Full wwPDB EM Validation Report

Sep 19, 2026 – 11:41 AM JST

PDB ID	:	7Y7F / pdb_00007y7f
EMDB ID	:	EMD-33663
Title	:	Structure of the Bacterial Ribosome with human tRNA Asp(ManQ34) and mRNA(GAC)
Authors	:	Ishiguro, K.; Yokoyama, T.; Shirouzu, M.; Suzuki, T.
Deposited on	:	2022-06-22
Resolution	:	2.43 Å(reported)
Based on initial model	:	7K00

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 (i) 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 (1)) were used in the production of this report:

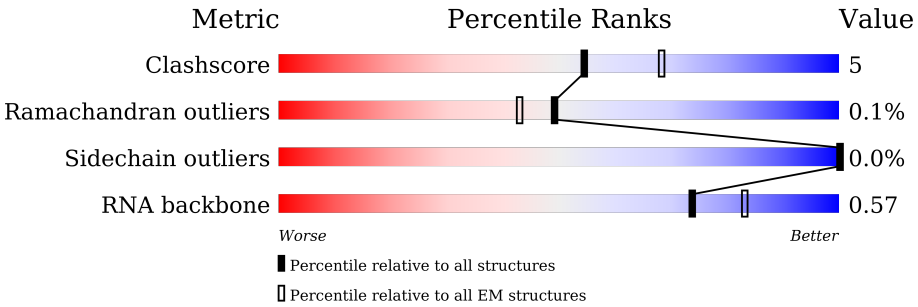
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.50

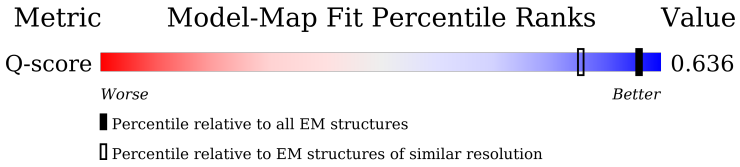
1 Overall quality at a glance

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

The reported resolution of this entry is 2.43 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	5787 (1.94 - 2.93)

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

Mol	Chain	Length	Quality of chain
1	A	1542	20% 67% 27%
2	B	241	93% 73% 20% 7%
3	C	233	40% 72% 16% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	206	78% 73% 26%
5	E	167	26% 80% 14% 7%
6	F	135	59% 58% 19% 24%
7	G	179	56% 70% 16% 15%
8	H	130	25% 82% 17%
9	I	130	45% 72% 25%
10	J	103	64% 65% 30% 5%
11	K	129	38% 77% 14% 9%
12	L	124	19% 91% 8%
13	M	118	55% 70% 25%
14	N	101	40% 82% 17%
15	O	89	42% 80% 19%
16	P	82	57% 77% 22%
17	Q	84	55% 81% 13% 6%
18	R	75	45% 76% 12% 12%
19	S	92	45% 71% 21% 9%
20	T	87	72% 85% 14%
21	U	71	89% 76% 23%
22	a	2904	10% 69% 23% 5%
23	b	120	12% 78% 21%
24	c	273	5% 86% 14%
25	d	209	13% 92% 8%
26	e	201	39% 83% 17%
27	f	179	63% 79% 20%
28	g	177	76% 74% 24%

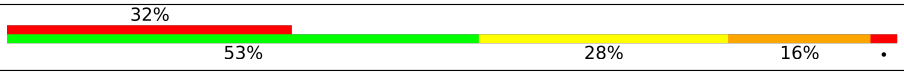
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	h	149	22% 20% 7% 72%
30	i	142	8% 90% 10%
31	j	123	14% 87% 13%
32	k	144	19% 92% 8%
33	l	136	6% 85% 15%
34	m	127	82% 11% 7%
35	n	117	35% 91% 8%
36	o	115	17% 87% 12%
37	p	118	5% 92% 7%
38	q	103	32% 88% 12%
39	r	110	11% 91% 9%
40	s	100	30% 78% 15% 7%
41	t	104	48% 81% 16%
42	u	94	34% 81% 19%
43	v	85	12% 88% 11%
44	w	78	18% 91% 8%
45	x	63	63% 83% 16%
46	y	59	12% 81% 17%
47	z	57	16% 84% 14%
48	0	55	22% 75% 18% 7%
49	1	46	91% 9%
50	2	65	5% 80% 15%
51	3	38	16% 92% 8%
52	4	70	81% 66% 20% 14%
53	X	35	17% 31% 6% 63%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	Z	77	
55	V	75	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 141929 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1520	32634	14562	5991	10561	1520	0	0

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

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

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

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

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

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

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

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

- Molecule 6 is a protein called 30S ribosomal protein S6, fully modified isoform.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP P0A7R9

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

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

- Molecule 30 is a protein called 50S ribosomal protein L13.

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

- Molecule 31 is a protein called 50S ribosomal protein L14.

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

- Molecule 32 is a protein called 50S ribosomal protein L15.

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

- Molecule 33 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	conflict	UNP P0ADY7

- Molecule 34 is a protein called 50S ribosomal protein L17.

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

- Molecule 35 is a protein called 50S ribosomal protein L18.

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

- Molecule 36 is a protein called 50S ribosomal protein L19.

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

- Molecule 37 is a protein called 50S ribosomal protein L20.

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

- Molecule 38 is a protein called 50S ribosomal protein L21.

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

- Molecule 39 is a protein called 50S ribosomal protein L22.

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

- Molecule 40 is a protein called 50S ribosomal protein L23.

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

- Molecule 41 is a protein called 50S ribosomal protein L24.

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

- Molecule 42 is a protein called 50S ribosomal protein L25.

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

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	84	Total	C	N	O	S	0	0
			628	388	126	113	1		

- Molecule 44 is a protein called 50S ribosomal protein L28.

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

- Molecule 45 is a protein called 50S ribosomal protein L29.

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

- Molecule 46 is a protein called 50S ribosomal protein L30.

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

- Molecule 47 is a protein called 50S ribosomal protein L32.

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

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	X	13	Total	C	N	O	P	0	0
			279	125	53	88	13		

- Molecule 54 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	Z	77	Total	C	N	O	P	S	0	0
			1645	734	297	536	77	1		

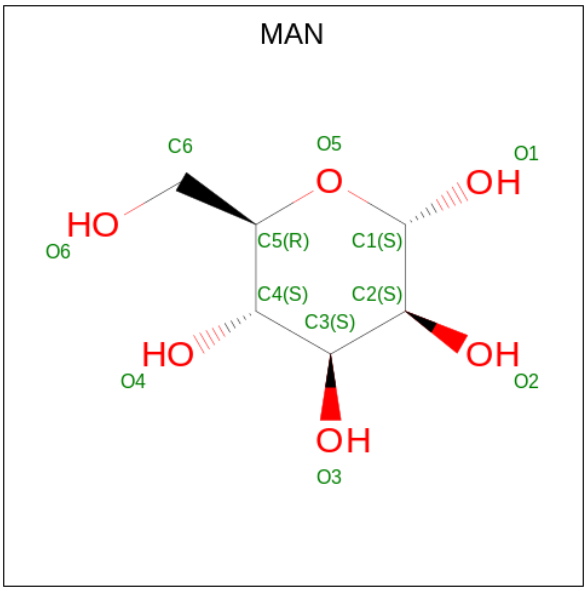
- Molecule 55 is a RNA chain called A-site tRNA-Asp.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	V	75	Total	C	N	O	P	0	0
			1612	726	283	529	74		

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

Mol	Chain	Residues	Atoms		AltConf
56	A	63	Total	Mg	0
			63	63	
56	a	185	Total	Mg	0
			185	185	
56	b	3	Total	Mg	0
			3	3	
56	c	1	Total	Mg	0
			1	1	
56	d	1	Total	Mg	0
			1	1	
56	z	1	Total	Mg	0
			1	1	
56	Z	3	Total	Mg	0
			3	3	
56	V	2	Total	Mg	0
			2	2	

- Molecule 57 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
57	V	1	Total	C	O	0
			11	6	5	

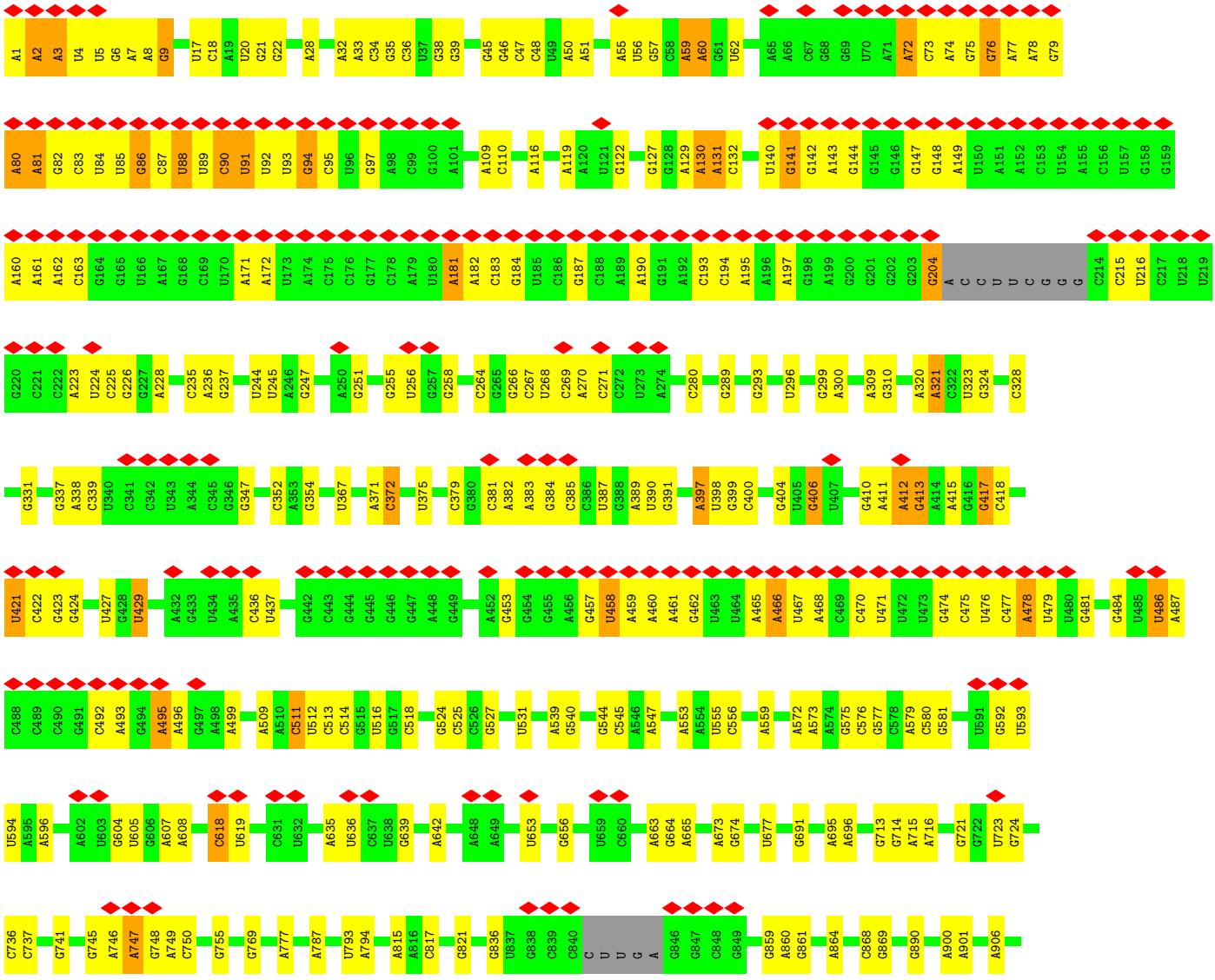
3 Residue-property plots (i)

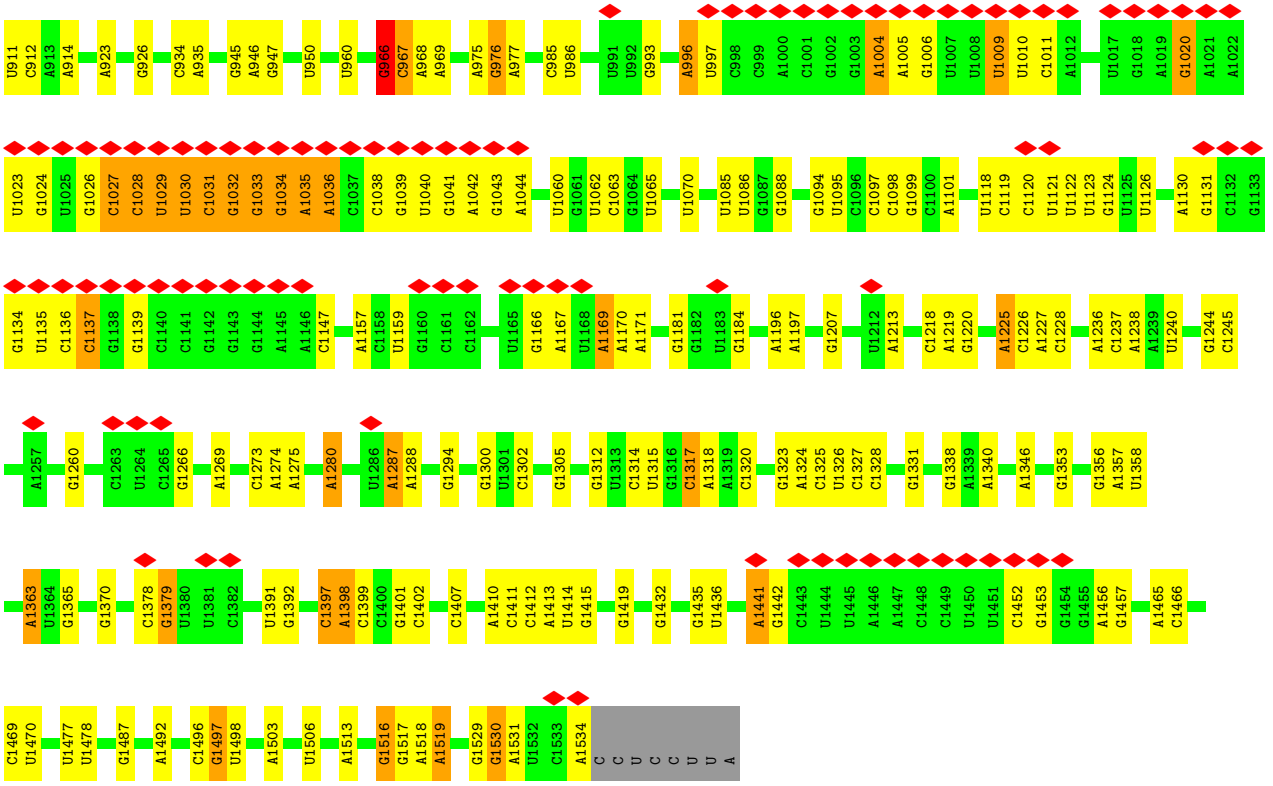
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S rRNA

Chain A:

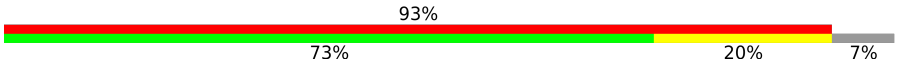


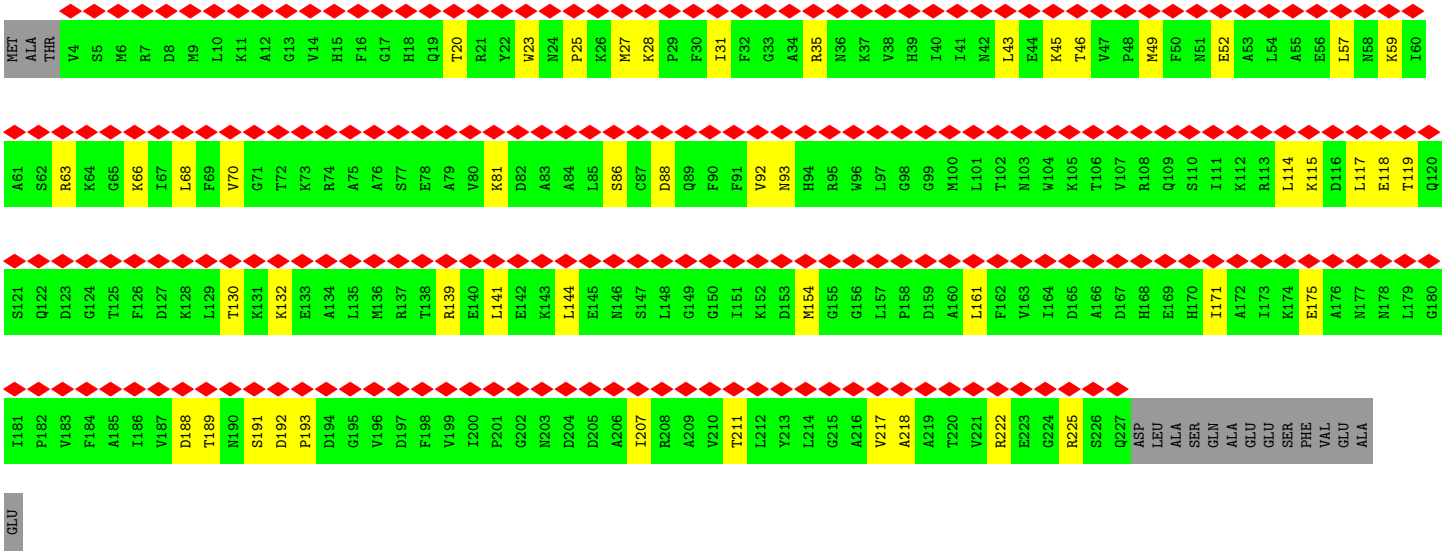




• Molecule 2: 30S ribosomal protein S2

Chain B:

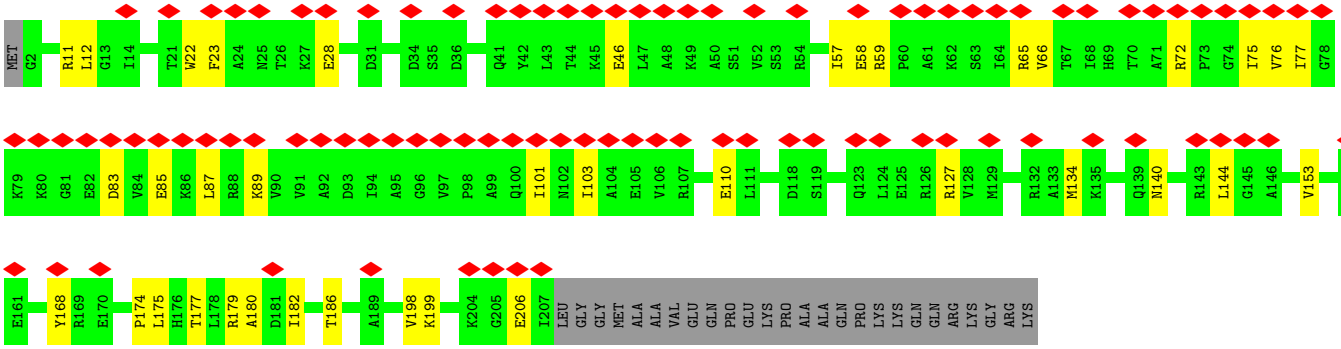




• Molecule 3: 30S ribosomal protein S3

Chain C:





• Molecule 4: 30S ribosomal protein S4

Chain D:

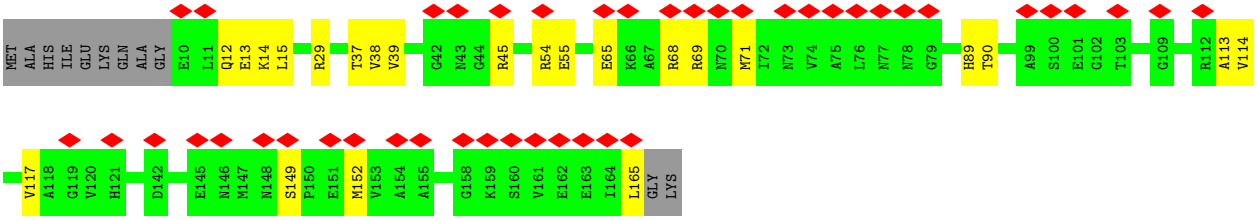




• Molecule 5: 30S ribosomal protein S5

Chain E:

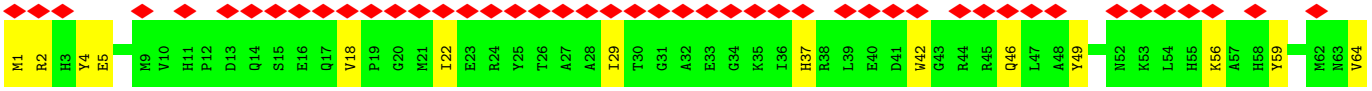


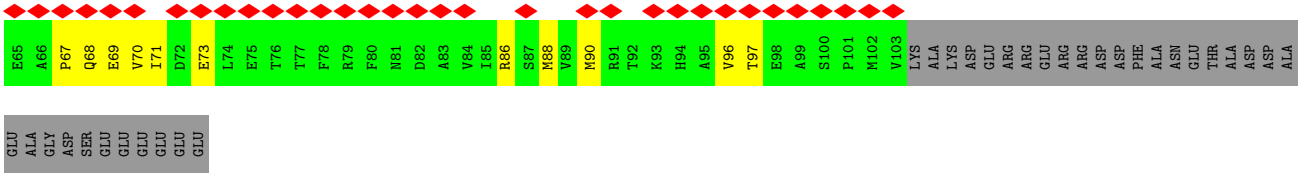


• Molecule 6: 30S ribosomal protein S6, fully modified isoform

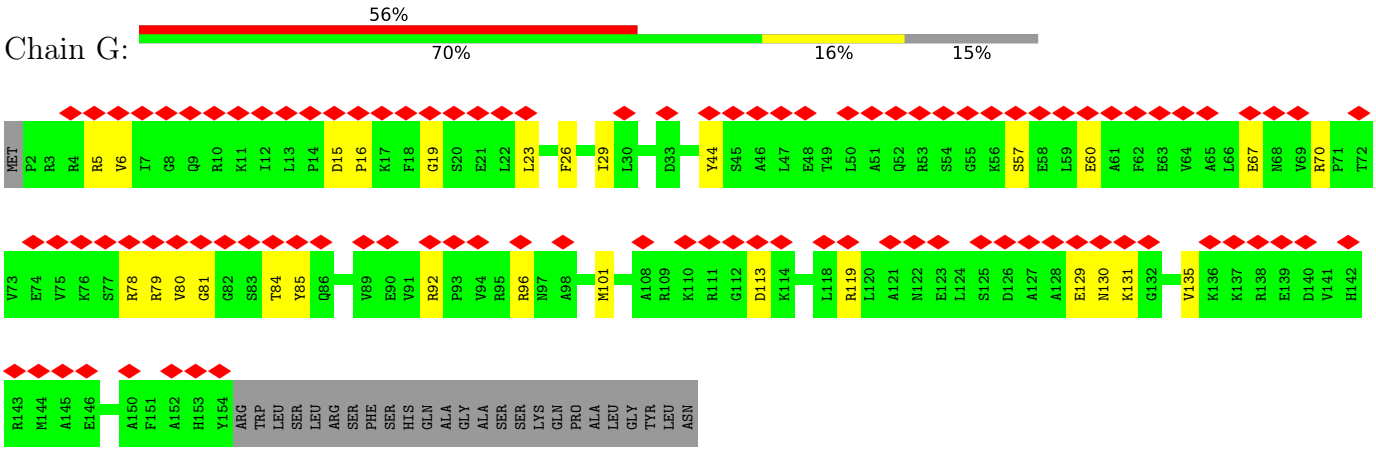
Chain F:



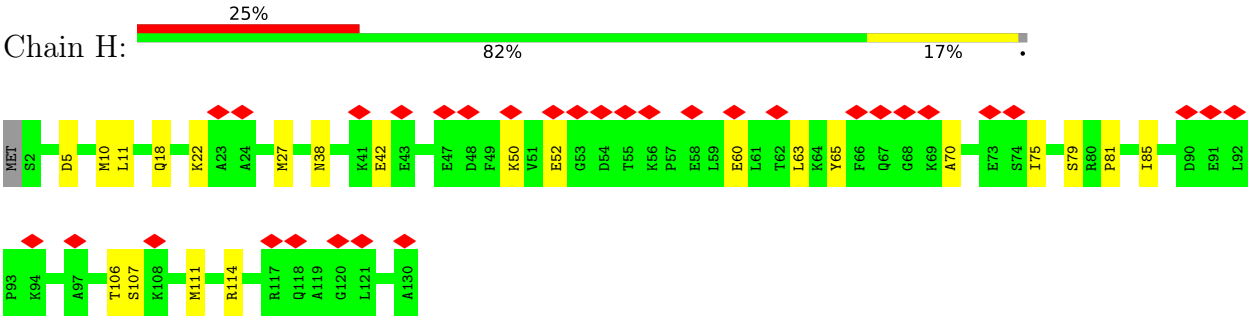




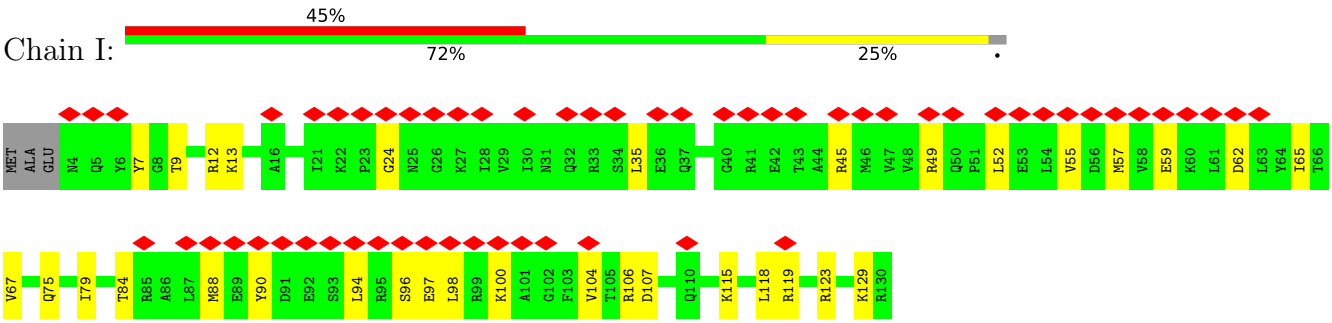
• Molecule 7: 30S ribosomal protein S7



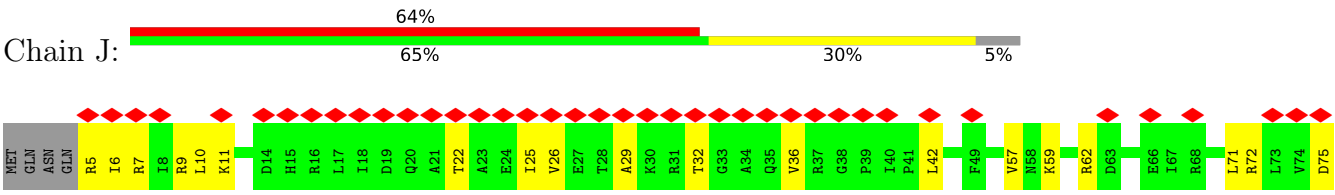
• Molecule 8: 30S ribosomal protein S8

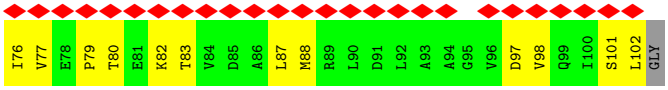


• Molecule 9: 30S ribosomal protein S9



• Molecule 10: 30S ribosomal protein S10

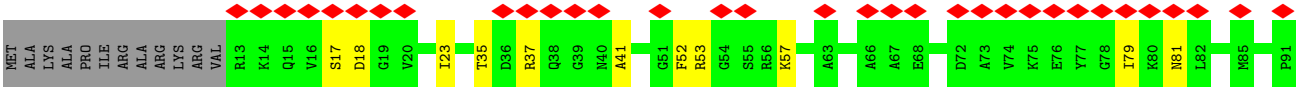


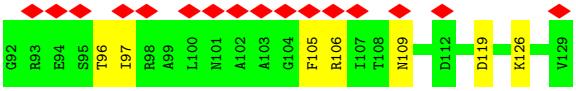


• Molecule 11: 30S ribosomal protein S11

Chain K:

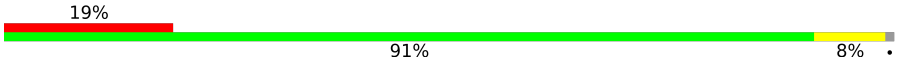


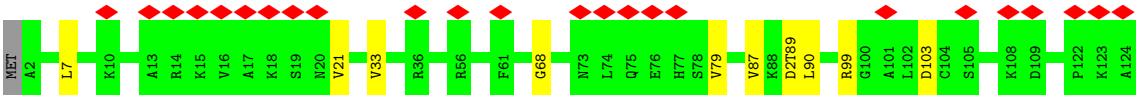




• Molecule 12: 30S ribosomal protein S12

Chain L:

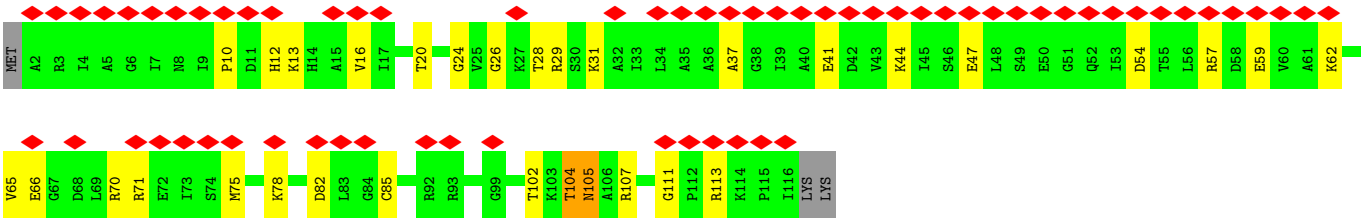




• Molecule 13: 30S ribosomal protein S13

Chain M:

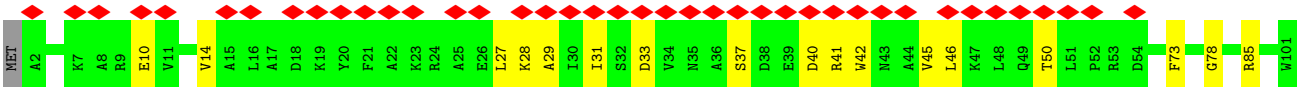




• Molecule 14: 30S ribosomal protein S14

Chain N:

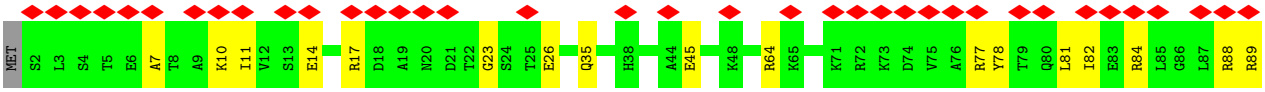




• Molecule 15: 30S ribosomal protein S15

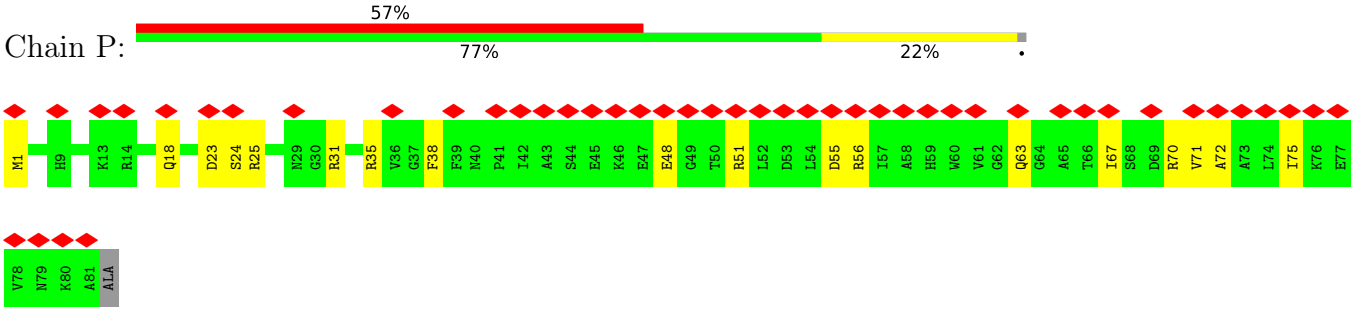
Chain O:





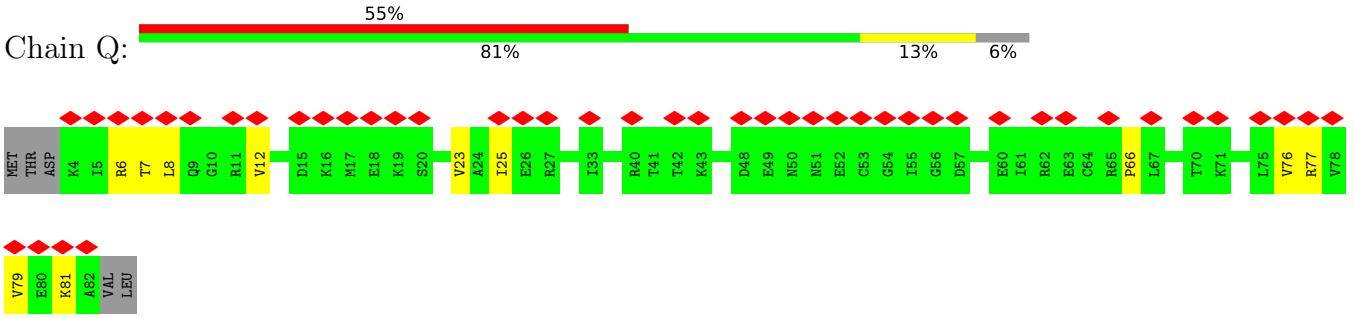
• Molecule 16: 30S ribosomal protein S16

Chain P:



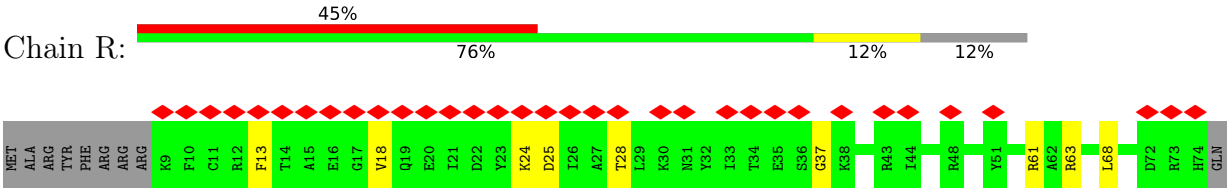
• Molecule 17: 30S ribosomal protein S17

Chain Q:



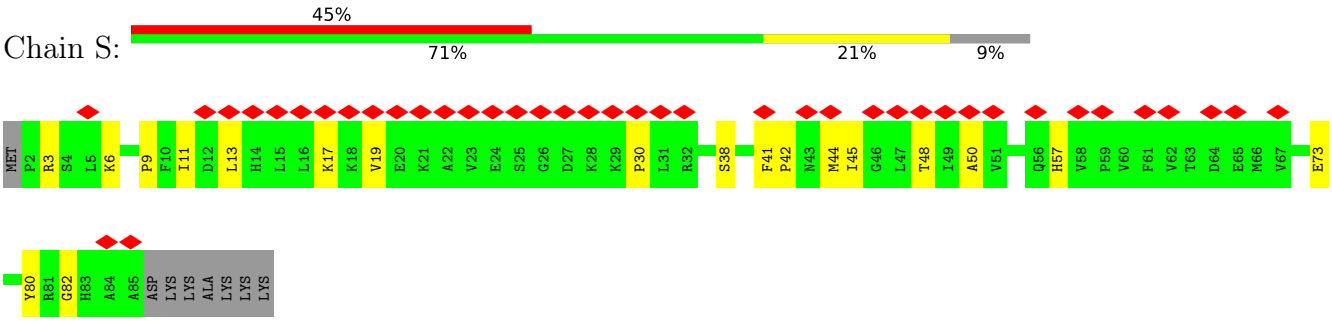
• Molecule 18: 30S ribosomal protein S18

Chain R:



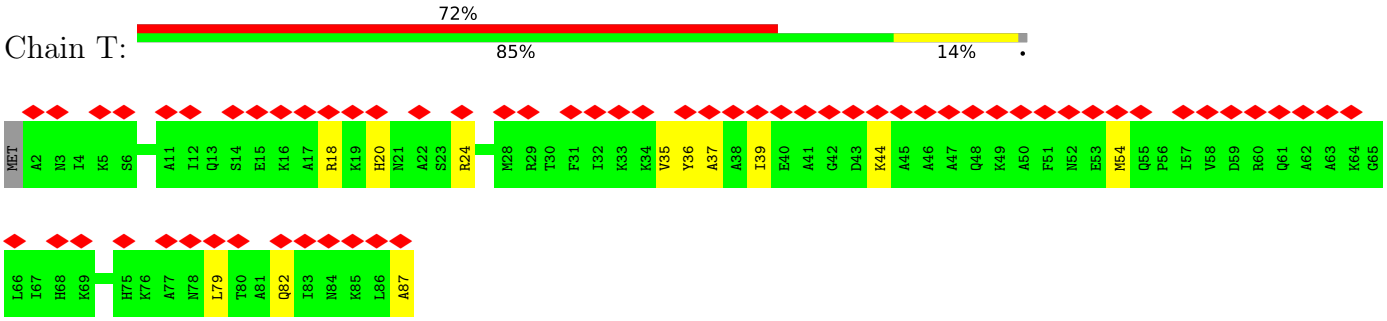
• Molecule 19: 30S ribosomal protein S19

Chain S:



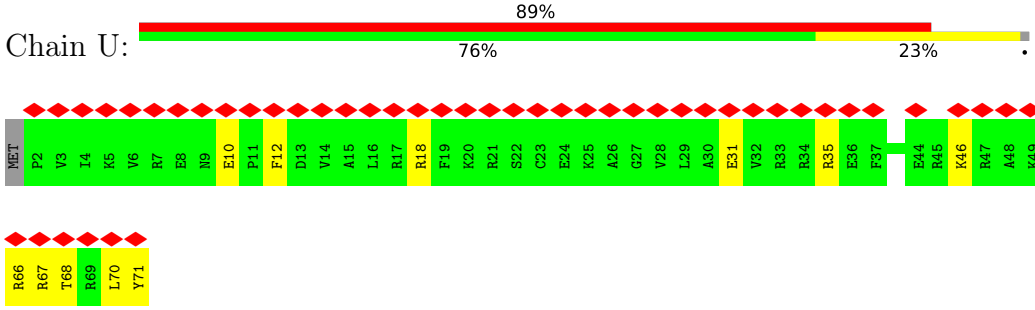
• Molecule 20: 30S ribosomal protein S20

Chain T:



• Molecule 21: 30S ribosomal protein S21

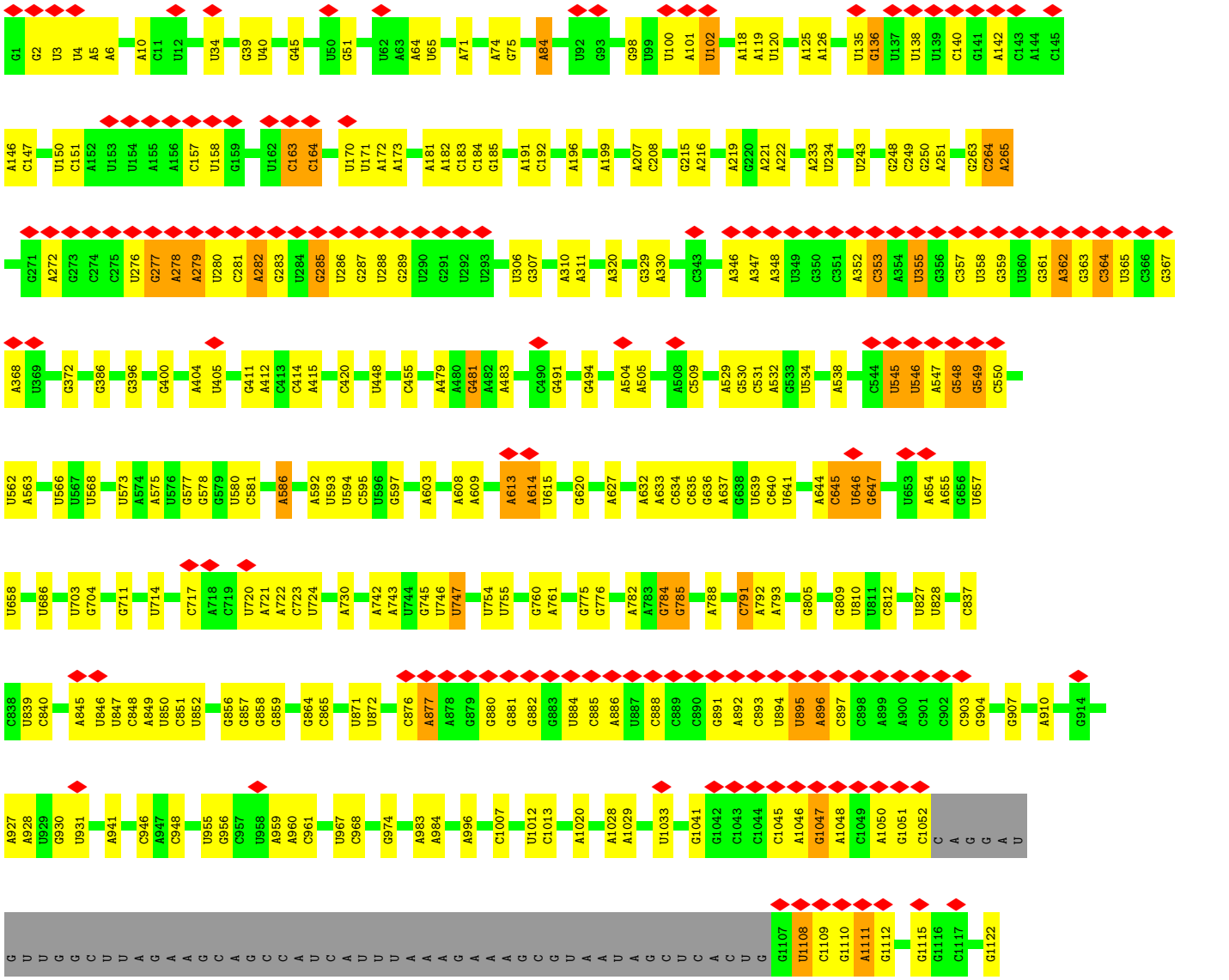
Chain U:

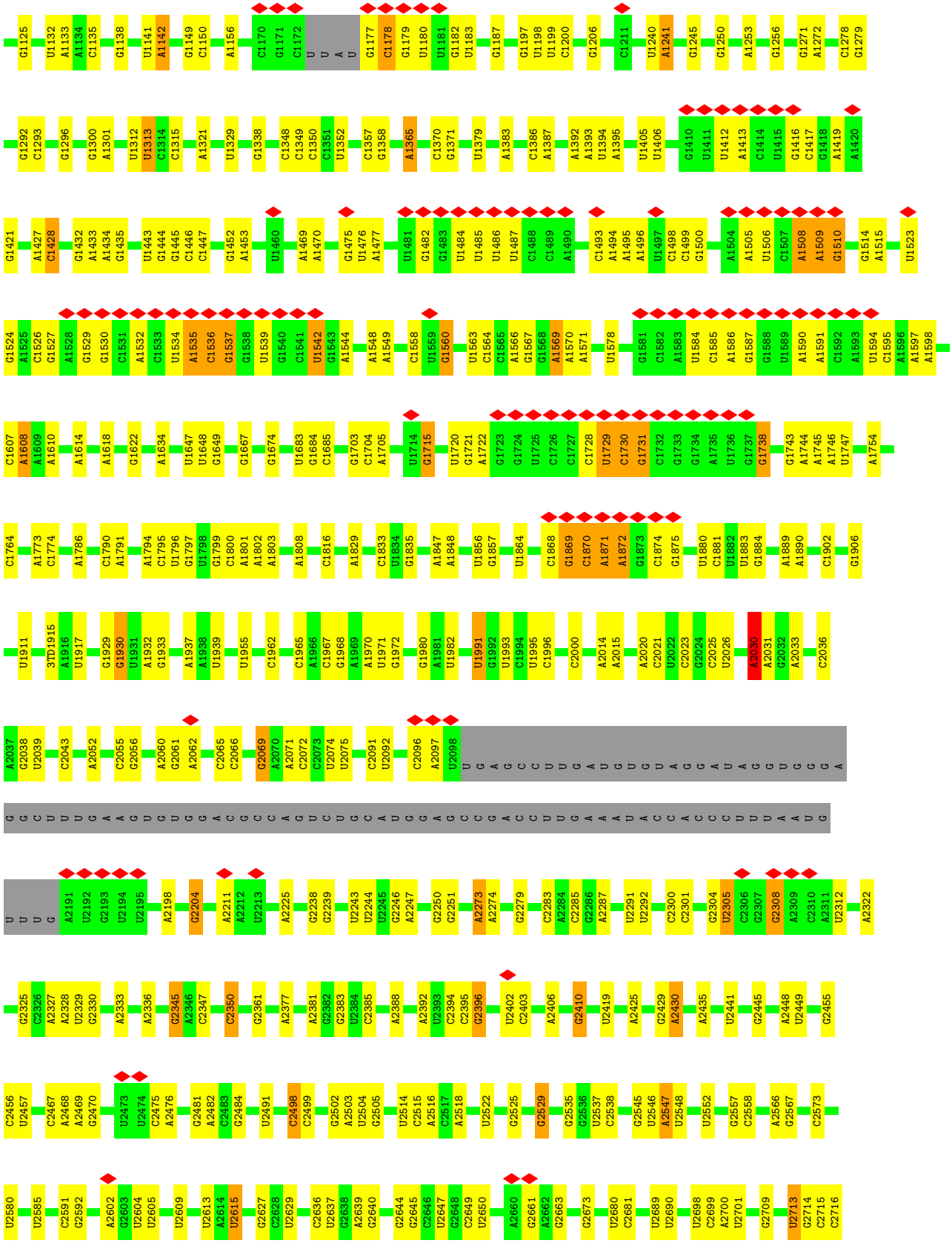


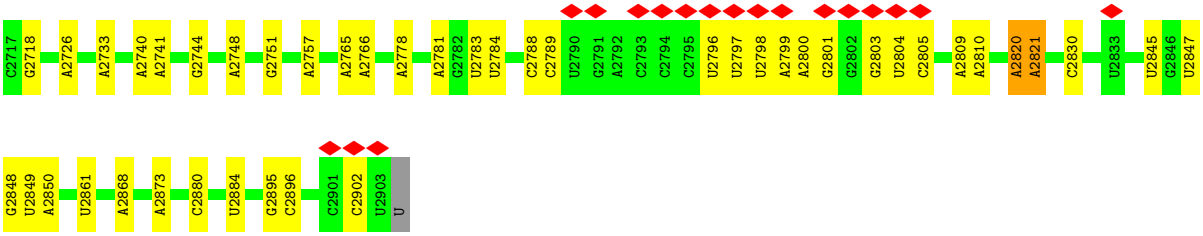
• Molecule 22: 23S rRNA

Chain a:





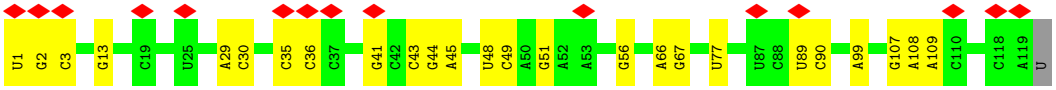




• Molecule 23: 5S rRNA

Chain b:

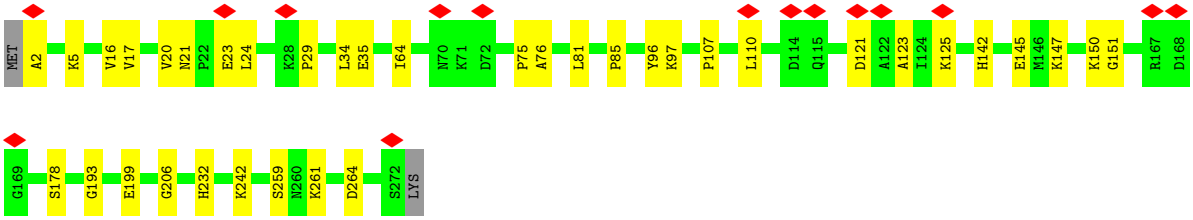




• Molecule 24: 50S ribosomal protein L2

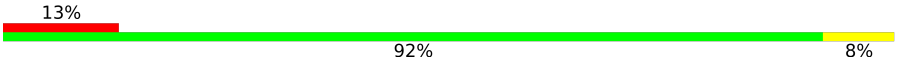
Chain c:

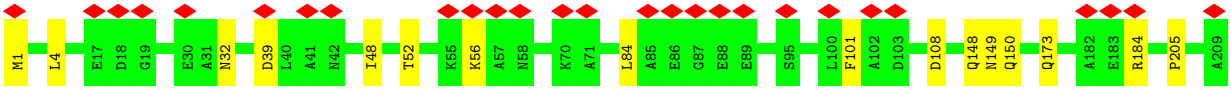




• Molecule 25: 50S ribosomal protein L3

Chain d:

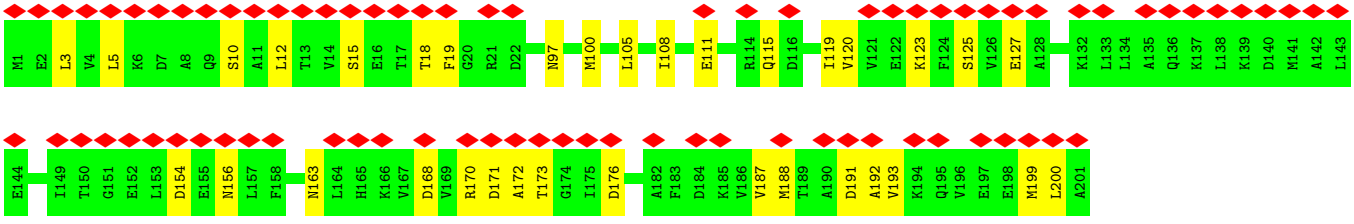




• Molecule 26: 50S ribosomal protein L4

Chain e:

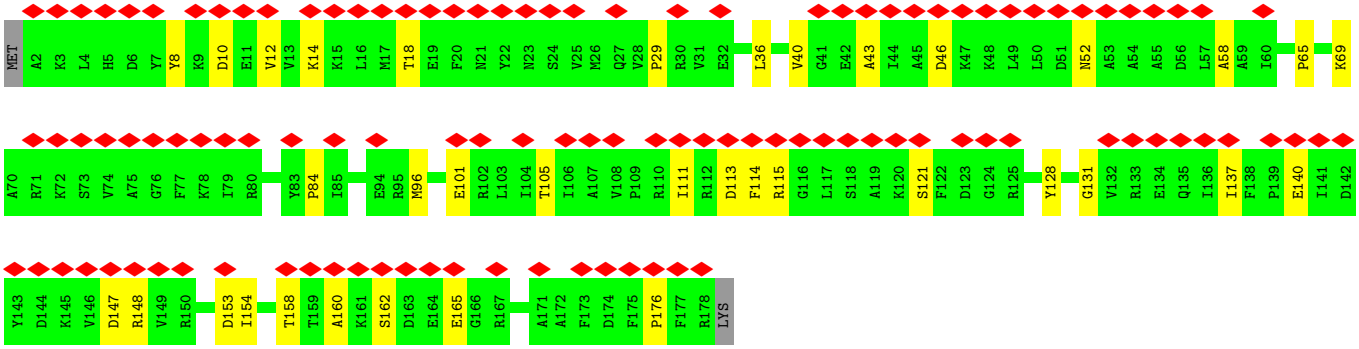




• Molecule 27: 50S ribosomal protein L5

Chain f:

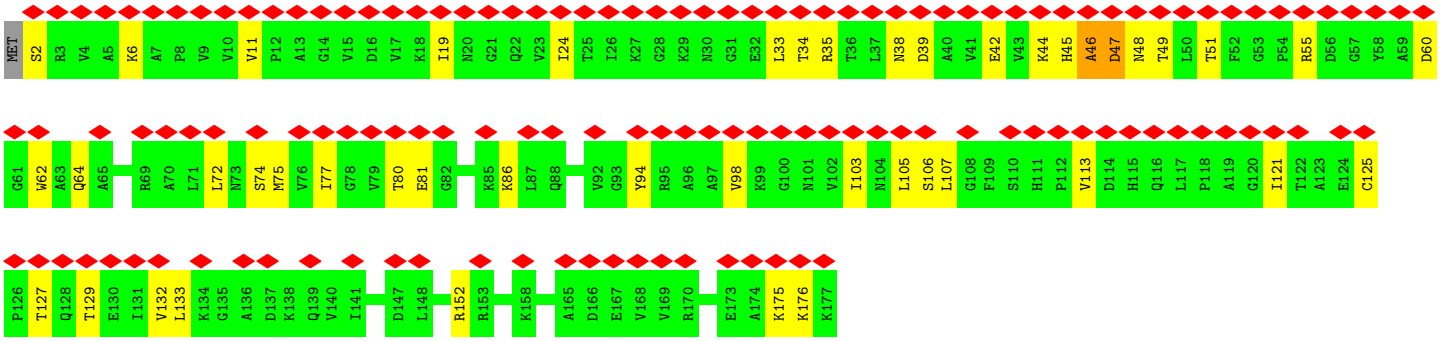




• Molecule 28: 50S ribosomal protein L6

Chain g:

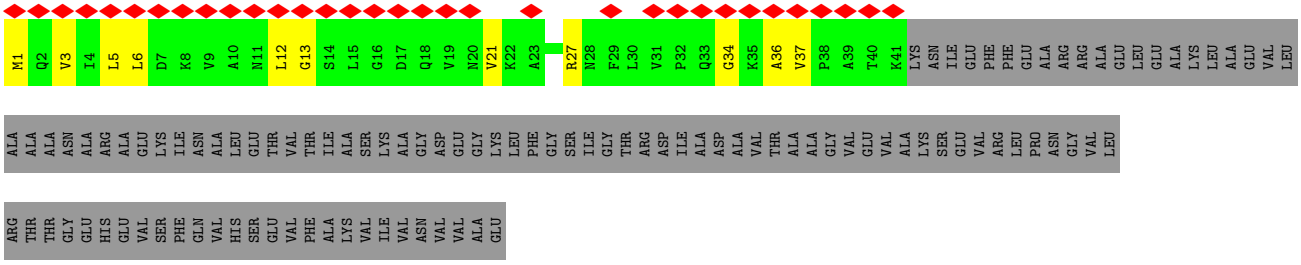




• Molecule 29: 50S ribosomal protein L9

Chain h:





• Molecule 30: 50S ribosomal protein L13

Chain i:

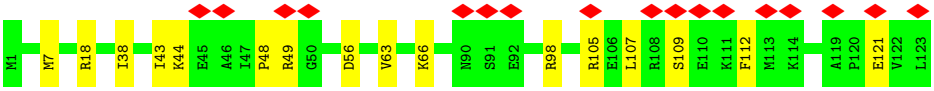




• Molecule 31: 50S ribosomal protein L14

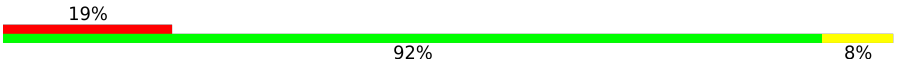
Chain j:

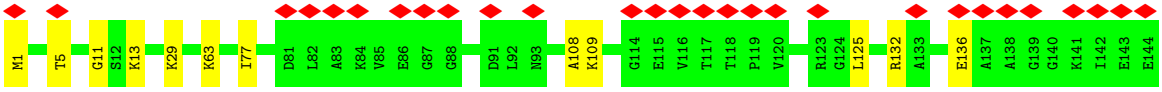




• Molecule 32: 50S ribosomal protein L15

Chain k:

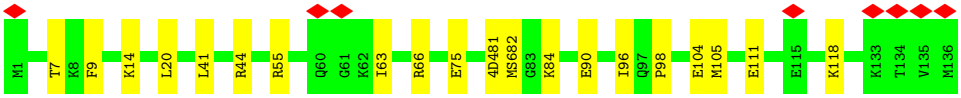




• Molecule 33: 50S ribosomal protein L16

Chain l:

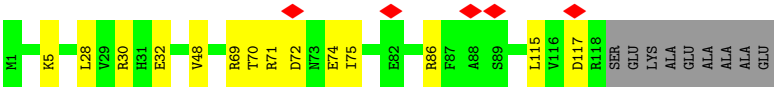




• Molecule 34: 50S ribosomal protein L17

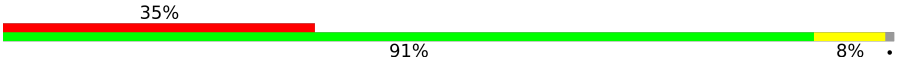
Chain m:

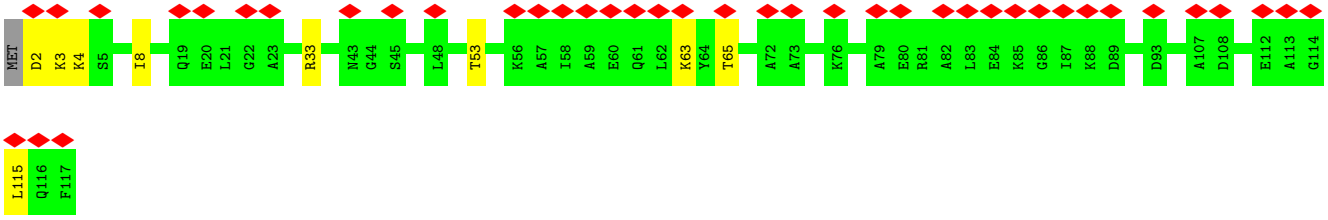




• Molecule 35: 50S ribosomal protein L18

Chain n:

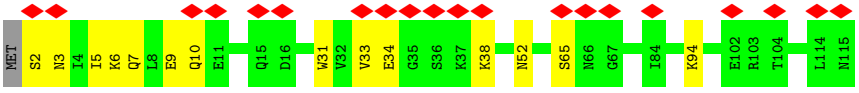




• Molecule 36: 50S ribosomal protein L19

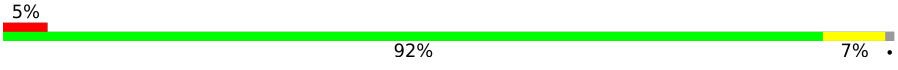
Chain o:

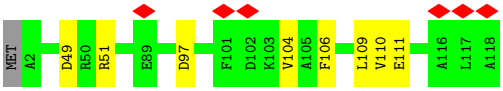




• Molecule 37: 50S ribosomal protein L20

Chain p:

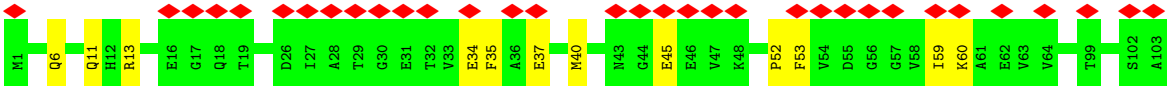




• Molecule 38: 50S ribosomal protein L21

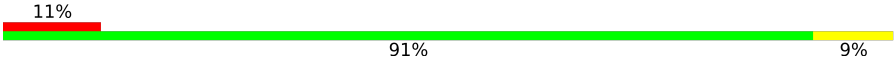
Chain q:

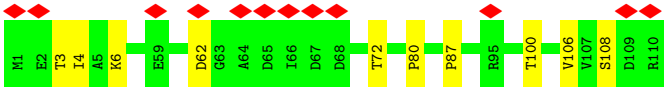




• Molecule 39: 50S ribosomal protein L22

Chain r:

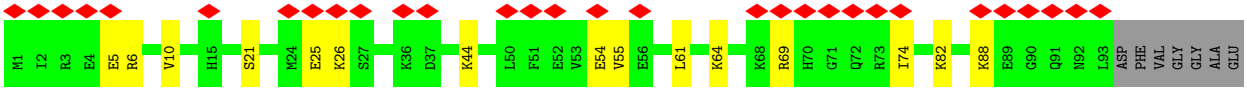




• Molecule 40: 50S ribosomal protein L23

Chain s:

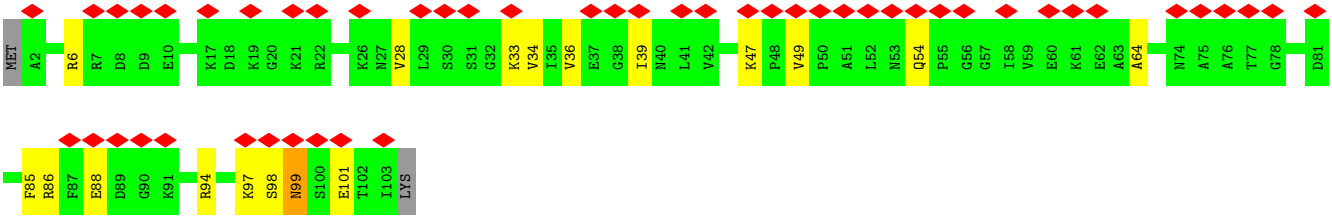




• Molecule 41: 50S ribosomal protein L24

Chain t:

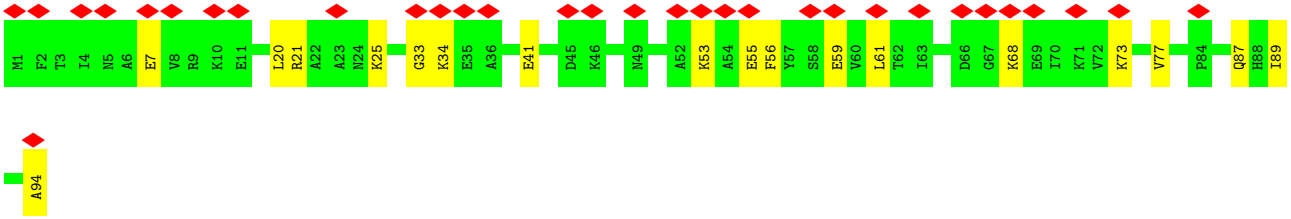




• Molecule 42: 50S ribosomal protein L25

Chain u:

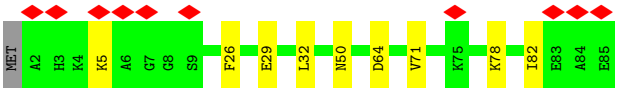




• Molecule 43: 50S ribosomal protein L27

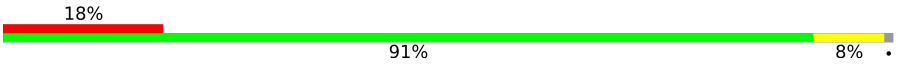
Chain v:

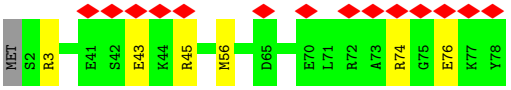




• Molecule 44: 50S ribosomal protein L28

Chain w:

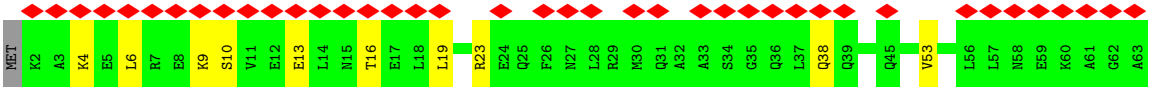




• Molecule 45: 50S ribosomal protein L29

Chain x:





• Molecule 46: 50S ribosomal protein L30

Chain y:

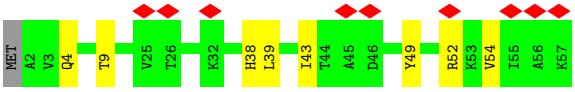




• Molecule 47: 50S ribosomal protein L32

Chain z:

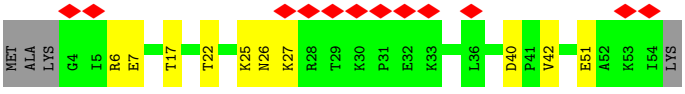




• Molecule 48: 50S ribosomal protein L33

Chain 0:





• Molecule 49: 50S ribosomal protein L34

Chain 1:

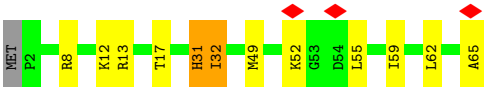




• Molecule 50: 50S ribosomal protein L35

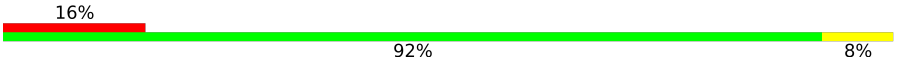
Chain 2:

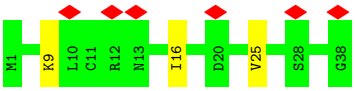




• Molecule 51: 50S ribosomal protein L36

Chain 3:

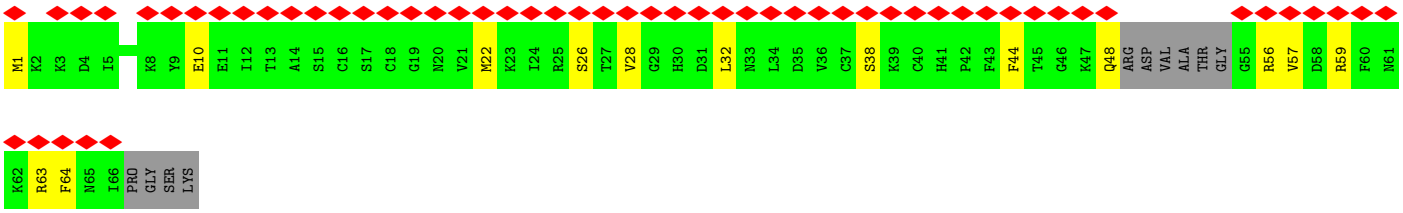




• Molecule 52: 50S ribosomal protein L31

Chain 4:

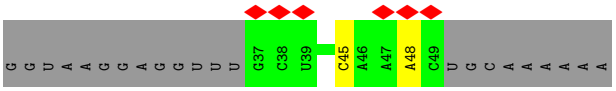




• Molecule 53: mRNA

Chain X:

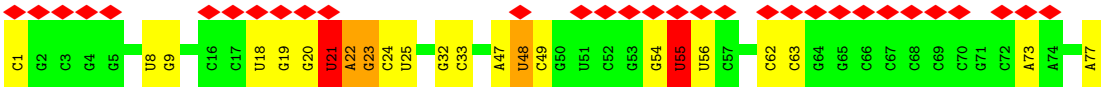




• Molecule 54: P-site tRNA-fMet

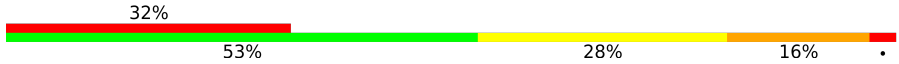
Chain Z:

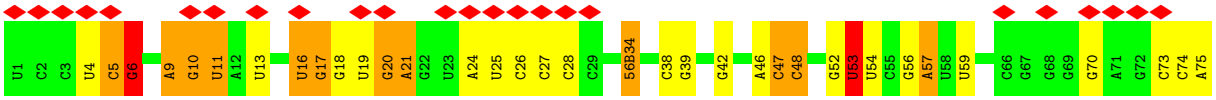




• Molecule 55: A-site tRNA-Asp

Chain V:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	247125	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.295	Depositor
Minimum map value	-0.144	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	439.10498, 439.10498, 439.10498	wwPDB
Map dimensions	530, 530, 530	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8285, 0.8285, 0.8285	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, OMC, 1MA, UR3, 5MU, 4OC, 2MG, IAS, 1MG, 6MZ, MAN, 2MA, MEQ, 3TD, 56B, 4D4, 4SU, H2U, MG, PSU, MA6, OMG, 5MC, OMU, D2T, MS6

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.55	0/36261	0.36	0/56559
2	B	0.24	0/1784	0.52	0/2403
3	C	0.45	0/1651	0.46	0/2225
4	D	0.35	0/1665	0.47	0/2227
5	E	0.47	0/1165	0.47	0/1568
6	F	0.40	0/858	0.44	0/1160
7	G	0.38	0/1219	0.47	0/1635
8	H	0.47	0/989	0.47	0/1326
9	I	0.46	0/1034	0.52	0/1375
10	J	0.43	0/796	0.54	0/1077
11	K	0.45	0/884	0.42	0/1191
12	L	0.48	0/960	0.47	0/1286
13	M	0.44	0/900	0.57	0/1204
14	N	0.46	0/817	0.48	0/1088
15	O	0.44	0/722	0.50	0/964
16	P	0.40	0/653	0.50	0/877
17	Q	0.43	0/650	0.46	0/871
18	R	0.47	0/553	0.52	0/742
19	S	0.42	0/685	0.46	0/922
20	T	0.37	0/676	0.44	0/895
21	U	0.30	0/597	0.52	0/792
22	a	0.65	0/65651	0.39	0/102413
23	b	0.53	0/2850	0.32	0/4444
24	c	0.57	0/2121	0.47	0/2852
25	d	0.55	0/1576	0.46	0/2119
26	e	0.48	0/1571	0.46	0/2113
27	f	0.41	0/1434	0.49	0/1926
28	g	0.39	0/1343	0.50	0/1816
29	h	0.33	0/306	0.58	1/413 (0.2%)
30	i	0.55	0/1152	0.49	0/1551
31	j	0.54	0/955	0.46	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
32	k	0.53	0/1062	0.50	0/1413
33	l	0.53	0/1073	0.42	0/1433
34	m	0.58	0/958	0.52	0/1281
35	n	0.44	0/902	0.46	0/1209
36	o	0.51	0/929	0.43	0/1242
37	p	0.61	0/960	0.45	0/1278
38	q	0.54	0/829	0.50	0/1107
39	r	0.54	0/864	0.44	0/1156
40	s	0.46	0/744	0.50	0/994
41	t	0.45	0/787	0.57	0/1051
42	u	0.48	0/766	0.52	0/1025
43	v	0.53	0/636	0.48	0/841
44	w	0.54	0/635	0.43	0/848
45	x	0.40	0/502	0.47	0/667
46	y	0.49	0/453	0.48	0/605
47	z	0.55	0/450	0.47	0/599
48	0	0.51	0/424	0.50	0/565
49	1	0.60	0/380	0.50	0/498
50	2	0.59	0/513	0.56	0/676
51	3	0.57	0/303	0.53	0/397
52	4	0.32	0/488	0.43	0/649
53	X	0.52	0/312	0.37	0/484
54	Z	0.46	0/1725	0.35	0/2687
55	V	0.45	0/1525	0.41	0/2375
All	All	0.57	0/152698	0.41	1/228393 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	M	0	2
28	g	0	2
50	2	0	1
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	h	13	GLY	N-CA-C	5.70	117.74	110.96

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	2	31	HIS	Peptide
13	M	104	THR	Peptide
13	M	65	VAL	Peptide
28	g	46	ALA	Peptide
28	g	47	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32634	0	16443	269	0
2	B	1753	0	1780	30	0
3	C	1624	0	1696	25	0
4	D	1643	0	1707	42	0
5	E	1152	0	1196	15	0
6	F	839	0	833	17	0
7	G	1203	0	1254	17	0
8	H	979	0	1031	13	0
9	I	1022	0	1070	27	0
10	J	786	0	828	24	0
11	K	877	0	884	11	0
12	L	957	0	1017	6	0
13	M	891	0	952	26	0
14	N	805	0	844	14	0
15	O	714	0	734	14	0
16	P	643	0	661	12	0
17	Q	641	0	682	10	0
18	R	544	0	565	6	0
19	S	668	0	693	17	0
20	T	670	0	719	10	0
21	U	589	0	629	14	0
22	a	59130	0	29766	340	0
23	b	2549	0	1291	10	0
24	c	2082	0	2154	23	0
25	d	1566	0	1618	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	e	1552	0	1619	22	0
27	f	1410	0	1444	28	0
28	g	1323	0	1371	31	0
29	h	303	0	327	6	0
30	i	1129	0	1162	11	0
31	j	946	0	1023	12	0
32	k	1053	0	1129	13	0
33	l	1075	0	1145	12	0
34	m	945	0	989	9	0
35	n	892	0	923	6	0
36	o	917	0	962	10	0
37	p	947	0	1019	7	0
38	q	816	0	839	8	0
39	r	857	0	922	6	0
40	s	738	0	807	11	0
41	t	779	0	831	11	0
42	u	753	0	780	14	0
43	v	628	0	642	5	0
44	w	625	0	652	4	0
45	x	501	0	531	7	0
46	y	449	0	488	7	0
47	z	444	0	458	7	0
48	0	417	0	451	7	0
49	1	377	0	418	4	0
50	2	504	0	572	9	0
51	3	302	0	343	2	0
52	4	480	0	482	16	0
53	X	279	0	142	1	0
54	Z	1645	0	842	10	0
55	V	1612	0	813	18	0
56	A	63	0	0	0	0
56	V	2	0	0	0	0
56	Z	3	0	0	0	0
56	a	185	0	0	0	0
56	b	3	0	0	0	0
56	c	1	0	0	0	0
56	d	1	0	0	0	0
56	z	1	0	0	0	0
57	V	11	0	10	0	0
All	All	141929	0	95183	1193	0

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

All (1193) 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)
22:a:1607:C:N4	22:a:1622:G:OP2	2.01	0.94
38:q:34:GLU:OE1	38:q:60:LYS:NZ	2.04	0.90
27:f:158:THR:HG22	27:f:160:ALA:H	1.36	0.89
22:a:881:G:O6	22:a:895:U:O4	1.90	0.88
22:a:881:G:H1	22:a:895:U:H3	1.17	0.88
1:A:76:G:N2	1:A:93:U:O2	2.12	0.81
26:e:108:ILE:HG23	32:k:1:MET:HE1	1.64	0.80
1:A:664:G:H22	1:A:741:G:H1	1.28	0.79
6:F:5:GLU:OE2	18:R:24:LYS:NZ	2.16	0.79
1:A:1034:G:O6	1:A:1035:A:N6	2.16	0.78
22:a:2304:G:H22	22:a:2312:U:H3	1.28	0.78
26:e:15:SER:HB2	26:e:18:THR:HG22	1.63	0.78
1:A:677:U:H3	1:A:713:G:H22	1.30	0.78
1:A:82:G:N1	1:A:89:U:N3	2.30	0.77
1:A:544:G:OP1	4:D:56:ARG:NH2	2.16	0.77
1:A:691:G:O6	11:K:57:LYS:NZ	2.17	0.77
7:G:79:ARG:HG2	7:G:84:THR:HG22	1.67	0.77
6:F:2:ARG:NH1	6:F:68:GLN:OE1	2.19	0.76
1:A:82:G:N2	1:A:89:U:O2	2.21	0.74
22:a:2796:U:H3	22:a:2799:A:H61	1.34	0.74
1:A:94:G:N1	1:A:97:G:O6	2.19	0.73
15:O:14:GLU:O	15:O:84:ARG:NH2	2.21	0.73
24:c:2:ALA:N	24:c:20:VAL:O	2.21	0.73
1:A:736:C:OP1	18:R:61:ARG:NH1	2.20	0.73
1:A:1038:C:H2'	1:A:1039:G:H8	1.54	0.73
36:o:2:SER:OG	36:o:3:ASN:N	2.22	0.73
2:B:188:ASP:OD1	2:B:189:THR:N	2.21	0.72
1:A:458:U:H2'	1:A:459:A:H8	1.53	0.72
23:b:51:G:OP1	35:n:63:LYS:NZ	2.20	0.72
8:H:50:LYS:NZ	8:H:52:GLU:OE1	2.19	0.72
1:A:512:U:P	4:D:44:ARG:HH22	2.12	0.72
23:b:77:U:OP1	42:u:21:ARG:NH2	2.23	0.72
24:c:75:PRO:HG2	24:c:97:LYS:HE2	1.72	0.71
21:U:62:ARG:HE	21:U:66:ARG:HH11	1.36	0.71
34:m:30:ARG:NH1	34:m:74:GLU:OE1	2.22	0.71
50:2:17:THR:HG21	50:2:49:MET:HE1	1.71	0.71
24:c:142:HIS:ND1	24:c:193:GLY:O	2.18	0.71
1:A:339:C:OP2	31:j:98:ARG:NH1	2.23	0.70
1:A:437:U:HO2'	4:D:120:HIS:HD1	1.38	0.70
19:S:11:ILE:HD12	19:S:38:SER:HB3	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:639:U:H2'	22:a:640:C:C6	2.26	0.70
1:A:673:A:H2'	1:A:674:G:C8	2.26	0.70
13:M:71:ARG:NH2	27:f:113:ASP:OD1	2.25	0.70
18:R:25:ASP:OD2	18:R:28:THR:OG1	2.06	0.70
28:g:33:LEU:HD11	28:g:75:MET:HB2	1.73	0.70
5:E:13:GLU:OE2	5:E:68:ARG:NH1	2.24	0.70
40:s:69:ARG:HG2	40:s:74:ILE:HG22	1.73	0.70
1:A:1086:U:H3	1:A:1099:G:H22	1.38	0.69
8:H:50:LYS:NZ	8:H:60:GLU:OE2	2.26	0.69
1:A:427:U:OP1	4:D:13:ARG:NH2	2.24	0.69
31:j:105:ARG:NH2	36:o:34:GLU:OE2	2.25	0.69
4:D:124:MET:HE3	4:D:146:ARG:HG2	1.73	0.69
22:a:278:A:N1	22:a:361:G:O2'	2.26	0.69
44:w:74:ARG:NH1	44:w:76:GLU:OE2	2.25	0.69
22:a:1508:A:O2'	22:a:1509:A:O4'	2.10	0.69
1:A:59:A:H3'	1:A:331:G:H22	1.58	0.68
15:O:88:ARG:NH2	22:a:714:U:OP2	2.24	0.68
24:c:107:PRO:HD2	24:c:110:LEU:HD22	1.75	0.68
42:u:20:LEU:HD21	42:u:41:GLU:HG3	1.75	0.68
4:D:174:ASP:OD2	4:D:177:LYS:NZ	2.27	0.68
1:A:946:A:H2'	1:A:947:G:C8	2.29	0.67
23:b:66:A:H61	23:b:107:G:H2'	1.59	0.67
30:i:125:TYR:OH	30:i:132:HIS:NE2	2.27	0.67
22:a:2796:U:H3	22:a:2799:A:N6	1.92	0.67
39:r:72:THR:HG21	39:r:108:SER:HB3	1.77	0.67
8:H:38:ASN:O	8:H:42:GLU:HG3	1.95	0.67
21:U:63:GLU:HG3	21:U:66:ARG:NH2	2.10	0.67
22:a:2204:G:OP2	24:c:147:LYS:NZ	2.25	0.67
4:D:95:GLU:OE1	4:D:100:ASN:ND2	2.25	0.66
26:e:188:MET:HE3	26:e:193:VAL:HG22	1.78	0.66
1:A:1397:C:OP2	5:E:29:ARG:NH2	2.29	0.66
23:b:1:U:H2'	23:b:2:G:H8	1.61	0.66
7:G:129:GLU:HB3	7:G:131:LYS:NZ	2.11	0.65
1:A:1328:C:H5"	13:M:28:THR:HG21	1.78	0.65
22:a:856:G:H2'	22:a:857:G:C8	2.31	0.65
10:J:71:LEU:O	10:J:72:ARG:NH1	2.27	0.65
9:I:12:ARG:HG3	9:I:13:LYS:H	1.61	0.65
1:A:299:G:H2'	1:A:300:A:C8	2.31	0.64
48:0:7:GLU:OE1	48:0:27:LYS:HE2	1.98	0.64
22:a:278:A:N6	22:a:362:A:N7	2.46	0.64
39:r:4:ILE:HG12	39:r:106:VAL:HG22	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:35:VAL:HG11	20:T:79:LEU:HD13	1.80	0.64
1:A:458:U:H2'	1:A:459:A:C8	2.33	0.64
1:A:89:U:H2'	1:A:90:C:C2	2.32	0.64
22:a:1417:C:O2'	22:a:1587:G:O2'	2.11	0.64
32:k:132:ARG:O	32:k:136:GLU:HG2	1.98	0.64
2:B:81:LYS:HB2	2:B:93:ASN:HD22	1.63	0.64
11:K:23:ILE:HG21	11:K:96:THR:HG21	1.80	0.64
28:g:86:LYS:HG2	28:g:132:VAL:HG12	1.80	0.64
25:d:1:MET:HG3	25:d:205:PRO:HG2	1.80	0.63
45:x:13:GLU:HA	45:x:16:THR:HG22	1.79	0.63
22:a:1296:G:OP1	22:a:2709:G:O2'	2.16	0.63
44:w:43:GLU:OE2	44:w:45:ARG:NE	2.28	0.63
41:t:33:LYS:HB3	41:t:64:ALA:HB1	1.79	0.63
4:D:169:THR:O	4:D:183:LYS:NZ	2.32	0.63
1:A:492:C:H2'	1:A:493:A:C8	2.34	0.63
6:F:1:MET:HE1	6:F:67:PRO:HD3	1.81	0.63
3:C:72:ARG:HE	3:C:75:ILE:HD12	1.64	0.63
2:B:117:LEU:HG	2:B:141:LEU:HD12	1.80	0.62
13:M:78:LYS:NZ	13:M:82:ASP:OD1	2.27	0.62
22:a:84:A:OP1	41:t:6:ARG:NH1	2.32	0.62
1:A:147:G:H2'	1:A:148:G:C8	2.34	0.62
1:A:437:U:H5"	4:D:152:GLN:HE21	1.64	0.62
1:A:1356:G:H2'	1:A:1357:A:C8	2.33	0.62
3:C:11:ARG:NH2	3:C:175:LEU:O	2.33	0.62
10:J:80:THR:HG22	10:J:82:LYS:H	1.65	0.62
32:k:77:ILE:HD11	32:k:108:ALA:HB1	1.81	0.62
6:F:29:ILE:HD13	6:F:64:VAL:HG11	1.80	0.62
40:s:5:GLU:N	40:s:5:GLU:OE1	2.32	0.62
16:P:55:ASP:OD1	16:P:56:ARG:N	2.32	0.62
22:a:358:U:H2'	22:a:359:G:H8	1.63	0.62
1:A:80:A:O2'	1:A:81:A:O5'	2.12	0.61
47:z:38:HIS:ND1	47:z:39:LEU:O	2.33	0.61
22:a:2522:U:O2'	22:a:2647:U:OP1	2.16	0.61
1:A:714:G:H2'	1:A:715:A:C8	2.35	0.61
1:A:1379:G:OP2	7:G:5:ARG:NH1	2.33	0.61
22:a:2547:A:H2'	22:a:2548:U:C6	2.35	0.61
1:A:1038:C:H2'	1:A:1039:G:C8	2.33	0.61
1:A:60:A:OP2	1:A:387:U:H4'	2.01	0.61
4:D:165:ARG:O	4:D:167:LYS:NZ	2.34	0.61
15:O:26:GLU:HG3	15:O:81:LEU:HD22	1.81	0.61
22:a:286:U:H2'	22:a:287:G:H8	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1469:A:H2'	22:a:1470:A:C8	2.36	0.60
22:a:2845:U:H5"	36:o:52:ASN:O	2.01	0.60
7:G:78:ARG:O	7:G:85:TYR:N	2.26	0.60
31:j:43:ILE:HD12	31:j:56:ASP:HB2	1.84	0.60
22:a:1156:A:C8	37:p:51:ARG:HG2	2.37	0.60
22:a:1548:A:H2'	22:a:1549:A:C8	2.36	0.60
29:h:5:LEU:HD11	29:h:12:LEU:HD12	1.84	0.60
1:A:695:A:H2'	1:A:696:A:C8	2.36	0.60
1:A:1040:U:H2'	1:A:1041:G:H8	1.66	0.60
22:a:1046:A:H3'	22:a:1047:G:H5'	1.82	0.60
1:A:204:G:H1'	1:A:465:A:N1	2.17	0.60
50:2:55:LEU:O	50:2:59:ILE:HG13	2.01	0.60
4:D:162:ALA:O	4:D:167:LYS:NZ	2.35	0.60
19:S:42:PRO:HB3	52:4:57:VAL:HG13	1.83	0.60
26:e:18:THR:HG23	26:e:19:PHE:HD1	1.67	0.60
27:f:147:ASP:OD1	27:f:148:ARG:N	2.33	0.60
41:t:28:VAL:HG22	41:t:34:VAL:HG12	1.83	0.60
22:a:1047:G:HO2'	22:a:1110:G:H1	1.50	0.59
26:e:18:THR:HG23	26:e:19:PHE:CD1	2.37	0.59
34:m:69:ARG:O	34:m:70:THR:OG1	2.17	0.59
38:q:6:GLN:HG2	38:q:11:GLN:HG2	1.84	0.59
26:e:123:LYS:NZ	26:e:125:SER:OG	2.35	0.59
5:E:15:LEU:HD12	5:E:37:THR:HG22	1.84	0.59
22:a:1722:A:N6	22:a:1738:G:O2'	2.34	0.59
1:A:337:G:H2'	1:A:338:A:C8	2.37	0.59
1:A:1273:C:H2'	1:A:1274:A:O4'	2.02	0.59
22:a:2788:C:H2'	22:a:2789:C:C6	2.37	0.59
9:I:88:MET:HE1	9:I:104:VAL:HG22	1.85	0.59
27:f:101:GLU:O	27:f:105:THR:OG1	2.17	0.59
5:E:65:GLU:OE2	5:E:69:ARG:NH2	2.30	0.59
10:J:6:ILE:HG22	10:J:102:LEU:HD13	1.84	0.59
42:u:21:ARG:NH1	42:u:87:GLN:O	2.36	0.59
55:V:20:G:O2'	55:V:21:A:OP1	2.21	0.59
1:A:76:G:H1	1:A:93:U:H3	0.72	0.59
1:A:131:A:H2'	1:A:132:C:C6	2.38	0.59
1:A:1317:C:OP2	14:N:28:LYS:NZ	2.28	0.58
9:I:75:GLN:O	9:I:79:ILE:HG12	2.03	0.58
5:E:149:SER:H	5:E:152:MET:HE3	1.67	0.58
5:E:13:GLU:HG2	5:E:39:VAL:HG12	1.85	0.58
42:u:33:GLY:C	42:u:34:LYS:HD3	2.29	0.58
1:A:375:U:OP1	16:P:70:ARG:NH1	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:TRP:CZ3	2:B:25:PRO:HA	2.38	0.58
6:F:49:TYR:OH	6:F:86:ARG:NH1	2.36	0.58
9:I:57:MET:HE1	9:I:90:TYR:CE2	2.39	0.58
22:a:534:U:O2'	37:p:49:ASP:OD2	2.11	0.58
22:a:1007:C:OP1	30:i:37:ARG:NH2	2.36	0.58
22:a:2250:G:OP1	33:l:84:LYS:NZ	2.34	0.58
22:a:1667:G:O2'	22:a:1991:U:O4	2.17	0.58
22:a:2000:C:OP1	34:m:5:LYS:NZ	2.34	0.58
3:C:177:THR:HG23	3:C:180:ALA:HB2	1.85	0.58
9:I:65:ILE:HG21	9:I:79:ILE:HD12	1.86	0.58
22:a:849:A:H2'	22:a:850:U:C6	2.38	0.58
41:t:98:SER:OG	41:t:98:SER:O	2.21	0.58
19:S:13:LEU:HD11	19:S:17:LYS:HE3	1.86	0.58
25:d:184:ARG:NH1	36:o:7:GLN:HE22	2.01	0.58
34:m:32:GLU:HG2	34:m:115:LEU:HD12	1.84	0.58
1:A:459:A:H2'	1:A:460:A:C8	2.39	0.58
22:a:2291:U:H2'	22:a:2292:U:C6	2.39	0.57
48:0:25:LYS:HG2	48:0:26:ASN:N	2.18	0.57
1:A:1126:U:OP1	10:J:7:ARG:NH2	2.37	0.57
23:b:66:A:N6	23:b:107:G:H2'	2.19	0.57
40:s:6:ARG:O	40:s:10:VAL:HG13	2.03	0.57
22:a:3:U:H2'	22:a:4:U:C6	2.39	0.57
22:a:2305:U:H5"	27:f:131:GLY:HA3	1.84	0.57
5:E:165:LEU:O	8:H:114:ARG:NH1	2.37	0.57
37:p:104:VAL:HG11	38:q:45:GLU:HG2	1.87	0.57
39:r:80:PRO:O	39:r:100:THR:OG1	2.23	0.57
1:A:1023:U:H2'	1:A:1024:G:H8	1.68	0.57
6:F:42:TRP:HB2	6:F:59:TYR:HB2	1.85	0.57
13:M:10:PRO:HG2	13:M:13:LYS:HE3	1.86	0.57
22:a:1802:A:H2'	22:a:1803:A:C8	2.39	0.57
52:4:59:ARG:NH2	52:4:63:ARG:HH21	2.02	0.57
22:a:2052:A:H4'	25:d:148:GLN:O	2.05	0.57
1:A:636:U:H5"	17:Q:6:ARG:HD3	1.86	0.57
11:K:35:THR:HG22	11:K:41:ALA:HA	1.87	0.57
22:a:549:G:H2'	22:a:550:C:C6	2.39	0.57
22:a:644:A:H2'	22:a:645:C:O4'	2.05	0.57
22:a:2285:C:OP2	48:0:6:ARG:NH1	2.37	0.57
22:a:2328:A:H2'	22:a:2329:U:C6	2.39	0.57
3:C:58:GLU:OE1	3:C:65:ARG:NH2	2.31	0.56
9:I:106:ARG:NH1	9:I:107:ASP:O	2.38	0.56
22:a:930:G:H1'	46:y:25:LEU:HD21	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:19:VAL:HG21	19:S:44:MET:HG2	1.87	0.56
22:a:2484:G:OP1	33:l:44:ARG:HD3	2.04	0.56
34:m:86:ARG:NH2	34:m:117:ASP:OD1	2.36	0.56
42:u:7:GLU:OE2	42:u:25:LYS:NZ	2.38	0.56
4:D:62:ARG:NH1	4:D:69:GLU:OE2	2.38	0.56
14:N:46:LEU:HD12	19:S:13:LEU:HD13	1.86	0.56
22:a:1730:C:H4'	22:a:1731:G:O5'	2.05	0.56
26:e:173:THR:HA	26:e:199:MET:HE1	1.87	0.56
4:D:99:ASP:OD2	4:D:133:ALA:HB1	2.05	0.56
26:e:105:LEU:HD23	26:e:200:LEU:HD21	1.87	0.56
1:A:1005:A:C2	1:A:1006:G:H1'	2.41	0.56
3:C:175:LEU:HD23	3:C:182:ILE:HD13	1.88	0.56
27:f:52:ASN:ND2	27:f:147:ASP:OD2	2.38	0.56
42:u:73:LYS:HG3	42:u:94:ALA:HB2	1.87	0.56
1:A:127:G:O2'	17:Q:6:ARG:NH2	2.34	0.56
1:A:950:U:O4	13:M:104:THR:HG21	2.06	0.56
1:A:1023:U:H2'	1:A:1024:G:C8	2.40	0.56
28:g:72:LEU:HA	28:g:75:MET:HG2	1.87	0.56
1:A:77:A:H2'	1:A:78:A:C8	2.40	0.56
16:P:23:ASP:OD1	16:P:24:SER:N	2.38	0.56
40:s:54:GLU:HB3	40:s:88:LYS:HD2	1.88	0.56
1:A:1098:C:O2'	21:U:71:TYR:O	2.21	0.56
22:a:545:U:O2'	22:a:548:G:N2	2.34	0.56
22:a:2030:6MZ:H2	22:a:2499:C:H5"	1.88	0.56
1:A:1314:C:OP1	19:S:6:LYS:NZ	2.36	0.56
22:a:286:U:H2'	22:a:287:G:C8	2.41	0.56
22:a:1141:U:H4'	22:a:1142:A:O4'	2.06	0.56
33:l:66:ARG:NH1	33:l:104:GLU:OE2	2.39	0.56
1:A:1130:A:H2'	1:A:1131:G:C8	2.41	0.55
16:P:48:GLU:OE1	16:P:51:ARG:NH2	2.39	0.55
1:A:1391:U:H2'	1:A:1392:G:C8	2.41	0.55
22:a:1870:C:O2'	22:a:1871:A:H8	1.89	0.55
1:A:82:G:O6	1:A:89:U:O4	2.25	0.55
22:a:249:C:O2	50:2:12:LYS:NZ	2.37	0.55
22:a:2327:A:H2'	22:a:2328:A:C8	2.41	0.55
22:a:2529:G:H4'	28:g:175:LYS:HE2	1.87	0.55
24:c:232:HIS:HA	24:c:242:LYS:HE3	1.88	0.55
1:A:406:G:H21	4:D:116:GLN:HE22	1.54	0.55
22:a:276:U:O2'	22:a:278:A:N7	2.37	0.55
13:M:71:ARG:NH2	27:f:115:ARG:HD3	2.21	0.55
22:a:285:G:H1	22:a:355:U:H3	1.52	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:894:U:H2'	22:a:895:U:C6	2.42	0.55
22:a:2698:U:H2'	22:a:2699:C:C6	2.41	0.55
5:E:45:ARG:HB3	5:E:71:MET:HE2	1.89	0.55
27:f:105:THR:HB	52:4:22:MET:HE1	1.87	0.55
1:A:976:G:OP2	1:A:1358:U:O2'	2.25	0.55
1:A:1530:G:H2'	1:A:1531:A:C8	2.42	0.55
22:a:182:A:H2'	22:a:183:C:H6	1.72	0.55
22:a:347:A:H2'	22:a:348:A:C8	2.42	0.55
45:x:6:LEU:HD21	45:x:53:VAL:HG22	1.89	0.55
51:3:9:LYS:HE3	51:3:16:ILE:HG12	1.88	0.55
10:J:7:ARG:HB2	10:J:101:SER:HB2	1.89	0.55
27:f:14:LYS:O	27:f:18:THR:HG23	2.07	0.55
43:v:5:LYS:HB3	54:Z:1:C:H1'	1.88	0.55
1:A:713:G:H2'	1:A:714:G:C8	2.41	0.54
15:O:64:ARG:HH22	15:O:89:ARG:C	2.15	0.54
22:a:1799:G:N7	24:c:178:SER:OG	2.39	0.54
35:n:4:LYS:O	35:n:8:ILE:HG12	2.06	0.54
22:a:414:C:H2'	22:a:415:A:C8	2.42	0.54
22:a:1051:G:H2'	22:a:1052:C:O4'	2.07	0.54
54:Z:1:C:N4	54:Z:73:A:H2	2.05	0.54
7:G:29:ILE:HD12	7:G:101:MET:HE2	1.90	0.54
22:a:593:U:H2'	22:a:594:U:C6	2.42	0.54
22:a:1902:C:H4'	24:c:242:LYS:O	2.07	0.54
4:D:87:GLY:HA3	4:D:197:GLU:HG3	1.90	0.54
19:S:9:PRO:HG3	52:4:64:PHE:CD2	2.43	0.54
1:A:269:C:H2'	1:A:270:A:C8	2.43	0.54
1:A:398:U:H2'	1:A:399:G:H8	1.72	0.54
9:I:96:SER:HB2	9:I:100:LYS:HZ1	1.72	0.54
22:a:2243:U:H2'	22:a:2244:U:C6	2.42	0.54
24:c:5:LYS:HD3	24:c:17:VAL:HG22	1.89	0.54
36:o:33:VAL:HG22	36:o:38:LYS:HB3	1.90	0.54
40:s:61:LEU:HD11	40:s:82:LYS:HD3	1.90	0.54
22:a:2537:U:H2'	22:a:2538:C:C6	2.43	0.54
26:e:5:LEU:HD13	26:e:10:SER:HB2	1.90	0.54
1:A:545:C:H5'	4:D:69:GLU:HB2	1.90	0.54
14:N:27:LEU:O	14:N:31:ILE:HG12	2.08	0.54
22:a:364:C:H2'	22:a:365:U:C6	2.43	0.54
26:e:170:ARG:NH2	26:e:176:ASP:OD1	2.39	0.54
28:g:33:LEU:CD1	28:g:75:MET:HB2	2.37	0.54
1:A:382:A:H2'	1:A:383:A:C8	2.43	0.54
51:3:16:ILE:HD13	51:3:25:VAL:HG22	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:A:H2'	1:A:1131:G:H8	1.71	0.54
2:B:66:LYS:NZ	2:B:154:MET:O	2.37	0.54
7:G:92:ARG:O	7:G:96:ARG:HG3	2.08	0.54
22:a:64:A:H2'	22:a:65:U:C6	2.43	0.54
7:G:15:ASP:OD1	7:G:23:LEU:HD23	2.08	0.53
19:S:41:PHE:HB2	19:S:44:MET:HE3	1.90	0.53
22:a:2091:C:O3'	44:w:56:MET:HE1	2.09	0.53
3:C:85:GLU:OE2	3:C:89:LYS:NZ	2.41	0.53
38:q:35:PHE:HB2	38:q:59:ILE:HB	1.91	0.53
1:A:1287:A:H2'	1:A:1288:A:C8	2.43	0.53
7:G:57:SER:OG	7:G:60:GLU:OE2	2.14	0.53
1:A:28:A:O2'	1:A:296:U:OP1	2.20	0.53
1:A:381:C:H2'	1:A:382:A:O4'	2.08	0.53
22:a:363:G:H2'	22:a:364:C:C6	2.44	0.53
22:a:547:A:H4'	22:a:548:G:H5'	1.89	0.53
23:b:1:U:H2'	23:b:2:G:C8	2.41	0.53
1:A:76:G:H2'	1:A:77:A:H8	1.74	0.53
1:A:91:U:H2'	1:A:92:U:C6	2.44	0.53
1:A:1062:U:H2'	1:A:1063:C:C6	2.43	0.53
1:A:1088:G:H4'	21:U:70:LEU:HD13	1.90	0.53
13:M:66:GLU:HB3	13:M:70:ARG:NH1	2.23	0.53
22:a:307:G:N1	22:a:310:A:OP2	2.39	0.53
52:4:59:ARG:HH22	52:4:63:ARG:HH21	1.57	0.53
1:A:17:U:H2'	1:A:18:C:C6	2.43	0.53
22:a:1870:C:HO2'	22:a:1871:A:H8	1.56	0.53
22:a:2481:G:HO2'	22:a:2482:A:H8	1.56	0.53
1:A:1031:C:O2'	1:A:1032:G:N2	2.42	0.53
1:A:1098:C:P	2:B:139:ARG:HH12	2.32	0.53
8:H:22:LYS:O	8:H:65:TYR:OH	2.27	0.53
22:a:881:G:H2'	22:a:882:G:H8	1.73	0.53
28:g:80:THR:OG1	28:g:81:GLU:OE1	2.16	0.53
29:h:34:GLY:O	29:h:36:ALA:N	2.41	0.53
41:t:49:VAL:O	41:t:54:GLN:HA	2.09	0.53
46:y:24:LEU:HD11	46:y:54:MET:SD	2.49	0.53
55:V:17:G:O2'	55:V:56:G:N2	2.29	0.53
2:B:114:LEU:HD12	2:B:144:LEU:HB3	1.91	0.53
16:P:67:ILE:HG23	16:P:71:VAL:HG13	1.91	0.53
22:a:956:G:N7	33:l:14:LYS:NZ	2.56	0.53
22:a:2830:C:H5"	25:d:56:LYS:HE3	1.91	0.53
50:2:62:LEU:HG	50:2:65:ALA:HB2	1.91	0.53
1:A:421:U:O2	3:C:127:ARG:NH2	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:A:H2'	1:A:461:A:H8	1.74	0.53
27:f:10:ASP:O	27:f:14:LYS:HE2	2.09	0.53
1:A:1225:A:H2'	1:A:1226:C:C5	2.44	0.52
14:N:29:ALA:O	14:N:33:ASP:HB2	2.09	0.52
19:S:45:ILE:HD12	19:S:45:ILE:H	1.75	0.52
30:i:125:TYR:HH	30:i:132:HIS:CD2	2.26	0.52
1:A:1010:U:H2'	1:A:1011:C:H6	1.74	0.52
3:C:174:PRO:HB2	3:C:177:THR:HG22	1.91	0.52
22:a:1494:A:H2'	22:a:1495:A:C8	2.45	0.52
16:P:18:GLN:OE1	16:P:35:ARG:NE	2.27	0.52
26:e:171:ASP:OD1	26:e:172:ALA:N	2.42	0.52
1:A:91:U:H2'	1:A:92:U:H6	1.75	0.52
18:R:37:GLY:O	18:R:63:ARG:NH2	2.40	0.52
22:a:347:A:H2'	22:a:348:A:H8	1.74	0.52
22:a:849:A:H2'	22:a:850:U:H6	1.73	0.52
22:a:1794:A:H2'	22:a:1795:C:C6	2.44	0.52
1:A:1218:C:H2'	1:A:1219:A:C8	2.44	0.52
9:I:57:MET:HE1	9:I:90:TYR:HE2	1.75	0.52
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.91	0.52
22:a:851:C:H2'	22:a:852:U:H6	1.75	0.52
22:a:1590:A:H2'	22:a:1591:A:C8	2.45	0.52
54:Z:24:C:H2'	54:Z:25:U:C6	2.45	0.52
54:Z:48:U:H5"	54:Z:49:C:H5'	1.92	0.52
1:A:1266:G:N2	1:A:1269:A:OP2	2.33	0.52
1:A:1314:C:H2'	1:A:1315:U:C6	2.44	0.52
15:O:26:GLU:OE2	15:O:77:ARG:NH1	2.40	0.52
26:e:154:ASP:OD1	26:e:154:ASP:N	2.43	0.52
1:A:1323:G:H2'	1:A:1324:A:C8	2.45	0.52
2:B:218:ALA:O	2:B:222:ARG:HG2	2.09	0.52
22:a:221:A:N1	22:a:265:A:O2'	2.42	0.52
1:A:1027:C:H3'	1:A:1028:C:H5	1.75	0.52
1:A:1356:G:H2'	1:A:1357:A:H8	1.74	0.52
3:C:23:PHE:CD1	10:J:97:ASP:HB2	2.45	0.52
22:a:1405:U:H2'	22:a:1406:U:C6	2.45	0.52
43:v:71:VAL:HG22	43:v:78:LYS:HD2	1.91	0.52
54:Z:54:G:H3'	54:Z:55:5MU:H73	1.91	0.52
1:A:38:G:H22	1:A:397:A:H5'	1.75	0.52
9:I:7:TYR:HH	9:I:9:THR:HG1	1.56	0.52
11:K:79:ILE:HB	11:K:105:PHE:HE1	1.75	0.52
22:a:851:C:H2'	22:a:852:U:C6	2.45	0.52
31:j:121:GLU:OE1	36:o:65:SER:OG	2.26	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:p:97:ASP:OD2	38:q:13:ARG:NE	2.40	0.52
41:t:36:VAL:HG13	41:t:39:ILE:HB	1.91	0.52
1:A:59:A:H3'	1:A:331:G:N2	2.23	0.51
1:A:187:G:N2	1:A:190:A:OP2	2.38	0.51
10:J:10:LEU:HD12	10:J:22:THR:HG22	1.91	0.51
22:a:1434:A:H2'	22:a:1435:G:C8	2.45	0.51
16:P:1:MET:O	16:P:24:SER:OG	2.24	0.51
22:a:172:A:H2'	22:a:173:A:C8	2.45	0.51
22:a:414:C:H2'	22:a:415:A:H8	1.76	0.51
22:a:1245:G:OP1	32:k:13:LYS:HE2	2.11	0.51
29:h:1:MET:N	29:h:21:VAL:O	2.44	0.51
1:A:309:A:H2'	1:A:310:G:H8	1.74	0.51
2:B:191:SER:OG	2:B:192:ASP:N	2.43	0.51
13:M:104:THR:HG22	13:M:105:ASN:N	2.25	0.51
22:a:243:U:OP2	50:2:8:ARG:NH1	2.43	0.51
22:a:1746:A:H2'	22:a:1747:U:C6	2.45	0.51
33:l:63:ILE:HD13	33:l:105:MET:HG3	1.91	0.51
1:A:76:G:O6	1:A:93:U:O4	2.28	0.51
6:F:46:GLN:OE1	6:F:56:LYS:NZ	2.41	0.51
8:H:10:MET:HG3	8:H:27:MET:SD	2.50	0.51
21:U:62:ARG:O	21:U:66:ARG:HG3	2.11	0.51
22:a:2:G:H2'	22:a:3:U:C6	2.46	0.51
22:a:639:U:H2'	22:a:640:C:H6	1.71	0.51
31:j:63:VAL:HG12	31:j:107:LEU:HD11	1.91	0.51
1:A:79:G:O6	1:A:80:A:N6	2.44	0.51
1:A:80:A:HO2'	1:A:81:A:P	2.32	0.51
21:U:31:GLU:O	21:U:35:ARG:HG2	2.10	0.51
22:a:892:A:H2'	22:a:893:C:O4'	2.11	0.51
22:a:1871:A:H2'	22:a:1872:A:C8	2.45	0.51
22:a:2273:A:H2'	22:a:2274:A:C8	2.45	0.51
1:A:1029:U:H1'	1:A:1033:G:O6	2.10	0.51
9:I:115:LYS:HB2	9:I:118:LEU:HD12	1.93	0.51
22:a:163:C:H2'	22:a:164:C:C6	2.46	0.51
22:a:1108:U:H2'	22:a:1109:C:C6	2.45	0.51
32:k:77:ILE:CD1	32:k:108:ALA:HB1	2.40	0.51
1:A:1:A:H2'	1:A:2:A:H5'	1.92	0.51
1:A:512:U:OP1	4:D:44:ARG:NH2	2.42	0.51
4:D:170:TRP:HA	4:D:184:ARG:NH1	2.26	0.51
16:P:72:ALA:O	16:P:75:ILE:HG22	2.10	0.51
22:a:876:C:H2'	22:a:877:A:O4'	2.11	0.51
26:e:97:ASN:HB2	26:e:100:MET:HG3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:U:H2'	1:A:391:G:H8	1.76	0.51
1:A:1166:G:N1	1:A:1169:A:OP2	2.44	0.51
4:D:28:ILE:HG23	4:D:34:ILE:HD11	1.92	0.51
40:s:44:LYS:HG3	40:s:55:VAL:HG21	1.92	0.51
28:g:38:ASN:OD1	28:g:39:ASP:N	2.44	0.51
11:K:17:SER:HA	11:K:79:ILE:HA	1.93	0.50
22:a:357:C:H2'	22:a:358:U:C6	2.46	0.50
43:v:26:PHE:O	43:v:29:GLU:HG3	2.10	0.50
55:V:5:C:H2'	55:V:6:2MG:O4'	2.10	0.50
3:C:134:MET:HE2	3:C:168:TYR:CD1	2.47	0.50
4:D:35:GLU:OE1	4:D:35:GLU:N	2.28	0.50
8:H:11:LEU:HD22	8:H:75:ILE:HD11	1.92	0.50
22:a:548:G:H2'	22:a:549:G:H1'	1.93	0.50
22:a:1529:G:H1	22:a:1542:U:H3	1.59	0.50
1:A:539:A:H2'	1:A:540:G:C8	2.46	0.50
22:a:1509:A:HO2'	22:a:1510:G:H8	1.57	0.50
22:a:1590:A:H2'	22:a:1591:A:H8	1.76	0.50
28:g:38:ASN:ND2	28:g:64:GLN:OE1	2.45	0.50
28:g:105:LEU:HB2	28:g:113:VAL:HG13	1.92	0.50
32:k:5:THR:HG22	32:k:5:THR:O	2.11	0.50
1:A:323:U:H2'	1:A:324:G:O4'	2.12	0.50
3:C:179:ARG:HB3	3:C:206:GLU:O	2.12	0.50
22:a:1864:U:OP1	22:a:2410:G:O2'	2.21	0.50
42:u:55:GLU:HB2	42:u:59:GLU:OE1	2.11	0.50
20:T:54:MET:HE2	20:T:79:LEU:HD12	1.93	0.50
22:a:1179:G:H2'	22:a:1180:U:C6	2.47	0.50
32:k:29:LYS:O	32:k:29:LYS:HG2	2.11	0.50
1:A:193:C:H2'	1:A:194:C:C6	2.47	0.50
8:H:106:THR:OG1	8:H:111:MET:HE3	2.12	0.50
22:a:172:A:H2'	22:a:173:A:H8	1.77	0.50
22:a:784:G:H5'	22:a:785:G:OP1	2.11	0.50
22:a:1149:G:H2'	22:a:1150:C:C6	2.47	0.50
55:V:52:G:H3'	55:V:53:5MU:H73	1.94	0.50
1:A:429:U:H3'	4:D:9:LEU:HD12	1.93	0.50
1:A:459:A:H2'	1:A:460:A:H8	1.75	0.50
1:A:1516:2MG:N1	1:A:1519:MA6:OP2	2.44	0.50
13:M:16:VAL:O	13:M:20:THR:HG23	2.12	0.50
17:Q:12:VAL:HG12	17:Q:23:VAL:HG22	1.93	0.50
22:a:102:U:O4	45:x:4:LYS:HG2	2.12	0.50
33:l:41:LEU:HG	33:l:96:ILE:HG13	1.93	0.50
14:N:46:LEU:O	14:N:50:THR:HG23	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:29:PRO:HG2	24:c:34:LEU:HD11	1.93	0.50
30:i:43:GLU:N	30:i:43:GLU:OE2	2.43	0.50
40:s:44:LYS:HG3	40:s:55:VAL:CG2	2.42	0.50
13:M:12:HIS:O	13:M:44:LYS:HD2	2.11	0.49
22:a:191:A:H2'	22:a:192:C:C6	2.46	0.49
22:a:871:U:H2'	22:a:872:U:C6	2.47	0.49
1:A:76:G:H2'	1:A:77:A:C8	2.47	0.49
22:a:1197:G:H2'	22:a:1198:U:H6	1.77	0.49
1:A:1006:G:O6	1:A:1023:U:O2	2.30	0.49
14:N:37:SER:O	14:N:41:ARG:HG3	2.12	0.49
22:a:568:U:H1'	22:a:2030:6MZ:H9C1	1.93	0.49
22:a:1365:A:OP1	44:w:3:ARG:NH2	2.43	0.49
1:A:575:G:O2'	1:A:821:G:OP2	2.25	0.49
2:B:57:LEU:HD13	2:B:217:VAL:HG13	1.94	0.49
22:a:358:U:H2'	22:a:359:G:C8	2.44	0.49
22:a:721:A:H2'	22:a:722:A:C8	2.47	0.49
22:a:1475:G:O2'	22:a:1514:G:O6	2.30	0.49
2:B:70:VAL:HG12	2:B:92:VAL:HB	1.95	0.49
13:M:66:GLU:HB3	13:M:70:ARG:HH12	1.78	0.49
46:y:4:THR:HA	46:y:38:ARG:O	2.13	0.49
1:A:545:C:OP1	4:D:58:LYS:NZ	2.46	0.49
1:A:1010:U:H2'	1:A:1011:C:C6	2.47	0.49
9:I:96:SER:OG	9:I:97:GLU:OE2	2.30	0.49
22:a:881:G:H2'	22:a:882:G:C8	2.46	0.49
24:c:261:LYS:HA	24:c:264:ASP:OD2	2.13	0.49
28:g:42:GLU:OE1	28:g:42:GLU:HA	2.13	0.49
1:A:748:G:H2'	1:A:749:A:H8	1.78	0.49
22:a:320:A:N3	26:e:163:ASN:ND2	2.50	0.49
22:a:1536:C:H1'	22:a:1537:G:N2	2.27	0.49
55:V:16:U:O2'	55:V:17:G:O5'	2.28	0.49
1:A:223:A:H2'	1:A:224:U:C6	2.48	0.49
1:A:412:A:O2'	1:A:413:G:H4'	2.13	0.49
2:B:28:LYS:O	2:B:31:ILE:HG22	2.13	0.49
2:B:88:ASP:OD2	2:B:225:ARG:NH1	2.46	0.49
3:C:28:GLU:N	3:C:28:GLU:OE1	2.46	0.49
10:J:5:ARG:HG2	10:J:77:VAL:HG12	1.95	0.49
22:a:483:A:OP1	41:t:47:LYS:NZ	2.46	0.49
22:a:657:U:H2'	22:a:658:U:C6	2.47	0.49
28:g:2:SER:O	28:g:6:LYS:HG2	2.13	0.49
1:A:85:U:O2	1:A:86:G:N2	2.45	0.49
1:A:996:A:H2'	1:A:997:U:C6	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:17:ARG:HG2	15:O:17:ARG:O	2.13	0.49
20:T:20:HIS:O	20:T:24:ARG:HG2	2.12	0.49
22:a:546:U:H3'	22:a:547:A:C8	2.46	0.49
42:u:7:GLU:N	42:u:7:GLU:OE1	2.46	0.49
1:A:460:A:H2'	1:A:461:A:C8	2.48	0.49
1:A:1226:C:H2'	13:M:102:THR:HG22	1.93	0.49
2:B:86:SER:O	2:B:222:ARG:NH2	2.46	0.49
22:a:184:C:H2'	22:a:185:G:H8	1.76	0.49
22:a:1870:C:O2'	22:a:1871:A:O4'	2.31	0.49
35:n:33:ARG:O	35:n:65:THR:HG23	2.12	0.49
35:n:53:THR:HB	35:n:65:THR:OG1	2.13	0.49
1:A:1029:U:O2'	1:A:1032:G:O6	2.31	0.48
5:E:38:VAL:HG11	5:E:114:VAL:HG22	1.94	0.48
22:a:306:U:H2'	22:a:307:G:O4'	2.12	0.48
30:i:96:ARG:HH22	30:i:98:GLU:CD	2.21	0.48
33:l:75:GLU:HG3	33:l:90:GLU:HG3	1.95	0.48
1:A:1530:G:N7	21:U:46:LYS:HE2	2.27	0.48
13:M:107:ARG:NH2	13:M:111:GLY:O	2.46	0.48
14:N:10:GLU:O	14:N:14:VAL:HG23	2.13	0.48
16:P:38:PHE:CE2	16:P:51:ARG:HG2	2.48	0.48
22:a:1614:A:C6	39:r:87:PRO:HB3	2.48	0.48
22:a:2204:G:H4'	24:c:150:LYS:HG3	1.95	0.48
27:f:162:SER:OG	27:f:165:GLU:HG3	2.14	0.48
1:A:79:G:N1	1:A:80:A:N1	2.61	0.48
1:A:437:U:O2'	4:D:120:HIS:ND1	2.34	0.48
3:C:22:TRP:HB3	3:C:59:ARG:HB2	1.94	0.48
18:R:13:PHE:HD1	18:R:18:VAL:HG21	1.77	0.48
21:U:64:ASN:HA	21:U:67:ARG:NH1	2.29	0.48
22:a:2680:U:O2'	22:a:2681:C:H5'	2.14	0.48
12:L:68:GLY:O	12:L:99:ARG:NH1	2.39	0.48
22:a:2030:6MZ:C2	22:a:2499:C:H5"	2.42	0.48
24:c:21:ASN:HB3	24:c:24:LEU:HG	1.96	0.48
10:J:29:ALA:O	10:J:32:THR:OG1	2.31	0.48
54:Z:22:A:H61	54:Z:47:A:H2'	1.78	0.48
1:A:171:A:H2'	1:A:172:A:C8	2.49	0.48
22:a:2065:C:H2'	22:a:2066:C:C6	2.49	0.48
22:a:2799:A:O2'	22:a:2801:G:OP2	2.29	0.48
28:g:127:THR:HG23	28:g:129:THR:H	1.78	0.48
1:A:56:U:H2'	1:A:57:G:C8	2.49	0.48
1:A:746:A:H2'	1:A:747:A:C8	2.49	0.48
1:A:967:5MC:OP2	1:A:968:A:O2'	2.24	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:THR:O	2:B:23:TRP:HD1	1.97	0.48
9:I:35:LEU:HG	9:I:45:ARG:HG2	1.94	0.48
22:a:586:A:N1	22:a:809:G:O2'	2.45	0.48
28:g:44:LYS:HG3	28:g:45:HIS:H	1.78	0.48
22:a:250:G:H2'	22:a:251:A:C8	2.48	0.48
22:a:1028:A:H2'	22:a:1029:A:C8	2.48	0.48
22:a:2537:U:H2'	22:a:2538:C:H6	1.78	0.48
1:A:470:C:H2'	1:A:471:U:H6	1.79	0.48
27:f:111:ILE:HD11	27:f:114:PHE:HD1	1.79	0.48
46:y:4:THR:HB	46:y:37:GLU:OE2	2.14	0.48
55:V:24:A:H2'	55:V:25:U:C6	2.48	0.48
55:V:27:C:H2'	55:V:28:C:H6	1.78	0.48
1:A:635:A:H2'	1:A:636:U:C6	2.49	0.48
1:A:1120:C:H2'	1:A:1121:U:H6	1.79	0.48
2:B:35:ARG:HB2	2:B:35:ARG:NH1	2.29	0.48
7:G:67:GLU:OE2	7:G:70:ARG:NH1	2.47	0.48
22:a:594:U:H2'	22:a:595:C:C6	2.49	0.48
22:a:1496:A:H2'	22:a:1498:C:C5	2.49	0.48
1:A:390:U:H2'	1:A:391:G:C8	2.49	0.47
8:H:18:GLN:NE2	8:H:70:ALA:HB1	2.29	0.47
15:O:35:GLN:HA	15:O:35:GLN:OE1	2.14	0.47
21:U:10:GLU:OE2	21:U:18:ARG:NH1	2.47	0.47
22:a:2:G:H2'	22:a:3:U:H6	1.78	0.47
22:a:1529:G:H2'	22:a:1530:G:H8	1.78	0.47
22:a:1563:U:H2'	22:a:1564:C:C6	2.49	0.47
22:a:2395:C:H2'	22:a:2396:G:O4'	2.14	0.47
22:a:2514:U:H2'	22:a:2515:C:C6	2.49	0.47
29:h:6:LEU:HD11	29:h:37:VAL:HG13	1.95	0.47
37:p:106:PHE:O	37:p:110:VAL:HG23	2.13	0.47
1:A:477:C:H2'	1:A:478:A:C8	2.49	0.47
10:J:10:LEU:HD22	10:J:98:VAL:HG22	1.97	0.47
22:a:2557:G:H2'	22:a:2558:C:C6	2.48	0.47
26:e:127:GLU:OE1	26:e:127:GLU:N	2.36	0.47
33:l:7:THR:OG1	33:l:9:PHE:O	2.30	0.47
1:A:470:C:H2'	1:A:471:U:C6	2.48	0.47
1:A:1244:G:H2'	1:A:1245:C:C6	2.50	0.47
13:M:71:ARG:O	13:M:75:MET:HG2	2.14	0.47
15:O:26:GLU:OE1	15:O:26:GLU:N	2.45	0.47
22:a:839:U:H2'	22:a:840:C:C6	2.50	0.47
55:V:57:1MA:O2'	55:V:59:U:OP2	2.29	0.47
1:A:946:A:H2'	1:A:947:G:H8	1.74	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:U:H2'	1:A:1041:G:C8	2.47	0.47
1:A:1530:G:H2'	1:A:1531:A:H8	1.79	0.47
22:a:126:A:OP1	49:1:45:SER:OG	2.30	0.47
22:a:703:U:H2'	22:a:704:G:O4'	2.15	0.47
22:a:1486:U:H2'	22:a:1487:U:C6	2.50	0.47
22:a:2038:G:H2'	22:a:2039:U:O4'	2.14	0.47
22:a:2799:A:O2'	22:a:2800:A:H5"	2.15	0.47
26:e:3:LEU:HD13	26:e:120:VAL:HG21	1.96	0.47
37:p:109:LEU:HD11	38:q:40:MET:HE1	1.95	0.47
1:A:864:A:H4'	5:E:90:THR:HG23	1.97	0.47
22:a:1433:A:H2'	22:a:1434:A:O4'	2.14	0.47
22:a:2430:A:N3	22:a:2430:A:H2'	2.29	0.47
30:i:17:VAL:HG23	30:i:137:PRO:HB2	1.96	0.47
1:A:87:C:H2'	1:A:88:U:C6	2.49	0.47
1:A:1441:A:N3	1:A:1441:A:H2'	2.29	0.47
21:U:62:ARG:NE	21:U:66:ARG:HH11	2.08	0.47
22:a:1443:U:H2'	22:a:1444:G:H8	1.80	0.47
22:a:1720:U:H2'	22:a:1721:G:O4'	2.15	0.47
22:a:2074:U:H2'	22:a:2075:U:C6	2.49	0.47
28:g:35:ARG:HB2	28:g:75:MET:HE1	1.95	0.47
28:g:94:TYR:HA	28:g:106:SER:O	2.15	0.47
46:y:16:ARG:HG3	46:y:54:MET:HE1	1.96	0.47
50:2:32:ILE:O	50:2:32:ILE:HG13	2.14	0.47
1:A:258:G:H5'	20:T:82:GLN:HE22	1.80	0.47
1:A:399:G:H2'	1:A:400:C:C6	2.49	0.47
2:B:81:LYS:HB2	2:B:93:ASN:ND2	2.28	0.47
4:D:196:ASN:HB2	4:D:199:LEU:HD12	1.97	0.47
7:G:130:ASN:HA	7:G:135:VAL:HG21	1.95	0.47
9:I:52:LEU:HA	9:I:55:VAL:HG12	1.96	0.47
9:I:67:VAL:HG11	9:I:79:ILE:HD11	1.97	0.47
22:a:367:G:H2'	22:a:368:A:C8	2.49	0.47
22:a:641:U:O2'	22:a:2350:C:OP1	2.33	0.47
22:a:848:C:H2'	22:a:849:A:H8	1.80	0.47
22:a:885:C:H2'	22:a:886:A:O4'	2.14	0.47
22:a:927:A:H2'	22:a:928:A:C8	2.50	0.47
22:a:959:A:H2'	22:a:960:A:C8	2.49	0.47
1:A:45:G:H2'	1:A:46:G:C8	2.50	0.47
22:a:1529:G:H2'	22:a:1530:G:C8	2.50	0.47
22:a:1570:A:H2'	22:a:1571:A:C8	2.49	0.47
22:a:1980:G:O2'	22:a:1982:U:OP2	2.28	0.47
28:g:11:VAL:HB	28:g:48:ASN:HB3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:l:111:GLU:CD	33:l:111:GLU:H	2.22	0.47
55:V:74:C:H2'	55:V:75:A:C8	2.50	0.47
6:F:90:MET:HE2	6:F:90:MET:HB3	1.63	0.47
20:T:18:ARG:NH1	20:T:18:ARG:HG2	2.30	0.47
22:a:84:A:N1	22:a:98:G:O2'	2.44	0.47
22:a:1278:C:H2'	22:a:1279:G:H8	1.80	0.47
31:j:18:ARG:HG3	31:j:18:ARG:HH11	1.80	0.47
42:u:68:LYS:N	42:u:68:LYS:HD2	2.30	0.47
55:V:21:A:H61	55:V:46:A:H2'	1.79	0.47
2:B:43:LEU:HA	2:B:46:THR:HB	1.97	0.47
4:D:48:LEU:HD22	4:D:52:GLY:HA3	1.96	0.47
4:D:105:MET:HA	4:D:173:VAL:HG21	1.96	0.47
13:M:107:ARG:NH2	13:M:113:ARG:HA	2.30	0.47
17:Q:6:ARG:HB2	17:Q:6:ARG:NH1	2.30	0.47
22:a:2455:G:H2'	22:a:2456:C:C6	2.50	0.47
38:q:52:PRO:HG2	38:q:53:PHE:CD2	2.50	0.47
42:u:20:LEU:HD11	42:u:41:GLU:HG2	1.97	0.47
1:A:411:A:H4'	1:A:412:A:O5'	2.15	0.46
1:A:486:U:H2'	1:A:487:A:H8	1.80	0.46
1:A:715:A:H2'	1:A:716:A:C8	2.51	0.46
13:M:24:GLY:O	13:M:29:ARG:NH1	2.47	0.46
22:a:1198:U:H2'	22:a:1199:U:C6	2.50	0.46
22:a:1932:A:H2'	22:a:1933:G:O4'	2.14	0.46
22:a:2014:A:H2'	22:a:2015:A:C8	2.49	0.46
2:B:68:LEU:HB3	2:B:161:LEU:HD12	1.96	0.46
9:I:12:ARG:O	9:I:13:LYS:C	2.59	0.46
22:a:372:G:O2'	22:a:400:G:O6	2.33	0.46
22:a:2071:A:H2'	22:a:2072:C:C6	2.50	0.46
1:A:62:U:OP1	1:A:385:C:O2'	2.33	0.46
9:I:94:LEU:HA	9:I:97:GLU:OE1	2.16	0.46
13:M:85:CYS:HB2	19:S:73:GLU:HG2	1.98	0.46
22:a:1585:C:H2'	22:a:1586:A:O4'	2.15	0.46
22:a:2713:U:O2'	22:a:2715:C:OP2	2.23	0.46
31:j:66:LYS:HB3	31:j:66:LYS:HE2	1.62	0.46
36:o:31:TRP:CE3	36:o:38:LYS:HE3	2.50	0.46
54:Z:22:A:H5'	54:Z:23:G:OP1	2.15	0.46
1:A:224:U:H2'	1:A:225:C:C6	2.51	0.46
1:A:264:C:O2'	17:Q:66:PRO:O	2.32	0.46
1:A:769:G:H4'	1:A:1513:A:H4'	1.97	0.46
1:A:900:A:H2'	1:A:901:A:C8	2.49	0.46
1:A:1280:A:OP1	10:J:9:ARG:NH1	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:597:G:O2'	32:k:11:GLY:O	2.27	0.46
22:a:848:C:H2'	22:a:849:A:C8	2.51	0.46
22:a:948:C:H1'	22:a:984:A:C8	2.50	0.46
22:a:1394:U:H2'	22:a:1395:A:O4'	2.15	0.46
26:e:111:GLU:O	26:e:115:GLN:HG3	2.15	0.46
47:z:52:ARG:CZ	47:z:54:VAL:HG12	2.46	0.46
1:A:59:A:H4'	1:A:60:A:OP2	2.15	0.46
13:M:71:ARG:CZ	27:f:115:ARG:HD3	2.45	0.46
22:a:742:A:H2'	22:a:743:A:C8	2.51	0.46
22:a:1412:U:H2'	22:a:1413:A:C8	2.51	0.46
42:u:77:VAL:HG22	42:u:89:ILE:HG12	1.97	0.46
1:A:35:G:H2'	1:A:36:C:C6	2.51	0.46
1:A:461:A:H2'	1:A:462:G:H8	1.79	0.46
6:F:4:TYR:CD1	6:F:71:ILE:HG13	2.51	0.46
11:K:81:ASN:HB3	11:K:106:ARG:NH1	2.31	0.46
22:a:1412:U:H2'	22:a:1413:A:H8	1.81	0.46
31:j:48:PRO:HB2	31:j:49:ARG:HD3	1.98	0.46
46:y:6:LYS:HB2	46:y:58:GLU:HB2	1.98	0.46
1:A:736:C:H2'	1:A:737:C:C6	2.50	0.46
1:A:923:A:O2'	1:A:1399:C:OP2	2.28	0.46
1:A:1326:U:H2'	1:A:1327:C:C6	2.51	0.46
3:C:46:GLU:HG2	3:C:87:LEU:HD21	1.98	0.46
4:D:100:ASN:O	4:D:104:ARG:HG2	2.16	0.46
22:a:2649:C:H2'	22:a:2650:U:H6	1.80	0.46
47:z:52:ARG:NH1	47:z:54:VAL:HG12	2.30	0.46
1:A:945:G:C2	1:A:946:A:C8	3.04	0.46
52:4:26:SER:OG	52:4:28:VAL:HG12	2.16	0.46
10:J:88:MET:HE2	10:J:88:MET:N	2.30	0.46
22:a:547:A:H4'	22:a:548:G:C5'	2.45	0.46
22:a:1386:C:H2'	22:a:1387:A:C8	2.51	0.46
28:g:24:ILE:O	28:g:34:THR:OG1	2.30	0.46
29:h:3:VAL:HG13	29:h:36:ALA:HB1	1.98	0.46
48:0:40:ASP:OD1	48:0:42:VAL:HG22	2.16	0.46
1:A:580:C:H2'	1:A:581:G:O4'	2.16	0.46
3:C:168:TYR:OH	5:E:55:GLU:OE1	2.29	0.46
4:D:69:GLU:OE1	4:D:204:TYR:OH	2.33	0.46
10:J:83:THR:O	10:J:87:LEU:HG	2.16	0.46
20:T:18:ARG:HG2	20:T:18:ARG:HH11	1.81	0.46
22:a:146:A:H2'	22:a:147:C:C6	2.51	0.46
22:a:903:C:H2'	22:a:904:G:H8	1.80	0.46
22:a:1728:C:H2'	22:a:1729:U:H5"	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2591:C:H2'	22:a:2592:G:C8	2.51	0.46
22:a:2804:U:H2'	22:a:2805:C:C6	2.50	0.46
25:d:4:LEU:HD12	25:d:101:PHE:HE2	1.81	0.46
26:e:12:LEU:HD23	26:e:12:LEU:H	1.80	0.46
27:f:131:GLY:HA2	27:f:153:ASP:HA	1.98	0.46
7:G:26:PHE:HA	7:G:101:MET:HE3	1.97	0.45
22:a:1315:C:O2'	22:a:1392:A:N3	2.46	0.45
55:V:17:G:HO2'	55:V:56:G:H22	1.57	0.45
1:A:129:A:H1'	1:A:130:A:C8	2.50	0.45
7:G:129:GLU:HB3	7:G:131:LYS:HZ3	1.77	0.45
13:M:59:GLU:OE2	13:M:62:LYS:NZ	2.49	0.45
22:a:207:A:H2'	22:a:208:C:O4'	2.17	0.45
22:a:1744:A:H3'	22:a:1745:A:H8	1.81	0.45
22:a:2025:C:H2'	22:a:2026:U:C6	2.51	0.45
28:g:46:ALA:O	28:g:49:THR:HG22	2.16	0.45
34:m:28:LEU:HD23	34:m:48:VAL:HG21	1.98	0.45
55:V:52:G:H2'	55:V:53:5MU:C6	2.51	0.45
1:A:215:C:H2'	1:A:216:U:C6	2.52	0.45
1:A:1236:A:H2'	1:A:1237:C:C6	2.51	0.45
4:D:198:HIS:O	4:D:202:GLU:HG3	2.17	0.45
5:E:12:GLN:HG3	5:E:117:VAL:HG12	1.98	0.45
8:H:79:SER:HB2	8:H:85:ILE:H	1.80	0.45
22:a:279:A:OP2	22:a:361:G:N2	2.49	0.45
22:a:645:C:O2'	22:a:646:U:H5'	2.15	0.45
22:a:1874:C:H2'	22:a:1875:G:O4'	2.16	0.45
22:a:2615:U:C2	47:z:4:GLN:HA	2.50	0.45
23:b:2:G:H2'	23:b:3:C:C6	2.52	0.45
1:A:72:A:H2'	1:A:72:A:N3	2.32	0.45
1:A:1496:C:H2'	1:A:1497:G:O4'	2.17	0.45
17:Q:77:ARG:NH1	17:Q:79:VAL:HG22	2.32	0.45
22:a:2469:A:H2'	22:a:2470:G:O4'	2.17	0.45
24:c:145:GLU:HG2	24:c:151:GLY:C	2.41	0.45
1:A:87:C:H2'	1:A:88:U:C5	2.51	0.45
1:A:384:G:H2'	1:A:385:C:C6	2.52	0.45
13:M:104:THR:HG22	13:M:105:ASN:H	1.82	0.45
20:T:44:LYS:NZ	20:T:87:ALA:HA	2.32	0.45
22:a:1889:A:H2'	22:a:1890:A:C8	2.52	0.45
22:a:2803:G:H2'	22:a:2804:U:C6	2.52	0.45
32:k:108:ALA:HB3	32:k:125:LEU:HD22	1.97	0.45
1:A:82:G:N1	1:A:89:U:C2	2.83	0.45
1:A:750:C:O2	15:O:23:GLY:HA3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1326:U:H2'	1:A:1327:C:H6	1.82	0.45
12:L:7:LEU:HD23	12:L:7:LEU:HA	1.79	0.45
22:a:277:G:H4'	22:a:278:A:C4	2.52	0.45
22:a:620:G:N3	22:a:620:G:H5'	2.32	0.45
22:a:2419:U:H4'	48:0:22:THR:HG21	1.99	0.45
27:f:121:SER:HB2	27:f:128:TYR:CE1	2.52	0.45
1:A:511:C:O3'	4:D:44:ARG:NH2	2.49	0.45
1:A:1060:U:OP1	14:N:85:ARG:NH2	2.39	0.45
10:J:6:ILE:HG12	10:J:76:ILE:HB	1.98	0.45
22:a:184:C:H2'	22:a:185:G:C8	2.52	0.45
22:a:2649:C:H2'	22:a:2650:U:C6	2.51	0.45
24:c:123:ALA:HB3	24:c:125:LYS:HE2	1.98	0.45
45:x:10:SER:H	45:x:13:GLU:CD	2.24	0.45
48:0:25:LYS:NZ	48:0:51:GLU:OE2	2.44	0.45
25:d:108:ASP:OD2	25:d:173:GLN:HA	2.17	0.45
1:A:77:A:H2'	1:A:78:A:H8	1.82	0.45
1:A:310:G:H5"	16:P:31:ARG:HB2	1.98	0.45
21:U:59:LYS:HB3	21:U:59:LYS:HE2	1.85	0.45
22:a:1292:G:H2'	22:a:1293:C:C6	2.52	0.45
22:a:2740:A:H2'	22:a:2741:A:C8	2.51	0.45
26:e:191:ASP:OD1	26:e:192:ALA:N	2.50	0.45
28:g:107:LEU:O	28:g:152:ARG:NH1	2.50	0.45
41:t:86:ARG:HD2	41:t:88:GLU:OE2	2.17	0.45
42:u:53:LYS:HB3	42:u:55:GLU:OE1	2.16	0.45
1:A:371:A:H2'	1:A:372:C:O4'	2.16	0.44
1:A:398:U:H2'	1:A:399:G:C8	2.51	0.44
1:A:859:G:H2'	1:A:860:A:C8	2.52	0.44
1:A:1318:A:H5"	19:S:3:ARG:NH2	2.32	0.44
10:J:76:ILE:HG22	10:J:79:PRO:HB3	1.99	0.44
12:L:33:VAL:HG22	12:L:79:VAL:HG22	1.99	0.44
55:V:10:G:O2'	55:V:11:U:OP1	2.31	0.44
7:G:113:ASP:HB2	7:G:119:ARG:HG3	2.00	0.44
9:I:24:GLY:HA3	9:I:62:ASP:CG	2.42	0.44
10:J:7:ARG:HD3	10:J:75:ASP:OD1	2.17	0.44
17:Q:81:LYS:HE2	17:Q:81:LYS:HB2	1.79	0.44
20:T:36:TYR:O	20:T:39:ILE:N	2.51	0.44
22:a:5:A:H2'	22:a:6:A:C8	2.52	0.44
22:a:494:G:H4'	39:r:6:LYS:HB2	1.99	0.44
24:c:259:SER:O	24:c:259:SER:OG	2.30	0.44
27:f:58:ALA:HB2	27:f:65:PRO:HD3	1.99	0.44
35:n:2:ASP:OD1	35:n:3:LYS:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:G:H2'	1:A:746:A:C8	2.53	0.44
1:A:748:G:H2'	1:A:749:A:C8	2.53	0.44
2:B:115:LYS:O	2:B:118:GLU:HG3	2.17	0.44
9:I:97:GLU:HA	9:I:100:LYS:HE2	1.99	0.44
19:S:13:LEU:O	19:S:17:LYS:HG2	2.17	0.44
22:a:1028:A:N6	22:a:1125:G:H2'	2.32	0.44
22:a:1484:U:H2'	22:a:1485:U:H6	1.83	0.44
22:a:1485:U:H2'	22:a:1486:U:H6	1.82	0.44
22:a:1526:C:H2'	22:a:1527:G:O4'	2.17	0.44
35:n:115:LEU:HD12	35:n:115:LEU:HA	1.79	0.44
36:o:5:ILE:O	36:o:9:GLU:HG3	2.17	0.44
41:t:85:PHE:CE1	41:t:94:ARG:HG2	2.52	0.44
43:v:50:ASN:HB2	43:v:82:ILE:HB	1.98	0.44
55:V:4:U:C2	55:V:5:C:C5	3.06	0.44
1:A:86:G:H21	1:A:87:C:N4	2.15	0.44
4:D:159:LEU:O	4:D:163:GLU:HG2	2.17	0.44
22:a:150:U:H2'	22:a:151:C:C6	2.53	0.44
22:a:1476:U:H2'	22:a:1477:A:H8	1.82	0.44
25:d:4:LEU:HD12	25:d:101:PHE:CE2	2.52	0.44
52:4:59:ARG:HH22	52:4:63:ARG:NH2	2.14	0.44
1:A:404:G:N7	4:D:2:ALA:HB3	2.33	0.44
1:A:868:C:H2'	1:A:869:G:O4'	2.16	0.44
22:a:1586:A:H2'	22:a:1587:G:O4'	2.18	0.44
27:f:176:PRO:HB3	52:4:44:PHE:CE1	2.53	0.44
31:j:38:ILE:HD11	31:j:112:PHE:HZ	1.81	0.44
1:A:140:U:H2'	1:A:141:G:O4'	2.18	0.44
1:A:1314:C:H2'	1:A:1315:U:H6	1.83	0.44
4:D:156:LYS:O	4:D:160:GLU:OE1	2.36	0.44
7:G:15:ASP:OD2	7:G:19:GLY:N	2.51	0.44
22:a:277:G:OP2	22:a:277:G:H8	2.00	0.44
22:a:2783:U:H2'	22:a:2784:U:C6	2.53	0.44
22:a:2820:A:N3	22:a:2820:A:H2'	2.32	0.44
28:g:24:ILE:HG12	28:g:72:LEU:HD11	2.00	0.44
28:g:176:LYS:HD2	28:g:176:LYS:HA	1.70	0.44
38:q:37:GLU:OE2	38:q:53:PHE:CZ	2.71	0.44
52:4:38:SER:HA	52:4:44:PHE:CD2	2.53	0.44
10:J:87:LEU:HB2	10:J:88:MET:HE2	1.99	0.44
21:U:64:ASN:O	21:U:68:THR:OG1	2.22	0.44
22:a:1883:U:H2'	22:a:1884:G:O4'	2.18	0.44
1:A:1398:A:H5'	1:A:1401:G:H4'	2.00	0.44
10:J:22:THR:HA	10:J:25:ILE:HG22	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:60:LEU:HA	21:U:63:GLU:OE1	2.17	0.44
22:a:2895:G:H2'	22:a:2896:C:C6	2.53	0.44
1:A:642:A:C5	8:H:107:SER:HA	2.52	0.43
9:I:84:THR:HG23	9:I:98:LEU:HD13	1.99	0.43
16:P:25:ARG:HE	16:P:25:ARG:HB2	1.62	0.43
22:a:754:U:H2'	22:a:755:U:C6	2.53	0.43
22:a:1499:C:C2	22:a:1500:G:C8	3.06	0.43
22:a:1930:G:O2'	22:a:1968:G:O6	2.30	0.43
24:c:23:GLU:HG2	24:c:81:LEU:HD12	1.98	0.43
1:A:1135:U:H2'	1:A:1137:C:C5	2.52	0.43
3:C:77:ILE:HD11	3:C:103:ILE:HG13	1.98	0.43
10:J:26:VAL:HG23	10:J:36:VAL:HG21	1.99	0.43
11:K:52:PHE:O	11:K:53:ARG:HD2	2.18	0.43
22:a:788:A:OP1	22:a:791:C:N4	2.37	0.43
22:a:1179:G:H2'	22:a:1180:U:H6	1.83	0.43
22:a:1428:C:C5	22:a:1569:A:H5"	2.53	0.43
26:e:168:ASP:OD1	26:e:170:ARG:NE	2.51	0.43
28:g:98:VAL:HG23	28:g:125:CYS:SG	2.58	0.43
1:A:465:A:H2'	1:A:466:A:C8	2.53	0.43
1:A:1318:A:H5"	19:S:3:ARG:HH22	1.83	0.43
1:A:1456:A:H2'	1:A:1457:G:O4'	2.18	0.43
3:C:186:THR:HG22	3:C:199:LYS:HG2	1.99	0.43
22:a:640:C:H2'	22:a:641:U:C6	2.54	0.43
22:a:1050:A:C2	22:a:2751:G:C4	3.06	0.43
22:a:1177:G:H2'	22:a:1178:C:C6	2.53	0.43
22:a:1432:G:H2'	22:a:1433:A:C8	2.53	0.43
24:c:35:GLU:OE2	24:c:64:ILE:HD11	2.18	0.43
27:f:43:ALA:HA	27:f:46:ASP:O	2.18	0.43
39:r:3:THR:OG1	39:r:62:ASP:OD2	2.34	0.43
52:4:28:VAL:HG21	52:4:32:LEU:HD11	2.00	0.43
1:A:524:G:H2'	1:A:525:C:C6	2.53	0.43
14:N:73:PHE:CZ	14:N:78:GLY:HA2	2.53	0.43
15:O:64:ARG:HD3	15:O:64:ARG:O	2.19	0.43
22:a:1505:A:H2'	22:a:1506:U:O4'	2.18	0.43
22:a:1527:G:N1	22:a:1544:A:OP2	2.41	0.43
22:a:2803:G:H2'	22:a:2804:U:H6	1.83	0.43
28:g:60:ASP:O	28:g:62:TRP:N	2.46	0.43
37:p:111:GLU:OE1	37:p:111:GLU:HA	2.19	0.43
40:s:74:ILE:O	40:s:74:ILE:HG13	2.19	0.43
1:A:1414:U:H2'	1:A:1415:G:H8	1.82	0.43
1:A:1435:G:H2'	1:A:1436:U:C6	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:LYS:HG2	2:B:63:ARG:HH12	1.83	0.43
4:D:9:LEU:HD13	4:D:32:CYS:HB3	1.99	0.43
11:K:97:ILE:HG22	21:U:12:PHE:HZ	1.83	0.43
20:T:79:LEU:HA	20:T:79:LEU:HD23	1.63	0.43
22:a:282:A:H2'	22:a:283:G:C8	2.53	0.43
22:a:1567:G:H2'	24:c:85:PRO:HG3	2.00	0.43
22:a:2394:C:H5"	32:k:63:LYS:HE2	2.00	0.43
23:b:29:A:H2'	23:b:30:C:C6	2.53	0.43
45:x:19:LEU:O	45:x:23:ARG:HG3	2.18	0.43
46:y:11:ARG:HG2	46:y:11:ARG:HH21	1.82	0.43
54:Z:22:A:N6	54:Z:47:A:H2'	2.34	0.43
1:A:79:G:C6	1:A:80:A:C6	3.06	0.43
17:Q:7:THR:O	17:Q:8:LEU:HD23	2.18	0.43
22:a:135:U:H2'	22:a:136:G:O4'	2.18	0.43
22:a:566:U:OP1	32:k:29:LYS:HE2	2.19	0.43
22:a:2329:U:H2'	22:a:2330:G:C8	2.53	0.43
30:i:114:LEU:HG	30:i:118:MET:HE3	2.01	0.43
41:t:99:ASN:O	41:t:101:GLU:N	2.52	0.43
54:Z:62:C:H2'	54:Z:63:C:H6	1.84	0.43
1:A:269:C:H2'	1:A:270:A:H8	1.81	0.43
1:A:966:2MG:HM21	9:I:129:LYS:HD2	2.00	0.43
1:A:1035:A:HO2'	1:A:1036:A:H2	1.65	0.43
1:A:1039:G:H2'	1:A:1040:U:C6	2.54	0.43
4:D:188:ARG:HA	4:D:188:ARG:HD2	1.78	0.43
5:E:14:LYS:HD2	5:E:113:ALA:HB1	2.00	0.43
22:a:1790:C:H2'	22:a:1791:A:C5	2.53	0.43
22:a:2627:G:O2'	22:a:2781:A:N1	2.48	0.43
22:a:2804:U:H2'	22:a:2805:C:H6	1.83	0.43
22:a:2820:A:O2'	22:a:2821:A:OP1	2.35	0.43
22:a:2847:U:H2'	22:a:2848:G:O4'	2.19	0.43
31:j:7:MET:HE3	31:j:7:MET:HB3	1.75	0.43
52:4:56:ARG:NH1	52:4:59:ARG:HD3	2.34	0.43
1:A:182:A:C4	1:A:184:G:C8	3.07	0.43
1:A:236:A:H2'	1:A:237:G:C8	2.54	0.43
1:A:592:G:H2'	1:A:593:U:C6	2.53	0.43
1:A:604:G:H2'	1:A:605:U:O4'	2.19	0.43
4:D:170:TRP:CD2	4:D:186:PRO:HB3	2.54	0.43
6:F:96:VAL:HG12	6:F:96:VAL:O	2.18	0.43
22:a:810:U:C4	32:k:29:LYS:O	2.72	0.43
22:a:837:C:H42	22:a:941:A:H62	1.66	0.43
22:a:2636:C:H2'	22:a:2637:U:C6	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2849:U:H4'	22:a:2868:A:C2	2.53	0.43
55:V:27:C:H2'	55:V:28:C:C6	2.54	0.43
9:I:84:THR:HG22	9:I:88:MET:HE3	2.00	0.43
22:a:857:G:H2'	22:a:858:G:O4'	2.19	0.43
22:a:864:G:O2'	22:a:865:C:H5'	2.18	0.43
22:a:1703:G:H2'	22:a:1704:C:C6	2.54	0.43
22:a:2698:U:H2'	22:a:2699:C:H6	1.84	0.43
40:s:25:GLU:HB2	40:s:26:LYS:HD2	2.01	0.43
1:A:2:A:O2'	1:A:3:A:C8	2.72	0.43
1:A:607:A:H2'	1:A:608:A:C8	2.54	0.43
1:A:1469:C:H2'	1:A:1470:U:O4'	2.18	0.43
10:J:7:ARG:HG3	10:J:7:ARG:HH11	1.83	0.43
12:L:79:VAL:O	12:L:103:ASP:HB2	2.19	0.43
18:R:68:LEU:HD23	18:R:68:LEU:HA	1.88	0.43
19:S:30:PRO:HB3	19:S:48:THR:HG23	2.00	0.43
22:a:1048:A:N7	22:a:1111:A:C6	2.87	0.43
22:a:2850:A:N7	22:a:2868:A:O2'	2.47	0.43
27:f:8:TYR:HA	27:f:12:VAL:HB	2.01	0.43
1:A:270:A:H2'	1:A:271:C:C6	2.54	0.42
1:A:1123:U:O2'	1:A:1124:G:H5'	2.19	0.42
3:C:22:TRP:CG	3:C:59:ARG:HD2	2.54	0.42
15:O:78:TYR:O	15:O:82:ILE:HG23	2.18	0.42
22:a:1349:C:C2	22:a:1350:C:C5	3.07	0.42
22:a:1754:A:C8	36:o:94:LYS:HE2	2.54	0.42
22:a:1796:U:H2'	22:a:1797:G:H8	1.84	0.42
1:A:131:A:H2'	1:A:132:C:H6	1.83	0.42
1:A:389:A:H3'	1:A:390:U:H6	1.84	0.42
1:A:553:A:H5"	12:L:21:VAL:HG21	2.01	0.42
1:A:1147:C:O2'	9:I:7:TYR:OH	2.28	0.42
4:D:9:LEU:O	4:D:13:ARG:HG3	2.20	0.42
7:G:16:PRO:HD2	7:G:44:TYR:OH	2.18	0.42
7:G:80:VAL:HG23	7:G:81:GLY:H	1.83	0.42
10:J:42:LEU:HB2	10:J:71:LEU:HB2	2.01	0.42
13:M:31:LYS:NZ	13:M:41:GLU:OE1	2.50	0.42
19:S:80:TYR:CZ	19:S:82:GLY:HA2	2.54	0.42
22:a:577:G:H2'	22:a:578:G:C8	2.55	0.42
22:a:1047:G:O2'	22:a:1110:G:N1	2.49	0.42
22:a:1485:U:H2'	22:a:1486:U:C6	2.54	0.42
27:f:140:GLU:OE1	27:f:140:GLU:N	2.49	0.42
1:A:244:U:O4	1:A:906:A:H1'	2.19	0.42
1:A:1009:U:H3	1:A:1020:G:H1	1.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1410:A:H2'	1:A:1411:C:C6	2.55	0.42
13:M:44:LYS:HB2	13:M:47:GLU:OE1	2.18	0.42
22:a:479:A:N3	22:a:481:G:H5"	2.33	0.42
22:a:1594:U:H2'	22:a:1595:C:C6	2.55	0.42
22:a:1684:G:H2'	22:a:1685:C:C6	2.54	0.42
30:i:99:ARG:HA	30:i:99:ARG:HD2	1.76	0.42
40:s:64:LYS:HD2	40:s:64:LYS:N	2.33	0.42
43:v:32:LEU:HA	43:v:64:ASP:OD1	2.19	0.42
55:V:16:U:H6	55:V:16:U:H2'	1.66	0.42
1:A:160:A:H2'	1:A:161:A:O4'	2.20	0.42
1:A:382:A:H2'	1:A:383:A:H8	1.83	0.42
1:A:1244:G:H2'	1:A:1245:C:H6	1.83	0.42
3:C:110:GLU:HG2	3:C:140:ASN:HB3	2.02	0.42
10:J:11:LYS:HG2	10:J:71:LEU:HD23	2.01	0.42
15:O:10:LYS:O	15:O:14:GLU:HG2	2.19	0.42
22:a:1683:U:H2'	22:a:1684:G:C8	2.54	0.42
22:a:1794:A:H2'	22:a:1795:C:H6	1.83	0.42
22:a:2345:G:N3	22:a:2381:A:H2'	2.34	0.42
26:e:127:GLU:O	26:e:156:ASN:ND2	2.52	0.42
1:A:88:U:H2'	1:A:89:U:C6	2.54	0.42
1:A:1004:A:H2'	1:A:1005:A:O4'	2.19	0.42
9:I:59:GLU:N	9:I:59:GLU:OE1	2.53	0.42
22:a:1534:U:O3'	22:a:1535:A:H2'	2.20	0.42
22:a:2308:G:H2'	22:a:2308:G:N3	2.34	0.42
22:a:2644:G:O2'	22:a:2645:G:H5'	2.19	0.42
27:f:40:VAL:HG13	27:f:40:VAL:O	2.19	0.42
33:l:118:LYS:HE3	33:l:118:LYS:HB3	1.70	0.42
48:0:17:THR:HB	48:0:42:VAL:HG21	2.02	0.42
54:Z:21:H2U:H2'	54:Z:21:H2U:H61	1.66	0.42
1:A:235:C:H2'	1:A:236:A:C8	2.55	0.42
1:A:860:A:H2'	1:A:861:G:O4'	2.19	0.42
1:A:985:C:H2'	1:A:986:U:C6	2.54	0.42
22:a:1199:U:H2'	22:a:1200:C:C6	2.54	0.42
22:a:1796:U:H2'	22:a:1797:G:C8	2.55	0.42
22:a:1880:U:H2'	22:a:1881:C:C6	2.55	0.42
22:a:2020:A:H5'	47:z:9:THR:HG21	2.02	0.42
22:a:2065:C:H2'	22:a:2066:C:H6	1.84	0.42
22:a:2545:G:H2'	22:a:2546:U:O4'	2.19	0.42
25:d:48:ILE:HG23	25:d:84:LEU:HD11	2.00	0.42
34:m:117:ASP:OD1	34:m:117:ASP:C	2.63	0.42
42:u:73:LYS:HB3	42:u:73:LYS:HE3	1.79	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:U:O2'	1:A:379:C:O2	2.37	0.42
1:A:663:A:H5'	1:A:836:G:OP1	2.19	0.42
1:A:1157:A:C2	1:A:1181:G:C4	3.08	0.42
6:F:88:MET:HE3	6:F:90:MET:SD	2.60	0.42
7:G:6:VAL:HG12	7:G:6:VAL:O	2.20	0.42
20:T:36:TYR:O	20:T:37:ALA:C	2.63	0.42
27:f:111:ILE:HG22	27:f:137:ILE:HG21	2.01	0.42
1:A:142:G:H3'	1:A:143:A:H8	1.84	0.42
1:A:404:G:OP2	4:D:115:ARG:NH2	2.39	0.42
1:A:911:U:H2'	1:A:912:C:C6	2.54	0.42
3:C:76:VAL:O	3:C:83:ASP:HB3	2.20	0.42
5:E:89:HIS:O	5:E:90:THR:C	2.63	0.42
13:M:54:ASP:OD1	13:M:57:ARG:NH1	2.53	0.42
22:a:170:U:H2'	22:a:171:U:C6	2.55	0.42
22:a:263:G:H2'	22:a:264:C:O4'	2.20	0.42
22:a:636:G:N7	32:k:109:LYS:HD3	2.35	0.42
22:a:1774:C:O2	22:a:1774:C:H2'	2.20	0.42
22:a:2392:A:OP2	50:2:31:HIS:NE2	2.40	0.42
28:g:44:LYS:HB3	28:g:51:THR:H	1.85	0.42
34:m:72:ASP:OD2	34:m:75:ILE:HB	2.20	0.42
1:A:8:A:H4'	1:A:9:G:OP1	2.20	0.42
1:A:410:G:H2'	1:A:429:U:C5	2.55	0.42
1:A:475:C:H2'	1:A:476:U:H6	1.85	0.42
1:A:1477:U:H2'	1:A:1478:U:C6	2.54	0.42
2:B:207:ILE:O	2:B:211:THR:HG23	2.20	0.42
10:J:59:LYS:HE2	10:J:62:ARG:NH2	2.35	0.42
22:a:967:U:H2'	22:a:968:C:C6	2.55	0.42
22:a:1197:G:H2'	22:a:1198:U:C6	2.53	0.42
24:c:199:GLU:CD	24:c:199:GLU:H	2.28	0.42
6:F:69:GLU:O	6:F:73:GLU:OE1	2.36	0.42
14:N:31:ILE:HD12	14:N:45:VAL:HG23	2.02	0.42
22:a:157:C:H2'	22:a:158:U:O4'	2.20	0.42
22:a:2020:A:H5'	47:z:9:THR:CG2	2.50	0.42
27:f:105:THR:HA	52:4:38:SER:HB3	2.02	0.42
28:g:33:LEU:C	28:g:33:LEU:HD12	2.45	0.42
40:s:21:SER:O	40:s:25:GLU:HG2	2.20	0.42
1:A:1412:C:H2'	1:A:1413:A:C8	2.54	0.41
2:B:171:ILE:O	2:B:175:GLU:HG3	2.20	0.41
6:F:67:PRO:O	6:F:70:VAL:HG12	2.19	0.41
22:a:64:A:H2'	22:a:65:U:H6	1.84	0.41
22:a:352:A:H2'	22:a:353:C:O4'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:632:A:H2'	22:a:633:A:C8	2.55	0.41
22:a:760:G:H2'	22:a:761:A:O4'	2.20	0.41
23:b:48:U:H2'	23:b:49:C:C6	2.54	0.41
45:x:38:GLN:H	45:x:38:GLN:HG2	1.61	0.41
49:1:25:LYS:HB3	49:1:25:LYS:HE3	1.86	0.41
55:V:25:U:H2'	55:V:26:C:H6	1.84	0.41
1:A:33:A:H2'	1:A:34:C:C6	2.55	0.41
1:A:109:A:H5'	1:A:110:C:C5	2.54	0.41
1:A:193:C:H2'	1:A:194:C:H6	1.85	0.41
1:A:410:G:OP1	4:D:26:ARG:NH1	2.46	0.41
2:B:115:LYS:O	2:B:119:THR:HG23	2.20	0.41
13:M:37:ALA:HB2	13:M:59:GLU:HG3	2.01	0.41
22:a:1138:G:N3	30:i:108:MET:HE2	2.35	0.41
22:a:1357:C:H2'	22:a:1358:G:O4'	2.21	0.41
22:a:1484:U:H2'	22:a:1485:U:C6	2.55	0.41
22:a:1486:U:H2'	22:a:1487:U:H6	1.83	0.41
22:a:1548:A:H2'	22:a:1549:A:H8	1.82	0.41
22:a:2300:C:H2'	22:a:2301:C:H6	1.85	0.41
27:f:115:ARG:HD2	52:4:48:GLN:NE2	2.36	0.41
22:a:362:A:C4	22:a:363:G:C8	3.09	0.41
22:a:2809:A:H2'	22:a:2810:A:C8	2.55	0.41
33:l:20:LEU:HD23	33:l:98:PRO:HG2	2.02	0.41
49:1:41:ARG:HH21	49:1:41:ARG:HG3	1.86	0.41
1:A:495:A:C2	1:A:496:A:C6	3.08	0.41
1:A:1118:U:H2'	1:A:1119:C:H6	1.85	0.41
1:A:1120:C:H2'	1:A:1121:U:C6	2.55	0.41
1:A:1219:A:H2'	1:A:1220:G:C8	2.56	0.41
6:F:4:TYR:HD2	6:F:90:MET:O	2.03	0.41
8:H:5:ASP:HB2	8:H:81:PRO:HG2	2.02	0.41
14:N:27:LEU:HA	14:N:27:LEU:HD23	1.79	0.41
22:a:1108:U:C2	22:a:1109:C:C5	3.09	0.41
22:a:2246:G:H2'	22:a:2247:A:C8	2.55	0.41
22:a:2470:G:OP1	33:l:55:ARG:NH1	2.52	0.41
22:a:2515:C:H2'	22:a:2516:A:H8	1.85	0.41
53:X:45:C:O2	55:V:34:56B:N2	2.54	0.41
2:B:27:MET:HE2	2:B:193:PRO:HD3	2.02	0.41
2:B:49:MET:HA	2:B:52:GLU:OE1	2.20	0.41
3:C:153:VAL:HG12	3:C:198:VAL:HG22	2.03	0.41
6:F:37:HIS:O	6:F:97:THR:HG22	2.20	0.41
22:a:1182:G:H2'	22:a:1183:U:O4'	2.20	0.41
22:a:1348:C:C5	22:a:1349:C:C5	3.09	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1419:A:O2'	22:a:1421:G:N7	2.43	0.41
23:b:43:C:H5"	52:4:1:MET:SD	2.60	0.41
27:f:36:LEU:HD22	27:f:154:ILE:HG12	2.01	0.41
1:A:181:A:N6	1:A:195:A:C8	2.89	0.41
1:A:736:C:H2'	1:A:737:C:H6	1.84	0.41
4:D:11:LEU:HB3	4:D:63:ARG:HG2	2.02	0.41
6:F:4:TYR:CE1	6:F:71:ILE:HG13	2.55	0.41
15:O:7:ALA:O	15:O:11:ILE:HG12	2.20	0.41
22:a:580:U:H2'	22:a:581:C:C6	2.56	0.41
22:a:720:U:H2'	22:a:721:A:C8	2.55	0.41
22:a:2700:A:H2'	22:a:2701:U:C6	2.56	0.41
22:a:2766:A:N3	22:a:2766:A:H2'	2.35	0.41
24:c:121:ASP:OD1	24:c:121:ASP:N	2.47	0.41
34:m:71:ARG:HA	34:m:71:ARG:HD2	1.77	0.41
52:4:10:GLU:OE1	52:4:10:GLU:N	2.54	0.41
1:A:255:G:H2'	1:A:256:U:C6	2.55	0.41
1:A:1363:A:O2'	1:A:1365:G:N7	2.38	0.41
22:a:1995:U:H3'	22:a:1996:C:H2'	2.02	0.41
22:a:2467:C:H2'	22:a:2468:A:O4'	2.20	0.41
28:g:103:ILE:HG22	28:g:105:LEU:HD22	2.03	0.41
36:o:6:LYS:O	36:o:10:GLN:HG2	2.21	0.41
1:A:320:A:H2'	1:A:321:A:O4'	2.21	0.41
1:A:1027:C:H3'	1:A:1028:C:C5	2.54	0.41
1:A:1042:A:O2'	1:A:1043:G:H5'	2.21	0.41
1:A:1169:A:H2'	1:A:1170:A:C8	2.56	0.41
1:A:1465:A:H2'	1:A:1466:C:C6	2.55	0.41
2:B:207:ILE:HD12	2:B:207:ILE:HA	1.93	0.41
3:C:57:ILE:HG12	3:C:66:VAL:HG12	2.03	0.41
14:N:42:TRP:O	14:N:46:LEU:HD23	2.20	0.41
22:a:613:A:H2'	22:a:614:A:O4'	2.21	0.41
22:a:723:C:H2'	22:a:724:U:O4'	2.21	0.41
22:a:1338:G:O2'	22:a:1393:A:N1	2.46	0.41
22:a:1444:G:C4	22:a:1445:G:C8	3.08	0.41
22:a:1558:C:O4'	22:a:1560:G:C8	2.73	0.41
28:g:42:GLU:OE2	28:g:55:ARG:NH1	2.54	0.41
28:g:74:SER:HA	28:g:77:ILE:HG22	2.03	0.41
1:A:1033:G:HO2'	1:A:1034:G:H8	1.61	0.41
1:A:1043:G:O2'	1:A:1044:A:H5"	2.21	0.41
1:A:1121:U:H2'	1:A:1122:U:C6	2.56	0.41
1:A:1121:U:H2'	1:A:1122:U:H6	1.86	0.41
2:B:130:THR:C	2:B:132:LYS:H	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:LEU:HA	3:C:12:LEU:HD23	1.88	0.41
4:D:117:LEU:HD23	4:D:117:LEU:HA	1.92	0.41
17:Q:25:ILE:HD12	17:Q:25:ILE:N	2.35	0.41
22:a:219:A:N3	22:a:234:U:O2'	2.44	0.41
22:a:1020:A:C2	22:a:1141:U:C2	3.07	0.41
22:a:1370:C:H2'	22:a:1371:G:O4'	2.21	0.41
22:a:2092:U:OP2	29:h:27:ARG:NH2	2.53	0.41
24:c:76:ALA:HB2	24:c:96:TYR:CD2	2.56	0.41
28:g:60:ASP:OD1	28:g:60:ASP:N	2.53	0.41
1:A:513:C:H2'	1:A:514:C:C6	2.56	0.41
1:A:1029:U:H4'	1:A:1030:U:C5	2.56	0.41
1:A:1031:C:HO2'	1:A:1032:G:N2	2.19	0.41
10:J:22:THR:O	10:J:26:VAL:HG12	2.21	0.41
14:N:41:ARG:NH2	19:S:6:LYS:O	2.53	0.41
16:P:67:ILE:CG2	16:P:71:VAL:HG13	2.51	0.41
17:Q:76:VAL:HG12	17:Q:77:ARG:HG2	2.03	0.41
22:a:1856:U:H2'	22:a:1857:G:O4'	2.21	0.41
22:a:1868:C:H2'	22:a:1869:G:O4'	2.21	0.41
27:f:96:MET:HE2	27:f:96:MET:HB3	1.98	0.41
28:g:19:ILE:HG12	28:g:24:ILE:HD13	2.03	0.41
28:g:121:ILE:CG2	28:g:133:LEU:HD12	2.51	0.41
30:i:96:ARG:HH21	30:i:96:ARG:HA	1.86	0.41
49:1:41:ARG:HG2	49:1:46:LYS:HD3	2.02	0.41
50:2:52:LYS:HE3	50:2:52:LYS:HB3	1.75	0.41
1:A:593:U:H2'	1:A:594:U:C6	2.56	0.40
5:E:54:ARG:HH11	5:E:54:ARG:HG3	1.86	0.40
11:K:126:LYS:HE2	11:K:126:LYS:HB2	1.82	0.40
12:L:87:VAL:HG13	12:L:90:LEU:HB2	2.04	0.40
22:a:3:U:H2'	22:a:4:U:H6	1.85	0.40
22:a:645:C:H2'	22:a:647:G:N7	2.36	0.40
22:a:895:U:O2'	22:a:896:A:H5'	2.21	0.40
22:a:1607:C:H4'	22:a:1608:A:O5'	2.21	0.40
24:c:16:VAL:HG22	24:c:206:GLY:HA3	2.03	0.40
41:t:97:LYS:O	41:t:98:SER:OG	2.37	0.40
42:u:56:PHE:CE2	42:u:61:LEU:HD21	2.55	0.40
52:4:56:ARG:HA	52:4:59:ARG:HG2	2.04	0.40
1:A:59:A:H5"	1:A:60:A:H5'	2.02	0.40
1:A:161:A:H2'	1:A:162:A:C8	2.56	0.40
1:A:459:A:C6	1:A:474:G:C6	3.10	0.40
1:A:618:C:H5'	1:A:619:U:H5"	2.04	0.40
3:C:110:GLU:HB2	3:C:144:LEU:HD22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:18:ASP:OD2	11:K:37:ARG:HD3	2.21	0.40
14:N:40:ASP:OD1	14:N:40:ASP:N	2.51	0.40
22:a:608:A:H2'	22:a:609:A:C8	2.56	0.40
22:a:2096:C:H2'	22:a:2097:A:H8	1.86	0.40
22:a:2639:A:H2'	22:a:2640:G:O4'	2.21	0.40
25:d:39:ASP:OD1	25:d:39:ASP:N	2.53	0.40
31:j:107:LEU:O	31:j:109:SER:N	2.55	0.40
1:A:20:U:H2'	1:A:21:G:O4'	2.21	0.40
4:D:206:LYS:HB3	4:D:206:LYS:HE2	1.92	0.40
8:H:18:GLN:OE1	8:H:63:LEU:HB3	2.21	0.40
9:I:45:ARG:HD2	9:I:49:ARG:NH2	2.36	0.40
9:I:88:MET:CE	9:I:104:VAL:HG22	2.51	0.40
9:I:119:ARG:HH21	9:I:123:ARG:CZ	2.34	0.40
13:M:78:LYS:HA	13:M:78:LYS:HD2	1.92	0.40
22:a:1240:U:O2'	22:a:1241:A:O5'	2.38	0.40
22:a:1312:U:H4'	22:a:1313:U:O5'	2.21	0.40
22:a:1715:G:O2'	22:a:1743:G:O6	2.35	0.40
1:A:73:C:C2	1:A:74:A:C8	3.08	0.40
1:A:417:G:H5'	1:A:418:C:OP2	2.22	0.40
1:A:555:U:H2'	1:A:556:C:C6	2.56	0.40
1:A:1324:A:H2'	1:A:1325:C:O4'	2.21	0.40
2:B:45:LYS:HG2	2:B:49:MET:HE3	2.04	0.40
11:K:37:ARG:HH11	11:K:37:ARG:HG3	1.86	0.40
15:O:45:GLU:O	15:O:45:GLU:HG2	2.21	0.40
22:a:39:G:H2'	22:a:40:U:C6	2.57	0.40
22:a:634:C:H2'	22:a:635:C:C6	2.56	0.40
22:a:1446:C:H2'	22:a:1447:C:C6	2.56	0.40
22:a:1597:A:H5"	22:a:1598:A:H5'	2.04	0.40
22:a:1704:C:H2'	22:a:1705:A:C8	2.56	0.40
27:f:29:PRO:HB3	27:f:160:ALA:HB2	2.02	0.40
27:f:69:LYS:HZ3	27:f:84:PRO:HG3	1.85	0.40
31:j:44:LYS:HA	31:j:44:LYS:HD3	1.86	0.40
45:x:9:LYS:HB3	45:x:13:GLU:CG	2.52	0.40
47:z:43:ILE:HG22	47:z:49:TYR:HB2	2.03	0.40
50:2:13:ARG:HH21	50:2:13:ARG:HD2	1.75	0.40
1:A:109:A:H5'	1:A:110:C:H5	1.86	0.40
1:A:399:G:H2'	1:A:400:C:H6	1.85	0.40
1:A:1097:C:O3'	2:B:139:ARG:NH2	2.50	0.40
3:C:66:VAL:CG2	3:C:101:ILE:HG12	2.52	0.40
6:F:18:VAL:O	6:F:22:ILE:HG13	2.21	0.40
9:I:55:VAL:HG23	9:I:94:LEU:HD22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:20:THR:HG22	13:M:26:GLY:O	2.22	0.40
22:a:1443:U:H2'	22:a:1444:G:C8	2.56	0.40
25:d:32:ASN:ND2	25:d:52:THR:HB	2.36	0.40
26:e:119:ILE:HB	26:e:187:VAL:HG22	2.04	0.40
30:i:58:ASN:HA	30:i:126:ALA:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	222/241 (92%)	206 (93%)	16 (7%)	0	100	100
3	C	204/233 (88%)	189 (93%)	15 (7%)	0	100	100
4	D	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
5	E	154/167 (92%)	146 (95%)	8 (5%)	0	100	100
6	F	101/135 (75%)	95 (94%)	6 (6%)	0	100	100
7	G	151/179 (84%)	142 (94%)	9 (6%)	0	100	100
8	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
9	I	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
10	J	96/103 (93%)	92 (96%)	3 (3%)	1 (1%)	12	13
11	K	113/129 (88%)	107 (95%)	6 (5%)	0	100	100
12	L	120/124 (97%)	113 (94%)	7 (6%)	0	100	100
13	M	113/118 (96%)	105 (93%)	7 (6%)	1 (1%)	14	16
14	N	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
15	O	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
16	P	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
17	Q	77/84 (92%)	76 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	64/75 (85%)	61 (95%)	3 (5%)	0	100	100
19	S	82/92 (89%)	78 (95%)	4 (5%)	0	100	100
20	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
24	c	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
25	d	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	24	29
26	e	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
27	f	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
28	g	174/177 (98%)	161 (92%)	12 (7%)	1 (1%)	21	25
29	h	39/149 (26%)	35 (90%)	4 (10%)	0	100	100
30	i	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
31	j	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
32	k	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
33	l	132/136 (97%)	128 (97%)	4 (3%)	0	100	100
34	m	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
35	n	114/117 (97%)	106 (93%)	8 (7%)	0	100	100
36	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
37	p	115/118 (98%)	115 (100%)	0	0	100	100
38	q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
39	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
40	s	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
41	t	100/104 (96%)	92 (92%)	7 (7%)	1 (1%)	12	13
42	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
43	v	82/85 (96%)	79 (96%)	3 (4%)	0	100	100
44	w	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
45	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
46	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
47	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
48	0	49/55 (89%)	49 (100%)	0	0	100	100
49	1	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
50	2	62/65 (95%)	57 (92%)	4 (6%)	1 (2%)	7	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
51	3	36/38 (95%)	36 (100%)	0	0	100 100
52	4	56/70 (80%)	51 (91%)	5 (9%)	0	100 100
All	All	5487/5913 (93%)	5249 (96%)	232 (4%)	6 (0%)	49 60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	57	VAL
13	M	105	ASN
25	d	149	ASN
50	2	32	ILE
28	g	47	ASP
41	t	99	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	186/199 (94%)	186 (100%)	0	100 100
3	C	170/190 (90%)	170 (100%)	0	100 100
4	D	172/173 (99%)	172 (100%)	0	100 100
5	E	119/126 (94%)	119 (100%)	0	100 100
6	F	90/116 (78%)	90 (100%)	0	100 100
7	G	126/147 (86%)	126 (100%)	0	100 100
8	H	104/105 (99%)	104 (100%)	0	100 100
9	I	105/107 (98%)	105 (100%)	0	100 100
10	J	86/90 (96%)	86 (100%)	0	100 100
11	K	89/98 (91%)	88 (99%)	1 (1%)	65 75
12	L	102/103 (99%)	102 (100%)	0	100 100
13	M	93/96 (97%)	93 (100%)	0	100 100
14	N	83/84 (99%)	83 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	76/77 (99%)	76 (100%)	0	100	100
16	P	65/65 (100%)	64 (98%)	1 (2%)	57	69
17	Q	73/78 (94%)	73 (100%)	0	100	100
18	R	57/65 (88%)	57 (100%)	0	100	100
19	S	72/79 (91%)	72 (100%)	0	100	100
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	60/61 (98%)	60 (100%)	0	100	100
24	c	216/218 (99%)	216 (100%)	0	100	100
25	d	163/163 (100%)	163 (100%)	0	100	100
26	e	165/165 (100%)	165 (100%)	0	100	100
27	f	148/150 (99%)	148 (100%)	0	100	100
28	g	137/138 (99%)	137 (100%)	0	100	100
29	h	32/114 (28%)	32 (100%)	0	100	100
30	i	116/116 (100%)	116 (100%)	0	100	100
31	j	104/104 (100%)	104 (100%)	0	100	100
32	k	103/103 (100%)	103 (100%)	0	100	100
33	l	107/107 (100%)	107 (100%)	0	100	100
34	m	98/103 (95%)	98 (100%)	0	100	100
35	n	86/87 (99%)	86 (100%)	0	100	100
36	o	99/100 (99%)	99 (100%)	0	100	100
37	p	89/90 (99%)	89 (100%)	0	100	100
38	q	84/84 (100%)	84 (100%)	0	100	100
39	r	93/93 (100%)	93 (100%)	0	100	100
40	s	80/84 (95%)	80 (100%)	0	100	100
41	t	83/85 (98%)	83 (100%)	0	100	100
42	u	78/78 (100%)	78 (100%)	0	100	100
43	v	61/63 (97%)	61 (100%)	0	100	100
44	w	67/68 (98%)	67 (100%)	0	100	100
45	x	54/55 (98%)	54 (100%)	0	100	100
46	y	48/49 (98%)	48 (100%)	0	100	100
47	z	47/48 (98%)	47 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	0	46/49 (94%)	46 (100%)	0	100	100
49	1	38/38 (100%)	38 (100%)	0	100	100
50	2	51/52 (98%)	51 (100%)	0	100	100
51	3	34/34 (100%)	34 (100%)	0	100	100
52	4	55/62 (89%)	55 (100%)	0	100	100
All	All	4575/4825 (95%)	4573 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	109	ASN
16	P	63	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	42	ASN
2	B	51	ASN
2	B	177	ASN
3	C	8	ASN
4	D	136	GLN
4	D	152	GLN
5	E	73	ASN
5	E	77	ASN
5	E	148	ASN
7	G	148	ASN
7	G	153	HIS
11	K	118	HIS
12	L	77	HIS
15	O	28	GLN
17	Q	50	ASN
25	d	42	ASN
25	d	49	GLN
26	e	115	GLN
27	f	27	GLN
29	h	11	ASN
33	l	13	HIS
34	m	73	ASN
36	o	52	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	o	66	ASN
37	p	81	ASN
39	r	31	GLN
42	u	75	GLN
43	v	12	ASN
43	v	50	ASN
43	v	57	HIS
44	w	36	HIS
52	4	61	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1517/1542 (98%)	198 (13%)	7 (0%)
22	a	2749/2904 (94%)	315 (11%)	0
23	b	118/120 (98%)	13 (11%)	0
53	X	12/35 (34%)	1 (8%)	0
54	Z	76/77 (98%)	10 (13%)	1 (1%)
55	V	74/75 (98%)	16 (21%)	3 (4%)
All	All	4546/4753 (95%)	553 (12%)	11 (0%)

All (553) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	3	A
1	A	4	U
1	A	5	U
1	A	6	G
1	A	7	A
1	A	9	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	55	A
1	A	59	A
1	A	60	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	72	A
1	A	75	G
1	A	76	G
1	A	80	A
1	A	81	A
1	A	83	C
1	A	84	U
1	A	86	G
1	A	88	U
1	A	90	C
1	A	91	U
1	A	94	G
1	A	95	C
1	A	116	A
1	A	119	A
1	A	122	G
1	A	130	A
1	A	131	A
1	A	141	G
1	A	144	G
1	A	149	A
1	A	163	C
1	A	181	A
1	A	183	C
1	A	197	A
1	A	204	G
1	A	226	G
1	A	228	A
1	A	245	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	268	U
1	A	280	C
1	A	289	G
1	A	293	G
1	A	321	A
1	A	328	C
1	A	347	G
1	A	352	C
1	A	354	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	367	U
1	A	372	C
1	A	397	A
1	A	406	G
1	A	412	A
1	A	413	G
1	A	415	A
1	A	417	G
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	429	U
1	A	436	C
1	A	453	G
1	A	457	G
1	A	458	U
1	A	466	A
1	A	467	U
1	A	468	A
1	A	478	A
1	A	479	U
1	A	481	G
1	A	484	G
1	A	486	U
1	A	495	A
1	A	499	A
1	A	509	A
1	A	511	C
1	A	518	C
1	A	531	U
1	A	547	A
1	A	559	A
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	579	A
1	A	596	A
1	A	618	C
1	A	639	G
1	A	653	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	656	G
1	A	665	A
1	A	721	G
1	A	723	U
1	A	724	G
1	A	747	A
1	A	755	G
1	A	777	A
1	A	787	A
1	A	793	U
1	A	794	A
1	A	815	A
1	A	817	C
1	A	890	G
1	A	914	A
1	A	926	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	966	2MG
1	A	969	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	993	G
1	A	996	A
1	A	1004	A
1	A	1009	U
1	A	1020	G
1	A	1027	C
1	A	1028	C
1	A	1029	U
1	A	1030	U
1	A	1031	C
1	A	1032	G
1	A	1033	G
1	A	1034	G
1	A	1036	A
1	A	1065	U
1	A	1070	U
1	A	1085	U
1	A	1094	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1095	U
1	A	1101	A
1	A	1134	G
1	A	1136	C
1	A	1137	C
1	A	1139	G
1	A	1159	U
1	A	1167	A
1	A	1169	A
1	A	1171	A
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1225	A
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1260	G
1	A	1275	A
1	A	1280	A
1	A	1287	A
1	A	1294	G
1	A	1300	G
1	A	1302	C
1	A	1305	G
1	A	1312	G
1	A	1317	C
1	A	1320	C
1	A	1331	G
1	A	1338	G
1	A	1340	A
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1370	G
1	A	1378	C
1	A	1379	G
1	A	1397	C
1	A	1398	A
1	A	1419	G
1	A	1432	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1441	A
1	A	1442	G
1	A	1452	C
1	A	1453	G
1	A	1487	G
1	A	1492	A
1	A	1497	G
1	A	1503	A
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
1	A	1534	A
22	a	10	A
22	a	34	U
22	a	45	G
22	a	51	G
22	a	71	A
22	a	74	A
22	a	75	G
22	a	84	A
22	a	100	U
22	a	101	A
22	a	102	U
22	a	118	A
22	a	119	A
22	a	120	U
22	a	125	A
22	a	136	G
22	a	138	U
22	a	140	C
22	a	142	A
22	a	163	C
22	a	164	C
22	a	181	A
22	a	196	A
22	a	199	A
22	a	215	G
22	a	216	A
22	a	222	A
22	a	233	A
22	a	248	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	264	C
22	a	265	A
22	a	272	A
22	a	277	G
22	a	278	A
22	a	279	A
22	a	280	U
22	a	281	C
22	a	282	A
22	a	285	G
22	a	288	U
22	a	289	G
22	a	311	A
22	a	329	G
22	a	330	A
22	a	346	A
22	a	353	C
22	a	355	U
22	a	362	A
22	a	364	C
22	a	386	G
22	a	396	G
22	a	404	A
22	a	405	U
22	a	411	G
22	a	412	A
22	a	420	C
22	a	448	U
22	a	455	C
22	a	481	G
22	a	491	G
22	a	504	A
22	a	505	A
22	a	509	C
22	a	529	A
22	a	530	G
22	a	531	C
22	a	532	A
22	a	538	A
22	a	545	U
22	a	546	U
22	a	548	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	549	G
22	a	562	U
22	a	563	A
22	a	573	U
22	a	575	A
22	a	586	A
22	a	592	A
22	a	603	A
22	a	613	A
22	a	614	A
22	a	615	U
22	a	627	A
22	a	637	A
22	a	645	C
22	a	646	U
22	a	647	G
22	a	654	A
22	a	655	A
22	a	686	U
22	a	711	G
22	a	717	C
22	a	730	A
22	a	747	5MU
22	a	775	G
22	a	776	G
22	a	782	A
22	a	784	G
22	a	785	G
22	a	791	C
22	a	792	A
22	a	793	A
22	a	805	G
22	a	812	C
22	a	827	U
22	a	828	U
22	a	845	A
22	a	846	U
22	a	847	U
22	a	859	G
22	a	877	A
22	a	880	G
22	a	884	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	888	C
22	a	891	G
22	a	895	U
22	a	896	A
22	a	897	C
22	a	907	G
22	a	910	A
22	a	931	U
22	a	946	C
22	a	961	C
22	a	974	G
22	a	983	A
22	a	996	A
22	a	1012	U
22	a	1013	C
22	a	1033	U
22	a	1041	G
22	a	1045	C
22	a	1047	G
22	a	1108	U
22	a	1111	A
22	a	1112	G
22	a	1115	G
22	a	1122	G
22	a	1132	U
22	a	1133	A
22	a	1135	C
22	a	1142	A
22	a	1178	C
22	a	1187	G
22	a	1206	G
22	a	1241	A
22	a	1250	G
22	a	1253	A
22	a	1256	G
22	a	1271	G
22	a	1272	A
22	a	1300	G
22	a	1301	A
22	a	1313	U
22	a	1321	A
22	a	1329	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	1352	U
22	a	1365	A
22	a	1379	U
22	a	1383	A
22	a	1416	G
22	a	1427	A
22	a	1428	C
22	a	1452	G
22	a	1453	A
22	a	1482	G
22	a	1493	C
22	a	1508	A
22	a	1509	A
22	a	1510	G
22	a	1515	A
22	a	1523	U
22	a	1524	G
22	a	1532	A
22	a	1535	A
22	a	1536	C
22	a	1537	G
22	a	1539	U
22	a	1542	U
22	a	1560	G
22	a	1566	A
22	a	1569	A
22	a	1578	U
22	a	1584	U
22	a	1608	A
22	a	1610	A
22	a	1634	A
22	a	1647	U
22	a	1648	U
22	a	1649	G
22	a	1674	G
22	a	1715	G
22	a	1729	U
22	a	1730	C
22	a	1731	G
22	a	1738	G
22	a	1764	C
22	a	1773	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	1786	A
22	a	1800	C
22	a	1801	A
22	a	1808	A
22	a	1816	C
22	a	1829	A
22	a	1833	C
22	a	1847	A
22	a	1848	A
22	a	1869	G
22	a	1870	C
22	a	1871	A
22	a	1872	A
22	a	1906	G
22	a	1929	G
22	a	1930	G
22	a	1937	A
22	a	1955	U
22	a	1965	C
22	a	1967	C
22	a	1970	A
22	a	1971	U
22	a	1972	G
22	a	1991	U
22	a	1993	U
22	a	2021	C
22	a	2023	C
22	a	2030	6MZ
22	a	2031	A
22	a	2033	A
22	a	2036	C
22	a	2043	C
22	a	2055	C
22	a	2056	G
22	a	2060	A
22	a	2061	G
22	a	2062	A
22	a	2069	G7M
22	a	2198	A
22	a	2204	G
22	a	2211	A
22	a	2225	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	2238	G
22	a	2239	G
22	a	2273	A
22	a	2279	G
22	a	2283	C
22	a	2287	A
22	a	2305	U
22	a	2308	G
22	a	2322	A
22	a	2325	G
22	a	2333	A
22	a	2336	A
22	a	2345	G
22	a	2347	C
22	a	2350	C
22	a	2361	G
22	a	2377	A
22	a	2383	G
22	a	2385	C
22	a	2388	A
22	a	2396	G
22	a	2402	U
22	a	2403	C
22	a	2406	A
22	a	2410	G
22	a	2425	A
22	a	2429	G
22	a	2430	A
22	a	2435	A
22	a	2441	U
22	a	2448	A
22	a	2475	C
22	a	2476	A
22	a	2491	U
22	a	2498	OMC
22	a	2502	G
22	a	2505	G
22	a	2518	A
22	a	2525	G
22	a	2529	G
22	a	2535	G
22	a	2547	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	2566	A
22	a	2567	G
22	a	2573	C
22	a	2585	U
22	a	2602	A
22	a	2609	U
22	a	2613	U
22	a	2615	U
22	a	2629	U
22	a	2661	G
22	a	2663	G
22	a	2673	G
22	a	2689	U
22	a	2690	U
22	a	2713	U
22	a	2714	G
22	a	2716	C
22	a	2718	G
22	a	2726	A
22	a	2733	A
22	a	2744	G
22	a	2748	A
22	a	2757	A
22	a	2765	A
22	a	2778	A
22	a	2797	U
22	a	2798	U
22	a	2820	A
22	a	2821	A
22	a	2861	U
22	a	2873	A
22	a	2880	C
22	a	2884	U
22	a	2902	C
23	b	13	G
23	b	35	C
23	b	36	C
23	b	41	G
23	b	44	G
23	b	45	A
23	b	56	G
23	b	67	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	b	89	U
23	b	90	C
23	b	99	A
23	b	108	A
23	b	109	A
53	X	48	A
54	Z	9	G
54	Z	18	U
54	Z	19	G
54	Z	21	H2U
54	Z	22	A
54	Z	23	G
54	Z	32	G
54	Z	48	U
54	Z	55	5MU
54	Z	77	A
55	V	5	C
55	V	6	2MG
55	V	9	1MA
55	V	11	U
55	V	16	U
55	V	17	G
55	V	18	G
55	V	20	G
55	V	21	A
55	V	39	G
55	V	42	G
55	V	47	5MC
55	V	48	5MC
55	V	53	5MU
55	V	70	G
55	V	73	C

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	59	A
1	A	80	A
1	A	1026	G
1	A	1028	C
1	A	1033	G
1	A	1035	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1240	U
54	Z	20	G
55	V	5	C
55	V	10	G
55	V	20	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	2MA	a	2503	22,56	22,25,26	3.67	10 (45%)	33,37,40	2.83	9 (27%)
54	H2U	Z	21	54	18,21,22	1.08	2 (11%)	21,30,33	0.83	1 (4%)
1	UR3	A	1498	1	19,22,23	2.46	6 (31%)	26,32,35	1.45	2 (7%)
55	5MC	V	48	55	18,22,23	3.50	8 (44%)	26,32,35	1.05	1 (3%)
1	4OC	A	1402	1,56	20,23,24	2.76	8 (40%)	26,32,35	0.98	2 (7%)
33	MS6	l	82	33	5,7,8	1.15	1 (20%)	2,7,9	1.90	1 (50%)
55	PSU	V	54	55	18,21,22	1.07	2 (11%)	22,30,33	1.96	4 (18%)
11	IAS	K	119	11	6,7,8	0.99	0	6,8,10	1.30	1 (16%)
22	PSU	a	955	22	18,21,22	1.17	3 (16%)	22,30,33	1.83	3 (13%)
55	5MU	V	53	55	19,22,23	4.40	7 (36%)	28,32,35	3.74	9 (32%)
22	PSU	a	2457	22	18,21,22	1.13	2 (11%)	22,30,33	2.04	4 (18%)
22	OMC	a	2498	22,56	19,22,23	2.59	7 (36%)	26,31,34	0.89	0
22	PSU	a	2580	22	18,21,22	1.26	2 (11%)	22,30,33	2.19	6 (27%)
1	MA6	A	1518	1	23,26,27	1.59	5 (21%)	34,38,41	2.29	13 (38%)
22	2MG	a	2445	22	23,26,27	2.43	7 (30%)	32,38,41	2.25	10 (31%)
1	5MC	A	967	1	18,22,23	3.59	8 (44%)	26,32,35	1.03	1 (3%)
22	2MG	a	1835	22	23,26,27	2.40	7 (30%)	32,38,41	2.17	9 (28%)
55	1MA	V	9	55	21,25,26	0.70	0	31,37,40	0.83	1 (3%)
33	4D4	l	81	33	9,11,12	1.82	2 (22%)	8,13,15	2.19	4 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	5MC	a	1962	22	18,22,23	3.34	7 (38%)	26,32,35	1.06	2 (7%)
1	MA6	A	1519	1	23,26,27	1.61	5 (21%)	34,38,41	2.33	12 (35%)
55	1MA	V	57	55	21,25,26	0.77	0	31,37,40	0.78	1 (3%)
1	2MG	A	1516	1	23,26,27	2.43	7 (30%)	32,38,41	2.33	10 (31%)
55	56B	V	34	57,55	29,35,36	2.91	11 (37%)	36,52,55	1.90	7 (19%)
1	2MG	A	966	1	23,26,27	2.52	6 (26%)	32,38,41	2.29	10 (31%)
25	MEQ	d	150	25	8,9,10	1.26	0	5,10,12	1.23	1 (20%)
1	5MC	A	1407	1	18,22,23	3.30	7 (38%)	26,32,35	1.09	2 (7%)
54	4SU	Z	8	54	18,21,22	3.97	8 (44%)	26,30,33	2.27	5 (19%)
22	6MZ	a	2030	22	22,25,26	2.70	5 (22%)	30,36,39	2.50	11 (36%)
22	H2U	a	2449	22	18,21,22	1.42	3 (16%)	21,30,33	0.93	1 (4%)
55	5MC	V	47	55	18,22,23	3.53	7 (38%)	26,32,35	1.12	2 (7%)
55	H2U	V	19	55	18,21,22	1.22	3 (16%)	21,30,33	1.00	0
22	PSU	a	746	22,56	18,21,22	1.13	3 (16%)	22,30,33	1.72	3 (13%)
22	PSU	a	2504	22	18,21,22	1.10	2 (11%)	22,30,33	1.92	4 (18%)
55	PSU	V	13	55	18,21,22	1.06	1 (5%)	22,30,33	1.90	5 (22%)
22	1MG	a	745	22	22,26,27	2.52	7 (31%)	33,39,42	1.69	6 (18%)
54	5MU	Z	55	54	19,22,23	4.57	7 (36%)	28,32,35	3.79	9 (32%)
22	G7M	a	2069	22	23,26,27	2.65	8 (34%)	35,39,42	1.73	10 (28%)
54	OMC	Z	33	54	19,22,23	2.73	7 (36%)	26,31,34	0.76	0
1	2MG	A	1207	1	23,26,27	2.45	7 (30%)	32,38,41	2.13	9 (28%)
22	6MZ	a	1618	22	22,25,26	2.65	5 (22%)	30,36,39	2.48	10 (33%)
22	3TD	a	1915	22	18,22,23	3.86	7 (38%)	22,32,35	1.93	4 (18%)
54	PSU	Z	56	54	18,21,22	0.97	1 (5%)	22,30,33	1.81	3 (13%)
22	OMG	a	2251	22,54	23,26,27	2.48	8 (34%)	33,38,41	1.92	8 (24%)
22	PSU	a	2604	22	18,21,22	1.08	2 (11%)	22,30,33	1.85	3 (13%)
22	PSU	a	1911	22	18,21,22	1.01	1 (5%)	22,30,33	1.86	3 (13%)
22	5MU	a	747	22	19,22,23	4.45	7 (36%)	28,32,35	3.88	9 (32%)
22	OMU	a	2552	22	19,22,23	2.56	6 (31%)	26,31,34	1.96	5 (19%)
1	PSU	A	516	1	18,21,22	1.06	3 (16%)	22,30,33	1.74	5 (22%)
12	D2T	L	89	12	7,9,10	1.29	0	6,11,13	2.11	3 (50%)
1	G7M	A	527	1	23,26,27	2.69	8 (34%)	35,39,42	1.71	9 (25%)
22	PSU	a	2605	22	18,21,22	1.11	2 (11%)	22,30,33	1.85	3 (13%)
55	5MC	V	38	55	18,22,23	3.48	7 (38%)	26,32,35	1.20	2 (7%)
22	5MU	a	1939	22	19,22,23	4.41	7 (36%)	28,32,35	3.84	9 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	PSU	a	1917	22	18,21,22	1.10	3 (16%)	22,30,33	1.85	3 (13%)
55	2MG	V	6	55	23,26,27	2.56	8 (34%)	32,38,41	2.17	9 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	2MA	a	2503	22,56	-	1/7/25/26	0/3/3/3
54	H2U	Z	21	54	-	7/7/38/39	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
55	5MC	V	48	55	-	2/7/25/26	0/2/2/2
1	4OC	A	1402	1,56	-	1/9/29/30	0/2/2/2
33	MS6	l	82	33	-	1/4/6/8	-
55	PSU	V	54	55	-	0/7/25/26	0/2/2/2
11	IAS	K	119	11	-	0/7/7/8	-
22	PSU	a	955	22	-	0/7/25/26	0/2/2/2
55	5MU	V	53	55	-	0/7/25/26	0/2/2/2
22	PSU	a	2457	22	-	0/7/25/26	0/2/2/2
22	OMC	a	2498	22,56	-	0/9/27/28	0/2/2/2
22	PSU	a	2580	22	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
22	2MG	a	2445	22	-	2/9/27/28	0/3/3/3
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
22	2MG	a	1835	22	-	0/9/27/28	0/3/3/3
55	1MA	V	9	55	-	2/7/25/26	0/3/3/3
33	4D4	l	81	33	-	6/11/12/14	-
22	5MC	a	1962	22	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	2/11/29/30	0/3/3/3
55	1MA	V	57	55	-	0/7/25/26	0/3/3/3
1	2MG	A	1516	1	-	0/9/27/28	0/3/3/3
55	56B	V	34	57,55	-	1/12/43/44	0/4/4/4
1	2MG	A	966	1	-	2/9/27/28	0/3/3/3
25	MEQ	d	150	25	-	2/8/9/11	-
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
54	4SU	Z	8	54	-	0/7/25/26	0/2/2/2
22	6MZ	a	2030	22	-	2/9/27/28	0/3/3/3
22	H2U	a	2449	22	-	0/7/38/39	0/2/2/2
55	5MC	V	47	55	-	3/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	H2U	V	19	55	-	4/7/38/39	0/2/2/2
22	PSU	a	746	22,56	-	1/7/25/26	0/2/2/2
22	PSU	a	2504	22	-	0/7/25/26	0/2/2/2
55	PSU	V	13	55	-	1/7/25/26	0/2/2/2
22	1MG	a	745	22	-	0/7/25/26	0/3/3/3
54	5MU	Z	55	54	-	2/7/25/26	0/2/2/2
22	G7M	a	2069	22	-	1/7/25/26	0/3/3/3
54	OMC	Z	33	54	-	0/9/27/28	0/2/2/2
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
22	6MZ	a	1618	22	-	0/9/27/28	0/3/3/3
22	3TD	a	1915	22	-	0/7/25/26	0/2/2/2
54	PSU	Z	56	54	-	0/7/25/26	0/2/2/2
22	OMG	a	2251	22,54	-	1/9/27/28	0/3/3/3
22	PSU	a	2604	22	-	0/7/25/26	0/2/2/2
22	PSU	a	1911	22	-	0/7/25/26	0/2/2/2
22	5MU	a	747	22	-	0/7/25/26	0/2/2/2
22	OMU	a	2552	22	-	0/9/27/28	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
12	D2T	L	89	12	-	2/7/12/14	-
1	G7M	A	527	1	-	2/7/25/26	0/3/3/3
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
55	5MC	V	38	55	-	0/7/25/26	0/2/2/2
22	5MU	a	1939	22	-	0/7/25/26	0/2/2/2
22	PSU	a	1917	22	-	0/7/25/26	0/2/2/2
55	2MG	V	6	55	-	1/9/27/28	0/3/3/3

All (273) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1915	3TD	C6-C5	11.62	1.48	1.35
22	a	2503	2MA	C4-N3	11.14	1.48	1.34
22	a	2030	6MZ	C6-N6	10.61	1.45	1.34
22	a	1618	6MZ	C6-N6	10.50	1.45	1.34
54	Z	55	5MU	C6-N1	10.43	1.55	1.38
54	Z	55	5MU	C2-N1	10.18	1.54	1.38
22	a	747	5MU	C6-N1	10.15	1.55	1.38
22	a	1939	5MU	C6-N1	9.94	1.55	1.38
55	V	53	5MU	C6-N1	9.88	1.54	1.38
22	a	747	5MU	C2-N1	9.50	1.53	1.38
55	V	53	5MU	C2-N1	9.32	1.53	1.38
1	A	967	5MC	C6-C5	9.12	1.49	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	Z	8	4SU	C4-N3	9.08	1.47	1.37
22	a	1939	5MU	C2-N1	9.01	1.52	1.38
55	V	47	5MC	C6-C5	8.95	1.49	1.34
55	V	48	5MC	C6-C5	8.92	1.49	1.34
55	V	38	5MC	C6-C5	8.74	1.49	1.34
54	Z	55	5MU	C4-C5	8.60	1.59	1.44
22	a	1962	5MC	C6-C5	8.55	1.48	1.34
1	A	1407	5MC	C6-C5	8.53	1.48	1.34
22	a	1939	5MU	C4-N3	-8.33	1.23	1.38
55	V	53	5MU	C4-C5	8.30	1.58	1.44
22	a	747	5MU	C4-C5	8.20	1.58	1.44
55	V	53	5MU	C4-N3	-8.19	1.23	1.38
22	a	1939	5MU	C4-C5	8.08	1.58	1.44
22	a	1915	3TD	C2-N1	8.07	1.47	1.37
22	a	747	5MU	C4-N3	-8.01	1.24	1.38
54	Z	55	5MU	C4-N3	-7.76	1.24	1.38
55	V	6	2MG	C2-N3	7.43	1.46	1.31
1	A	966	2MG	C2-N3	7.17	1.45	1.31
54	Z	8	4SU	C2-N1	7.16	1.49	1.38
55	V	34	56B	C14-C13	6.90	1.52	1.32
1	A	967	5MC	C4-N3	6.78	1.45	1.34
55	V	47	5MC	C4-N3	6.73	1.45	1.34
1	A	1207	2MG	C2-N3	6.72	1.44	1.31
55	V	38	5MC	C4-N3	6.65	1.45	1.34
55	V	48	5MC	C4-N3	6.62	1.45	1.34
22	a	2503	2MA	C2-N3	6.61	1.45	1.34
22	a	1835	2MG	C2-N3	6.61	1.44	1.31
1	A	1516	2MG	C2-N3	6.56	1.44	1.31
22	a	2445	2MG	C2-N3	6.55	1.44	1.31
22	a	2251	OMG	C4-N3	6.46	1.49	1.34
22	a	1962	5MC	C4-N3	6.35	1.44	1.34
54	Z	8	4SU	C2-N3	6.30	1.49	1.38
55	V	6	2MG	C4-N3	6.29	1.49	1.34
54	Z	55	5MU	C6-C5	6.19	1.44	1.34
1	A	966	2MG	C4-N3	6.18	1.48	1.34
1	A	967	5MC	C2-N3	6.12	1.48	1.36
1	A	1498	UR3	C2-N1	6.09	1.47	1.38
1	A	527	G7M	C2-N2	6.09	1.48	1.34
55	V	47	5MC	C2-N3	6.08	1.48	1.36
55	V	38	5MC	C2-N3	6.03	1.48	1.36
22	a	1939	5MU	C6-C5	5.99	1.44	1.34
1	A	1402	4OC	C4-N3	5.97	1.43	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C4-N3	5.94	1.48	1.34
1	A	1407	5MC	C4-N3	5.93	1.44	1.34
55	V	34	56B	O11-C11	-5.89	1.29	1.43
1	A	527	G7M	C4-N3	5.88	1.48	1.34
22	a	747	5MU	C6-C5	5.85	1.44	1.34
55	V	48	5MC	C2-N3	5.84	1.48	1.36
22	a	2069	G7M	C2-N2	5.82	1.48	1.34
22	a	2069	G7M	C5-N7	-5.78	1.32	1.39
22	a	2503	2MA	C2-N1	5.78	1.44	1.34
54	Z	8	4SU	C6-C5	5.76	1.48	1.35
22	a	2445	2MG	C4-N3	5.74	1.47	1.34
1	A	1516	2MG	C4-N3	5.72	1.47	1.34
54	Z	33	OMC	C2-N3	5.69	1.47	1.36
55	V	34	56B	C4-N3	5.69	1.47	1.34
22	a	1962	5MC	C2-N3	5.69	1.47	1.36
22	a	745	1MG	C4-N3	5.66	1.47	1.34
1	A	1402	4OC	C6-C5	5.63	1.48	1.35
54	Z	33	OMC	C6-C5	5.62	1.48	1.35
55	V	53	5MU	C6-C5	5.61	1.43	1.34
54	Z	8	4SU	C4-S4	-5.61	1.57	1.68
22	a	1835	2MG	C4-N3	5.60	1.47	1.34
22	a	2069	G7M	C4-N3	5.55	1.47	1.34
1	A	1498	UR3	C6-C5	5.54	1.47	1.35
22	a	2552	OMU	C2-N1	5.53	1.47	1.38
1	A	1407	5MC	C2-N3	5.53	1.47	1.36
22	a	2552	OMU	C2-N3	5.48	1.47	1.38
22	a	745	1MG	C2-N3	5.47	1.44	1.34
22	a	745	1MG	C2-N2	5.39	1.43	1.34
55	V	34	56B	C11-C10	5.35	1.62	1.54
22	a	2498	OMC	C2-N3	5.34	1.47	1.36
22	a	2552	OMU	C6-C5	5.33	1.47	1.35
22	a	2498	OMC	C6-C5	5.31	1.47	1.35
22	a	1915	3TD	C6-N1	5.28	1.45	1.36
22	a	2503	2MA	C6-N6	-5.24	1.21	1.34
1	A	1402	4OC	C2-N3	5.17	1.46	1.36
1	A	527	G7M	C5-N7	-5.16	1.33	1.39
1	A	527	G7M	C2-N3	5.06	1.45	1.33
55	V	34	56B	C2-N3	4.98	1.45	1.33
54	Z	8	4SU	C5-C4	4.89	1.48	1.42
22	a	2503	2MA	C5-C6	4.83	1.54	1.41
22	a	2251	OMG	C2-N3	4.67	1.44	1.33
1	A	967	5MC	C6-N1	4.66	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2069	G7M	C2-N3	4.65	1.44	1.33
55	V	47	5MC	C6-N1	4.62	1.45	1.38
55	V	48	5MC	C6-N1	4.61	1.45	1.38
54	Z	33	OMC	C4-N4	4.53	1.44	1.33
55	V	6	2MG	C2-N1	4.48	1.43	1.36
22	a	2251	OMG	C2-N2	4.46	1.44	1.34
1	A	966	2MG	C2-N1	4.45	1.43	1.36
55	V	38	5MC	C6-N1	4.34	1.45	1.38
55	V	34	56B	C2-N2	4.31	1.44	1.34
1	A	1407	5MC	C6-N1	4.30	1.45	1.38
54	Z	33	OMC	C4-N3	4.28	1.43	1.34
22	a	1962	5MC	C6-N1	4.25	1.45	1.38
22	a	2498	OMC	C4-N4	4.25	1.43	1.33
1	A	1207	2MG	C2-N1	4.25	1.43	1.36
1	A	1516	2MG	C2-N1	4.19	1.43	1.36
22	a	2498	OMC	C4-N3	3.99	1.42	1.34
1	A	1498	UR3	C2-N3	3.98	1.46	1.39
1	A	1402	4OC	C4-N4	3.97	1.44	1.35
22	a	1915	3TD	C2-N3	3.94	1.47	1.38
55	V	38	5MC	C4-N4	3.93	1.44	1.34
1	A	1519	MA6	C5-C4	-3.93	1.31	1.39
1	A	967	5MC	C4-N4	3.88	1.44	1.34
1	A	967	5MC	C2-N1	3.87	1.48	1.40
22	a	1835	2MG	C2-N1	3.86	1.42	1.36
22	a	2251	OMG	C5-N7	-3.86	1.31	1.39
55	V	47	5MC	C4-N4	3.85	1.44	1.34
55	V	48	5MC	C4-N4	3.85	1.44	1.34
54	Z	33	OMC	C2-N1	3.78	1.48	1.40
22	a	2445	2MG	C5-N7	-3.78	1.31	1.39
1	A	1518	MA6	C5-C4	-3.76	1.32	1.39
55	V	48	5MC	C2-N1	3.70	1.48	1.40
22	a	1618	6MZ	C5-C4	-3.69	1.32	1.39
22	a	2552	OMU	O2-C2	-3.67	1.16	1.23
22	a	745	1MG	C5-N7	-3.67	1.32	1.39
22	a	2445	2MG	C2-N1	3.65	1.42	1.36
22	a	2030	6MZ	C5-C4	-3.65	1.32	1.39
22	a	2503	2MA	C5-N7	-3.64	1.32	1.39
22	a	1835	2MG	C5-N7	-3.60	1.32	1.39
55	V	47	5MC	C2-N1	3.58	1.47	1.40
22	a	2498	OMC	C2-N1	3.57	1.47	1.40
22	a	1962	5MC	C4-N4	3.55	1.43	1.34
1	A	1407	5MC	C4-N4	3.53	1.43	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1402	4OC	O2-C2	-3.52	1.17	1.23
22	a	2498	OMC	O2-C2	-3.49	1.17	1.23
22	a	2449	H2U	C4-N3	-3.47	1.31	1.37
55	V	34	56B	C5-C6	3.44	1.51	1.44
54	Z	8	4SU	O2-C2	-3.43	1.16	1.23
22	a	2449	H2U	C2-N3	-3.42	1.31	1.38
1	A	1516	2MG	C5-N7	-3.40	1.32	1.39
55	V	38	5MC	C2-N1	3.37	1.47	1.40
1	A	527	G7M	C5-C6	3.36	1.52	1.43
33	l	81	4D4	OB-CB	-3.36	1.36	1.43
22	a	2251	OMG	O6-C6	-3.35	1.17	1.23
1	A	966	2MG	C5-N7	-3.33	1.32	1.39
1	A	1207	2MG	C5-N7	-3.30	1.32	1.39
22	a	2552	OMU	O4-C4	-3.30	1.18	1.24
55	V	6	2MG	C5-N7	-3.29	1.32	1.39
1	A	1407	5MC	O2-C2	-3.28	1.17	1.23
1	A	1402	4OC	C2-N1	3.28	1.47	1.40
1	A	1402	4OC	C5-C4	3.27	1.47	1.40
54	Z	33	OMC	O2-C2	-3.24	1.17	1.23
1	A	1518	MA6	C5-N7	-3.20	1.33	1.39
55	V	34	56B	C11-C12	3.19	1.59	1.53
22	a	2069	G7M	O6-C6	-3.16	1.17	1.23
22	a	2069	G7M	C5-C6	3.16	1.52	1.43
22	a	2445	2MG	O6-C6	-3.14	1.17	1.23
1	A	1519	MA6	C5-N7	-3.14	1.33	1.39
55	V	34	56B	O6-C6	-3.13	1.17	1.23
1	A	1407	5MC	C2-N1	3.08	1.46	1.40
1	A	1519	MA6	C8-N9	-3.08	1.32	1.37
22	a	1962	5MC	C2-N1	3.07	1.46	1.40
22	a	1962	5MC	O2-C2	-3.07	1.18	1.23
55	V	19	H2U	C4-N3	-3.05	1.32	1.37
22	a	1835	2MG	O6-C6	-3.04	1.17	1.23
22	a	1939	5MU	O2-C2	-3.02	1.17	1.23
22	a	2503	2MA	C6-N1	3.01	1.39	1.35
22	a	745	1MG	O6-C6	-2.96	1.16	1.23
22	a	745	1MG	C4-N9	-2.96	1.30	1.38
1	A	527	G7M	O6-C6	-2.95	1.18	1.23
55	V	19	H2U	C2-N3	-2.93	1.32	1.38
1	A	1518	MA6	C8-N9	-2.92	1.32	1.37
22	a	2030	6MZ	C8-N9	-2.92	1.32	1.37
1	A	1498	UR3	O2-C2	-2.91	1.17	1.22
55	V	13	PSU	C6-C5	2.90	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1498	UR3	O4-C4	-2.87	1.17	1.23
22	a	2030	6MZ	C5-N7	-2.84	1.33	1.39
22	a	1618	6MZ	C5-N7	-2.84	1.33	1.39
22	a	1618	6MZ	C8-N9	-2.82	1.32	1.37
1	A	1516	2MG	O6-C6	-2.81	1.18	1.23
54	Z	8	4SU	C6-N1	2.79	1.44	1.38
22	a	747	5MU	O2-C2	-2.78	1.18	1.23
1	A	967	5MC	O2-C2	-2.77	1.18	1.23
55	V	38	5MC	O2-C2	-2.77	1.18	1.23
54	Z	56	PSU	C6-C5	2.73	1.38	1.35
54	Z	21	H2U	C2-N3	-2.71	1.33	1.38
55	V	48	5MC	O2-C2	-2.69	1.18	1.23
1	A	1207	2MG	O6-C6	-2.68	1.18	1.23
55	V	53	5MU	O2-C2	-2.67	1.18	1.23
55	V	47	5MC	O2-C2	-2.65	1.18	1.23
22	a	2580	PSU	O4'-C1'	-2.64	1.40	1.43
22	a	2251	OMG	C4-N9	-2.63	1.31	1.38
22	a	2449	H2U	C2-N1	-2.63	1.31	1.35
1	A	1516	2MG	C4-N9	-2.62	1.31	1.38
1	A	966	2MG	O6-C6	-2.61	1.18	1.23
1	A	1519	MA6	C4-N9	-2.60	1.31	1.37
54	Z	33	OMC	C6-N1	2.59	1.44	1.38
22	a	2251	OMG	C8-N9	-2.58	1.31	1.37
1	A	1518	MA6	C6-N6	2.57	1.44	1.36
22	a	1835	2MG	C4-N9	-2.57	1.31	1.38
1	A	1518	MA6	C4-N9	-2.56	1.32	1.37
1	A	1519	MA6	C6-N6	2.55	1.44	1.36
54	Z	21	H2U	C4-N3	-2.54	1.33	1.37
22	a	2445	2MG	C4-N9	-2.54	1.31	1.38
55	V	54	PSU	C6-C5	2.53	1.38	1.35
22	a	1939	5MU	O4-C4	-2.52	1.18	1.23
1	A	1207	2MG	C4-N9	-2.52	1.31	1.38
22	a	1915	3TD	O4-C4	-2.50	1.17	1.23
1	A	1402	4OC	C6-N1	2.48	1.44	1.38
55	V	6	2MG	O6-C6	-2.48	1.18	1.23
22	a	1915	3TD	O2-C2	-2.46	1.18	1.23
33	l	82	MS6	CB-CA	2.46	1.56	1.53
22	a	1917	PSU	C4-C5	-2.43	1.37	1.44
22	a	2504	PSU	C6-C5	2.42	1.38	1.35
1	A	527	G7M	C2-N1	2.42	1.43	1.37
22	a	747	5MU	O4-C4	-2.42	1.19	1.23
55	V	34	56B	C5-C4	-2.40	1.36	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2580	PSU	C4-C5	-2.40	1.37	1.44
22	a	2251	OMG	C5-C6	2.39	1.53	1.44
55	V	53	5MU	O4-C4	-2.36	1.19	1.23
22	a	2503	2MA	C5-C4	-2.36	1.34	1.39
22	a	746	PSU	C4-C5	-2.34	1.37	1.44
22	a	2503	2MA	C8-N9	-2.33	1.33	1.37
1	A	966	2MG	C5-C6	2.33	1.53	1.44
1	A	516	PSU	C6-C5	2.32	1.38	1.35
22	a	955	PSU	C4-C5	-2.32	1.37	1.44
1	A	516	PSU	C4-C5	-2.30	1.37	1.44
22	a	2605	PSU	C4-C5	-2.30	1.37	1.44
55	V	6	2MG	C5-C6	2.30	1.52	1.44
1	A	1516	2MG	C5-C6	2.28	1.52	1.44
1	A	1498	UR3	C6-N1	2.28	1.43	1.38
54	Z	55	5MU	O2-C2	-2.25	1.18	1.23
22	a	2552	OMU	C4-N3	2.25	1.42	1.38
22	a	2030	6MZ	C6-N1	-2.25	1.31	1.35
1	A	1207	2MG	C5-C6	2.24	1.52	1.44
22	a	745	1MG	C5-C6	2.23	1.51	1.45
22	a	746	PSU	O4'-C1'	-2.23	1.40	1.43
33	l	81	4D4	CD-NE	-2.23	1.41	1.46
22	a	2498	OMC	C6-N1	2.22	1.43	1.38
55	V	34	56B	C2-N1	2.21	1.43	1.37
22	a	2604	PSU	C4-C5	-2.20	1.37	1.44
22	a	1911	PSU	C4-C5	-2.20	1.37	1.44
22	a	2069	G7M	C4-N9	-2.19	1.32	1.38
22	a	1917	PSU	C6-C5	2.19	1.37	1.35
22	a	2504	PSU	C4-C5	-2.19	1.37	1.44
22	a	2069	G7M	C2-N1	2.14	1.43	1.37
22	a	1835	2MG	C5-C6	2.14	1.52	1.44
54	Z	55	5MU	O4-C4	-2.14	1.19	1.23
22	a	955	PSU	C6-C5	2.13	1.37	1.35
1	A	516	PSU	O4'-C1'	-2.12	1.40	1.43
22	a	2457	PSU	C4-C5	-2.11	1.38	1.44
22	a	2457	PSU	O4'-C1'	-2.10	1.40	1.43
22	a	2445	2MG	C5-C6	2.10	1.52	1.44
1	A	527	G7M	C6-N1	2.09	1.42	1.38
55	V	54	PSU	C4-C5	-2.09	1.38	1.44
55	V	6	2MG	C4-N9	-2.09	1.32	1.38
55	V	19	H2U	C2-N1	-2.07	1.32	1.35
22	a	2503	2MA	CM2-C2	2.05	1.55	1.49
22	a	1915	3TD	C4-N3	2.05	1.44	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1618	6MZ	C5-C6	-2.04	1.36	1.41
22	a	2605	PSU	C6-C5	2.03	1.37	1.35
22	a	955	PSU	O4'-C1'	-2.03	1.41	1.43
22	a	2604	PSU	C6-C5	2.03	1.37	1.35
55	V	6	2MG	C6-N1	2.01	1.42	1.38
1	A	967	5MC	CM5-C5	2.01	1.55	1.50
22	a	1917	PSU	O4'-C1'	-2.00	1.41	1.43
55	V	48	5MC	CM5-C5	2.00	1.55	1.50
22	a	746	PSU	C6-C5	2.00	1.37	1.35

All (279) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	747	5MU	C5-C4-N3	13.04	126.44	115.31
54	Z	55	5MU	C5-C4-N3	12.86	126.29	115.31
22	a	1939	5MU	C5-C4-N3	12.81	126.24	115.31
55	V	53	5MU	C5-C4-N3	12.55	126.02	115.31
22	a	747	5MU	C5-C6-N1	-10.98	112.04	123.34
54	Z	55	5MU	C5-C6-N1	-10.80	112.22	123.34
22	a	1939	5MU	C5-C6-N1	-10.78	112.25	123.34
55	V	53	5MU	C5-C6-N1	-10.51	112.53	123.34
22	a	2503	2MA	C5-C4-N3	-8.44	117.69	127.19
54	Z	8	4SU	C4-N3-C2	-7.94	119.63	127.34
1	A	966	2MG	C2-N3-C4	6.89	120.59	112.04
22	a	2503	2MA	C4-N9-C1'	-6.69	110.66	126.59
22	a	2445	2MG	C2-N3-C4	6.60	120.23	112.04
22	a	2503	2MA	C1'-N9-C8	6.53	141.88	127.14
22	a	1835	2MG	C2-N3-C4	6.49	120.08	112.04
1	A	1516	2MG	C2-N3-C4	6.44	120.03	112.04
22	a	1915	3TD	N1-C2-N3	6.38	121.18	116.14
1	A	1207	2MG	C2-N3-C4	6.23	119.76	112.04
55	V	6	2MG	C2-N3-C4	6.21	119.74	112.04
22	a	2552	OMU	C4-N3-C2	-6.12	118.51	126.58
55	V	34	56B	C5-C4-N3	-6.05	120.44	127.52
1	A	1519	MA6	N1-C2-N3	-6.01	119.21	128.60
22	a	2030	6MZ	C9-N6-C6	-5.97	117.73	122.87
22	a	2580	PSU	N1-C2-N3	5.85	121.75	115.13
1	A	1518	MA6	N1-C2-N3	-5.78	119.56	128.60
22	a	2030	6MZ	N1-C2-N3	-5.78	119.56	128.60
22	a	1618	6MZ	N1-C2-N3	-5.72	119.65	128.60
22	a	2503	2MA	N3-C4-N9	5.69	134.88	126.99
1	A	1498	UR3	C4-N3-C2	-5.62	119.27	124.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	966	2MG	C5-C4-N3	-5.59	119.40	128.46
22	a	747	5MU	O4-C4-C5	-5.59	118.43	124.90
54	Z	55	5MU	O4-C4-C5	-5.54	118.48	124.90
22	a	2457	PSU	N1-C2-N3	5.50	121.36	115.13
1	A	1516	2MG	C2-N1-C6	-5.46	118.20	124.48
22	a	1618	6MZ	C5-C4-N3	-5.41	119.70	126.75
22	a	1939	5MU	C4-N3-C2	-5.37	120.40	127.35
22	a	2251	OMG	C5-C4-N3	-5.35	119.78	128.46
22	a	747	5MU	C4-N3-C2	-5.34	120.43	127.35
22	a	1835	2MG	C5-C4-N3	-5.34	119.80	128.46
54	Z	8	4SU	C5-C4-N3	5.25	119.56	114.69
54	Z	55	5MU	C4-N3-C2	-5.21	120.61	127.35
55	V	53	5MU	O4-C4-C5	-5.18	118.90	124.90
55	V	6	2MG	C5-C4-N3	-5.18	120.06	128.46
22	a	2605	PSU	C4-N3-C2	-5.17	118.90	126.34
22	a	2457	PSU	C4-N3-C2	-5.16	118.90	126.34
55	V	54	PSU	N1-C2-N3	5.15	120.97	115.13
22	a	1911	PSU	C4-N3-C2	-5.15	118.92	126.34
22	a	2445	2MG	C5-C4-N3	-5.14	120.12	128.46
22	a	1939	5MU	O4-C4-C5	-5.13	118.95	124.90
22	a	2580	PSU	C4-N3-C2	-5.13	118.95	126.34
22	a	2445	2MG	C2-N1-C6	-5.10	118.61	124.48
22	a	2504	PSU	N1-C2-N3	5.08	120.88	115.13
1	A	1516	2MG	C5-C4-N3	-5.06	120.25	128.46
22	a	1835	2MG	C2-N1-C6	-5.06	118.66	124.48
1	A	966	2MG	C2-N1-C6	-5.02	118.71	124.48
22	a	2604	PSU	C4-N3-C2	-5.00	119.13	126.34
22	a	2030	6MZ	N9-C8-N7	-5.00	107.07	113.91
22	a	2552	OMU	N3-C2-N1	4.99	121.52	114.89
22	a	1939	5MU	N3-C2-N1	4.98	121.50	114.89
55	V	13	PSU	N1-C2-N3	4.98	120.77	115.13
22	a	2504	PSU	C4-N3-C2	-4.97	119.17	126.34
55	V	54	PSU	C4-N3-C2	-4.96	119.20	126.34
55	V	53	5MU	C4-N3-C2	-4.93	120.97	127.35
22	a	955	PSU	C4-N3-C2	-4.91	119.27	126.34
22	a	746	PSU	C4-N3-C2	-4.88	119.30	126.34
22	a	1917	PSU	C4-N3-C2	-4.88	119.30	126.34
22	a	1618	6MZ	C9-N6-C6	-4.88	118.67	122.87
54	Z	56	PSU	C4-N3-C2	-4.86	119.33	126.34
1	A	1519	MA6	N9-C8-N7	-4.86	107.27	113.91
22	a	955	PSU	N1-C2-N3	4.78	120.54	115.13
22	a	1618	6MZ	N9-C8-N7	-4.73	107.44	113.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1207	2MG	C5-C4-N3	-4.72	120.81	128.46
22	a	2605	PSU	N1-C2-N3	4.69	120.45	115.13
55	V	13	PSU	C4-N3-C2	-4.65	119.64	126.34
22	a	2030	6MZ	C5-C4-N3	-4.64	120.70	126.75
1	A	1518	MA6	C5-C4-N3	-4.63	120.71	126.75
22	a	2604	PSU	N1-C2-N3	4.62	120.36	115.13
55	V	6	2MG	C2-N1-C6	-4.61	119.17	124.48
22	a	1917	PSU	N1-C2-N3	4.59	120.33	115.13
22	a	1911	PSU	N1-C2-N3	4.54	120.28	115.13
1	A	1518	MA6	N9-C8-N7	-4.54	107.71	113.91
1	A	516	PSU	C4-N3-C2	-4.50	119.85	126.34
54	Z	56	PSU	N1-C2-N3	4.50	120.23	115.13
1	A	1519	MA6	C2-N1-C6	4.46	122.29	111.75
22	a	747	5MU	N3-C2-N1	4.46	120.81	114.89
1	A	1518	MA6	C2-N1-C6	4.45	122.26	111.75
1	A	1519	MA6	C5-C4-N3	-4.44	120.96	126.75
1	A	1207	2MG	C2-N1-C6	-4.43	119.38	124.48
22	a	745	1MG	C5-C4-N3	-4.42	121.28	128.46
22	a	2251	OMG	C2-N3-C4	4.38	120.10	112.30
54	Z	55	5MU	N3-C2-N1	4.38	120.70	114.89
55	V	53	5MU	N3-C2-N1	4.32	120.63	114.89
22	a	2069	G7M	C2-N3-C4	4.27	119.91	112.30
22	a	1915	3TD	C4-N3-C2	-4.27	119.98	124.61
22	a	746	PSU	N1-C2-N3	4.24	119.94	115.13
55	V	34	56B	C2-N3-C4	4.21	119.80	112.30
1	A	1518	MA6	C4-C5-C6	4.18	120.56	115.88
55	V	38	5MC	C5-C6-N1	-4.13	119.09	123.34
1	A	516	PSU	N1-C2-N3	4.13	119.81	115.13
1	A	527	G7M	C2-N3-C4	4.11	119.63	112.30
55	V	34	56B	C7-C5-C4	-4.08	107.94	112.66
22	a	2069	G7M	C5-C6-N1	4.06	120.27	111.79
1	A	527	G7M	C5-C6-N1	4.03	120.20	111.79
55	V	53	5MU	C5M-C5-C6	-3.96	117.56	122.85
55	V	53	5MU	C5M-C5-C4	3.95	123.12	118.77
1	A	1519	MA6	C4-C5-C6	3.85	120.19	115.88
22	a	1618	6MZ	C2-N3-C4	3.82	120.77	111.75
22	a	747	5MU	C5M-C5-C6	-3.82	117.75	122.85
54	Z	8	4SU	N3-C2-N1	3.80	119.93	114.89
1	A	527	G7M	C5-C4-N3	-3.76	120.94	128.15
55	V	6	2MG	N9-C4-N3	3.73	133.43	125.94
22	a	1939	5MU	C5M-C5-C6	-3.72	117.88	122.85
22	a	1618	6MZ	C4-C5-C6	3.71	119.69	116.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	Z	8	4SU	C5-C4-S4	-3.68	119.73	124.47
22	a	2503	2MA	N9-C8-N7	-3.66	108.91	113.91
55	V	48	5MC	C5-C6-N1	-3.66	119.58	123.34
1	A	1407	5MC	C5-C6-N1	-3.65	119.58	123.34
55	V	47	5MC	C5-C6-N1	-3.62	119.61	123.34
22	a	2030	6MZ	C2-N3-C4	3.60	120.25	111.75
1	A	966	2MG	N9-C4-N3	3.59	133.15	125.94
22	a	747	5MU	C5M-C5-C4	3.58	122.71	118.77
33	l	81	4D4	NH1-CZ-NE	3.58	127.45	119.19
22	a	1939	5MU	C5M-C5-C4	3.57	122.70	118.77
1	A	1519	MA6	C5-N7-C8	3.56	108.57	103.51
22	a	2069	G7M	C5-C4-N3	-3.53	121.37	128.15
22	a	2552	OMU	C5-C4-N3	3.49	120.07	114.84
22	a	2030	6MZ	C5-N7-C8	3.48	108.45	103.51
54	Z	55	5MU	C5M-C5-C6	-3.48	118.21	122.85
22	a	2069	G7M	O6-C6-C5	-3.45	120.28	128.06
22	a	2580	PSU	C6-N1-C2	-3.44	119.17	122.68
22	a	2251	OMG	N9-C4-N3	3.42	132.80	125.94
1	A	1516	2MG	N9-C8-N7	-3.41	106.98	113.39
22	a	745	1MG	C2-N3-C4	3.40	119.63	111.98
22	a	1962	5MC	C5-C6-N1	-3.40	119.84	123.34
22	a	2445	2MG	N9-C8-N7	-3.39	107.00	113.39
12	L	89	D2T	OD2-CG-CB	3.39	120.47	113.15
1	A	1518	MA6	C5-N7-C8	3.39	108.32	103.51
1	A	1519	MA6	C2-N3-C4	3.37	119.71	111.75
22	a	1835	2MG	N9-C4-N3	3.36	132.69	125.94
22	a	2445	2MG	N9-C4-N3	3.36	132.68	125.94
1	A	1207	2MG	N9-C8-N7	-3.35	107.08	113.39
1	A	527	G7M	O6-C6-C5	-3.34	120.52	128.06
22	a	1618	6MZ	N3-C4-N9	3.33	132.57	127.08
55	V	34	56B	C7-C8-N9	-3.31	107.81	111.06
22	a	745	1MG	N9-C8-N7	-3.29	107.20	113.39
1	A	1518	MA6	C2-N3-C4	3.28	119.50	111.75
22	a	2251	OMG	C2-N1-C6	-3.26	119.15	125.10
55	V	6	2MG	N9-C8-N7	-3.21	107.35	113.39
1	A	1518	MA6	N1-C6-N6	-3.20	113.58	117.08
22	a	1618	6MZ	C5-N7-C8	3.19	108.04	103.51
55	V	34	56B	C2-N1-C6	-3.19	119.29	125.10
22	a	1939	5MU	O2-C2-N1	-3.16	118.59	122.79
1	A	527	G7M	C2-N1-C6	-3.15	119.36	125.10
22	a	2445	2MG	C5-C6-N1	3.14	121.17	113.19
12	L	89	D2T	OD1-CG-CB	-3.13	115.89	122.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	2503	2MA	N3-C2-N1	-3.12	119.97	125.72
1	A	1207	2MG	N9-C4-N3	3.11	132.19	125.94
54	Z	55	5MU	C5M-C5-C4	3.11	122.19	118.77
22	a	745	1MG	C5-C6-N1	3.09	120.89	114.91
22	a	2251	OMG	N9-C8-N7	-3.07	107.61	113.39
55	V	13	PSU	O2-C2-N1	-3.05	119.43	122.79
22	a	2069	G7M	C2-N1-C6	-3.05	119.53	125.10
1	A	966	2MG	N9-C8-N7	-3.03	107.68	113.39
22	a	2457	PSU	O2-C2-N1	-3.02	119.46	122.79
55	V	54	PSU	O2-C2-N1	-3.01	119.48	122.79
22	a	2503	2MA	C6-C5-C4	3.01	121.23	117.18
1	A	1516	2MG	C5-C6-N1	2.98	120.77	113.19
33	l	81	4D4	NE-CZ-NH2	-2.98	115.45	120.70
1	A	966	2MG	C5-C6-N1	2.96	120.72	113.19
1	A	1519	MA6	N1-C6-N6	-2.95	113.86	117.08
55	V	38	5MC	CM5-C5-C6	-2.94	118.93	122.85
1	A	1516	2MG	CM2-N2-C2	-2.93	117.39	123.86
1	A	1516	2MG	N9-C4-N3	2.91	131.78	125.94
22	a	1835	2MG	C5-C6-N1	2.90	120.56	113.19
1	A	1519	MA6	C4-C5-N7	-2.86	107.13	110.62
1	A	527	G7M	N9-C4-N3	2.85	131.67	125.94
22	a	746	PSU	O2-C2-N1	-2.84	119.66	122.79
22	a	1835	2MG	N9-C8-N7	-2.82	108.08	113.39
22	a	2580	PSU	O2-C2-N1	-2.82	119.69	122.79
1	A	1516	2MG	O6-C6-C5	-2.81	119.13	126.60
55	V	6	2MG	C5-C6-N1	2.80	120.31	113.19
1	A	1207	2MG	C5-C6-N1	2.79	120.29	113.19
22	a	2503	2MA	C5-N7-C8	2.78	107.46	103.51
22	a	2552	OMU	O2-C2-N1	-2.78	119.09	122.79
22	a	1939	5MU	O4-C4-N3	-2.77	114.81	120.12
55	V	34	56B	N9-C4-N3	2.76	131.47	125.94
1	A	516	PSU	O2-C2-N1	-2.75	119.77	122.79
1	A	966	2MG	O6-C6-C5	-2.74	119.32	126.60
22	a	1911	PSU	O2-C2-N1	-2.74	119.77	122.79
22	a	2251	OMG	C5-C6-N1	2.73	120.13	113.19
22	a	2030	6MZ	C4-C5-N7	-2.73	107.29	110.62
22	a	2604	PSU	O2-C2-N1	-2.72	119.79	122.79
22	a	2457	PSU	C6-N1-C2	-2.72	119.91	122.68
1	A	1207	2MG	O6-C6-C5	-2.71	119.41	126.60
33	l	81	4D4	CB-CA-C	-2.71	107.45	111.77
1	A	1518	MA6	C4-C5-N7	-2.69	107.35	110.62
22	a	745	1MG	N9-C4-N3	2.67	131.30	125.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	V	6	2MG	O6-C6-C5	-2.67	119.52	126.60
22	a	2030	6MZ	C4-C5-C6	2.66	118.87	116.81
22	a	1915	3TD	C6-C5-C4	2.66	120.06	118.22
33	l	82	MS6	CE-SD-CG	2.64	109.48	100.40
1	A	967	5MC	C5-C6-N1	-2.64	120.62	123.34
55	V	53	5MU	O4-C4-N3	-2.63	115.08	120.12
22	a	1618	6MZ	C4-N9-C8	2.62	108.57	105.73
22	a	2504	PSU	O2-C2-N1	-2.62	119.91	122.79
55	V	13	PSU	C6-N1-C2	-2.61	120.01	122.68
22	a	745	1MG	C1'-N9-C8	-2.61	119.27	126.70
22	a	747	5MU	O4-C4-N3	-2.60	115.13	120.12
22	a	2445	2MG	CM2-N2-C2	-2.59	118.13	123.86
22	a	2580	PSU	O4'-C1'-C2'	2.58	108.78	105.14
54	Z	55	5MU	O4-C4-N3	-2.55	115.22	120.12
22	a	2552	OMU	O4-C4-C5	-2.53	120.70	125.16
22	a	2030	6MZ	C5-C4-N9	2.53	108.72	105.78
22	a	2030	6MZ	C4-N9-C8	2.52	108.46	105.73
22	a	1835	2MG	O6-C6-C5	-2.52	119.92	126.60
22	a	2251	OMG	O6-C6-C5	-2.51	119.95	126.60
1	A	527	G7M	CN7-N7-C5	2.50	129.87	126.77
22	a	2069	G7M	CN7-N7-C5	2.50	129.87	126.77
55	V	53	5MU	O2-C2-N1	-2.49	119.47	122.79
1	A	1519	MA6	C4-N9-C8	2.49	108.42	105.73
55	V	54	PSU	C6-N1-C2	-2.48	120.15	122.68
54	Z	56	PSU	O2-C2-N1	-2.48	120.06	122.79
22	a	2504	PSU	C6-N1-C2	-2.47	120.16	122.68
22	a	747	5MU	O2-C2-N1	-2.45	119.53	122.79
22	a	1618	6MZ	C5-C6-N1	2.45	120.81	118.20
1	A	1519	MA6	C5-C4-N9	2.43	108.61	105.78
54	Z	55	5MU	O2-C2-N1	-2.40	119.59	122.79
1	A	1407	5MC	CM5-C5-C6	-2.40	119.64	122.85
33	l	81	4D4	O-C-CA	-2.40	118.49	124.78
1	A	1516	2MG	C1'-N9-C4	-2.39	119.42	126.50
22	a	2251	OMG	C1'-N9-C4	-2.39	119.42	126.50
55	V	34	56B	C11-C12-C13	2.38	105.11	102.81
1	A	1402	4OC	C6-C5-C4	2.38	119.87	116.96
1	A	1518	MA6	C5-C4-N9	2.37	108.54	105.78
1	A	1207	2MG	N1-C2-N3	-2.37	120.29	123.95
22	a	2069	G7M	N9-C4-N3	2.36	130.68	125.94
55	V	6	2MG	CM2-N2-C2	-2.35	118.66	123.86
22	a	1917	PSU	O2-C2-N1	-2.35	120.21	122.79
55	V	57	1MA	C6-C5-N7	-2.35	127.93	132.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	955	PSU	C6-N1-C2	-2.33	120.31	122.68
1	A	966	2MG	CM2-N2-C2	-2.32	118.74	123.86
1	A	966	2MG	N1-C2-N3	-2.31	120.38	123.95
22	a	2445	2MG	O6-C6-C5	-2.30	120.49	126.60
22	a	1835	2MG	CM2-N2-C2	-2.29	118.81	123.86
12	L	89	D2T	O-C-CA	-2.28	118.79	124.78
22	a	2445	2MG	N1-C2-N3	-2.26	120.45	123.95
54	Z	21	H2U	C5-C6-N1	-2.26	104.16	111.61
22	a	1962	5MC	CM5-C5-C6	-2.25	119.84	122.85
1	A	1518	MA6	N3-C4-N9	2.22	130.74	127.08
55	V	9	1MA	C6-C5-N7	-2.22	128.16	132.20
22	a	2449	H2U	C4-N3-C2	-2.21	123.96	125.79
55	V	6	2MG	N1-C2-N3	-2.20	120.55	123.95
22	a	2445	2MG	C8-N7-C5	2.20	108.22	104.24
1	A	1207	2MG	CM2-N2-C2	-2.19	119.02	123.86
1	A	1516	2MG	C8-N7-C5	2.19	108.21	104.24
1	A	516	PSU	O4'-C1'-C2'	2.19	108.23	105.14
1	A	1518	MA6	C4-N9-C8	2.17	108.08	105.73
25	d	150	MEQ	OE1-CD-CG	2.17	125.99	122.02
1	A	516	PSU	C6-N1-C2	-2.16	120.47	122.68
22	a	2580	PSU	C6-C5-C4	2.16	119.71	118.20
22	a	2069	G7M	N9-C8-N7	-2.16	106.86	112.21
22	a	2069	G7M	N2-C2-N1	2.16	121.31	116.71
55	V	13	PSU	C6-C5-C4	2.15	119.70	118.20
54	Z	8	4SU	O2-C2-N1	-2.14	119.94	122.79
1	A	1518	MA6	C5-C6-N6	2.13	129.01	125.30
55	V	47	5MC	CM5-C5-C6	-2.12	120.01	122.85
22	a	2030	6MZ	N3-C4-N9	2.12	130.58	127.08
1	A	966	2MG	C8-N7-C5	2.12	108.08	104.24
1	A	527	G7M	N9-C8-N7	-2.11	106.98	112.21
11	K	119	IAS	OXT-C-CA	2.11	120.57	113.38
1	A	1402	4OC	O2-C2-N3	-2.08	118.95	122.33
22	a	1915	3TD	O4'-C1'-C2'	2.07	108.06	105.14
22	a	1835	2MG	N1-C2-N3	-2.04	120.80	123.95
22	a	2605	PSU	C5-C4-N3	2.04	121.19	116.58
1	A	1519	MA6	N3-C4-N9	2.03	130.43	127.08
22	a	2069	G7M	CN7-N7-C8	-2.02	121.72	124.84
1	A	527	G7M	CN7-N7-C8	-2.02	121.72	124.84
22	a	2503	2MA	N6-C6-N1	2.01	119.87	117.03
1	A	1498	UR3	C3U-N3-C2	2.00	120.83	117.31

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	L	89	D2T	CG-CB-SB-CB1
33	l	81	4D4	CA-CB-CG-CD
54	Z	21	H2U	O4'-C1'-N1-C6
54	Z	21	H2U	C2'-C1'-N1-C2
54	Z	21	H2U	C2'-C1'-N1-C6
22	a	2251	OMG	C1'-C2'-O2'-CM2
55	V	9	1MA	C3'-C4'-C5'-O5'
55	V	19	H2U	O4'-C1'-N1-C6
55	V	34	56B	C11-C10-N10-C9
55	V	47	5MC	C3'-C4'-C5'-O5'
55	V	48	5MC	O4'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
22	a	2030	6MZ	O4'-C4'-C5'-O5'
22	a	2030	6MZ	C3'-C4'-C5'-O5'
55	V	9	1MA	O4'-C4'-C5'-O5'
55	V	48	5MC	C3'-C4'-C5'-O5'
54	Z	55	5MU	C3'-C4'-C5'-O5'
54	Z	55	5MU	O4'-C4'-C5'-O5'
25	d	150	MEQ	NE2-CD-CG-CB
25	d	150	MEQ	OE1-CD-CG-CB
33	l	81	4D4	OB-CB-CG-CD
55	V	19	H2U	C2'-C1'-N1-C6
22	a	2445	2MG	C3'-C4'-C5'-O5'
55	V	47	5MC	O4'-C4'-C5'-O5'
1	A	527	G7M	C3'-C4'-C5'-O5'
22	a	2445	2MG	O4'-C4'-C5'-O5'
55	V	19	H2U	C2'-C1'-N1-C2
33	l	82	MS6	CB-CG-SD-CE
33	l	81	4D4	NE-CD-CG-CB
1	A	966	2MG	C3'-C4'-C5'-O5'
54	Z	21	H2U	C3'-C4'-C5'-O5'
55	V	19	H2U	O4'-C1'-N1-C2
54	Z	21	H2U	C4'-C5'-O5'-P
54	Z	21	H2U	O4'-C4'-C5'-O5'
55	V	13	PSU	C3'-C4'-C5'-O5'
55	V	47	5MC	C4'-C5'-O5'-P
33	l	81	4D4	CG-CD-NE-CZ
33	l	81	4D4	N-CA-CB-CG
12	L	89	D2T	CA-CB-SB-CB1
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	966	2MG	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
55	V	6	2MG	C3'-C4'-C5'-O5'
1	A	527	G7M	O4'-C4'-C5'-O5'
22	a	746	PSU	O4'-C1'-C5-C6
22	a	2069	G7M	O4'-C4'-C5'-O5'
54	Z	21	H2U	O4'-C1'-N1-C2
22	a	2503	2MA	O4'-C4'-C5'-O5'
33	l	81	4D4	O-C-CA-CB

There are no ring outliers.

11 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	Z	21	H2U	1	0
55	V	53	5MU	2	0
1	A	967	5MC	1	0
1	A	1519	MA6	1	0
55	V	57	1MA	1	0
1	A	1516	2MG	1	0
55	V	34	56B	1	0
1	A	966	2MG	1	0
22	a	2030	6MZ	3	0
54	Z	55	5MU	1	0
55	V	6	2MG	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 260 ligands modelled in this entry, 259 are monoatomic - leaving 1 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	$\#\|Z\|>2$
57	MAN	V	103	55	11,11,12	2.06	5 (45%)	15,15,17	1.20	1 (6%)

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
57	MAN	V	103	55	-	1/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	V	103	MAN	C4-C5	3.57	1.60	1.53
57	V	103	MAN	O2-C2	-2.90	1.37	1.43
57	V	103	MAN	O3-C3	-2.51	1.37	1.43
57	V	103	MAN	O5-C1	-2.47	1.39	1.43
57	V	103	MAN	O4-C4	-2.31	1.37	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	V	103	MAN	O5-C1-C2	-2.03	107.63	110.77

There are no chirality outliers.

All (1) torsion outliers are listed below:

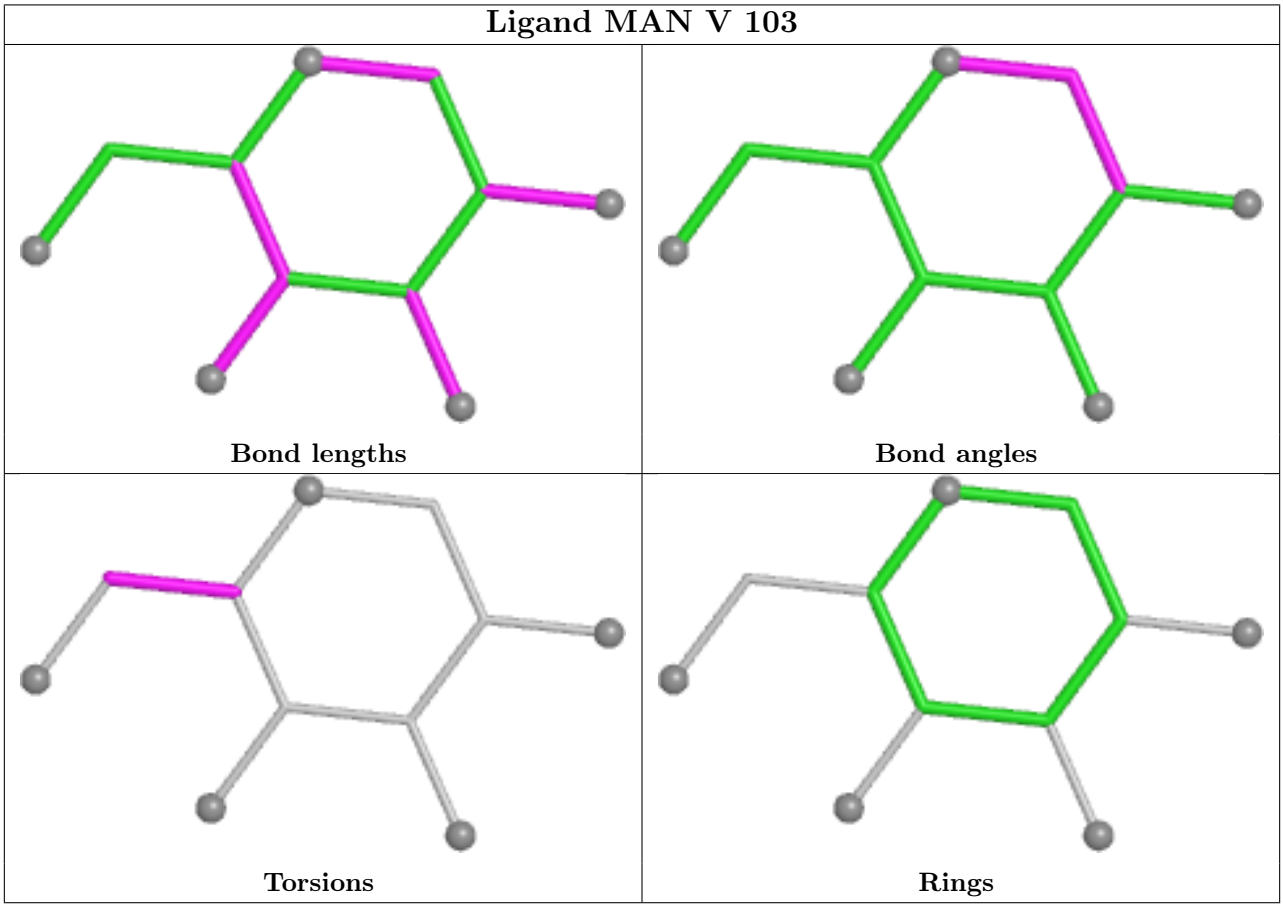
Mol	Chain	Res	Type	Atoms
57	V	103	MAN	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

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



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	119:IAS	CG	120:GLY	N	1.19

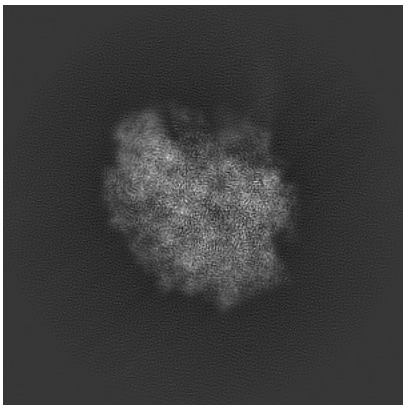
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33663. These allow visual inspection of the internal detail of the map and identification of artifacts.

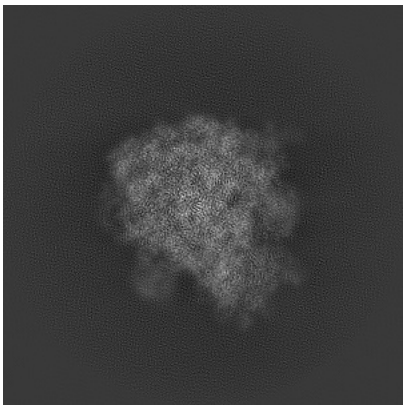
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

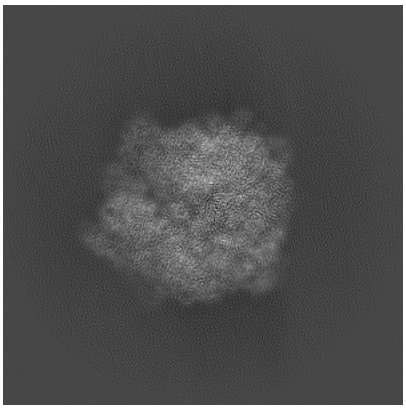
6.1.1 Primary map



X

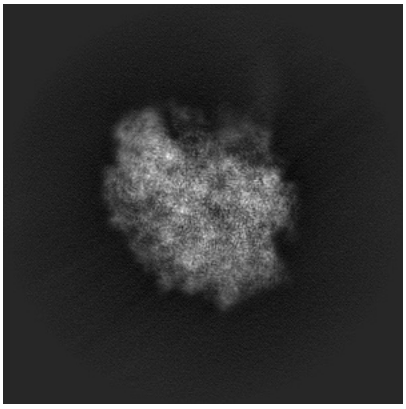


Y

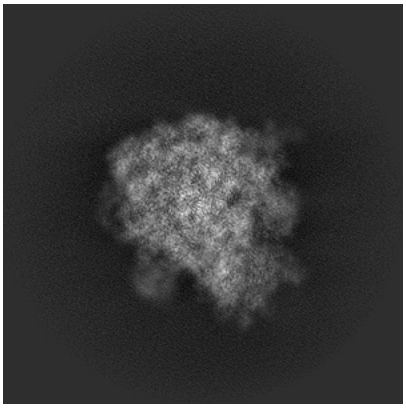


Z

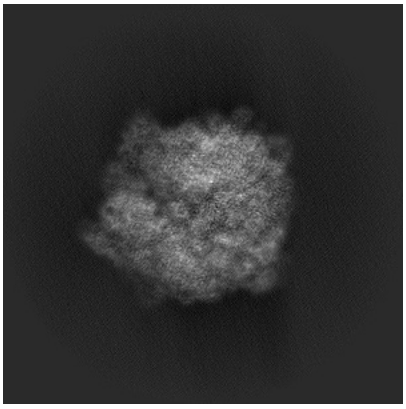
6.1.2 Raw map



X



Y

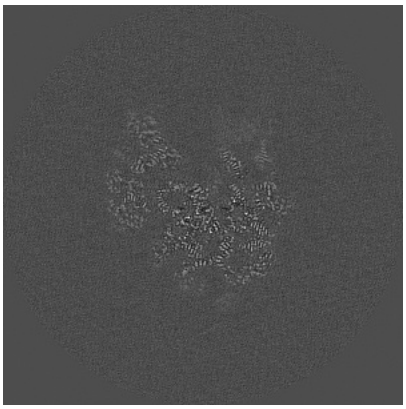


Z

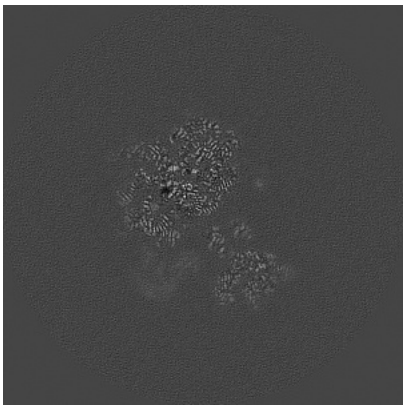
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

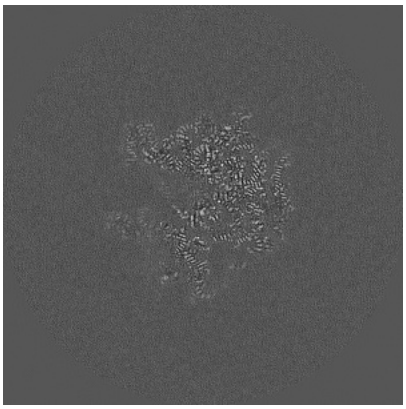
6.2.1 Primary map



X Index: 265

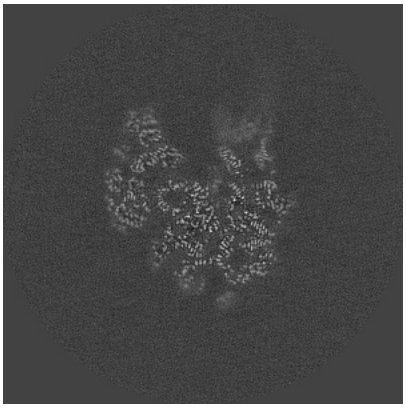


Y Index: 265

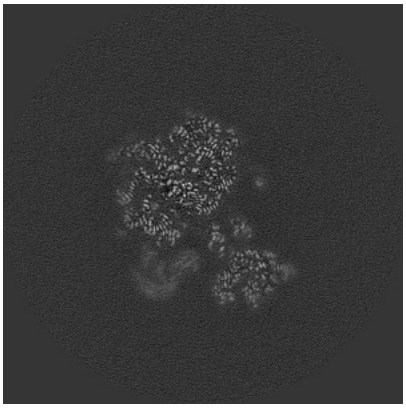


Z Index: 265

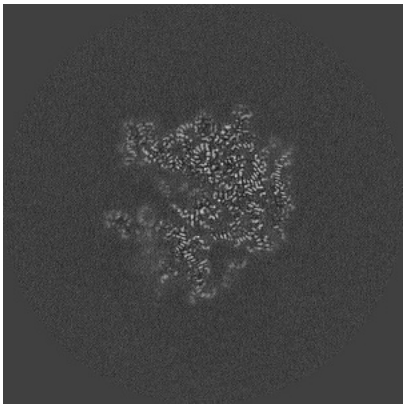
6.2.2 Raw map



X Index: 265



Y Index: 265

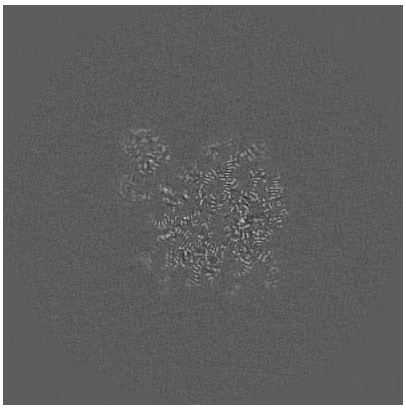


Z Index: 265

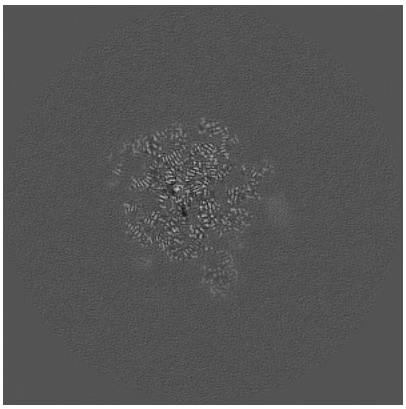
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

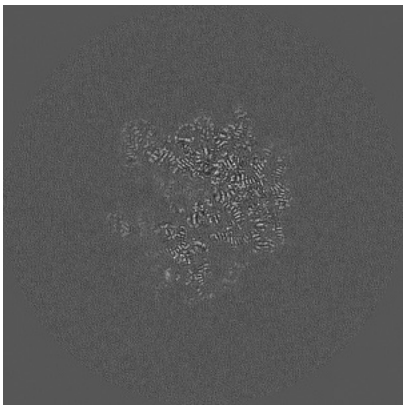
6.3.1 Primary map



X Index: 297

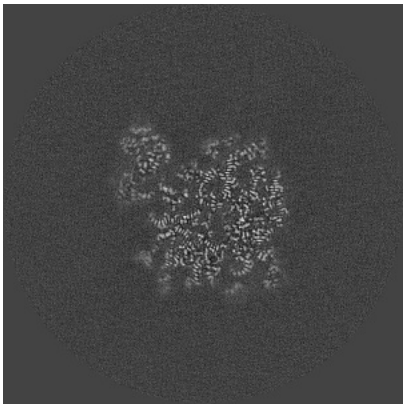


Y Index: 318

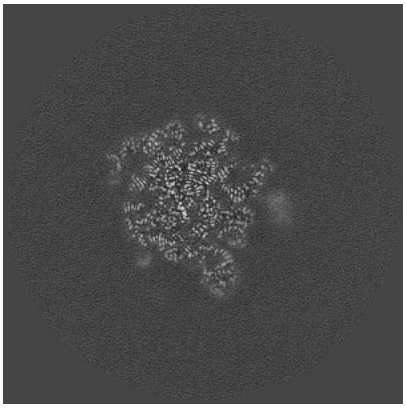


Z Index: 268

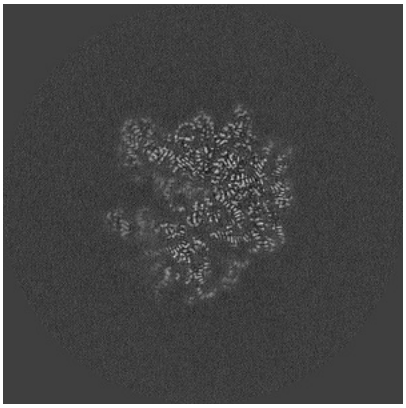
6.3.2 Raw map



X Index: 297



Y Index: 320

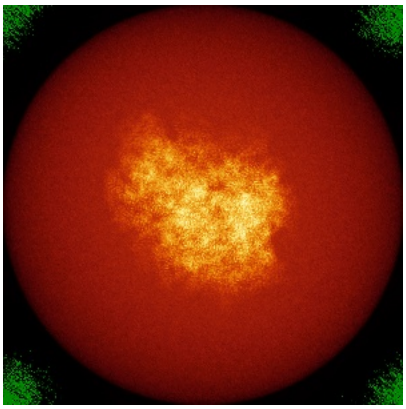


Z Index: 268

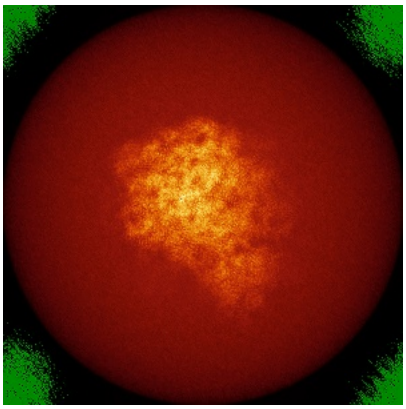
The images above show the largest variance slices of the map in three orthogonal directions.

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

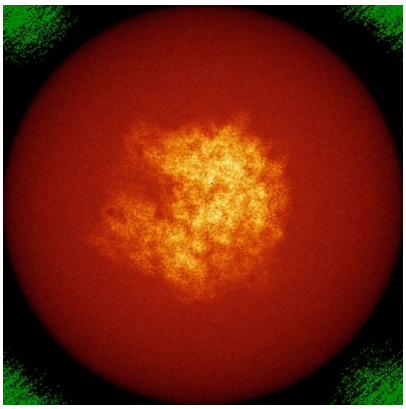
6.4.1 Primary map



X

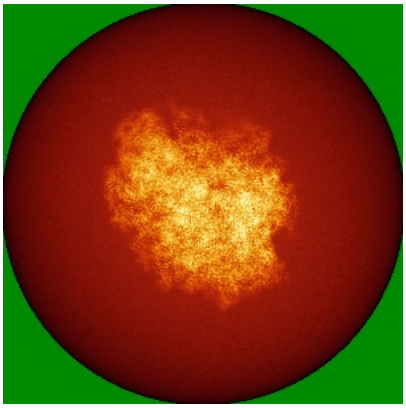


Y

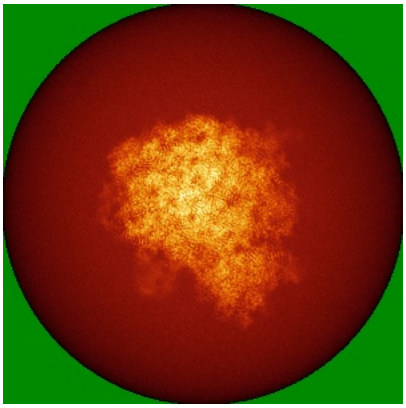


Z

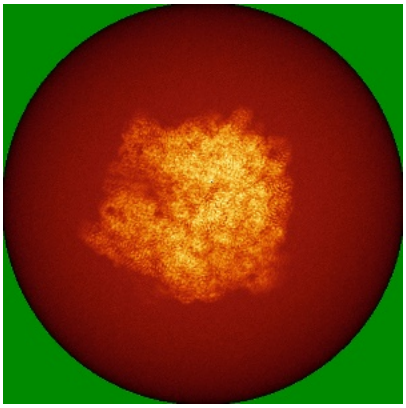
6.4.2 Raw map



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 0.04. 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.

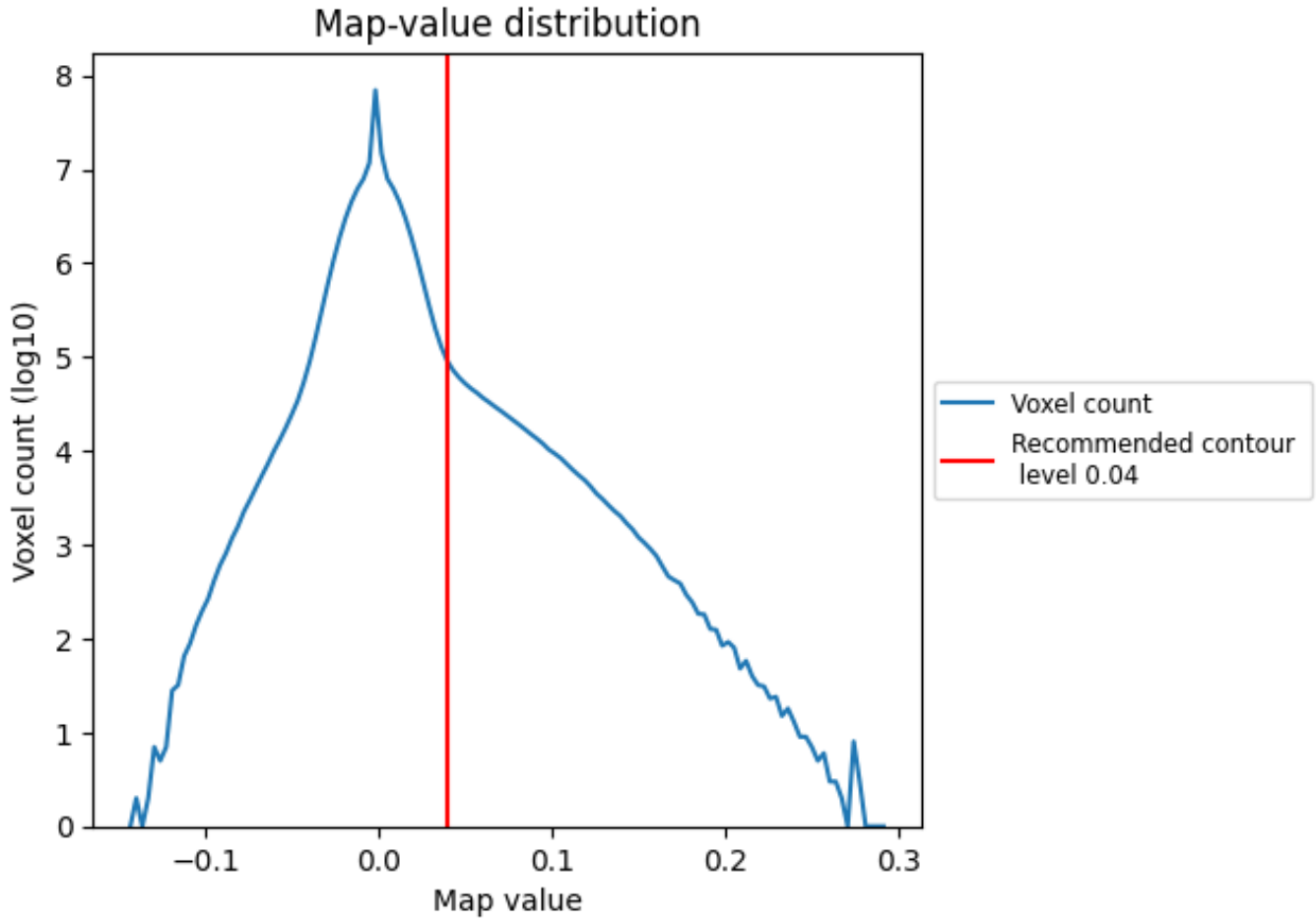
6.6 Mask visualisation (i)

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

7 Map analysis

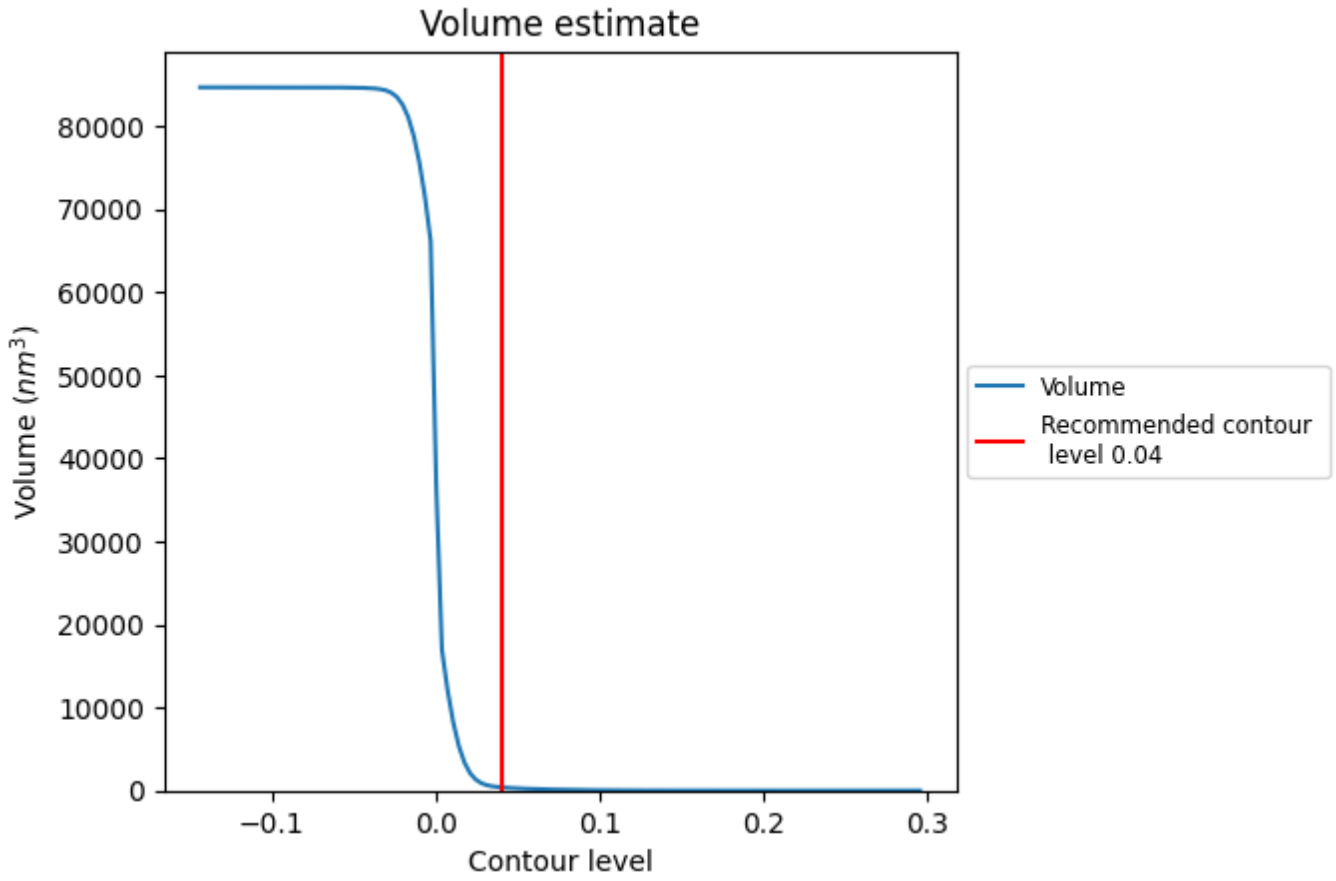
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

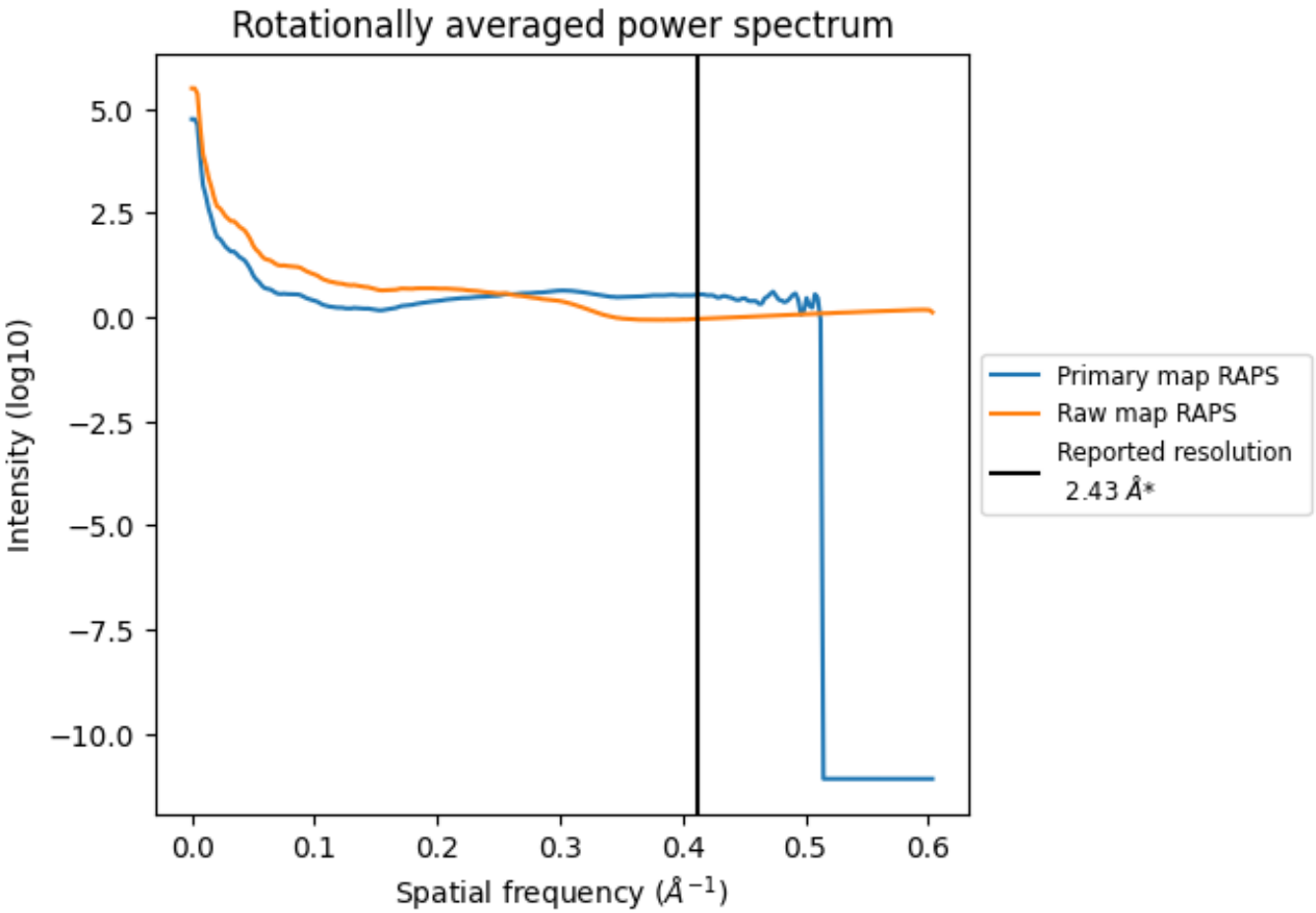
7.2 Volume estimate



The volume at the recommended contour level is 386 nm^3; this corresponds to an approximate mass of 349 kDa.

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

7.3 Rotationally averaged power spectrum (i)

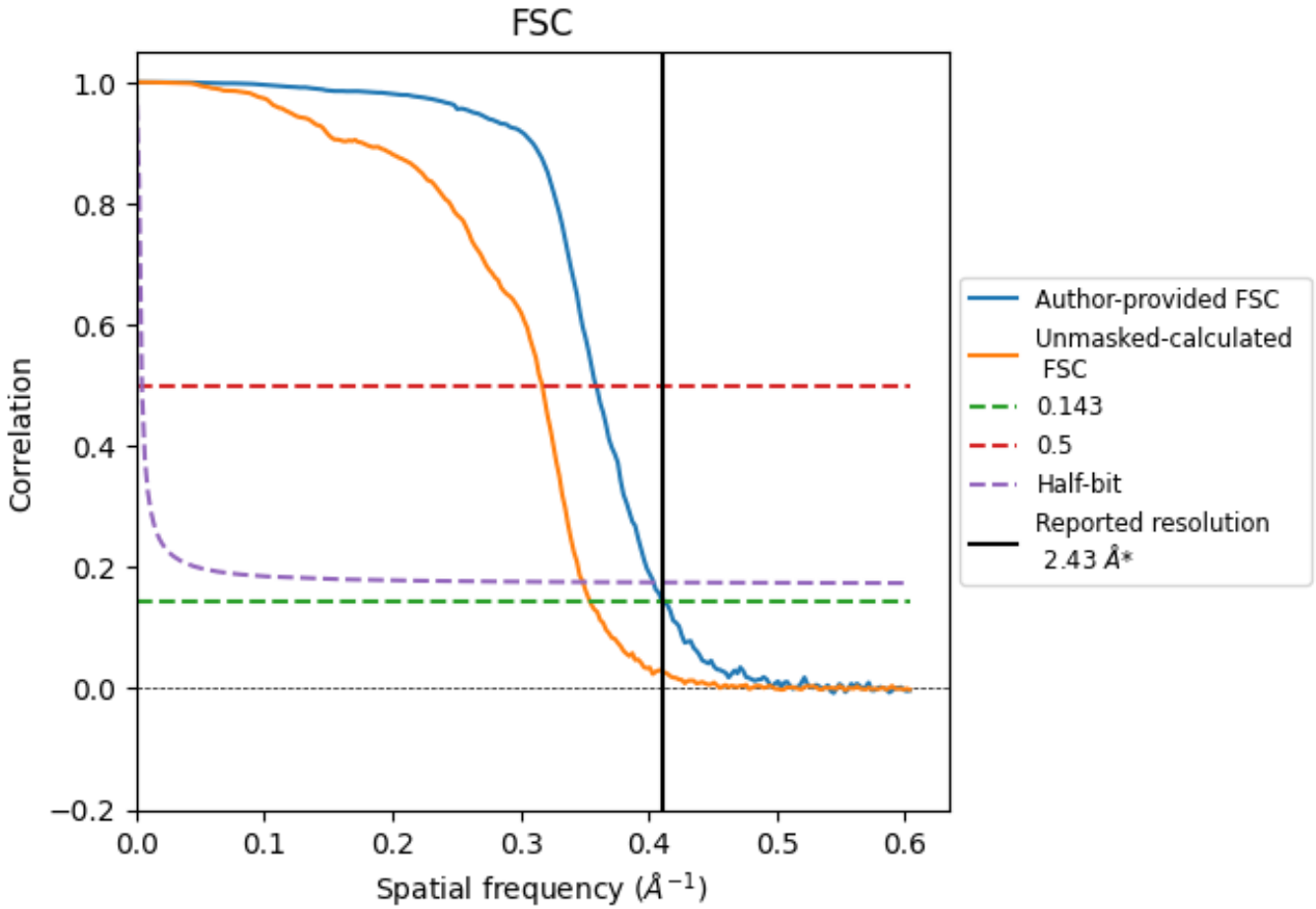


*Reported resolution corresponds to spatial frequency of 0.412 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.412 Å^{-1}

8.2 Resolution estimates (i)

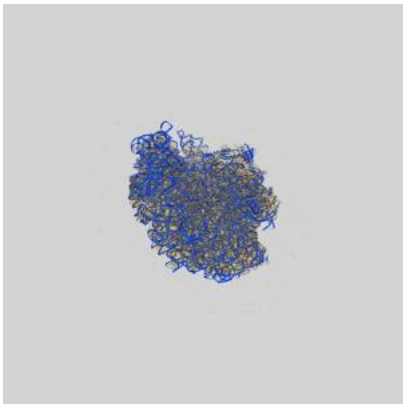
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.43	-	-
Author-provided FSC curve	2.42	2.79	2.48
Unmasked-calculated*	2.82	3.16	2.87

*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 2.82 differs from the reported value 2.43 by more than 10 %

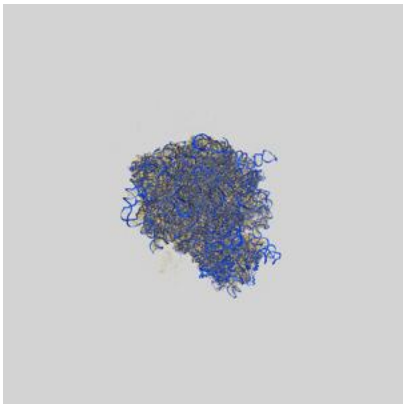
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33663 and PDB model 7Y7F. Per-residue inclusion information can be found in section 3 on page 16.

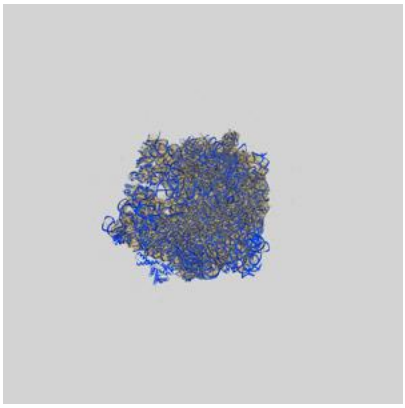
9.1 Map-model overlay



X



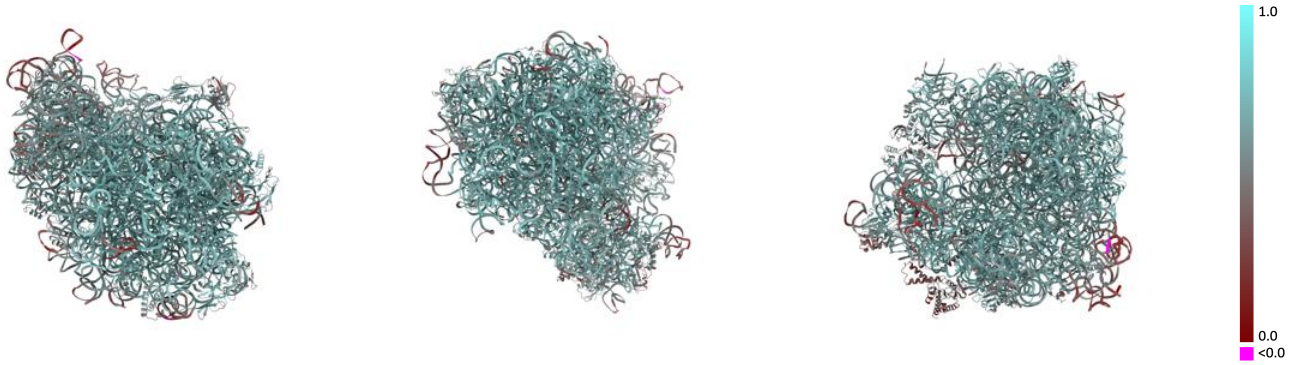
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

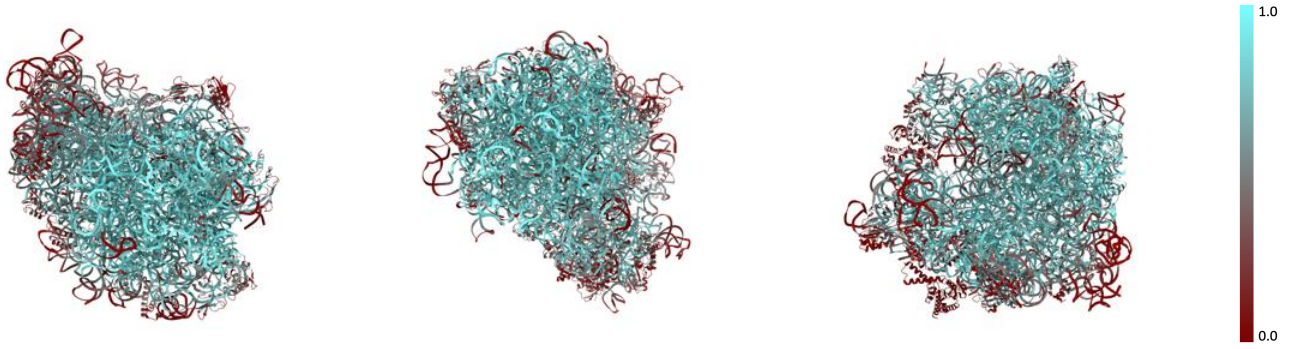
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

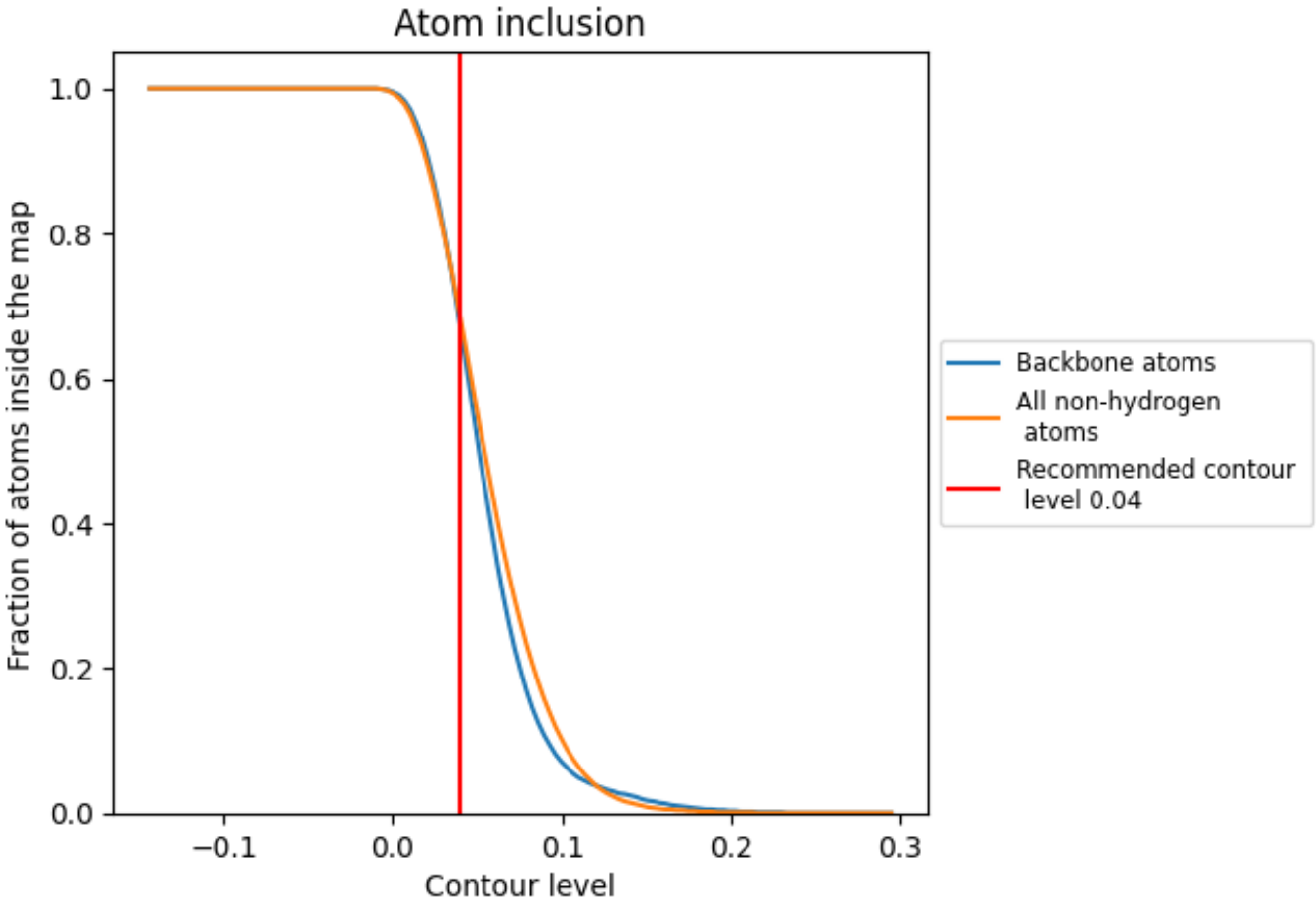
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 68% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6830	0.6360
0	0.6500	0.6520
1	0.9100	0.7100
2	0.8660	0.7000
3	0.7640	0.6610
4	0.1230	0.4540
A	0.6690	0.6220
B	0.0090	0.3660
C	0.4820	0.6050
D	0.2430	0.5520
E	0.5970	0.6490
F	0.2600	0.5260
G	0.3280	0.5500
H	0.5760	0.6410
I	0.4360	0.5930
J	0.3150	0.5140
K	0.4810	0.6030
L	0.6610	0.6530
M	0.4100	0.5980
N	0.5260	0.6210
O	0.5250	0.6100
P	0.3620	0.5670
Q	0.3900	0.5840
R	0.4400	0.5800
S	0.4480	0.6000
T	0.3040	0.5540
U	0.1700	0.4740
V	0.5250	0.5790
X	0.5660	0.6110
Z	0.5090	0.5620
a	0.8100	0.6670
b	0.6840	0.6340
c	0.8300	0.7090
d	0.7690	0.6890
e	0.5590	0.6290



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	0.3380	0.5580
g	0.2460	0.5180
h	0.1630	0.5140
i	0.7830	0.6740
j	0.7420	0.6790
k	0.7010	0.6660
l	0.8050	0.6950
m	0.8580	0.7000
n	0.5350	0.6270
o	0.6940	0.6630
p	0.8480	0.7080
q	0.6210	0.6380
r	0.7390	0.6710
s	0.5320	0.5950
t	0.4000	0.5590
u	0.5490	0.6190
v	0.7830	0.6830
w	0.7450	0.6760
x	0.3170	0.5460
y	0.7440	0.6610
z	0.7370	0.6790