



Full wwPDB EM Validation Report ⓘ

May 4, 2026 – 11:55 AM EDT

PDB ID : 9PII / pdb_00009pii
EMDB ID : EMD-71668
Title : E. coli 70S ribosome bound to Sarecycline
Authors : Devarkar, S.C.; Lomakin, I.B.; Bunick, C.G.
Deposited on : 2025-07-10
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

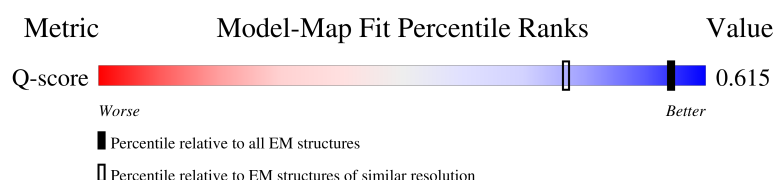
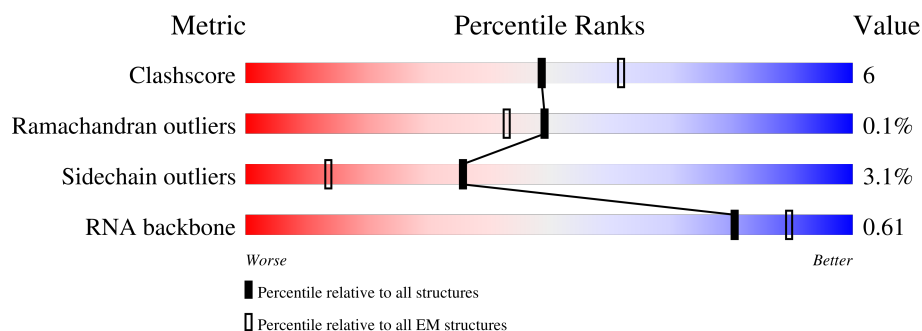
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




The reported resolution of this entry is 2.40 Å.

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









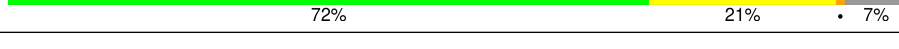

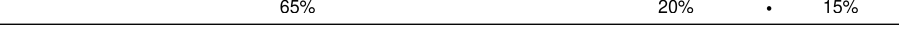
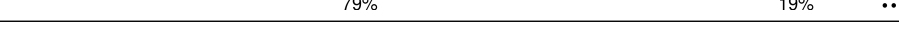
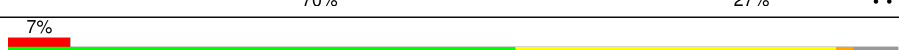

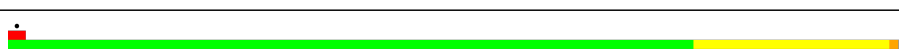

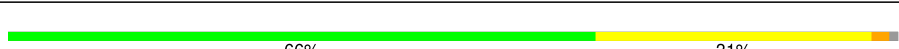





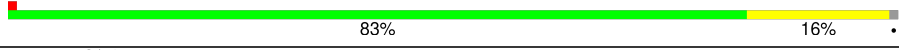
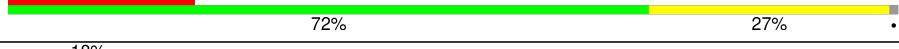



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

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

Mol	Chain	Length	Quality of chain
1	0	55	
2	1	46	
3	2	65	









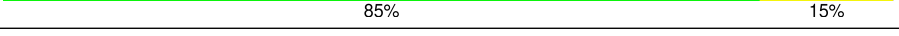

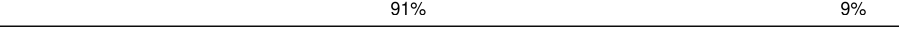
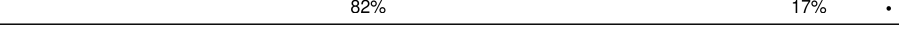

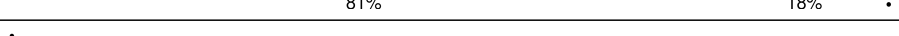

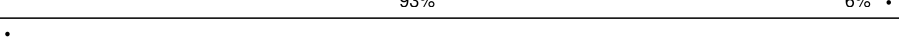
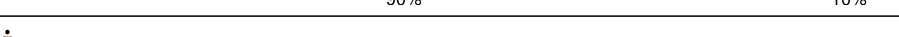

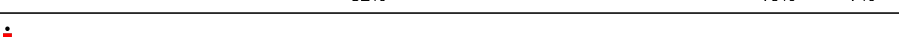






Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	A	1542	
7	B	241	
8	C	233	
9	D	206	
10	E	167	
11	F	135	
12	G	179	
13	H	130	
14	I	130	
15	J	103	
16	K	129	
17	L	124	
18	M	118	
19	N	101	
20	O	89	
21	P	82	
22	Q	84	
23	R	75	
24	S	92	
25	T	87	
26	U	71	
27	X	22	
28	Z	75	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	a	2904	
30	b	120	
31	c	273	
32	d	209	
33	e	201	
34	f	179	
35	g	177	
36	h	149	
37	i	142	
38	j	123	
39	k	144	
40	l	136	
41	m	127	
42	n	117	
43	o	115	
44	p	118	
45	q	103	
46	r	110	
47	s	100	
48	t	104	
49	u	94	
50	v	85	
51	w	78	
52	x	63	
53	y	59	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	z	57	<div><div></div><div>93%</div><div>5% •</div></div>

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 141212 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

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

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1500	Total	C	N	O	P	0	0
			32211	14373	5919	10419	1500		

- Molecule 7 is a protein called 30S ribosomal protein S2.

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

- Molecule 8 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 11 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 12 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 13 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 16 is a protein called 30S ribosomal protein S11.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 19 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 20 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 21 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 22 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 23 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 24 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 25 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 26 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 27 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	10	Total	C	N	O	P	0	0
			211	95	35	71	10		

- Molecule 28 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	75	Total	C	N	O	P	S	
			1605	716	291	522	75	1	
								0	0

- Molecule 29 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	2753	Total	C	N	O	P		
			59130	26384	10897	19096	2753		
								0	0

- Molecule 30 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	119	Total	C	N	O	P		
			2549	1135	466	829	119		
								0	0

- Molecule 31 is a protein called 50S ribosomal protein L2.

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

- Molecule 32 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	209	Total	C	N	O	S		
			1566	980	288	294	4		
								0	0

- Molecule 33 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 36 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 37 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 38 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 40 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 41 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 42 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 43 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called Ribosomal protein L21.

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

- Molecule 46 is a protein called 50S ribosomal protein L22.

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

- Molecule 47 is a protein called 50S ribosomal protein L23.

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

- Molecule 48 is a protein called 50S ribosomal protein L24.

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

- Molecule 49 is a protein called Large ribosomal subunit protein bL25.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

- Molecule 51 is a protein called 50S ribosomal protein L28.

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

- Molecule 52 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 53 is a protein called 50S ribosomal protein L30.

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

- Molecule 54 is a protein called 50S ribosomal protein L32.

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

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	3	1	Total	Zn	0
			1	1	

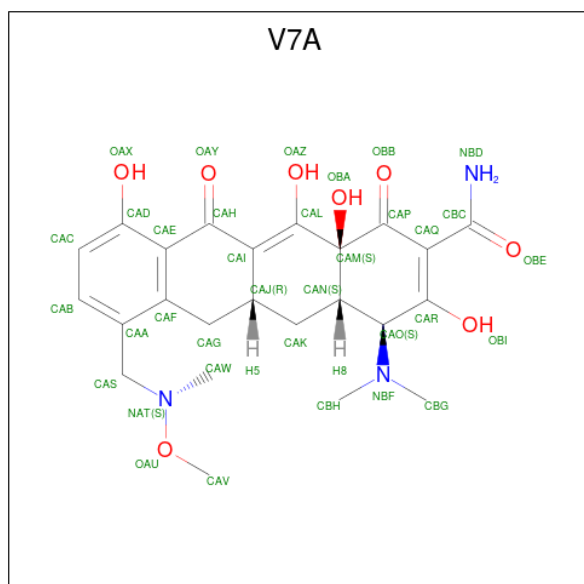
- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	A	62	Total	Mg	0
			62	62	
56	a	211	Total	Mg	0
			211	211	
56	b	5	Total	Mg	0
			5	5	
56	m	1	Total	Mg	0
			1	1	
56	p	2	Total	Mg	0
			2	2	

- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
57	A	24	Total	K	0
			24	24	
57	a	75	Total	K	0
			75	75	
57	b	1	Total	K	0
			1	1	

- Molecule 58 is Sarecycline (CCD ID: V7A) (formula: C₂₄H₂₉N₃O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
58	A	1	Total	C	N	O	0
			35	24	3	8	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
58	a	1	Total	C	N	O	0
			35	24	3	8	

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		AltConf
59	0	1	Total	O	0
			1	1	
59	1	3	Total	O	0
			3	3	
59	2	3	Total	O	0
			3	3	
59	3	1	Total	O	0
			1	1	
59	A	123	Total	O	0
			123	123	
59	O	1	Total	O	0
			1	1	
59	U	1	Total	O	0
			1	1	
59	a	1091	Total	O	0
			1091	1091	
59	b	14	Total	O	0
			14	14	
59	c	6	Total	O	0
			6	6	
59	d	5	Total	O	0
			5	5	
59	e	5	Total	O	0
			5	5	
59	i	2	Total	O	0
			2	2	
59	k	2	Total	O	0
			2	2	
59	l	1	Total	O	0
			1	1	
59	m	5	Total	O	0
			5	5	
59	o	1	Total	O	0
			1	1	
59	p	4	Total	O	0
			4	4	

Continued on next page...


Continued from previous page...

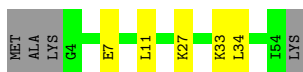
Mol	Chain	Residues	Atoms		AltConf
59	q	7	Total 7	O 7	0
59	r	2	Total 2	O 2	0
59	s	2	Total 2	O 2	0
59	v	1	Total 1	O 1	0
59	y	2	Total 2	O 2	0
59	z	3	Total 3	O 3	0

3 Residue-property plots [i](#)

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

- Molecule 1: 50S ribosomal protein L33

Chain 0: 




- Molecule 2: 50S ribosomal protein L34

Chain 1: 




- Molecule 3: 50S ribosomal protein L35

Chain 2: 



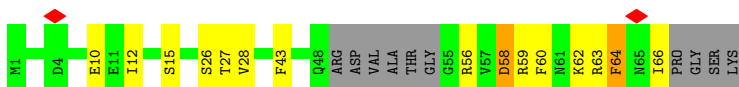
- Molecule 4: 50S ribosomal protein L36

Chain 3: 



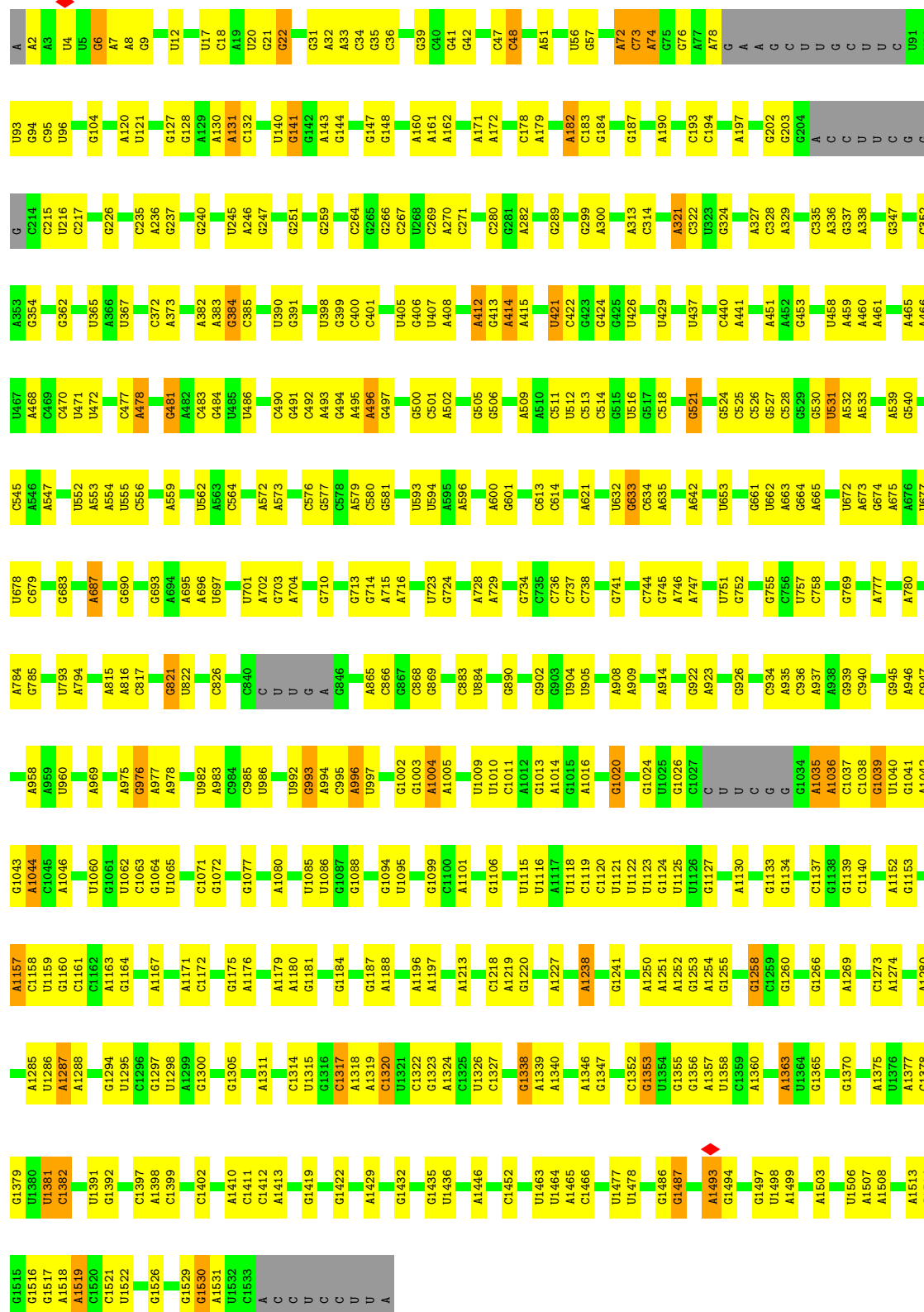
- Molecule 5: 50S ribosomal protein L31

Chain 4: 

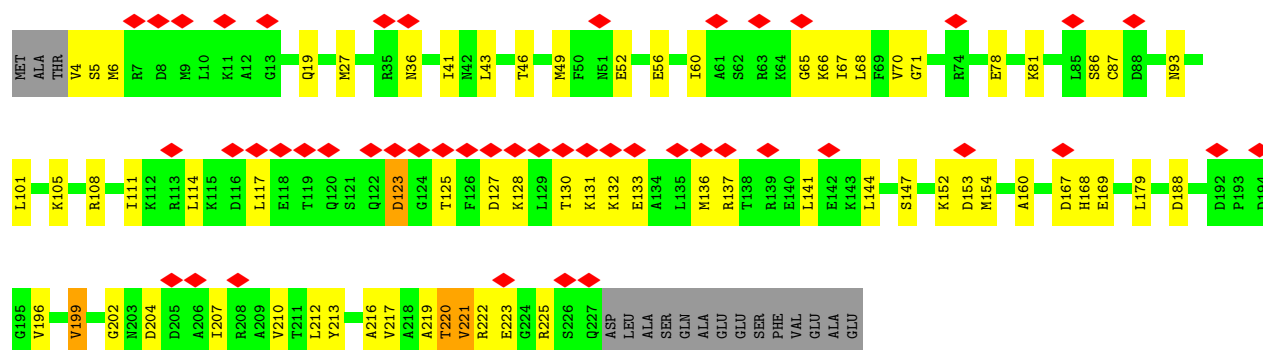


- Molecule 6: 16S rRNA

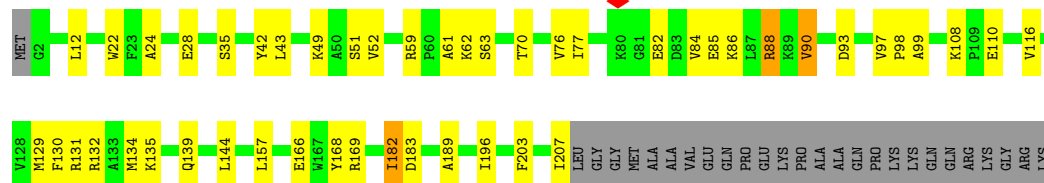
Chain A:  64% 30%



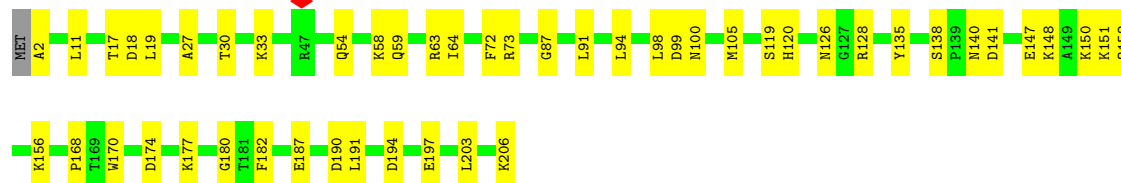
• Molecule 7: 30S ribosomal protein S2



- Molecule 8: Small ribosomal subunit protein uS3



- Molecule 9: Small ribosomal subunit protein uS4

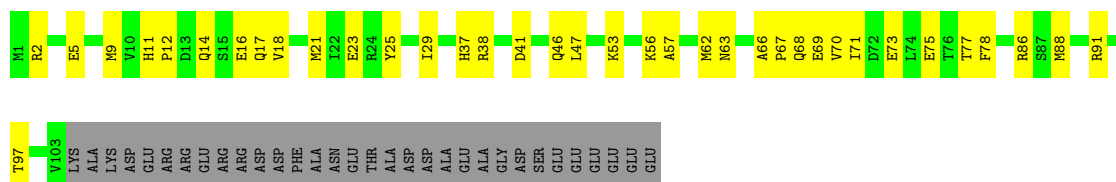


- Molecule 10: Small ribosomal subunit protein uS5

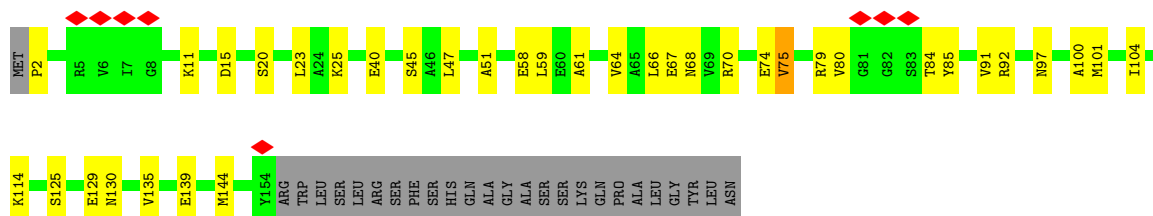


- Molecule 11: Small ribosomal subunit protein bS6

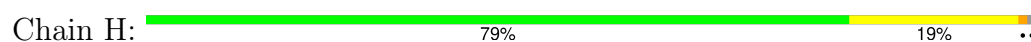




- Molecule 12: Small ribosomal subunit protein uS7



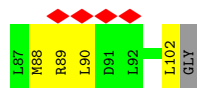
- Molecule 13: Small ribosomal subunit protein uS8



- Molecule 14: Small ribosomal subunit protein uS9

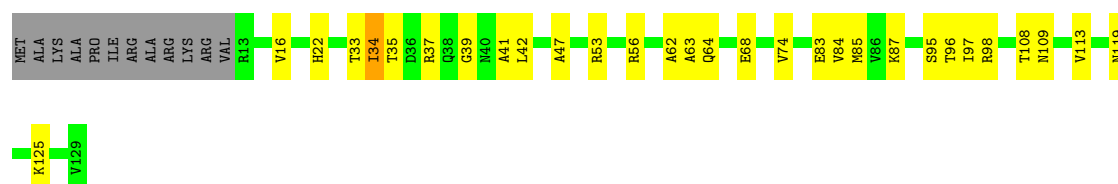


- Molecule 15: Small ribosomal subunit protein uS10

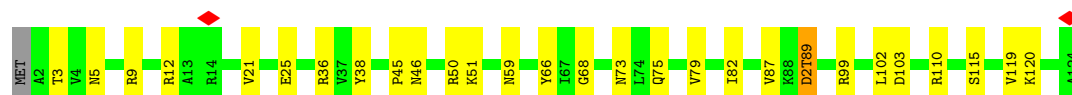
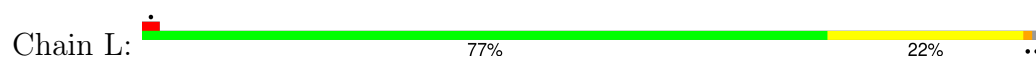


- Molecule 16: 30S ribosomal protein S11

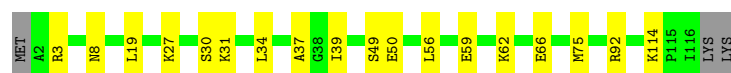
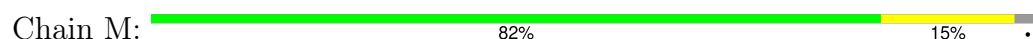




- Molecule 17: Small ribosomal subunit protein uS12



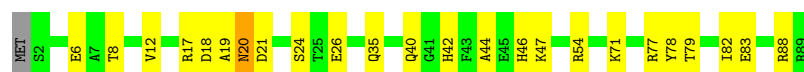
- Molecule 18: Small ribosomal subunit protein uS13



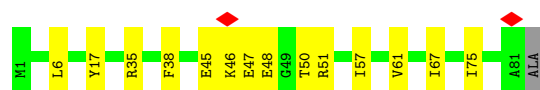
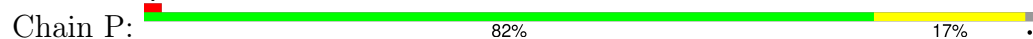
- Molecule 19: Small ribosomal subunit protein uS14



- Molecule 20: Small ribosomal subunit protein uS15



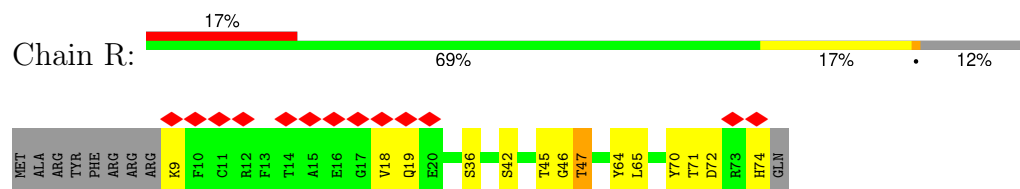
- Molecule 21: Small ribosomal subunit protein bS16



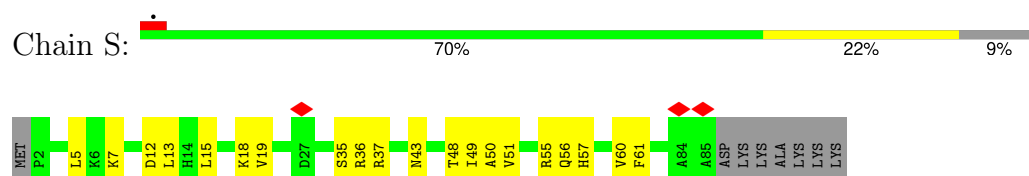
- Molecule 22: Small ribosomal subunit protein uS17



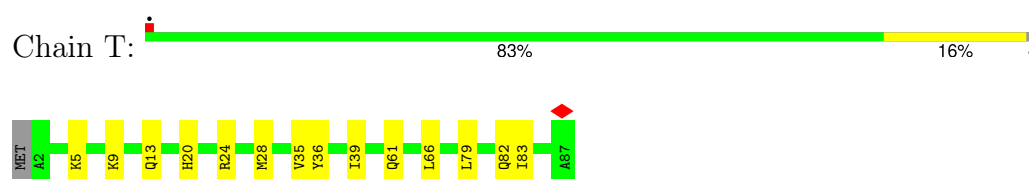
- Molecule 23: Small ribosomal subunit protein bS18



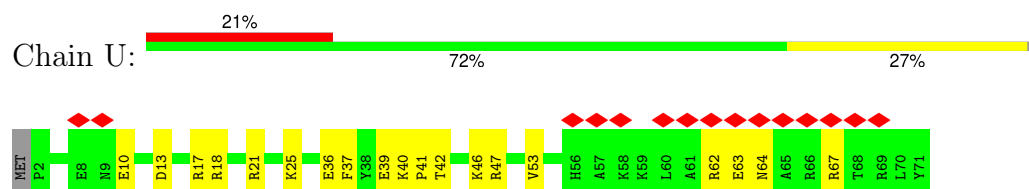
- Molecule 24: Small ribosomal subunit protein uS19



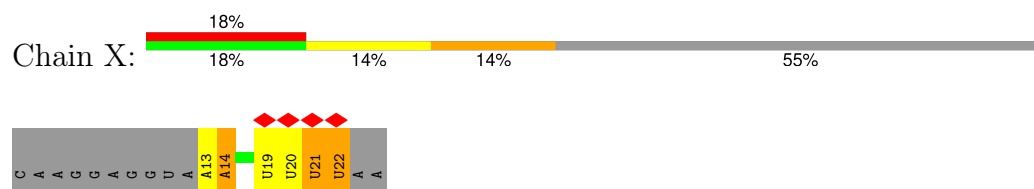
- Molecule 25: Small ribosomal subunit protein bS20



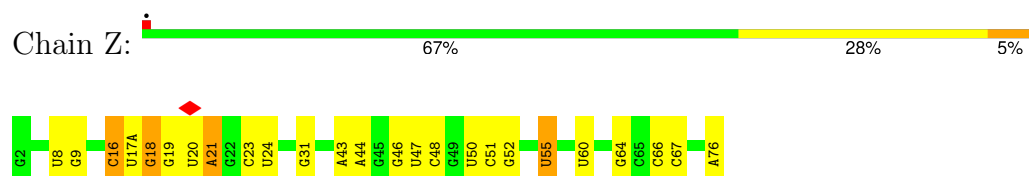
- Molecule 26: Small ribosomal subunit protein bS21



- Molecule 27: mRNA



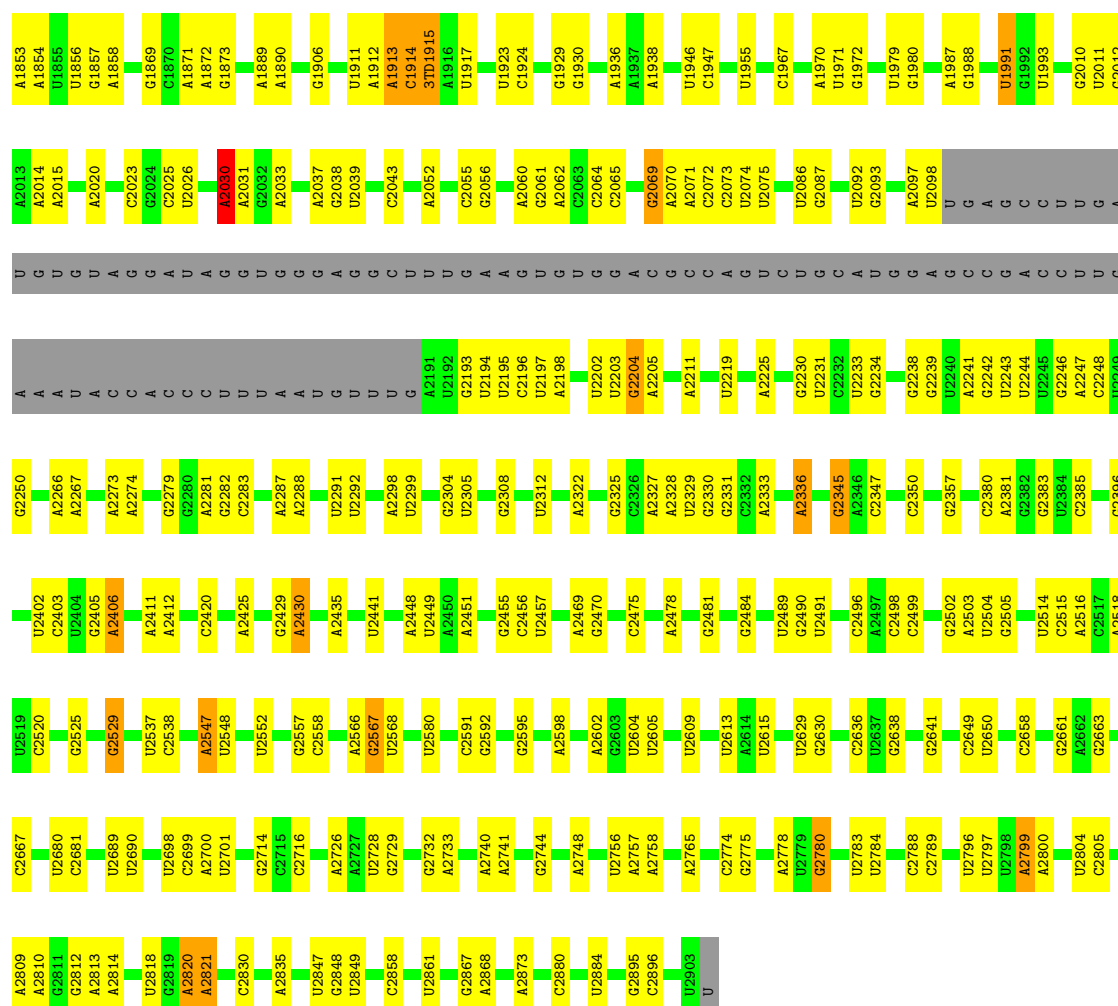
- Molecule 28: P-site tRNA



- Molecule 29: 23S rRNA







• Molecule 30: 5S rRNA

Chain b: 72% 25% ..



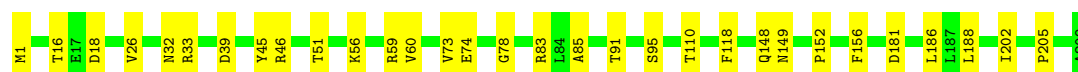
• Molecule 31: 50S ribosomal protein L2

Chain c: 89% 11% .



• Molecule 32: 50S ribosomal protein L3

Chain d: 85% 15%



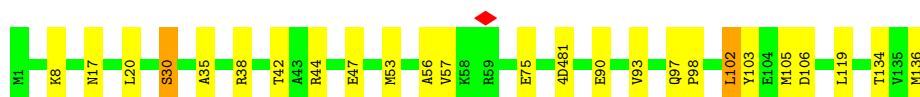
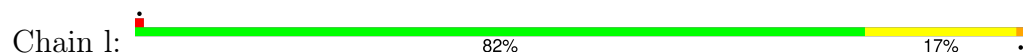
- Chain j: 92% 8%



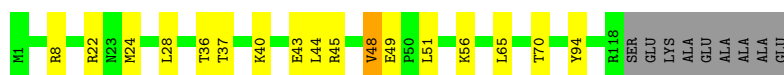
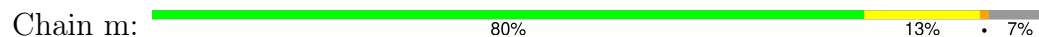
- Molecule 39: Large ribosomal subunit protein uL15



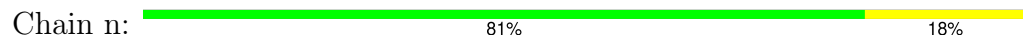
- Molecule 40: 50S ribosomal protein L16



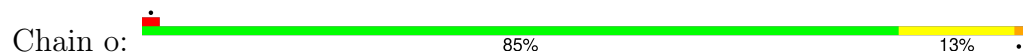
- Molecule 41: Large ribosomal subunit protein bL17



- Molecule 42: Large ribosomal subunit protein uL18



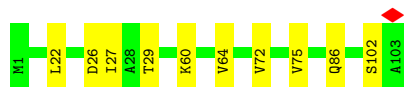
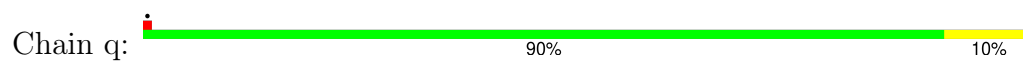
- Molecule 43: Large ribosomal subunit protein bL19



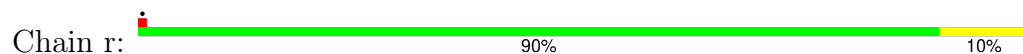
- Molecule 44: 50S ribosomal protein L20



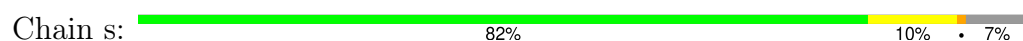
- Molecule 45: Ribosomal protein L21



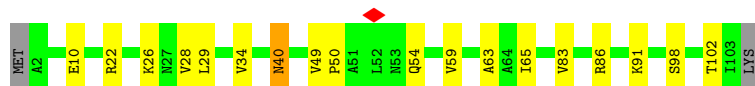
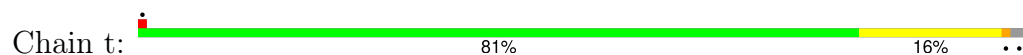
- Molecule 46: 50S ribosomal protein L22



- Molecule 47: 50S ribosomal protein L23



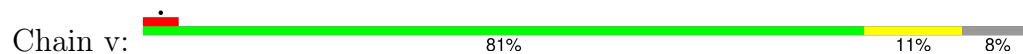
- Molecule 48: 50S ribosomal protein L24



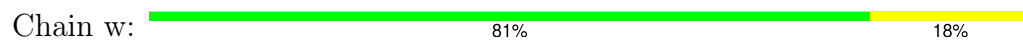
- Molecule 49: Large ribosomal subunit protein bL25




- Molecule 50: 50S ribosomal protein L27

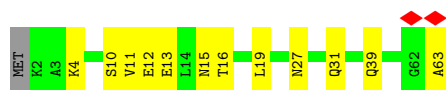


- Molecule 51: 50S ribosomal protein L28




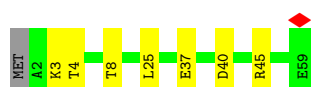
- Molecule 52: Large ribosomal subunit protein uL29

Chain x:  79% 19%



- Molecule 53: 50S ribosomal protein L30

Chain y:  86% 12%



- Molecule 54: 50S ribosomal protein L32

Chain z:  93% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	234706	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.743	Depositor
Minimum map value	-0.230	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	470.80002, 470.80002, 470.80002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, UR3, MA6, 2MA, MEQ, OMU, 5MU, G7M, V7A, 3TD, 6MZ, 5MC, 4SU, 1MG, 2MG, D2T, ZN, PSU, K, MG, OMG, 4OC, 4D4, H2U

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	0	0.20	0/424	0.38	0/565
2	1	0.24	0/380	0.29	0/498
3	2	0.22	0/513	0.29	0/676
4	3	0.22	0/303	0.25	0/397
5	4	0.17	0/488	0.38	0/649
6	A	0.22	0/35787	0.28	0/55816
7	B	0.16	0/1784	0.39	0/2403
8	C	0.16	0/1651	0.32	0/2225
9	D	0.16	0/1665	0.27	0/2227
10	E	0.20	0/1165	0.35	0/1568
11	F	0.22	0/858	0.44	0/1160
12	G	0.17	0/1219	0.34	0/1635
13	H	0.20	0/989	0.38	0/1326
14	I	0.17	0/1034	0.36	0/1375
15	J	0.21	0/796	0.47	0/1077
16	K	0.19	0/893	0.34	0/1205
17	L	0.24	0/960	0.40	0/1286
18	M	0.18	0/900	0.38	0/1204
19	N	0.28	0/817	0.48	0/1088
20	O	0.20	0/722	0.39	0/964
21	P	0.19	0/653	0.35	0/877
22	Q	0.18	0/650	0.32	0/871
23	R	0.19	0/553	0.34	0/742
24	S	0.18	0/685	0.39	0/922
25	T	0.21	0/676	0.33	0/895
26	U	0.15	0/597	0.29	0/792
27	X	0.17	0/235	0.24	0/363
28	Z	0.23	0/1703	0.32	0/2655
29	a	0.29	0/65651	0.33	0/102413
30	b	0.21	0/2850	0.24	0/4444
31	c	0.26	0/2121	0.37	1/2852 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	d	0.23	0/1576	0.30	0/2119
33	e	0.21	0/1571	0.29	0/2113
34	f	0.16	0/1434	0.31	0/1926
35	g	0.23	0/1343	0.44	0/1816
36	h	0.18	0/306	0.53	0/413
37	i	0.22	0/1152	0.31	0/1551
38	j	0.23	0/955	0.31	0/1279
39	k	0.21	0/1062	0.27	0/1413
40	l	0.25	0/1081	0.36	0/1443
41	m	0.24	0/958	0.35	0/1281
42	n	0.18	0/902	0.33	0/1209
43	o	0.23	0/929	0.34	0/1242
44	p	0.24	0/960	0.30	0/1278
45	q	0.24	0/829	0.47	0/1107
46	r	0.22	0/864	0.33	0/1156
47	s	0.22	0/744	0.42	0/994
48	t	0.21	0/787	0.42	0/1051
49	u	0.20	0/766	0.32	0/1025
50	v	0.21	0/593	0.29	0/785
51	w	0.23	0/635	0.29	0/848
52	x	0.23	0/502	0.49	0/667
53	y	0.20	0/453	0.30	0/605
54	z	0.22	0/450	0.31	0/599
All	All	0.25	0/150574	0.32	1/225090 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	146	MET	N-CA-C	-5.39	107.25	113.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	417	0	451	3	0
2	1	377	0	418	3	0
3	2	504	0	572	8	0
4	3	302	0	340	3	0
5	4	480	0	482	11	0
6	A	32211	0	16225	283	0
7	B	1753	0	1780	42	0
8	C	1624	0	1696	34	0
9	D	1643	0	1707	29	0
10	E	1152	0	1196	24	0
11	F	839	0	833	29	0
12	G	1203	0	1254	28	0
13	H	979	0	1031	14	0
14	I	1022	0	1070	30	0
15	J	786	0	828	32	0
16	K	877	0	887	20	0
17	L	957	0	1017	18	0
18	M	891	0	952	12	0
19	N	805	0	844	30	0
20	O	714	0	734	19	0
21	P	643	0	661	10	0
22	Q	641	0	682	9	0
23	R	544	0	565	10	0
24	S	668	0	693	17	0
25	T	670	0	719	11	0
26	U	589	0	629	12	0
27	X	211	0	106	5	0
28	Z	1605	0	818	11	0
29	a	59130	0	29757	404	0
30	b	2549	0	1288	20	0
31	c	2082	0	2154	17	0
32	d	1566	0	1618	19	0
33	e	1552	0	1619	7	0
34	f	1410	0	1444	18	0
35	g	1323	0	1371	32	0
36	h	303	0	327	9	0
37	i	1129	0	1162	16	0
38	j	946	0	1023	7	0
39	k	1053	0	1129	7	0
40	l	1075	0	1154	14	0
41	m	945	0	989	10	0
42	n	892	0	923	13	0
43	o	917	0	962	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	p	947	0	1019	4	0
45	q	816	0	839	2	0
46	r	857	0	922	6	0
47	s	738	0	807	10	0
48	t	779	0	831	9	0
49	u	753	0	780	19	0
50	v	586	0	596	5	0
51	w	625	0	652	7	0
52	x	501	0	531	10	0
53	y	449	0	488	4	0
54	z	444	0	458	2	0
55	3	1	0	0	0	0
56	A	62	0	0	0	0
56	a	211	0	0	0	0
56	b	5	0	0	0	0
56	m	1	0	0	0	0
56	p	2	0	0	0	0
57	A	24	0	0	0	0
57	a	75	0	0	0	0
57	b	1	0	0	0	0
58	A	35	0	0	0	0
58	a	35	0	0	1	0
59	0	1	0	0	0	0
59	1	3	0	0	0	0
59	2	3	0	0	1	0
59	3	1	0	0	0	0
59	A	123	0	0	0	0
59	O	1	0	0	0	0
59	U	1	0	0	0	0
59	a	1091	0	0	0	0
59	b	14	0	0	0	0
59	c	6	0	0	0	0
59	d	5	0	0	0	0
59	e	5	0	0	0	0
59	i	2	0	0	0	0
59	k	2	0	0	0	0
59	l	1	0	0	0	0
59	m	5	0	0	0	0
59	o	1	0	0	0	0
59	p	4	0	0	0	0
59	q	7	0	0	0	0
59	r	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	s	2	0	0	0	0
59	v	1	0	0	0	0
59	y	2	0	0	0	0
59	z	3	0	0	0	0
All	All	141212	0	94033	1323	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 6.

All (1323) 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)
29:a:881:G:H1	29:a:895:U:H3	1.09	0.97
6:A:1086:U:H3	6:A:1099:G:H22	1.21	0.88
5:4:60:PHE:O	5:4:64:PHE:HB2	1.76	0.85
5:4:59:ARG:HA	5:4:62:LYS:HD3	1.59	0.82
29:a:1047:G:HO2'	29:a:1110:G:H1	1.26	0.82
6:A:76:G:H1	6:A:93:U:H3	1.27	0.80
14:I:84:THR:HG23	14:I:98:LEU:HD13	1.64	0.79
35:g:10:VAL:HG13	35:g:48:ASN:HD22	1.47	0.78
37:i:96:ARG:NH2	37:i:98:GLU:OE2	2.20	0.75
6:A:1026:G:O6	6:A:1035:A:N1	2.20	0.74
34:f:119:ALA:HB1	34:f:167:ARG:HH12	1.53	0.74
42:n:88:LYS:NZ	42:n:89:ASP:OD2	2.20	0.74
15:J:10:LEU:HB3	15:J:18:ILE:HD11	1.69	0.74
5:4:59:ARG:NH2	6:A:1311:A:OP1	2.21	0.73
6:A:673:A:H2'	6:A:674:G:C8	2.22	0.73
47:s:38:ALA:O	47:s:81:LYS:NZ	2.21	0.73
6:A:1493:A:H1'	29:a:1913:A:H61	1.54	0.72
15:J:28:THR:HG21	15:J:90:LEU:HD21	1.71	0.72
29:a:1802:A:H2'	29:a:1803:A:C8	2.24	0.72
30:b:117:G:OP1	42:n:56:LYS:NZ	2.23	0.72
7:B:133:GLU:HA	7:B:136:MET:HG3	1.71	0.72
33:e:97:ASN:HB2	33:e:100:MET:HG3	1.69	0.72
31:c:107:PRO:HD2	31:c:110:LEU:HD22	1.72	0.71
6:A:1124:G:N2	6:A:1125:U:O4	2.22	0.71
46:r:4:ILE:HG13	46:r:106:VAL:HG22	1.71	0.71
38:j:110:GLU:OE2	38:j:110:GLU:N	2.22	0.71
18:M:50:GLU:N	18:M:50:GLU:OE2	2.24	0.71
8:C:110:GLU:HB2	8:C:144:LEU:HD22	1.73	0.70
14:I:59:GLU:OE2	14:I:59:GLU:N	2.24	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:7:GLU:OE1	1:0:27:LYS:HE3	1.91	0.70
5:4:10:GLU:OE1	5:4:10:GLU:N	2.24	0.70
17:L:25:GLU:OE1	17:L:59:ASN:ND2	2.23	0.70
19:N:26:GLU:O	19:N:30:ILE:HD12	1.91	0.70
6:A:202:G:H21	6:A:466:A:H61	1.39	0.70
26:U:13:ASP:OD1	26:U:17:ARG:NH2	2.25	0.70
6:A:1381:U:H1'	12:G:79:ARG:HH12	1.56	0.69
9:D:126:ASN:ND2	9:D:141:ASP:OD1	2.25	0.69
7:B:86:SER:O	7:B:222:ARG:NH2	2.26	0.69
31:c:199:GLU:OE1	31:c:199:GLU:N	2.21	0.69
10:E:13:GLU:OE2	10:E:68:ARG:NH1	2.25	0.68
29:a:546:U:H3'	29:a:547:A:H8	1.57	0.68
26:U:40:LYS:HD2	26:U:42:THR:HG22	1.74	0.68
41:m:22:ARG:HG2	41:m:70:THR:HA	1.75	0.68
23:R:45:THR:HG1	23:R:47:THR:HG1	1.38	0.68
15:J:8:ILE:HD11	15:J:74:VAL:HB	1.75	0.68
6:A:1060:U:H5''	15:J:53:ILE:HD12	1.75	0.68
7:B:217:VAL:O	7:B:221:VAL:HG12	1.93	0.68
29:a:848:C:H2'	29:a:849:A:H8	1.59	0.68
42:n:50:ALA:O	42:n:81:ARG:NH1	2.27	0.68
9:D:11:LEU:HD13	9:D:63:ARG:HG2	1.76	0.68
35:g:2:SER:OG	35:g:3:ARG:N	2.22	0.68
29:a:286:U:H2'	29:a:287:G:C8	2.29	0.67
29:a:993:G:OP2	44:p:51:ARG:NH2	2.27	0.67
26:U:64:ASN:HA	26:U:67:ARG:HH12	1.59	0.67
7:B:133:GLU:O	7:B:137:ARG:HG2	1.93	0.67
29:a:1047:G:N2	29:a:1110:G:O2'	2.28	0.67
36:h:7:ASP:OD1	36:h:8:LYS:N	2.27	0.67
30:b:66:A:H61	30:b:107:G:H2'	1.59	0.67
40:l:20:LEU:HD13	49:u:81:PRO:HG2	1.76	0.67
29:a:1392:A:N6	47:s:18:GLU:OE1	2.24	0.66
9:D:147:GLU:HA	9:D:150:LYS:HG3	1.77	0.66
15:J:6:ILE:HD11	15:J:102:LEU:HD23	1.78	0.66
11:F:16:GLU:OE2	11:F:16:GLU:N	2.20	0.66
28:Z:21:A:H61	28:Z:46:G:H2'	1.60	0.66
6:A:946:A:H2'	6:A:947:G:C8	2.31	0.66
29:a:639:U:H2'	29:a:640:C:C6	2.30	0.66
37:i:95:ARG:HG3	37:i:95:ARG:HH11	1.60	0.66
6:A:147:G:H2'	6:A:148:G:C8	2.31	0.65
32:d:1:MET:HB3	32:d:205:PRO:HG2	1.79	0.65
7:B:219:ALA:O	7:B:223:GLU:HG2	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1071:C:H2'	6:A:1072:G:H8	1.62	0.65
6:A:1106:G:O2'	8:C:169:ARG:NH1	2.31	0.65
6:A:1152:A:OP1	15:J:70:HIS:ND1	2.30	0.65
12:G:15:ASP:HB3	12:G:20:SER:H	1.62	0.65
38:j:43:ILE:HD12	38:j:56:ASP:HB2	1.78	0.65
6:A:203:G:O2'	6:A:465:A:N1	2.29	0.64
6:A:1356:G:H2'	6:A:1357:A:C8	2.31	0.64
12:G:67:GLU:OE1	12:G:70:ARG:NH2	2.27	0.64
30:b:1:U:H2'	30:b:2:G:H8	1.62	0.64
16:K:56:ARG:HG3	16:K:56:ARG:HH11	1.61	0.64
24:S:50:ALA:HB1	24:S:57:HIS:HB3	1.78	0.64
43:o:5:ILE:O	43:o:9:GLU:HG3	1.98	0.64
48:t:10:GLU:OE2	48:t:22:ARG:NH1	2.29	0.64
8:C:135:LYS:O	8:C:139:GLN:HG2	1.97	0.64
16:K:83:GLU:HG2	16:K:109:ASN:HB2	1.80	0.64
51:w:74:ARG:NH2	51:w:76:GLU:OE1	2.31	0.64
29:a:139:U:H5''	29:a:140:C:H5	1.62	0.64
31:c:133:ARG:NH1	31:c:187:ASP:OD1	2.31	0.64
8:C:63:SER:HB3	8:C:98:PRO:HG2	1.78	0.64
9:D:27:ALA:HB3	9:D:30:THR:HG23	1.78	0.64
12:G:74:GLU:HG2	12:G:91:VAL:HG22	1.78	0.64
19:N:89:MET:HE2	19:N:89:MET:HA	1.80	0.64
29:a:546:U:H3'	29:a:547:A:C8	2.32	0.64
26:U:21:ARG:O	26:U:25:LYS:HG2	1.97	0.64
29:a:2328:A:H2'	29:a:2329:U:C6	2.33	0.64
39:k:82:LEU:HD22	39:k:90:VAL:HG21	1.79	0.64
29:a:100:U:O2	48:t:91:LYS:NZ	2.30	0.63
29:a:1469:A:H2'	29:a:1470:A:C8	2.34	0.63
15:J:66:GLU:HB2	19:N:99:ALA:HB2	1.80	0.63
35:g:173:GLU:N	35:g:173:GLU:OE1	2.32	0.63
7:B:108:ARG:HA	7:B:111:ILE:HG22	1.80	0.63
29:a:307:G:N1	29:a:310:A:OP2	2.28	0.63
7:B:131:LYS:HD2	7:B:131:LYS:O	1.99	0.63
6:A:492:C:H2'	6:A:493:A:C8	2.33	0.62
35:g:22:GLN:NE2	35:g:41:VAL:O	2.32	0.62
16:K:22:HIS:HB2	16:K:33:THR:HG22	1.80	0.62
46:r:1:MET:HA	46:r:1:MET:HE2	1.81	0.62
37:i:128:ASN:O	37:i:128:ASN:ND2	2.31	0.62
13:H:47:GLU:HG3	13:H:64:LYS:HB3	1.82	0.62
48:t:86:ARG:NH2	48:t:102:THR:OG1	2.33	0.62
26:U:10:GLU:OE2	26:U:18:ARG:NH2	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:880:G:H2'	29:a:881:G:C8	2.35	0.62
10:E:151:GLU:OE2	10:E:151:GLU:N	2.24	0.62
49:u:35:GLU:N	49:u:35:GLU:OE2	2.32	0.62
6:A:35:G:N3	17:L:115:SER:OG	2.33	0.61
6:A:539:A:H2'	6:A:540:G:C8	2.35	0.61
8:C:77:ILE:HA	8:C:84:VAL:HG13	1.81	0.61
6:A:713:G:H2'	6:A:714:G:C8	2.35	0.61
16:K:64:GLN:O	16:K:68:GLU:HG3	2.00	0.61
14:I:28:ILE:HG21	14:I:35:LEU:HB2	1.81	0.61
29:a:286:U:H2'	29:a:287:G:H8	1.64	0.61
37:i:125:TYR:OH	37:i:132:HIS:NE2	2.34	0.61
29:a:138:U:H4'	47:s:1:MET:HE1	1.82	0.61
29:a:191:A:H2'	29:a:192:C:C6	2.36	0.61
6:A:555:U:H2'	6:A:556:C:C6	2.35	0.61
6:A:714:G:H2'	6:A:715:A:C8	2.35	0.61
15:J:12:ALA:HB2	15:J:18:ILE:HD13	1.83	0.61
36:h:37:VAL:HG22	36:h:38:PRO:HD2	1.83	0.61
29:a:197:A:N6	29:a:2430:A:O2'	2.34	0.61
37:i:114:LEU:HG	37:i:118:MET:HE3	1.83	0.61
8:C:130:PHE:O	8:C:134:MET:HG3	2.01	0.61
19:N:24:ARG:NH1	19:N:55:SER:OG	2.33	0.61
8:C:62:LYS:N	8:C:62:LYS:HE2	2.16	0.61
35:g:60:ASP:OD1	35:g:60:ASP:N	2.27	0.61
29:a:1816:C:N4	31:c:35:GLU:OE1	2.29	0.60
6:A:1218:C:H2'	6:A:1219:A:C8	2.36	0.60
6:A:674:G:H2'	6:A:675:A:H8	1.66	0.60
20:O:8:THR:O	20:O:12:VAL:HG23	2.01	0.60
30:b:9:G:HO2'	42:n:45:SER:HG	1.47	0.60
7:B:213:TYR:O	7:B:217:VAL:HG23	2.01	0.60
31:c:203:ARG:HG3	31:c:203:ARG:HH11	1.66	0.60
42:n:60:GLU:OE1	42:n:61:GLN:NE2	2.34	0.60
6:A:664:G:H22	6:A:741:G:H1	1.50	0.60
6:A:677:U:H3	6:A:713:G:H22	1.46	0.60
25:T:39:ILE:HD11	25:T:83:ILE:HG13	1.82	0.60
35:g:11:VAL:N	35:g:48:ASN:O	2.32	0.60
13:H:29:SER:HB3	13:H:57:PRO:HB2	1.82	0.60
29:a:75:G:H22	29:a:111:A:H2	1.50	0.60
29:a:2728:U:HO2'	29:a:2729:G:H8	1.49	0.60
29:a:1590:A:H2'	29:a:1591:A:H8	1.65	0.60
52:x:11:VAL:O	52:x:15:ASN:ND2	2.31	0.60
6:A:36:C:OP1	17:L:120:LYS:NZ	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:127:G:O2'	22:Q:6:ARG:NH1	2.35	0.59
29:a:568:U:H1'	29:a:2030:6MZ:H9C1	1.82	0.59
6:A:1363:A:O2'	6:A:1365:G:N7	2.35	0.59
38:j:106:GLU:OE2	38:j:106:GLU:N	2.34	0.59
6:A:1360:A:OP2	19:N:75:ARG:NH2	2.35	0.59
15:J:19:ASP:OD1	15:J:20:GLN:N	2.35	0.59
29:a:593:U:H2'	29:a:594:U:C6	2.37	0.59
29:a:1796:U:H2'	29:a:1797:G:H8	1.67	0.59
9:D:72:PHE:HE1	9:D:94:LEU:HD11	1.66	0.59
20:O:26:GLU:OE2	20:O:77:ARG:NH1	2.35	0.59
29:a:2243:U:H2'	29:a:2244:U:C6	2.37	0.59
51:w:72:ARG:NH1	51:w:78:TYR:OH	2.35	0.59
52:x:27:ASN:O	52:x:31:GLN:HG3	2.02	0.59
29:a:1590:A:H2'	29:a:1591:A:C8	2.37	0.59
50:v:70:GLU:HG3	50:v:72:LYS:HG3	1.83	0.59
15:J:8:ILE:CD1	15:J:74:VAL:HB	2.33	0.59
29:a:279:A:N6	29:a:361:G:H1'	2.17	0.59
29:a:2071:A:H2'	29:a:2072:C:C6	2.38	0.59
29:a:111:A:H4'	52:x:63:ALA:HB1	1.83	0.59
6:A:337:G:H2'	6:A:338:A:C8	2.38	0.59
29:a:856:G:H2'	29:a:857:G:C8	2.38	0.59
34:f:14:LYS:O	34:f:18:THR:HG23	2.01	0.59
45:q:75:VAL:HG22	45:q:86:GLN:HG2	1.85	0.59
7:B:87:CYS:SG	7:B:221:VAL:HG13	2.43	0.58
15:J:42:LEU:HB2	15:J:71:LEU:HB3	1.86	0.58
29:a:278:A:OP2	29:a:361:G:N2	2.35	0.58
49:u:11:GLU:N	49:u:11:GLU:OE2	2.35	0.58
6:A:1298:U:OP2	12:G:114:LYS:NZ	2.34	0.58
29:a:2667:C:N3	35:g:110:SER:OG	2.35	0.58
32:d:46:ARG:NH1	32:d:85:ALA:O	2.35	0.58
29:a:1115:G:O2'	29:a:1116:G:O5'	2.20	0.58
8:C:86:LYS:O	8:C:90:VAL:HG22	2.04	0.58
6:A:1530:G:O6	26:U:46:LYS:NZ	2.37	0.58
6:A:384:G:H2'	6:A:385:C:C6	2.39	0.58
14:I:55:VAL:HG11	14:I:87:LEU:HD11	1.84	0.58
6:A:437:U:H4'	9:D:152:GLN:HE21	1.69	0.58
10:E:13:GLU:HG2	10:E:39:VAL:HG12	1.86	0.58
6:A:1323:G:H2'	6:A:1324:A:C8	2.38	0.57
14:I:21:ILE:HG12	14:I:63:LEU:HD22	1.84	0.57
29:a:1746:A:H2'	29:a:1747:U:C6	2.39	0.57
33:e:1:MET:HB3	33:e:14:VAL:HG23	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:53:ARG:HH21	24:S:37:ARG:NH2	2.00	0.57
34:f:38:MET:HE3	34:f:57:LEU:HB2	1.85	0.57
52:x:13:GLU:HA	52:x:16:THR:HG22	1.85	0.57
29:a:189:G:OP2	51:w:14:THR:HG21	2.03	0.57
29:a:476:G:N1	29:a:479:A:OP2	2.34	0.57
14:I:65:ILE:HG21	14:I:79:ILE:HG12	1.87	0.57
29:a:2205:A:H61	29:a:2219:U:H3	1.52	0.57
20:O:18:ASP:OD1	20:O:19:ALA:N	2.37	0.57
37:i:43:GLU:N	37:i:43:GLU:OE2	2.38	0.57
42:n:4:LYS:O	42:n:8:ILE:HG12	2.03	0.57
6:A:459:A:H2'	6:A:460:A:C8	2.39	0.57
9:D:87:GLY:HA3	9:D:197:GLU:HG3	1.86	0.57
12:G:51:ALA:HB2	12:G:58:GLU:HG3	1.86	0.57
35:g:44:LYS:HE3	35:g:44:LYS:HA	1.87	0.57
40:l:75:GLU:HG3	40:l:90:GLU:HG3	1.86	0.57
6:A:460:A:H2'	6:A:461:A:H8	1.68	0.57
7:B:68:LEU:HD22	7:B:154:MET:HE1	1.86	0.57
16:K:56:ARG:HG3	16:K:56:ARG:NH1	2.20	0.57
29:a:2086:U:H2'	29:a:2087:G:C8	2.40	0.57
30:b:1:U:H2'	30:b:2:G:C8	2.39	0.57
29:a:608:A:H2'	29:a:609:A:C8	2.39	0.57
29:a:1527:G:N1	29:a:1544:A:OP2	2.33	0.56
6:A:1377:A:OP1	12:G:92:ARG:NH2	2.38	0.56
13:H:69:LYS:NZ	13:H:69:LYS:HB3	2.20	0.56
29:a:1047:G:O2'	29:a:1110:G:N1	2.36	0.56
29:a:2291:U:H2'	29:a:2292:U:C6	2.39	0.56
5:4:26:SER:OG	5:4:27:THR:N	2.38	0.56
6:A:524:G:H2'	6:A:525:C:C6	2.40	0.56
6:A:1062:U:H2'	6:A:1063:C:C6	2.40	0.56
20:O:71:LYS:HD3	20:O:78:TYR:CE2	2.40	0.56
29:a:2430:A:N3	29:a:2430:A:H2'	2.20	0.56
34:f:145:LYS:HD2	34:f:145:LYS:N	2.20	0.56
6:A:1005:A:N6	6:A:1024:G:O2'	2.38	0.56
17:L:73:ASN:O	17:L:75:GLN:NE2	2.39	0.56
6:A:187:G:N2	6:A:190:A:OP2	2.35	0.56
6:A:459:A:H2'	6:A:460:A:H8	1.70	0.56
10:E:115:LEU:HD13	10:E:123:VAL:HG11	1.87	0.56
29:a:1405:U:H2'	29:a:1406:U:C6	2.40	0.56
7:B:56:GLU:O	7:B:60:ILE:HD12	2.06	0.56
15:J:10:LEU:HB2	15:J:72:ARG:HB2	1.86	0.56
6:A:56:U:H2'	6:A:57:G:C8	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1255:G:O2'	6:A:1258:G:N3	2.33	0.56
10:E:61:GLN:O	10:E:65:GLU:HG2	2.05	0.56
29:a:2469:A:N6	29:a:2481:G:O2'	2.35	0.56
11:F:18:VAL:HA	11:F:21:MET:HE3	1.88	0.56
34:f:119:ALA:O	34:f:167:ARG:NH2	2.38	0.56
42:n:56:LYS:O	42:n:60:GLU:HG3	2.05	0.56
47:s:3:ARG:NH2	47:s:5:GLU:OE2	2.39	0.56
28:Z:50:U:H2'	28:Z:51:C:C6	2.40	0.56
29:a:1000:A:H2'	29:a:1001:A:C8	2.41	0.56
4:3:16:ILE:HD13	4:3:25:VAL:HG22	1.87	0.56
7:B:123:ASP:OD1	7:B:125:THR:OG1	2.23	0.56
6:A:690:G:O6	16:K:53:ARG:NH2	2.39	0.55
24:S:48:THR:HG22	24:S:61:PHE:HD1	1.71	0.55
6:A:131:A:H2'	6:A:132:C:C6	2.41	0.55
29:a:964:C:O2'	29:a:2273:A:N3	2.37	0.55
6:A:1086:U:H3	6:A:1099:G:N2	2.00	0.55
20:O:78:TYR:O	20:O:82:ILE:HG23	2.07	0.55
6:A:1412:C:H2'	6:A:1413:A:C8	2.42	0.55
10:E:44:GLY:O	10:E:74:VAL:N	2.37	0.55
32:d:110:THR:HG23	32:d:202:ILE:HB	1.87	0.55
48:t:28:VAL:HG22	48:t:34:VAL:HG12	1.88	0.55
12:G:70:ARG:NH1	12:G:97:ASN:OD1	2.39	0.55
19:N:46:LEU:HD12	24:S:13:LEU:HD13	1.89	0.55
29:a:851:C:H2'	29:a:852:U:C6	2.42	0.55
6:A:17:U:H2'	6:A:18:C:C6	2.42	0.55
6:A:235:C:H2'	6:A:236:A:H8	1.71	0.55
8:C:35:SER:OG	8:C:59:ARG:NH2	2.40	0.55
12:G:68:ASN:OD1	12:G:130:ASN:ND2	2.39	0.55
29:a:219:A:N3	29:a:234:U:O2'	2.37	0.55
29:a:882:G:O6	29:a:894:U:O2	2.24	0.55
32:d:16:THR:OG1	32:d:18:ASP:OD1	2.23	0.55
41:m:8:ARG:HD2	41:m:43:GLU:HG2	1.89	0.55
6:A:56:U:H2'	6:A:57:G:H8	1.72	0.55
7:B:65:GLY:O	7:B:225:ARG:NH2	2.36	0.55
29:a:155:A:H2'	29:a:156:A:C8	2.42	0.55
6:A:481:G:O2'	6:A:483:C:N4	2.39	0.55
19:N:46:LEU:HB3	24:S:13:LEU:HD22	1.89	0.55
6:A:460:A:H2'	6:A:461:A:C8	2.42	0.55
6:A:1077:G:N2	6:A:1080:A:OP2	2.35	0.55
11:F:5:GLU:OE1	11:F:63:ASN:ND2	2.37	0.54
18:M:30:SER:O	18:M:34:LEU:HD23	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:1733:G:H2'	29:a:1734:G:H8	1.71	0.54
10:E:159:LYS:HD3	10:E:163:GLU:OE1	2.08	0.54
11:F:73:GLU:O	11:F:77:THR:HG22	2.07	0.54
22:Q:76:VAL:HG12	22:Q:77:ARG:HG2	1.90	0.54
38:j:58:LEU:HD11	38:j:86:LEU:HD13	1.88	0.54
6:A:996:A:H2'	6:A:997:U:C6	2.42	0.54
10:E:93:ARG:HG3	10:E:93:ARG:HH11	1.72	0.54
41:m:24:MET:HE1	41:m:40:LYS:HD3	1.90	0.54
15:J:40:ILE:CD1	15:J:73:LEU:HB3	2.37	0.54
15:J:65:TYR:HB3	19:N:96:LEU:HD11	1.90	0.54
29:a:96:C:OP1	52:x:39:GLN:NE2	2.40	0.54
6:A:1071:C:H2'	6:A:1072:G:C8	2.43	0.54
6:A:1513:A:H2'	6:A:1514:G:C8	2.42	0.54
7:B:153:ASP:OD1	7:B:153:ASP:N	2.41	0.54
14:I:114:LYS:NZ	14:I:118:LEU:O	2.41	0.54
30:b:66:A:N6	30:b:107:G:H2'	2.23	0.54
6:A:1251:A:H2'	6:A:1252:A:C8	2.43	0.54
18:M:66:GLU:OE2	18:M:66:GLU:HA	2.08	0.54
29:a:2074:U:H2'	29:a:2075:U:C6	2.43	0.54
5:4:58:ASP:OD1	5:4:58:ASP:N	2.41	0.54
6:A:1391:U:H2'	6:A:1392:G:C8	2.42	0.54
29:a:2052:A:H4'	32:d:148:GLN:O	2.08	0.54
31:c:167:ARG:HG3	31:c:172:VAL:HG12	1.89	0.54
35:g:149:ARG:NH1	35:g:167:GLU:OE2	2.41	0.54
39:k:132:ARG:HG3	39:k:142:ILE:HD12	1.90	0.54
6:A:235:C:H2'	6:A:236:A:C8	2.43	0.54
6:A:269:C:H2'	6:A:270:A:C8	2.42	0.54
11:F:2:ARG:HD3	11:F:91:ARG:NH1	2.23	0.54
19:N:42:TRP:O	19:N:46:LEU:HD22	2.07	0.54
29:a:1597:A:H5''	29:a:1598:A:H5'	1.89	0.54
26:U:62:ARG:HH12	26:U:63:GLU:HB2	1.73	0.53
29:a:848:C:H2'	29:a:849:A:C8	2.42	0.53
29:a:876:C:H2'	29:a:877:A:O4'	2.07	0.53
35:g:164:TYR:HB2	35:g:167:GLU:HB2	1.90	0.53
40:l:38:ARG:HB2	40:l:98:PRO:HD3	1.90	0.53
7:B:114:LEU:HD13	7:B:144:LEU:HB3	1.88	0.53
19:N:49:GLN:NE2	24:S:12:ASP:HA	2.24	0.53
29:a:279:A:H2'	29:a:280:U:O4'	2.08	0.53
29:a:1198:U:H2'	29:a:1199:U:C6	2.43	0.53
29:a:2246:G:H2'	29:a:2247:A:C8	2.44	0.53
29:a:2547:A:H2'	29:a:2548:U:C6	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:h:11:ASN:O	36:h:11:ASN:ND2	2.41	0.53
40:l:35:ALA:HB2	40:l:102:LEU:HD21	1.91	0.53
10:E:101:GLU:CD	10:E:101:GLU:H	2.15	0.53
29:a:538:A:O2'	37:i:9:GLU:OE1	2.25	0.53
29:a:813:U:H2'	29:a:814:C:C6	2.44	0.53
6:A:923:A:O2'	6:A:1399:C:OP2	2.24	0.53
29:a:833:A:H2'	29:a:834:G:C8	2.43	0.53
29:a:1432:G:H2'	29:a:1433:A:C8	2.43	0.53
29:a:1889:A:H2'	29:a:1890:A:C8	2.43	0.53
20:O:6:GLU:CD	20:O:6:GLU:H	2.17	0.53
29:a:2788:C:H2'	29:a:2789:C:C6	2.44	0.53
44:p:86:ALA:HB2	44:p:116:ALA:HB2	1.89	0.53
6:A:1038:C:H2'	6:A:1039:G:H8	1.72	0.53
7:B:67:ILE:HD12	7:B:160:ALA:HB3	1.90	0.53
17:L:110:ARG:HB3	17:L:119:VAL:HG21	1.91	0.53
29:a:475:C:O2	29:a:479:A:N6	2.34	0.53
29:a:851:C:H2'	29:a:852:U:H6	1.74	0.53
11:F:46:GLN:HG3	11:F:56:LYS:NZ	2.23	0.53
19:N:46:LEU:O	19:N:50:THR:HG22	2.09	0.53
29:a:84:A:N1	29:a:98:G:O2'	2.41	0.53
29:a:1028:A:H2'	29:a:1029:A:C8	2.43	0.53
29:a:1654:A:O2'	32:d:118:PHE:O	2.25	0.53
29:a:2514:U:H2'	29:a:2515:C:C6	2.44	0.53
6:A:683:G:N2	16:K:39:GLY:O	2.42	0.53
6:A:745:G:H2'	6:A:746:A:C8	2.44	0.53
19:N:79:LEU:HB2	19:N:84:VAL:HG23	1.91	0.53
21:P:61:VAL:HG22	21:P:67:ILE:HD11	1.90	0.53
29:a:5:A:H2'	29:a:6:A:C8	2.44	0.53
29:a:64:A:H2'	29:a:65:U:C6	2.43	0.53
37:i:95:ARG:HG2	37:i:96:ARG:HG2	1.91	0.53
6:A:382:A:H2'	6:A:383:A:C8	2.44	0.52
18:M:75:MET:HE3	18:M:75:MET:O	2.09	0.52
22:Q:53:CYS:SG	22:Q:75:LEU:HD11	2.49	0.52
29:a:1794:A:H2'	29:a:1795:C:C6	2.44	0.52
32:d:181:ASP:HB3	32:d:186:LEU:HB2	1.90	0.52
40:l:30:SER:OG	40:l:106:ASP:OD1	2.25	0.52
48:t:50:PRO:O	48:t:54:GLN:NE2	2.34	0.52
6:A:746:A:H2'	6:A:747:A:C8	2.44	0.52
11:F:69:GLU:CD	11:F:69:GLU:H	2.16	0.52
29:a:742:A:H2'	29:a:743:A:C8	2.43	0.52
41:m:24:MET:HG2	41:m:44:LEU:HD22	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:729:G:H5''	29:a:730:A:H5''	1.91	0.52
36:h:34:GLY:O	36:h:36:ALA:N	2.42	0.52
40:l:17:ASN:O	40:l:38:ARG:NH1	2.42	0.52
9:D:99:ASP:OD1	9:D:100:ASN:N	2.42	0.52
11:F:38:ARG:HB3	11:F:63:ASN:HB2	1.92	0.52
29:a:306:U:H2'	29:a:307:G:O4'	2.09	0.52
29:a:880:G:H2'	29:a:881:G:H8	1.74	0.52
6:A:715:A:H2'	6:A:716:A:C8	2.44	0.52
6:A:945:G:C2	6:A:946:A:C8	2.97	0.52
11:F:46:GLN:HG3	11:F:56:LYS:HZ2	1.74	0.52
29:a:191:A:H2'	29:a:192:C:H6	1.72	0.52
29:a:279:A:H61	29:a:361:G:H1'	1.74	0.52
29:a:2848:G:O2'	29:a:2867:G:N2	2.31	0.52
11:F:11:HIS:HB3	11:F:14:GLN:HG2	1.92	0.52
25:T:20:HIS:O	25:T:24:ARG:HG2	2.10	0.52
29:a:364:C:H2'	29:a:365:U:C6	2.45	0.52
35:g:22:GLN:HE22	35:g:55:ARG:HH21	1.57	0.52
1:0:11:LEU:HD21	1:0:34:LEU:HD23	1.91	0.52
6:A:539:A:H2'	6:A:540:G:H8	1.74	0.52
15:J:37:ARG:HB2	15:J:75:ASP:HB2	1.91	0.52
31:c:199:GLU:H	31:c:199:GLU:CD	2.14	0.52
42:n:15:ARG:NH2	42:n:95:SER:OG	2.43	0.52
6:A:501:C:H2'	6:A:502:A:C8	2.45	0.52
6:A:1013:G:N2	6:A:1016:A:OP2	2.31	0.52
6:A:1266:G:N2	6:A:1269:A:OP2	2.26	0.52
8:C:51:SER:O	8:C:51:SER:OG	2.25	0.52
19:N:32:SER:O	19:N:33:ASP:C	2.53	0.52
29:a:1720:U:H2'	29:a:1721:G:O4'	2.09	0.52
29:a:2820:A:O2'	29:a:2821:A:OP1	2.27	0.52
31:c:21:ASN:HB3	31:c:24:LEU:HG	1.90	0.52
5:4:56:ARG:O	5:4:59:ARG:HG3	2.09	0.52
29:a:151:C:H2'	29:a:152:A:H8	1.75	0.52
29:a:594:U:H2'	29:a:595:C:C6	2.45	0.52
29:a:1386:C:H2'	29:a:1387:A:C8	2.45	0.52
6:A:662:U:H2'	6:A:663:A:C8	2.45	0.51
6:A:908:A:H2'	6:A:909:A:H8	1.75	0.51
12:G:100:ALA:O	12:G:104:ILE:HG13	2.09	0.51
29:a:1747:U:H2'	29:a:1748:C:C6	2.45	0.51
8:C:131:ARG:NH1	8:C:166:GLU:OE2	2.43	0.51
11:F:88:MET:HE2	23:R:64:TYR:CD2	2.45	0.51
29:a:1548:A:H2'	29:a:1549:A:C8	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:1796:U:H2'	29:a:1797:G:C8	2.44	0.51
32:d:56:LYS:HB2	32:d:59:ARG:HB2	1.93	0.51
6:A:426:U:OP1	9:D:33:LYS:NZ	2.28	0.51
6:A:530:G:C5	27:X:22:U:H2'	2.46	0.51
6:A:1009:U:H3	6:A:1020:G:H1	1.58	0.51
7:B:167:ASP:OD1	7:B:168:HIS:N	2.43	0.51
29:a:910:A:H2'	29:a:911:A:C8	2.45	0.51
28:Z:16:C:O2'	28:Z:60:U:O3'	2.27	0.51
29:a:155:A:H2'	29:a:156:A:H8	1.76	0.51
29:a:639:U:H2'	29:a:640:C:H6	1.73	0.51
29:a:1443:U:H2'	29:a:1444:G:H8	1.76	0.51
5:4:60:PHE:O	5:4:64:PHE:CB	2.54	0.51
6:A:335:C:H2'	6:A:336:A:H8	1.75	0.51
25:T:35:VAL:HG11	25:T:79:LEU:HD13	1.93	0.51
29:a:1197:G:H2'	29:a:1198:U:H6	1.76	0.51
41:m:24:MET:HB3	41:m:44:LEU:HD13	1.93	0.51
6:A:744:C:H2'	6:A:745:G:H8	1.74	0.51
14:I:28:ILE:HD11	14:I:63:LEU:HD12	1.93	0.51
29:a:347:A:H2'	29:a:348:A:C8	2.46	0.51
29:a:581:C:H2'	29:a:582:A:C8	2.46	0.51
6:A:216:U:H2'	6:A:217:C:C6	2.44	0.51
29:a:1149:G:H2'	29:a:1150:C:C6	2.45	0.51
43:o:37:LYS:HE3	43:o:38:LYS:H	1.76	0.51
10:E:81:LEU:HB3	10:E:147:MET:SD	2.50	0.51
17:L:36:ARG:HG2	17:L:38:TYR:CD1	2.46	0.51
19:N:23:LYS:HD2	19:N:26:GLU:OE1	2.11	0.51
53:y:40:ASP:OD2	53:y:45:ARG:NH2	2.36	0.51
6:A:384:G:H2'	6:A:385:C:H6	1.75	0.51
6:A:1273:C:H2'	6:A:1274:A:O4'	2.11	0.51
17:L:68:GLY:O	17:L:99:ARG:NH1	2.44	0.51
29:a:272:A:H2'	29:a:273:G:C8	2.45	0.51
29:a:272:A:H2'	29:a:273:G:H8	1.75	0.51
29:a:543:G:H1	29:a:550:C:H42	1.58	0.51
29:a:1914:C:H2'	29:a:1915:3TD:H6	1.93	0.51
29:a:2641:G:H5''	37:i:78:THR:HB	1.93	0.51
33:e:111:GLU:O	33:e:115:GLN:HG3	2.11	0.51
6:A:908:A:H2'	6:A:909:A:C8	2.45	0.51
6:A:1218:C:H2'	6:A:1219:A:H8	1.73	0.51
24:S:15:LEU:O	24:S:19:VAL:HG12	2.10	0.51
29:a:1506:U:H2'	29:a:1507:C:H6	1.76	0.51
29:a:1808:A:H3'	29:a:1809:A:C8	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:z:43:ILE:HG22	54:z:49:TYR:HB2	1.93	0.51
28:Z:24:U:O2'	29:a:1923:U:OP1	2.29	0.50
29:a:807:U:OP2	39:k:41:ARG:NH2	2.43	0.50
31:c:29:PRO:HG2	31:c:34:LEU:HD11	1.93	0.50
42:n:12:THR:O	42:n:16:ARG:HG2	2.11	0.50
49:u:40:ILE:HD12	49:u:42:LEU:HD21	1.93	0.50
8:C:182:ILE:HD13	8:C:203:PHE:HB2	1.93	0.50
9:D:17:THR:OG1	9:D:18:ASP:N	2.43	0.50
14:I:41:ARG:NE	14:I:43:THR:OG1	2.44	0.50
29:a:597:G:O2'	39:k:11:GLY:O	2.26	0.50
29:a:1168:G:H2'	29:a:1169:A:C8	2.47	0.50
30:b:51:G:OP1	42:n:63:LYS:NZ	2.38	0.50
6:A:939:G:H2'	6:A:940:C:C6	2.47	0.50
23:R:71:THR:OG1	23:R:72:ASP:N	2.45	0.50
29:a:1594:U:H2'	29:a:1595:C:C6	2.45	0.50
29:a:1856:U:H2'	29:a:1857:G:O4'	2.11	0.50
29:a:2025:C:H2'	29:a:2026:U:C6	2.46	0.50
35:g:76:VAL:HG12	35:g:77:ILE:HD13	1.93	0.50
6:A:674:G:H2'	6:A:675:A:C8	2.45	0.50
12:G:11:LYS:HE3	12:G:11:LYS:HA	1.94	0.50
29:a:309:A:N3	29:a:329:G:O2'	2.42	0.50
29:a:1353:A:H2'	29:a:1354:A:C8	2.46	0.50
31:c:78:VAL:HG21	31:c:110:LEU:HD21	1.94	0.50
6:A:451:A:H61	6:A:481:G:H5'	1.77	0.50
8:C:12:LEU:HD11	19:N:91:GLY:HA2	1.93	0.50
9:D:148:LYS:O	9:D:151:LYS:NZ	2.44	0.50
29:a:102:U:C4	52:x:4:LYS:NZ	2.79	0.50
29:a:871:U:H2'	29:a:872:U:C6	2.46	0.50
29:a:2658:C:OP1	35:g:160:LYS:NZ	2.44	0.50
6:A:1314:C:H2'	6:A:1315:U:C6	2.45	0.50
10:E:14:LYS:HB2	10:E:14:LYS:NZ	2.27	0.50
21:P:57:ILE:HG21	21:P:75:ILE:HD11	1.94	0.50
29:a:849:A:H2'	29:a:850:U:H6	1.77	0.50
38:j:114:LYS:O	38:j:118:LEU:HD12	2.12	0.50
15:J:18:ILE:O	15:J:22:THR:HG23	2.11	0.50
18:M:27:LYS:O	18:M:31:LYS:HG3	2.11	0.50
29:a:645:C:H2'	29:a:647:G:N7	2.27	0.50
29:a:1225:G:H2'	29:a:1226:A:C8	2.47	0.50
6:A:1250:A:H2'	6:A:1251:A:C8	2.47	0.50
6:A:1494:G:HO2'	29:a:1912:A:HO2'	1.60	0.50
6:A:470:C:H2'	6:A:471:U:H6	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:816:A:OP1	6:A:1526:G:O2'	2.30	0.50
6:A:1157:A:H5'	6:A:1158:C:C6	2.46	0.50
7:B:41:ILE:HD13	7:B:202:GLY:HA2	1.94	0.50
23:R:9:LYS:HD3	23:R:46:GLY:HA2	1.94	0.50
29:a:172:A:H2'	29:a:173:A:C8	2.47	0.50
29:a:2064:C:H2'	29:a:2065:C:C6	2.47	0.50
29:a:2070:A:H2'	29:a:2071:A:C8	2.47	0.50
29:a:2092:U:OP2	36:h:27:ARG:NH1	2.44	0.50
29:a:2345:G:N3	29:a:2381:A:H2'	2.27	0.50
29:a:2591:C:H2'	29:a:2592:G:C8	2.47	0.50
52:x:12:GLU:H	52:x:12:GLU:CD	2.18	0.50
6:A:8:A:N6	9:D:206:LYS:HB2	2.26	0.49
12:G:79:ARG:HA	12:G:84:THR:HA	1.94	0.49
17:L:79:VAL:O	17:L:103:ASP:HB2	2.12	0.49
29:a:411:G:OP2	29:a:2406:A:O2'	2.29	0.49
29:a:2291:U:OP1	29:a:2380:C:O2'	2.30	0.49
50:v:15:ASP:OD1	50:v:16:SER:N	2.45	0.49
6:A:269:C:H2'	6:A:270:A:H8	1.76	0.49
6:A:1477:U:H2'	6:A:1478:U:C6	2.47	0.49
20:O:21:ASP:OD1	20:O:24:SER:HB3	2.11	0.49
26:U:40:LYS:HG2	26:U:41:PRO:HD2	1.92	0.49
29:a:1183:U:H2'	29:a:1184:U:C6	2.47	0.49
30:b:112:G:H2'	30:b:113:C:H6	1.76	0.49
6:A:701:U:OP1	6:A:702:A:O2'	2.19	0.49
6:A:728:A:H2'	6:A:729:A:C8	2.48	0.49
6:A:996:A:H2'	6:A:997:U:H6	1.76	0.49
8:C:24:ALA:HB1	8:C:28:GLU:HG2	1.94	0.49
11:F:71:ILE:O	11:F:75:GLU:HG3	2.12	0.49
37:i:95:ARG:HG3	37:i:95:ARG:NH1	2.27	0.49
6:A:35:G:H2'	6:A:36:C:C6	2.48	0.49
6:A:1163:A:H2'	6:A:1164:G:H8	1.77	0.49
6:A:1355:G:H2'	6:A:1356:G:H8	1.77	0.49
18:M:49:SER:OG	18:M:50:GLU:OE2	2.23	0.49
29:a:2557:G:H2'	29:a:2558:C:C6	2.48	0.49
29:a:849:A:H2'	29:a:850:U:C6	2.47	0.49
29:a:1469:A:H2'	29:a:1470:A:H8	1.77	0.49
29:a:2804:U:H2'	29:a:2805:C:C6	2.47	0.49
35:g:127:THR:OG1	35:g:128:GLN:N	2.46	0.49
36:h:8:LYS:NZ	36:h:13:GLY:O	2.43	0.49
49:u:75:GLN:HB2	49:u:92:VAL:HG23	1.94	0.49
3:2:16:LYS:HE3	3:2:20:GLY:HA2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:104:G:N7	25:T:9:LYS:NZ	2.60	0.49
29:a:1790:C:H2'	29:a:1791:A:C5	2.47	0.49
41:m:56:LYS:NZ	41:m:94:TYR:OH	2.41	0.49
6:A:362:G:N2	6:A:365:U:OP2	2.41	0.49
19:N:33:ASP:C	19:N:35:ASN:N	2.69	0.49
29:a:1853:A:H2'	29:a:1854:A:C8	2.48	0.49
29:a:2331:G:O2'	29:a:2336:A:N1	2.40	0.49
29:a:2567:G:H2'	29:a:2568:U:C6	2.47	0.49
29:a:2636:C:O2'	32:d:45:TYR:OH	2.26	0.49
29:a:2847:U:H2'	29:a:2848:G:O4'	2.13	0.49
30:b:48:U:H2'	30:b:49:C:C6	2.48	0.49
6:A:1238:A:H2	6:A:1241:G:N3	2.10	0.49
6:A:1314:C:H2'	6:A:1315:U:H6	1.78	0.49
11:F:88:MET:HE2	23:R:64:TYR:HD2	1.78	0.49
19:N:53:ARG:HH21	24:S:37:ARG:HH21	1.59	0.49
29:a:1486:U:H2'	29:a:1487:U:H6	1.78	0.49
29:a:2799:A:O2'	29:a:2800:A:H5''	2.12	0.49
6:A:1435:G:H2'	6:A:1436:U:C6	2.47	0.49
8:C:70:THR:HG21	8:C:76:VAL:HG21	1.93	0.49
48:t:98:SER:OG	48:t:98:SER:O	2.30	0.49
6:A:501:C:H2'	6:A:502:A:H8	1.78	0.49
21:P:35:ARG:HG2	21:P:35:ARG:HH11	1.78	0.49
29:a:720:U:H2'	29:a:721:A:C8	2.48	0.49
6:A:1397:C:OP2	10:E:29:ARG:NH2	2.33	0.48
27:X:13:A:H2'	27:X:14:A:H8	1.78	0.48
11:F:16:GLU:H	11:F:16:GLU:CD	2.14	0.48
29:a:58:G:O2'	29:a:73:A:N1	2.45	0.48
30:b:48:U:H2'	30:b:49:C:H6	1.77	0.48
6:A:922:G:H2'	6:A:923:A:C8	2.48	0.48
6:A:1318:A:OP1	24:S:7:LYS:NZ	2.46	0.48
10:E:80:THR:OG1	10:E:81:LEU:N	2.47	0.48
17:L:3:THR:HG22	17:L:5:ASN:H	1.78	0.48
29:a:1443:U:H2'	29:a:1444:G:C8	2.48	0.48
29:a:1703:G:H2'	29:a:1704:C:C6	2.48	0.48
29:a:1794:A:H2'	29:a:1795:C:H6	1.79	0.48
34:f:8:TYR:HB2	34:f:173:PHE:CZ	2.48	0.48
6:A:437:U:HO2'	9:D:120:HIS:HD1	1.58	0.48
6:A:1507:A:H2'	6:A:1508:A:C8	2.47	0.48
11:F:88:MET:HE3	23:R:65:LEU:HG	1.96	0.48
19:N:63:ARG:NH1	19:N:68:GLY:O	2.45	0.48
29:a:1168:G:H2'	29:a:1169:A:H8	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:1735:A:H2'	29:a:1736:U:C6	2.49	0.48
6:A:407:U:H2'	6:A:408:A:C8	2.49	0.48
8:C:61:ALA:C	8:C:62:LYS:HE2	2.38	0.48
23:R:9:LYS:HA	23:R:46:GLY:HA3	1.94	0.48
29:a:1614:A:C2	46:r:93:ALA:HB2	2.49	0.48
29:a:1746:A:H2'	29:a:1747:U:H6	1.77	0.48
29:a:2830:C:H5''	32:d:56:LYS:HE3	1.95	0.48
6:A:1516:2MG:N2	6:A:1519:MA6:OP2	2.43	0.48
29:a:2:G:H2'	29:a:3:U:C6	2.49	0.48
29:a:545:U:H3'	29:a:546:U:H5'	1.94	0.48
29:a:644:A:H2'	29:a:645:C:O4'	2.13	0.48
32:d:39:ASP:OD1	32:d:39:ASP:N	2.47	0.48
50:v:59:LEU:HD12	50:v:80:ILE:HD12	1.96	0.48
6:A:299:G:H2'	6:A:300:A:C8	2.49	0.48
6:A:1043:G:O2'	6:A:1044:A:O5'	2.22	0.48
14:I:55:VAL:HG21	14:I:87:LEU:HD21	1.95	0.48
14:I:88:MET:HG3	14:I:98:LEU:HD12	1.94	0.48
29:a:414:C:H2'	29:a:415:A:C8	2.48	0.48
29:a:832:U:H2'	29:a:833:A:C8	2.48	0.48
29:a:839:U:H2'	29:a:840:C:C6	2.49	0.48
29:a:1570:A:H2'	29:a:1571:A:C8	2.48	0.48
29:a:2698:U:H2'	29:a:2699:C:C6	2.48	0.48
20:O:79:THR:O	20:O:83:GLU:OE1	2.32	0.48
25:T:24:ARG:HB2	25:T:66:LEU:HD22	1.94	0.48
29:a:365:U:H2'	29:a:366:C:C6	2.48	0.48
29:a:1704:C:H2'	29:a:1705:A:C8	2.49	0.48
29:a:2202:U:O2'	29:a:2204:G:OP1	2.30	0.48
52:x:12:GLU:OE2	52:x:12:GLU:N	2.29	0.48
6:A:904:U:H2'	6:A:905:U:C6	2.49	0.48
13:H:5:ASP:HB2	13:H:81:PRO:HG2	1.95	0.48
14:I:115:LYS:HB2	14:I:118:LEU:HD12	1.94	0.48
20:O:42:HIS:CE1	20:O:46:HIS:HD2	2.32	0.48
29:a:753:A:H2'	29:a:754:U:H6	1.79	0.48
38:j:121:GLU:OE1	43:o:65:SER:OG	2.27	0.48
6:A:1375:A:OP1	12:G:25:LYS:NZ	2.35	0.48
12:G:20:SER:HB3	12:G:23:LEU:HB2	1.96	0.48
15:J:21:ALA:O	15:J:24:GLU:HG3	2.13	0.48
29:a:2014:A:H2'	29:a:2015:A:C8	2.48	0.48
29:a:2327:A:H2'	29:a:2328:A:C8	2.49	0.48
29:a:2809:A:H2'	29:a:2810:A:C8	2.49	0.48
35:g:45:HIS:O	35:g:46:ALA:HB3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:t:50:PRO:HA	48:t:54:GLN:HG3	1.95	0.48
6:A:780:A:H5'	16:K:125:LYS:HD3	1.96	0.47
8:C:108:LYS:HB3	8:C:144:LEU:HD23	1.96	0.47
10:E:38:VAL:HG11	10:E:114:VAL:HG22	1.94	0.47
16:K:34:ILE:HG21	16:K:74:VAL:HG11	1.95	0.47
19:N:33:ASP:C	19:N:35:ASN:H	2.22	0.47
26:U:36:GLU:HG2	26:U:37:PHE:CD2	2.49	0.47
29:a:1357:C:H2'	29:a:1358:G:O4'	2.13	0.47
6:A:579:A:O2'	20:O:54:ARG:NH1	2.47	0.47
6:A:769:G:H4'	6:A:1513:A:H4'	1.96	0.47
7:B:133:GLU:N	7:B:133:GLU:OE1	2.47	0.47
13:H:96:MET:HE2	13:H:130:ALA:HB1	1.96	0.47
27:X:13:A:H2'	27:X:14:A:C8	2.49	0.47
29:a:299:A:N3	29:a:319:G:O2'	2.44	0.47
29:a:634:C:H2'	29:a:635:C:C6	2.48	0.47
29:a:2247:A:H2'	29:a:2248:C:H6	1.79	0.47
31:c:157:SER:O	31:c:160:THR:OG1	2.29	0.47
49:u:34:LYS:N	49:u:35:GLU:OE2	2.47	0.47
11:F:69:GLU:CD	11:F:69:GLU:N	2.73	0.47
29:a:1179:G:H2'	29:a:1180:U:C6	2.49	0.47
29:a:1486:U:H2'	29:a:1487:U:C6	2.49	0.47
29:a:2812:G:H2'	29:a:2813:A:C8	2.48	0.47
33:e:136:GLN:NE2	33:e:140:ASP:OD1	2.47	0.47
49:u:64:VAL:HG22	49:u:69:GLU:HG2	1.95	0.47
6:A:1004:A:H5'	6:A:1024:G:H22	1.80	0.47
6:A:1014:A:C2	6:A:1219:A:H1'	2.49	0.47
8:C:82:GLU:O	8:C:86:LYS:HD3	2.14	0.47
14:I:42:GLU:OE2	14:I:45:ARG:NH1	2.48	0.47
29:a:5:A:H2'	29:a:6:A:H8	1.76	0.47
29:a:1292:G:H2'	29:a:1293:C:C6	2.50	0.47
29:a:2193:G:H2'	29:a:2194:U:C6	2.50	0.47
29:a:2780:G:OP2	37:i:120:ARG:HD3	2.14	0.47
6:A:1410:A:H2'	6:A:1411:C:C6	2.50	0.47
18:M:3:ARG:HG2	18:M:8:ASN:ND2	2.30	0.47
18:M:59:GLU:O	18:M:62:LYS:HG3	2.14	0.47
19:N:22:ALA:O	19:N:26:GLU:OE2	2.33	0.47
29:a:2246:G:H2'	29:a:2247:A:H8	1.79	0.47
7:B:6:MET:HE3	7:B:43:LEU:HB2	1.96	0.47
29:a:1429:G:H2'	29:a:1430:G:H8	1.80	0.47
29:a:1534:U:H1'	29:a:1537:G:H1	1.79	0.47
29:a:1946:U:H2'	29:a:1947:C:C6	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:h:8:LYS:HG2	36:h:14:SER:HA	1.95	0.47
2:l:1:MET:SD	29:a:752:A:H3'	2.55	0.47
6:A:236:A:H2'	6:A:237:G:H8	1.80	0.47
6:A:562:U:H1'	17:L:12:ARG:HB3	1.96	0.47
6:A:696:A:H2'	6:A:697:U:H6	1.79	0.47
6:A:993:G:H2'	6:A:995:C:H41	1.79	0.47
6:A:1317:C:OP1	19:N:56:SER:OG	2.32	0.47
8:C:42:TYR:OH	8:C:90:VAL:HG21	2.15	0.47
9:D:54:GLN:HB3	9:D:203:LEU:HB2	1.97	0.47
15:J:40:ILE:HD11	15:J:73:LEU:HB3	1.95	0.47
20:O:79:THR:HG22	20:O:83:GLU:OE1	2.14	0.47
29:a:29:U:H2'	29:a:30:G:C8	2.50	0.47
29:a:588:U:H2'	29:a:589:U:C6	2.49	0.47
29:a:667:U:H2'	29:a:668:A:O4'	2.15	0.47
29:a:721:A:H2'	29:a:722:A:C8	2.49	0.47
29:a:1494:A:H2'	29:a:1495:A:C8	2.49	0.47
29:a:2233:U:H2'	29:a:2234:G:C8	2.50	0.47
30:b:112:G:H2'	30:b:113:C:C6	2.50	0.47
35:g:50:LEU:HD12	35:g:50:LEU:HA	1.79	0.47
6:A:236:A:H2'	6:A:237:G:C8	2.50	0.47
6:A:1119:C:OP1	14:I:85:ARG:NH1	2.45	0.47
15:J:6:ILE:HB	15:J:76:ILE:HB	1.97	0.47
15:J:40:ILE:HD12	15:J:40:ILE:O	2.14	0.47
28:Z:23:C:H2'	28:Z:24:U:C6	2.49	0.47
29:a:52:A:H2'	29:a:53:A:C8	2.50	0.47
29:a:250:G:H2'	29:a:251:A:C8	2.50	0.47
29:a:288:U:H2'	29:a:289:G:H8	1.80	0.47
29:a:784:G:H5'	29:a:785:G:OP1	2.15	0.47
29:a:1682:G:H2'	29:a:1683:U:C6	2.49	0.47
3:2:17:THR:HG21	3:2:49:MET:HE1	1.97	0.47
8:C:157:LEU:HD23	8:C:196:ILE:HD13	1.96	0.47
12:G:135:VAL:O	12:G:139:GLU:HG3	2.15	0.47
29:a:1442:U:H2'	29:a:1443:U:C6	2.50	0.47
35:g:41:VAL:HA	35:g:53:GLY:O	2.15	0.47
6:A:270:A:H2'	6:A:271:C:C6	2.50	0.47
6:A:405:U:O4	9:D:2:ALA:N	2.48	0.47
6:A:821:G:H2'	6:A:822:U:C6	2.50	0.47
6:A:993:G:O2'	6:A:994:A:N7	2.48	0.47
9:D:128:ARG:HB3	9:D:128:ARG:NH1	2.31	0.47
29:a:581:C:H2'	29:a:582:A:H8	1.79	0.47
29:a:1141:U:H4'	29:a:1142:A:O4'	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:1266:G:O2'	29:a:2012:G:O6	2.24	0.47
29:a:2649:C:H2'	29:a:2650:U:H6	1.78	0.47
6:A:399:G:H2'	6:A:400:C:C6	2.51	0.46
14:I:19:VAL:HG11	14:I:83:ILE:HG12	1.97	0.46
29:a:544:C:H3'	29:a:545:U:C6	2.50	0.46
6:A:1287:A:H2'	6:A:1288:A:C8	2.50	0.46
9:D:194:ASP:OD1	9:D:194:ASP:N	2.35	0.46
12:G:79:ARG:O	12:G:79:ARG:HD3	2.14	0.46
15:J:52:LEU:HD23	15:J:62:ARG:HD3	1.97	0.46
24:S:12:ASP:OD2	24:S:35:SER:OG	2.28	0.46
40:l:53:MET:HE1	40:l:103:TYR:CG	2.50	0.46
6:A:1347:G:O6	14:I:12:ARG:NH2	2.47	0.46
6:A:1355:G:H2'	6:A:1356:G:C8	2.51	0.46
15:J:52:LEU:HD21	15:J:59:LYS:HD2	1.96	0.46
26:U:39:GLU:OE1	26:U:47:ARG:NH2	2.44	0.46
29:a:495:G:H21	46:r:61:ASN:HD21	1.61	0.46
6:A:1130:A:O2'	14:I:5:GLN:OE1	2.28	0.46
11:F:25:TYR:CE2	11:F:78:PHE:HE1	2.33	0.46
14:I:57:MET:HA	14:I:60:LYS:CE	2.45	0.46
17:L:50:ARG:HB3	17:L:66:TYR:HE1	1.79	0.46
28:Z:43:A:H2'	28:Z:44:A:C8	2.50	0.46
29:a:284:U:O2	29:a:356:G:O6	2.33	0.46
29:a:2273:A:H2'	29:a:2274:A:C8	2.50	0.46
29:a:2700:A:H2'	29:a:2701:U:C6	2.51	0.46
6:A:672:U:H2'	6:A:673:A:C8	2.50	0.46
29:a:1667:G:O2'	29:a:1991:U:O4	2.30	0.46
29:a:2638:G:OP2	32:d:83:ARG:NH2	2.49	0.46
30:b:30:C:H2'	30:b:31:C:H5'	1.98	0.46
6:A:1163:A:H2'	6:A:1164:G:C8	2.50	0.46
14:I:52:LEU:HA	14:I:55:VAL:HG12	1.97	0.46
23:R:19:GLN:OE1	23:R:19:GLN:N	2.46	0.46
29:a:64:A:H2'	29:a:65:U:H6	1.81	0.46
29:a:78:U:H2'	29:a:79:C:C6	2.50	0.46
29:a:881:G:N2	29:a:895:U:O2	2.35	0.46
31:c:145:GLU:HB2	31:c:188:CYS:HB3	1.98	0.46
41:m:51:LEU:HD11	41:m:70:THR:HG21	1.98	0.46
6:A:34:C:H2'	6:A:35:G:H8	1.81	0.46
6:A:477:C:H2'	6:A:478:A:C8	2.50	0.46
7:B:130:THR:C	7:B:132:LYS:H	2.22	0.46
8:C:134:MET:HE2	8:C:168:TYR:HD2	1.80	0.46
13:H:5:ASP:OD2	13:H:8:ALA:HB3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:L:9:ARG:HB2	17:L:9:ARG:NH1	2.31	0.46
29:a:181:A:H2'	29:a:182:A:C8	2.50	0.46
29:a:2097:A:H2'	29:a:2098:U:C6	2.51	0.46
29:a:2595:G:N2	29:a:2598:A:OP2	2.43	0.46
35:g:127:THR:CG2	35:g:130:GLU:HG2	2.46	0.46
40:l:47:GLU:OE2	40:l:47:GLU:HA	2.15	0.46
47:s:3:ARG:HB3	47:s:5:GLU:OE1	2.15	0.46
6:A:407:U:H2'	6:A:408:A:H8	1.79	0.46
6:A:552:U:H2'	6:A:553:A:H8	1.81	0.46
6:A:744:C:H2'	6:A:745:G:C8	2.50	0.46
6:A:985:C:H2'	6:A:986:U:C6	2.50	0.46
10:E:62:LYS:O	10:E:66:LYS:HG3	2.16	0.46
29:a:419:U:H2'	29:a:420:C:C6	2.50	0.46
32:d:33:ARG:NH2	32:d:74:GLU:O	2.47	0.46
6:A:6:G:O2'	6:A:7:A:H8	1.99	0.46
11:F:37:HIS:HB3	11:F:97:THR:HG23	1.97	0.46
29:a:534:U:O2'	44:p:49:ASP:OD2	2.25	0.46
6:A:580:C:H2'	6:A:581:G:O4'	2.16	0.46
6:A:1120:C:H2'	6:A:1121:U:H6	1.81	0.46
16:K:22:HIS:CE1	16:K:85:MET:HE2	2.51	0.46
28:Z:21:A:N6	28:Z:46:G:H2'	2.30	0.46
29:a:182:A:H2'	29:a:183:C:H6	1.80	0.46
29:a:580:U:H2'	29:a:581:C:C6	2.51	0.46
37:i:102:GLU:HG2	37:i:119:PHE:HZ	1.81	0.46
44:p:114:LYS:HA	44:p:117:LEU:HD12	1.98	0.46
6:A:946:A:H2'	6:A:947:G:H8	1.75	0.45
6:A:958:A:C6	24:S:55:ARG:HG2	2.52	0.45
6:A:1320:C:O2	24:S:36:ARG:NH2	2.48	0.45
6:A:1530:G:H2'	6:A:1531:A:C8	2.51	0.45
8:C:90:VAL:HA	8:C:93:ASP:OD2	2.16	0.45
10:E:93:ARG:HG3	10:E:93:ARG:NH1	2.30	0.45
12:G:75:VAL:HG21	12:G:144:MET:HG2	1.98	0.45
22:Q:11:ARG:HE	22:Q:11:ARG:HB2	1.52	0.45
29:a:511:U:C2'	29:a:512:G:H5'	2.46	0.45
29:a:522:A:H2'	29:a:523:C:C6	2.51	0.45
6:A:178:C:C2	6:A:179:A:C8	3.04	0.45
6:A:593:U:H2'	6:A:594:U:C6	2.52	0.45
29:a:645:C:O2'	29:a:646:U:H5'	2.15	0.45
29:a:973:A:H5'	29:a:1188:U:H1'	1.98	0.45
29:a:2484:G:OP1	40:l:44:ARG:NE	2.49	0.45
29:a:2774:C:H2'	29:a:2775:G:O4'	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:v:78:LYS:HB2	50:v:78:LYS:HE2	1.69	0.45
6:A:390:U:H2'	6:A:391:G:C8	2.51	0.45
6:A:1040:U:H2'	6:A:1041:G:H8	1.82	0.45
6:A:1356:G:H2'	6:A:1357:A:H8	1.77	0.45
13:H:11:LEU:HD22	13:H:75:ILE:HD11	1.99	0.45
20:O:18:ASP:OD1	20:O:20:ASN:N	2.42	0.45
20:O:44:ALA:O	20:O:47:LYS:NZ	2.43	0.45
29:a:414:C:H2'	29:a:415:A:H8	1.81	0.45
29:a:1444:G:H2'	29:a:1445:G:H8	1.80	0.45
29:a:2241:A:H2'	29:a:2242:G:C8	2.52	0.45
29:a:2529:G:H5'	35:g:175:LYS:HB3	1.98	0.45
43:o:54:GLY:O	43:o:57:SER:OG	2.29	0.45
6:A:12:U:H4'	6:A:526:C:H4'	1.99	0.45
6:A:335:C:H2'	6:A:336:A:C8	2.52	0.45
6:A:976:G:OP2	6:A:1358:U:O2'	2.34	0.45
7:B:219:ALA:O	7:B:222:ARG:HG2	2.16	0.45
13:H:22:LYS:O	13:H:65:TYR:OH	2.32	0.45
13:H:48:ASP:OD1	13:H:49:PHE:N	2.48	0.45
20:O:40:GLN:OE1	20:O:40:GLN:HA	2.17	0.45
29:a:3:U:H2'	29:a:4:U:C6	2.51	0.45
29:a:739:A:H1'	29:a:740:C:H5	1.82	0.45
29:a:2329:U:H2'	29:a:2330:G:C8	2.52	0.45
30:b:106:G:H2'	30:b:107:G:O4'	2.16	0.45
35:g:19:ILE:HG23	35:g:24:ILE:HD11	1.98	0.45
50:v:44:LYS:HB2	50:v:44:LYS:HE3	1.66	0.45
3:2:52:LYS:HE3	3:2:52:LYS:HB3	1.60	0.45
6:A:171:A:H2'	6:A:172:A:C8	2.51	0.45
8:C:116:VAL:O	8:C:120:ILE:HG13	2.17	0.45
9:D:19:LEU:HD22	9:D:64:ILE:HG13	1.98	0.45
16:K:84:VAL:HG11	16:K:97:ILE:HG12	1.98	0.45
29:a:709:U:H2'	29:a:710:U:C6	2.52	0.45
29:a:1248:G:OP1	33:e:44:ARG:NH1	2.44	0.45
29:a:2783:U:H2'	29:a:2784:U:C6	2.52	0.45
29:a:2895:G:H2'	29:a:2896:C:C6	2.52	0.45
37:i:69:ARG:HG2	37:i:90:GLU:OE1	2.16	0.45
37:i:96:ARG:HA	37:i:96:ARG:NE	2.32	0.45
7:B:111:ILE:HD11	7:B:152:LYS:HA	1.98	0.45
8:C:88:ARG:NH2	8:C:99:ALA:O	2.47	0.45
12:G:66:LEU:O	12:G:70:ARG:HG3	2.17	0.45
14:I:34:SER:OG	14:I:35:LEU:N	2.49	0.45
29:a:1198:U:H2'	29:a:1199:U:H6	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:2193:G:H2'	29:a:2194:U:H6	1.82	0.45
29:a:2312:U:H5'	34:f:85:ILE:HD11	1.99	0.45
42:n:115:LEU:HD23	42:n:115:LEU:HA	1.85	0.45
6:A:1220:G:P	19:N:53:ARG:HH22	2.40	0.45
15:J:90:LEU:HD23	15:J:90:LEU:HA	1.71	0.45
39:k:82:LEU:HD13	39:k:120:VAL:HG11	1.97	0.45
6:A:41:G:H2'	6:A:42:G:H8	1.82	0.45
29:a:151:C:H2'	29:a:152:A:C8	2.51	0.45
29:a:594:U:H2'	29:a:595:C:H6	1.82	0.45
6:A:600:A:H2'	6:A:601:G:C8	2.52	0.45
7:B:117:LEU:HD23	7:B:141:LEU:HB2	1.98	0.45
15:J:18:ILE:HA	15:J:18:ILE:HD12	1.69	0.45
16:K:37:ARG:HG3	16:K:37:ARG:HH11	1.82	0.45
19:N:27:LEU:HD21	19:N:47:LYS:HB3	1.98	0.45
21:P:45:GLU:OE1	21:P:45:GLU:N	2.50	0.45
29:a:756:A:H2'	29:a:757:G:O4'	2.17	0.45
29:a:1599:U:H2'	29:a:1600:C:C6	2.52	0.45
32:d:51:THR:OG1	32:d:78:GLY:O	2.32	0.45
35:g:90:VAL:HG22	35:g:160:LYS:HA	1.99	0.45
36:h:4:ILE:O	36:h:4:ILE:HD12	2.17	0.45
49:u:34:LYS:HA	49:u:34:LYS:HD3	1.63	0.45
5:4:43:PHE:CD1	5:4:43:PHE:C	2.95	0.45
6:A:140:U:H2'	6:A:141:G:O4'	2.16	0.45
6:A:324:G:N1	6:A:327:A:OP2	2.50	0.45
13:H:7:ILE:O	13:H:11:LEU:HG	2.17	0.45
15:J:78:GLU:O	15:J:78:GLU:HG2	2.17	0.45
25:T:39:ILE:HG21	25:T:82:GLN:HG2	1.98	0.45
29:a:2455:G:H2'	29:a:2456:C:C6	2.52	0.45
31:c:16:VAL:HG22	31:c:206:GLY:HA3	1.99	0.45
34:f:73:SER:OG	34:f:81:GLN:N	2.50	0.45
6:A:246:A:C2	6:A:282:A:C5	3.05	0.44
6:A:1253:G:H2'	6:A:1254:A:H8	1.83	0.44
7:B:127:ASP:HB2	7:B:128:LYS:NZ	2.32	0.44
25:T:5:LYS:HE2	25:T:5:LYS:HB3	1.76	0.44
29:a:582:A:H2'	29:a:583:G:C8	2.52	0.44
29:a:668:A:H2'	29:a:670:A:H62	1.82	0.44
29:a:753:A:H2'	29:a:754:U:C6	2.52	0.44
29:a:2514:U:H2'	29:a:2515:C:H6	1.82	0.44
48:t:26:LYS:HD3	48:t:26:LYS:HA	1.83	0.44
3:2:34:THR:OG1	29:a:2420:C:OP1	2.35	0.44
6:A:72:A:H2'	6:A:72:A:N3	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:390:U:H2'	6:A:391:G:H8	1.82	0.44
6:A:737:C:H2'	6:A:738:C:H6	1.82	0.44
6:A:1382:C:O4'	12:G:79:ARG:NH2	2.49	0.44
6:A:1513:A:H2'	6:A:1514:G:H8	1.83	0.44
9:D:98:LEU:HB2	9:D:135:TYR:HB3	1.98	0.44
12:G:97:ASN:O	12:G:101:MET:HG3	2.18	0.44
19:N:27:LEU:O	19:N:31:ILE:HG12	2.17	0.44
29:a:397:U:H5''	51:w:32:ASN:HB2	2.00	0.44
29:a:645:C:H2'	29:a:647:G:C8	2.52	0.44
29:a:708:G:H2'	29:a:709:U:C6	2.52	0.44
29:a:1387:A:H2'	29:a:1388:G:H8	1.82	0.44
29:a:1506:U:H2'	29:a:1507:C:C6	2.52	0.44
29:a:1733:G:H2'	29:a:1734:G:C8	2.52	0.44
49:u:70:ILE:HG22	49:u:72:VAL:HG13	1.99	0.44
6:A:490:C:C2	6:A:491:G:C8	3.05	0.44
9:D:174:ASP:OD1	9:D:177:LYS:N	2.45	0.44
10:E:77:ASN:HB2	10:E:82:GLN:NE2	2.33	0.44
11:F:25:TYR:O	11:F:29:ILE:HD12	2.17	0.44
22:Q:16:LYS:HE3	22:Q:16:LYS:HB2	1.70	0.44
29:a:544:C:H3'	29:a:545:U:H6	1.83	0.44
40:l:134:THR:HG22	40:l:136:MET:H	1.81	0.44
6:A:264:C:O2'	22:Q:66:PRO:O	2.31	0.44
6:A:1035:A:C4	6:A:1036:A:C2	3.06	0.44
6:A:1465:A:H2'	6:A:1466:C:C6	2.52	0.44
8:C:49:LYS:HA	8:C:49:LYS:HD2	1.84	0.44
10:E:108:GLY:C	10:E:112:ARG:HG3	2.43	0.44
12:G:23:LEU:HD12	12:G:23:LEU:HA	1.88	0.44
24:S:5:LEU:HD23	24:S:5:LEU:HA	1.79	0.44
29:a:1747:U:H2'	29:a:1748:C:H6	1.81	0.44
29:a:2591:C:H2'	29:a:2592:G:H8	1.81	0.44
32:d:26:VAL:HG22	32:d:188:LEU:HD22	1.99	0.44
49:u:55:GLU:OE2	49:u:55:GLU:N	2.22	0.44
4:3:2:LYS:NZ	29:a:2478:A:OP2	2.27	0.44
6:A:1175:G:H2'	6:A:1176:A:H8	1.81	0.44
8:C:134:MET:HE2	8:C:168:TYR:CD2	2.51	0.44
10:E:96:MET:HE3	10:E:96:MET:HB2	1.80	0.44
11:F:47:LEU:HD21	11:F:57:ALA:HB3	2.00	0.44
19:N:10:GLU:O	19:N:14:VAL:HG12	2.17	0.44
29:a:2230:G:H2'	29:a:2231:U:C6	2.52	0.44
29:a:2649:C:H2'	29:a:2650:U:C6	2.51	0.44
30:b:34:A:H4'	30:b:35:C:H5	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:l:57:VAL:HG11	40:l:105:MET:SD	2.57	0.44
53:y:4:THR:OG1	53:y:37:GLU:HG2	2.17	0.44
4:3:19:ARG:NE	29:a:2756:U:OP2	2.50	0.44
6:A:1038:C:H2'	6:A:1039:G:C8	2.51	0.44
6:A:1253:G:H2'	6:A:1254:A:C8	2.53	0.44
6:A:1352:C:H2'	6:A:1353:G:C8	2.53	0.44
6:A:1486:G:H2'	6:A:1487:G:O4'	2.18	0.44
7:B:219:ALA:HA	7:B:222:ARG:HG2	1.99	0.44
14:I:114:LYS:NZ	14:I:115:LYS:O	2.50	0.44
18:M:37:ALA:HB2	18:M:59:GLU:HG3	1.99	0.44
29:a:1199:U:H2'	29:a:1200:C:H6	1.83	0.44
29:a:2849:U:H4'	29:a:2868:A:C2	2.53	0.44
6:A:736:C:H2'	6:A:737:C:C6	2.51	0.44
6:A:737:C:H2'	6:A:738:C:C6	2.52	0.44
29:a:632:A:H2'	29:a:633:A:C8	2.52	0.44
29:a:1378:A:O2'	29:a:1380:G:N7	2.51	0.44
12:G:40:GLU:OE1	14:I:41:ARG:NH2	2.51	0.44
29:a:500:G:N1	29:a:503:A:OP2	2.46	0.44
29:a:1496:A:H2'	29:a:1498:C:C5	2.52	0.44
29:a:1680:U:H2'	29:a:1681:G:O4'	2.17	0.44
29:a:1727:C:H2'	29:a:1728:C:C6	2.53	0.44
29:a:2038:G:H2'	29:a:2039:U:O4'	2.18	0.44
49:u:72:VAL:HB	49:u:91:PHE:HB3	2.00	0.44
6:A:73:C:C2	6:A:74:A:C8	3.05	0.44
6:A:259:G:OP1	25:T:36:TYR:OH	2.31	0.44
6:A:1530:G:N7	26:U:46:LYS:NZ	2.65	0.44
8:C:129:MET:HG2	8:C:132:ARG:H	1.82	0.44
18:M:92:ARG:HG2	29:a:888:C:C6	2.53	0.44
29:a:146:A:H2'	29:a:147:C:C6	2.52	0.44
29:a:493:G:H2'	29:a:494:G:O4'	2.17	0.44
29:a:1736:U:H2'	29:a:1737:G:O4'	2.18	0.44
29:a:2020:A:H5'	54:z:9:THR:CG2	2.48	0.44
37:i:102:GLU:HG2	37:i:119:PHE:CZ	2.52	0.44
51:w:3:ARG:O	51:w:12:PRO:HD3	2.17	0.44
5:4:62:LYS:HG2	5:4:63:ARG:N	2.31	0.43
6:A:1004:A:H3'	6:A:1024:G:H22	1.82	0.43
10:E:108:GLY:O	10:E:112:ARG:HG3	2.18	0.43
29:a:1599:U:H2'	29:a:1600:C:H6	1.83	0.43
37:i:89:PHE:HE1	37:i:100:VAL:HG11	1.83	0.43
6:A:321:A:H2'	6:A:322:C:C6	2.53	0.43
6:A:471:U:H2'	6:A:472:U:H6	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:545:C:OP1	9:D:58:LYS:NZ	2.51	0.43
6:A:710:G:OP1	11:F:53:LYS:HE3	2.17	0.43
6:A:757:U:H2'	6:A:758:C:O4'	2.18	0.43
6:A:1010:U:H2'	6:A:1011:C:C6	2.53	0.43
7:B:19:GLN:OE1	7:B:19:GLN:N	2.39	0.43
7:B:188:ASP:HB2	7:B:204:ASP:OD2	2.18	0.43
16:K:34:ILE:HB	16:K:74:VAL:HG21	2.00	0.43
28:Z:76:A:H2'	29:a:2451:A:H1'	1.99	0.43
29:a:17:G:H2'	29:a:18:U:C6	2.53	0.43
29:a:1340:U:OP1	47:s:19:LYS:NZ	2.47	0.43
29:a:1387:A:H2'	29:a:1388:G:C8	2.53	0.43
29:a:2411:A:H2'	29:a:2412:A:C8	2.54	0.43
32:d:186:LEU:HD21	43:o:4:ILE:HG21	1.99	0.43
47:s:5:GLU:OE1	47:s:5:GLU:N	2.33	0.43
6:A:20:U:H2'	6:A:21:G:O4'	2.19	0.43
6:A:634:C:H2'	6:A:635:A:H8	1.83	0.43
6:A:695:A:H2'	6:A:696:A:C8	2.54	0.43
7:B:66:LYS:C	7:B:67:ILE:HD13	2.43	0.43
10:E:72:ILE:HD13	10:E:145:GLU:HG3	1.99	0.43
14:I:123:ARG:NH1	14:I:124:ARG:O	2.43	0.43
22:Q:24:ALA:C	22:Q:25:ILE:HD13	2.42	0.43
24:S:55:ARG:HD2	24:S:56:GLN:NE2	2.33	0.43
29:a:296:U:H2'	29:a:297:G:C8	2.53	0.43
29:a:548:G:H2'	29:a:549:G:C8	2.54	0.43
29:a:1703:G:H2'	29:a:1704:C:H6	1.83	0.43
49:u:53:LYS:HE2	49:u:53:LYS:HB2	1.90	0.43
6:A:471:U:H2'	6:A:472:U:C6	2.53	0.43
6:A:1157:A:C2	6:A:1181:G:C4	3.06	0.43
7:B:43:LEU:HA	7:B:46:THR:HB	2.01	0.43
10:E:101:GLU:CD	10:E:101:GLU:N	2.76	0.43
18:M:114:LYS:HB3	18:M:114:LYS:HE3	1.79	0.43
25:T:9:LYS:HE2	25:T:13:GLN:HE21	1.84	0.43
29:a:1172:C:H2'	29:a:1172:C:O2	2.18	0.43
29:a:1802:A:H2'	29:a:1803:A:H8	1.80	0.43
29:a:2804:U:H2'	29:a:2805:C:H6	1.82	0.43
30:b:42:C:C5	34:f:66:LEU:HD22	2.53	0.43
32:d:152:PRO:HG3	32:d:156:PHE:CZ	2.52	0.43
6:A:161:A:H2'	6:A:162:A:C8	2.54	0.43
6:A:513:C:H2'	6:A:514:C:C6	2.53	0.43
6:A:553:A:H2'	6:A:554:A:C8	2.54	0.43
29:a:75:G:H2'	29:a:75:G:N3	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:138:U:H2'	29:a:140:C:C4	2.54	0.43
29:a:930:G:H1'	53:y:25:LEU:HD21	2.01	0.43
29:a:1434:A:H2'	29:a:1435:G:C8	2.53	0.43
29:a:1534:U:O3'	29:a:1535:A:H2'	2.18	0.43
29:a:1987:A:H2'	29:a:1988:G:H8	1.84	0.43
10:E:149:SER:OG	10:E:152:MET:HG3	2.19	0.43
12:G:47:LEU:HD23	12:G:47:LEU:HA	1.82	0.43
29:a:2281:A:O2'	29:a:2282:G:H5'	2.18	0.43
31:c:35:GLU:HG3	31:c:64:ILE:HD11	2.00	0.43
35:g:47:ASP:N	35:g:47:ASP:OD1	2.52	0.43
42:n:83:LEU:HD23	42:n:83:LEU:HA	1.72	0.43
3:2:55:LEU:HD12	3:2:55:LEU:HA	1.84	0.43
6:A:401:C:O2'	6:A:621:A:N3	2.44	0.43
6:A:470:C:H2'	6:A:471:U:C6	2.54	0.43
6:A:1160:G:C2	6:A:1161:C:C6	3.07	0.43
6:A:1179:A:H2'	6:A:1180:A:O4'	2.19	0.43
14:I:116:VAL:HG11	15:J:62:ARG:HG3	2.00	0.43
29:a:796:C:H2'	29:a:797:G:C8	2.54	0.43
29:a:1889:A:H2'	29:a:1890:A:H8	1.83	0.43
30:b:14:U:OP2	30:b:70:C:O2'	2.34	0.43
35:g:19:ILE:HG12	35:g:24:ILE:HG13	2.00	0.43
35:g:44:LYS:HB3	35:g:45:HIS:H	1.69	0.43
6:A:553:A:H2'	6:A:554:A:H8	1.84	0.43
6:A:687:A:C2	6:A:704:A:C5	3.07	0.43
15:J:67:ILE:HG13	19:N:96:LEU:HD13	2.00	0.43
21:P:38:PHE:CE1	21:P:51:ARG:HB3	2.54	0.43
29:a:288:U:H2'	29:a:289:G:C8	2.54	0.43
29:a:832:U:H2'	29:a:833:A:H8	1.83	0.43
43:o:7:GLN:C	43:o:7:GLN:OE1	2.62	0.43
6:A:600:A:H2'	6:A:601:G:H8	1.84	0.43
6:A:1122:U:H2'	6:A:1123:U:C6	2.54	0.43
6:A:1287:A:N3	6:A:1353:G:O2'	2.42	0.43
7:B:71:GLY:O	7:B:93:ASN:HA	2.18	0.43
16:K:63:ALA:HB1	16:K:96:THR:HG23	2.01	0.43
19:N:93:ILE:HG22	19:N:96:LEU:HB2	1.99	0.43
20:O:17:ARG:O	20:O:17:ARG:NE	2.51	0.43
29:a:499:U:H2'	29:a:500:G:O4'	2.17	0.43
29:a:518:G:H2'	29:a:519:U:C6	2.54	0.43
34:f:83:TYR:HD1	34:f:84:PRO:HD2	1.83	0.43
47:s:26:LYS:HD2	47:s:26:LYS:HA	1.82	0.43
6:A:215:C:H2'	6:A:216:U:C6	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:35:GLN:HA	20:O:35:GLN:OE1	2.19	0.43
23:R:70:TYR:HB2	23:R:74:HIS:NE2	2.34	0.43
27:X:21:U:H2'	27:X:22:U:H4'	2.01	0.43
29:a:1045:C:H4'	29:a:1047:G:H5''	2.01	0.43
29:a:2037:A:H2'	29:a:2038:G:C8	2.54	0.43
29:a:2820:A:N3	29:a:2820:A:H2'	2.33	0.43
43:o:13:MET:HE3	43:o:13:MET:HB2	1.77	0.43
49:u:48:MET:HA	49:u:51:GLN:HG3	2.01	0.43
51:w:59:ILE:HG12	51:w:67:VAL:HG21	2.00	0.43
6:A:672:U:H2'	6:A:673:A:H8	1.84	0.42
7:B:137:ARG:HG2	7:B:137:ARG:H	1.73	0.42
8:C:28:GLU:OE1	8:C:28:GLU:N	2.46	0.42
21:P:35:ARG:HG2	21:P:35:ARG:NH1	2.33	0.42
29:a:77:G:H2'	29:a:78:U:C6	2.54	0.42
29:a:172:A:H2'	29:a:173:A:H8	1.84	0.42
29:a:2304:G:H22	29:a:2312:U:H3	1.65	0.42
53:y:3:LYS:HE3	53:y:3:LYS:HB3	1.72	0.42
6:A:33:A:H2'	6:A:34:C:C6	2.54	0.42
6:A:642:A:C5	13:H:107:SER:HA	2.53	0.42
6:A:936:C:C2	6:A:937:A:C8	3.07	0.42
6:A:1118:U:H1'	6:A:1179:A:C5	2.54	0.42
11:F:67:PRO:HG2	11:F:70:VAL:HG12	2.01	0.42
14:I:58:VAL:HB	14:I:59:GLU:OE2	2.19	0.42
24:S:15:LEU:HA	24:S:18:LYS:HG3	2.01	0.42
29:a:1563:U:H2'	29:a:1564:C:C6	2.54	0.42
29:a:2469:A:H2'	29:a:2470:G:O4'	2.18	0.42
34:f:134:GLU:N	34:f:134:GLU:OE1	2.53	0.42
46:r:109:ASP:OD1	46:r:110:ARG:N	2.51	0.42
6:A:1294:G:H2'	6:A:1295:U:C6	2.54	0.42
15:J:8:ILE:HD12	15:J:8:ILE:O	2.19	0.42
20:O:88:ARG:HH21	29:a:716:A:P	2.41	0.42
29:a:150:U:H2'	29:a:151:C:C6	2.54	0.42
29:a:359:G:H2'	29:a:360:U:H6	1.84	0.42
29:a:878:A:N7	29:a:899:A:H2	2.16	0.42
29:a:1394:U:H2'	29:a:1395:A:O4'	2.20	0.42
29:a:2537:U:H2'	29:a:2538:C:C6	2.54	0.42
52:x:10:SER:OG	52:x:12:GLU:OE2	2.25	0.42
5:4:12:ILE:C	5:4:12:ILE:HD12	2.44	0.42
6:A:494:G:O2'	6:A:496:A:H1'	2.19	0.42
6:A:784:A:H2'	6:A:785:G:C8	2.54	0.42
11:F:66:ALA:HB3	11:F:71:ILE:HD11	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:67:PRO:O	11:F:71:ILE:HG12	2.20	0.42
23:R:65:LEU:HD23	23:R:65:LEU:HA	1.84	0.42
29:a:969:G:H2'	29:a:970:U:C6	2.54	0.42
3:2:54:ASP:HB3	39:k:57:LEU:HD22	2.02	0.42
6:A:412:A:O2'	6:A:414:A:H5''	2.20	0.42
20:O:20:ASN:HD22	20:O:20:ASN:HA	1.66	0.42
21:P:45:GLU:O	21:P:46:LYS:HB3	2.19	0.42
21:P:45:GLU:C	21:P:47:GLU:H	2.28	0.42
22:Q:57:ASP:OD1	22:Q:81:LYS:HD3	2.18	0.42
31:c:272:SER:O	31:c:272:SER:OG	2.20	0.42
40:l:56:ALA:HB2	40:l:119:LEU:HD12	2.01	0.42
6:A:512:U:H2'	6:A:513:C:C6	2.54	0.42
6:A:751:U:H2'	6:A:752:G:O4'	2.19	0.42
7:B:49:MET:HA	7:B:52:GLU:HG2	2.02	0.42
9:D:105:MET:SD	9:D:180:GLY:HA3	2.60	0.42
9:D:156:LYS:H	9:D:156:LYS:HG2	1.59	0.42
11:F:23:GLU:N	11:F:23:GLU:OE2	2.52	0.42
14:I:34:SER:HB3	14:I:37:GLN:HE22	1.84	0.42
17:L:102:LEU:H	17:L:102:LEU:HG	1.61	0.42
34:f:33:LYS:HG3	34:f:157:THR:HB	2.01	0.42
34:f:69:LYS:HB3	34:f:69:LYS:HE3	1.81	0.42
43:o:53:ARG:HD3	43:o:53:ARG:HA	1.83	0.42
49:u:90:ASP:OD1	49:u:90:ASP:N	2.53	0.42
6:A:41:G:H2'	6:A:42:G:C8	2.55	0.42
6:A:313:A:H2'	6:A:314:C:C6	2.55	0.42
7:B:27:MET:HE3	7:B:27:MET:HB3	1.72	0.42
7:B:207:ILE:HA	7:B:210:VAL:HG22	2.02	0.42
8:C:42:TYR:CD1	8:C:42:TYR:C	2.97	0.42
8:C:121:THR:HG23	8:C:189:ALA:HB2	2.01	0.42
29:a:156:A:H2'	29:a:157:C:C6	2.55	0.42
29:a:657:U:H2'	29:a:658:U:C6	2.55	0.42
29:a:1485:U:H2'	29:a:1486:U:H6	1.84	0.42
29:a:2298:A:H2'	29:a:2299:U:O4'	2.20	0.42
43:o:44:GLU:OE1	43:o:87:LYS:HG3	2.19	0.42
1:0:33:LYS:HA	1:0:33:LYS:HD3	1.79	0.42
2:1:29:GLN:NE2	29:a:210:C:OP1	2.50	0.42
6:A:337:G:H2'	6:A:338:A:H8	1.80	0.42
6:A:613:C:H2'	6:A:614:C:C6	2.54	0.42
29:a:2:G:H2'	29:a:3:U:H6	1.84	0.42
29:a:1182:G:H2'	29:a:1183:U:O4'	2.20	0.42
29:a:1281:G:H2'	29:a:1282:U:C6	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:1710:G:H4'	29:a:2858:C:O2	2.20	0.42
35:g:39:ASP:OD1	35:g:39:ASP:N	2.49	0.42
6:A:437:U:O2'	9:D:120:HIS:ND1	2.42	0.42
6:A:978:A:C4	6:A:1319:A:C2	3.08	0.42
6:A:1326:U:H2'	6:A:1327:C:C6	2.55	0.42
8:C:85:GLU:O	8:C:88:ARG:HG3	2.20	0.42
11:F:11:HIS:ND1	11:F:12:PRO:HD2	2.35	0.42
11:F:17:GLN:HA	11:F:17:GLN:OE1	2.19	0.42
24:S:43:ASN:C	24:S:43:ASN:OD1	2.62	0.42
29:a:1689:A:H2'	29:a:1690:A:C8	2.55	0.42
29:a:2194:U:H2'	29:a:2195:U:H6	1.84	0.42
29:a:2740:A:H2'	29:a:2741:A:C8	2.55	0.42
41:m:45:ARG:O	41:m:49:GLU:HG3	2.20	0.42
6:A:72:A:H2'	6:A:73:C:H5'	2.02	0.42
6:A:528:C:H41	17:L:46:ASN:CG	2.28	0.42
7:B:70:VAL:HG12	7:B:169:GLU:HG3	2.01	0.42
15:J:22:THR:O	15:J:25:ILE:HG22	2.20	0.42
15:J:84:VAL:O	15:J:88:MET:HG2	2.20	0.42
29:a:598:U:H2'	29:a:599:A:H8	1.83	0.42
29:a:1636:U:H2'	29:a:1637:A:C8	2.54	0.42
29:a:2728:U:O2'	29:a:2729:G:H8	2.02	0.42
30:b:23:G:H2'	30:b:24:G:C8	2.55	0.42
6:A:182:A:C4	6:A:184:G:C8	3.08	0.41
6:A:1115:U:H2'	6:A:1116:U:C6	2.55	0.41
6:A:1463:U:H2'	6:A:1464:U:C6	2.55	0.41
9:D:91:LEU:HD23	9:D:91:LEU:HA	1.80	0.41
14:I:91:ASP:O	14:I:94:LEU:HD12	2.20	0.41
18:M:39:ILE:HD12	18:M:56:LEU:HD21	2.02	0.41
29:a:181:A:H2'	29:a:182:A:H8	1.84	0.41
29:a:880:G:C2	29:a:898:C:C2	3.08	0.41
29:a:1572:A:H2'	29:a:1573:G:H8	1.85	0.41
29:a:2515:C:H2'	29:a:2516:A:H8	1.84	0.41
34:f:114:PHE:HZ	34:f:176:PRO:HB2	1.85	0.41
38:j:114:LYS:HB2	38:j:114:LYS:HE2	1.70	0.41
46:r:74:ILE:HD12	46:r:105:VAL:HG22	2.02	0.41
6:A:678:U:H2'	6:A:679:C:H6	1.85	0.41
6:A:1133:G:H2'	6:A:1134:G:O4'	2.20	0.41
6:A:1338:G:H2'	6:A:1339:A:C8	2.55	0.41
6:A:1521:C:H2'	6:A:1522:U:C6	2.54	0.41
10:E:85:VAL:HG23	10:E:96:MET:HE3	2.01	0.41
16:K:35:THR:HG22	16:K:41:ALA:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:L:89:D2T:H7	17:L:89:D2T:H4	1.93	0.41
29:a:361:G:H8	29:a:361:G:OP2	2.03	0.41
29:a:2455:G:H2'	29:a:2456:C:H6	1.85	0.41
40:l:42:THR:HG22	40:l:93:VAL:HG12	2.01	0.41
45:q:26:ASP:O	45:q:27:ILE:HD13	2.19	0.41
6:A:521:G:OP2	17:L:51:LYS:NZ	2.50	0.41
6:A:982:U:H4'	6:A:983:A:O4'	2.21	0.41
7:B:196:VAL:HB	7:B:199:VAL:HG12	2.02	0.41
13:H:3:MET:HE2	13:H:3:MET:HA	2.03	0.41
14:I:28:ILE:HD13	14:I:63:LEU:HB2	2.01	0.41
16:K:34:ILE:HG22	16:K:42:LEU:HD12	2.02	0.41
28:Z:18:G:O6	28:Z:55:PSU:H1'	2.20	0.41
29:a:1542:U:H2'	29:a:1543:G:O4'	2.21	0.41
29:a:2242:G:H2'	29:a:2243:U:O4'	2.20	0.41
35:g:52:PHE:CE2	35:g:69:ARG:HA	2.55	0.41
49:u:31:TYR:HE2	49:u:90:ASP:HB3	1.85	0.41
6:A:21:G:H2'	6:A:22:G:C8	2.55	0.41
6:A:321:A:H2'	6:A:322:C:H6	1.85	0.41
12:G:125:SER:O	12:G:129:GLU:HG2	2.20	0.41
13:H:90:ASP:OD1	13:H:90:ASP:N	2.32	0.41
14:I:94:LEU:HA	14:I:97:GLU:OE2	2.20	0.41
16:K:37:ARG:NH2	16:K:83:GLU:OE2	2.53	0.41
29:a:116:C:O2'	29:a:126:A:N3	2.49	0.41
29:a:742:A:H2'	29:a:743:A:H8	1.86	0.41
29:a:1485:U:H2'	29:a:1486:U:C6	2.56	0.41
29:a:1677:A:H2'	29:a:1678:A:C8	2.55	0.41
29:a:2011:U:H2'	29:a:2012:G:O4'	2.19	0.41
34:f:57:LEU:O	34:f:61:SER:OG	2.38	0.41
39:k:77:ILE:HD12	39:k:108:ALA:HB1	2.02	0.41
48:t:40:ASN:O	48:t:63:ALA:N	2.49	0.41
6:A:1026:G:O6	6:A:1035:A:C6	2.72	0.41
21:P:6:LEU:HB3	21:P:17:TYR:HB3	2.03	0.41
28:Z:51:C:H2'	28:Z:52:G:H8	1.85	0.41
29:a:871:U:H2'	29:a:872:U:H6	1.85	0.41
29:a:2196:C:H2'	29:a:2197:U:C6	2.55	0.41
35:g:18:LYS:HB2	35:g:25:THR:OG1	2.21	0.41
47:s:39:THR:OG1	47:s:42:GLU:HG3	2.20	0.41
49:u:30:ILE:HD11	49:u:40:ILE:HD13	2.02	0.41
6:A:865:A:H2'	6:A:866:C:C6	2.55	0.41
6:A:883:C:O2'	6:A:884:U:H5'	2.21	0.41
7:B:81:LYS:HB2	7:B:93:ASN:HD22	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:80:VAL:HG21	12:G:85:TYR:CE2	2.56	0.41
17:L:82:ILE:O	17:L:82:ILE:HG13	2.18	0.41
29:a:2405:G:O2'	29:a:2411:A:N6	2.53	0.41
29:a:2609:U:H5	58:a:3008:V7A:OAX	2.03	0.41
29:a:2813:A:H2'	29:a:2814:A:C8	2.55	0.41
31:c:155:ALA:HB2	31:c:162:VAL:HG23	2.03	0.41
35:g:16:ASP:OD1	35:g:16:ASP:C	2.64	0.41
6:A:513:C:H2'	6:A:514:C:H6	1.86	0.41
9:D:168:PRO:HB3	9:D:170:TRP:CH2	2.56	0.41
16:K:47:ALA:HB1	16:K:62:ALA:HB1	2.03	0.41
16:K:87:LYS:HB2	16:K:113:VAL:HG23	2.01	0.41
19:N:83:LYS:HD2	19:N:83:LYS:HA	1.89	0.41
29:a:287:G:H1	29:a:353:C:H42	1.67	0.41
29:a:542:C:H2'	29:a:543:G:C8	2.56	0.41
29:a:1447:C:H2'	29:a:1448:G:H8	1.86	0.41
29:a:2072:C:H2'	29:a:2073:C:H6	1.85	0.41
29:a:2489:U:H2'	29:a:2490:G:O4'	2.20	0.41
29:a:2783:U:H2'	29:a:2784:U:H6	1.86	0.41
34:f:128:TYR:HE2	34:f:130:MET:HE2	1.86	0.41
6:A:215:C:H2'	6:A:216:U:H6	1.85	0.41
6:A:555:U:H2'	6:A:556:C:H6	1.82	0.41
6:A:826:C:O2	13:H:16:ASN:ND2	2.54	0.41
6:A:1010:U:H2'	6:A:1011:C:H6	1.85	0.41
6:A:1063:C:OP2	6:A:1064:G:O2'	2.33	0.41
21:P:48:GLU:OE1	21:P:51:ARG:NH2	2.52	0.41
22:Q:31:HIS:CE1	22:Q:33:ILE:HD12	2.56	0.41
29:a:1641:A:H2'	29:a:1642:G:O4'	2.21	0.41
29:a:2680:U:O2'	29:a:2681:C:H5'	2.21	0.41
31:c:43:ARG:HA	31:c:48:ARG:O	2.20	0.41
34:f:162:SER:HB3	34:f:165:GLU:OE1	2.20	0.41
2:1:26:ASN:CG	29:a:682:G:H5'	2.45	0.41
6:A:678:U:H2'	6:A:679:C:C6	2.56	0.41
6:A:693:G:C8	27:X:13:A:H1'	2.56	0.41
6:A:1036:A:H2'	6:A:1037:C:O4'	2.21	0.41
6:A:1040:U:H2'	6:A:1041:G:C8	2.56	0.41
6:A:1319:A:C8	6:A:1323:G:C5	3.09	0.41
7:B:4:VAL:HG11	7:B:212:LEU:HD21	2.02	0.41
7:B:101:LEU:HB3	7:B:179:LEU:HD12	2.03	0.41
8:C:22:TRP:CG	8:C:59:ARG:HD2	2.56	0.41
9:D:138:SER:O	9:D:141:ASP:HB2	2.21	0.41
12:G:61:ALA:HA	12:G:64:VAL:HG12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:I:55:VAL:CG2	14:I:94:LEU:HD22	2.51	0.41
15:J:86:ALA:HA	15:J:89:ARG:HH11	1.85	0.41
16:K:98:ARG:HG2	16:K:98:ARG:HH11	1.85	0.41
19:N:96:LEU:HD12	19:N:96:LEU:HA	1.88	0.41
28:Z:66:C:H2'	28:Z:67:C:H6	1.86	0.41
29:a:52:A:H2'	29:a:53:A:H8	1.86	0.41
29:a:157:C:H2'	29:a:158:U:O4'	2.20	0.41
29:a:302:C:H2'	29:a:303:G:H8	1.86	0.41
29:a:608:A:H2'	29:a:609:A:H8	1.83	0.41
29:a:693:A:H2'	29:a:694:U:C6	2.56	0.41
29:a:813:U:H2'	29:a:814:C:H6	1.85	0.41
29:a:903:C:H2'	29:a:904:G:H8	1.85	0.41
29:a:1326:U:O2'	29:a:2010:G:O2'	2.39	0.41
29:a:1923:U:H2'	29:a:1924:C:C6	2.56	0.41
29:a:2700:A:H2'	29:a:2701:U:H6	1.86	0.41
30:b:29:A:H2'	30:b:30:C:C6	2.55	0.41
35:g:24:ILE:HG21	35:g:72:LEU:HD11	2.03	0.41
41:m:28:LEU:HD23	41:m:48:VAL:HG21	2.02	0.41
42:n:28:VAL:HG21	42:n:92:PHE:CZ	2.55	0.41
47:s:69:ARG:HB2	47:s:69:ARG:CZ	2.51	0.41
6:A:160:A:H2'	6:A:161:A:O4'	2.20	0.41
6:A:500:G:H2'	6:A:501:C:C6	2.55	0.41
6:A:632:U:H5''	6:A:633:G:C8	2.56	0.41
6:A:1465:A:H2'	6:A:1466:C:H6	1.86	0.41
7:B:78:GLU:H	7:B:78:GLU:CD	2.20	0.41
15:J:11:LYS:HG2	15:J:71:LEU:CD1	2.51	0.41
17:L:36:ARG:HG2	17:L:38:TYR:HD1	1.84	0.41
25:T:61:GLN:OE1	25:T:61:GLN:HA	2.21	0.41
26:U:62:ARG:HH11	26:U:62:ARG:HG3	1.86	0.41
29:a:1013:C:H2'	29:a:1014:A:H8	1.85	0.41
29:a:1048:A:N7	29:a:1111:A:C6	2.89	0.41
29:a:1327:A:H2'	29:a:1328:A:O4'	2.21	0.41
29:a:1361:G:H2'	29:a:1362:C:C6	2.55	0.41
29:a:1410:G:H2'	29:a:1411:U:C6	2.55	0.41
29:a:1571:A:H2'	29:a:1572:A:C8	2.55	0.41
29:a:1979:U:O2'	29:a:1980:G:H5'	2.21	0.41
29:a:2250:G:O2'	29:a:2496:C:OP1	2.38	0.41
29:a:2266:A:H4'	29:a:2267:A:N3	2.36	0.41
33:e:168:ASP:OD1	33:e:169:VAL:N	2.54	0.41
35:g:43:VAL:HG13	35:g:52:PHE:CE1	2.56	0.41
49:u:20:LEU:HD22	49:u:25:LYS:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:31:G:O2'	6:A:48:C:N4	2.54	0.40
6:A:421:U:O2	8:C:127:ARG:NH1	2.54	0.40
6:A:440:C:C2	6:A:441:A:C8	3.09	0.40
8:C:43:LEU:HD23	8:C:43:LEU:HA	1.89	0.40
11:F:9:MET:SD	11:F:86:ARG:HB3	2.61	0.40
12:G:66:LEU:HD23	12:G:66:LEU:HA	1.90	0.40
24:S:49:ILE:HG22	24:S:51:VAL:HG22	2.03	0.40
25:T:28:MET:HE3	25:T:28:MET:HB3	1.82	0.40
29:a:598:U:H2'	29:a:599:A:C8	2.56	0.40
30:b:5:U:OP1	30:b:61:G:O2'	2.35	0.40
32:d:32:ASN:N	32:d:32:ASN:HD22	2.19	0.40
36:h:34:GLY:C	36:h:36:ALA:H	2.29	0.40
40:l:17:ASN:OD1	40:l:97:GLN:NE2	2.47	0.40
3:2:55:LEU:O	3:2:59:ILE:HG13	2.22	0.40
6:A:2:A:H1'	6:A:613:C:O2'	2.21	0.40
6:A:193:C:H2'	6:A:194:C:C6	2.56	0.40
6:A:505:G:H2'	6:A:506:G:C8	2.55	0.40
6:A:530:G:H3'	6:A:531:U:H5'	2.03	0.40
6:A:1410:A:H2'	6:A:1411:C:H6	1.86	0.40
11:F:41:ASP:C	11:F:41:ASP:OD1	2.64	0.40
29:a:305:C:H2'	29:a:306:U:C6	2.57	0.40
29:a:1198:U:C2	29:a:1199:U:C5	3.08	0.40
29:a:1656:C:H2'	29:a:1657:U:H6	1.86	0.40
35:g:9:VAL:HG21	35:g:73:ASN:HA	2.03	0.40
35:g:17:VAL:HG12	35:g:26:ILE:HG13	2.03	0.40
43:o:60:THR:HG23	43:o:73:VAL:HG22	2.03	0.40
51:w:54:LYS:HE3	51:w:54:LYS:HB2	1.95	0.40
3:2:23:LYS:NZ	59:2:101:HOH:O	2.35	0.40
6:A:868:C:H2'	6:A:869:G:O4'	2.21	0.40
6:A:1171:A:H2'	6:A:1172:C:C6	2.57	0.40
6:A:1377:A:H2'	12:G:2:PRO:HD3	2.03	0.40
20:O:88:ARG:NH2	29:a:716:A:OP2	2.54	0.40
29:a:78:U:H2'	29:a:79:C:H6	1.87	0.40
29:a:723:C:H2'	29:a:724:U:O4'	2.21	0.40
29:a:959:A:H2'	29:a:960:A:C8	2.56	0.40
29:a:984:A:N3	29:a:984:A:H2'	2.37	0.40
29:a:1282:U:H2'	29:a:1283:G:O4'	2.21	0.40
29:a:1441:G:H2'	29:a:1442:U:C6	2.56	0.40
29:a:1751:U:H2'	29:a:1752:C:C6	2.57	0.40
30:b:2:G:H2'	30:b:3:C:H6	1.86	0.40
32:d:56:LYS:O	32:d:60:VAL:HG23	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:e:14:VAL:HA	33:e:197:GLU:OE2	2.21	0.40
49:u:31:TYR:CE2	49:u:90:ASP:HB3	2.57	0.40
49:u:53:LYS:HB3	49:u:55:GLU:OE2	2.21	0.40
52:x:19:LEU:HD23	52:x:19:LEU:HA	1.84	0.40
6:A:1319:A:C8	6:A:1323:G:C6	3.09	0.40
7:B:216:ALA:O	7:B:220:THR:OG1	2.39	0.40
9:D:187:GLU:N	9:D:190:ASP:OD2	2.40	0.40
29:a:363:G:H2'	29:a:364:C:C6	2.56	0.40
29:a:570:G:H2'	29:a:2030:6MZ:N7	2.37	0.40
29:a:579:G:H2'	29:a:580:U:C6	2.56	0.40
29:a:898:C:H2'	29:a:899:A:O4'	2.21	0.40
29:a:1278:C:H2'	29:a:1279:G:H8	1.86	0.40
29:a:2796:U:O2'	29:a:2797:U:H2'	2.22	0.40
34:f:3:LYS:HB2	34:f:3:LYS:HE3	1.93	0.40
43:o:15:GLN:OE1	43:o:15:GLN:HA	2.22	0.40
6:A:1152:A:H2'	6:A:1153:G:H8	1.87	0.40
6:A:1187:G:H2'	6:A:1188:A:C8	2.57	0.40
9:D:140:ASN:N	9:D:182:PHE:O	2.48	0.40
29:a:445:C:H2'	29:a:446:G:O4'	2.21	0.40
29:a:2030:6MZ:C2	29:a:2499:C:H5''	2.52	0.40
29:a:2757:A:C2	29:a:2758:A:C8	3.09	0.40
29:a:2813:A:H2'	29:a:2814:A:H8	1.87	0.40
41:m:36:THR:OG1	41:m:37:THR:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	52 (93%)	4 (7%)	0	100	100
7	B	222/241 (92%)	209 (94%)	13 (6%)	0	100	100
8	C	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
9	D	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
10	E	154/167 (92%)	148 (96%)	6 (4%)	0	100	100
11	F	101/135 (75%)	97 (96%)	4 (4%)	0	100	100
12	G	151/179 (84%)	140 (93%)	11 (7%)	0	100	100
13	H	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
14	I	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
15	J	96/103 (93%)	91 (95%)	4 (4%)	1 (1%)	12	20
16	K	115/129 (89%)	110 (96%)	5 (4%)	0	100	100
17	L	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
18	M	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
19	N	98/101 (97%)	95 (97%)	2 (2%)	1 (1%)	12	20
20	O	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
21	P	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
22	Q	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
23	R	64/75 (85%)	61 (95%)	3 (5%)	0	100	100
24	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100
25	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
26	U	68/71 (96%)	68 (100%)	0	0	100	100
31	c	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
32	d	206/209 (99%)	201 (98%)	4 (2%)	1 (0%)	24	37
33	e	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
34	f	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
35	g	174/177 (98%)	163 (94%)	10 (6%)	1 (1%)	21	32
36	h	39/149 (26%)	32 (82%)	7 (18%)	0	100	100
37	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
38	j	121/123 (98%)	119 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	k	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
40	l	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
41	m	116/127 (91%)	109 (94%)	7 (6%)	0	100	100
42	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
43	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
44	p	115/118 (98%)	115 (100%)	0	0	100	100
45	q	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
46	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
47	s	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
48	t	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
49	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
50	v	76/85 (89%)	75 (99%)	1 (1%)	0	100	100
51	w	75/78 (96%)	75 (100%)	0	0	100	100
52	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
53	y	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
54	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	5484/5913 (93%)	5294 (96%)	186 (3%)	4 (0%)	49	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	J	57	VAL
32	d	149	ASN
35	g	46	ALA
19	N	33	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	46 (100%)	0	100	100
2	1	38/38 (100%)	37 (97%)	1 (3%)	40	63
3	2	51/52 (98%)	49 (96%)	2 (4%)	28	48
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	55/62 (89%)	50 (91%)	5 (9%)	9	14
7	B	186/199 (94%)	178 (96%)	8 (4%)	26	44
8	C	170/190 (90%)	163 (96%)	7 (4%)	27	46
9	D	172/173 (99%)	168 (98%)	4 (2%)	44	66
10	E	119/126 (94%)	115 (97%)	4 (3%)	32	54
11	F	90/116 (78%)	88 (98%)	2 (2%)	45	67
12	G	126/147 (86%)	123 (98%)	3 (2%)	43	65
13	H	104/105 (99%)	98 (94%)	6 (6%)	18	32
14	I	105/107 (98%)	104 (99%)	1 (1%)	68	84
15	J	86/90 (96%)	83 (96%)	3 (4%)	32	53
16	K	90/99 (91%)	85 (94%)	5 (6%)	19	33
17	L	102/103 (99%)	99 (97%)	3 (3%)	37	60
18	M	93/96 (97%)	92 (99%)	1 (1%)	65	82
19	N	83/84 (99%)	80 (96%)	3 (4%)	31	52
20	O	76/77 (99%)	75 (99%)	1 (1%)	61	80
21	P	65/65 (100%)	64 (98%)	1 (2%)	57	77
22	Q	73/78 (94%)	72 (99%)	1 (1%)	59	79
23	R	57/65 (88%)	53 (93%)	4 (7%)	14	24
24	S	72/79 (91%)	71 (99%)	1 (1%)	59	79
25	T	65/66 (98%)	65 (100%)	0	100	100
26	U	60/61 (98%)	59 (98%)	1 (2%)	53	74
31	c	216/218 (99%)	214 (99%)	2 (1%)	70	85
32	d	163/163 (100%)	160 (98%)	3 (2%)	51	73
33	e	165/165 (100%)	156 (94%)	9 (6%)	19	34
34	f	148/150 (99%)	139 (94%)	9 (6%)	17	30
35	g	137/138 (99%)	124 (90%)	13 (10%)	8	13
36	h	32/114 (28%)	31 (97%)	1 (3%)	35	57
37	i	116/116 (100%)	113 (97%)	3 (3%)	40	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	j	104/104 (100%)	103 (99%)	1 (1%)	68	84
39	k	103/103 (100%)	100 (97%)	3 (3%)	37	60
40	l	108/108 (100%)	105 (97%)	3 (3%)	38	60
41	m	98/103 (95%)	96 (98%)	2 (2%)	48	70
42	n	86/87 (99%)	84 (98%)	2 (2%)	44	66
43	o	99/100 (99%)	98 (99%)	1 (1%)	68	84
44	p	89/90 (99%)	88 (99%)	1 (1%)	65	82
45	q	84/84 (100%)	78 (93%)	6 (7%)	13	23
46	r	93/93 (100%)	91 (98%)	2 (2%)	45	67
47	s	80/84 (95%)	79 (99%)	1 (1%)	61	80
48	t	83/85 (98%)	77 (93%)	6 (7%)	13	23
49	u	78/78 (100%)	75 (96%)	3 (4%)	29	49
50	v	58/63 (92%)	57 (98%)	1 (2%)	53	74
51	w	67/68 (98%)	64 (96%)	3 (4%)	24	42
52	x	54/55 (98%)	54 (100%)	0	100	100
53	y	48/49 (98%)	47 (98%)	1 (2%)	47	69
54	z	47/48 (98%)	47 (100%)	0	100	100
All	All	4574/4827 (95%)	4431 (97%)	143 (3%)	36	57

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	43	THR
3	2	54	ASP
3	2	55	LEU
5	4	15	SER
5	4	28	VAL
5	4	58	ASP
5	4	64	PHE
5	4	66	ILE
7	B	5	SER
7	B	36	ASN
7	B	105	LYS
7	B	123	ASP
7	B	147	SER
7	B	199	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	B	220	THR
7	B	221	VAL
8	C	52	VAL
8	C	88	ARG
8	C	90	VAL
8	C	97	VAL
8	C	182	ILE
8	C	183	ASP
8	C	207	ILE
9	D	59	GLN
9	D	73	ARG
9	D	119	SER
9	D	191	LEU
10	E	43	ASN
10	E	134	ILE
10	E	149	SER
10	E	164	ILE
11	F	62	MET
11	F	68	GLN
12	G	45	SER
12	G	59	LEU
12	G	75	VAL
13	H	25	VAL
13	H	40	LEU
13	H	55	THR
13	H	73	GLU
13	H	74	SER
13	H	90	ASP
14	I	94	LEU
15	J	18	ILE
15	J	25	ILE
15	J	36	VAL
16	K	16	VAL
16	K	34	ILE
16	K	95	SER
16	K	108	THR
16	K	119	ASN
17	L	21	VAL
17	L	45	PRO
17	L	87	VAL
18	M	19	LEU
19	N	35	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	N	37	SER
19	N	40	ASP
20	O	20	ASN
21	P	50	THR
22	Q	29	VAL
23	R	18	VAL
23	R	36	SER
23	R	42	SER
23	R	47	THR
24	S	60	VAL
26	U	53	VAL
31	c	4	VAL
31	c	137	VAL
32	d	73	VAL
32	d	91	THR
32	d	95	SER
33	e	55	SER
33	e	80	SER
33	e	125	SER
33	e	126	VAL
33	e	132	LYS
33	e	153	LEU
33	e	191	ASP
33	e	197	GLU
33	e	198	GLU
34	f	69	LYS
34	f	83	TYR
34	f	101	GLU
34	f	104	ILE
34	f	136	ILE
34	f	137	ILE
34	f	149	VAL
34	f	175	PHE
34	f	178	ARG
35	g	29	LYS
35	g	34	THR
35	g	39	ASP
35	g	43	VAL
35	g	60	ASP
35	g	67	THR
35	g	76	VAL
35	g	79	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	g	84	THR
35	g	90	VAL
35	g	92	VAL
35	g	127	THR
35	g	171	THR
36	h	40	THR
37	i	10	THR
37	i	11	VAL
37	i	64	VAL
38	j	76	VAL
39	k	76	GLU
39	k	106	GLU
39	k	136	GLU
40	l	8	LYS
40	l	30	SER
40	l	102	LEU
41	m	48	VAL
41	m	65	LEU
42	n	54	VAL
42	n	78	VAL
43	o	5	ILE
44	p	13	ARG
45	q	22	LEU
45	q	29	THR
45	q	60	LYS
45	q	64	VAL
45	q	72	VAL
45	q	102	SER
46	r	12	SER
46	r	108	SER
47	s	26	LYS
48	t	29	LEU
48	t	40	ASN
48	t	49	VAL
48	t	59	VAL
48	t	65	ILE
48	t	83	VAL
49	u	59	GLU
49	u	68	LYS
49	u	90	ASP
50	v	10	THR
51	w	2	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	w	35	SER
51	w	42	SER
53	y	8	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	26	ASN
4	3	13	ASN
5	4	20	ASN
5	4	33	ASN
8	C	8	ASN
8	C	123	GLN
10	E	43	ASN
10	E	73	ASN
10	E	132	ASN
10	E	146	ASN
11	F	94	HIS
18	M	12	HIS
19	N	35	ASN
19	N	49	GLN
19	N	66	GLN
22	Q	51	ASN
23	R	54	GLN
25	T	3	ASN
25	T	13	GLN
31	c	21	ASN
31	c	25	HIS
31	c	134	ASN
32	d	140	HIS
33	e	9	GLN
33	e	41	GLN
33	e	136	GLN
33	e	156	ASN
35	g	22	GLN
35	g	48	ASN
36	h	20	ASN
43	o	66	ASN
44	p	44	GLN
45	q	82	HIS
46	r	61	ASN
47	s	28	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	u	12	GLN
53	y	9	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	9/22 (40%)	5 (55%)	0
28	Z	74/75 (98%)	11 (14%)	2 (2%)
29	a	2749/2904 (94%)	283 (10%)	0
30	b	118/120 (98%)	9 (7%)	0
6	A	1495/1542 (96%)	177 (11%)	2 (0%)
All	All	4445/4663 (95%)	485 (10%)	4 (0%)

All (485) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	4	U
6	A	6	G
6	A	9	G
6	A	22	G
6	A	32	A
6	A	39	G
6	A	47	C
6	A	48	C
6	A	51	A
6	A	72	A
6	A	73	C
6	A	74	A
6	A	78	A
6	A	94	G
6	A	95	C
6	A	96	U
6	A	120	A
6	A	121	U
6	A	128	G
6	A	130	A
6	A	131	A
6	A	141	G
6	A	143	A
6	A	144	G
6	A	182	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	183	C
6	A	197	A
6	A	226	G
6	A	240	G
6	A	245	U
6	A	247	G
6	A	251	G
6	A	266	G
6	A	267	C
6	A	280	C
6	A	289	G
6	A	321	A
6	A	328	C
6	A	329	A
6	A	347	G
6	A	352	C
6	A	354	G
6	A	367	U
6	A	372	C
6	A	373	A
6	A	384	G
6	A	398	U
6	A	406	G
6	A	412	A
6	A	413	G
6	A	414	A
6	A	415	A
6	A	421	U
6	A	422	C
6	A	424	G
6	A	429	U
6	A	453	G
6	A	458	U
6	A	468	A
6	A	478	A
6	A	481	G
6	A	484	G
6	A	486	U
6	A	495	A
6	A	496	A
6	A	497	G
6	A	509	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	511	C
6	A	518	C
6	A	521	G
6	A	531	U
6	A	532	A
6	A	533	A
6	A	547	A
6	A	559	A
6	A	564	C
6	A	572	A
6	A	573	A
6	A	576	C
6	A	577	G
6	A	596	A
6	A	633	G
6	A	653	U
6	A	661	G
6	A	665	A
6	A	687	A
6	A	703	G
6	A	723	U
6	A	724	G
6	A	734	G
6	A	755	G
6	A	777	A
6	A	793	U
6	A	794	A
6	A	815	A
6	A	817	C
6	A	821	G
6	A	890	G
6	A	902	G
6	A	914	A
6	A	926	G
6	A	934	C
6	A	935	A
6	A	960	U
6	A	969	A
6	A	975	A
6	A	976	G
6	A	977	A
6	A	992	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	993	G
6	A	996	A
6	A	1002	G
6	A	1003	G
6	A	1004	A
6	A	1020	G
6	A	1036	A
6	A	1039	G
6	A	1042	A
6	A	1044	A
6	A	1046	A
6	A	1065	U
6	A	1085	U
6	A	1088	G
6	A	1094	G
6	A	1095	U
6	A	1101	A
6	A	1127	G
6	A	1137	C
6	A	1139	G
6	A	1140	C
6	A	1157	A
6	A	1159	U
6	A	1167	A
6	A	1184	G
6	A	1196	A
6	A	1197	A
6	A	1213	A
6	A	1227	A
6	A	1238	A
6	A	1258	G
6	A	1260	G
6	A	1280	A
6	A	1285	A
6	A	1286	U
6	A	1287	A
6	A	1297	G
6	A	1300	G
6	A	1305	G
6	A	1317	C
6	A	1320	C
6	A	1322	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	1338	G
6	A	1340	A
6	A	1346	A
6	A	1353	G
6	A	1363	A
6	A	1370	G
6	A	1378	C
6	A	1379	G
6	A	1381	U
6	A	1382	C
6	A	1398	A
6	A	1419	G
6	A	1422	G
6	A	1429	A
6	A	1432	G
6	A	1446	A
6	A	1452	C
6	A	1487	G
6	A	1493	A
6	A	1497	G
6	A	1499	A
6	A	1503	A
6	A	1506	U
6	A	1517	G
6	A	1529	G
6	A	1530	G
27	X	14	A
27	X	19	U
27	X	20	U
27	X	21	U
27	X	22	U
28	Z	9	G
28	Z	16	C
28	Z	17(A)	U
28	Z	18	G
28	Z	19	G
28	Z	20	U
28	Z	21	A
28	Z	31	G
28	Z	47	U
28	Z	48	C
28	Z	64	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	a	10	A
29	a	15	G
29	a	34	U
29	a	35	G
29	a	45	G
29	a	51	G
29	a	61	C
29	a	63	A
29	a	71	A
29	a	74	A
29	a	75	G
29	a	84	A
29	a	101	A
29	a	102	U
29	a	118	A
29	a	119	A
29	a	120	U
29	a	136	G
29	a	139	U
29	a	140	C
29	a	142	A
29	a	163	C
29	a	181	A
29	a	196	A
29	a	199	A
29	a	215	G
29	a	216	A
29	a	222	A
29	a	233	A
29	a	248	G
29	a	272	A
29	a	278	A
29	a	279	A
29	a	281	C
29	a	311	A
29	a	329	G
29	a	330	A
29	a	356	G
29	a	362	A
29	a	367	G
29	a	386	G
29	a	396	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	a	405	U
29	a	411	G
29	a	425	G
29	a	481	G
29	a	491	G
29	a	505	A
29	a	508	A
29	a	509	C
29	a	529	A
29	a	530	G
29	a	532	A
29	a	545	U
29	a	546	U
29	a	547	A
29	a	548	G
29	a	563	A
29	a	573	U
29	a	575	A
29	a	603	A
29	a	614	A
29	a	615	U
29	a	627	A
29	a	637	A
29	a	645	C
29	a	646	U
29	a	647	G
29	a	654	A
29	a	655	A
29	a	685	A
29	a	686	U
29	a	730	A
29	a	747	5MU
29	a	764	A
29	a	775	G
29	a	776	G
29	a	782	A
29	a	784	G
29	a	785	G
29	a	805	G
29	a	812	C
29	a	827	U
29	a	828	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	a	846	U
29	a	847	U
29	a	859	G
29	a	869	G
29	a	885	C
29	a	888	C
29	a	890	C
29	a	891	G
29	a	893	C
29	a	895	U
29	a	896	A
29	a	897	C
29	a	899	A
29	a	910	A
29	a	931	U
29	a	946	C
29	a	961	C
29	a	974	G
29	a	983	A
29	a	996	A
29	a	1009	A
29	a	1012	U
29	a	1013	C
29	a	1026	G
29	a	1033	U
29	a	1047	G
29	a	1108	U
29	a	1111	A
29	a	1112	G
29	a	1116	G
29	a	1128	G
29	a	1130	U
29	a	1132	U
29	a	1133	A
29	a	1135	C
29	a	1142	A
29	a	1212	G
29	a	1236	G
29	a	1250	G
29	a	1253	A
29	a	1256	G
29	a	1271	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	a	1272	A
29	a	1273	U
29	a	1300	G
29	a	1301	A
29	a	1321	A
29	a	1329	U
29	a	1352	U
29	a	1365	A
29	a	1379	U
29	a	1383	A
29	a	1395	A
29	a	1416	G
29	a	1428	C
29	a	1434	A
29	a	1452	G
29	a	1482	G
29	a	1493	C
29	a	1508	A
29	a	1509	A
29	a	1510	G
29	a	1515	A
29	a	1524	G
29	a	1535	A
29	a	1536	C
29	a	1537	G
29	a	1566	A
29	a	1569	A
29	a	1578	U
29	a	1583	A
29	a	1584	U
29	a	1585	C
29	a	1586	A
29	a	1607	C
29	a	1609	A
29	a	1647	U
29	a	1648	U
29	a	1674	G
29	a	1715	G
29	a	1729	U
29	a	1730	C
29	a	1732	C
29	a	1738	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	a	1764	C
29	a	1773	A
29	a	1786	A
29	a	1791	A
29	a	1800	C
29	a	1801	A
29	a	1807	G
29	a	1808	A
29	a	1816	C
29	a	1829	A
29	a	1848	A
29	a	1858	A
29	a	1869	G
29	a	1871	A
29	a	1872	A
29	a	1873	G
29	a	1906	G
29	a	1913	A
29	a	1914	C
29	a	1929	G
29	a	1930	G
29	a	1936	A
29	a	1938	A
29	a	1955	U
29	a	1967	C
29	a	1970	A
29	a	1971	U
29	a	1972	G
29	a	1991	U
29	a	1993	U
29	a	2023	C
29	a	2030	6MZ
29	a	2031	A
29	a	2033	A
29	a	2043	C
29	a	2055	C
29	a	2056	G
29	a	2060	A
29	a	2061	G
29	a	2062	A
29	a	2069	G7M
29	a	2093	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	a	2198	A
29	a	2203	U
29	a	2204	G
29	a	2211	A
29	a	2225	A
29	a	2238	G
29	a	2239	G
29	a	2279	G
29	a	2283	C
29	a	2287	A
29	a	2288	A
29	a	2305	U
29	a	2308	G
29	a	2322	A
29	a	2325	G
29	a	2333	A
29	a	2336	A
29	a	2345	G
29	a	2347	C
29	a	2350	C
29	a	2357	G
29	a	2383	G
29	a	2385	C
29	a	2396	G
29	a	2402	U
29	a	2403	C
29	a	2406	A
29	a	2425	A
29	a	2429	G
29	a	2430	A
29	a	2435	A
29	a	2441	U
29	a	2448	A
29	a	2475	C
29	a	2491	U
29	a	2498	OMC
29	a	2502	G
29	a	2505	G
29	a	2518	A
29	a	2520	C
29	a	2525	G
29	a	2529	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	a	2547	A
29	a	2566	A
29	a	2567	G
29	a	2602	A
29	a	2613	U
29	a	2615	U
29	a	2629	U
29	a	2630	G
29	a	2661	G
29	a	2663	G
29	a	2689	U
29	a	2690	U
29	a	2714	G
29	a	2716	C
29	a	2726	A
29	a	2732	G
29	a	2733	A
29	a	2744	G
29	a	2748	A
29	a	2765	A
29	a	2778	A
29	a	2780	G
29	a	2799	A
29	a	2818	U
29	a	2820	A
29	a	2821	A
29	a	2835	A
29	a	2861	U
29	a	2873	A
29	a	2880	C
29	a	2884	U
30	b	9	G
30	b	16	G
30	b	35	C
30	b	56	G
30	b	67	G
30	b	89	U
30	b	90	C
30	b	99	A
30	b	109	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	182	A
6	A	1035	A
28	Z	16	C
28	Z	17(A)	U

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

42 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$
6	2MG	A	966	6	23,26,27	0.51	0	33,38,41	0.51	0
6	PSU	A	516	6,56	18,21,22	1.08	1 (5%)	21,30,33	1.91	5 (23%)
28	4SU	Z	8	28	18,21,22	3.85	8 (44%)	25,30,33	2.32	5 (20%)
29	PSU	a	2457	29	18,21,22	1.08	2 (11%)	21,30,33	2.01	6 (28%)
29	6MZ	a	1618	29	22,25,26	2.24	7 (31%)	29,36,39	2.42	10 (34%)
6	G7M	A	527	6	23,26,27	0.73	1 (4%)	34,39,42	0.64	1 (2%)
6	UR3	A	1498	6	19,22,23	2.73	8 (42%)	26,32,35	1.63	3 (11%)
29	PSU	a	1911	29	18,21,22	1.06	1 (5%)	21,30,33	1.96	5 (23%)
29	3TD	a	1915	29	19,22,23	4.11	7 (36%)	23,32,35	1.79	3 (13%)
29	5MC	a	1962	29,57	19,22,23	0.66	0	26,32,35	0.68	0
29	OMC	a	2498	29,56	19,22,23	0.64	0	25,31,34	0.70	0
6	2MG	A	1207	6	23,26,27	0.47	0	33,38,41	0.52	0
29	2MA	a	2503	29,56,57	22,25,26	0.84	1 (4%)	32,37,40	1.20	4 (12%)
28	5MC	Z	32	28	19,22,23	0.65	0	26,32,35	0.69	0
6	2MG	A	1516	6	23,26,27	0.53	0	33,38,41	0.74	0
29	2MG	a	2445	29	23,26,27	0.58	0	33,38,41	0.45	0
6	5MC	A	1407	6	19,22,23	0.65	0	26,32,35	0.68	0
29	2MG	a	1835	29	23,26,27	0.52	0	33,38,41	0.44	0
40	4D4	l	81	40	9,11,12	2.03	2 (22%)	7,13,15	1.88	3 (42%)
6	4OC	A	1402	6	20,23,24	3.19	8 (40%)	25,32,35	0.90	1 (4%)
32	MEQ	d	150	32	8,9,10	0.87	0	5,10,12	0.67	0
6	MA6	A	1519	6	23,26,27	0.29	0	33,38,41	0.74	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	D2T	L	89	17	8,9,10	1.56	1 (12%)	6,11,13	1.90	2 (33%)
28	PSU	Z	55	28	18,21,22	1.10	1 (5%)	21,30,33	1.94	5 (23%)
29	6MZ	a	2030	29	22,25,26	2.29	7 (31%)	29,36,39	2.47	13 (44%)
29	OMG	a	2251	29,28,57	23,26,27	0.56	0	32,38,41	0.44	0
29	OMU	a	2552	29,57	19,22,23	2.96	7 (36%)	25,31,34	1.90	5 (20%)
29	PSU	a	2580	29	18,21,22	1.11	3 (16%)	21,30,33	1.98	5 (23%)
29	H2U	a	2449	29	18,21,22	0.54	0	19,30,33	1.13	1 (5%)
6	5MC	A	967	6	19,22,23	0.60	0	26,32,35	0.63	0
28	5MU	Z	54	28	19,22,23	0.38	0	27,32,35	0.63	0
29	PSU	a	746	29,56	18,21,22	1.10	1 (5%)	21,30,33	1.87	3 (14%)
29	1MG	a	745	29	23,26,27	2.85	8 (34%)	33,39,42	1.69	6 (18%)
29	PSU	a	1917	29	18,21,22	1.06	1 (5%)	21,30,33	1.95	4 (19%)
29	PSU	a	955	29	18,21,22	1.07	1 (5%)	21,30,33	2.03	4 (19%)
6	MA6	A	1518	6	23,26,27	0.30	0	33,38,41	0.64	1 (3%)
29	5MU	a	747	29	19,22,23	0.48	0	27,32,35	0.72	1 (3%)
29	PSU	a	2605	29	18,21,22	1.07	1 (5%)	21,30,33	1.95	4 (19%)
29	PSU	a	2604	29	18,21,22	1.04	1 (5%)	21,30,33	2.01	5 (23%)
29	5MU	a	1939	29,57	19,22,23	0.57	0	27,32,35	0.47	0
29	PSU	a	2504	29,57	18,21,22	1.12	1 (5%)	21,30,33	1.94	4 (19%)
29	G7M	a	2069	29,57	23,26,27	2.61	9 (39%)	34,39,42	2.35	11 (32%)

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
6	2MG	A	966	6	-	0/9/27/28	0/3/3/3
6	PSU	A	516	6,56	-	0/7/25/26	0/2/2/2
28	4SU	Z	8	28	-	0/7/25/26	0/2/2/2
29	PSU	a	2457	29	-	0/7/25/26	0/2/2/2
29	6MZ	a	1618	29	-	0/9/27/28	0/3/3/3
6	G7M	A	527	6	-	2/7/25/26	0/3/3/3
6	UR3	A	1498	6	-	0/7/25/26	0/2/2/2
29	PSU	a	1911	29	-	0/7/25/26	0/2/2/2
29	3TD	a	1915	29	-	0/7/25/26	0/2/2/2
29	5MC	a	1962	29,57	-	0/7/25/26	0/2/2/2
29	OMC	a	2498	29,56	-	1/9/27/28	0/2/2/2
6	2MG	A	1207	6	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	2MA	a	2503	29,56,57	-	2/7/25/26	0/3/3/3
28	5MC	Z	32	28	-	0/7/25/26	0/2/2/2
6	2MG	A	1516	6	-	0/9/27/28	0/3/3/3
29	2MG	a	2445	29	-	1/9/27/28	0/3/3/3
6	5MC	A	1407	6	-	0/7/25/26	0/2/2/2
29	2MG	a	1835	29	-	0/9/27/28	0/3/3/3
40	4D4	l	81	40	-	4/11/12/14	-
6	4OC	A	1402	6	-	1/9/29/30	0/2/2/2
32	MEQ	d	150	32	-	2/8/9/11	-
6	MA6	A	1519	6	-	0/11/29/30	0/3/3/3
17	D2T	L	89	17	-	4/7/12/14	-
28	PSU	Z	55	28	-	0/7/25/26	0/2/2/2
29	6MZ	a	2030	29	-	2/9/27/28	0/3/3/3
29	OMG	a	2251	29,28,57	-	1/9/27/28	0/3/3/3
29	OMU	a	2552	29,57	-	1/9/27/28	0/2/2/2
29	PSU	a	2580	29	-	0/7/25/26	0/2/2/2
29	H2U	a	2449	29	-	0/7/38/39	0/2/2/2
6	5MC	A	967	6	-	0/7/25/26	0/2/2/2
28	5MU	Z	54	28	-	0/7/25/26	0/2/2/2
29	PSU	a	746	29,56	-	2/7/25/26	0/2/2/2
29	1MG	a	745	29	-	0/7/25/26	0/3/3/3
29	PSU	a	1917	29	-	0/7/25/26	0/2/2/2
29	PSU	a	955	29	-	0/7/25/26	0/2/2/2
6	MA6	A	1518	6	-	0/11/29/30	0/3/3/3
29	5MU	a	747	29	-	0/7/25/26	0/2/2/2
29	PSU	a	2605	29	-	0/7/25/26	0/2/2/2
29	PSU	a	2604	29	-	0/7/25/26	0/2/2/2
29	5MU	a	1939	29,57	-	0/7/25/26	0/2/2/2
29	PSU	a	2504	29,57	-	2/7/25/26	0/2/2/2
29	G7M	a	2069	29,57	-	2/7/25/26	0/3/3/3

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	1915	3TD	C6-C5	12.83	1.49	1.35
29	a	1915	3TD	C2-N1	9.11	1.48	1.37
28	Z	8	4SU	C4-N3	8.56	1.46	1.37
29	a	1618	6MZ	C6-N6	7.96	1.43	1.34
29	a	745	1MG	C2-N3	7.80	1.45	1.33
29	a	2030	6MZ	C6-N6	7.80	1.43	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1402	4OC	C4-N3	7.22	1.44	1.32
6	A	1498	UR3	C2-N1	7.06	1.48	1.38
28	Z	8	4SU	C2-N3	7.02	1.50	1.38
29	a	2552	OMU	C2-N3	6.99	1.50	1.38
29	a	2552	OMU	C2-N1	6.90	1.49	1.38
29	a	745	1MG	C4-N3	6.45	1.49	1.34
28	Z	8	4SU	C2-N1	6.42	1.48	1.38
6	A	1402	4OC	C6-C5	6.29	1.49	1.35
29	a	2069	G7M	C4-N3	6.14	1.48	1.34
6	A	1402	4OC	C2-N3	6.10	1.48	1.36
29	a	745	1MG	C2-N2	6.06	1.44	1.34
6	A	1498	UR3	C6-C5	6.03	1.49	1.35
29	a	2552	OMU	C6-C5	5.98	1.48	1.35
28	Z	8	4SU	C6-C5	5.73	1.48	1.35
29	a	2069	G7M	C5-N7	-5.49	1.32	1.39
29	a	1915	3TD	C6-N1	5.32	1.45	1.36
28	Z	8	4SU	C4-S4	-5.31	1.59	1.68
40	l	81	4D4	CZ-NE	4.99	1.42	1.33
6	A	1402	4OC	C4-N4	4.88	1.46	1.36
29	a	1915	3TD	C2-N3	4.86	1.48	1.38
28	Z	8	4SU	C5-C4	4.84	1.48	1.42
6	A	1498	UR3	C2-N3	4.83	1.48	1.39
29	a	2069	G7M	C2-N3	4.80	1.44	1.33
29	a	2069	G7M	C2-N2	4.53	1.44	1.34
6	A	1402	4OC	C2-N1	4.02	1.48	1.40
29	a	2552	OMU	C4-N3	3.98	1.45	1.38
6	A	1402	4OC	C5-C4	3.78	1.49	1.41
29	a	2030	6MZ	C5-N7	-3.63	1.32	1.39
28	Z	55	PSU	C6-C5	3.61	1.39	1.35
29	a	2504	PSU	C6-C5	3.58	1.39	1.35
29	a	2069	G7M	C5-C6	3.58	1.53	1.43
29	a	1618	6MZ	C5-N7	-3.53	1.32	1.39
17	L	89	D2T	CB-CA	-3.46	1.53	1.54
29	a	745	1MG	C2-N1	3.44	1.43	1.37
29	a	1911	PSU	C6-C5	3.32	1.39	1.35
29	a	746	PSU	C6-C5	3.30	1.38	1.35
29	a	1917	PSU	C6-C5	3.28	1.38	1.35
6	A	516	PSU	C6-C5	3.28	1.38	1.35
29	a	2605	PSU	C6-C5	3.24	1.38	1.35
29	a	955	PSU	C6-C5	3.22	1.38	1.35
6	A	1402	4OC	C6-N1	3.19	1.45	1.38
29	a	745	1MG	C5-N7	-3.16	1.32	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Z	8	4SU	C6-N1	3.13	1.45	1.38
29	a	2580	PSU	C6-C5	3.12	1.38	1.35
29	a	2604	PSU	C6-C5	3.11	1.38	1.35
29	a	2030	6MZ	C5-C4	-3.10	1.33	1.39
29	a	2457	PSU	C6-C5	3.06	1.38	1.35
29	a	745	1MG	C5-C6	3.00	1.53	1.45
6	A	1402	4OC	O2-C2	-2.98	1.18	1.23
6	A	1498	UR3	C6-N1	2.95	1.45	1.38
29	a	1618	6MZ	C5-C4	-2.83	1.34	1.39
29	a	2069	G7M	O6-C6	-2.79	1.18	1.23
29	a	2030	6MZ	C6-N1	-2.79	1.30	1.35
40	l	81	4D4	CZ-NH1	2.74	1.44	1.34
28	Z	8	4SU	O2-C2	-2.73	1.18	1.23
29	a	2069	G7M	C4-N9	-2.64	1.31	1.38
6	A	527	G7M	C8-N7	2.58	1.37	1.33
6	A	1498	UR3	O4-C4	-2.55	1.18	1.23
29	a	2069	G7M	C2-N1	2.51	1.43	1.37
29	a	1618	6MZ	C6-N1	-2.50	1.31	1.35
29	a	1915	3TD	O2-C2	-2.50	1.18	1.23
29	a	2503	2MA	C6-N6	-2.50	1.27	1.34
29	a	2552	OMU	C6-N1	2.46	1.44	1.38
29	a	2030	6MZ	C8-N9	-2.39	1.33	1.37
29	a	1915	3TD	C4-N3	2.36	1.45	1.40
29	a	2030	6MZ	C9-N6	-2.29	1.41	1.45
6	A	1498	UR3	C4-N3	2.29	1.45	1.40
29	a	1618	6MZ	C8-N9	-2.27	1.33	1.37
29	a	745	1MG	O6-C6	-2.25	1.18	1.23
29	a	2580	PSU	O4'-C1'	-2.25	1.40	1.43
6	A	1498	UR3	O2-C2	-2.25	1.18	1.22
29	a	1618	6MZ	C9-N6	-2.23	1.41	1.45
29	a	2069	G7M	C6-N1	2.20	1.43	1.38
29	a	2030	6MZ	C5-C6	-2.20	1.36	1.41
6	A	1498	UR3	C5-C4	2.15	1.49	1.43
29	a	2552	OMU	C5-C4	2.14	1.48	1.43
29	a	745	1MG	C4-N9	-2.14	1.32	1.38
29	a	1915	3TD	O4-C4	-2.14	1.18	1.23
29	a	1618	6MZ	C5-C6	-2.10	1.36	1.41
29	a	2580	PSU	C4-C5	-2.08	1.38	1.44
29	a	2552	OMU	O4-C4	-2.05	1.20	1.24
29	a	2457	PSU	C4-C5	-2.00	1.38	1.44

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	Z	8	4SU	C4-N3-C2	-7.86	119.78	127.31
29	a	2069	G7M	C1'-N9-C4	6.03	144.29	126.49
29	a	2552	OMU	C4-N3-C2	-5.98	119.19	126.61
6	A	1498	UR3	C4-N3-C2	-5.82	119.90	124.58
29	a	1915	3TD	N1-C2-N3	5.69	120.26	116.13
29	a	1618	6MZ	N1-C2-N3	-5.65	120.03	128.58
29	a	2069	G7M	C1'-N9-C8	-5.64	107.70	126.74
29	a	2030	6MZ	N1-C2-N3	-5.39	120.43	128.58
29	a	1618	6MZ	C5-C4-N3	-5.38	119.30	126.72
29	a	955	PSU	N1-C2-N3	5.27	120.73	115.17
29	a	2030	6MZ	C5-C4-N3	-5.25	119.49	126.72
28	Z	8	4SU	C5-C4-N3	5.25	119.63	114.75
29	a	2604	PSU	C4-N3-C2	-5.14	119.29	126.37
29	a	745	1MG	C5-C4-N3	-5.09	120.29	128.39
29	a	2604	PSU	N1-C2-N3	5.07	120.51	115.17
29	a	746	PSU	C4-N3-C2	-5.06	119.40	126.37
29	a	2457	PSU	N1-C2-N3	5.06	120.50	115.17
29	a	2504	PSU	N1-C2-N3	5.00	120.45	115.17
29	a	2605	PSU	C4-N3-C2	-4.99	119.50	126.37
29	a	1911	PSU	C4-N3-C2	-4.99	119.50	126.37
29	a	2605	PSU	N1-C2-N3	4.99	120.43	115.17
29	a	955	PSU	C4-N3-C2	-4.98	119.52	126.37
29	a	2457	PSU	C4-N3-C2	-4.97	119.52	126.37
28	Z	55	PSU	C4-N3-C2	-4.94	119.57	126.37
29	a	1917	PSU	N1-C2-N3	4.92	120.36	115.17
29	a	1917	PSU	C4-N3-C2	-4.87	119.67	126.37
29	a	2504	PSU	C4-N3-C2	-4.84	119.71	126.37
29	a	1911	PSU	N1-C2-N3	4.82	120.25	115.17
28	Z	55	PSU	N1-C2-N3	4.80	120.23	115.17
29	a	2580	PSU	N1-C2-N3	4.80	120.23	115.17
29	a	2580	PSU	C4-N3-C2	-4.73	119.85	126.37
6	A	516	PSU	C4-N3-C2	-4.73	119.86	126.37
29	a	746	PSU	N1-C2-N3	4.68	120.11	115.17
6	A	516	PSU	N1-C2-N3	4.64	120.07	115.17
29	a	2030	6MZ	C9-N6-C6	-4.41	118.76	122.85
29	a	2069	G7M	C2-N3-C4	4.29	119.70	112.30
29	a	2030	6MZ	N9-C8-N7	-4.29	107.84	113.94
29	a	1618	6MZ	N9-C8-N7	-4.21	107.96	113.94
29	a	1915	3TD	C4-N3-C2	-4.19	120.18	124.61
29	a	2069	G7M	CN7-N7-C5	4.12	131.93	126.80
28	Z	8	4SU	C5-C4-S4	-4.05	119.68	124.31
29	a	1618	6MZ	C9-N6-C6	-3.97	119.17	122.85
29	a	2552	OMU	N3-C2-N1	3.96	120.04	114.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	2552	OMU	C5-C4-N3	3.91	120.27	114.80
28	Z	8	4SU	N3-C2-N1	3.90	119.96	114.89
29	a	2069	G7M	C5-C6-N1	3.88	119.87	111.84
29	a	2030	6MZ	C4-C5-C6	3.73	119.88	116.78
6	A	1498	UR3	C5-C4-N3	3.69	119.89	115.04
40	l	81	4D4	NE-CZ-NH2	3.63	126.91	120.67
29	a	1618	6MZ	C4-C5-C6	3.61	119.78	116.78
29	a	1618	6MZ	N3-C4-N9	3.55	133.20	127.17
29	a	1618	6MZ	C2-N3-C4	3.55	120.50	111.83
29	a	745	1MG	C2-N3-C4	3.50	119.85	111.98
29	a	2069	G7M	C5-C4-N3	-3.49	121.56	128.15
29	a	2449	H2U	C5-C4-N3	-3.46	113.01	116.69
29	a	2069	G7M	O6-C6-C5	-3.42	120.38	128.01
29	a	2030	6MZ	C2-N3-C4	3.41	120.16	111.83
29	a	2503	2MA	C5-C4-N3	-3.32	123.68	127.18
29	a	2069	G7M	CN7-N7-C8	-3.27	119.84	124.79
29	a	2580	PSU	O2-C2-N1	-3.08	119.61	122.79
29	a	2030	6MZ	N3-C4-N9	3.07	132.38	127.17
29	a	745	1MG	N9-C4-N3	3.06	132.08	125.95
29	a	2552	OMU	O4-C4-C5	-3.05	119.90	125.16
29	a	2030	6MZ	C5-N7-C8	3.04	108.22	103.45
29	a	745	1MG	N9-C8-N7	-3.02	107.80	113.40
29	a	1618	6MZ	C5-N7-C8	3.00	108.17	103.45
29	a	1917	PSU	O2-C2-N1	-2.95	119.74	122.79
29	a	955	PSU	O2-C2-N1	-2.92	119.77	122.79
29	a	2069	G7M	C2-N1-C6	-2.91	119.83	125.11
29	a	746	PSU	O2-C2-N1	-2.86	119.83	122.79
29	a	2030	6MZ	C4-N9-C1'	-2.86	119.95	126.63
29	a	955	PSU	C6-N1-C2	-2.84	120.06	122.69
6	A	1519	MA6	C2-N1-C6	2.83	118.75	111.83
29	a	2457	PSU	O2-C2-N1	-2.83	119.87	122.79
6	A	516	PSU	O2-C2-N1	-2.81	119.89	122.79
6	A	1518	MA6	C2-N1-C6	2.80	118.68	111.83
29	a	1911	PSU	O2-C2-N1	-2.80	119.90	122.79
29	a	745	1MG	C5-C6-N1	2.76	120.11	115.02
17	L	89	D2T	O-C-CA	-2.72	117.77	124.77
29	a	2504	PSU	O2-C2-N1	-2.66	120.05	122.79
29	a	2604	PSU	O2-C2-N1	-2.65	120.05	122.79
29	a	2580	PSU	C6-N1-C2	-2.63	120.25	122.69
29	a	2504	PSU	C6-N1-C2	-2.60	120.28	122.69
28	Z	55	PSU	O2-C2-N1	-2.59	120.12	122.79
29	a	2580	PSU	O4'-C1'-C2'	2.57	108.70	105.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	1618	6MZ	C5-C6-N1	2.56	120.90	118.15
29	a	1917	PSU	C6-N1-C2	-2.56	120.31	122.69
29	a	2457	PSU	C6-N1-C2	-2.56	120.31	122.69
29	a	2503	2MA	C2-N1-C6	2.54	122.01	118.10
17	L	89	D2T	OD1-CG-CB	-2.54	117.12	122.44
29	a	2030	6MZ	C5-C6-N1	2.53	120.87	118.15
29	a	2503	2MA	N3-C2-N1	-2.46	121.43	125.77
6	A	516	PSU	O4'-C1'-C2'	2.42	108.50	105.15
29	a	2552	OMU	O2-C2-N1	-2.41	119.66	122.80
6	A	516	PSU	C6-N1-C2	-2.35	120.51	122.69
29	a	2503	2MA	CM2-C2-N1	2.35	120.65	117.13
29	a	2605	PSU	C6-N1-C2	-2.34	120.52	122.69
29	a	2030	6MZ	C1'-N9-C8	2.34	132.29	127.09
40	l	81	4D4	O-C-CA	-2.33	118.79	124.77
29	a	2604	PSU	C6-C5-C4	2.30	119.72	118.17
28	Z	55	PSU	C6-N1-C2	-2.26	120.59	122.69
29	a	2069	G7M	N2-C2-N1	2.25	121.51	116.76
29	a	1911	PSU	C6-C5-C4	2.24	119.68	118.17
29	a	2030	6MZ	C4-C5-N7	-2.22	108.05	110.58
29	a	2457	PSU	C6-C5-C4	2.19	119.65	118.17
29	a	1911	PSU	C6-N1-C2	-2.18	120.67	122.69
40	l	81	4D4	NH1-CZ-NE	-2.18	114.32	119.27
6	A	527	G7M	N9-C8-N7	-2.18	107.19	112.48
29	a	1915	3TD	C6-C5-C4	2.18	119.65	118.19
29	a	2604	PSU	C6-N1-C2	-2.17	120.67	122.69
6	A	1402	4OC	C6-C5-C4	2.15	119.59	117.00
29	a	2605	PSU	O2-C2-N1	-2.13	120.59	122.79
29	a	2030	6MZ	C5-C4-N9	2.13	108.13	105.81
29	a	745	1MG	C8-N7-C5	2.11	108.02	104.26
29	a	2069	G7M	N9-C8-N7	-2.11	107.36	112.48
29	a	1618	6MZ	C4-N9-C8	2.10	107.95	105.74
6	A	1498	UR3	C6-N1-C2	-2.08	120.10	121.80
28	Z	8	4SU	O2-C2-N1	-2.08	120.09	122.80
28	Z	55	PSU	C6-C5-C4	2.07	119.57	118.17
29	a	2457	PSU	O4'-C1'-C2'	2.02	107.94	105.15
29	a	747	5MU	C1'-N1-C2	2.01	121.20	117.59

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	L	89	D2T	CA-CB-CG-OD1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	L	89	D2T	CA-CB-CG-OD2
40	l	81	4D4	CA-CB-CG-CD
29	a	2504	PSU	O4'-C4'-C5'-O5'
32	d	150	MEQ	OE1-CD-CG-CB
32	d	150	MEQ	NE2-CD-CG-CB
6	A	527	G7M	C3'-C4'-C5'-O5'
29	a	2030	6MZ	O4'-C4'-C5'-O5'
29	a	2030	6MZ	C3'-C4'-C5'-O5'
40	l	81	4D4	OB-CB-CG-CD
6	A	527	G7M	O4'-C4'-C5'-O5'
29	a	2504	PSU	C3'-C4'-C5'-O5'
6	A	1402	4OC	O4'-C4'-C5'-O5'
17	L	89	D2T	CG-CB-SB-CB1
40	l	81	4D4	CG-CD-NE-CZ
29	a	2552	OMU	C3'-C2'-O2'-CM2
29	a	2445	2MG	C3'-C4'-C5'-O5'
29	a	2503	2MA	C4'-C5'-O5'-P
29	a	2069	G7M	C4'-C5'-O5'-P
29	a	2498	OMC	O4'-C4'-C5'-O5'
17	L	89	D2T	SB-CB-CG-OD2
29	a	2251	OMG	C1'-C2'-O2'-CM2
29	a	746	PSU	O4'-C1'-C5-C6
29	a	2069	G7M	O4'-C4'-C5'-O5'
29	a	746	PSU	C2'-C1'-C5-C6
29	a	2503	2MA	O4'-C1'-N9-C8
40	l	81	4D4	NE-CD-CG-CB

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	a	1915	3TD	1	0
6	A	1516	2MG	1	0
6	A	1519	MA6	1	0
17	L	89	D2T	1	0
28	Z	55	PSU	1	0
29	a	2030	6MZ	3	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 384 ligands modelled in this entry, 382 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	V7A	A	1674	56	37,38,38	1.10	2 (5%)	43,60,60	0.96	4 (9%)
58	V7A	a	3008	-	37,38,38	1.11	2 (5%)	43,60,60	1.21	5 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	V7A	A	1674	56	-	2/13/72/72	0/4/4/4
58	V7A	a	3008	-	-	7/13/72/72	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	a	3008	V7A	CBC-NBD	5.03	1.48	1.33
58	A	1674	V7A	CBC-NBD	4.93	1.47	1.33
58	a	3008	V7A	OAY-CAH	2.25	1.28	1.23
58	A	1674	V7A	OAY-CAH	2.25	1.27	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	a	3008	V7A	CAF-CAG-CAJ	3.58	117.86	113.12
58	a	3008	V7A	CAH-CAI-CAL	2.26	120.59	118.80
58	A	1674	V7A	CAH-CAI-CAL	2.11	120.47	118.80
58	A	1674	V7A	OAZ-CAL-CAM	2.10	116.41	113.37
58	a	3008	V7A	OAZ-CAL-CAI	-2.08	119.49	123.52
58	A	1674	V7A	OAZ-CAL-CAI	-2.06	119.53	123.52
58	a	3008	V7A	CAW-NAT-CAS	2.05	113.26	110.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	A	1674	V7A	CAW-NAT-CAS	2.04	113.24	110.19
58	a	3008	V7A	CAM-CAL-CAI	2.03	125.12	123.06

There are no chirality outliers.

All (9) torsion outliers are listed below:

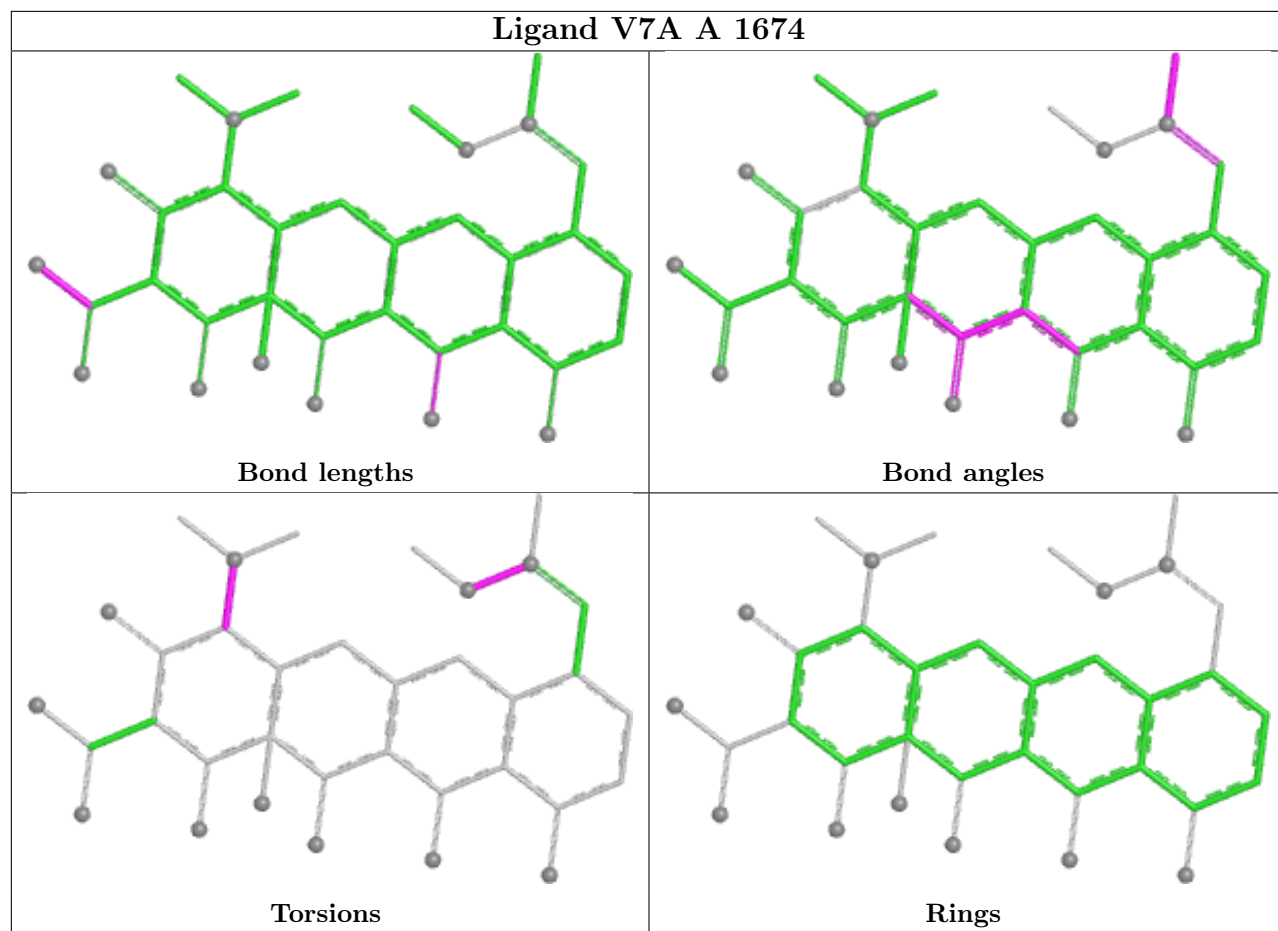
Mol	Chain	Res	Type	Atoms
58	A	1674	V7A	CAN-CAO-NBF-CBG
58	a	3008	V7A	CAF-CAA-CAS-NAT
58	a	3008	V7A	CAN-CAO-NBF-CBG
58	a	3008	V7A	CAR-CAO-NBF-CBG
58	a	3008	V7A	CAR-CAO-NBF-CBH
58	a	3008	V7A	CAB-CAA-CAS-NAT
58	a	3008	V7A	CAN-CAO-NBF-CBH
58	A	1674	V7A	CAW-NAT-OAU-CAV
58	a	3008	V7A	CAA-CAS-NAT-OAU

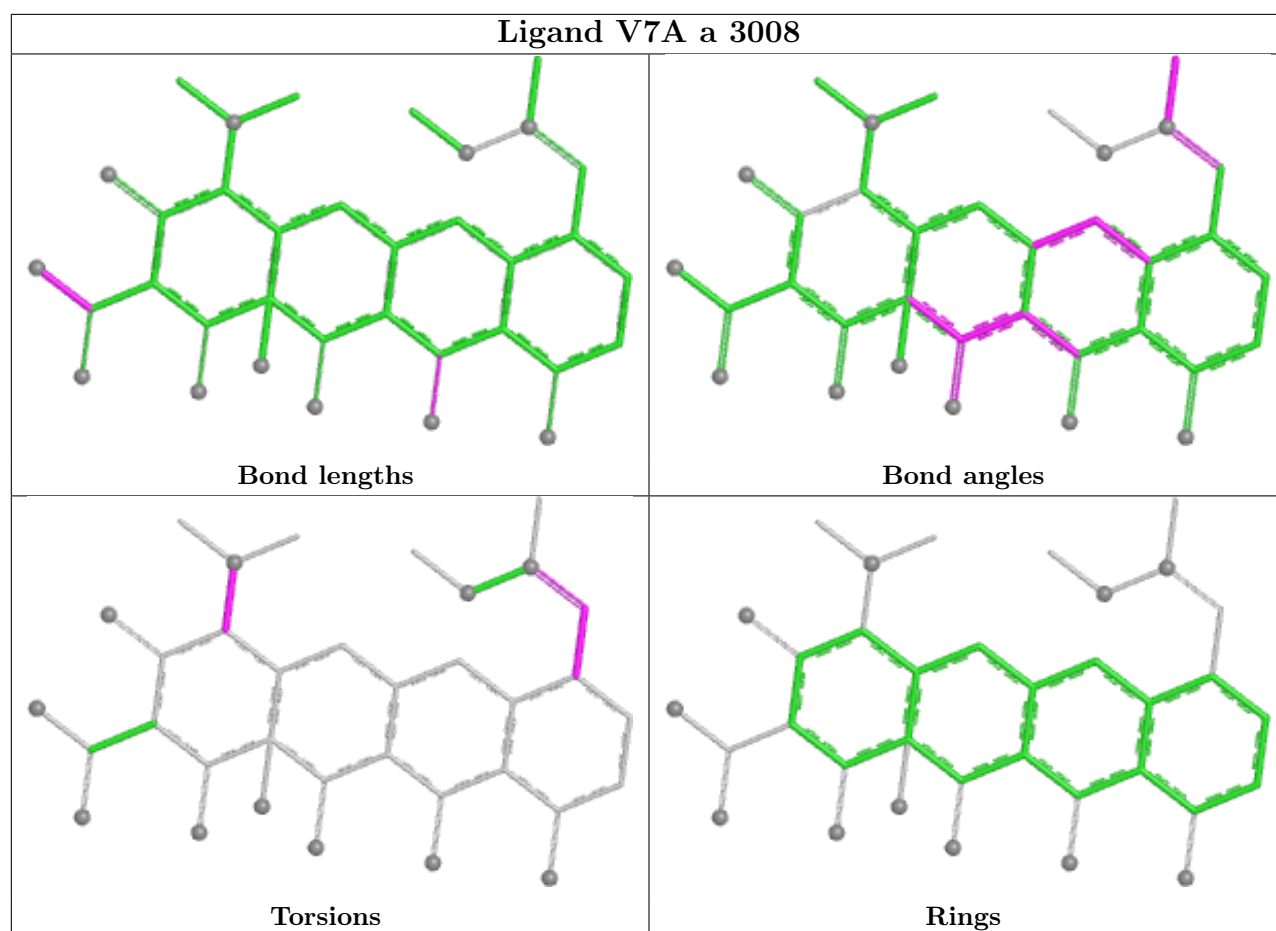
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	a	3008	V7A	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

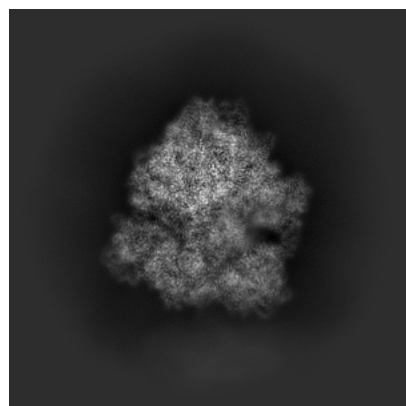
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71668. These allow visual inspection of the internal detail of the map and identification of artifacts.

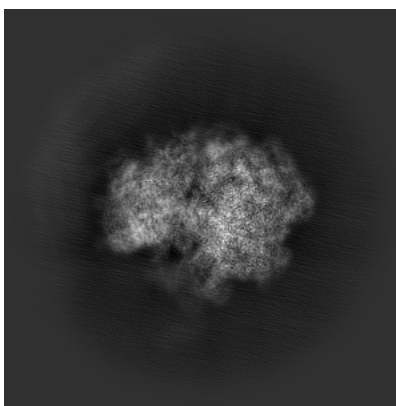
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

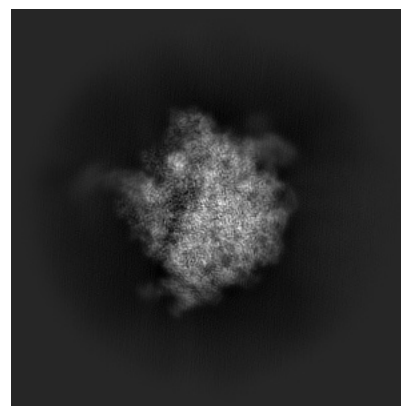
6.1.1 Primary map



X

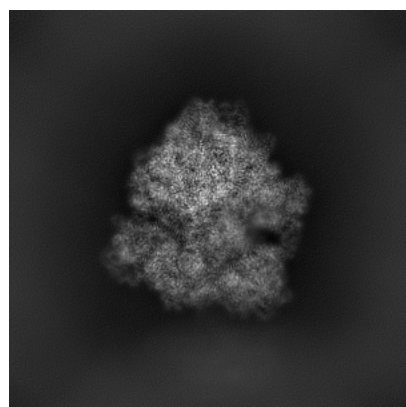


Y

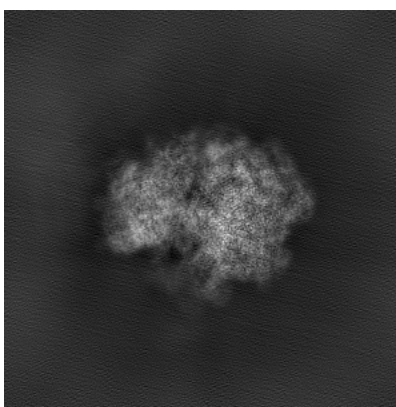


Z

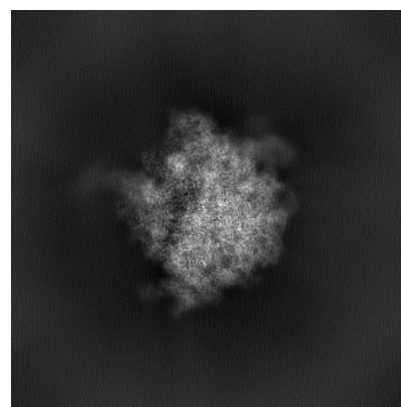
6.1.2 Raw map



X



Y

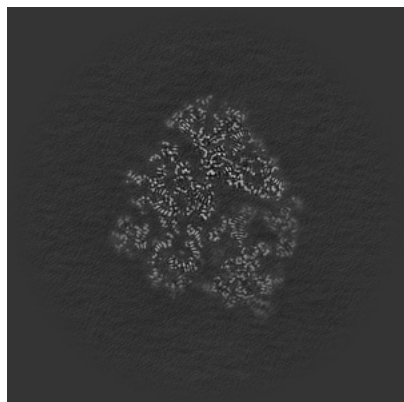


Z

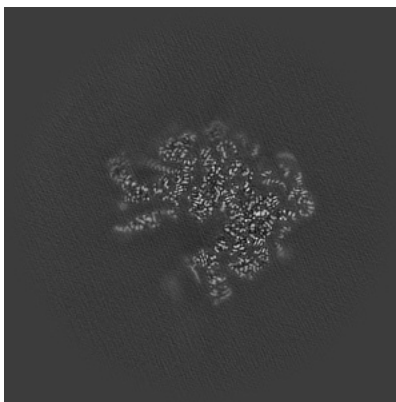
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

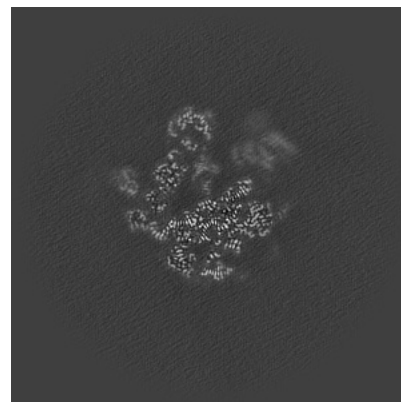
6.2.1 Primary map



X Index: 220

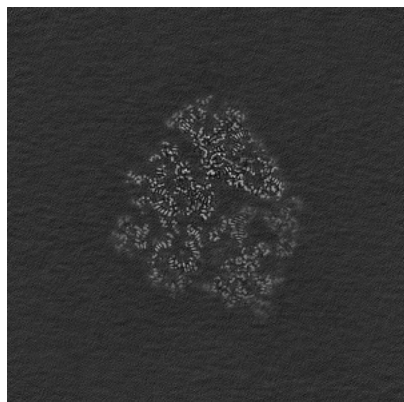


Y Index: 220

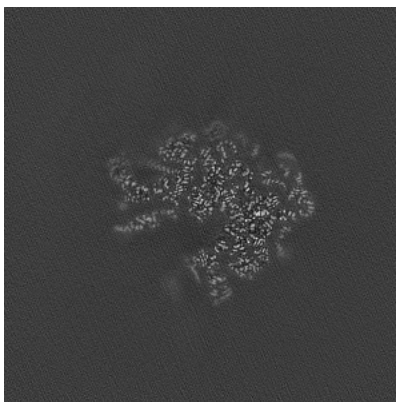


Z Index: 220

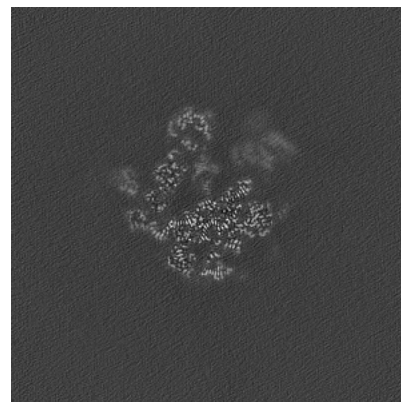
6.2.2 Raw map



X Index: 220



Y Index: 220

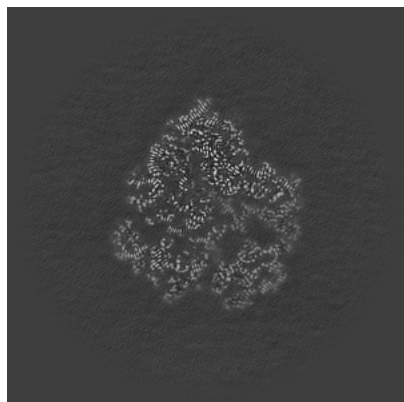


Z Index: 220

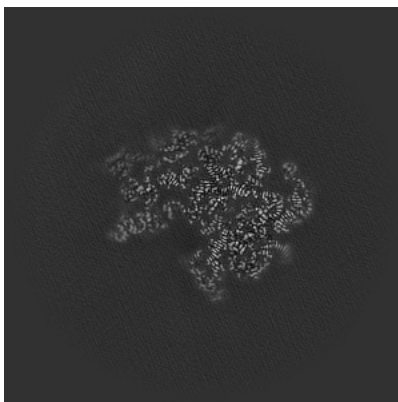
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

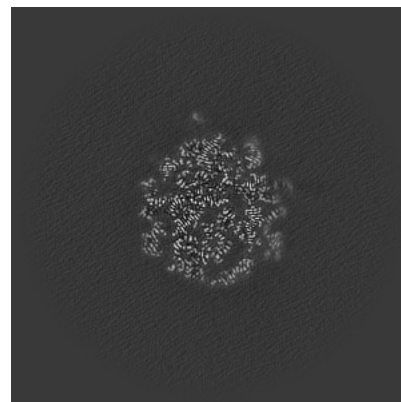
6.3.1 Primary map



X Index: 213

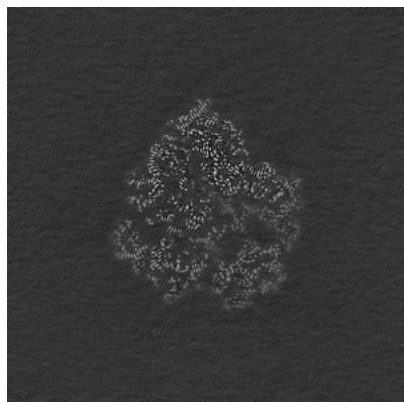


Y Index: 213

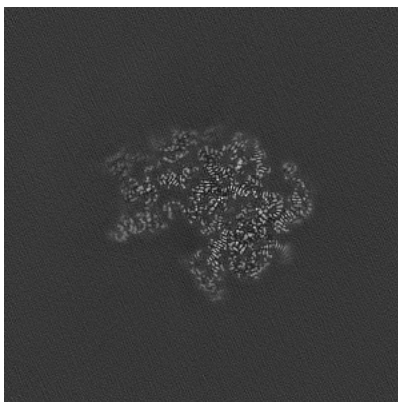


Z Index: 258

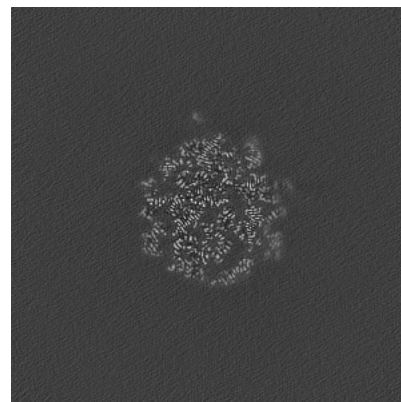
6.3.2 Raw map



X Index: 213



Y Index: 213

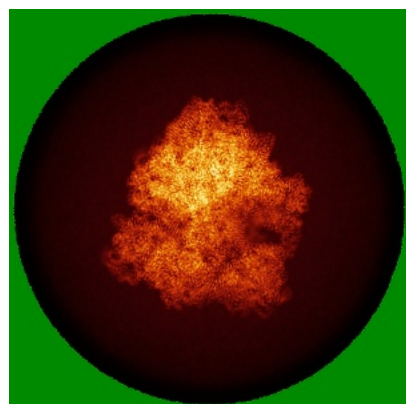


Z Index: 258

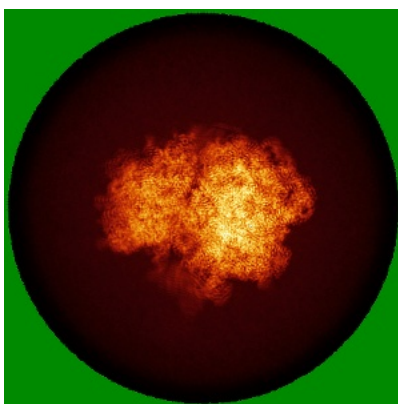
The images above show the largest variance slices of the map in three orthogonal directions.

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

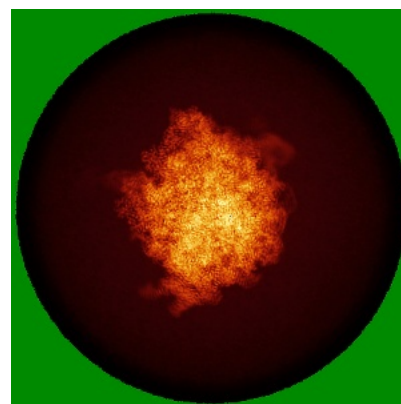
6.4.1 Primary map



X

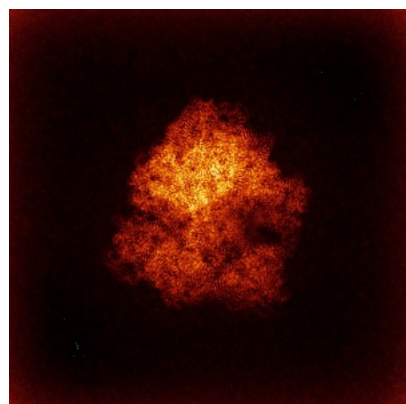


Y

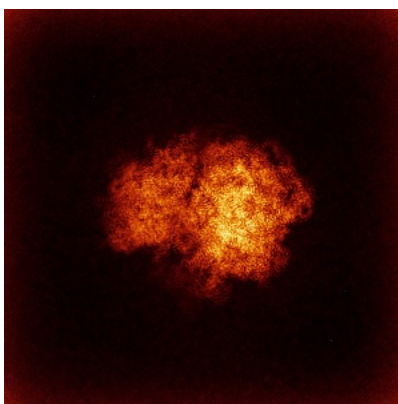


Z

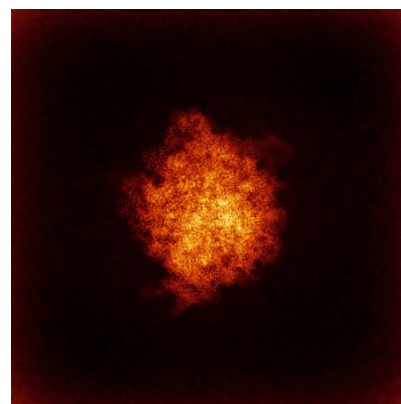
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



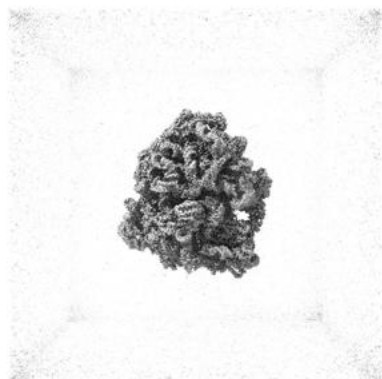
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

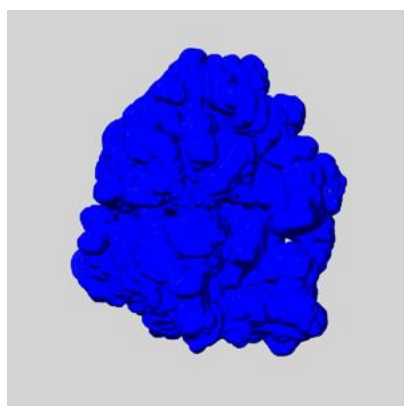
6.6 Mask visualisation [i](#)

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

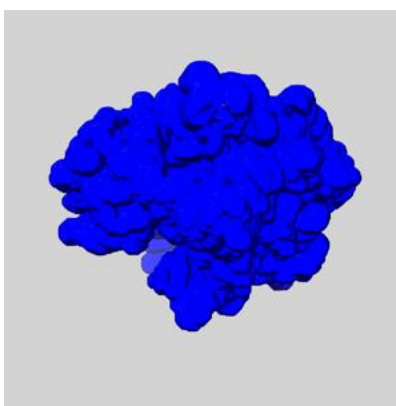
A mask typically either:

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

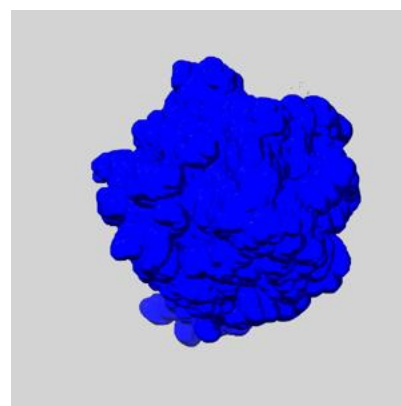
6.6.1 emd_71668_msk_1.map [i](#)



X



Y

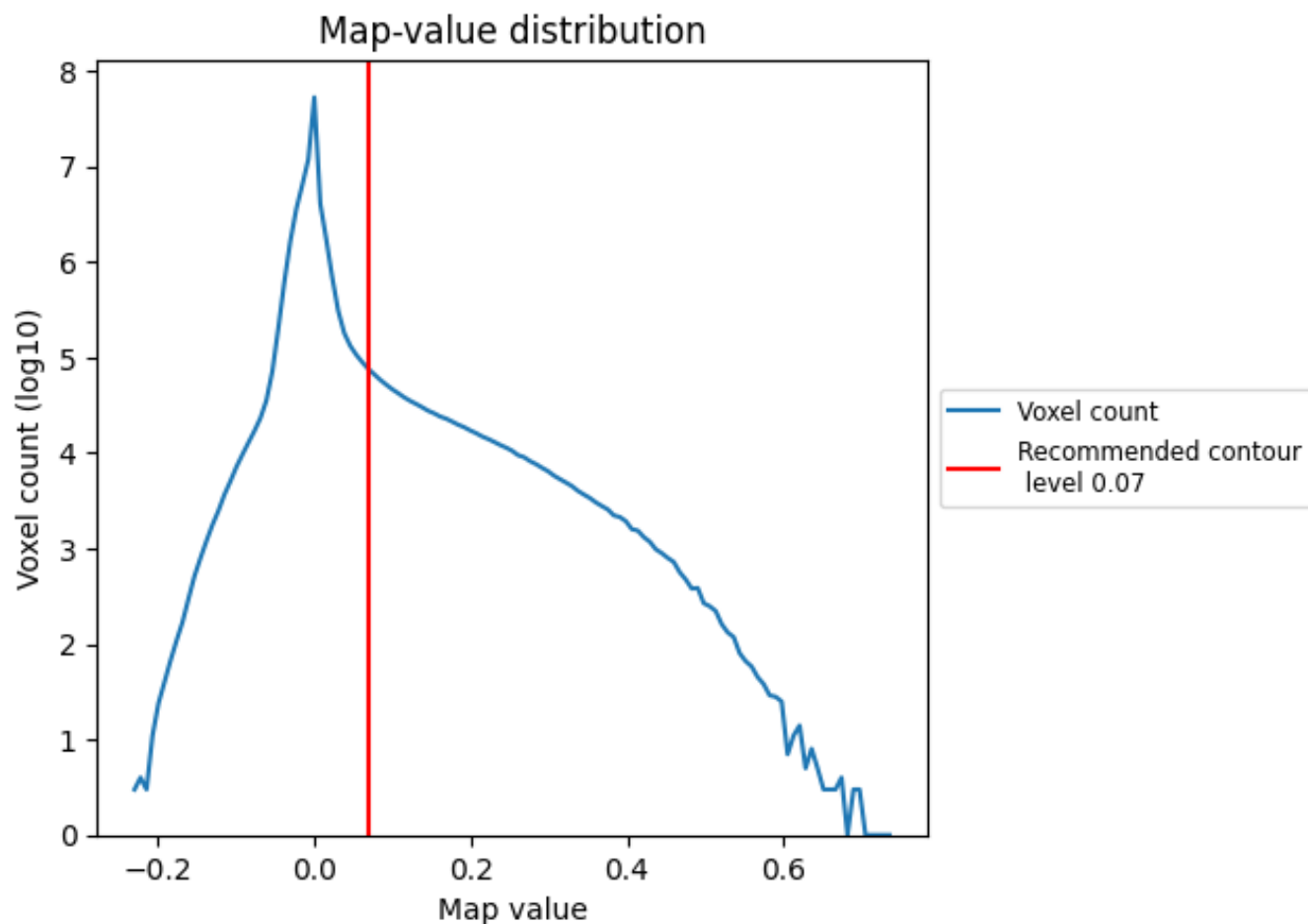


Z

7 Map analysis [i](#)

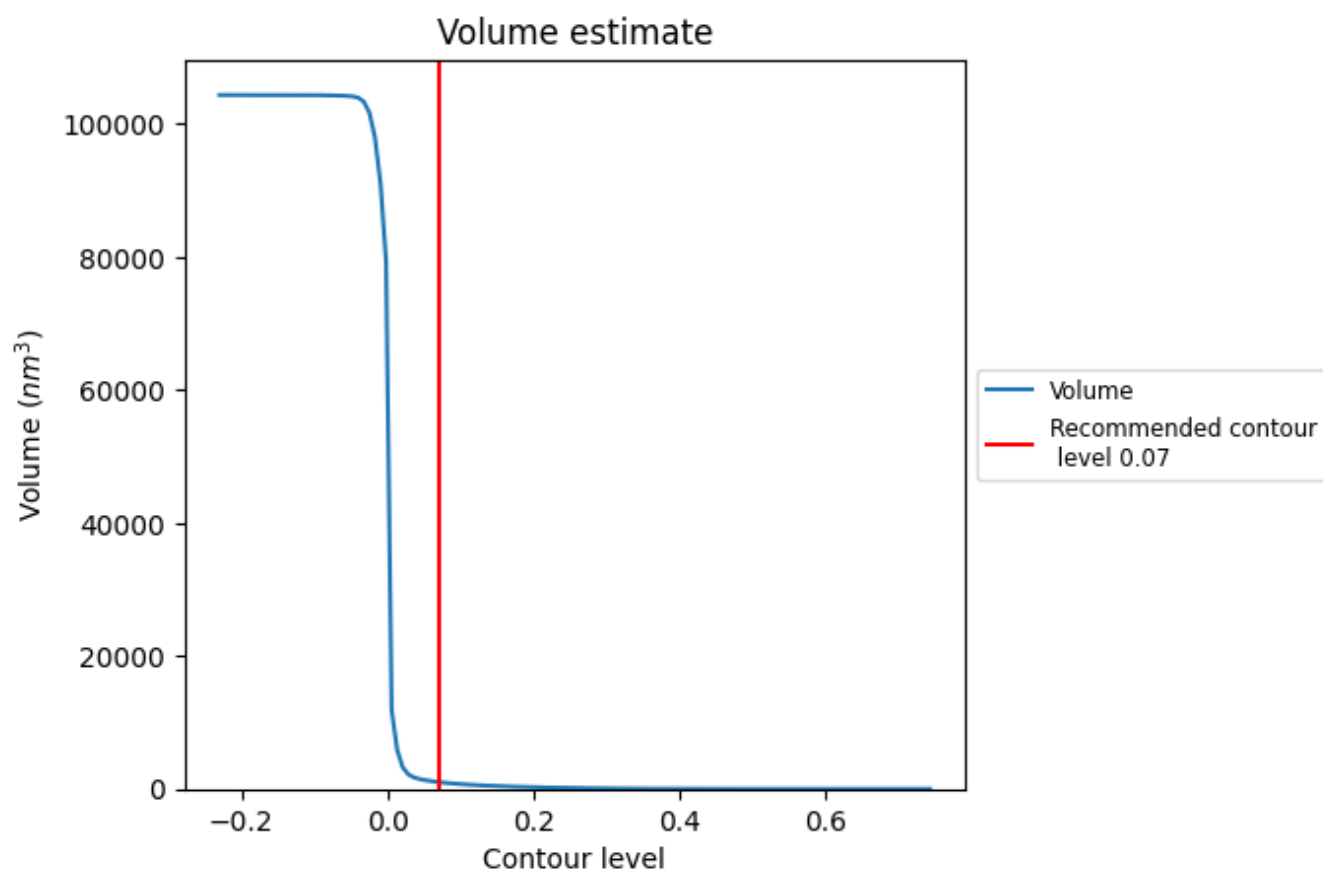
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

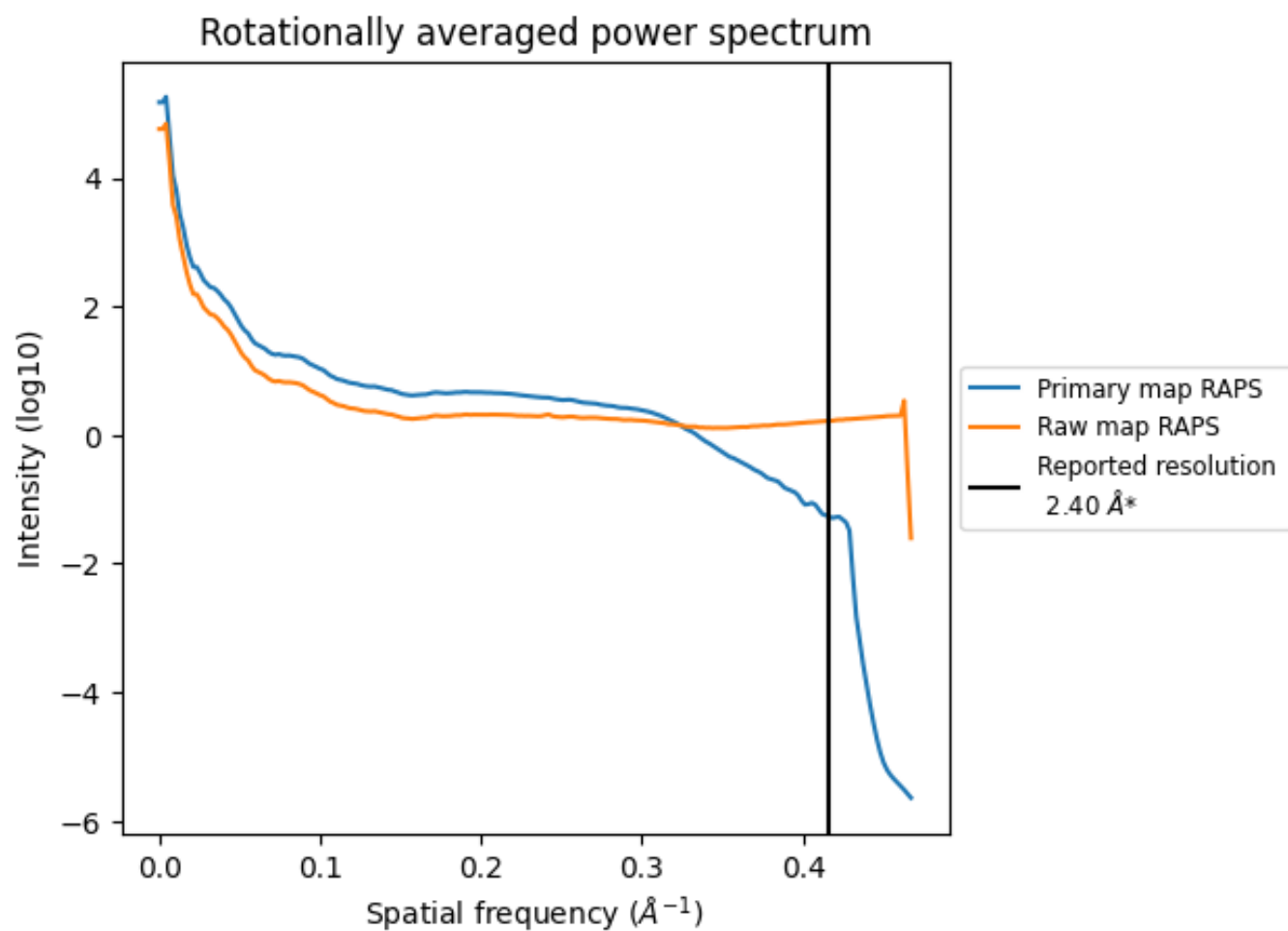
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1031 nm^3 ; this corresponds to an approximate mass of 931 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 ⓘ

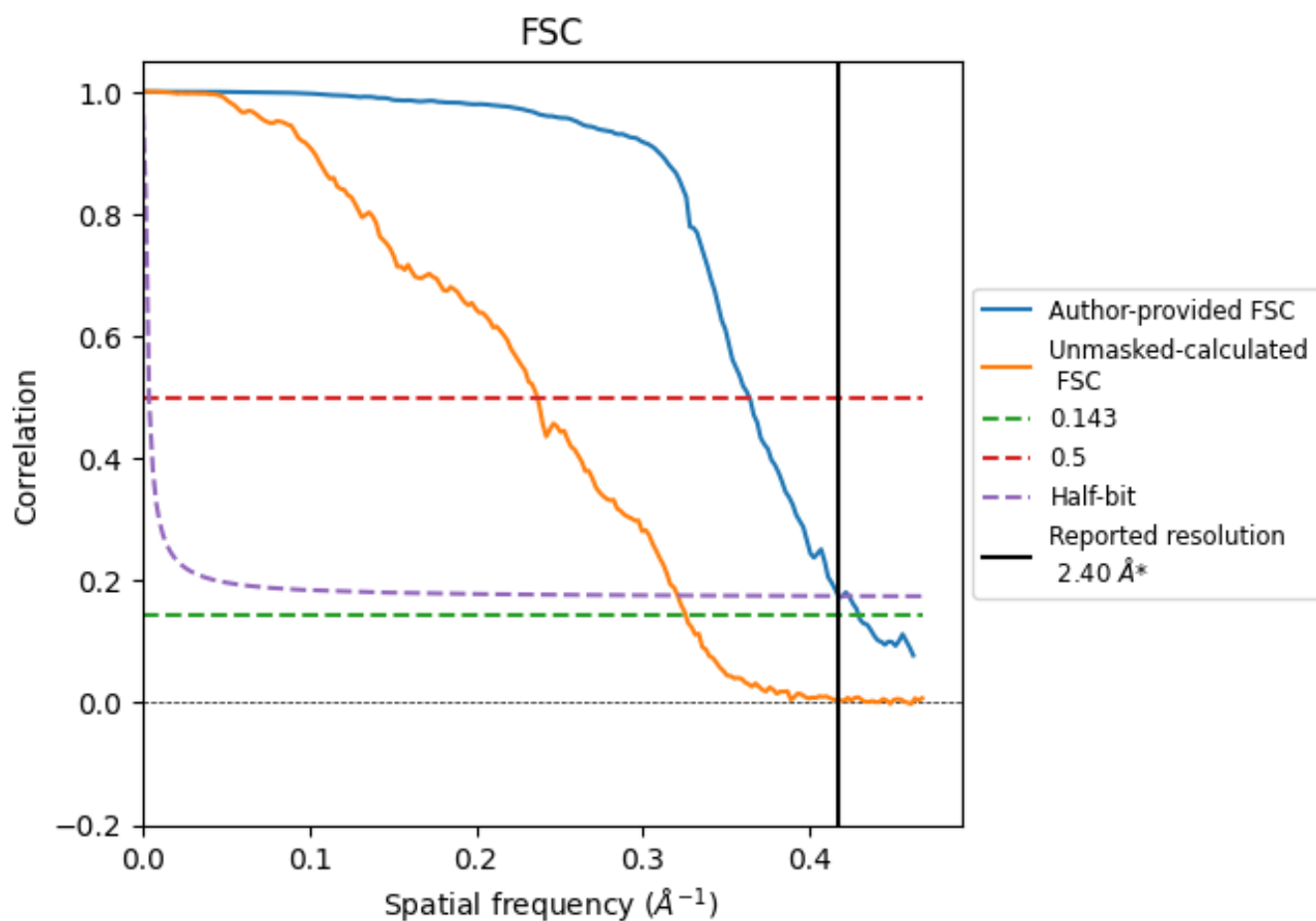


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8.2 Resolution estimates [i](#)

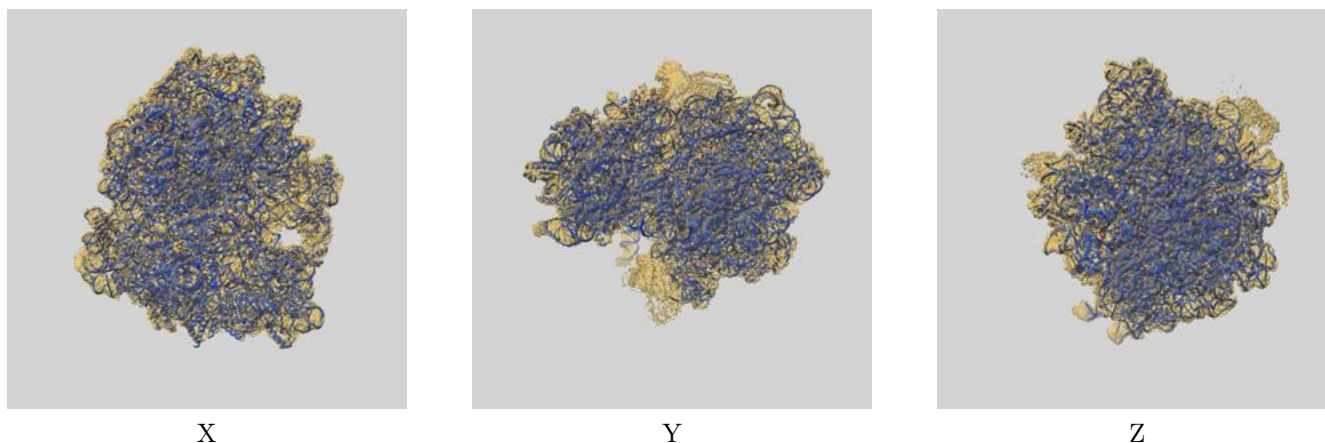
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.33	2.75	2.40
Unmasked-calculated*	3.07	4.23	3.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.07 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

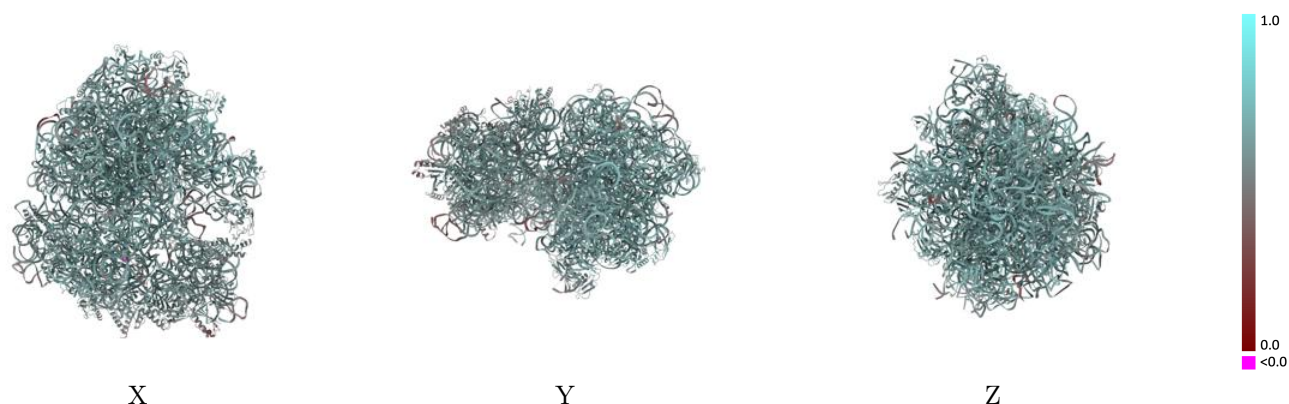
This section contains information regarding the fit between EMDB map EMD-71668 and PDB model 9PII. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



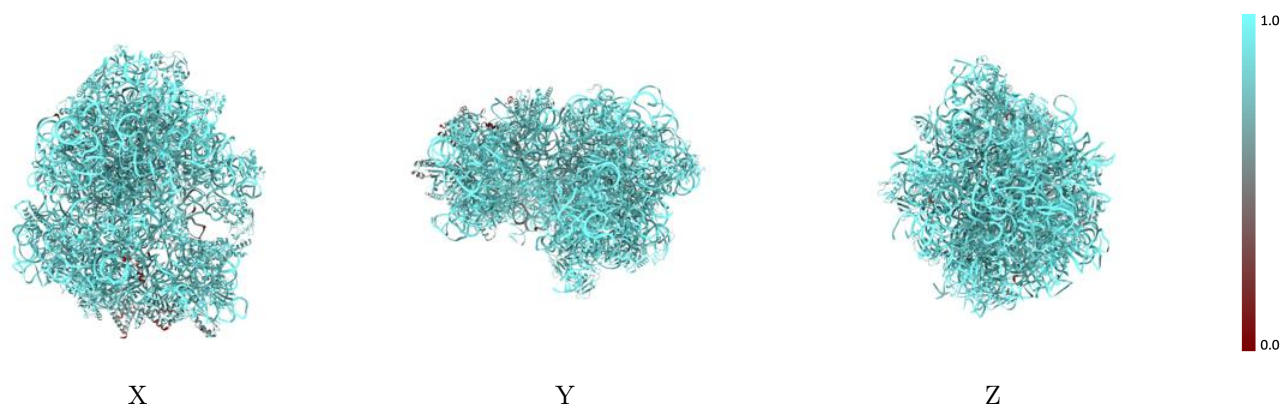
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



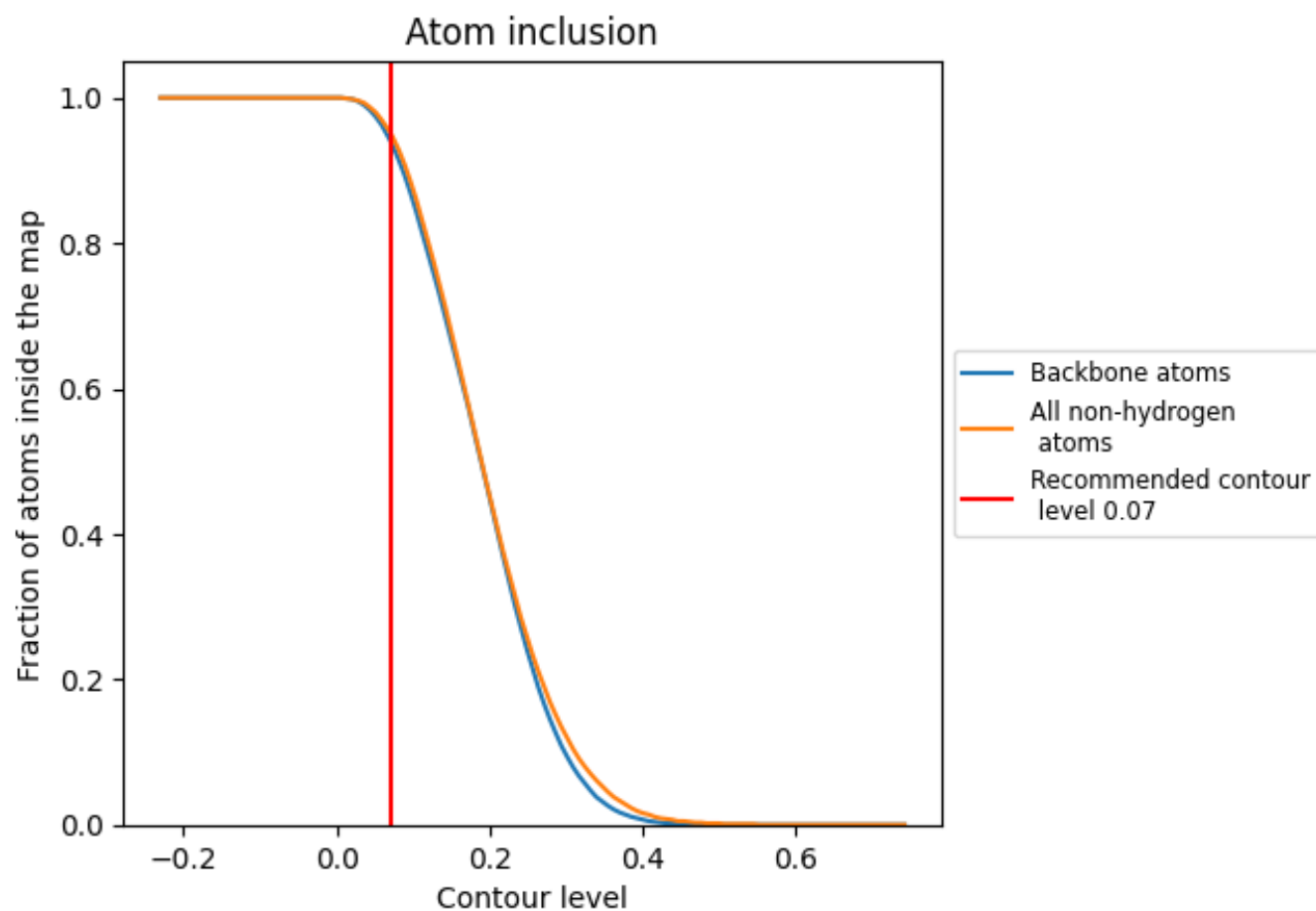
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ









































The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9530	 0.6150
0	 0.9170	 0.6300
1	 0.9690	 0.6570
2	 0.9650	 0.6580
3	 0.9320	 0.6400
4	 0.7920	 0.5290
A	 0.9840	 0.6010
B	 0.6030	 0.5340
C	 0.8560	 0.5800
D	 0.8790	 0.5860
E	 0.9140	 0.6160
F	 0.8670	 0.5700
G	 0.8110	 0.5540
H	 0.9200	 0.6150
I	 0.8970	 0.5670
J	 0.7570	 0.5270
K	 0.8900	 0.5960
L	 0.9070	 0.6190
M	 0.8780	 0.5760
N	 0.8710	 0.5730
O	 0.9230	 0.5970
P	 0.9370	 0.6030
Q	 0.8990	 0.6080
R	 0.7630	 0.5610
S	 0.8240	 0.5520
T	 0.9050	 0.5970
U	 0.6560	 0.5430
X	 0.6020	 0.4460
Z	 0.8620	 0.5670
a	 0.9870	 0.6320
b	 0.9830	 0.6050
c	 0.9610	 0.6560
d	 0.9570	 0.6480
e	 0.9260	 0.6240
f	 0.8730	 0.5690



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g	 0.8640	 0.5650
h	 0.8030	 0.5640
i	 0.9520	 0.6430
j	 0.9290	 0.6410
k	 0.9440	 0.6380
l	 0.9360	 0.6360
m	 0.9700	 0.6490
n	 0.9370	 0.6090
o	 0.9170	 0.6340
p	 0.9700	 0.6530
q	 0.9400	 0.6300
r	 0.9410	 0.6410
s	 0.9150	 0.6130
t	 0.9150	 0.5940
u	 0.9130	 0.6100
v	 0.9390	 0.6460
w	 0.9450	 0.6410
x	 0.9040	 0.5820
y	 0.9220	 0.6340
z	 0.9390	 0.6420