	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:F2:47:LYS:H	27:F2:47:LYS:HD2	1.62	0.64
1:A1:1005:A:H61	1:A1:1024:G:H1'	1.62	0.64
1:A1:1071:C:H2'	1:A1:1072:G:H8	1.62	0.64
1:A1:1130:A:H2'	1:A1:1131:G:H8	1.62	0.64
5:E1:154:ALA:HB3	5:E1:161:VAL:HG12	1.72	0.64
22:A2:881:G:H3'	22:A2:882:G:C8	2.33	0.64
22:A2:2900:A:O5'	22:A2:2900:A:H8	1.80	0.64
1:A1:82:G:N2	1:A1:89:U:OP1	2.31	0.64
27:F2:104:ILE:O	27:F2:108:VAL:CG1	2.46	0.64
22:A2:1061:U:OP2	30:I2:10:LYS:NZ	2.31	0.63
1:A1:269:C:H2'	1:A1:270:A:H8	1.63	0.63
12:L1:59:ASN:OD1	12:L1:61:PHE:HD1	1.81	0.63
1:A1:946:A:H2'	1:A1:947:G:C8	2.33	0.63
22:A2:882:G:H22	22:A2:895:U:H2'	1.61	0.63
28:G2:47:ASP:O	28:G2:49:THR:N	2.29	0.63
1:A1:1004:A:N6	1:A1:1025:U:H5'	2.13	0.63
1:A1:1494:G:H8	22:A2:1913:A:C2	2.11	0.63
6:F1:1:MET:HG2	6:F1:65:GLU:HG2	1.80	0.63
3:C1:110:GLU:HB2	3:C1:144:LEU:HD12	1.81	0.63
14:N1:10:GLU:HG3	14:N1:63:ARG:HD2	1.81	0.63
22:A2:134:G:C5	22:A2:135:U:C4	2.86	0.63
12:L1:55:VAL:HG21	12:L1:80:ILE:HD11	1.80	0.63
1:A1:923:A:O2'	1:A1:1399:C:OP2	2.16	0.63
1:A1:1494:G:C8	22:A2:1913:A:H2	2.14	0.62
1:A1:1084:G:OP2	1:A1:1085:U:O2'	2.13	0.62
9:I1:58:VAL:HG12	9:I1:59:GLU:HG3	1.81	0.62
22:A2:568:U:H1'	22:A2:2030:6MZ:H9C1	1.81	0.62
22:A2:790:U:O2'	22:A2:791:C:C5	2.53	0.62
32:K2:121:GLU:OE1	37:P2:65:SER:OG	2.17	0.62
22:A2:1:G:O6	22:A2:2902:C:N3	2.32	0.62
5:E1:105:ILE:O	5:E1:112:ARG:NH2	2.33	0.62
22:A2:1248:G:OP1	26:E2:44:ARG:NH2	2.33	0.62
27:F2:136:ILE:HD13	27:F2:143:TYR:HD1	1.64	0.62
37:P2:91:ALA:HB2	37:P2:113:ARG:HA	1.80	0.62
1:A1:1474:U:H4'	22:A2:1701:A:N3	2.15	0.62
8:H1:77:ARG:NH1	8:H1:79:SER:O	2.32	0.62
16:P1:50:THR:CG2	16:P1:78:VAL:CG2	2.77	0.62
5:E1:159:LYS:NZ	5:E1:159:LYS:HB3	2.13	0.62
27:F2:4:LEU:HA	27:F2:7:TYR:HB3	1.81	0.62
1:A1:492:C:H2'	1:A1:493:A:C8	2.35	0.62
1:A1:521:G:H4'	12:L1:70:GLU:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A2:139:U:C5	41:T2:1:MET:CE	2.83	0.62
22:A2:881:G:C6	22:A2:882:G:C6	2.87	0.62
1:A1:202:G:HO2'	1:A1:468:A:H8	1.47	0.61
7:G1:50:LEU:HG	7:G1:50:LEU:O	1.99	0.61
27:F2:103:LEU:CA	27:F2:107:ALA:HB2	2.28	0.61
1:A1:147:G:H2'	1:A1:148:G:C8	2.34	0.61
12:L1:110:ARG:NH1	12:L1:112:GLN:O	2.32	0.61
1:A1:1086:U:O2'	1:A1:1087:G:C8	2.50	0.61
22:A2:1826:G:O2'	22:A2:1971:U:OP2	2.18	0.61
25:D2:33:ARG:NH1	25:D2:53:GLY:O	2.33	0.61
13:M1:7:ILE:HD12	27:F2:112:ARG:CG	2.30	0.61
22:A2:355:U:H2'	22:A2:356:G:H8	1.65	0.61
22:A2:881:G:H3'	22:A2:882:G:H8	1.66	0.61
1:A1:1062:U:H2'	1:A1:1063:C:C6	2.36	0.61
21:U1:4:ILE:HG13	21:U1:19:PHE:HA	1.82	0.61
1:A1:890:G:O2'	1:A1:906:A:N6	2.34	0.61
8:H1:74:SER:OG	8:H1:130:ALA:HB3	2.01	0.61
27:F2:103:LEU:CB	27:F2:107:ALA:HB2	2.31	0.61
41:T2:11:LEU:O	46:Y2:29:ARG:NH1	2.31	0.61
1:A1:1005:A:H2'	1:A1:1006:G:H8	1.65	0.61
1:A1:1059:C:O3'	14:N1:85:ARG:NH2	2.34	0.61
30:I2:100:LYS:HB2	30:I2:141:GLU:HB2	1.81	0.61
13:M1:3:ARG:HH12	27:F2:110:ARG:CG	2.14	0.60
1:A1:50:A:O2'	1:A1:360:G:N2	2.34	0.60
1:A1:411:A:OP1	4:D1:26:ARG:NH2	2.33	0.60
22:A2:84:A:N1	22:A2:98:G:O2'	2.32	0.60
22:A2:144:A:H2'	22:A2:145:C:C6	2.36	0.60
1:A1:626:G:O2'	16:P1:51:ARG:NH1	2.33	0.60
1:A1:714:G:H2'	1:A1:715:A:C8	2.36	0.60
8:H1:11:LEU:HD22	8:H1:75:ILE:HD11	1.83	0.60
13:M1:7:ILE:CD1	27:F2:112:ARG:CB	2.66	0.60
29:H2:132:TYR:N	29:H2:133:GLU:HB2	2.16	0.60
22:A2:1115:G:HO2'	22:A2:1116:G:P	2.24	0.60
22:A2:1115:G:O2'	22:A2:1116:G:O5'	2.16	0.60
39:R2:51:VAL:HG12	39:R2:52:PRO:HD3	1.83	0.60
1:A1:1086:U:OP2	1:A1:1086:U:H6	1.84	0.60
30:I2:110:ALA:O	30:I2:114:ALA:N	2.34	0.60
27:F2:103:LEU:C	27:F2:107:ALA:HB3	2.22	0.60
1:A1:713:G:H2'	1:A1:714:G:C8	2.37	0.60
1:A1:999:C:H2'	1:A1:1000:A:H8	1.66	0.60
1:A1:1323:G:H2'	1:A1:1324:A:C8	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A2:136:G:C5	22:A2:137:U:C5	2.89	0.60
22:A2:1112:G:H2'	22:A2:1113:U:C6	2.37	0.60
1:A1:208:U:H6	1:A1:211:G:H1	1.48	0.60
22:A2:1049:C:HO2'	22:A2:1114:C:P	2.24	0.60
19:S1:16:LEU:O	19:S1:20:GLU:HG3	2.01	0.59
28:G2:35:ARG:HD3	28:G2:71:LEU:HD23	1.82	0.59
22:A2:63:A:C2	41:T2:70:HIS:CE1	2.90	0.59
22:A2:2324:U:H3'	22:A2:2325:G:C5'	2.32	0.59
1:A1:1018:G:N3	1:A1:1018:G:H2'	2.18	0.59
5:E1:161:VAL:HG23	5:E1:161:VAL:O	2.02	0.59
6:F1:86:ARG:NH1	18:R1:64:TYR:O	2.35	0.59
1:A1:269:C:H2'	1:A1:270:A:C8	2.38	0.59
1:A1:1321:U:O2'	19:S1:78:ARG:NH2	2.34	0.59
27:F2:101:GLU:HA	27:F2:104:ILE:HG22	1.83	0.59
47:Z2:41:THR:HG22	47:Z2:43:ALA:H	1.67	0.59
13:M1:3:ARG:CZ	27:F2:110:ARG:HD3	2.33	0.59
28:G2:87:LEU:HB2	28:G2:131:ILE:HG23	1.85	0.59
35:N2:29:VAL:HG21	35:N2:75:ILE:HG23	1.84	0.59
43:V2:4:ILE:HG12	43:V2:50:MET:HE1	1.83	0.59
12:L1:34:CYS:HA	12:L1:55:VAL:HG22	1.83	0.59
18:R1:23:TYR:HE2	18:R1:65:LEU:CD1	2.15	0.59
24:C2:29:PRO:HG2	24:C2:34:LEU:HD11	1.85	0.59
1:A1:1218:C:H2'	1:A1:1219:A:C8	2.38	0.59
22:A2:1049:C:C1'	22:A2:1113:U:O2'	2.48	0.59
27:F2:136:ILE:O	27:F2:136:ILE:CG2	2.48	0.59
17:Q1:17:MET:CE	17:Q1:20:SER:OG	2.50	0.59
1:A1:843:U:OP1	1:A1:846:G:N2	2.36	0.59
22:A2:45:G:H5'	22:A2:46:G:H5'	1.85	0.59
22:A2:894:U:N3	22:A2:895:U:C4	2.70	0.59
28:G2:127:THR:HG23	28:G2:130:GLU:HB2	1.85	0.59
1:A1:1053:G:N7	1:A1:1200:C:H5'	2.18	0.59
22:A2:143:C:O5'	22:A2:143:C:H6	1.86	0.59
22:A2:1869:G:HO2'	22:A2:1871:A:H2	1.49	0.59
27:F2:75:ALA:O	27:F2:78:LYS:N	2.34	0.59
28:G2:127:THR:OG1	28:G2:128:GLN:N	2.35	0.59
1:A1:674:G:H2'	1:A1:675:A:C8	2.38	0.58
5:E1:154:ALA:HB1	5:E1:161:VAL:HG12	1.79	0.58
22:A2:807:U:OP2	33:L2:41:ARG:NH1	2.36	0.58
27:F2:65:PRO:HA	27:F2:89:VAL:HG22	1.85	0.58
1:A1:376:G:H5''	16:P1:5:ARG:HB2	1.84	0.58
1:A1:999:C:H2'	1:A1:1000:A:C8	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A2:134:G:C5	22:A2:135:U:C5	2.92	0.58
1:A1:1494:G:C1'	22:A2:1913:A:N3	2.67	0.58
5:E1:61:GLN:O	5:E1:65:GLU:HG3	2.04	0.58
10:J1:16:ARG:NH2	10:J1:19:ASP:OD2	2.37	0.58
22:A2:884:U:N3	22:A2:893:C:C2	2.68	0.58
27:F2:134:GLU:CD	27:F2:149:VAL:CG1	2.72	0.58
27:F2:141:ILE:HG23	27:F2:141:ILE:O	2.04	0.58
22:A2:1527:G:N1	22:A2:1544:A:OP2	2.32	0.58
1:A1:1077:G:N2	1:A1:1080:A:OP2	2.35	0.58
22:A2:894:U:C2	22:A2:895:U:C5	2.92	0.58
1:A1:71:A:H61	1:A1:99:C:H1'	1.68	0.58
13:M1:66:GLU:O	13:M1:69:LEU:N	2.37	0.58
22:A2:320:A:N3	26:E2:163:ASN:ND2	2.50	0.57
34:M2:20:LEU:HD13	43:V2:81:PRO:HG2	1.86	0.57
4:D1:87:GLY:HA3	4:D1:197:GLU:HG3	1.86	0.57
29:H2:103:ASN:O	29:H2:105:LYS:N	2.37	0.57
1:A1:337:G:H2'	1:A1:338:A:C8	2.39	0.57
22:A2:883:G:N1	22:A2:894:U:N3	2.35	0.57
18:R1:23:TYR:CE2	18:R1:65:LEU:CD1	2.88	0.57
1:A1:1494:G:H8	22:A2:1913:A:H2	1.51	0.57
1:A1:81:A:N6	1:A1:86:G:H1	2.02	0.57
1:A1:842:U:O2'	1:A1:846:G:N1	2.37	0.57
6:F1:22:ILE:O	6:F1:26:THR:HG23	2.04	0.57
6:F1:38:ARG:NH1	6:F1:98:GLU:O	2.37	0.57
28:G2:19:ILE:HG13	28:G2:24:ILE:HD12	1.87	0.57
27:F2:134:GLU:OE2	27:F2:149:VAL:CG1	2.52	0.57
9:I1:57:MET:HG2	9:I1:61:LEU:HD12	1.87	0.57
15:O1:89:ARG:NH1	22:A2:715:A:H5''	2.20	0.57
22:A2:139:U:C5	41:T2:1:MET:HE1	2.40	0.57
1:A1:1314:C:H2'	1:A1:1315:U:C6	2.40	0.57
9:I1:52:LEU:HD21	9:I1:63:LEU:HD11	1.87	0.57
43:V2:58:SER:OG	43:V2:59:GLU:OE1	2.20	0.57
5:E1:11:LEU:HD12	5:E1:11:LEU:C	2.24	0.57
1:A1:384:G:H2'	1:A1:385:C:C6	2.39	0.56
1:A1:1477:U:H2'	1:A1:1478:U:C6	2.40	0.56
9:I1:51:PRO:HD3	9:I1:80:ARG:HG3	1.87	0.56
22:A2:2315:G:H2'	22:A2:2316:G:H8	1.69	0.56
27:F2:35:THR:HG23	27:F2:155:THR:HG23	1.87	0.56
36:O2:99:TYR:OH	36:O2:111:ARG:NH1	2.38	0.56
27:F2:117:LEU:HB2	27:F2:176:PRO:O	2.05	0.56
4:D1:48:LEU:HD21	4:D1:56:ARG:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J1:52:LEU:HD22	10:J1:59:LYS:HA	1.87	0.56
28:G2:42:GLU:HB3	28:G2:55:ARG:HE	1.70	0.56
29:H2:22:ALA:HA	29:H2:86:THR:HA	1.88	0.56
30:I2:100:LYS:HA	30:I2:139:VAL:O	2.05	0.56
1:A1:21:G:H2'	1:A1:22:G:C8	2.40	0.56
1:A1:337:G:H2'	1:A1:338:A:H8	1.70	0.56
1:A1:1151:A:HO2'	1:A1:1152:A:H8	1.51	0.56
15:O1:39:LEU:HD22	15:O1:39:LEU:H	1.70	0.56
22:A2:271:G:O2'	22:A2:272:A:O5'	2.22	0.56
22:A2:2193:G:O5'	22:A2:2193:G:H8	1.88	0.56
24:C2:227:PRO:HA	24:C2:233:GLY:HA2	1.87	0.56
34:M2:77:PRO:HG2	34:M2:80:VAL:HG21	1.88	0.56
1:A1:972:C:O2'	10:J1:57:VAL:HG12	2.06	0.56
14:N1:79:LEU:HB2	14:N1:84:VAL:HG23	1.87	0.56
27:F2:110:ARG:HB3	27:F2:137:ILE:CG2	2.28	0.56
34:M2:75:GLU:HB2	34:M2:90:GLU:HG3	1.86	0.56
1:A1:77:A:H2'	1:A1:78:A:C8	2.40	0.56
1:A1:235:C:H2'	1:A1:236:A:H8	1.71	0.56
1:A1:297:G:N2	1:A1:300:A:OP2	2.34	0.56
24:C2:79:GLU:OE2	24:C2:101:ARG:NE	2.39	0.56
28:G2:155:GLU:OE1	28:G2:160:LYS:N	2.33	0.56
30:I2:19:ASN:HA	30:I2:39:CYS:SG	2.46	0.56
1:A1:1356:G:H2'	1:A1:1357:A:H8	1.71	0.56
26:E2:136:GLN:NE2	26:E2:140:ASP:OD1	2.38	0.56
1:A1:976:G:OP2	1:A1:1358:U:O2'	2.23	0.56
22:A2:1040:A:H61	22:A2:1115:G:H1	1.54	0.56
1:A1:996:A:H2'	1:A1:997:U:H6	1.71	0.56
22:A2:2898:U:O2'	22:A2:2899:A:H5'	2.06	0.55
40:S2:4:ILE:HG12	40:S2:106:VAL:HG22	1.89	0.55
40:S2:83:LYS:HD2	40:S2:95:ARG:HE	1.71	0.55
1:A1:17:U:H2'	1:A1:18:C:C6	2.42	0.55
13:M1:7:ILE:HG13	13:M1:8:ASN:H	1.70	0.55
22:A2:411:G:OP2	22:A2:2406:A:O2'	2.23	0.55
27:F2:111:ILE:HA	27:F2:137:ILE:HD12	1.87	0.55
4:D1:8:LYS:HB3	4:D1:21:LEU:HB3	1.88	0.55
47:Z2:37:GLU:O	47:Z2:38:ARG:NH1	2.39	0.55
6:F1:38:ARG:HB3	6:F1:63:ASN:HB2	1.87	0.55
9:I1:57:MET:HG3	9:I1:60:LYS:HB2	1.89	0.55
13:M1:3:ARG:HH12	27:F2:110:ARG:HG2	1.70	0.55
1:A1:552:U:H2'	1:A1:553:A:H8	1.71	0.55
1:A1:1432:G:H3'	37:P2:106:LYS:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M1:3:ARG:NH2	27:F2:110:ARG:HD3	2.22	0.55
27:F2:126:GLY:O	27:F2:158:THR:OG1	2.23	0.55
34:M2:25:ASP:OD1	34:M2:25:ASP:N	2.38	0.55
1:A1:335:C:O2'	1:A1:1433:A:N3	2.37	0.55
27:F2:104:ILE:HG23	27:F2:105:THR:HG23	1.88	0.55
34:M2:66:ARG:NH1	34:M2:104:GLU:OE1	2.39	0.55
32:K2:110:GLU:HA	32:K2:113:MET:HG2	1.89	0.55
1:A1:447:G:N1	1:A1:486:U:OP2	2.38	0.55
1:A1:579:A:O2'	15:O1:54:ARG:NH1	2.36	0.55
1:A1:1211:U:H1'	1:A1:1213:A:C2	2.42	0.55
1:A1:1412:C:H2'	1:A1:1413:A:C8	2.42	0.55
3:C1:11:ARG:NH2	3:C1:177:THR:O	2.40	0.55
7:G1:102:ARG:O	7:G1:106:GLU:HG2	2.07	0.55
22:A2:597:G:O2'	33:L2:11:GLY:O	2.24	0.55
22:A2:2194:U:O5'	22:A2:2194:U:H6	1.90	0.55
1:A1:460:A:H2'	1:A1:461:A:H8	1.72	0.54
22:A2:134:G:C6	22:A2:135:U:N3	2.76	0.54
22:A2:2314:A:OP1	27:F2:88:LYS:NZ	2.41	0.54
1:A1:81:A:H61	1:A1:86:G:H1	1.55	0.54
1:A1:231:U:H2'	1:A1:232:G:H8	1.73	0.54
1:A1:1060:U:H2'	1:A1:1061:G:H8	1.73	0.54
9:I1:36:GLU:OE2	9:I1:49:ARG:NH2	2.41	0.54
12:L1:49:LEU:O	12:L1:51:LYS:NZ	2.34	0.54
13:M1:66:GLU:C	13:M1:68:ASP:N	2.51	0.54
16:P1:19:VAL:HG21	16:P1:52:LEU:CG	2.36	0.54
22:A2:1266:G:O2'	22:A2:2012:G:O6	2.21	0.54
54:A2:3001:DIO:CAR	54:A2:3001:DIO:CBN	2.86	0.54
1:A1:346:G:OP1	37:P2:39:ARG:NH1	2.39	0.54
15:O1:79:THR:O	15:O1:83:GLU:HG3	2.08	0.54
22:A2:370:G:O2'	22:A2:424:G:OP1	2.20	0.54
1:A1:1513:A:H2'	1:A1:1514:G:C8	2.43	0.54
22:A2:2097:A:N1	22:A2:2192:U:C4	2.76	0.54
1:A1:335:C:H2'	1:A1:336:A:H8	1.73	0.54
1:A1:846:G:H2'	1:A1:847:G:C8	2.42	0.54
7:G1:101:MET:O	7:G1:105:VAL:HG23	2.08	0.54
16:P1:47:GLU:H	16:P1:47:GLU:CD	2.11	0.54
22:A2:894:U:HO2'	22:A2:895:U:P	2.29	0.54
22:A2:2032:G:N2	25:D2:151:THR:OG1	2.40	0.54
26:E2:157:LEU:HG	26:E2:169:VAL:HG11	1.89	0.54
1:A1:1287:A:H2'	1:A1:1288:A:C8	2.43	0.54
22:A2:790:U:O2'	22:A2:791:C:C6	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:E2:118:LEU:HD11	26:E2:188:MET:HG3	1.90	0.54
1:A1:1071:C:H2'	1:A1:1072:G:C8	2.42	0.54
1:A1:1320:C:O2	19:S1:36:ARG:NH1	2.41	0.54
11:K1:109:ASN:OD1	21:U1:5:LYS:HA	2.08	0.54
22:A2:141:G:N3	22:A2:141:G:H5''	2.23	0.54
34:M2:110:GLU:OE2	34:M2:114:ARG:NH2	2.41	0.54
1:A1:1027:C:H2'	1:A1:1028:C:C6	2.43	0.54
9:I1:41:ARG:NE	9:I1:43:THR:OG1	2.38	0.54
22:A2:668:A:H2'	22:A2:670:A:H62	1.73	0.54
31:J2:45:THR:HG22	38:Q2:64:ARG:HH21	1.73	0.54
1:A1:96:U:HO2'	1:A1:97:G:H8	1.56	0.54
1:A1:407:U:H2'	1:A1:408:A:C8	2.43	0.54
12:L1:33:VAL:O	12:L1:55:VAL:HG13	2.07	0.54
22:A2:1494:A:O2'	22:A2:1495:A:OP1	2.26	0.54
22:A2:2646:C:OP2	22:A2:2732:G:O2'	2.25	0.54
1:A1:113:G:H2'	1:A1:114:U:C6	2.43	0.53
13:M1:66:GLU:O	13:M1:68:ASP:CA	2.52	0.53
16:P1:50:THR:HG21	16:P1:78:VAL:HG23	1.90	0.53
26:E2:17:THR:O	26:E2:21:ARG:NH2	2.41	0.53
23:B2:40:U:N3	23:B2:44:G:OP2	2.29	0.53
1:A1:1130:A:H2'	1:A1:1131:G:C8	2.41	0.53
9:I1:114:LYS:NZ	9:I1:115:LYS:O	2.41	0.53
13:M1:6:GLY:O	13:M1:8:ASN:N	2.41	0.53
22:A2:2172:U:H4'	22:A2:2173:A:H5'	1.90	0.53
22:A2:1871:A:O2'	22:A2:1872:A:O5'	2.27	0.53
24:C2:5:LYS:NZ	24:C2:14:ARG:O	2.40	0.53
1:A1:880:C:OP1	12:L1:9:ARG:NH1	2.42	0.53
12:L1:53:CYS:HB3	12:L1:67:ILE:HD11	1.91	0.53
16:P1:6:LEU:HB3	16:P1:17:TYR:HB3	1.89	0.53
42:U2:81:ASP:OD2	42:U2:96:PHE:HB3	2.09	0.53
1:A1:455:G:H2'	1:A1:456:A:C8	2.43	0.53
1:A1:946:A:H2'	1:A1:947:G:H8	1.71	0.53
1:A1:421:U:C2	3:C1:127:ARG:NH2	2.77	0.53
2:B1:187:VAL:CG2	2:B1:199:VAL:HG13	2.39	0.53
1:A1:1355:G:H2'	1:A1:1356:G:C8	2.44	0.53
8:H1:102:ALA:HB3	8:H1:113:ASP:HB3	1.91	0.53
16:P1:4:ILE:HG12	16:P1:21:VAL:HG22	1.91	0.53
1:A1:1038:C:H2'	1:A1:1039:G:H8	1.74	0.53
12:L1:3:THR:HG22	12:L1:5:ASN:H	1.71	0.53
22:A2:882:G:C6	22:A2:883:G:C8	2.97	0.53
22:A2:894:U:C4	22:A2:895:U:O4	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:V2:45:ASP:OD1	43:V2:45:ASP:N	2.42	0.53
22:A2:1007:C:OP1	31:J2:37:ARG:NH2	2.42	0.53
37:P2:63:LYS:HE2	37:P2:65:SER:HB2	1.91	0.53
43:V2:11:GLU:N	43:V2:11:GLU:OE1	2.42	0.53
1:A1:407:U:H2'	1:A1:408:A:H8	1.75	0.52
1:A1:1005:A:N6	1:A1:1024:G:H1'	2.24	0.52
22:A2:1:G:O6	22:A2:2902:C:C4	2.62	0.52
22:A2:881:G:C2'	22:A2:882:G:C8	2.92	0.52
22:A2:142:A:H2'	22:A2:143:C:C6	2.44	0.52
41:T2:89:GLU:CD	41:T2:89:GLU:H	2.13	0.52
1:A1:677:U:H3	1:A1:713:G:H22	1.58	0.52
1:A1:1355:G:H2'	1:A1:1356:G:H8	1.74	0.52
1:A1:1530:G:H2'	1:A1:1531:A:C8	2.45	0.52
15:O1:39:LEU:H	15:O1:39:LEU:CD2	2.22	0.52
22:A2:136:G:O5'	22:A2:136:G:H8	1.91	0.52
22:A2:155:A:H2'	22:A2:156:A:C8	2.45	0.52
22:A2:1141:U:H4'	22:A2:1142:A:O4'	2.10	0.52
22:A2:1105:U:H2'	22:A2:1106:G:H8	1.75	0.52
22:A2:1796:U:H2'	22:A2:1797:G:C8	2.45	0.52
22:A2:2291:U:OP1	22:A2:2380:C:O2'	2.26	0.52
15:O1:89:ARG:HH22	22:A2:715:A:H5''	1.68	0.52
24:C2:107:PRO:HD2	24:C2:110:LEU:HD22	1.91	0.52
28:G2:123:ALA:HB1	28:G2:131:ILE:HD11	1.92	0.52
1:A1:821:G:H2'	1:A1:822:U:C6	2.45	0.52
14:N1:41:ARG:O	14:N1:43:ASN:ND2	2.43	0.52
22:A2:2857:G:N2	22:A2:2860:A:OP2	2.35	0.52
44:W2:65:GLY:HA2	44:W2:85:GLU:HG2	1.92	0.52
1:A1:34:C:H2'	1:A1:35:G:H8	1.74	0.52
1:A1:1239:A:H62	1:A1:1299:A:N6	2.08	0.52
7:G1:113:ASP:OD2	7:G1:122:ASN:ND2	2.35	0.52
22:A2:141:G:N3	22:A2:141:G:C3'	2.73	0.52
22:A2:2788:C:O2'	22:A2:2809:A:N3	2.38	0.52
22:A2:2469:A:H4'	34:M2:55:ARG:CD	2.33	0.52
1:A1:56:U:H2'	1:A1:57:G:C8	2.45	0.52
1:A1:555:U:H2'	1:A1:556:C:C6	2.45	0.52
1:A1:757:U:OP1	1:A1:822:U:O2'	2.28	0.52
1:A1:1507:A:H2'	1:A1:1508:A:C8	2.44	0.52
9:I1:47:VAL:HG13	9:I1:80:ARG:HD3	1.90	0.52
22:A2:881:G:C3'	22:A2:882:G:C8	2.93	0.52
22:A2:882:G:H22	22:A2:895:U:C2'	2.23	0.52
27:F2:34:ILE:HG12	27:F2:96:MET:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:235:C:H2'	1:A1:236:A:C8	2.44	0.51
1:A1:1101:A:OP2	2:B1:95:ARG:NH1	2.43	0.51
22:A2:894:U:O2'	22:A2:895:U:P	2.68	0.51
1:A1:131:A:H2'	1:A1:132:C:C6	2.46	0.51
1:A1:1119:C:H2'	1:A1:1120:C:H6	1.75	0.51
22:A2:143:C:H2'	22:A2:144:A:C8	2.45	0.51
7:G1:79:ARG:HH21	7:G1:84:THR:HA	1.74	0.51
23:B2:51:G:OP1	36:O2:63:LYS:NZ	2.37	0.51
1:A1:41:G:H2'	1:A1:42:G:H8	1.74	0.51
1:A1:410:G:OP2	4:D1:31:LYS:NZ	2.41	0.51
1:A1:460:A:H2'	1:A1:461:A:C8	2.46	0.51
1:A1:1391:U:H2'	1:A1:1392:G:C8	2.46	0.51
4:D1:54:GLN:HB3	4:D1:203:LEU:HB2	1.91	0.51
5:E1:13:GLU:OE1	5:E1:68:ARG:NH1	2.43	0.51
8:H1:29:SER:HB3	8:H1:57:PRO:HB2	1.91	0.51
22:A2:2757:A:N1	28:G2:67:THR:HG21	2.26	0.51
6:F1:55:HIS:O	6:F1:56:LYS:HB2	2.11	0.51
19:S1:29:LYS:HE2	19:S1:29:LYS:H	1.76	0.51
22:A2:894:U:C2	22:A2:895:U:C6	2.98	0.51
1:A1:1213:A:O2'	1:A1:1215:G:N7	2.39	0.51
1:A1:1513:A:H2'	1:A1:1514:G:H8	1.75	0.51
22:A2:463:G:N2	22:A2:466:A:OP2	2.37	0.51
22:A2:2315:G:H2'	22:A2:2316:G:C8	2.44	0.51
1:A1:945:G:C2	1:A1:946:A:C8	2.98	0.51
1:A1:1055:A:O2'	3:C1:161:GLU:O	2.22	0.51
27:F2:108:VAL:CG1	27:F2:109:PRO:CD	2.61	0.51
41:T2:28:ASN:ND2	41:T2:88:LYS:O	2.43	0.51
1:A1:486:U:H2'	1:A1:487:A:H8	1.75	0.51
1:A1:501:C:H2'	1:A1:502:A:H8	1.76	0.51
9:I1:55:VAL:HG21	9:I1:94:LEU:HD13	1.93	0.51
12:L1:79:VAL:O	12:L1:103:ASP:HB2	2.11	0.51
22:A2:612:G:H2'	22:A2:614:A:C8	2.45	0.51
23:B2:66:A:H61	23:B2:107:G:H2'	1.76	0.51
12:L1:110:ARG:HB2	12:L1:119:VAL:HG21	1.93	0.51
16:P1:52:LEU:CD1	16:P1:52:LEU:N	2.73	0.51
22:A2:743:A:O2'	22:A2:1659:G:OP1	2.28	0.51
22:A2:1046:A:H4'	29:H2:58:THR:HG21	1.91	0.51
22:A2:1172:C:C5	22:A2:1173:U:H1'	2.46	0.51
33:L2:91:ASP:OD1	33:L2:93:ASN:N	2.43	0.51
1:A1:390:U:H2'	1:A1:391:G:C8	2.46	0.50
2:B1:187:VAL:HG13	2:B1:191:SER:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:K2:107:LEU:HB2	32:K2:116:ILE:HD11	1.93	0.50
1:A1:1299:A:N3	1:A1:1299:A:H2'	2.25	0.50
22:A2:1059:G:H4'	30:I2:117:MET:HE2	1.93	0.50
22:A2:1796:U:H2'	22:A2:1797:G:H8	1.76	0.50
1:A1:455:G:H2'	1:A1:456:A:H8	1.76	0.50
25:D2:3:GLY:HA3	25:D2:204:LYS:HG2	1.93	0.50
1:A1:837:U:H2'	1:A1:838:G:H8	1.76	0.50
16:P1:44:SER:N	16:P1:47:GLU:OE1	2.28	0.50
22:A2:534:U:O2'	38:Q2:49:ASP:OD2	2.25	0.50
22:A2:1715:G:O2'	22:A2:1743:G:O6	2.20	0.50
22:A2:2469:A:N6	22:A2:2481:G:O2'	2.44	0.50
24:C2:133:ARG:O	24:C2:167:ARG:NH2	2.45	0.50
24:C2:245:VAL:HG12	24:C2:251:GLN:HA	1.94	0.50
3:C1:35:SER:OG	3:C1:59:ARG:NH2	2.40	0.50
1:A1:490:C:H2'	1:A1:491:G:H8	1.77	0.50
22:A2:611:C:N4	22:A2:612:G:N1	2.59	0.50
22:A2:1808:A:H3'	22:A2:1809:A:C8	2.47	0.50
22:A2:2052:A:H4'	25:D2:148:GLN:O	2.11	0.50
25:D2:77:ARG:NH2	25:D2:200:ASP:OD1	2.45	0.50
1:A1:31:G:O2'	1:A1:48:C:N4	2.45	0.50
1:A1:769:G:H4'	1:A1:1513:A:H4'	1.93	0.50
1:A1:1277:C:O2'	1:A1:1279:G:H8	1.94	0.50
13:M1:3:ARG:HH22	27:F2:110:ARG:HD3	1.75	0.50
22:A2:278:A:OP2	22:A2:361:G:N1	2.45	0.50
22:A2:613:A:H4'	22:A2:614:A:H5''	1.94	0.50
22:A2:1506:U:H2'	22:A2:1507:C:C6	2.46	0.50
30:I2:100:LYS:HB3	30:I2:141:GLU:HB2	1.93	0.50
1:A1:56:U:H2'	1:A1:57:G:H8	1.76	0.50
16:P1:51:ARG:O	16:P1:51:ARG:HG2	2.11	0.50
22:A2:611:C:C6	22:A2:612:G:N7	2.79	0.50
22:A2:2848:G:O2'	22:A2:2867:G:N2	2.33	0.50
22:A2:2899:A:H2'	22:A2:2900:A:C8	2.46	0.50
22:A2:1090:A:N1	22:A2:1101:U:O2	2.45	0.50
22:A2:1587:G:H2'	22:A2:1588:G:H8	1.77	0.50
1:A1:41:G:H2'	1:A1:42:G:C8	2.47	0.49
1:A1:501:C:H2'	1:A1:502:A:C8	2.47	0.49
18:R1:21:ILE:HD13	18:R1:55:LEU:HG	1.94	0.49
22:A2:1042:G:N2	22:A2:1114:C:H1'	2.26	0.49
22:A2:2591:C:H2'	22:A2:2592:G:C8	2.48	0.49
1:A1:160:A:H2'	1:A1:161:A:O4'	2.12	0.49
1:A1:562:U:H5''	1:A1:563:A:C5	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:996:A:H2'	1:A1:997:U:C6	2.47	0.49
18:R1:23:TYR:CE2	18:R1:65:LEU:HD11	2.48	0.49
22:A2:2898:U:C2	22:A2:2899:A:N7	2.80	0.49
27:F2:121:SER:OG	27:F2:129:SER:O	2.29	0.49
1:A1:19:A:H5''	5:E1:91:GLY:HA3	1.93	0.49
1:A1:429:U:H5'	4:D1:9:LEU:HD12	1.95	0.49
1:A1:1166:G:N1	1:A1:1169:A:OP2	2.45	0.49
2:B1:68:LEU:HD13	2:B1:154:MET:HE1	1.94	0.49
15:O1:39:LEU:N	15:O1:39:LEU:CD2	2.75	0.49
22:A2:784:G:H5'	22:A2:785:G:OP1	2.12	0.49
29:H2:131:THR:OG1	29:H2:133:GLU:O	2.19	0.49
37:P2:49:ALA:HB3	37:P2:60:THR:HG23	1.92	0.49
1:A1:715:A:H2'	1:A1:716:A:C8	2.48	0.49
2:B1:61:ALA:HB2	2:B1:221:VAL:HG23	1.93	0.49
22:A2:355:U:H2'	22:A2:356:G:C8	2.47	0.49
43:V2:9:ARG:HG2	43:V2:41:GLU:HG3	1.94	0.49
1:A1:1251:A:H2'	1:A1:1252:A:C8	2.47	0.49
4:D1:124:MET:HG3	4:D1:146:ARG:HG2	1.94	0.49
11:K1:23:ILE:HD13	11:K1:96:THR:OG1	2.12	0.49
24:C2:72:ASP:OD2	24:C2:189:ARG:NH1	2.33	0.49
1:A1:182:A:N1	1:A1:223:A:O2'	2.45	0.49
1:A1:1410:A:H2'	1:A1:1411:C:C6	2.47	0.49
5:E1:157:ARG:NH2	8:H1:43:GLU:HB3	2.28	0.49
10:J1:18:ILE:O	10:J1:22:THR:OG1	2.29	0.49
22:A2:136:G:C6	22:A2:137:U:C4	3.01	0.49
22:A2:191:A:H2'	22:A2:192:C:C6	2.47	0.49
22:A2:729:G:C6	24:C2:207:LYS:HB2	2.47	0.49
22:A2:1172:C:C6	22:A2:1173:U:H1'	2.48	0.49
36:O2:15:ARG:NH2	36:O2:95:SER:HB2	2.27	0.49
1:A1:166:U:H2'	1:A1:167:A:H8	1.78	0.49
1:A1:539:A:H2'	1:A1:540:G:C8	2.47	0.49
2:B1:93:ASN:H	2:B1:93:ASN:HD22	1.60	0.49
10:J1:92:LEU:HD12	10:J1:98:VAL:HG21	1.94	0.49
22:A2:1590:A:H2'	22:A2:1591:A:C8	2.48	0.49
27:F2:44:ILE:HG21	27:F2:79:ILE:HG22	1.94	0.49
1:A1:951:G:OP2	13:M1:101:ARG:NH2	2.44	0.49
1:A1:1029:U:H2'	1:A1:1031:C:C2	2.47	0.49
1:A1:1376:U:H2'	1:A1:1377:A:C8	2.47	0.49
12:L1:40:THR:HB	12:L1:90:LEU:HD11	1.93	0.49
22:A2:1113:U:H6	22:A2:1113:U:O5'	1.96	0.49
22:A2:1794:A:H2'	22:A2:1795:C:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A2:2313:C:H5''	27:F2:88:LYS:HD3	1.95	0.49
27:F2:129:SER:HA	27:F2:155:THR:HA	1.94	0.49
1:A1:216:U:H2'	1:A1:217:C:C6	2.48	0.49
1:A1:855:U:OP2	1:A1:871:U:N3	2.38	0.49
3:C1:156:ARG:H	3:C1:163:ALA:HA	1.77	0.49
19:S1:50:ALA:HB1	19:S1:57:HIS:HB3	1.95	0.49
22:A2:1170:C:H2'	22:A2:1171:G:O4'	2.13	0.49
32:K2:40:LYS:HE3	32:K2:57:VAL:HG12	1.94	0.49
1:A1:932:C:OP1	7:G1:4:ARG:HB3	2.12	0.49
1:A1:1038:C:H2'	1:A1:1039:G:C8	2.48	0.49
4:D1:95:GLU:O	4:D1:100:ASN:ND2	2.46	0.49
4:D1:110:THR:H	4:D1:113:GLU:HG2	1.78	0.49
17:Q1:7:THR:OG1	17:Q1:8:LEU:N	2.46	0.49
18:R1:48:ARG:HB2	18:R1:51:TYR:HD2	1.77	0.49
1:A1:1047:G:H5''	14:N1:4:GLN:HG3	1.95	0.48
1:A1:1087:G:N3	1:A1:1087:G:H2'	2.27	0.48
22:A2:134:G:H2'	22:A2:135:U:O4'	2.13	0.48
22:A2:144:A:H2'	22:A2:145:C:H6	1.77	0.48
1:A1:1273:C:H2'	1:A1:1274:A:O4'	2.14	0.48
22:A2:141:G:N3	22:A2:141:G:C5'	2.76	0.48
22:A2:1870:C:O2'	22:A2:1871:A:N3	2.36	0.48
24:C2:232:HIS:HA	24:C2:242:LYS:HD2	1.95	0.48
27:F2:4:LEU:HD13	27:F2:97:TRP:HE3	1.79	0.48
27:F2:108:VAL:N	27:F2:109:PRO:CD	2.77	0.48
33:L2:132:ARG:HG3	33:L2:142:ILE:HD12	1.94	0.48
1:A1:949:A:N7	13:M1:105:ASN:ND2	2.61	0.48
13:M1:16:VAL:HB	13:M1:41:GLU:HG2	1.95	0.48
22:A2:612:G:O5'	22:A2:612:G:H8	1.96	0.48
22:A2:896:A:C8	22:A2:896:A:H3'	2.48	0.48
22:A2:1590:A:H2'	22:A2:1591:A:H8	1.77	0.48
24:C2:123:ALA:O	24:C2:128:ASN:ND2	2.41	0.48
27:F2:75:ALA:C	27:F2:78:LYS:H	2.15	0.48
1:A1:33:A:H2'	1:A1:34:C:C6	2.48	0.48
1:A1:111:G:H1	1:A1:330:C:H41	1.61	0.48
12:L1:33:VAL:CG1	12:L1:77:HIS:HA	2.43	0.48
31:J2:125:TYR:OH	31:J2:132:HIS:NE2	2.45	0.48
43:V2:72:VAL:HG12	43:V2:93:ARG:HA	1.95	0.48
22:A2:2000:C:OP1	35:N2:5:LYS:NZ	2.35	0.48
1:A1:1475:G:H4'	22:A2:1689:A:H4'	1.94	0.48
16:P1:53:ASP:O	16:P1:57:ILE:HG13	2.13	0.48
29:H2:66:GLY:O	29:H2:67:THR:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H1:25:VAL:HG13	8:H1:63:LEU:HD11	1.95	0.48
15:O1:88:ARG:NE	15:O1:88:ARG:CA	2.73	0.48
22:A2:1083:U:H4'	29:H2:42:ARG:NH1	2.28	0.48
30:I2:21:SER:HB3	30:I2:22:PRO:HD3	1.96	0.48
1:A1:335:C:H2'	1:A1:336:A:C8	2.49	0.48
4:D1:19:LEU:HD22	4:D1:64:ILE:HG13	1.95	0.48
22:A2:2514:U:H2'	22:A2:2515:C:C6	2.48	0.48
27:F2:136:ILE:HD11	27:F2:146:VAL:HG21	1.95	0.48
28:G2:101:ASN:ND2	28:G2:116:GLN:OE1	2.47	0.48
1:A1:87:C:H2'	1:A1:88:U:H4'	1.96	0.48
1:A1:358:U:H2'	1:A1:359:G:H8	1.76	0.48
4:D1:61:VAL:HG21	4:D1:200:ILE:HD11	1.96	0.48
7:G1:56:LYS:O	7:G1:60:GLU:HB2	2.14	0.48
14:N1:64:CYS:HB2	14:N1:80:SER:HB3	1.96	0.48
1:A1:356:A:N3	1:A1:368:U:O2'	2.33	0.48
10:J1:35:GLN:HB2	10:J1:78:GLU:OE1	2.14	0.48
27:F2:79:ILE:HD12	27:F2:79:ILE:O	2.14	0.48
1:A1:339:C:H2'	1:A1:340:U:C6	2.49	0.47
1:A1:653:U:HO2'	1:A1:654:G:H8	1.62	0.47
5:E1:90:THR:OG1	5:E1:135:ASN:ND2	2.46	0.47
15:O1:3:LEU:HG	15:O1:35:GLN:HG3	1.95	0.47
1:A1:1314:C:H2'	1:A1:1315:U:H6	1.78	0.47
6:F1:40:GLU:OE1	6:F1:100:SER:OG	2.22	0.47
18:R1:26:ILE:HG22	18:R1:30:LYS:HE3	1.96	0.47
22:A2:546:U:O2'	22:A2:548:G:OP2	2.27	0.47
22:A2:1177:G:H2'	22:A2:1178:C:C6	2.49	0.47
22:A2:2243:U:H2'	22:A2:2244:U:C6	2.49	0.47
45:X2:6:GLN:O	45:X2:74:ARG:NH1	2.47	0.47
6:F1:19:PRO:O	6:F1:23:GLU:HG3	2.15	0.47
22:A2:630:G:N2	22:A2:633:A:OP2	2.33	0.47
26:E2:119:ILE:HB	26:E2:187:VAL:HG22	1.97	0.47
27:F2:108:VAL:N	27:F2:109:PRO:HD2	2.29	0.47
29:H2:68:PRO:HD2	29:H2:69:PHE:CE2	2.49	0.47
43:V2:2:PHE:HB2	43:V2:61:LEU:HD22	1.95	0.47
44:W2:26:PHE:N	44:W2:29:GLU:OE1	2.36	0.47
16:P1:38:PHE:CZ	16:P1:51:ARG:HB3	2.48	0.47
22:A2:1651:G:OP1	35:N2:40:LYS:NZ	2.41	0.47
22:A2:2162:G:H5''	22:A2:2171:A:H2'	1.95	0.47
30:I2:22:PRO:HB2	30:I2:23:PRO:HD3	1.96	0.47
1:A1:500:G:H2'	1:A1:501:C:C6	2.49	0.47
11:K1:83:GLU:HG3	11:K1:109:ASN:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A2:2251:OMG:HM23	22:A2:2251:OMG:H1'	1.70	0.47
41:T2:33:LYS:HG2	41:T2:80:TRP:CZ3	2.49	0.47
3:C1:155:GLY:HA2	3:C1:163:ALA:HB1	1.95	0.47
26:E2:171:ASP:OD1	26:E2:172:ALA:N	2.45	0.47
1:A1:35:G:H2'	1:A1:36:C:C6	2.49	0.47
1:A1:89:U:O2'	1:A1:90:C:H5''	2.15	0.47
1:A1:111:G:H1	1:A1:330:C:N4	2.13	0.47
1:A1:363:A:N6	12:L1:27:CYS:SG	2.88	0.47
1:A1:1005:A:H2'	1:A1:1006:G:C8	2.47	0.47
1:A1:1073:U:O2'	2:B1:105:LYS:HE2	2.15	0.47
6:F1:74:LEU:HD23	6:F1:74:LEU:HA	1.80	0.47
9:I1:9:THR:O	9:I1:85:ARG:HD2	2.15	0.47
13:M1:65:VAL:O	13:M1:66:GLU:CB	2.62	0.47
22:A2:307:G:N1	22:A2:310:A:OP2	2.45	0.47
22:A2:340:A:O2'	26:E2:162:ARG:NH1	2.47	0.47
22:A2:476:G:N1	22:A2:479:A:OP2	2.48	0.47
22:A2:611:C:C5	22:A2:612:G:N7	2.82	0.47
22:A2:896:A:H3'	22:A2:896:A:H8	1.80	0.47
22:A2:1105:U:H2'	22:A2:1106:G:C8	2.49	0.47
22:A2:2576:G:O2'	22:A2:2579:C:OP2	2.25	0.47
24:C2:163:GLN:OE1	24:C2:175:ARG:NH1	2.40	0.47
25:D2:129:THR:HG22	25:D2:130:GLN:O	2.15	0.47
27:F2:68:THR:N	27:F2:86:GLY:O	2.37	0.47
27:F2:103:LEU:O	27:F2:107:ALA:HB3	2.14	0.47
30:I2:20:PRO:HB2	30:I2:23:PRO:HD2	1.97	0.47
30:I2:113:LYS:O	30:I2:117:MET:HG2	2.15	0.47
33:L2:123:ARG:NE	33:L2:143:GLU:OE2	2.46	0.47
45:X2:3:ARG:O	45:X2:12:PRO:HD3	2.15	0.47
1:A1:421:U:O2	3:C1:127:ARG:NH2	2.48	0.47
1:A1:532:A:N6	3:C1:156:ARG:HH12	2.13	0.47
1:A1:859:G:H2'	1:A1:860:A:C8	2.50	0.47
1:A1:1250:A:H2'	1:A1:1251:A:C8	2.50	0.47
5:E1:154:ALA:HB1	5:E1:161:VAL:CG1	2.41	0.47
22:A2:400:G:N7	45:X2:57:ARG:NH1	2.54	0.47
22:A2:881:G:C3'	22:A2:882:G:H8	2.26	0.47
22:A2:2099:U:O2'	22:A2:2100:G:H5'	2.14	0.47
22:A2:2532:G:N2	22:A2:2663:G:O2'	2.48	0.47
1:A1:215:C:H2'	1:A1:216:U:C6	2.50	0.47
1:A1:358:U:H2'	1:A1:359:G:C8	2.49	0.47
1:A1:839:C:H2'	1:A1:840:C:C6	2.50	0.47
1:A1:881:G:P	12:L1:9:ARG:HH22	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M1:3:ARG:HH22	27:F2:110:ARG:CD	2.28	0.47
22:A2:881:G:C5	22:A2:882:G:C6	3.02	0.47
22:A2:2377:A:H2'	22:A2:2378:A:C8	2.50	0.47
28:G2:68:ALA:O	28:G2:72:LEU:HD12	2.15	0.47
28:G2:164:TYR:HB2	28:G2:167:GLU:HG2	1.97	0.47
30:I2:19:ASN:N	30:I2:20:PRO:HD2	2.29	0.47
1:A1:950:U:H2'	1:A1:951:G:C8	2.50	0.47
22:A2:2305:U:H5''	27:F2:131:GLY:HA3	1.97	0.47
1:A1:481:G:O2'	1:A1:483:C:N4	2.47	0.46
1:A1:554:A:H2'	1:A1:555:U:C6	2.50	0.46
1:A1:1085:U:H3'	1:A1:1086:U:C6	2.50	0.46
1:A1:1347:G:N7	9:I1:13:LYS:HE2	2.31	0.46
6:F1:14:GLN:NE2	6:F1:83:ALA:HB2	2.30	0.46
7:G1:150:ALA:HB2	11:K1:61:PHE:HD2	1.80	0.46
20:T1:44:LYS:HG2	20:T1:87:ALA:HB3	1.97	0.46
30:I2:12:GLN:HA	30:I2:56:PRO:HA	1.96	0.46
1:A1:545:C:H5'	4:D1:69:GLU:CB	2.45	0.46
1:A1:1309:G:N7	13:M1:98:ARG:NH2	2.63	0.46
11:K1:64:GLN:HG3	11:K1:99:ALA:HB2	1.97	0.46
22:A2:2720:U:OP1	37:P2:53:ARG:NH2	2.48	0.46
29:H2:29:ASP:OD1	29:H2:30:SER:N	2.48	0.46
1:A1:215:C:H2'	1:A1:216:U:H6	1.81	0.46
1:A1:983:A:H5''	1:A1:984:C:OP2	2.15	0.46
5:E1:30:ILE:HG23	5:E1:54:ARG:NH2	2.30	0.46
5:E1:115:LEU:HD13	5:E1:123:VAL:HG11	1.97	0.46
8:H1:39:VAL:HG21	8:H1:110:VAL:HG12	1.96	0.46
15:O1:89:ARG:HD3	22:A2:716:A:P	2.56	0.46
21:U1:22:SER:HA	21:U1:25:LYS:HG2	1.97	0.46
22:A2:281:C:H2'	22:A2:282:A:C8	2.49	0.46
36:O2:52:SER:OG	36:O2:54:VAL:HG22	2.15	0.46
36:O2:64:TYR:HB3	36:O2:67:ASN:ND2	2.31	0.46
1:A1:360:G:H2'	1:A1:361:G:C8	2.50	0.46
4:D1:129:VAL:HG21	4:D1:146:ARG:NE	2.31	0.46
10:J1:54:SER:OG	10:J1:55:PRO:HD2	2.15	0.46
22:A2:593:U:H2'	22:A2:594:U:C6	2.51	0.46
22:A2:1870:C:O2'	22:A2:1871:A:O5'	2.34	0.46
6:F1:11:HIS:NE2	6:F1:54:LEU:HD11	2.30	0.46
22:A2:882:G:C5	22:A2:883:G:C8	3.03	0.46
25:D2:181:ASP:HB3	25:D2:186:LEU:HB2	1.98	0.46
27:F2:166:GLY:O	27:F2:170:LEU:HD12	2.15	0.46
29:H2:54:VAL:HG22	29:H2:81:LEU:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:J2:58:ASN:HD21	31:J2:128:ASN:ND2	2.13	0.46
43:V2:65:VAL:HG22	43:V2:66:ASP:OD1	2.15	0.46
1:A1:404:G:N7	4:D1:2:ALA:HB3	2.30	0.46
1:A1:459:A:H2'	1:A1:460:A:H8	1.80	0.46
1:A1:751:U:H2'	1:A1:752:G:O4'	2.16	0.46
1:A1:1198:G:N2	10:J1:55:PRO:CG	2.79	0.46
3:C1:142:MET:HG3	3:C1:170:GLU:HG2	1.97	0.46
22:A2:287:G:H2'	22:A2:288:U:C6	2.51	0.46
22:A2:350:G:H2'	22:A2:351:C:O4'	2.15	0.46
22:A2:479:A:N3	22:A2:481:G:H5''	2.30	0.46
22:A2:577:G:O2'	22:A2:1254:A:OP1	2.33	0.46
22:A2:811:U:H2'	33:L2:21:ARG:HA	1.98	0.46
22:A2:1405:U:H2'	22:A2:1406:U:C6	2.50	0.46
22:A2:2314:A:H2'	22:A2:2315:G:H8	1.81	0.46
28:G2:2:SER:O	28:G2:6:LYS:N	2.44	0.46
36:O2:95:SER:O	36:O2:95:SER:OG	2.26	0.46
1:A1:532:A:O2'	1:A1:533:A:OP1	2.29	0.46
22:A2:144:A:O2'	22:A2:145:C:H5'	2.14	0.46
22:A2:1736:U:H2'	22:A2:1737:G:O4'	2.16	0.46
22:A2:2097:A:C2'	22:A2:2098:U:H5'	2.45	0.46
22:A2:2189:U:H2'	22:A2:2190:G:O4'	2.16	0.46
29:H2:85:VAL:HG22	29:H2:92:ALA:HB2	1.98	0.46
1:A1:195:A:N3	1:A1:222:C:O2'	2.43	0.46
1:A1:380:G:N2	1:A1:383:A:OP2	2.35	0.46
1:A1:579:A:H2'	1:A1:580:C:C6	2.51	0.46
1:A1:604:G:H2'	1:A1:605:U:O4'	2.16	0.46
1:A1:1266:G:N2	1:A1:1269:A:OP2	2.35	0.46
22:A2:1183:U:H2'	22:A2:1184:U:C6	2.51	0.46
22:A2:1219:U:H2'	22:A2:1220:G:C8	2.51	0.46
30:I2:35:ILE:CG2	30:I2:36:MET:N	2.79	0.46
1:A1:323:U:H2'	1:A1:324:G:O4'	2.15	0.46
1:A1:592:G:H2'	1:A1:593:U:C6	2.51	0.46
1:A1:712:A:H2'	1:A1:713:G:C8	2.50	0.46
1:A1:908:A:H2'	1:A1:909:A:C8	2.51	0.46
22:A2:1028:A:N3	22:A2:2486:C:O2'	2.43	0.46
22:A2:1874:C:H2'	22:A2:1875:G:O4'	2.16	0.46
22:A2:2291:U:H2'	22:A2:2292:U:C6	2.51	0.46
27:F2:104:ILE:C	27:F2:108:VAL:HG12	2.36	0.46
27:F2:150:ARG:NH1	27:F2:150:ARG:CG	2.74	0.46
1:A1:237:G:H5''	17:Q1:27:ARG:NH2	2.31	0.46
1:A1:946:A:O2'	1:A1:1333:A:N3	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1074:G:O2'	1:A1:1101:A:N1	2.37	0.46
6:F1:9:MET:HE3	6:F1:86:ARG:HG2	1.97	0.46
6:F1:101:PRO:HA	6:F1:104:LYS:HB3	1.98	0.46
22:A2:851:C:H2'	22:A2:852:U:C6	2.51	0.46
22:A2:964:C:O2'	22:A2:2273:A:N3	2.42	0.46
24:C2:252:THR:OG1	24:C2:253:LYS:N	2.49	0.46
44:W2:33:ALA:N	44:W2:64:ASP:OD1	2.48	0.46
1:A1:264:C:O2'	17:Q1:66:PRO:O	2.28	0.45
1:A1:821:G:H2'	1:A1:822:U:H6	1.81	0.45
2:B1:83:ALA:HB2	2:B1:214:LEU:HB3	1.98	0.45
7:G1:78:ARG:HG2	7:G1:80:VAL:HG23	1.98	0.45
22:A2:286:U:H2'	22:A2:287:G:C8	2.51	0.45
22:A2:1563:U:H2'	22:A2:1564:C:C6	2.51	0.45
29:H2:82:ILE:HD12	29:H2:84:TYR:CE2	2.51	0.45
30:I2:86:ILE:HD13	30:I2:138:LEU:HD21	1.97	0.45
32:K2:10:VAL:HG12	32:K2:12:ASP:H	1.80	0.45
36:O2:15:ARG:HH21	36:O2:95:SER:HB2	1.81	0.45
7:G1:150:ALA:HB2	11:K1:61:PHE:CD2	2.50	0.45
12:L1:88:LYS:O	12:L1:90:LEU:N	2.48	0.45
19:S1:4:SER:O	19:S1:5:LEU:O	2.34	0.45
19:S1:6:LYS:HA	19:S1:6:LYS:HD2	1.37	0.45
22:A2:2298:A:H2'	22:A2:2299:U:O4'	2.16	0.45
1:A1:1084:G:H3'	1:A1:1085:U:H2'	1.99	0.45
1:A1:1180:A:OP2	9:I1:99:ARG:NH2	2.37	0.45
1:A1:1291:U:H2'	1:A1:1292:G:H8	1.80	0.45
1:A1:1417:G:O2'	1:A1:1483:A:N6	2.47	0.45
1:A1:1437:A:H2'	1:A1:1438:G:H8	1.80	0.45
2:B1:132:LYS:HE2	2:B1:132:LYS:HB2	1.73	0.45
4:D1:28:ILE:HD12	4:D1:34:ILE:HG13	1.98	0.45
4:D1:156:LYS:HE3	4:D1:156:LYS:HB3	1.63	0.45
6:F1:36:ILE:HG12	6:F1:64:VAL:HG12	1.97	0.45
13:M1:45:ILE:O	13:M1:48:LEU:HB2	2.16	0.45
22:A2:896:A:C8	22:A2:896:A:C3'	2.99	0.45
22:A2:2799:A:O2'	22:A2:2800:A:H5''	2.16	0.45
27:F2:136:ILE:HD13	27:F2:143:TYR:CD1	2.47	0.45
28:G2:86:LYS:HG2	28:G2:132:VAL:HG22	1.98	0.45
1:A1:29:U:O2'	1:A1:30:U:H5'	2.15	0.45
1:A1:554:A:H2'	1:A1:555:U:H6	1.81	0.45
13:M1:7:ILE:O	13:M1:8:ASN:C	2.55	0.45
22:A2:281:C:H2'	22:A2:282:A:H8	1.81	0.45
22:A2:570:G:H2'	22:A2:2030:6MZ:N7	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:D2:1:MET:HB3	25:D2:205:PRO:HG2	1.99	0.45
1:A1:1004:A:H61	1:A1:1025:U:H5'	1.81	0.45
1:A1:1030:U:H4'	1:A1:1031:C:C5	2.51	0.45
1:A1:1297:G:O2'	7:G1:114:LYS:NZ	2.46	0.45
1:A1:1492:A:H2'	1:A1:1492:A:N3	2.32	0.45
22:A2:930:G:H1'	47:Z2:25:LEU:HD21	1.99	0.45
22:A2:1009:A:N3	22:A2:1153:C:O2'	2.48	0.45
22:A2:1040:A:N6	22:A2:1115:G:H1	2.14	0.45
27:F2:40:VAL:HG11	27:F2:43:ALA:HB2	1.99	0.45
40:S2:83:LYS:HD2	40:S2:95:ARG:HH11	1.81	0.45
1:A1:384:G:H2'	1:A1:385:C:H6	1.80	0.45
1:A1:494:G:O2'	1:A1:496:A:H1'	2.16	0.45
11:K1:29:ASN:OD1	11:K1:30:THR:N	2.47	0.45
14:N1:47:LYS:HE2	14:N1:47:LYS:HB2	1.74	0.45
15:O1:89:ARG:NH1	22:A2:715:A:C5'	2.79	0.45
15:O1:89:ARG:CD	22:A2:716:A:OP2	2.65	0.45
22:A2:280:U:H2'	22:A2:281:C:C6	2.52	0.45
22:A2:548:G:H5''	22:A2:549:G:H5'	1.98	0.45
22:A2:1607:C:N4	22:A2:1621:U:OP2	2.50	0.45
42:U2:89:ASP:N	42:U2:89:ASP:OD1	2.49	0.45
1:A1:214:C:C2	1:A1:215:C:C5	3.05	0.45
1:A1:973:G:H4'	10:J1:56:HIS:O	2.16	0.45
1:A1:1316:G:N1	1:A1:1319:A:OP2	2.44	0.45
1:A1:1436:U:O4	1:A1:1437:A:N6	2.50	0.45
13:M1:66:GLU:OE1	13:M1:66:GLU:HA	2.16	0.45
19:S1:19:VAL:O	19:S1:23:VAL:HG13	2.17	0.45
27:F2:43:ALA:HA	27:F2:49:LEU:HD11	1.99	0.45
1:A1:413:G:H1'	1:A1:428:G:H21	1.82	0.45
1:A1:676:A:H2'	1:A1:677:U:H6	1.82	0.45
6:F1:10:VAL:HG21	6:F1:18:VAL:HG22	1.97	0.45
22:A2:172:A:H2'	22:A2:173:A:C8	2.52	0.45
22:A2:639:U:H2'	22:A2:640:C:C6	2.52	0.45
22:A2:2098:U:C2'	22:A2:2099:U:H5'	2.47	0.45
22:A2:2304:G:H22	22:A2:2312:U:H3	1.65	0.45
30:I2:18:ALA:C	30:I2:20:PRO:HD2	2.37	0.45
36:O2:88:LYS:HB2	36:O2:88:LYS:HE2	1.71	0.45
1:A1:22:G:O2'	1:A1:913:A:N1	2.44	0.45
1:A1:618:C:H5'	1:A1:619:U:H5''	1.99	0.45
1:A1:920:U:H2'	1:A1:921:U:C6	2.52	0.45
1:A1:1404:C:H2'	1:A1:1405:G:C8	2.52	0.45
2:B1:122:GLN:O	2:B1:125:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A2:1182:G:H2'	22:A2:1183:U:O4'	2.17	0.45
22:A2:2233:U:H2'	22:A2:2234:G:C8	2.52	0.45
24:C2:16:VAL:HG22	24:C2:206:GLY:HA3	1.99	0.45
41:T2:18:GLU:O	41:T2:22:THR:HG22	2.17	0.45
1:A1:78:A:H2'	1:A1:79:G:O4'	2.17	0.45
22:A2:2788:C:H2'	22:A2:2789:C:C6	2.52	0.45
40:S2:84:ARG:O	40:S2:96:ILE:N	2.44	0.45
1:A1:838:G:H2'	1:A1:839:C:C6	2.52	0.44
1:A1:1160:G:OP1	2:B1:132:LYS:NZ	2.50	0.44
1:A1:1458:G:H5''	20:T1:26:SER:HB2	1.99	0.44
22:A2:1494:A:H2'	22:A2:1495:A:C8	2.52	0.44
22:A2:1868:C:H2'	22:A2:1869:G:O4'	2.16	0.44
22:A2:2537:U:H2'	22:A2:2538:C:C6	2.52	0.44
22:A2:2793:C:H2'	22:A2:2794:C:C6	2.52	0.44
1:A1:166:U:H2'	1:A1:167:A:C8	2.52	0.44
1:A1:1008:U:H2'	1:A1:1009:U:C2	2.52	0.44
19:S1:5:LEU:H	19:S1:5:LEU:HG	1.45	0.44
22:A2:286:U:H2'	22:A2:287:G:H8	1.82	0.44
22:A2:568:U:O4	39:R2:81:LYS:NZ	2.48	0.44
22:A2:2328:A:H2'	22:A2:2329:U:C6	2.52	0.44
23:B2:48:U:H4'	36:O2:100:HIS:HD2	1.82	0.44
24:C2:37:ASN:HB2	24:C2:62:TYR:HB2	1.99	0.44
27:F2:36:LEU:HD22	27:F2:154:ILE:HG12	1.99	0.44
36:O2:59:ALA:HA	36:O2:62:LEU:HD12	1.98	0.44
1:A1:539:A:H2'	1:A1:540:G:H8	1.83	0.44
1:A1:1072:G:H2'	1:A1:1073:U:C6	2.53	0.44
6:F1:14:GLN:OE1	6:F1:83:ALA:HA	2.17	0.44
22:A2:883:G:C4	22:A2:895:U:O2	2.70	0.44
22:A2:1028:A:N6	22:A2:1125:G:H2'	2.33	0.44
24:C2:28:LYS:HA	24:C2:28:LYS:HD2	1.82	0.44
28:G2:28:GLY:HA3	28:G2:79:VAL:HB	2.00	0.44
29:H2:50:VAL:HG22	29:H2:85:VAL:HG13	1.98	0.44
36:O2:33:ARG:O	36:O2:65:THR:HG23	2.18	0.44
1:A1:322:C:H2'	1:A1:323:U:C6	2.52	0.44
18:R1:72:ASP:OD1	18:R1:72:ASP:N	2.50	0.44
22:A2:351:C:H2'	22:A2:352:A:O4'	2.17	0.44
22:A2:543:G:H2'	22:A2:544:C:O4'	2.18	0.44
27:F2:103:LEU:C	27:F2:107:ALA:H	2.20	0.44
29:H2:132:TYR:HB3	29:H2:133:GLU:HG2	1.98	0.44
37:P2:60:THR:HB	37:P2:73:VAL:HG22	1.98	0.44
1:A1:545:C:H5'	4:D1:69:GLU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1026:G:H2'	1:A1:1026:G:N3	2.32	0.44
3:C1:20:SER:OG	3:C1:40:ARG:NH2	2.49	0.44
4:D1:91:LEU:HB3	4:D1:191:LEU:CD1	2.47	0.44
7:G1:58:GLU:O	7:G1:61:ALA:N	2.51	0.44
14:N1:23:LYS:HG3	14:N1:24:ARG:N	2.32	0.44
30:I2:99:GLY:O	30:I2:139:VAL:HG22	2.18	0.44
1:A1:74:A:H2'	1:A1:75:G:O4'	2.17	0.44
1:A1:390:U:H2'	1:A1:391:G:H8	1.81	0.44
1:A1:1480:A:H2'	1:A1:1481:U:O4'	2.18	0.44
7:G1:49:THR:O	7:G1:53:ARG:HG3	2.17	0.44
12:L1:108:LYS:HB2	12:L1:108:LYS:HE2	1.81	0.44
22:A2:134:G:C2	22:A2:135:U:C2	3.05	0.44
22:A2:137:U:O2	22:A2:137:U:H2'	2.18	0.44
22:A2:1113:U:C6	22:A2:1113:U:O5'	2.70	0.44
22:A2:2822:G:O6	35:N2:2:ARG:NH1	2.50	0.44
29:H2:119:PRO:HG2	29:H2:122:GLN:HB2	1.98	0.44
1:A1:1119:C:OP1	9:I1:85:ARG:NH1	2.48	0.44
5:E1:11:LEU:C	5:E1:11:LEU:CD1	2.85	0.44
14:N1:41:ARG:NE	14:N1:41:ARG:HA	2.32	0.44
14:N1:53:ARG:O	14:N1:59:ARG:HD3	2.18	0.44
22:A2:1746:A:H2'	22:A2:1747:U:C6	2.53	0.44
27:F2:30:ARG:HG3	27:F2:30:ARG:HH11	1.83	0.44
41:T2:69:ARG:O	41:T2:69:ARG:HG2	2.18	0.44
1:A1:1446:A:O2'	1:A1:1447:A:H5'	2.18	0.44
13:M1:7:ILE:HG13	13:M1:8:ASN:N	2.33	0.44
22:A2:2161:C:H4'	22:A2:2173:A:P	2.58	0.44
22:A2:2193:G:O5'	22:A2:2193:G:C8	2.71	0.44
22:A2:2845:U:H5''	37:P2:52:ASN:O	2.18	0.44
25:D2:25:THR:HG21	25:D2:193:VAL:HG22	1.99	0.44
29:H2:132:TYR:H	29:H2:133:GLU:HB2	1.82	0.44
35:N2:30:ARG:NH2	35:N2:74:GLU:OE1	2.40	0.44
36:O2:2:ASP:OD1	36:O2:2:ASP:N	2.51	0.44
1:A1:538:G:H2'	1:A1:539:A:H8	1.83	0.44
1:A1:918:A:H2'	1:A1:919:A:C8	2.53	0.44
4:D1:170:TRP:HB3	4:D1:184:ARG:NH1	2.32	0.44
22:A2:796:C:H2'	22:A2:797:G:C8	2.53	0.44
22:A2:871:U:H2'	22:A2:872:U:C6	2.53	0.44
30:I2:80:LEU:CD2	30:I2:101:ILE:HD13	2.48	0.44
39:R2:34:GLU:OE1	39:R2:60:LYS:HG2	2.17	0.44
1:A1:299:G:H2'	1:A1:300:A:C8	2.53	0.43
1:A1:977:A:O2'	1:A1:979:C:OP2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1175:G:H2'	1:A1:1176:A:H8	1.83	0.43
2:B1:35:ARG:O	2:B1:38:VAL:HG22	2.17	0.43
12:L1:59:ASN:OD1	12:L1:61:PHE:CD1	2.67	0.43
37:P2:34:GLU:OE1	37:P2:34:GLU:N	2.50	0.43
1:A1:406:G:H5'	4:D1:5:LEU:HD22	2.00	0.43
1:A1:1236:A:H2'	1:A1:1237:C:C6	2.53	0.43
22:A2:1181:U:H2'	22:A2:1182:G:C8	2.54	0.43
22:A2:2255:G:H2'	22:A2:2256:G:H8	1.83	0.43
24:C2:161:TYR:HB3	24:C2:194:GLU:HB2	1.98	0.43
30:I2:20:PRO:HB2	30:I2:23:PRO:CG	2.47	0.43
35:N2:96:ARG:HD3	35:N2:98:LEU:HD21	2.00	0.43
1:A1:470:C:H2'	1:A1:471:U:C6	2.54	0.43
1:A1:532:A:H61	3:C1:156:ARG:HH12	1.65	0.43
1:A1:677:U:O2	1:A1:777:A:O2'	2.33	0.43
1:A1:985:C:H2'	1:A1:986:U:C6	2.54	0.43
1:A1:1028:C:N4	1:A1:1029:U:O2	2.51	0.43
7:G1:135:VAL:HG13	7:G1:138:ARG:HH12	1.82	0.43
8:H1:114:ARG:HE	8:H1:114:ARG:HB2	1.62	0.43
22:A2:898:C:H2'	22:A2:899:A:O4'	2.18	0.43
22:A2:1847:A:O2'	22:A2:1848:A:H8	1.79	0.43
22:A2:2595:G:N2	22:A2:2598:A:OP2	2.40	0.43
25:D2:39:ASP:OD1	25:D2:39:ASP:N	2.51	0.43
33:L2:90:VAL:HG22	33:L2:122:VAL:HA	1.99	0.43
42:U2:96:PHE:CE2	42:U2:103:ILE:HG12	2.53	0.43
1:A1:559:A:H4'	1:A1:560:A:H3'	2.00	0.43
1:A1:768:A:H4'	1:A1:1523:G:N2	2.32	0.43
4:D1:3:ARG:HE	4:D1:3:ARG:HB3	1.63	0.43
10:J1:54:SER:CB	10:J1:58:ASN:HB2	2.49	0.43
22:A2:672:C:OP2	33:L2:42:SER:OG	2.29	0.43
22:A2:1536:C:H4'	22:A2:1537:G:C4	2.54	0.43
22:A2:2688:G:N1	22:A2:2720:U:OP2	2.32	0.43
1:A1:4:U:HO2'	1:A1:5:U:P	2.40	0.43
1:A1:202:G:O2'	1:A1:468:A:H8	2.02	0.43
1:A1:371:A:H2'	1:A1:372:C:O4'	2.18	0.43
1:A1:763:G:H2'	1:A1:764:C:C6	2.54	0.43
1:A1:1060:U:H5''	10:J1:53:ILE:HD12	2.01	0.43
1:A1:1144:G:N2	1:A1:1146:A:H62	2.17	0.43
3:C1:86:LYS:O	3:C1:90:VAL:HG22	2.18	0.43
22:A2:2329:U:H2'	22:A2:2330:G:C8	2.53	0.43
23:B2:24:G:N7	23:B2:56:G:H2'	2.33	0.43
37:P2:88:ARG:HH21	37:P2:112:GLU:HB2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:156:C:H2'	1:A1:157:U:O4'	2.19	0.43
1:A1:356:A:O2'	1:A1:367:U:O2'	2.26	0.43
1:A1:978:A:C2	1:A1:1319:A:C4	3.06	0.43
1:A1:1226:C:H2'	13:M1:102:THR:HB	1.99	0.43
10:J1:85:ASP:O	10:J1:89:ARG:HD3	2.17	0.43
13:M1:65:VAL:O	13:M1:66:GLU:HB2	2.18	0.43
14:N1:21:PHE:HA	14:N1:25:ALA:HB3	2.01	0.43
22:A2:1939:5MU:OP1	22:A2:2604:PSU:O2'	2.37	0.43
25:D2:97:SER:OG	25:D2:98:VAL:N	2.51	0.43
29:H2:64:VAL:HG13	29:H2:69:PHE:HB2	2.01	0.43
30:I2:18:ALA:O	30:I2:19:ASN:CB	2.67	0.43
40:S2:90:LYS:HB2	40:S2:92:ARG:NH1	2.33	0.43
1:A1:116:A:H61	1:A1:313:A:H1'	1.84	0.43
1:A1:211:G:C6	1:A1:212:G:H1'	2.54	0.43
1:A1:434:U:H2'	1:A1:435:A:C8	2.54	0.43
1:A1:458:U:H2'	1:A1:459:A:H8	1.84	0.43
1:A1:649:A:H2'	1:A1:650:G:O4'	2.18	0.43
1:A1:904:U:H2'	1:A1:905:U:C6	2.53	0.43
1:A1:939:G:H2'	1:A1:940:C:C6	2.54	0.43
4:D1:58:LYS:HD3	4:D1:203:LEU:HD23	2.00	0.43
7:G1:51:ALA:HB2	7:G1:58:GLU:HG3	1.99	0.43
7:G1:113:ASP:HB2	7:G1:119:ARG:HG3	1.99	0.43
8:H1:7:ILE:O	8:H1:11:LEU:HG	2.18	0.43
12:L1:33:VAL:C	12:L1:55:VAL:HG13	2.38	0.43
22:A2:813:U:H2'	22:A2:814:C:C6	2.54	0.43
27:F2:104:ILE:HD11	27:F2:176:PRO:HD3	2.00	0.43
28:G2:155:GLU:OE1	28:G2:159:GLY:N	2.52	0.43
32:K2:71:ARG:HD3	32:K2:71:ARG:HA	1.85	0.43
1:A1:73:C:O2'	1:A1:74:A:H8	2.01	0.43
1:A1:413:G:O5'	1:A1:414:A:H5'	2.18	0.43
1:A1:524:G:H2'	1:A1:525:C:C6	2.54	0.43
1:A1:555:U:H2'	1:A1:556:C:H6	1.82	0.43
1:A1:1007:U:N3	1:A1:1023:U:O2	2.51	0.43
1:A1:1070:U:H2'	1:A1:1071:C:C6	2.53	0.43
1:A1:1352:C:H2'	1:A1:1353:G:C8	2.54	0.43
4:D1:167:LYS:HD3	4:D1:167:LYS:N	2.34	0.43
22:A2:136:G:O5'	22:A2:136:G:C8	2.70	0.43
22:A2:143:C:O5'	22:A2:143:C:C6	2.70	0.43
22:A2:586:A:N1	22:A2:809:G:O2'	2.46	0.43
22:A2:2188:U:H2'	22:A2:2189:U:O4'	2.19	0.43
22:A2:2273:A:H2'	22:A2:2274:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:F2:35:THR:HA	27:F2:90:THR:HA	2.01	0.43
32:K2:24:VAL:HG13	32:K2:33:ALA:HB2	2.01	0.43
40:S2:11:ARG:HD2	40:S2:100:THR:HG22	2.00	0.43
1:A1:303:A:H2'	1:A1:304:U:O4'	2.19	0.43
1:A1:363:A:C6	12:L1:28:PRO:HD2	2.54	0.43
1:A1:461:A:H2'	1:A1:462:G:H8	1.84	0.43
1:A1:593:U:H2'	1:A1:594:U:H6	1.84	0.43
1:A1:600:A:H2'	1:A1:601:G:C8	2.54	0.43
1:A1:1037:C:H2'	1:A1:1038:C:H6	1.82	0.43
1:A1:1228:C:P	13:M1:107:ARG:HH22	2.42	0.43
3:C1:153:VAL:HG12	3:C1:198:VAL:HG22	2.00	0.43
9:I1:25:ASN:HB3	9:I1:62:ASP:OD1	2.19	0.43
22:A2:134:G:O6	22:A2:135:U:O4	2.36	0.43
22:A2:2339:C:H2'	22:A2:2340:A:C8	2.53	0.43
23:B2:1:U:H2'	23:B2:2:G:H8	1.83	0.43
23:B2:48:U:H4'	36:O2:100:HIS:CD2	2.54	0.43
27:F2:54:ALA:HB1	27:F2:65:PRO:HG2	2.01	0.43
36:O2:108:ASP:HA	36:O2:111:ARG:HB2	2.00	0.43
1:A1:216:U:H2'	1:A1:217:C:H6	1.84	0.43
1:A1:859:G:H2'	1:A1:860:A:H8	1.84	0.43
1:A1:1014:A:C2	1:A1:1219:A:H1'	2.53	0.43
5:E1:14:LYS:HE3	5:E1:14:LYS:HB2	1.65	0.43
5:E1:157:ARG:HH21	8:H1:43:GLU:HB3	1.83	0.43
23:B2:42:C:N3	27:F2:90:THR:HG22	2.33	0.43
30:I2:56:PRO:HG2	30:I2:72:LYS:HB2	2.01	0.43
36:O2:115:LEU:HD12	36:O2:115:LEU:HA	1.85	0.43
46:Y2:42:LEU:O	46:Y2:46:VAL:HG12	2.19	0.43
1:A1:593:U:H2'	1:A1:594:U:C6	2.54	0.42
1:A1:1070:U:H2'	1:A1:1071:C:H6	1.85	0.42
3:C1:150:LYS:HG3	3:C1:201:TRP:CE3	2.54	0.42
4:D1:62:ARG:HE	4:D1:62:ARG:HB3	1.67	0.42
13:M1:66:GLU:C	13:M1:68:ASP:H	2.17	0.42
16:P1:18:GLN:OE1	16:P1:35:ARG:NE	2.42	0.42
22:A2:278:A:N1	22:A2:361:G:O2'	2.49	0.42
22:A2:594:U:H2'	22:A2:595:C:C6	2.54	0.42
22:A2:1199:U:H1'	38:Q2:4:VAL:HG22	2.01	0.42
22:A2:1441:G:H2'	22:A2:1442:U:C6	2.54	0.42
22:A2:2193:G:H2'	22:A2:2194:U:C6	2.54	0.42
27:F2:150:ARG:H	27:F2:150:ARG:HG3	1.46	0.42
28:G2:105:LEU:HB2	28:G2:113:VAL:HG13	2.01	0.42
1:A1:427:U:O2'	1:A1:541:G:OP1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:757:U:H2'	1:A1:758:C:O4'	2.19	0.42
1:A1:1034:G:C2	1:A1:1035:A:C8	3.07	0.42
1:A1:1037:C:H2'	1:A1:1038:C:C6	2.53	0.42
1:A1:1179:A:H2'	1:A1:1180:A:O4'	2.19	0.42
22:A2:57:C:H2'	22:A2:58:G:O4'	2.19	0.42
22:A2:708:G:N2	22:A2:724:U:H1'	2.34	0.42
22:A2:2314:A:H2'	22:A2:2315:G:C8	2.53	0.42
22:A2:2808:G:O2'	22:A2:2890:G:O6	2.29	0.42
30:I2:20:PRO:HB2	30:I2:23:PRO:HG2	2.01	0.42
30:I2:86:ILE:CD1	30:I2:138:LEU:HD21	2.49	0.42
30:I2:114:ALA:CB	30:I2:125:MET:SD	3.07	0.42
1:A1:171:A:H2'	1:A1:172:A:C8	2.55	0.42
1:A1:399:G:H2'	1:A1:400:C:C6	2.53	0.42
1:A1:505:G:H2'	1:A1:506:G:C8	2.55	0.42
1:A1:642:A:C8	8:H1:107:SER:HA	2.54	0.42
4:D1:87:GLY:O	4:D1:91:LEU:HD12	2.19	0.42
10:J1:10:LEU:HD23	10:J1:98:VAL:HG22	2.01	0.42
22:A2:544:C:H2'	22:A2:545:U:O4'	2.19	0.42
22:A2:1420:A:C5	22:A2:2211:A:C6	3.07	0.42
22:A2:2333:A:P	44:W2:77:ARG:HH22	2.42	0.42
22:A2:2389:G:H5''	22:A2:2390:U:O4'	2.19	0.42
28:G2:153:ARG:HB2	28:G2:153:ARG:CZ	2.49	0.42
42:U2:14:LEU:HD11	42:U2:71:ALA:HB2	2.01	0.42
45:X2:65:ASP:OD1	45:X2:66:THR:N	2.53	0.42
1:A1:409:U:H2'	1:A1:410:G:O4'	2.18	0.42
1:A1:1005:A:N6	1:A1:1006:G:O6	2.53	0.42
2:B1:101:LEU:HB3	2:B1:179:LEU:HD12	2.02	0.42
13:M1:6:GLY:O	13:M1:7:ILE:C	2.58	0.42
21:U1:41:PRO:HA	21:U1:44:GLU:HG2	2.00	0.42
22:A2:207:A:H2'	22:A2:208:C:O4'	2.18	0.42
22:A2:1172:C:H3'	22:A2:1173:U:C4'	2.49	0.42
22:A2:2728:U:O2'	22:A2:2729:G:H8	2.03	0.42
27:F2:38:MET:HE2	27:F2:87:CYS:SG	2.59	0.42
42:U2:47:LYS:HE2	42:U2:47:LYS:HB3	1.88	0.42
1:A1:254:G:N2	17:Q1:18:GLU:OE2	2.45	0.42
1:A1:911:U:H2'	1:A1:912:C:C6	2.54	0.42
1:A1:1141:C:HO2'	1:A1:1142:G:P	2.42	0.42
1:A1:1169:A:H2'	1:A1:1170:A:C8	2.55	0.42
1:A1:1399:C:O2	1:A1:1502:A:N6	2.53	0.42
4:D1:140:ASN:N	4:D1:182:PHE:O	2.53	0.42
11:K1:31:ILE:HG12	11:K1:46:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M1:3:ARG:HH22	27:F2:110:ARG:NE	2.15	0.42
14:N1:41:ARG:HH21	14:N1:43:ASN:HA	1.85	0.42
22:A2:2698:U:H2'	22:A2:2699:C:C6	2.54	0.42
23:B2:48:U:H2'	23:B2:49:C:C6	2.54	0.42
27:F2:175:PHE:HB3	27:F2:177:PHE:CE1	2.55	0.42
1:A1:36:C:O2'	12:L1:114:ARG:NH2	2.53	0.42
1:A1:236:A:H2'	1:A1:237:G:C8	2.54	0.42
1:A1:602:A:H2'	1:A1:603:U:C6	2.55	0.42
13:M1:86:TYR:O	13:M1:90:ARG:HG2	2.19	0.42
21:U1:14:VAL:HG12	21:U1:17:ARG:HH22	1.85	0.42
22:A2:483:A:O2'	42:U2:57:GLY:N	2.49	0.42
22:A2:721:A:H2'	22:A2:722:A:C8	2.55	0.42
28:G2:72:LEU:HA	28:G2:75:MET:HB2	2.01	0.42
1:A1:212:G:H2'	1:A1:213:G:C8	2.55	0.42
1:A1:1095:U:H2'	1:A1:1096:C:C6	2.55	0.42
1:A1:1464:U:H2'	1:A1:1465:A:H8	1.84	0.42
2:B1:186:ILE:HD13	2:B1:200:ILE:HB	2.01	0.42
3:C1:169:ARG:HE	3:C1:169:ARG:HB3	1.55	0.42
6:F1:2:ARG:HD3	6:F1:91:ARG:NH2	2.33	0.42
33:L2:77:ILE:HD13	33:L2:108:ALA:HB1	2.02	0.42
44:W2:17:GLU:O	44:W2:19:LYS:NZ	2.52	0.42
1:A1:439:U:O4'	4:D1:120:HIS:HA	2.20	0.42
1:A1:580:C:H2'	1:A1:581:G:O4'	2.19	0.42
1:A1:599:C:H2'	1:A1:600:A:H8	1.84	0.42
5:E1:154:ALA:HB3	5:E1:161:VAL:CG1	2.43	0.42
16:P1:44:SER:C	16:P1:46:LYS:H	2.23	0.42
22:A2:139:U:C5	41:T2:1:MET:SD	3.13	0.42
22:A2:612:G:H1'	22:A2:616:A:H61	1.84	0.42
27:F2:121:SER:OG	27:F2:121:SER:O	2.35	0.42
28:G2:155:GLU:H	28:G2:155:GLU:HG3	1.68	0.42
1:A1:109:A:H5'	1:A1:110:C:C5	2.55	0.42
1:A1:600:A:H2'	1:A1:601:G:H8	1.85	0.42
1:A1:672:U:H2'	1:A1:673:A:C8	2.55	0.42
1:A1:824:G:H2'	1:A1:825:A:H8	1.85	0.42
2:B1:104:TRP:HA	2:B1:107:VAL:HG22	2.01	0.42
4:D1:168:PRO:HG2	4:D1:171:LEU:HB2	2.02	0.42
14:N1:27:LEU:O	14:N1:31:ILE:HG12	2.20	0.42
22:A2:2481:G:HO2'	22:A2:2482:A:H8	1.65	0.42
28:G2:38:ASN:HD22	28:G2:64:GLN:CD	2.23	0.42
43:V2:46:LYS:HE3	43:V2:46:LYS:HB2	1.79	0.42
1:A1:592:G:H2'	1:A1:593:U:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:860:A:H2'	1:A1:861:G:O4'	2.20	0.42
7:G1:27:VAL:HG11	7:G1:40:GLU:HG3	2.02	0.42
7:G1:58:GLU:O	7:G1:59:LEU:C	2.58	0.42
9:I1:24:GLY:O	9:I1:25:ASN:HB2	2.20	0.42
21:U1:8:GLU:HG3	21:U1:9:ASN:OD1	2.19	0.42
22:A2:225:C:H2'	22:A2:226:A:O4'	2.20	0.42
22:A2:1930:G:O2'	22:A2:1968:G:O6	2.33	0.42
27:F2:56:ASP:O	27:F2:60:ILE:HG12	2.20	0.42
28:G2:50:LEU:HD23	28:G2:50:LEU:HA	1.87	0.42
31:J2:117:ALA:HA	31:J2:120:ARG:HH21	1.85	0.42
43:V2:63:ILE:HD12	43:V2:72:VAL:HG21	2.01	0.42
1:A1:34:C:H2'	1:A1:35:G:C8	2.55	0.41
1:A1:76:G:C5	1:A1:77:A:C8	3.08	0.41
1:A1:1125:U:C5	10:J1:40:ILE:HG21	2.55	0.41
1:A1:1313:U:H2'	1:A1:1314:C:C6	2.55	0.41
9:I1:39:PHE:O	9:I1:45:ARG:NE	2.45	0.41
28:G2:54:PRO:HG3	28:G2:62:TRP:CE2	2.54	0.41
29:H2:38:MET:O	29:H2:41:LEU:N	2.53	0.41
1:A1:35:G:H2'	1:A1:36:C:H6	1.85	0.41
1:A1:601:G:H2'	1:A1:602:A:C8	2.55	0.41
1:A1:1072:G:N2	2:B1:106:THR:HG21	2.35	0.41
1:A1:1486:G:H2'	1:A1:1487:G:O4'	2.20	0.41
2:B1:112:LYS:HB2	2:B1:112:LYS:HE3	1.60	0.41
3:C1:150:LYS:HB3	3:C1:169:ARG:HG2	2.02	0.41
5:E1:62:LYS:O	5:E1:66:LYS:HG3	2.21	0.41
22:A2:714:U:H1'	22:A2:717:C:H5	1.86	0.41
22:A2:2375:G:N2	22:A2:2378:A:OP2	2.47	0.41
28:G2:10:VAL:HA	28:G2:49:THR:HA	2.02	0.41
1:A1:71:A:N3	1:A1:72:A:C8	2.88	0.41
1:A1:255:G:H2'	1:A1:256:U:C6	2.55	0.41
1:A1:1315:U:H2'	1:A1:1316:G:O4'	2.19	0.41
1:A1:1435:G:H2'	1:A1:1436:U:C6	2.55	0.41
22:A2:364:C:H2'	22:A2:365:U:C6	2.56	0.41
22:A2:2162:G:OP1	22:A2:2171:A:H2'	2.20	0.41
29:H2:51:TYR:OH	29:H2:53:ARG:NH1	2.53	0.41
32:K2:38:ILE:HD11	32:K2:112:PHE:HZ	1.85	0.41
1:A1:1096:C:H2'	1:A1:1097:C:H6	1.86	0.41
1:A1:1463:U:H2'	1:A1:1464:U:C6	2.55	0.41
2:B1:129:LEU:C	2:B1:131:LYS:H	2.23	0.41
4:D1:159:LEU:O	4:D1:163:GLU:HG3	2.21	0.41
22:A2:358:U:H2'	22:A2:359:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A2:1084:A:C6	22:A2:1085:A:C6	3.08	0.41
22:A2:1385:A:O2'	22:A2:1396:U:O2	2.39	0.41
22:A2:1475:G:O2'	22:A2:1514:G:O6	2.34	0.41
22:A2:2129:C:N4	22:A2:2130:U:O4	2.54	0.41
27:F2:8:TYR:HA	27:F2:12:VAL:HG22	2.03	0.41
27:F2:175:PHE:HB3	27:F2:177:PHE:HE1	1.85	0.41
29:H2:52:MET:HE1	29:H2:96:PHE:HZ	1.85	0.41
31:J2:31:GLU:OE2	31:J2:35:ARG:NE	2.51	0.41
1:A1:185:U:H2'	1:A1:186:C:C6	2.56	0.41
1:A1:279:A:H5''	1:A1:281:G:O4'	2.21	0.41
1:A1:1107:C:C4	1:A1:1108:G:C8	3.08	0.41
5:E1:44:GLY:O	5:E1:74:VAL:N	2.43	0.41
9:I1:124:ARG:HG2	9:I1:125:PRO:HD2	2.02	0.41
13:M1:68:ASP:O	13:M1:72:GLU:HG3	2.21	0.41
22:A2:742:A:H2'	22:A2:743:A:C8	2.56	0.41
22:A2:984:A:N3	22:A2:984:A:H2'	2.35	0.41
34:M2:50:ARG:O	34:M2:53:MET:HG2	2.20	0.41
1:A1:1013:G:N2	1:A1:1016:A:OP2	2.39	0.41
1:A1:1025:U:H5''	1:A1:1026:G:O5'	2.20	0.41
11:K1:52:PHE:HD1	11:K1:56:ARG:HB3	1.86	0.41
22:A2:1174:U:H5'	22:A2:1175:A:OP2	2.20	0.41
22:A2:1278:C:H2'	22:A2:1279:G:C8	2.56	0.41
22:A2:1482:G:H1'	22:A2:1509:A:N6	2.32	0.41
22:A2:2321:U:H5'	22:A2:2322:A:OP2	2.21	0.41
36:O2:43:ASN:OD1	36:O2:45:SER:OG	2.29	0.41
36:O2:60:GLU:H	36:O2:60:GLU:HG2	1.72	0.41
1:A1:254:G:H2'	1:A1:255:G:H8	1.85	0.41
1:A1:486:U:H2'	1:A1:487:A:C8	2.55	0.41
12:L1:79:VAL:O	12:L1:79:VAL:HG13	2.20	0.41
22:A2:287:G:H2'	22:A2:288:U:H6	1.85	0.41
22:A2:2098:U:C2	22:A2:2191:A:C2	3.09	0.41
27:F2:67:ILE:HD13	27:F2:87:CYS:HB3	2.02	0.41
27:F2:94:GLU:HA	27:F2:97:TRP:HD1	1.85	0.41
31:J2:110:PRO:O	31:J2:115:GLY:HA3	2.21	0.41
1:A1:187:G:N2	1:A1:190:A:OP2	2.50	0.41
1:A1:320:A:H2'	1:A1:321:A:C8	2.55	0.41
1:A1:398:U:H2'	1:A1:399:G:H8	1.86	0.41
10:J1:57:VAL:HB	10:J1:58:ASN:H	1.59	0.41
11:K1:89:PRO:HB3	21:U1:32:VAL:CG2	2.51	0.41
22:A2:278:A:N6	22:A2:362:A:N7	2.69	0.41
22:A2:322:A:OP2	26:E2:163:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A2:1223:G:C6	22:A2:1227:G:C6	3.08	0.41
22:A2:1799:G:O2'	24:C2:180:GLU:OE2	2.24	0.41
22:A2:2114:A:OP2	22:A2:2115:G:C6	2.73	0.41
28:G2:18:LYS:NZ	28:G2:20:ASN:HB2	2.36	0.41
1:A1:285:C:H2'	1:A1:286:C:C6	2.56	0.41
1:A1:458:U:H2'	1:A1:459:A:C8	2.56	0.41
1:A1:1267:C:O2	1:A1:1327:C:H4'	2.21	0.41
6:F1:47:LEU:HD21	6:F1:57:ALA:HB3	2.03	0.41
14:N1:35:ASN:OD1	14:N1:35:ASN:N	2.53	0.41
14:N1:42:TRP:HD1	14:N1:43:ASN:N	2.19	0.41
22:A2:882:G:C2	22:A2:883:G:C8	3.08	0.41
22:A2:1278:C:H2'	22:A2:1279:G:H8	1.86	0.41
22:A2:1932:A:H2'	22:A2:1933:G:O4'	2.21	0.41
23:B2:78:A:H2'	23:B2:79:G:O4'	2.21	0.41
23:B2:118:C:H2'	23:B2:119:A:C8	2.56	0.41
24:C2:155:ALA:HB2	24:C2:162:VAL:HG23	2.03	0.41
26:E2:2:GLU:HB3	26:E2:11:ALA:HB1	2.03	0.41
26:E2:6:LYS:HE2	26:E2:6:LYS:HA	2.02	0.41
27:F2:32:GLU:N	27:F2:32:GLU:OE2	2.53	0.41
27:F2:42:GLU:H	27:F2:42:GLU:HG3	1.72	0.41
27:F2:103:LEU:HA	27:F2:107:ALA:H	1.85	0.41
28:G2:117:LEU:HD13	28:G2:117:LEU:HA	1.88	0.41
29:H2:103:ASN:C	29:H2:105:LYS:H	2.24	0.41
41:T2:33:LYS:HE2	41:T2:80:TRP:CE3	2.56	0.41
1:A1:6:G:H4'	1:A1:298:A:H4'	2.02	0.41
1:A1:109:A:H5'	1:A1:110:C:H5	1.86	0.41
1:A1:214:C:H2'	1:A1:215:C:H6	1.86	0.41
1:A1:266:G:H3'	17:Q1:69:LYS:HB2	2.03	0.41
1:A1:276:G:H5'	17:Q1:17:MET:SD	2.61	0.41
1:A1:476:U:H2'	1:A1:477:C:C6	2.55	0.41
1:A1:601:G:H2'	1:A1:602:A:H8	1.86	0.41
1:A1:691:G:O2'	1:A1:797:C:H4'	2.21	0.41
1:A1:993:G:O2'	1:A1:994:A:N7	2.54	0.41
1:A1:1494:G:C8	22:A2:1913:A:N3	2.88	0.41
2:B1:166:ALA:HB2	2:B1:185:ALA:HB1	2.03	0.41
4:D1:49:SER:O	4:D1:53:VAL:HG23	2.20	0.41
11:K1:14:LYS:CD	11:K1:14:LYS:H	2.34	0.41
11:K1:26:SER:O	11:K1:90:GLY:HA3	2.20	0.41
22:A2:458:G:O2'	22:A2:469:G:O6	2.32	0.41
22:A2:634:C:H2'	22:A2:635:C:C6	2.56	0.41
22:A2:880:G:C2	22:A2:881:G:H1'	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A2:979:A:H2'	22:A2:982:C:H42	1.85	0.41
22:A2:1394:U:H4'	22:A2:1603:A:H4'	2.03	0.41
22:A2:2484:G:OP1	34:M2:44:ARG:NH2	2.49	0.41
27:F2:103:LEU:O	27:F2:108:VAL:N	2.54	0.41
33:L2:77:ILE:CD1	33:L2:108:ALA:HB1	2.51	0.41
41:T2:26:LYS:HE2	41:T2:26:LYS:HA	2.02	0.41
1:A1:339:C:H2'	1:A1:340:U:H6	1.86	0.40
1:A1:553:A:H5''	12:L1:21:VAL:HG21	2.02	0.40
1:A1:1143:G:H2'	1:A1:1144:G:C8	2.56	0.40
9:I1:34:SER:HB3	9:I1:37:GLN:HG3	2.03	0.40
10:J1:78:GLU:O	10:J1:78:GLU:HG2	2.21	0.40
22:A2:861:A:H2'	22:A2:862:G:O4'	2.20	0.40
22:A2:1357:C:H2'	22:A2:1358:G:O4'	2.20	0.40
22:A2:1871:A:H1'	22:A2:1872:A:H5'	2.02	0.40
22:A2:1881:C:H2'	22:A2:1882:U:O4'	2.21	0.40
22:A2:2116:G:C6	22:A2:2171:A:N6	2.84	0.40
25:D2:99:GLU:H	25:D2:99:GLU:HG3	1.74	0.40
25:D2:157:LYS:HE3	25:D2:157:LYS:HB2	1.85	0.40
32:K2:63:VAL:HG12	32:K2:107:LEU:HD11	2.03	0.40
1:A1:321:A:H2'	1:A1:322:C:C6	2.56	0.40
1:A1:1409:C:H2'	1:A1:1410:A:H8	1.87	0.40
1:A1:1460:C:C2	1:A1:1461:G:C8	3.09	0.40
12:L1:114:ARG:HB3	12:L1:119:VAL:HB	2.03	0.40
22:A2:493:G:H2'	22:A2:494:G:O4'	2.21	0.40
22:A2:1370:C:H2'	22:A2:1371:G:O4'	2.22	0.40
22:A2:1430:G:H2'	22:A2:1431:A:O4'	2.21	0.40
22:A2:1450:G:C6	22:A2:1451:C:N4	2.89	0.40
22:A2:2095:A:C2	22:A2:2195:U:N3	2.89	0.40
25:D2:186:LEU:HD13	37:P2:8:LEU:HD11	2.04	0.40
31:J2:58:ASN:HD21	31:J2:128:ASN:HD22	1.69	0.40
1:A1:246:A:N1	1:A1:278:G:O2'	2.42	0.40
1:A1:459:A:H2'	1:A1:460:A:C8	2.56	0.40
1:A1:471:U:H2'	1:A1:472:U:C6	2.56	0.40
1:A1:553:A:H2'	1:A1:554:A:H8	1.87	0.40
1:A1:838:G:H2'	1:A1:839:C:H6	1.87	0.40
1:A1:916:U:H2'	1:A1:917:G:H8	1.86	0.40
1:A1:1512:U:H2'	1:A1:1513:A:C8	2.56	0.40
3:C1:155:GLY:O	3:C1:196:ILE:HG12	2.21	0.40
7:G1:74:GLU:HG2	7:G1:91:VAL:HG22	2.03	0.40
10:J1:7:ARG:HE	10:J1:7:ARG:HB3	1.66	0.40
11:K1:52:PHE:CE2	11:K1:65:VAL:HG11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M1:55:THR:O	13:M1:59:GLU:HG2	2.21	0.40
22:A2:1414:C:H2'	22:A2:1415:U:O4'	2.21	0.40
27:F2:10:ASP:OD1	27:F2:11:GLU:N	2.54	0.40
1:A1:113:G:H2'	1:A1:114:U:H6	1.85	0.40
1:A1:1121:U:H2'	1:A1:1122:U:C6	2.56	0.40
1:A1:1530:G:H2'	1:A1:1531:A:H8	1.86	0.40
13:M1:65:VAL:O	13:M1:65:VAL:HG23	2.21	0.40
14:N1:9:ARG:O	14:N1:13:ARG:HG3	2.22	0.40
22:A2:1:G:H2'	22:A2:2:G:H8	1.85	0.40
22:A2:882:G:C6	22:A2:883:G:C5	3.10	0.40
22:A2:2194:U:O5'	22:A2:2194:U:C6	2.71	0.40
28:G2:48:ASN:ND2	28:G2:48:ASN:O	2.54	0.40
36:O2:89:ASP:OD1	36:O2:89:ASP:N	2.54	0.40
1:A1:1165:U:H2'	1:A1:1166:G:O4'	2.21	0.40
1:A1:1481:U:H2'	1:A1:1482:G:C8	2.56	0.40
7:G1:78:ARG:CZ	7:G1:80:VAL:HG21	2.52	0.40
22:A2:645:C:H2'	22:A2:647:G:C8	2.57	0.40
22:A2:1132:U:H3'	22:A2:1133:A:H5''	2.04	0.40
28:G2:121:ILE:N	28:G2:121:ILE:HD12	2.35	0.40
42:U2:4:LYS:O	42:U2:94:ARG:NH2	2.50	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B1	222/224 (99%)	209 (94%)	13 (6%)	0	100	100
3	C1	204/206 (99%)	197 (97%)	7 (3%)	0	100	100
4	D1	203/205 (99%)	201 (99%)	2 (1%)	0	100	100
5	E1	153/155 (99%)	147 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F1	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
7	G1	149/151 (99%)	140 (94%)	8 (5%)	1 (1%)	19	31
8	H1	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
9	I1	125/127 (98%)	113 (90%)	12 (10%)	0	100	100
10	J1	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	13	21
11	K1	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
12	L1	118/123 (96%)	112 (95%)	4 (3%)	2 (2%)	7	12
13	M1	112/114 (98%)	105 (94%)	3 (3%)	4 (4%)	3	4
14	N1	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
15	O1	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
16	P1	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
17	Q1	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
18	R1	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
19	S1	77/79 (98%)	75 (97%)	1 (1%)	1 (1%)	10	16
20	T1	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
21	U1	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
24	C2	269/271 (99%)	265 (98%)	4 (2%)	0	100	100
25	D2	206/209 (99%)	201 (98%)	4 (2%)	1 (0%)	25	40
26	E2	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
27	F2	175/177 (99%)	163 (93%)	11 (6%)	1 (1%)	22	35
28	G2	174/176 (99%)	168 (97%)	5 (3%)	1 (1%)	22	35
29	H2	133/135 (98%)	107 (80%)	19 (14%)	7 (5%)	1	2
30	I2	132/134 (98%)	117 (89%)	11 (8%)	4 (3%)	3	5
31	J2	140/142 (99%)	140 (100%)	0	0	100	100
32	K2	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
33	L2	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
34	M2	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
35	N2	123/125 (98%)	117 (95%)	6 (5%)	0	100	100
36	O2	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
37	P2	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
38	Q2	115/117 (98%)	115 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	R2	101/103 (98%)	96 (95%)	4 (4%)	1 (1%)	13	21
40	S2	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
41	T2	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
42	U2	100/102 (98%)	95 (95%)	5 (5%)	0	100	100
43	V2	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
44	W2	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
45	X2	75/77 (97%)	75 (100%)	0	0	100	100
46	Y2	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
47	Z2	56/58 (97%)	56 (100%)	0	0	100	100
48	a2	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
49	b2	49/51 (96%)	49 (100%)	0	0	100	100
50	c2	44/46 (96%)	44 (100%)	0	0	100	100
51	d2	62/64 (97%)	58 (94%)	3 (5%)	1 (2%)	8	13
52	e2	36/38 (95%)	36 (100%)	0	0	100	100
All	All	5630/5733 (98%)	5429 (96%)	176 (3%)	25 (0%)	32	46

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J1	57	VAL
12	L1	44	LYS
13	M1	7	ILE
13	M1	67	GLY
19	S1	5	LEU
29	H2	67	THR
29	H2	104	ALA
29	H2	106	PHE
30	I2	15	ALA
30	I2	19	ASN
12	L1	42	PRO
13	M1	8	ASN
13	M1	66	GLU
25	D2	149	ASN
29	H2	108	VAL
30	I2	25	GLY
29	H2	124	ASP
30	I2	23	PRO

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Mol	Chain	Res	Type
51	d2	32	ILE
7	G1	54	SER
29	H2	130	PRO
28	G2	47	ASP
29	H2	68	PRO
27	F2	110	ARG
39	R2	52	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B1	186/186 (100%)	176 (95%)	10 (5%)	18	32
3	C1	170/170 (100%)	165 (97%)	5 (3%)	37	58
4	D1	172/172 (100%)	167 (97%)	5 (3%)	37	58
5	E1	118/118 (100%)	115 (98%)	3 (2%)	42	64
6	F1	92/92 (100%)	91 (99%)	1 (1%)	70	84
7	G1	124/124 (100%)	110 (89%)	14 (11%)	4	7
8	H1	104/104 (100%)	101 (97%)	3 (3%)	37	58
9	I1	105/105 (100%)	98 (93%)	7 (7%)	13	22
10	J1	87/87 (100%)	79 (91%)	8 (9%)	7	12
11	K1	90/90 (100%)	88 (98%)	2 (2%)	47	68
12	L1	102/102 (100%)	99 (97%)	3 (3%)	37	58
13	M1	92/92 (100%)	84 (91%)	8 (9%)	8	13
14	N1	83/83 (100%)	79 (95%)	4 (5%)	21	36
15	O1	76/76 (100%)	75 (99%)	1 (1%)	65	80
16	P1	65/65 (100%)	64 (98%)	1 (2%)	60	77
17	Q1	74/74 (100%)	71 (96%)	3 (4%)	26	43
18	R1	48/48 (100%)	47 (98%)	1 (2%)	48	70
19	S1	70/70 (100%)	64 (91%)	6 (9%)	8	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	T1	65/65 (100%)	64 (98%)	1 (2%)	60	77
21	U1	48/48 (100%)	46 (96%)	2 (4%)	25	42
24	C2	216/216 (100%)	213 (99%)	3 (1%)	62	79
25	D2	163/163 (100%)	160 (98%)	3 (2%)	54	73
26	E2	165/165 (100%)	158 (96%)	7 (4%)	25	42
27	F2	148/148 (100%)	127 (86%)	21 (14%)	2	4
28	G2	137/137 (100%)	125 (91%)	12 (9%)	8	12
29	H2	103/103 (100%)	100 (97%)	3 (3%)	37	58
30	I2	104/104 (100%)	103 (99%)	1 (1%)	73	85
31	J2	116/116 (100%)	112 (97%)	4 (3%)	32	51
32	K2	104/104 (100%)	102 (98%)	2 (2%)	52	72
33	L2	103/103 (100%)	101 (98%)	2 (2%)	52	72
34	M2	108/108 (100%)	104 (96%)	4 (4%)	29	48
35	N2	102/102 (100%)	101 (99%)	1 (1%)	73	85
36	O2	87/87 (100%)	85 (98%)	2 (2%)	45	67
37	P2	99/99 (100%)	93 (94%)	6 (6%)	15	27
38	Q2	89/89 (100%)	89 (100%)	0	100	100
39	R2	84/84 (100%)	83 (99%)	1 (1%)	67	82
40	S2	93/93 (100%)	91 (98%)	2 (2%)	47	68
41	T2	80/80 (100%)	77 (96%)	3 (4%)	28	47
42	U2	83/83 (100%)	79 (95%)	4 (5%)	21	36
43	V2	78/78 (100%)	76 (97%)	2 (3%)	41	63
44	W2	57/58 (98%)	56 (98%)	1 (2%)	54	73
45	X2	67/67 (100%)	65 (97%)	2 (3%)	36	56
46	Y2	54/54 (100%)	52 (96%)	2 (4%)	29	48
47	Z2	48/48 (100%)	46 (96%)	2 (4%)	25	42
48	a2	47/47 (100%)	46 (98%)	1 (2%)	48	70
49	b2	45/46 (98%)	44 (98%)	1 (2%)	47	68
50	c2	38/38 (100%)	36 (95%)	2 (5%)	19	33
51	d2	51/51 (100%)	47 (92%)	4 (8%)	10	17
52	e2	34/34 (100%)	33 (97%)	1 (3%)	37	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4674/4676 (100%)	4487 (96%)	187 (4%)	29	44

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B1	5	SER
2	B1	23	TRP
2	B1	37	LYS
2	B1	57	LEU
2	B1	90	PHE
2	B1	93	ASN
2	B1	121	SER
2	B1	128	LYS
2	B1	194	ASP
2	B1	197	ASP
3	C1	35	SER
3	C1	107	ARG
3	C1	165	THR
3	C1	169	ARG
3	C1	185	ASN
4	D1	144	SER
4	D1	148	LYS
4	D1	167	LYS
4	D1	194	ASP
4	D1	197	GLU
5	E1	22	SER
5	E1	159	LYS
5	E1	163	GLU
6	F1	33	GLU
7	G1	3	ARG
7	G1	7	ILE
7	G1	10	ARG
7	G1	11	LYS
7	G1	25	LYS
7	G1	30	LEU
7	G1	45	SER
7	G1	52	GLN
7	G1	56	LYS
7	G1	72	THR
7	G1	77	SER
7	G1	84	THR
7	G1	118	LEU

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Mol	Chain	Res	Type
7	G1	136	LYS
8	H1	79	SER
8	H1	89	LYS
8	H1	94	LYS
9	I1	15	SER
9	I1	33	ARG
9	I1	52	LEU
9	I1	57	MET
9	I1	93	SER
9	I1	95	ARG
9	I1	99	ARG
10	J1	16	ARG
10	J1	22	THR
10	J1	35	GLN
10	J1	57	VAL
10	J1	71	LEU
10	J1	75	ASP
10	J1	77	VAL
10	J1	101	SER
11	K1	14	LYS
11	K1	119	ASN
12	L1	43	LYS
12	L1	78	SER
12	L1	103	ASP
13	M1	11	ASP
13	M1	49	SER
13	M1	54	ASP
13	M1	66	GLU
13	M1	68	ASP
13	M1	75	MET
13	M1	107	ARG
13	M1	114	LYS
14	N1	37	SER
14	N1	40	ASP
14	N1	42	TRP
14	N1	100	SER
15	O1	88	ARG
16	P1	1	MET
17	Q1	28	PHE
17	Q1	57	ASP
17	Q1	72	SER
18	R1	42	SER

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Mol	Chain	Res	Type
19	S1	5	LEU
19	S1	6	LYS
19	S1	7	LYS
19	S1	17	LYS
19	S1	29	LYS
19	S1	48	THR
20	T1	24	ARG
21	U1	25	LYS
21	U1	56	HIS
24	C2	10	SER
24	C2	38	SER
24	C2	133	ARG
25	D2	43	ASP
25	D2	95	SER
25	D2	97	SER
26	E2	7	ASP
26	E2	15	SER
26	E2	21	ARG
26	E2	61	ARG
26	E2	75	SER
26	E2	122	GLU
26	E2	155	GLU
27	F2	4	LEU
27	F2	14	LYS
27	F2	19	GLU
27	F2	24	SER
27	F2	33	LYS
27	F2	35	THR
27	F2	42	GLU
27	F2	47	LYS
27	F2	51	ASP
27	F2	74	VAL
27	F2	98	GLU
27	F2	108	VAL
27	F2	110	ARG
27	F2	111	ILE
27	F2	130	MET
27	F2	141	ILE
27	F2	150	ARG
27	F2	155	THR
27	F2	162	SER
27	F2	175	PHE

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Mol	Chain	Res	Type
27	F2	178	ARG
28	G2	2	SER
28	G2	32	GLU
28	G2	34	THR
28	G2	42	GLU
28	G2	84	THR
28	G2	99	LYS
28	G2	127	THR
28	G2	130	GLU
28	G2	131	ILE
28	G2	167	GLU
28	G2	173	GLU
28	G2	176	LYS
29	H2	16	SER
29	H2	71	CYS
29	H2	105	LYS
30	I2	59	ILE
31	J2	5	THR
31	J2	12	LYS
31	J2	90	GLU
31	J2	142	ILE
32	K2	91	SER
32	K2	109	SER
33	L2	84	LYS
33	L2	118	THR
34	M2	53	MET
34	M2	55	ARG
34	M2	58	LYS
34	M2	59	ARG
35	N2	2	ARG
36	O2	24	THR
36	O2	95	SER
37	P2	6	LYS
37	P2	36	SER
37	P2	60	THR
37	P2	76	THR
37	P2	83	SER
37	P2	104	THR
39	R2	71	LYS
40	S2	70	LYS
40	S2	95	ARG
41	T2	1	MET

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Mol	Chain	Res	Type
41	T2	49	LYS
41	T2	93	LEU
42	U2	27	ASN
42	U2	68	SER
42	U2	86	ARG
42	U2	89	ASP
43	V2	34	LYS
43	V2	59	GLU
44	W2	11	ARG
45	X2	42	SER
45	X2	48	THR
46	Y2	34	SER
46	Y2	49	ASP
47	Z2	12	SER
47	Z2	37	GLU
48	a2	11	SER
49	b2	17	THR
50	c2	8	SER
50	c2	25	LYS
51	d2	15	LYS
51	d2	31	HIS
51	d2	32	ILE
51	d2	52	LYS
52	e2	20	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
2	B1	93	ASN
2	B1	146	ASN
2	B1	227	GLN
3	C1	41	GLN
3	C1	100	GLN
3	C1	139	GLN
4	D1	36	GLN
4	D1	164	GLN
5	E1	70	ASN
5	E1	83	HIS
5	E1	135	ASN
5	E1	146	ASN
6	F1	17	GLN
6	F1	63	ASN

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Mol	Chain	Res	Type
6	F1	68	GLN
7	G1	148	ASN
10	J1	56	HIS
10	J1	58	ASN
12	L1	112	GLN
14	N1	43	ASN
14	N1	60	GLN
15	O1	40	GLN
17	Q1	9	GLN
20	T1	13	GLN
24	C2	134	ASN
26	E2	9	GLN
26	E2	90	GLN
28	G2	104	ASN
28	G2	111	HIS
28	G2	115	HIS
31	J2	128	ASN
34	M2	3	GLN
36	O2	100	HIS
37	P2	41	GLN
37	P2	66	ASN
38	Q2	81	ASN
41	T2	70	HIS
42	U2	27	ASN
42	U2	46	GLN
43	V2	87	GLN
46	Y2	58	ASN
50	c2	29	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	1513/1534 (98%)	226 (14%)	6 (0%)
22	A2	2888/2897 (99%)	381 (13%)	15 (0%)
23	B2	119/120 (99%)	7 (5%)	0
53	f2	75/76 (98%)	27 (36%)	0
All	All	4595/4627 (99%)	641 (13%)	21 (0%)

All (641) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	4	U
1	A1	5	U
1	A1	6	G
1	A1	9	G
1	A1	39	G
1	A1	44	A
1	A1	47	C
1	A1	48	C
1	A1	51	A
1	A1	52	C
1	A1	54	C
1	A1	71	A
1	A1	72	A
1	A1	74	A
1	A1	75	G
1	A1	78	A
1	A1	80	A
1	A1	81	A
1	A1	82	G
1	A1	83	C
1	A1	84	U
1	A1	85	U
1	A1	86	G
1	A1	87	C
1	A1	88	U
1	A1	89	U
1	A1	90	C
1	A1	91	U
1	A1	92	U
1	A1	95	C
1	A1	97	G
1	A1	108	G
1	A1	120	A
1	A1	121	U
1	A1	130	A
1	A1	131	A
1	A1	160	A
1	A1	163	C
1	A1	164	G
1	A1	173	U
1	A1	181	A
1	A1	183	C
1	A1	188	C

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Mol	Chain	Res	Type
1	A1	197	A
1	A1	205	A
1	A1	208	U
1	A1	210	C
1	A1	211	G
1	A1	212	G
1	A1	213	G
1	A1	214	C
1	A1	245	U
1	A1	247	G
1	A1	251	G
1	A1	266	G
1	A1	267	C
1	A1	279	A
1	A1	280	C
1	A1	289	G
1	A1	321	A
1	A1	328	C
1	A1	329	A
1	A1	330	C
1	A1	332	G
1	A1	348	G
1	A1	352	C
1	A1	354	G
1	A1	367	U
1	A1	372	C
1	A1	373	A
1	A1	384	G
1	A1	406	G
1	A1	411	A
1	A1	412	A
1	A1	413	G
1	A1	414	A
1	A1	421	U
1	A1	422	C
1	A1	424	G
1	A1	429	U
1	A1	458	U
1	A1	465	A
1	A1	467	U
1	A1	468	A
1	A1	481	G

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Mol	Chain	Res	Type
1	A1	482	A
1	A1	484	G
1	A1	486	U
1	A1	493	A
1	A1	495	A
1	A1	497	G
1	A1	509	A
1	A1	510	A
1	A1	511	C
1	A1	515	G
1	A1	518	C
1	A1	521	G
1	A1	526	C
1	A1	532	A
1	A1	533	A
1	A1	547	A
1	A1	562	U
1	A1	564	C
1	A1	572	A
1	A1	573	A
1	A1	576	C
1	A1	577	G
1	A1	618	C
1	A1	633	G
1	A1	650	G
1	A1	653	U
1	A1	665	A
1	A1	687	A
1	A1	703	G
1	A1	721	G
1	A1	723	U
1	A1	734	G
1	A1	748	G
1	A1	755	G
1	A1	777	A
1	A1	793	U
1	A1	794	A
1	A1	799	G
1	A1	815	A
1	A1	817	C
1	A1	821	G
1	A1	828	U

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Mol	Chain	Res	Type
1	A1	832	G
1	A1	841	C
1	A1	843	U
1	A1	845	A
1	A1	870	U
1	A1	884	U
1	A1	914	A
1	A1	926	G
1	A1	927	G
1	A1	934	C
1	A1	935	A
1	A1	960	U
1	A1	969	A
1	A1	975	A
1	A1	976	G
1	A1	977	A
1	A1	978	A
1	A1	983	A
1	A1	992	U
1	A1	993	G
1	A1	1004	A
1	A1	1008	U
1	A1	1009	U
1	A1	1010	U
1	A1	1024	G
1	A1	1025	U
1	A1	1026	G
1	A1	1027	C
1	A1	1028	C
1	A1	1029	U
1	A1	1030	U
1	A1	1031	C
1	A1	1032	G
1	A1	1033	G
1	A1	1054	C
1	A1	1065	U
1	A1	1084	G
1	A1	1085	U
1	A1	1086	U
1	A1	1088	G
1	A1	1094	G
1	A1	1095	U

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Mol	Chain	Res	Type
1	A1	1101	A
1	A1	1124	G
1	A1	1136	C
1	A1	1137	C
1	A1	1138	G
1	A1	1139	G
1	A1	1140	C
1	A1	1141	C
1	A1	1142	G
1	A1	1151	A
1	A1	1152	A
1	A1	1158	C
1	A1	1159	U
1	A1	1167	A
1	A1	1168	U
1	A1	1184	G
1	A1	1196	A
1	A1	1197	A
1	A1	1200	C
1	A1	1212	U
1	A1	1213	A
1	A1	1225	A
1	A1	1227	A
1	A1	1238	A
1	A1	1239	A
1	A1	1279	G
1	A1	1280	A
1	A1	1285	A
1	A1	1286	U
1	A1	1287	A
1	A1	1302	C
1	A1	1305	G
1	A1	1317	C
1	A1	1320	C
1	A1	1346	A
1	A1	1353	G
1	A1	1363	A
1	A1	1364	U
1	A1	1368	A
1	A1	1370	G
1	A1	1378	C
1	A1	1394	A

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Mol	Chain	Res	Type
1	A1	1419	G
1	A1	1430	A
1	A1	1432	G
1	A1	1441	A
1	A1	1442	G
1	A1	1446	A
1	A1	1487	G
1	A1	1492	A
1	A1	1493	A
1	A1	1497	G
1	A1	1503	A
1	A1	1506	U
1	A1	1529	G
1	A1	1530	G
1	A1	1534	A
22	A2	10	A
22	A2	15	G
22	A2	34	U
22	A2	45	G
22	A2	46	G
22	A2	58	G
22	A2	71	A
22	A2	74	A
22	A2	75	G
22	A2	84	A
22	A2	101	A
22	A2	102	U
22	A2	118	A
22	A2	119	A
22	A2	120	U
22	A2	125	A
22	A2	135	U
22	A2	137	U
22	A2	138	U
22	A2	139	U
22	A2	140	C
22	A2	141	G
22	A2	142	A
22	A2	157	C
22	A2	163	C
22	A2	165	A
22	A2	181	A

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Mol	Chain	Res	Type
22	A2	196	A
22	A2	199	A
22	A2	216	A
22	A2	221	A
22	A2	222	A
22	A2	248	G
22	A2	266	G
22	A2	272	A
22	A2	276	U
22	A2	285	G
22	A2	302	C
22	A2	311	A
22	A2	329	G
22	A2	330	A
22	A2	352	A
22	A2	353	C
22	A2	361	G
22	A2	362	A
22	A2	372	G
22	A2	386	G
22	A2	396	G
22	A2	399	U
22	A2	403	U
22	A2	406	G
22	A2	411	G
22	A2	412	A
22	A2	424	G
22	A2	425	G
22	A2	479	A
22	A2	481	G
22	A2	491	G
22	A2	504	A
22	A2	505	A
22	A2	509	C
22	A2	529	A
22	A2	530	G
22	A2	532	A
22	A2	544	C
22	A2	546	U
22	A2	547	A
22	A2	548	G
22	A2	549	G

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Mol	Chain	Res	Type
22	A2	550	C
22	A2	563	A
22	A2	573	U
22	A2	575	A
22	A2	603	A
22	A2	613	A
22	A2	614	A
22	A2	615	U
22	A2	627	A
22	A2	637	A
22	A2	645	C
22	A2	647	G
22	A2	654	A
22	A2	655	A
22	A2	685	A
22	A2	686	U
22	A2	717	C
22	A2	730	A
22	A2	747	5MU
22	A2	775	G
22	A2	776	G
22	A2	782	A
22	A2	784	G
22	A2	785	G
22	A2	790	U
22	A2	791	C
22	A2	792	A
22	A2	805	G
22	A2	812	C
22	A2	827	U
22	A2	828	U
22	A2	845	A
22	A2	846	U
22	A2	847	U
22	A2	858	G
22	A2	859	G
22	A2	878	A
22	A2	881	G
22	A2	883	G
22	A2	884	U
22	A2	885	C
22	A2	895	U

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Mol	Chain	Res	Type
22	A2	896	A
22	A2	897	C
22	A2	910	A
22	A2	914	G
22	A2	927	A
22	A2	931	U
22	A2	946	C
22	A2	961	C
22	A2	974	G
22	A2	983	A
22	A2	996	A
22	A2	1012	U
22	A2	1013	C
22	A2	1026	G
22	A2	1033	U
22	A2	1040	A
22	A2	1046	A
22	A2	1047	G
22	A2	1070	A
22	A2	1083	U
22	A2	1084	A
22	A2	1088	A
22	A2	1090	A
22	A2	1112	G
22	A2	1114	C
22	A2	1116	G
22	A2	1119	U
22	A2	1132	U
22	A2	1133	A
22	A2	1135	C
22	A2	1141	U
22	A2	1142	A
22	A2	1168	G
22	A2	1171	G
22	A2	1173	U
22	A2	1174	U
22	A2	1175	A
22	A2	1176	U
22	A2	1212	G
22	A2	1236	G
22	A2	1238	G
22	A2	1253	A

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Mol	Chain	Res	Type
22	A2	1256	G
22	A2	1271	G
22	A2	1272	A
22	A2	1300	G
22	A2	1301	A
22	A2	1329	U
22	A2	1345	C
22	A2	1352	U
22	A2	1365	A
22	A2	1379	U
22	A2	1383	A
22	A2	1416	G
22	A2	1417	C
22	A2	1421	G
22	A2	1428	C
22	A2	1434	A
22	A2	1435	G
22	A2	1452	G
22	A2	1459	G
22	A2	1476	U
22	A2	1482	G
22	A2	1490	A
22	A2	1493	C
22	A2	1494	A
22	A2	1495	A
22	A2	1497	U
22	A2	1509	A
22	A2	1510	G
22	A2	1515	A
22	A2	1524	G
22	A2	1529	G
22	A2	1533	C
22	A2	1534	U
22	A2	1535	A
22	A2	1536	C
22	A2	1537	G
22	A2	1566	A
22	A2	1569	A
22	A2	1578	U
22	A2	1583	A
22	A2	1584	U
22	A2	1585	C

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Mol	Chain	Res	Type
22	A2	1607	C
22	A2	1608	A
22	A2	1647	U
22	A2	1648	U
22	A2	1649	G
22	A2	1674	G
22	A2	1715	G
22	A2	1729	U
22	A2	1730	C
22	A2	1738	G
22	A2	1744	A
22	A2	1764	C
22	A2	1773	A
22	A2	1776	G
22	A2	1791	A
22	A2	1800	C
22	A2	1801	A
22	A2	1808	A
22	A2	1811	G
22	A2	1816	C
22	A2	1829	A
22	A2	1870	C
22	A2	1871	A
22	A2	1872	A
22	A2	1873	G
22	A2	1906	G
22	A2	1913	A
22	A2	1914	C
22	A2	1929	G
22	A2	1930	G
22	A2	1936	A
22	A2	1955	U
22	A2	1960	A
22	A2	1967	C
22	A2	1970	A
22	A2	1971	U
22	A2	1972	G
22	A2	1991	U
22	A2	1993	U
22	A2	1997	C
22	A2	2023	C
22	A2	2031	A

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Mol	Chain	Res	Type
22	A2	2033	A
22	A2	2043	C
22	A2	2055	C
22	A2	2056	G
22	A2	2060	A
22	A2	2061	G
22	A2	2062	A
22	A2	2069	G7M
22	A2	2093	G
22	A2	2098	U
22	A2	2099	U
22	A2	2101	A
22	A2	2105	U
22	A2	2108	A
22	A2	2111	U
22	A2	2112	G
22	A2	2113	U
22	A2	2115	G
22	A2	2116	G
22	A2	2117	A
22	A2	2118	U
22	A2	2119	A
22	A2	2123	G
22	A2	2126	A
22	A2	2127	G
22	A2	2128	G
22	A2	2131	U
22	A2	2132	U
22	A2	2133	G
22	A2	2134	A
22	A2	2136	G
22	A2	2137	U
22	A2	2145	C
22	A2	2146	C
22	A2	2147	A
22	A2	2148	G
22	A2	2149	U
22	A2	2159	G
22	A2	2160	C
22	A2	2161	C
22	A2	2162	G
22	A2	2163	A

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Mol	Chain	Res	Type
22	A2	2164	C
22	A2	2165	C
22	A2	2167	U
22	A2	2168	G
22	A2	2169	A
22	A2	2170	A
22	A2	2171	A
22	A2	2172	U
22	A2	2173	A
22	A2	2177	C
22	A2	2178	C
22	A2	2179	C
22	A2	2181	U
22	A2	2185	U
22	A2	2187	U
22	A2	2188	U
22	A2	2190	G
22	A2	2192	U
22	A2	2193	G
22	A2	2194	U
22	A2	2195	U
22	A2	2198	A
22	A2	2204	G
22	A2	2211	A
22	A2	2225	A
22	A2	2238	G
22	A2	2239	G
22	A2	2268	A
22	A2	2279	G
22	A2	2283	C
22	A2	2287	A
22	A2	2288	A
22	A2	2297	A
22	A2	2305	U
22	A2	2308	G
22	A2	2322	A
22	A2	2325	G
22	A2	2327	A
22	A2	2333	A
22	A2	2334	U
22	A2	2336	A
22	A2	2345	G

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Mol	Chain	Res	Type
22	A2	2347	C
22	A2	2350	C
22	A2	2383	G
22	A2	2385	C
22	A2	2402	U
22	A2	2406	A
22	A2	2425	A
22	A2	2435	A
22	A2	2441	U
22	A2	2445	2MG
22	A2	2448	A
22	A2	2476	A
22	A2	2478	A
22	A2	2491	U
22	A2	2502	G
22	A2	2504	PSU
22	A2	2505	G
22	A2	2518	A
22	A2	2525	G
22	A2	2529	G
22	A2	2535	G
22	A2	2547	A
22	A2	2566	A
22	A2	2567	G
22	A2	2585	U
22	A2	2602	A
22	A2	2609	U
22	A2	2613	U
22	A2	2615	U
22	A2	2629	U
22	A2	2663	G
22	A2	2689	U
22	A2	2690	U
22	A2	2714	G
22	A2	2716	C
22	A2	2726	A
22	A2	2732	G
22	A2	2733	A
22	A2	2744	G
22	A2	2748	A
22	A2	2765	A
22	A2	2778	A

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Mol	Chain	Res	Type
22	A2	2798	U
22	A2	2818	U
22	A2	2820	A
22	A2	2821	A
22	A2	2832	U
22	A2	2835	A
22	A2	2849	U
22	A2	2861	U
22	A2	2867	G
22	A2	2873	A
22	A2	2879	A
22	A2	2880	C
22	A2	2884	U
22	A2	2885	G
22	A2	2886	A
22	A2	2891	U
22	A2	2901	C
22	A2	2903	U
23	B2	9	G
23	B2	35	C
23	B2	42	C
23	B2	56	G
23	B2	89	U
23	B2	90	C
23	B2	109	A
53	f2	6	G
53	f2	7	G
53	f2	8	4SU
53	f2	9	G
53	f2	14	A
53	f2	17	C
53	f2	17(A)	U
53	f2	18	G
53	f2	19	G
53	f2	20	U
53	f2	21	A
53	f2	22	G
53	f2	31	G
53	f2	42	G
53	f2	48	C
53	f2	55	PSU
53	f2	56	C

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Mol	Chain	Res	Type
53	f2	57	A
53	f2	58	A
53	f2	59	A
53	f2	63	G
53	f2	65	C
53	f2	66	C
53	f2	67	C
53	f2	68	C
53	f2	70	G
53	f2	76	A

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A1	4	U
1	A1	428	G
1	A1	532	A
1	A1	1024	G
1	A1	1031	C
1	A1	1211	U
22	A2	100	U
22	A2	549	G
22	A2	784	G
22	A2	790	U
22	A2	894	U
22	A2	1046	A
22	A2	1113	U
22	A2	1494	A
22	A2	1535	A
22	A2	2099	U
22	A2	2118	U
22	A2	2127	G
22	A2	2130	U
22	A2	2158	A
22	A2	2193	G

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

30 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
22	5MC	A2	1962	22	18,22,23	2.01	6 (33%)	26,32,35	1.16	2 (7%)
22	PSU	A2	2605	22	18,21,22	2.39	8 (44%)	22,30,33	1.87	4 (18%)
34	4D4	M2	81	34	9,11,12	2.03	2 (22%)	8,13,15	2.10	4 (50%)
25	MEQ	D2	150[A]	25	8,9,10	0.95	0	5,10,12	0.66	0
22	2MG	A2	1835	22	18,26,27	3.37	7 (38%)	16,38,41	1.35	3 (18%)
53	PSU	f2	55	53	18,21,22	2.37	5 (27%)	22,30,33	3.19	12 (54%)
53	5MU	f2	54	53	19,22,23	2.68	6 (31%)	28,32,35	3.28	14 (50%)
22	PSU	A2	2604	22	18,21,22	2.40	8 (44%)	22,30,33	1.87	4 (18%)
22	2MG	A2	2445	22	18,26,27	3.39	7 (38%)	16,38,41	1.30	3 (18%)
22	PSU	A2	2504	22	18,21,22	2.39	8 (44%)	22,30,33	1.89	4 (18%)
22	G7M	A2	2069	22	20,26,27	2.24	5 (25%)	17,39,42	0.71	0
53	5MC	f2	32	53	18,22,23	0.97	2 (11%)	26,32,35	1.29	3 (11%)
22	PSU	A2	1911	22	18,21,22	2.32	8 (44%)	22,30,33	1.84	4 (18%)
22	OMG	A2	2251	53,22	18,26,27	2.46	5 (27%)	19,38,41	1.15	3 (15%)
22	OMC	A2	2498	22	19,22,23	1.90	6 (31%)	26,31,34	0.96	1 (3%)
22	PSU	A2	2580	22	18,21,22	2.47	10 (55%)	22,30,33	1.90	5 (22%)
22	6MZ	A2	1618	22	18,25,26	1.98	1 (5%)	16,36,39	2.19	4 (25%)
22	3TD	A2	1915	22	18,22,23	2.73	7 (38%)	22,32,35	1.89	2 (9%)
22	PSU	A2	746	22	18,21,22	2.37	9 (50%)	22,30,33	1.80	4 (18%)
22	2MA	A2	2503	22	19,25,26	1.20	1 (5%)	21,37,40	1.85	3 (14%)
53	4SU	f2	8	53	18,21,22	5.37	13 (72%)	26,30,33	5.68	15 (57%)
22	OMU	A2	2552	22	19,22,23	2.68	7 (36%)	26,31,34	1.86	6 (23%)
22	H2U	A2	2449	22	18,21,22	4.07	5 (27%)	21,30,33	5.20	7 (33%)
22	PSU	A2	955	22	18,21,22	2.44	8 (44%)	22,30,33	1.85	4 (18%)
22	5MU	A2	1939	22	19,22,23	2.67	7 (36%)	28,32,35	3.95	10 (35%)
22	1MG	A2	745	22	18,26,27	2.80	4 (22%)	19,39,42	1.28	3 (15%)
22	5MU	A2	747	22	19,22,23	2.58	7 (36%)	28,32,35	3.81	11 (39%)
22	PSU	A2	2457	22	18,21,22	2.46	8 (44%)	22,30,33	1.90	4 (18%)
22	PSU	A2	1917	22	18,21,22	2.32	8 (44%)	22,30,33	1.82	4 (18%)
22	6MZ	A2	2030	22	18,25,26	1.98	1 (5%)	16,36,39	2.59	4 (25%)



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
22	5MC	A2	1962	22	-	2/7/25/26	0/2/2/2
22	PSU	A2	2605	22	-	0/7/25/26	0/2/2/2
34	4D4	M2	81	34	-	3/11/12/14	-
25	MEQ	D2	150[A]	25	-	4/8/9/11	-
22	2MG	A2	1835	22	-	0/5/27/28	0/3/3/3
53	PSU	f2	55	53	-	5/7/25/26	0/2/2/2
53	5MU	f2	54	53	-	0/7/25/26	0/2/2/2
22	PSU	A2	2604	22	-	0/7/25/26	0/2/2/2
22	2MG	A2	2445	22	-	2/5/27/28	0/3/3/3
22	PSU	A2	2504	22	-	2/7/25/26	0/2/2/2
22	G7M	A2	2069	22	-	1/3/25/26	0/3/3/3
53	5MC	f2	32	53	-	0/7/25/26	0/2/2/2
22	PSU	A2	1911	22	-	0/7/25/26	0/2/2/2
22	OMG	A2	2251	53,22	-	1/5/27/28	0/3/3/3
22	OMC	A2	2498	22	-	0/9/27/28	0/2/2/2
22	PSU	A2	2580	22	-	0/7/25/26	0/2/2/2
22	6MZ	A2	1618	22	-	0/5/27/28	0/3/3/3
22	3TD	A2	1915	22	-	0/7/25/26	0/2/2/2
22	PSU	A2	746	22	-	2/7/25/26	0/2/2/2
22	2MA	A2	2503	22	-	1/3/25/26	0/3/3/3
53	4SU	f2	8	53	-	0/7/25/26	0/2/2/2
22	OMU	A2	2552	22	-	0/9/27/28	0/2/2/2
22	H2U	A2	2449	22	-	0/7/38/39	0/2/2/2
22	PSU	A2	955	22	-	0/7/25/26	0/2/2/2
22	5MU	A2	1939	22	-	0/7/25/26	0/2/2/2
22	1MG	A2	745	22	-	0/3/25/26	0/3/3/3
22	5MU	A2	747	22	-	0/7/25/26	0/2/2/2
22	PSU	A2	2457	22	-	0/7/25/26	0/2/2/2
22	PSU	A2	1917	22	-	0/7/25/26	0/2/2/2
22	6MZ	A2	2030	22	-	2/5/27/28	0/3/3/3

All (179) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	f2	8	4SU	C4-S4	-14.35	1.41	1.68
53	f2	8	4SU	C4-N3	-10.75	1.26	1.37
22	A2	2449	H2U	O4-C4	10.10	1.43	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A2	1835	2MG	O6-C6	9.24	1.42	1.23
22	A2	2445	2MG	O6-C6	9.16	1.41	1.23
22	A2	745	1MG	O6-C6	9.03	1.40	1.22
22	A2	1915	3TD	O4-C4	8.17	1.40	1.23
22	A2	2449	H2U	C2-N1	8.08	1.47	1.35
22	A2	2449	H2U	O2-C2	8.07	1.37	1.23
22	A2	2552	OMU	O4-C4	7.89	1.39	1.24
22	A2	1618	6MZ	C6-N6	7.88	1.47	1.35
22	A2	2030	6MZ	C6-N6	7.75	1.47	1.35
53	f2	8	4SU	C5-C4	-7.67	1.32	1.42
22	A2	1939	5MU	C2-N1	-6.47	1.28	1.38
53	f2	8	4SU	C2-N3	-6.46	1.26	1.38
22	A2	2251	OMG	O6-C6	6.41	1.36	1.23
22	A2	2069	G7M	O6-C6	6.32	1.36	1.23
22	A2	2449	H2U	C2-N3	6.14	1.48	1.38
22	A2	747	5MU	C2-N1	-6.10	1.28	1.38
53	f2	54	5MU	C2-N3	-6.01	1.27	1.38
53	f2	55	PSU	C2-N1	-5.71	1.29	1.36
22	A2	1835	2MG	C2-N2	5.69	1.46	1.33
22	A2	2445	2MG	C2-N2	5.64	1.45	1.33
22	A2	1835	2MG	CM2-N2	5.35	1.55	1.45
53	f2	55	PSU	C2-N3	-5.30	1.28	1.37
53	f2	54	5MU	C6-N1	-5.30	1.29	1.38
22	A2	2445	2MG	CM2-N2	5.22	1.54	1.45
53	f2	54	5MU	C4-N3	-5.12	1.29	1.38
22	A2	745	1MG	C2-N2	5.06	1.43	1.34
22	A2	2251	OMG	C6-N1	-5.05	1.30	1.37
22	A2	2580	PSU	C1'-C5	-4.84	1.39	1.50
22	A2	2604	PSU	C1'-C5	-4.81	1.39	1.50
22	A2	2457	PSU	C1'-C5	-4.80	1.39	1.50
22	A2	2445	2MG	C6-N1	-4.80	1.30	1.37
22	A2	2069	G7M	C2-N2	4.76	1.45	1.34
34	M2	81	4D4	CZ-NE	4.74	1.42	1.33
22	A2	1939	5MU	C2-N3	-4.73	1.29	1.38
22	A2	2449	H2U	C4-N3	4.73	1.45	1.37
22	A2	1917	PSU	C1'-C5	-4.71	1.39	1.50
22	A2	955	PSU	C1'-C5	-4.70	1.39	1.50
22	A2	2605	PSU	C1'-C5	-4.69	1.39	1.50
22	A2	746	PSU	C1'-C5	-4.68	1.39	1.50
22	A2	2504	PSU	C1'-C5	-4.67	1.39	1.50
22	A2	1911	PSU	C1'-C5	-4.66	1.39	1.50
22	A2	2498	OMC	C4-N4	4.65	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A2	1939	5MU	C6-N1	-4.62	1.30	1.38
22	A2	1835	2MG	C6-N1	-4.60	1.31	1.37
22	A2	747	5MU	C2-N3	-4.58	1.29	1.38
22	A2	2552	OMU	C2-N1	-4.55	1.31	1.38
22	A2	2251	OMG	C2-N2	4.53	1.45	1.34
22	A2	747	5MU	C6-N1	-4.46	1.30	1.38
53	f2	8	4SU	O2-C2	-4.44	1.14	1.23
53	f2	8	4SU	C2'-C1'	-4.39	1.39	1.53
22	A2	1962	5MC	C4-N4	4.17	1.45	1.34
22	A2	2069	G7M	C6-N1	-4.16	1.31	1.37
22	A2	2457	PSU	C4-N3	-4.03	1.31	1.38
22	A2	2580	PSU	C4-N3	-4.03	1.31	1.38
22	A2	1962	5MC	C2-N1	-4.02	1.31	1.40
22	A2	955	PSU	C2-N1	-4.01	1.31	1.36
22	A2	1915	3TD	C2-N1	-3.99	1.31	1.37
22	A2	2457	PSU	C2-N1	-3.96	1.31	1.36
22	A2	955	PSU	C4-N3	-3.96	1.31	1.38
22	A2	2605	PSU	C4-N3	-3.93	1.31	1.38
22	A2	1915	3TD	C4-N3	-3.89	1.32	1.40
22	A2	2504	PSU	C4-N3	-3.89	1.31	1.38
22	A2	2580	PSU	C2-N1	-3.89	1.31	1.36
22	A2	2445	2MG	C5-C6	-3.89	1.39	1.47
22	A2	2604	PSU	C4-N3	-3.86	1.31	1.38
22	A2	2552	OMU	C4-N3	-3.83	1.31	1.38
22	A2	1962	5MC	C6-N1	-3.83	1.31	1.38
22	A2	2504	PSU	C2-N1	-3.82	1.31	1.36
22	A2	1835	2MG	C5-C6	-3.81	1.39	1.47
22	A2	2604	PSU	C2-N1	-3.80	1.31	1.36
22	A2	2605	PSU	C2-N1	-3.79	1.31	1.36
22	A2	746	PSU	C4-N3	-3.77	1.31	1.38
22	A2	2457	PSU	C2-N3	-3.75	1.31	1.37
22	A2	1911	PSU	C4-N3	-3.75	1.31	1.38
22	A2	745	1MG	C6-N1	-3.75	1.32	1.39
22	A2	2503	2MA	C6-N6	3.74	1.47	1.34
22	A2	2605	PSU	C2-N3	-3.74	1.31	1.37
22	A2	2552	OMU	C2-N3	-3.73	1.31	1.38
22	A2	2498	OMC	C2-N1	-3.72	1.31	1.40
22	A2	1917	PSU	C4-N3	-3.72	1.31	1.38
22	A2	746	PSU	C2-N1	-3.70	1.31	1.36
22	A2	955	PSU	C2-N3	-3.69	1.31	1.37
22	A2	2580	PSU	C2-N3	-3.66	1.31	1.37
22	A2	2604	PSU	C2-N3	-3.65	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A2	1911	PSU	C2-N1	-3.64	1.31	1.36
22	A2	2504	PSU	C2-N3	-3.63	1.31	1.37
22	A2	1917	PSU	C2-N1	-3.63	1.31	1.36
22	A2	1939	5MU	C4-N3	-3.59	1.32	1.38
22	A2	746	PSU	C2-N3	-3.53	1.31	1.37
22	A2	747	5MU	C6-C5	3.52	1.40	1.34
22	A2	1939	5MU	C6-C5	3.51	1.40	1.34
22	A2	1917	PSU	C2-N3	-3.48	1.31	1.37
53	f2	54	5MU	O4'-C4'	-3.47	1.37	1.45
22	A2	747	5MU	C4-N3	-3.47	1.32	1.38
22	A2	2445	2MG	C2-N1	-3.46	1.31	1.36
53	f2	8	4SU	O4'-C4'	-3.46	1.37	1.45
22	A2	1911	PSU	C2-N3	-3.42	1.31	1.37
22	A2	1835	2MG	C2-N1	-3.27	1.31	1.36
53	f2	55	PSU	O3'-C3'	3.20	1.50	1.43
22	A2	1915	3TD	C6-C5	3.10	1.38	1.35
22	A2	1915	3TD	C2-N3	-3.07	1.31	1.38
53	f2	8	4SU	C6-N1	-3.06	1.30	1.38
34	M2	81	4D4	CZ-NH2	3.03	1.44	1.32
22	A2	1962	5MC	O2-C2	-3.02	1.18	1.23
22	A2	1939	5MU	O4-C4	-3.00	1.17	1.23
22	A2	1939	5MU	O2-C2	-3.00	1.17	1.23
22	A2	2498	OMC	O2-C2	-2.99	1.18	1.23
22	A2	2605	PSU	O4-C4	-2.99	1.17	1.23
22	A2	2457	PSU	O4-C4	-2.98	1.17	1.23
22	A2	955	PSU	O4-C4	-2.97	1.17	1.23
22	A2	747	5MU	O4-C4	-2.97	1.17	1.23
22	A2	1911	PSU	C6-C5	2.95	1.38	1.35
22	A2	2580	PSU	O4-C4	-2.93	1.18	1.23
53	f2	54	5MU	C3'-C4'	-2.93	1.45	1.53
22	A2	1917	PSU	C6-C5	2.90	1.38	1.35
53	f2	8	4SU	C1'-N1	-2.90	1.39	1.47
22	A2	2504	PSU	C6-C5	2.90	1.38	1.35
22	A2	747	5MU	O2-C2	-2.89	1.17	1.23
22	A2	2604	PSU	O4-C4	-2.89	1.18	1.23
22	A2	746	PSU	C6-C5	2.89	1.38	1.35
22	A2	2504	PSU	O4-C4	-2.88	1.18	1.23
22	A2	746	PSU	O4-C4	-2.85	1.18	1.23
53	f2	55	PSU	C4-N3	-2.82	1.33	1.38
22	A2	2604	PSU	C6-C5	2.81	1.38	1.35
22	A2	2069	G7M	C2-N1	-2.78	1.30	1.37
22	A2	955	PSU	C6-C5	2.77	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A2	1911	PSU	O4-C4	-2.75	1.18	1.23
22	A2	2580	PSU	C6-N1	-2.75	1.31	1.36
22	A2	2580	PSU	C6-C5	2.74	1.38	1.35
22	A2	2457	PSU	C6-C5	2.74	1.38	1.35
22	A2	2552	OMU	O2-C2	-2.72	1.18	1.23
22	A2	2605	PSU	C6-C5	2.72	1.38	1.35
22	A2	955	PSU	C6-N1	-2.72	1.31	1.36
53	f2	32	5MC	C6-N1	-2.70	1.33	1.38
22	A2	745	1MG	C5-C6	-2.69	1.39	1.47
22	A2	2457	PSU	C6-N1	-2.65	1.31	1.36
53	f2	8	4SU	C2-N1	-2.64	1.34	1.38
22	A2	1917	PSU	O4-C4	-2.64	1.18	1.23
53	f2	55	PSU	C6-N1	-2.64	1.31	1.36
53	f2	54	5MU	C4-C5	-2.63	1.40	1.44
22	A2	2605	PSU	C6-N1	-2.61	1.31	1.36
22	A2	2604	PSU	C6-N1	-2.60	1.31	1.36
22	A2	2457	PSU	O2-C2	-2.59	1.18	1.23
22	A2	2504	PSU	C6-N1	-2.59	1.31	1.36
22	A2	2580	PSU	O2-C2	-2.56	1.18	1.23
22	A2	2552	OMU	C6-N1	-2.55	1.31	1.38
22	A2	955	PSU	O2-C2	-2.55	1.18	1.23
22	A2	2251	OMG	C5-C6	-2.55	1.42	1.47
22	A2	1917	PSU	C6-N1	-2.54	1.32	1.36
22	A2	2498	OMC	C6-N1	-2.51	1.31	1.38
22	A2	1911	PSU	C6-N1	-2.49	1.32	1.36
22	A2	2605	PSU	O2-C2	-2.47	1.18	1.23
53	f2	8	4SU	O4'-C1'	-2.47	1.36	1.42
22	A2	1915	3TD	O2-C2	-2.45	1.18	1.23
22	A2	2504	PSU	O2-C2	-2.45	1.18	1.23
22	A2	1962	5MC	C2-N3	-2.44	1.31	1.36
22	A2	2604	PSU	O2-C2	-2.44	1.18	1.23
22	A2	2498	OMC	C2-N3	-2.42	1.31	1.36
22	A2	746	PSU	C6-N1	-2.41	1.32	1.36
22	A2	2552	OMU	C5-C4	-2.41	1.38	1.43
22	A2	1915	3TD	C6-N1	-2.39	1.32	1.36
22	A2	1917	PSU	O2-C2	-2.38	1.18	1.23
53	f2	32	5MC	C6-C5	2.35	1.38	1.34
22	A2	1911	PSU	O2-C2	-2.34	1.18	1.23
22	A2	746	PSU	O2-C2	-2.34	1.18	1.23
53	f2	8	4SU	C3'-C4'	-2.30	1.47	1.53
22	A2	2580	PSU	O4'-C1'	-2.30	1.40	1.43
22	A2	2251	OMG	C5-C4	-2.25	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A2	1962	5MC	C6-C5	2.22	1.38	1.34
22	A2	746	PSU	O4'-C1'	-2.18	1.40	1.43
22	A2	2445	2MG	C4-N3	-2.12	1.32	1.37
53	f2	8	4SU	O2'-C2'	-2.11	1.38	1.43
22	A2	2069	G7M	C5-C6	-2.09	1.40	1.45
22	A2	1835	2MG	C4-N3	-2.03	1.32	1.37
22	A2	2580	PSU	C4-C5	-2.01	1.38	1.44
22	A2	2498	OMC	C5-C4	-2.00	1.38	1.42

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A2	2449	H2U	C4-N3-C2	-15.23	113.16	125.79
53	f2	8	4SU	C5-C4-N3	14.84	128.45	114.69
53	f2	8	4SU	C4-N3-C2	-12.97	114.73	127.34
22	A2	2449	H2U	O2-C2-N1	-11.49	108.68	123.11
53	f2	8	4SU	C2'-C1'-N1	-9.54	86.20	113.22
22	A2	1939	5MU	C4-N3-C2	-9.13	115.53	127.35
53	f2	55	PSU	C6-C5-C4	-9.10	111.83	118.20
53	f2	8	4SU	C5-C4-S4	-8.84	113.08	124.47
53	f2	8	4SU	C6-C5-C4	-8.57	112.53	119.95
22	A2	747	5MU	C4-N3-C2	-8.56	116.27	127.35
22	A2	747	5MU	C5M-C5-C4	8.48	128.10	118.77
22	A2	1939	5MU	N3-C2-N1	8.44	126.09	114.89
53	f2	54	5MU	O4-C4-C5	-8.35	115.22	124.90
22	A2	1939	5MU	C5-C6-N1	-8.33	114.77	123.34
53	f2	8	4SU	N3-C2-N1	8.26	125.86	114.89
22	A2	747	5MU	N3-C2-N1	8.22	125.80	114.89
22	A2	1939	5MU	C5M-C5-C4	8.09	127.67	118.77
22	A2	2449	H2U	O4-C4-N3	-7.92	107.72	120.28
53	f2	54	5MU	C5-C4-N3	7.44	121.66	115.31
22	A2	747	5MU	C5-C6-N1	-7.32	115.81	123.34
22	A2	2449	H2U	O2-C2-N3	-7.19	108.11	121.50
22	A2	1915	3TD	N1-C2-N3	6.99	121.65	116.14
22	A2	1939	5MU	C5-C4-N3	6.87	121.18	115.31
22	A2	2503	2MA	C2-N3-C4	6.61	120.89	115.52
22	A2	747	5MU	C5M-C5-C6	-6.57	114.07	122.85
22	A2	2449	H2U	O4-C4-C5	-6.54	108.19	122.17
22	A2	1939	5MU	C5M-C5-C6	-6.51	114.16	122.85
22	A2	2030	6MZ	C9-N6-C6	-6.46	117.30	122.87
22	A2	747	5MU	C5-C4-N3	6.46	120.83	115.31
53	f2	54	5MU	C4-N3-C2	-6.43	119.02	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A2	2449	H2U	N3-C2-N1	-6.07	110.24	116.65
22	A2	2580	PSU	N1-C2-N3	5.74	121.64	115.13
22	A2	2504	PSU	N1-C2-N3	5.72	121.61	115.13
22	A2	2457	PSU	N1-C2-N3	5.71	121.60	115.13
22	A2	2604	PSU	N1-C2-N3	5.62	121.50	115.13
22	A2	955	PSU	N1-C2-N3	5.57	121.44	115.13
53	f2	55	PSU	O3'-C3'-C4'	5.57	127.14	111.05
22	A2	1917	PSU	N1-C2-N3	5.56	121.44	115.13
22	A2	2605	PSU	N1-C2-N3	5.56	121.42	115.13
22	A2	2552	OMU	N3-C2-N1	5.51	122.21	114.89
22	A2	1911	PSU	N1-C2-N3	5.51	121.37	115.13
53	f2	54	5MU	N3-C2-N1	5.45	122.12	114.89
22	A2	746	PSU	N1-C2-N3	5.43	121.28	115.13
53	f2	8	4SU	O2-C2-N1	-5.35	115.67	122.79
22	A2	2030	6MZ	C2-N1-C6	5.24	121.08	116.59
53	f2	8	4SU	O3'-C3'-C2'	5.22	128.71	111.82
22	A2	2030	6MZ	N3-C2-N1	-4.92	120.99	128.68
22	A2	1618	6MZ	C2-N1-C6	4.81	120.71	116.59
22	A2	2552	OMU	C4-N3-C2	-4.76	120.31	126.58
22	A2	1618	6MZ	C9-N6-C6	-4.75	118.78	122.87
22	A2	1618	6MZ	N3-C2-N1	-4.71	121.31	128.68
53	f2	8	4SU	C6-N1-C2	-4.66	115.03	120.99
53	f2	32	5MC	C5-C6-N1	-4.29	118.92	123.34
53	f2	55	PSU	C2'-C3'-C4'	-4.24	94.40	102.64
22	A2	1939	5MU	O2-C2-N1	-4.24	117.15	122.79
22	A2	1962	5MC	C5-C6-N1	-4.23	118.99	123.34
53	f2	55	PSU	N1-C2-N3	4.18	119.86	115.13
22	A2	2605	PSU	C4-N3-C2	-4.12	120.40	126.34
22	A2	2457	PSU	C4-N3-C2	-4.09	120.44	126.34
22	A2	746	PSU	C4-N3-C2	-4.06	120.50	126.34
22	A2	2604	PSU	C4-N3-C2	-4.05	120.50	126.34
22	A2	2504	PSU	C4-N3-C2	-4.04	120.51	126.34
22	A2	1939	5MU	O4-C4-N3	-4.00	112.44	120.12
22	A2	955	PSU	C4-N3-C2	-3.92	120.68	126.34
22	A2	1911	PSU	C4-N3-C2	-3.92	120.69	126.34
53	f2	55	PSU	O4'-C1'-C2'	-3.91	99.64	105.14
22	A2	1917	PSU	C4-N3-C2	-3.90	120.72	126.34
22	A2	2580	PSU	C4-N3-C2	-3.89	120.73	126.34
22	A2	747	5MU	O4-C4-N3	-3.87	112.69	120.12
53	f2	54	5MU	O4'-C4'-C3'	-3.74	97.72	105.11
53	f2	54	5MU	C3'-C2'-C1'	-3.68	94.44	101.43
34	M2	81	4D4	NE-CZ-NH2	-3.60	114.37	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A2	1915	3TD	C4-N3-C2	-3.51	120.80	124.61
22	A2	747	5MU	O2-C2-N1	-3.46	118.19	122.79
53	f2	54	5MU	C2'-C1'-N1	-3.44	103.48	113.22
22	A2	745	1MG	C5-C6-N1	3.38	118.98	113.90
53	f2	54	5MU	O2'-C2'-C3'	3.34	122.62	111.82
53	f2	55	PSU	O2'-C2'-C3'	-3.33	101.05	111.82
53	f2	8	4SU	C3'-C2'-C1'	3.32	107.74	101.43
22	A2	2504	PSU	O2-C2-N1	-3.29	119.17	122.79
22	A2	955	PSU	O2-C2-N1	-3.24	119.23	122.79
22	A2	1835	2MG	C5-C6-N1	3.17	119.56	113.95
22	A2	2580	PSU	O2-C2-N1	-3.17	119.30	122.79
34	M2	81	4D4	NH1-CZ-NE	3.16	126.48	119.19
22	A2	2457	PSU	O2-C2-N1	-3.14	119.34	122.79
22	A2	2503	2MA	C5-C6-N1	-3.13	118.95	121.01
53	f2	54	5MU	O3'-C3'-C2'	3.13	121.93	111.82
22	A2	1911	PSU	O2-C2-N1	-3.05	119.44	122.79
22	A2	2552	OMU	O2-C2-N1	-3.04	118.74	122.79
22	A2	746	PSU	O2-C2-N1	-3.03	119.45	122.79
53	f2	55	PSU	O2'-C2'-C1'	3.02	118.44	111.23
22	A2	1917	PSU	O2-C2-N1	-3.01	119.48	122.79
22	A2	2445	2MG	C5-C6-N1	3.00	119.24	113.95
22	A2	747	5MU	C1'-N1-C6	-2.98	116.17	121.12
22	A2	747	5MU	O2-C2-N3	-2.95	116.01	121.50
22	A2	1939	5MU	C6-N1-C2	2.93	124.27	121.30
22	A2	2604	PSU	O2-C2-N1	-2.92	119.58	122.79
22	A2	2498	OMC	O2-C2-N3	-2.89	117.62	122.33
22	A2	2251	OMG	C8-N7-C5	2.84	108.40	102.99
22	A2	2605	PSU	O2-C2-N1	-2.81	119.69	122.79
53	f2	54	5MU	C2'-C3'-C4'	2.75	107.99	102.64
53	f2	8	4SU	O2'-C2'-C3'	2.73	120.66	111.82
22	A2	1835	2MG	C8-N7-C5	2.73	108.19	102.99
22	A2	745	1MG	C8-N7-C5	2.73	108.19	102.99
53	f2	8	4SU	O4'-C1'-C2'	-2.73	100.70	106.64
22	A2	2445	2MG	C8-N7-C5	2.71	108.14	102.99
53	f2	8	4SU	C1'-N1-C2	2.70	122.46	117.57
53	f2	54	5MU	C5'-C4'-C3'	-2.69	105.10	115.18
22	A2	2552	OMU	C5-C6-N1	-2.67	117.33	121.81
22	A2	2030	6MZ	C4-C5-N7	-2.66	106.62	109.40
22	A2	2552	OMU	C5-C4-N3	2.62	118.76	114.84
53	f2	32	5MC	C5-C4-N3	-2.61	118.86	121.67
53	f2	55	PSU	O2-C2-N1	-2.56	119.97	122.79
22	A2	1939	5MU	O2-C2-N3	-2.55	116.75	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	f2	55	PSU	C4-N3-C2	-2.51	122.72	126.34
22	A2	2552	OMU	O4-C4-C5	-2.51	120.75	125.16
22	A2	2457	PSU	C5-C6-N1	-2.51	118.35	122.11
22	A2	2604	PSU	C5-C6-N1	-2.47	118.41	122.11
22	A2	746	PSU	C5-C6-N1	-2.46	118.42	122.11
22	A2	2605	PSU	C5-C6-N1	-2.46	118.42	122.11
34	M2	81	4D4	CB-CA-C	-2.45	107.85	111.77
53	f2	8	4SU	C4'-O4'-C1'	2.44	114.86	109.47
22	A2	2251	OMG	C5-C6-N1	2.38	118.16	113.95
22	A2	1911	PSU	C5-C6-N1	-2.33	118.61	122.11
22	A2	2449	H2U	C5-C4-N3	-2.33	114.03	116.65
53	f2	8	4SU	O4'-C4'-C3'	-2.32	100.53	105.11
22	A2	2504	PSU	C5-C6-N1	-2.30	118.65	122.11
22	A2	745	1MG	O6-C6-C5	-2.26	120.18	124.19
53	f2	54	5MU	C5-C6-N1	-2.26	121.02	123.34
22	A2	1917	PSU	C5-C6-N1	-2.25	118.73	122.11
53	f2	32	5MC	CM5-C5-C6	-2.25	119.85	122.85
22	A2	2445	2MG	CM2-N2-C2	-2.24	118.91	123.86
22	A2	2580	PSU	C5-C6-N1	-2.21	118.79	122.11
22	A2	2503	2MA	N3-C2-N1	-2.21	121.70	125.73
22	A2	955	PSU	C5-C6-N1	-2.21	118.80	122.11
22	A2	1835	2MG	CM2-N2-C2	-2.20	119.00	123.86
22	A2	2580	PSU	O4'-C1'-C2'	2.19	108.23	105.14
22	A2	1618	6MZ	C4-C5-N7	-2.15	107.16	109.40
22	A2	747	5MU	C6-N1-C2	2.13	123.45	121.30
34	M2	81	4D4	O-C-CA	-2.10	119.27	124.78
53	f2	55	PSU	C5'-C4'-C3'	2.08	122.97	115.18
53	f2	55	PSU	C4'-O4'-C1'	2.06	113.73	108.55
53	f2	54	5MU	O2-C2-N3	-2.06	117.67	121.50
53	f2	55	PSU	C3'-C2'-C1'	2.04	104.01	101.64
53	f2	54	5MU	C6-C5-C4	-2.02	116.34	118.03
22	A2	1962	5MC	C5-C4-N3	-2.02	119.50	121.67
22	A2	2251	OMG	C2-N1-C6	-2.01	121.40	125.10

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	D2	150[A]	MEQ	N-CA-CB-CG
34	M2	81	4D4	NE-CD-CG-CB
22	A2	746	PSU	C2'-C1'-C5-C4
22	A2	2251	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
53	f2	55	PSU	C2'-C1'-C5-C4
53	f2	55	PSU	C2'-C1'-C5-C6
22	A2	2030	6MZ	O4'-C4'-C5'-O5'
22	A2	2030	6MZ	C3'-C4'-C5'-O5'
22	A2	2445	2MG	C3'-C4'-C5'-O5'
22	A2	2504	PSU	O4'-C4'-C5'-O5'
22	A2	2504	PSU	C3'-C4'-C5'-O5'
53	f2	55	PSU	C3'-C4'-C5'-O5'
53	f2	55	PSU	O4'-C4'-C5'-O5'
22	A2	2445	2MG	O4'-C4'-C5'-O5'
34	M2	81	4D4	OB-CB-CG-CD
25	D2	150[A]	MEQ	C-CA-CB-CG
34	M2	81	4D4	CA-CB-CG-CD
25	D2	150[A]	MEQ	OE1-CD-CG-CB
25	D2	150[A]	MEQ	NE2-CD-CG-CB
53	f2	55	PSU	O4'-C1'-C5-C4
22	A2	1962	5MC	C2'-C1'-N1-C6
22	A2	2503	2MA	O4'-C4'-C5'-O5'
22	A2	1962	5MC	O4'-C1'-N1-C6
22	A2	746	PSU	O4'-C1'-C5-C6
22	A2	2069	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A2	2604	PSU	1	0
22	A2	2251	OMG	1	0
22	A2	1939	5MU	1	0
22	A2	2030	6MZ	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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
54	DI0	A2	3001	-	58,61,61	1.62	11 (18%)	77,92,92	1.65	20 (25%)

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
54	DI0	A2	3001	-	-	10/70/121/121	0/3/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	A2	3001	DI0	CAF-CAE	-5.60	1.39	1.51
54	A2	3001	DI0	OBI-CAG	-4.12	1.33	1.43
54	A2	3001	DI0	OAU-CBG	-3.41	1.38	1.44
54	A2	3001	DI0	OAY-CAC	-3.13	1.35	1.43
54	A2	3001	DI0	CBC-CBB	2.86	1.58	1.54
54	A2	3001	DI0	OAU-CAB	-2.79	1.34	1.41
54	A2	3001	DI0	CAP-CAH	2.66	1.60	1.55
54	A2	3001	DI0	CAI-CAK	2.49	1.57	1.54
54	A2	3001	DI0	CAD-CAW	-2.49	1.50	1.54
54	A2	3001	DI0	OBJ-CAP	-2.28	1.40	1.44
54	A2	3001	DI0	OBL-CAX	-2.25	1.38	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	A2	3001	DI0	OAL-CAW-CBT	4.88	116.70	107.40
54	A2	3001	DI0	CBT-CAW-CAD	-4.69	106.31	115.20
54	A2	3001	DI0	OBK-CAN-CAX	4.22	110.07	103.81
54	A2	3001	DI0	CAP-CAH-CAJ	-3.35	109.30	114.05
54	A2	3001	DI0	CBR-CAP-CBC	-2.75	106.45	111.09
54	A2	3001	DI0	CCB-OBK-CAN	-2.68	111.95	117.55
54	A2	3001	DI0	CBV-CBB-CBC	-2.64	106.45	112.45
54	A2	3001	DI0	CBP-CAJ-CAC	-2.51	106.89	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	A2	3001	DI0	CAF-CAC-CAJ	-2.37	106.20	113.05
54	A2	3001	DI0	OBI-CAG-CAO	-2.35	105.59	109.77
54	A2	3001	DI0	OBJ-CAP-CAH	2.22	111.80	107.59
54	A2	3001	DI0	OBK-CAN-CAT	-2.22	109.41	112.96
54	A2	3001	DI0	OAY-CAR-CAT	2.13	112.68	109.01
54	A2	3001	DI0	CBO-CAI-CAA	-2.12	107.97	112.94
54	A2	3001	DI0	CBO-CAI-CAK	-2.11	109.52	112.02
54	A2	3001	DI0	OAU-CAB-CAG	-2.08	105.95	110.35
54	A2	3001	DI0	OBK-CAN-CBQ	-2.07	107.48	110.92
54	A2	3001	DI0	CAN-CAX-CAZ	-2.06	107.98	111.14
54	A2	3001	DI0	OAM-CAH-CAJ	-2.04	108.48	111.54
54	A2	3001	DI0	OAM-CAB-OAU	-2.03	105.02	110.67

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	A2	3001	DI0	NAQ-CBA-CBS-OBW
54	A2	3001	DI0	NAQ-CAK-CBB-CBC
54	A2	3001	DI0	CAJ-CAH-CAP-OBJ
54	A2	3001	DI0	OBX-CCC-CCD-OBW
54	A2	3001	DI0	OAL-CAW-CBT-CCF
54	A2	3001	DI0	CAD-CAW-OAL-CAE
54	A2	3001	DI0	CBA-CBS-OBW-CCD
54	A2	3001	DI0	CAJ-CAC-CAF-CBN
54	A2	3001	DI0	CAD-CAW-CBT-CCF
54	A2	3001	DI0	NAQ-CAK-CBB-CBV

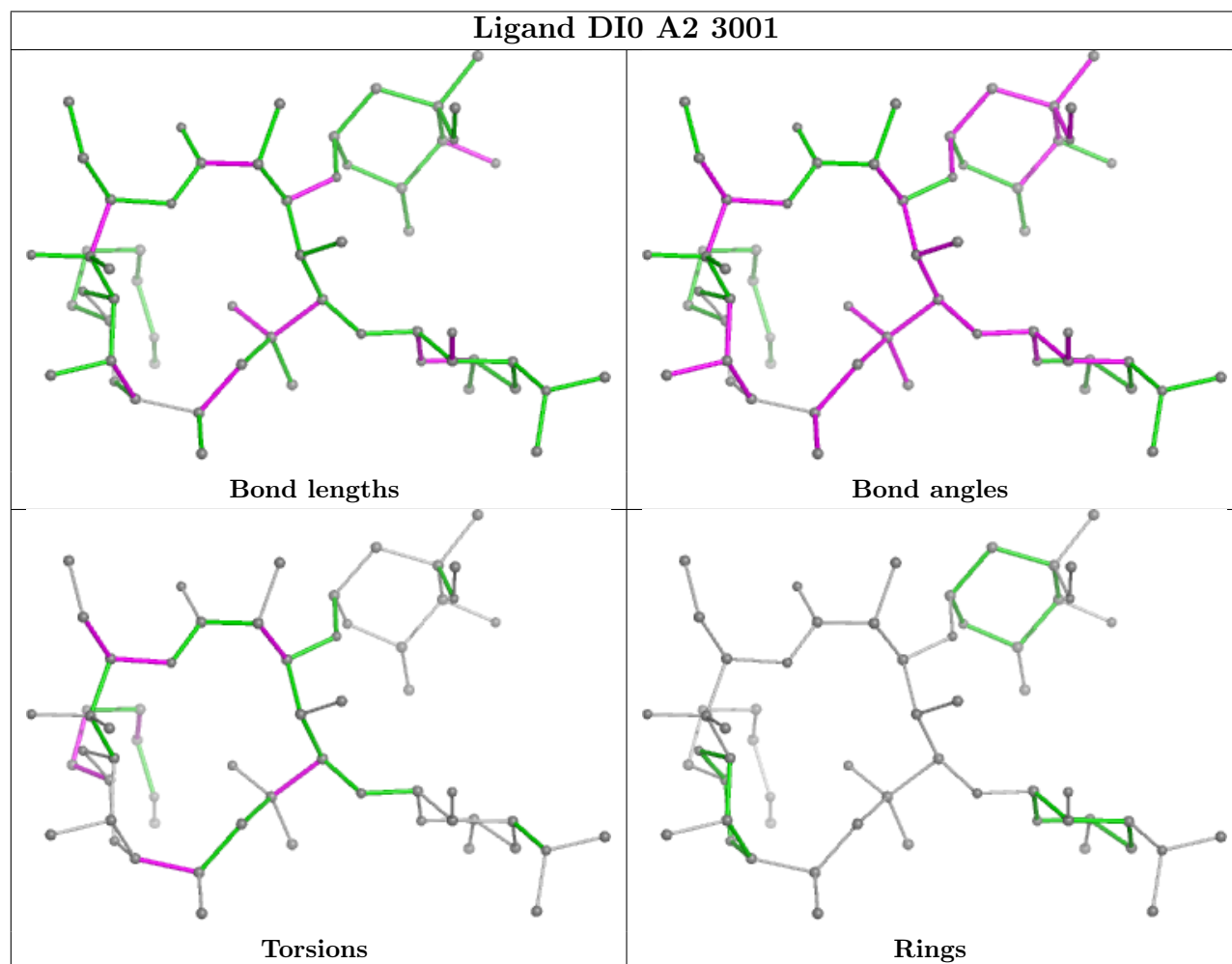
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	A2	3001	DI0	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	A2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A2	885:C	O3'	892:A	P	11.25

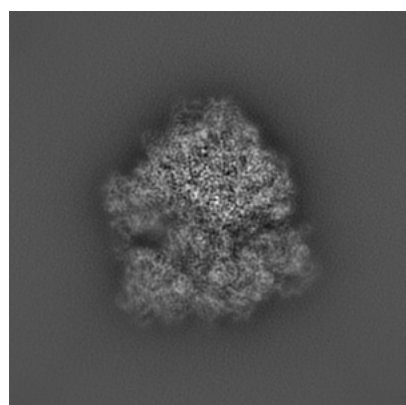
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10656. These allow visual inspection of the internal detail of the map and identification of artifacts.

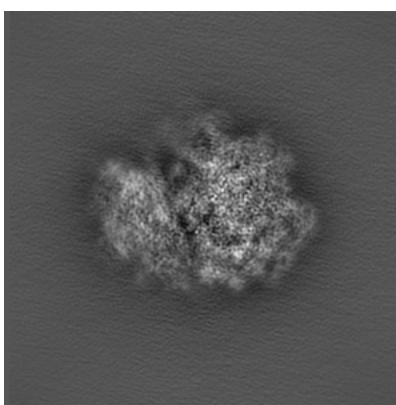
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

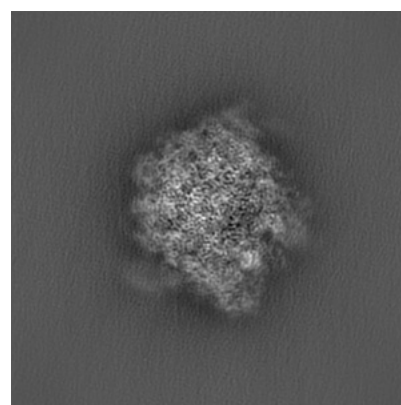
#### 6.1.1 Primary map



X



Y

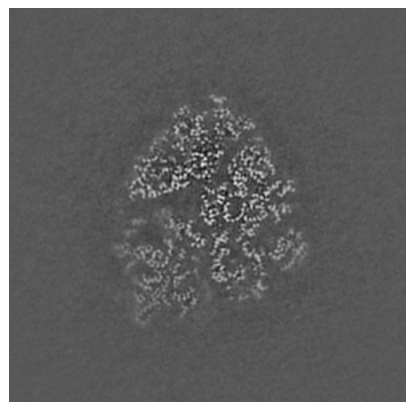


Z

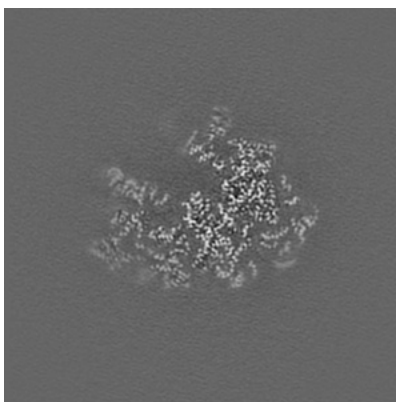
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

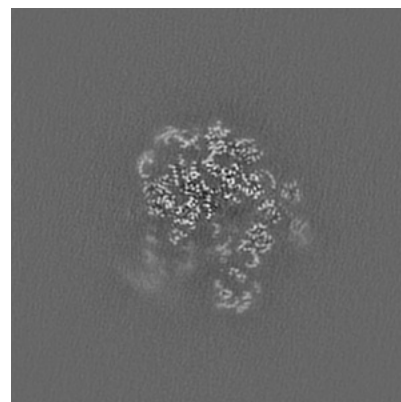
#### 6.2.1 Primary map



X Index: 256



Y Index: 256



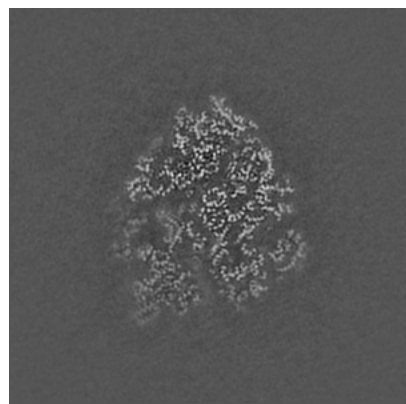
Z Index: 256



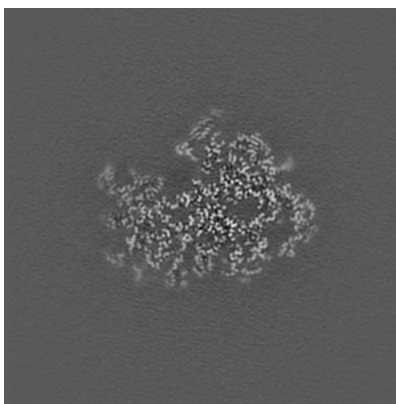
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

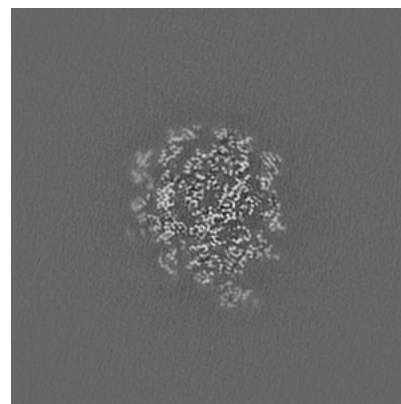
### 6.3.1 Primary map



X Index: 259



Y Index: 271

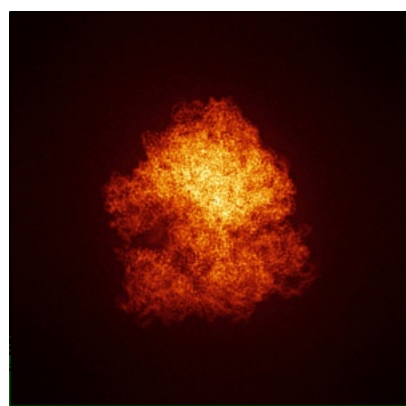


Z Index: 297

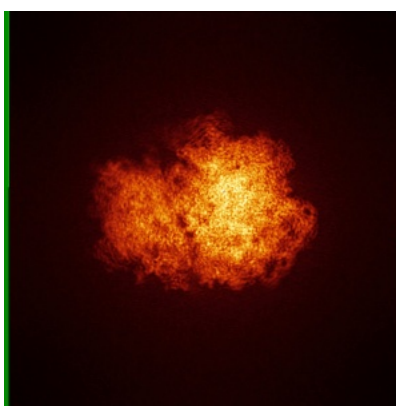
The images above show the largest variance slices of the map in three orthogonal directions.

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

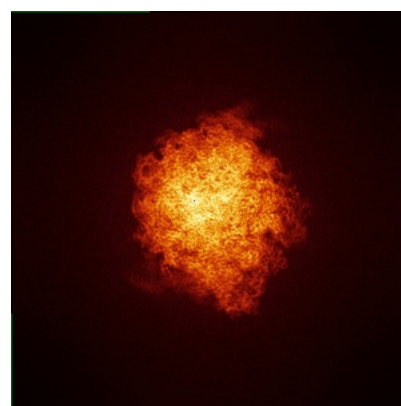
### 6.4.1 Primary map



X



Y



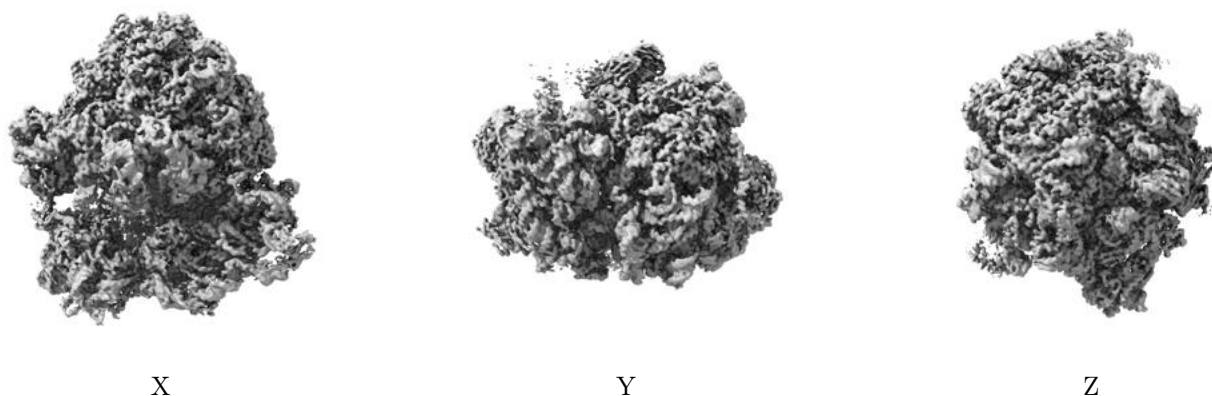
Z

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



## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

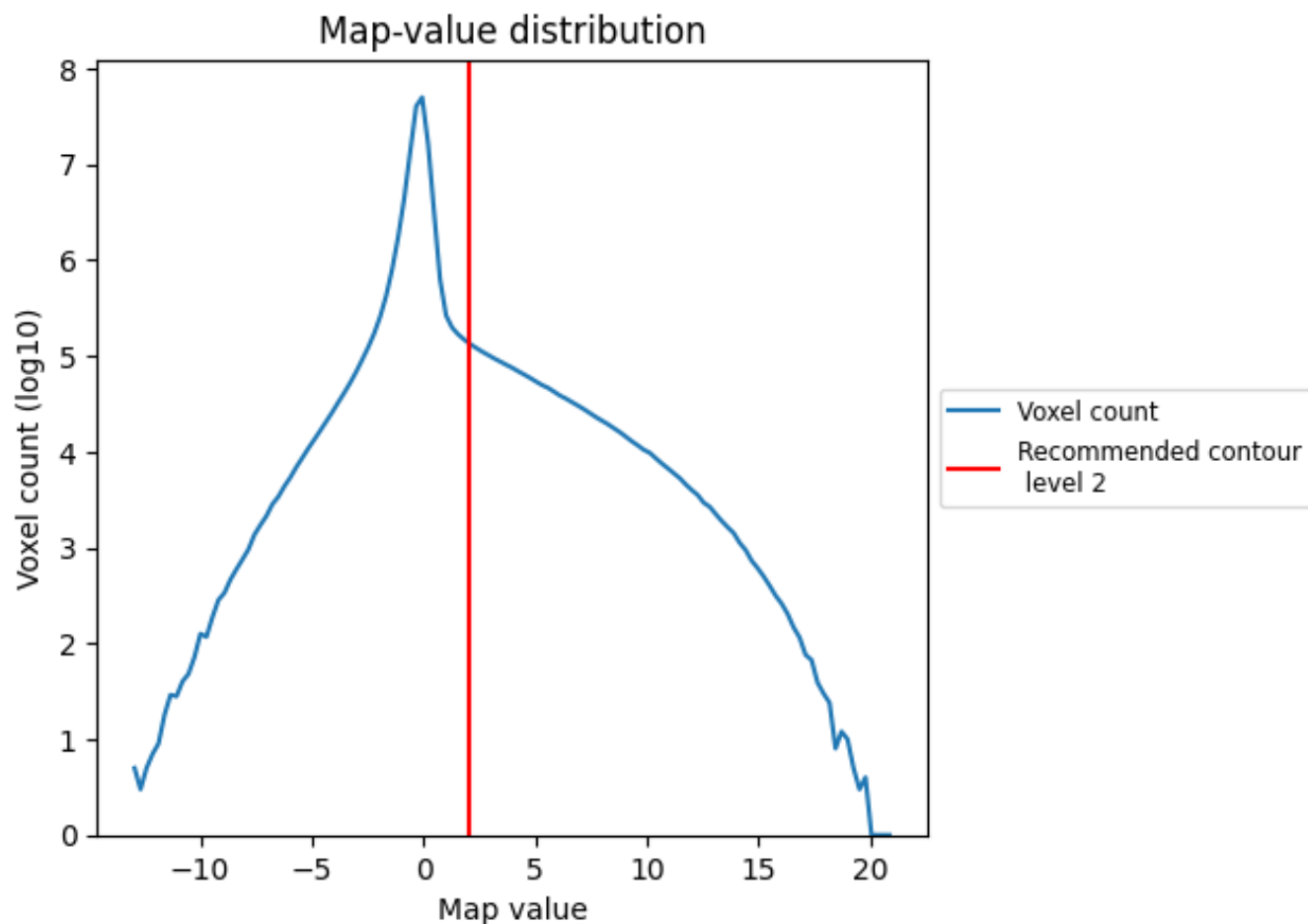
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

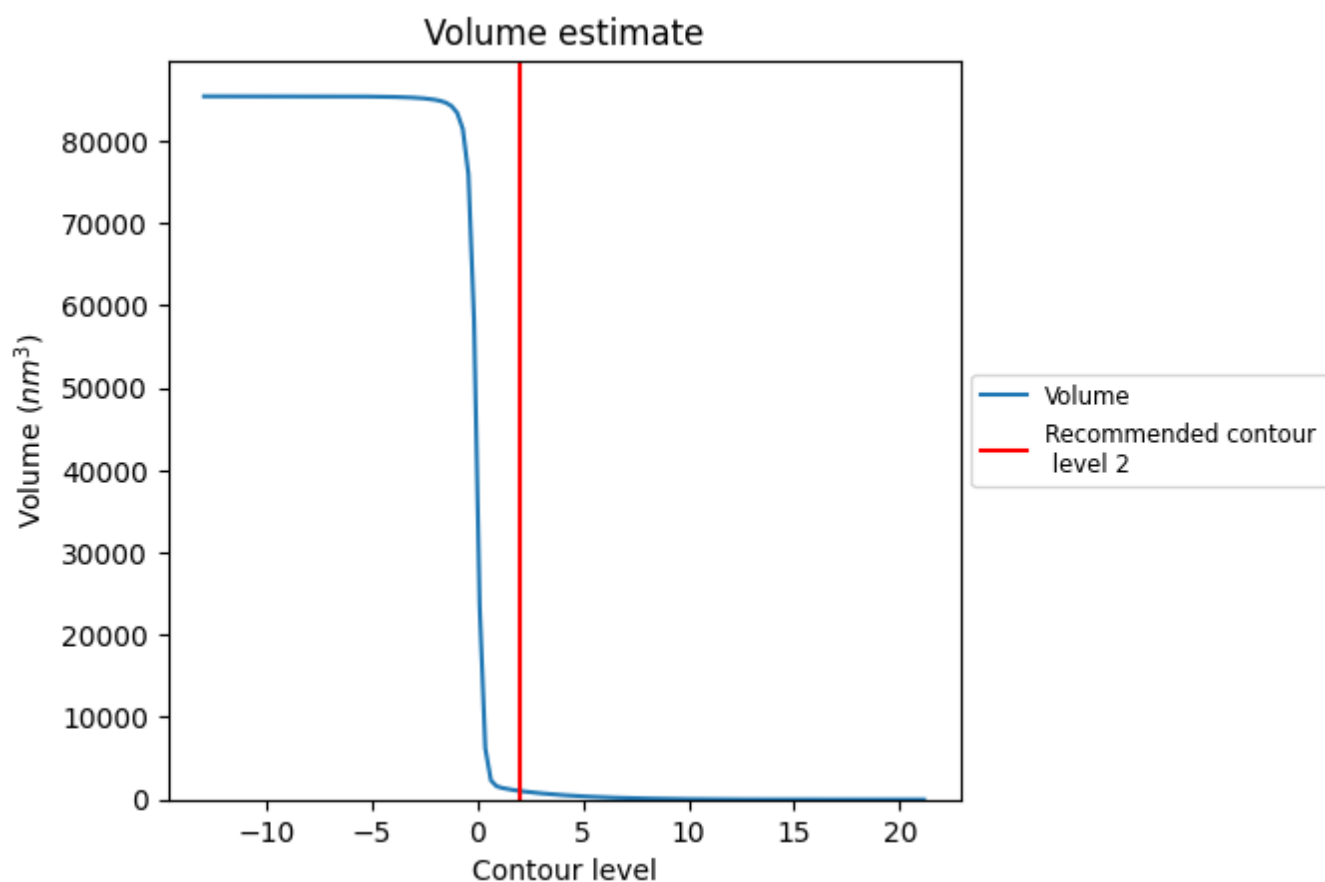
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

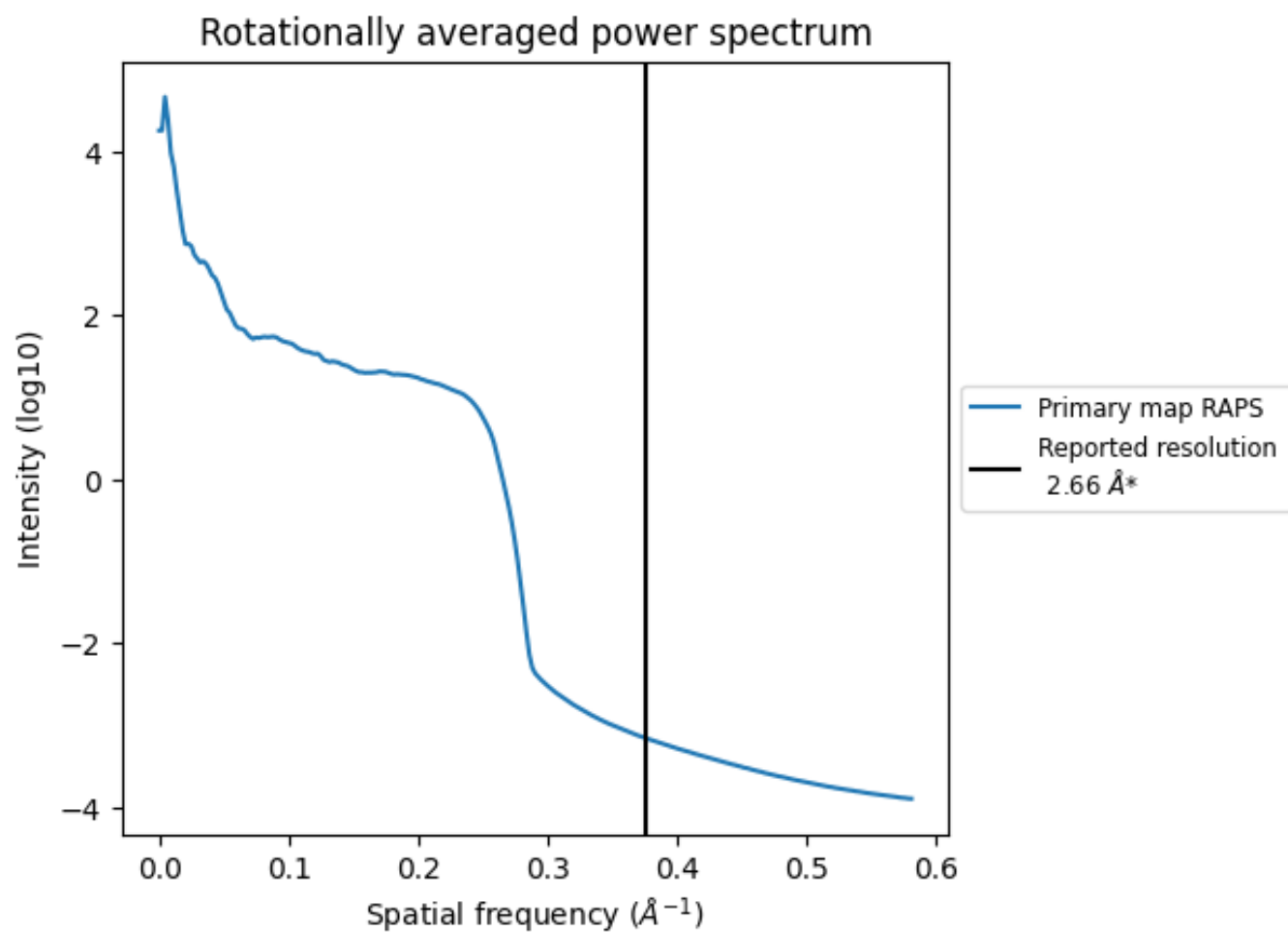
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1051  $\text{nm}^3$ ; this corresponds to an approximate mass of 949 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.376 Å<sup>-1</sup>

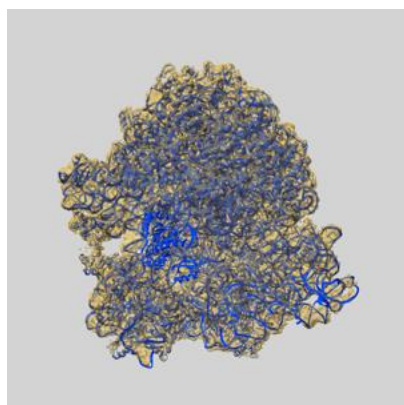
## 8 Fourier-Shell correlation

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

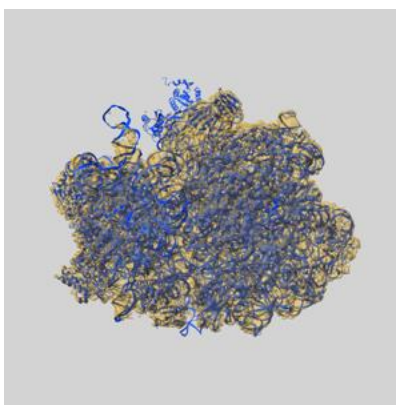
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10656 and PDB model 6XZA. Per-residue inclusion information can be found in section 3 on page 14.

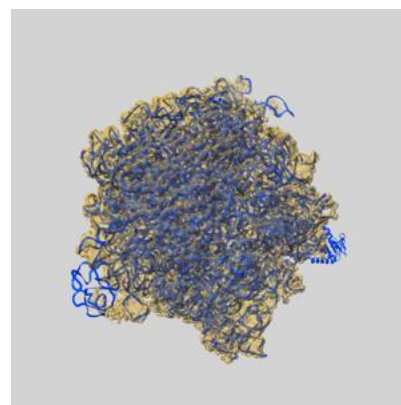
### 9.1 Map-model overlay [i](#)



X



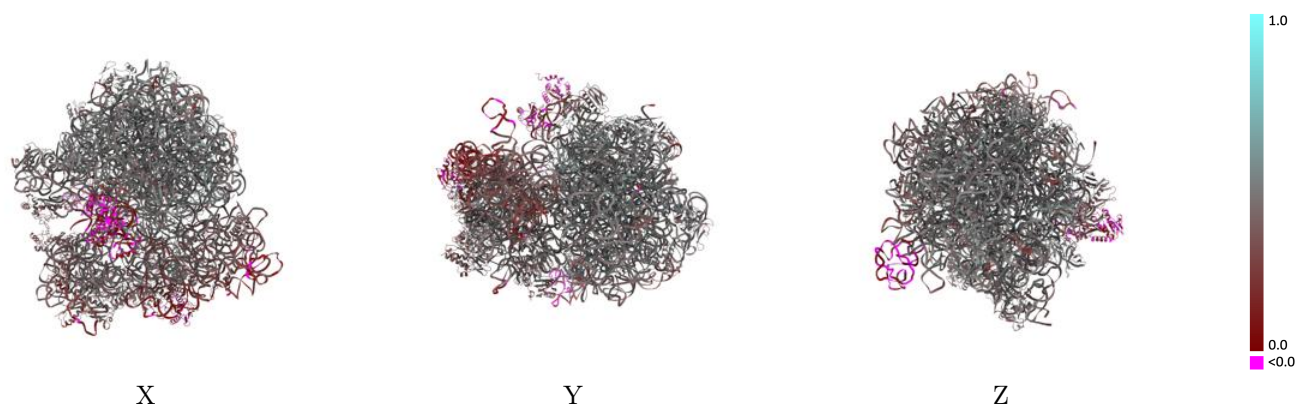
Y



Z

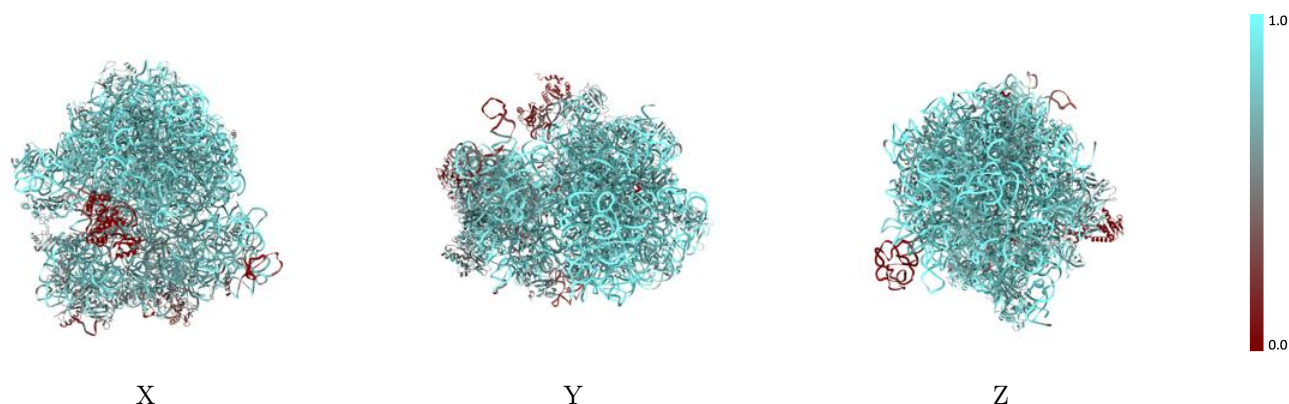
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



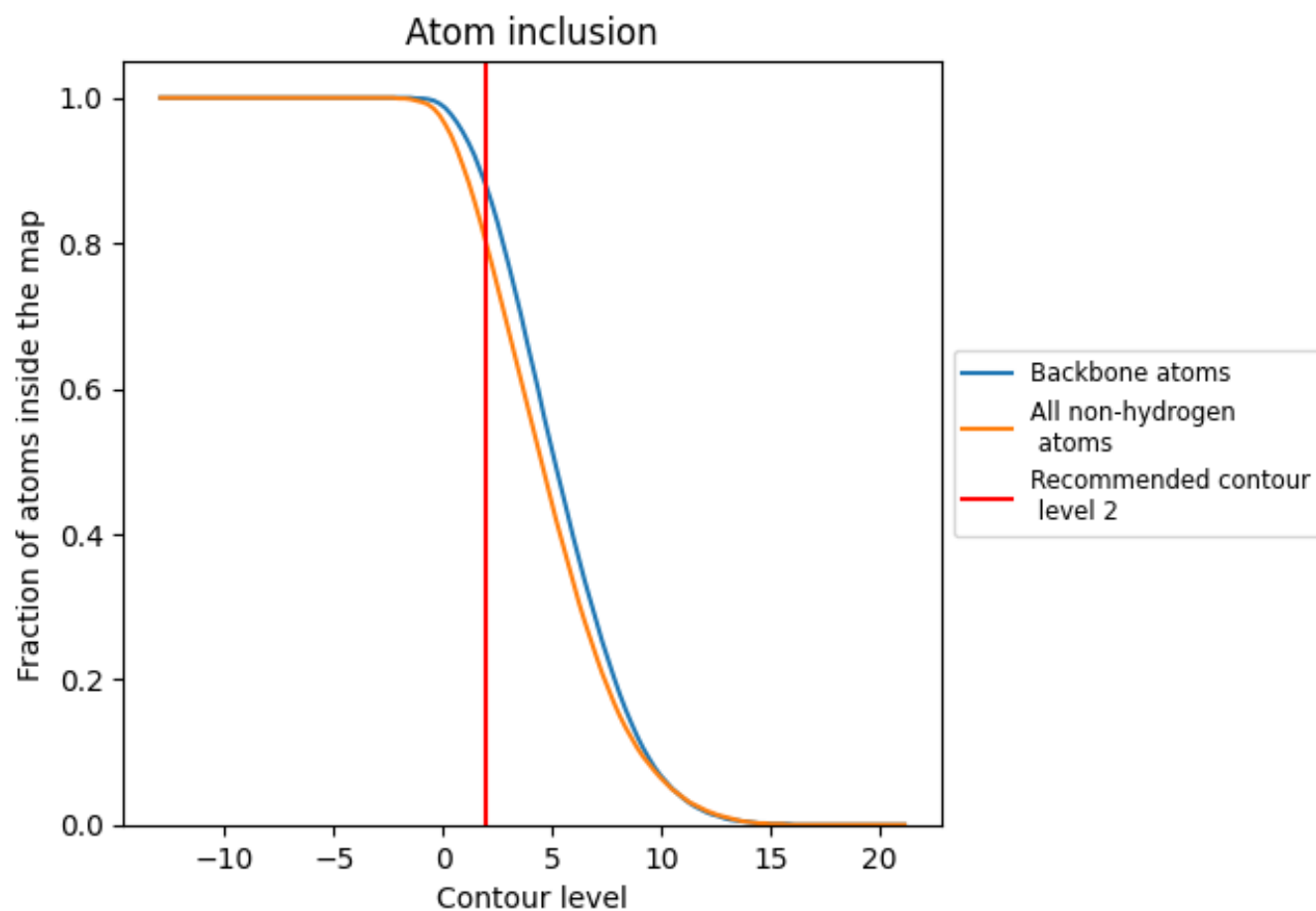
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 88% of all backbone atoms, 80% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7980	 0.4120
A1	 0.8190	 0.3750
A2	 0.8820	 0.4380
B1	 0.5530	 0.3670
B2	 0.9330	 0.4360
C1	 0.6020	 0.4170
C2	 0.8010	 0.4990
D1	 0.3680	 0.1710
D2	 0.7780	 0.4910
E1	 0.6950	 0.4350
E2	 0.7540	 0.4680
F1	 0.6630	 0.3780
F2	 0.6620	 0.3820
G1	 0.5510	 0.3500
G2	 0.6880	 0.4110
H1	 0.6940	 0.4400
H2	 0.0060	 0.0420
I1	 0.5510	 0.3670
I2	 0.0130	 0.0650
J1	 0.4750	 0.3570
J2	 0.7830	 0.4760
K1	 0.6870	 0.4000
K2	 0.7590	 0.4980
L1	 0.5560	 0.3160
L2	 0.8000	 0.4760
M1	 0.6030	 0.3660
M2	 0.7840	 0.4840
N1	 0.5790	 0.3580
N2	 0.7700	 0.4820
O1	 0.7290	 0.4150
O2	 0.7470	 0.4320
P1	 0.5650	 0.3300
P2	 0.7670	 0.4790
Q1	 0.5860	 0.2850
Q2	 0.8020	 0.4860



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Chain	Atom inclusion	Q-score
R1	 0.7050	 0.4240
R2	 0.7900	 0.4800
S1	 0.5970	 0.3460
S2	 0.7570	 0.4820
T1	 0.6020	 0.3090
T2	 0.7260	 0.4500
U1	 0.4600	 0.3450
U2	 0.7400	 0.4620
V2	 0.7490	 0.4520
W2	 0.7890	 0.4920
X2	 0.8090	 0.4760
Y2	 0.7380	 0.4130
Z2	 0.7620	 0.4750
a2	 0.7920	 0.4810
b2	 0.7120	 0.4600
c2	 0.7800	 0.4840
d2	 0.7960	 0.5070
e2	 0.7330	 0.4860
f2	 0.8080	 0.4160