



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:53 PM UTC

PDB ID : 5H5U / pdb_00005h5u
EMDB ID : EMD-6667
Title : Mechanistic insights into the alternative translation termination by ArfA and RF2
Authors : Ma, C.; Kurita, D.; Li, N.; Chen, Y.; Himeno, H.; Gao, N.
Deposited on : 2016-11-09
Resolution : 3.01 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

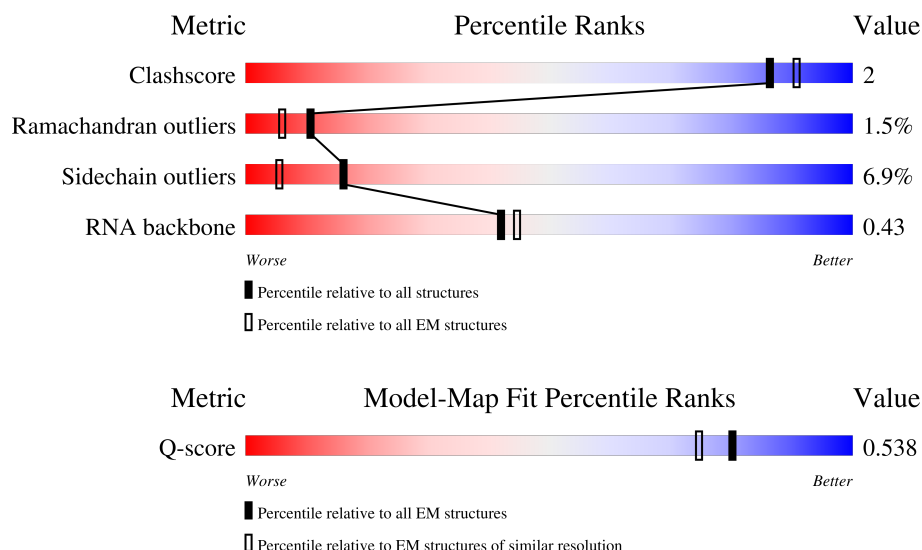
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.01 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	13882 (2.51 - 3.51)

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

Mol	Chain	Length	Quality of chain
1	1	86	92% 7% .
2	2	70	69% 11% 20%
3	3	72	47% 12% . 38%

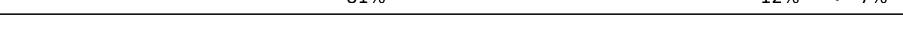
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Mol	Chain	Length	Quality of chain
4	4	365	
5	5	76	
6	7	6	
7	A	2903	
8	B	120	
9	C	272	
10	D	209	
11	E	201	
12	F	178	
13	G	176	
14	H	149	
15	I	164	
16	J	141	
17	K	142	
18	L	123	
19	M	144	
20	N	136	
21	O	127	
22	P	117	
23	Q	114	
24	R	117	
25	S	103	
26	T	110	
27	U	100	
28	V	103	

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Mol	Chain	Length	Quality of chain
29	W	94	
30	X	84	
31	Y	77	
32	Z	63	
33	a	58	
34	b	56	
35	c	54	
36	d	46	
37	e	64	
38	f	38	
39	h	1534	
40	i	240	
41	j	232	
42	k	205	
43	l	166	
44	m	135	
45	n	178	
46	o	129	
47	p	129	
48	q	103	
49	r	128	
50	s	123	
51	t	117	
52	u	100	
53	v	88	

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Mol	Chain	Length	Quality of chain
54	w	82	84% 15%
55	x	83	81% 12%
56	y	74	69% 5% 26%
57	z	91	74% 12%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 148128 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 2 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 3 is a protein called Alternative ribosome-rescue factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	45	Total	C	N	O	S	0	0
			369	229	76	63	1		

- Molecule 4 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	357	Total	C	N	O	S	0	0
			2829	1740	499	580	10		

- Molecule 5 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	76	Total	C	N	O	P	0	0
			1620	723	294	528	75		

- Molecule 6 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	6	Total	C	N	O	P	0	0
			127	57	22	42	6		

- Molecule 7 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	2897	Total	C	N	O	P	3	0
			62240	27765	11457	20119	2899		

- Molecule 8 is a RNA chain called 5S Ribosomal RNA.

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

- Molecule 9 is a protein called 50S ribosomal protein L2.

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

- Molecule 10 is a protein called 50S ribosomal protein L3.

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

- Molecule 11 is a protein called 50S ribosomal protein L4.

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

- Molecule 12 is a protein called 50S ribosomal protein L5.

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

- Molecule 13 is a protein called 50S ribosomal protein L6.

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

- Molecule 14 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	148	Total	C	N	O	S	0	0
			1101	694	196	210	1		

- Molecule 15 is a protein called 50S ribosomal protein L10.

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

- Molecule 16 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	71	Total	C	N	O	S	0	0
			509	313	93	100	3		

- Molecule 17 is a protein called 50S ribosomal protein L13.

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

- Molecule 18 is a protein called 50S ribosomal protein L14.

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

- Molecule 19 is a protein called 50S ribosomal protein L15.

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

- Molecule 20 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	136	Total	C	N	O	S	1	0
			1082	691	208	177	6		

- Molecule 21 is a protein called 50S ribosomal protein L17.

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

- Molecule 22 is a protein called 50S ribosomal protein L18.

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

- Molecule 23 is a protein called 50S ribosomal protein L19.

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

- Molecule 24 is a protein called 50S ribosomal protein L20.

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

- Molecule 25 is a protein called 50S ribosomal protein L21.

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

- Molecule 26 is a protein called 50S ribosomal protein L22.

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

- Molecule 27 is a protein called 50S ribosomal protein L23.

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

- Molecule 28 is a protein called 50S ribosomal protein L24.

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

- Molecule 29 is a protein called 50S ribosomal protein L25.

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

- Molecule 30 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	X	76	Total	C	N	O	S	
			591	365	121	104	1	0

- Molecule 31 is a protein called 50S ribosomal protein L28.

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

- Molecule 32 is a protein called 50S ribosomal protein L29.

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

- Molecule 33 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	a	58	Total	C	N	O	S	
			463	290	90	81	2	0

- Molecule 34 is a protein called 50S ribosomal protein L32.

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

- Molecule 35 is a protein called 50S ribosomal protein L33.

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

- Molecule 36 is a protein called 50S ribosomal protein L34.

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

- Molecule 37 is a protein called 50S ribosomal protein L35.

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

- Molecule 38 is a protein called 50S ribosomal protein L36.

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

- Molecule 39 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	1534	Total	C	N	O	P	0	0
			32917	14681	6041	10661	1534		

- Molecule 40 is a protein called 30S ribosomal protein S2.

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

- Molecule 41 is a protein called 30S ribosomal protein S3.

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

- Molecule 42 is a protein called 30S ribosomal protein S4.

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

- Molecule 43 is a protein called 30S ribosomal protein S5.

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

- Molecule 44 is a protein called 30S ribosomal protein S6.

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

- Molecule 45 is a protein called 30S ribosomal protein S7.

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

- Molecule 46 is a protein called 30S ribosomal protein S8.

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

- Molecule 47 is a protein called 30S ribosomal protein S9.

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

- Molecule 48 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 49 is a protein called 30S ribosomal protein S11.

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

- Molecule 50 is a protein called 30S ribosomal protein S12.

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

- Molecule 51 is a protein called 30S ribosomal protein S13.

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

- Molecule 52 is a protein called 30S ribosomal protein S14.

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

- Molecule 53 is a protein called 30S ribosomal protein S15.

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

- Molecule 54 is a protein called 30S ribosomal protein S16.

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

- Molecule 55 is a protein called 30S ribosomal protein S17.

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

- Molecule 56 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	y	55	Total	C	N	O	0	0
			455	288	86	81		

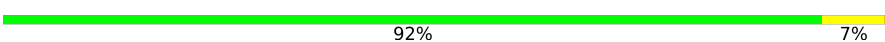
- Molecule 57 is a protein called 30S ribosomal protein S19.

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

3 Residue-property plots

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

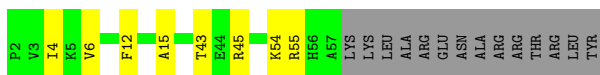
- Molecule 1: 30S ribosomal protein S20

Chain 1: 

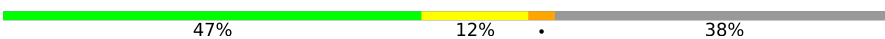


- Molecule 2: 30S ribosomal protein S21

Chain 2: 



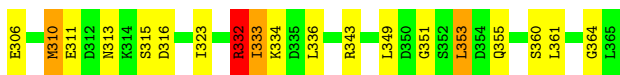
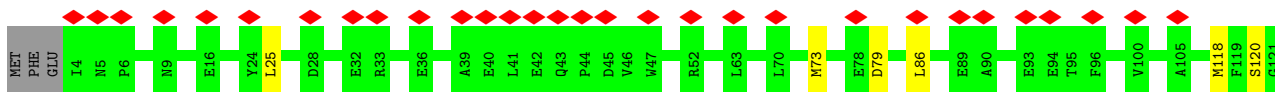
- Molecule 3: Alternative ribosome-rescue factor A

Chain 3: 



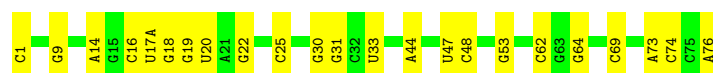
- Molecule 4: Peptide chain release factor 2

Chain 4: 



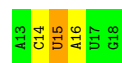
- Molecule 5: P-site tRNA

Chain 5:  70% 30%



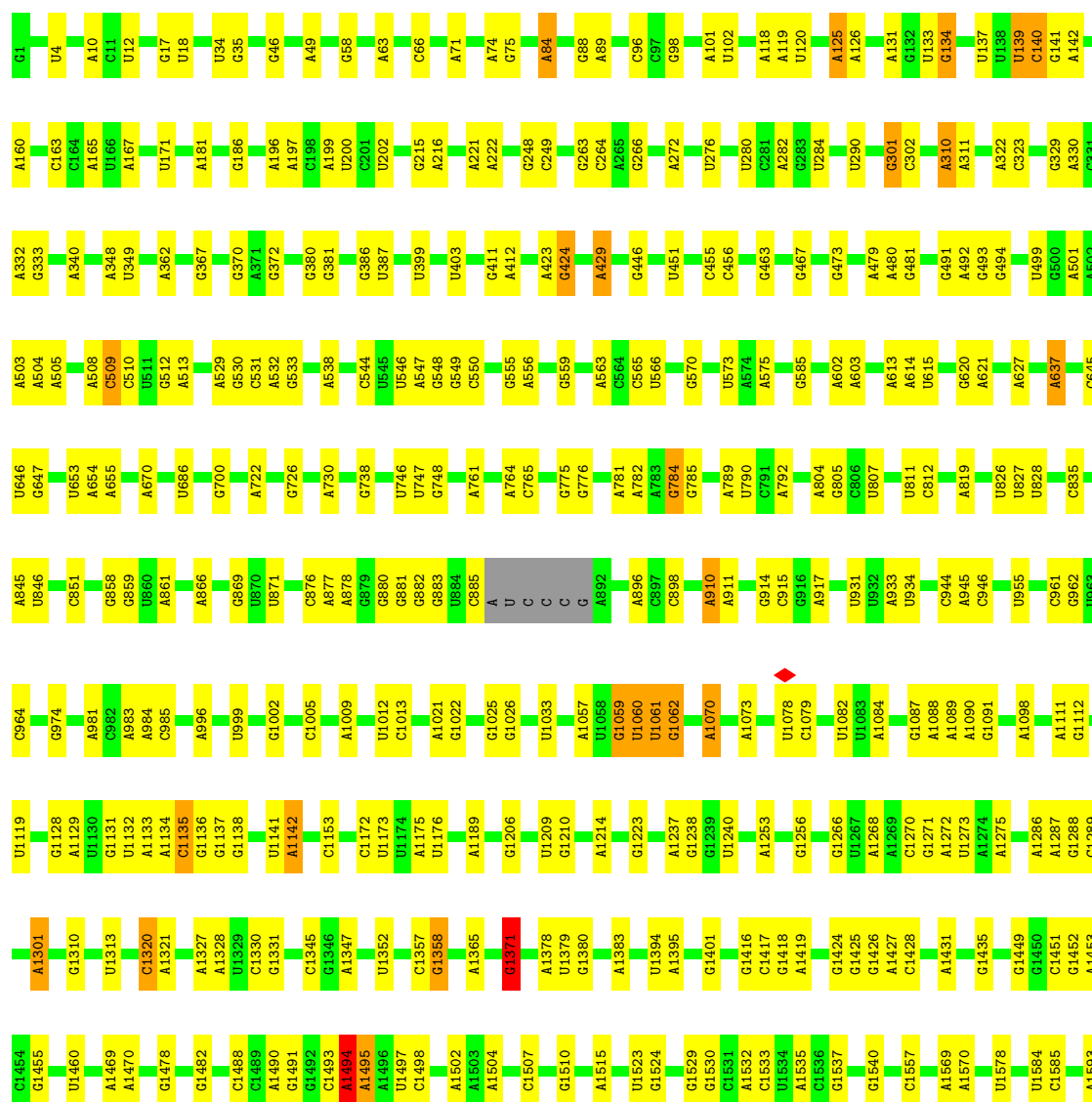
• Molecule 6: mRNA

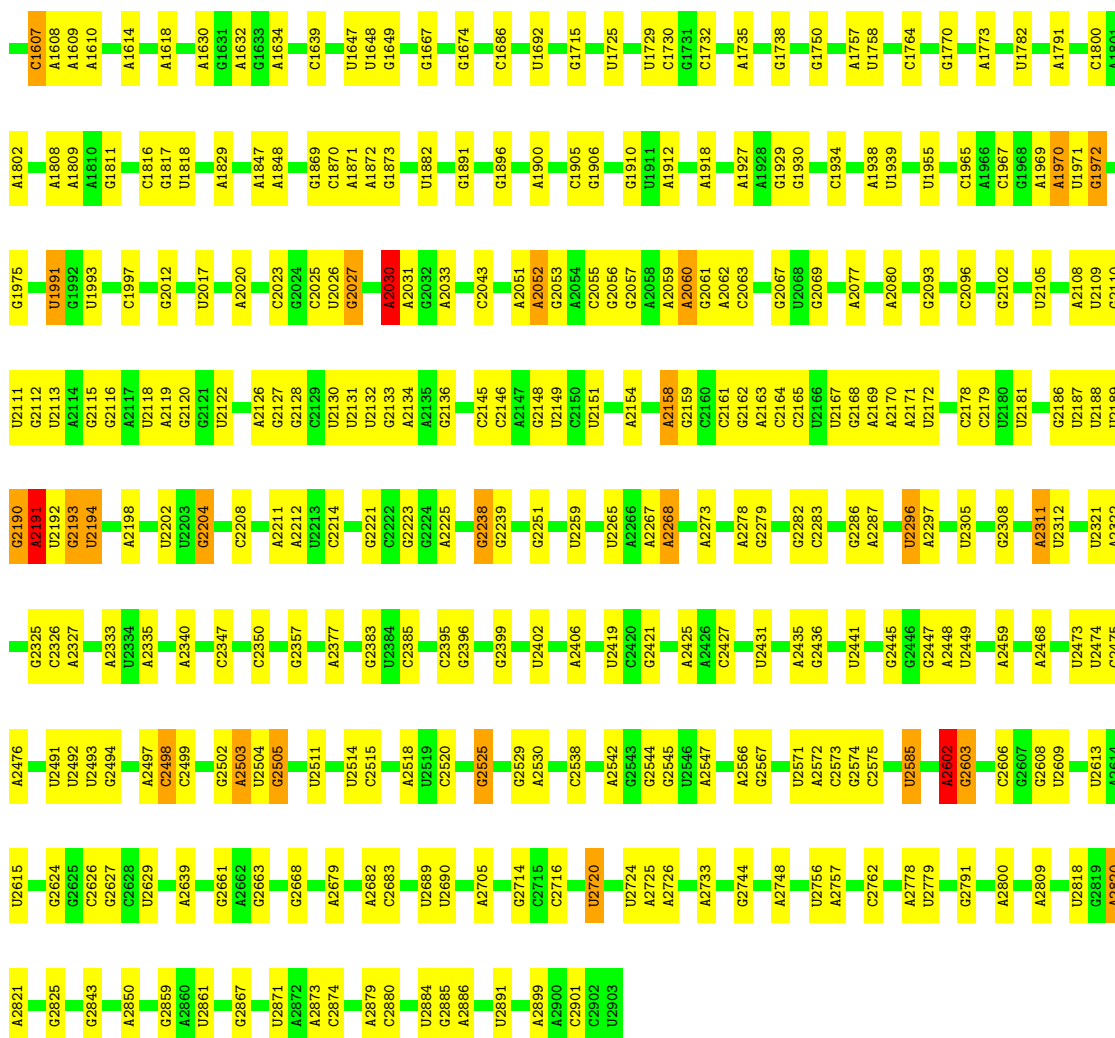
Chain 7:  50% 33% 17%



• Molecule 7: 23S rRNA

Chain A:  76% 22% .

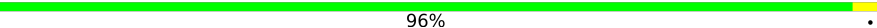




Chain D:  87% 11% .



- Molecule 11: 50S ribosomal protein L4

Chain E:  96% .



- Molecule 12: 50S ribosomal protein L5

Chain F:  87% 11% ..

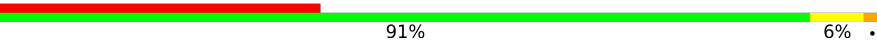


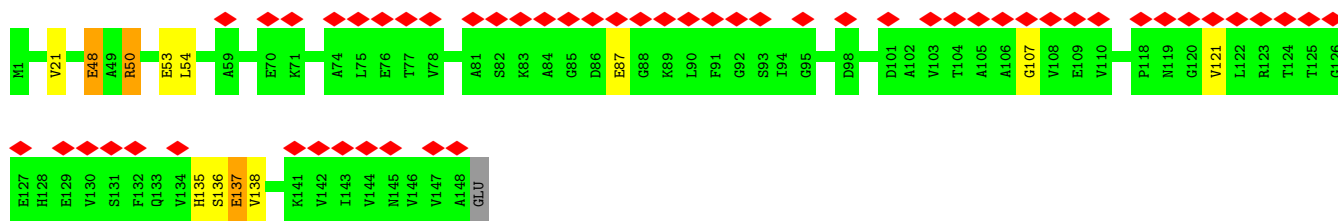
- Molecule 13: 50S ribosomal protein L6

Chain G:  89% 10% .



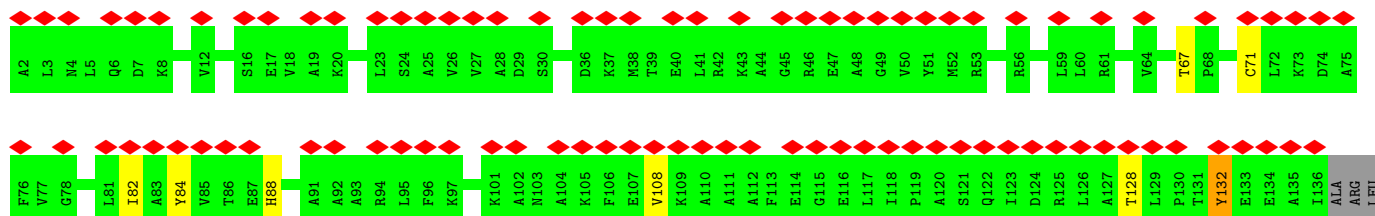
- Molecule 14: 50S ribosomal protein L9

Chain H:  36% 91% 6% ..



- Molecule 15: 50S ribosomal protein L10

Chain I:  55% 77% 18%



- Molecule 16: 50S ribosomal protein L11



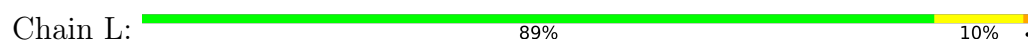
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-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

[illegible]

- Molecule 17: 50S ribosomal protein L13

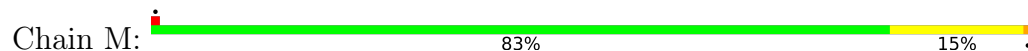


- Molecule 18: 50S ribosomal protein L14



Item	Count
M1	1
M7	2
L8	2
R17	2
I22	2
I41	2
K44	2
L58	2
R70	3
S75	2
D80	2
R105	2
R108	2
S109	2
E110	2
L123	2

- Molecule 19: 50S ribosomal protein L15



F1		S7	K14	R21	G22	I23	G24	S25	G45	V46	G53	S68	I77	R78	L112	V116	R123	G124	R125	R126	V127	T128	K129	G130	A131	R132	A133	A134	F144
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- Molecule 20: 50S ribosomal protein L16



M1
L2
Q3
R6
L33
R59
P77
L78
A79
V80
R81
M82
K86
M105
T129
M136

- Molecule 21: 50S ribosomal protein L17



- Molecule 22: 50S ribosomal protein L18

Chain P:  91% 7%



- Molecule 23: 50S ribosomal protein L19

Chain Q:  89% 11%



- Molecule 24: 50S ribosomal protein L20

Chain R:  91% 7%



- Molecule 25: 50S ribosomal protein L21

Chain S:  77% 19%



- Molecule 26: 50S ribosomal protein L22

Chain T:  88% 11%



- Molecule 27: 50S ribosomal protein L23

Chain U:  77% 14% 7%



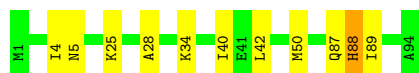
- Molecule 28: 50S ribosomal protein L24

Chain V:  79% 17%



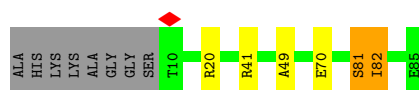
- Molecule 29: 50S ribosomal protein L25

Chain W:  88% 11%



- Molecule 30: 50S ribosomal protein L27

Chain X:  83% 5% 10%



- Molecule 31: 50S ribosomal protein L28

Chain Y:  82% 14%



- Molecule 32: 50S ribosomal protein L29

Chain Z:  90% 8%



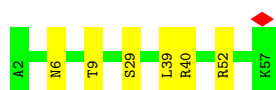
- Molecule 33: 50S ribosomal protein L30

Chain a:  88% 12%



- Molecule 34: 50S ribosomal protein L32

Chain b:  89% 11%



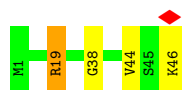
- Molecule 35: 50S ribosomal protein L33

Chain c:  80% 13% 6%



- Molecule 36: 50S ribosomal protein L34

Chain d:  91% 7%



- Molecule 37: 50S ribosomal protein L35

Chain e:  91% 9%



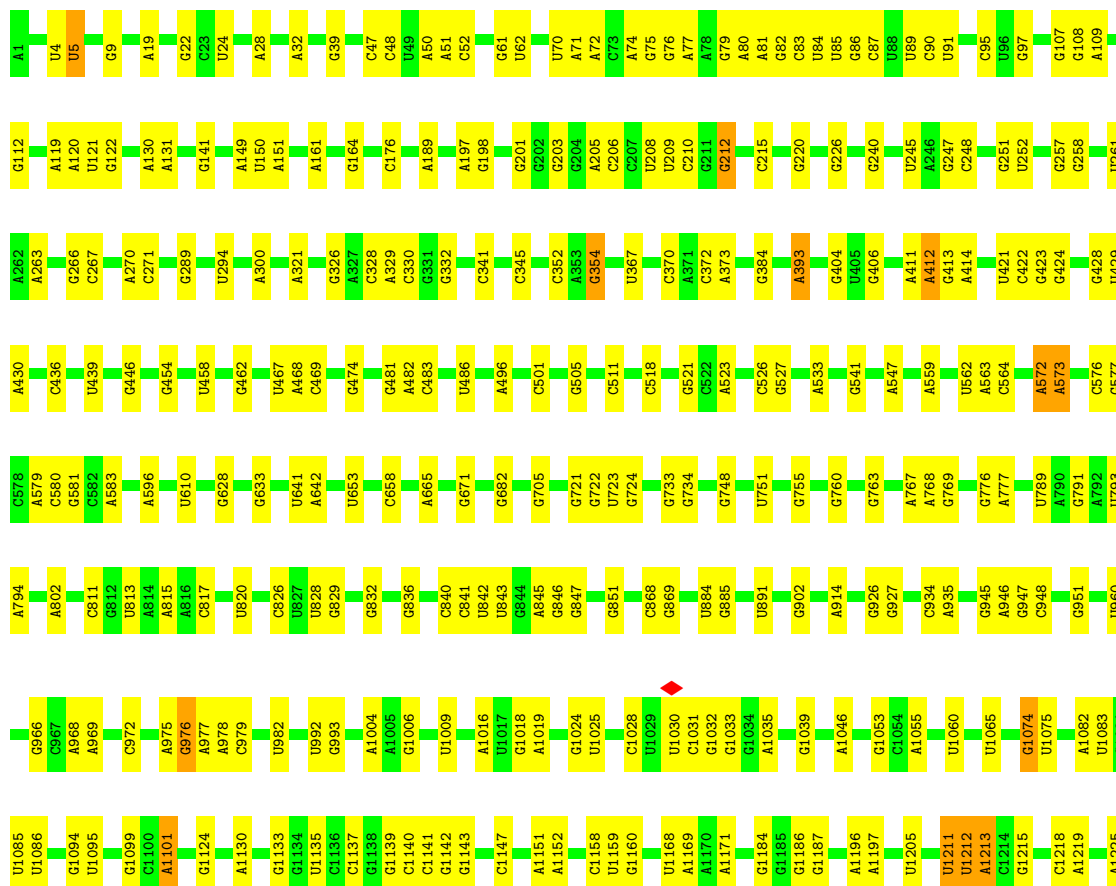
- Molecule 38: 50S ribosomal protein L36

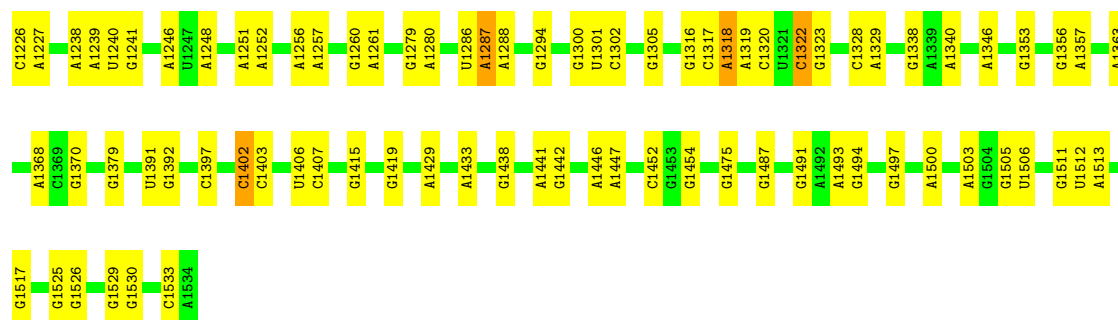
Chain f:  92% 8%



- Molecule 39: 16S rRNA

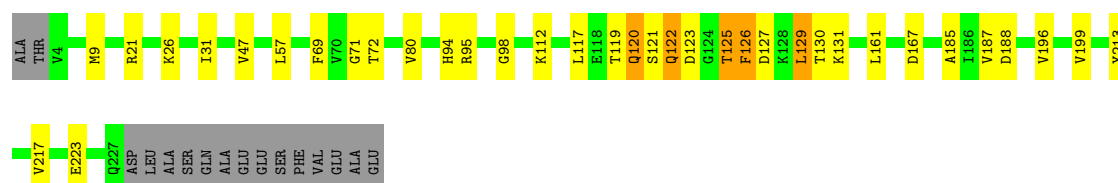
Chain h:  76% 23%





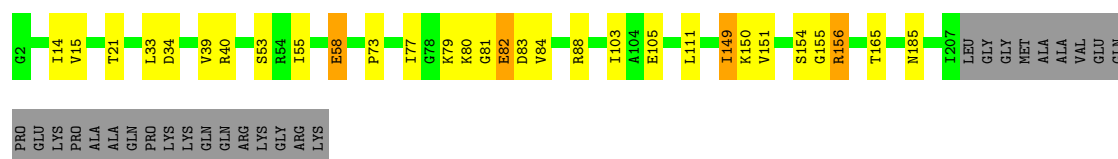
• Molecule 40: 30S ribosomal protein S2

Chain i: 78% 13% 7%



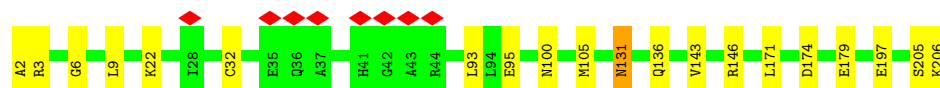
• Molecule 41: 30S ribosomal protein S3

Chain j: 76% 11% 11%



• Molecule 42: 30S ribosomal protein S4

Chain k: 90% 9%



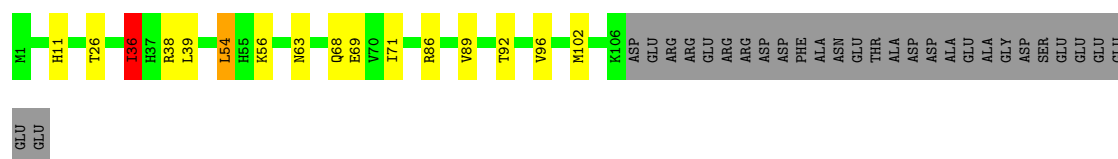
• Molecule 43: 30S ribosomal protein S5

Chain l: 81% 12% 7%

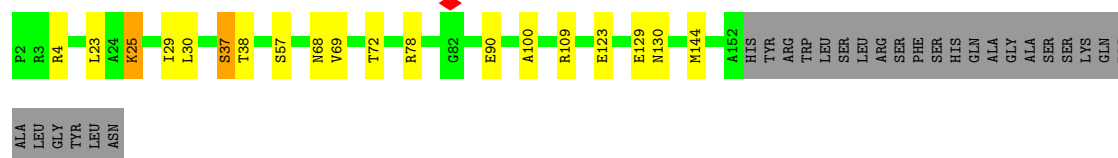


• Molecule 44: 30S ribosomal protein S6

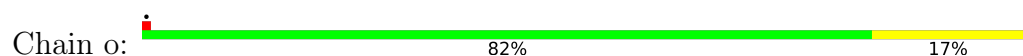
Chain m: 67% 10% 21%



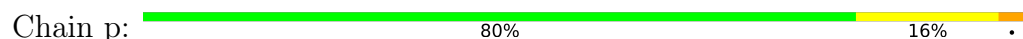
- Molecule 45: 30S ribosomal protein S7



- Molecule 46: 30S ribosomal protein S8



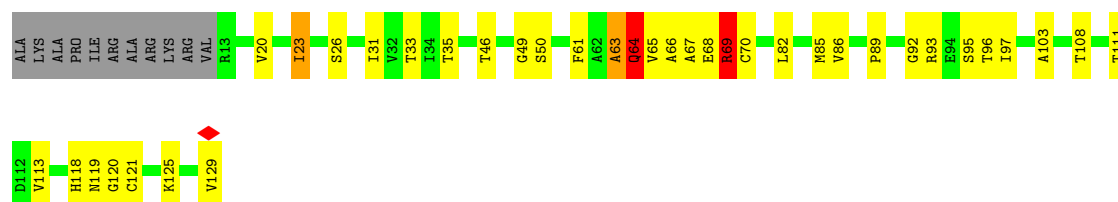
- Molecule 47: 30S ribosomal protein S9



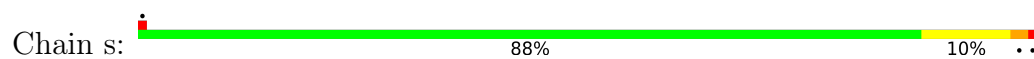
- Molecule 48: 30S ribosomal protein S10



- Molecule 49: 30S ribosomal protein S11



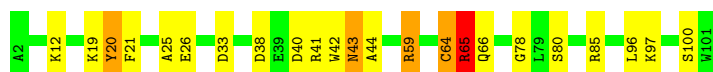
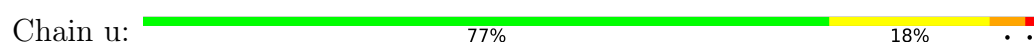
- Molecule 50: 30S ribosomal protein S12



- Molecule 51: 30S ribosomal protein S13



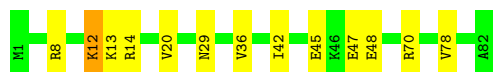
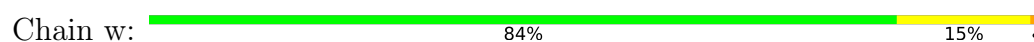
- Molecule 52: 30S ribosomal protein S14



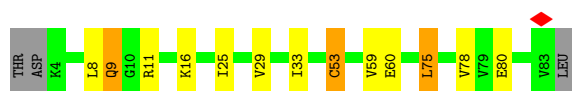
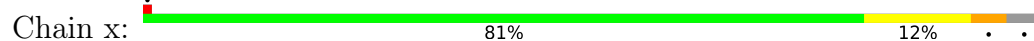
- Molecule 53: 30S ribosomal protein S15



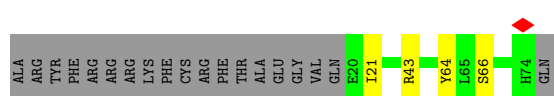
- Molecule 54: 30S ribosomal protein S16



- Molecule 55: 30S ribosomal protein S17



- Molecule 56: 30S ribosomal protein S18



- Molecule 57: 30S ribosomal protein S19



PRO	R3	S4	L5	K6	K7	G8	F9	F10	I11	L15	D27	S38	T39	T63	R78	R81	GLY	HIS	ALA	ALA	ASP	LYS	LYS	ALA	LYS	LYS	LYS
-----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13693	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.456	Depositor
Minimum map value	-0.203	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.026	Depositor
Map size ($\text{\AA}$)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.56	0/676	0.89	0/895
2	2	0.62	0/472	0.85	0/627
3	3	0.60	0/375	0.89	0/494
4	4	0.64	1/2868 (0.0%)	0.81	4/3861 (0.1%)
5	5	0.41	0/1810	0.75	1/2821 (0.0%)
6	7	0.48	0/141	1.07	1/217 (0.5%)
7	A	0.41	0/69735	0.78	62/108791 (0.1%)
8	B	0.40	0/2872	0.71	0/4478
9	C	0.58	0/2121	0.87	1/2852 (0.0%)
10	D	0.60	0/1586	0.84	1/2134 (0.0%)
11	E	0.52	0/1571	0.78	0/2113
12	F	0.57	0/1434	0.77	0/1926
13	G	0.59	0/1343	0.81	1/1816 (0.1%)
14	H	0.67	0/1112	0.76	1/1503 (0.1%)
15	I	0.69	0/1037	0.77	0/1402
16	J	0.68	0/511	0.84	0/683
17	K	0.56	0/1152	0.83	0/1551
18	L	0.56	0/955	0.80	0/1279
19	M	0.56	0/1062	0.84	0/1413
20	N	0.60	0/1104	0.80	0/1474
21	O	0.62	0/1006	0.89	0/1345
22	P	0.53	0/910	0.85	1/1219 (0.1%)
23	Q	0.55	0/929	0.77	0/1242
24	R	0.60	0/960	0.93	0/1278
25	S	0.54	0/829	0.77	2/1107 (0.2%)
26	T	0.62	0/864	0.82	0/1156
27	U	0.61	0/744	0.82	0/994
28	V	0.53	0/787	0.76	0/1051
29	W	0.54	0/766	0.76	0/1025
30	X	0.64	0/598	0.87	1/790 (0.1%)
31	Y	0.59	0/635	0.83	0/848
32	Z	0.50	0/502	0.90	0/667
33	a	0.53	0/467	0.84	0/623
34	b	0.56	0/450	0.83	0/599

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	c	0.59	0/421	0.79	0/561
36	d	0.65	0/380	1.10	0/498
37	e	0.55	0/513	0.84	0/676
38	f	0.50	0/303	0.77	0/397
39	h	0.41	0/36859	0.78	24/57501 (0.0%)
40	i	0.58	0/1784	0.82	0/2403
41	j	0.60	0/1651	0.83	0/2225
42	k	0.57	0/1665	0.81	2/2227 (0.1%)
43	l	0.63	0/1157	0.87	0/1557
44	m	0.62	0/881	0.88	0/1189
45	n	0.62	0/1195	0.86	0/1602
46	o	0.55	0/989	0.84	0/1326
47	p	0.59	0/1034	0.84	0/1375
48	q	0.59	0/805	0.81	1/1089 (0.1%)
49	r	0.59	0/893	0.88	1/1205 (0.1%)
50	s	0.65	0/969	0.84	1/1300 (0.1%)
51	t	0.62	0/892	0.85	1/1193 (0.1%)
52	u	0.60	0/817	0.83	0/1088
53	v	0.54	0/722	0.85	0/964
54	w	0.62	0/659	0.84	0/884
55	x	0.56	0/657	0.71	0/881
56	y	0.66	0/462	0.88	0/621
57	z	0.62	0/652	0.81	0/877
All	All	0.47	1/160744 (0.0%)	0.79	106/239913 (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
1	1	0	1
2	2	0	1
3	3	0	4
4	4	0	6
9	C	0	6
10	D	0	3
11	E	0	3
12	F	0	4
13	G	0	6
14	H	0	1
15	I	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
18	L	0	1
19	M	0	2
20	N	0	2
21	O	0	1
22	P	0	1
23	Q	0	2
25	S	0	3
26	T	0	1
27	U	0	3
28	V	0	1
29	W	0	1
31	Y	0	2
32	Z	0	1
35	c	0	2
36	d	0	1
40	i	0	4
41	j	0	4
42	k	0	4
43	l	0	1
44	m	0	2
45	n	0	3
46	o	0	4
47	p	0	5
48	q	0	3
49	r	0	4
50	s	0	1
51	t	0	4
52	u	0	3
53	v	0	1
54	w	0	2
55	x	0	1
56	y	0	1
57	z	0	2
All	All	0	111

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	332	ARG	CA-C	5.81	1.59	1.53

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1607	C	C2'-C3'-O3'	11.61	126.92	109.50
39	h	1211	U	C2'-C3'-O3'	9.06	123.08	109.50
4	4	332	ARG	N-CA-C	8.97	120.46	108.07
7	A	2030	A	C2'-C3'-O3'	8.84	122.76	109.50
39	h	428	G	C4'-C3'-O3'	8.83	122.64	109.40
13	G	121	ILE	N-CA-C	8.63	121.44	109.45
14	H	48	GLU	N-CA-C	-8.33	102.28	111.36
7	A	2191	A	C4'-C3'-O3'	8.29	121.83	109.40
49	r	63	ALA	N-CA-C	-8.26	100.15	112.04
7	A	2497	A	C2'-C3'-O3'	8.13	121.69	109.50
7	A	1270	C	C2'-C3'-O3'	-8.08	101.58	113.70
7	A	2820	A	C4'-C3'-O3'	-8.01	100.98	113.00
6	7	15	U	C2'-C3'-O3'	7.53	120.80	109.50
7	A	509	C	C2'-C3'-O3'	-7.43	102.56	113.70
7	A	2498	C	C2'-C3'-O3'	7.19	124.48	113.70
39	h	1151	A	C2'-C3'-O3'	7.19	120.28	109.50
7	A	1494	A	C2'-C3'-O3'	7.12	124.38	113.70
7	A	1418	G	C4'-C3'-O3'	-7.04	102.44	113.00
25	S	51	VAL	C-N-CD	7.03	136.07	120.60
7	A	2498	C	C4'-C3'-O3'	6.97	123.46	113.00
7	A	2602	A	C4'-C3'-O3'	6.96	119.83	109.40
30	X	82	ILE	N-CA-C	6.79	117.26	107.88
39	h	573	A	C4'-C3'-O3'	-6.77	102.85	113.00
39	h	813	U	C4'-C3'-O3'	-6.75	102.87	113.00
7	A	2296	U	C4'-C3'-O3'	6.72	119.48	109.40
7	A	1142	A	C2'-C3'-O3'	-6.67	99.50	109.50
39	h	1493	A	C2'-C3'-O3'	6.49	119.23	109.50
7	A	1431	A	C3'-C2'-O2'	6.49	120.43	110.70
7	A	1301	A	C2'-C3'-O3'	-6.45	99.82	109.50
7	A	1770	G	C3'-C2'-O2'	6.38	120.27	110.70
7	A	2311	A	C2'-C3'-O3'	6.35	119.03	109.50
7	A	1692	U	C4'-C3'-O3'	-6.29	103.57	113.00
50	s	89	ASP	N-CA-C	-6.29	97.41	110.80
7	A	494	G	C3'-C2'-O2'	6.20	120.00	110.70
10	D	186	LEU	N-CA-C	6.19	119.62	110.46
5	5	1	C	C5'-C4'-C3'	6.16	125.25	116.00
39	h	1525	G	C1'-C2'-O2'	6.15	117.63	108.40
7	A	2025	C	C4'-C3'-O3'	-6.14	103.80	113.00
7	A	2238	G	C2'-C3'-O3'	6.11	118.67	109.50
7	A	2017	U	C2'-C3'-O3'	-6.04	104.64	113.70
39	h	563	A	C4'-C3'-O3'	-6.00	104.01	113.00
7	A	2067	G	C2'-C3'-O3'	5.95	118.42	109.50
7	A	1135	C	C2'-C3'-O3'	-5.87	104.89	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	761	A	C4'-C3'-O3'	-5.86	104.20	113.00
39	h	370	C	C3'-C2'-O2'	5.86	119.49	110.70
25	S	53	PHE	N-CA-C	5.84	118.23	110.53
39	h	24	U	C3'-C2'-O2'	5.83	119.45	110.70
7	A	781	A	C4'-C3'-O3'	-5.83	104.26	113.00
7	A	1328	A	C4'-C3'-O3'	-5.82	104.28	113.00
7	A	2679	A	C3'-C2'-O2'	5.82	119.43	110.70
39	h	1186	G	C3'-C2'-O2'	5.78	119.37	110.70
22	P	99	TYR	N-CA-C	-5.76	99.74	108.67
7	A	463	G	C1'-C2'-O2'	5.74	117.00	108.40
7	A	2265	U	C4'-C3'-O3'	-5.71	104.44	113.00
48	q	53	ILE	CB-CA-C	5.67	116.05	111.06
7	A	301	G	C2'-C3'-O3'	5.64	117.97	109.50
7	A	944	C	C4'-C3'-O3'	-5.63	104.56	113.00
39	h	483	C	C1'-C2'-O2'	5.63	116.84	108.40
7	A	17	G	C3'-C2'-O2'	5.63	119.14	110.70
9	C	171	TYR	N-CA-C	5.58	118.73	110.46
39	h	1205	U	C3'-C2'-O2'	5.55	119.03	110.70
7	A	2724	U	C4'-C3'-O3'	-5.54	104.68	113.00
7	A	1273	U	C4'-C3'-O3'	-5.53	104.70	113.00
7	A	826	U	C2'-C3'-O3'	-5.52	105.42	113.70
7	A	2538	C	C3'-C2'-O2'	5.50	118.95	110.70
7	A	423	A	C2'-C3'-O3'	-5.48	105.48	113.70
39	h	776	G	C4'-C3'-O3'	-5.46	104.81	113.00
7	A	784	G	C2'-C3'-O3'	-5.45	105.53	113.70
39	h	1493	A	C4'-C3'-O3'	5.44	117.57	109.40
7	A	784	G	C4'-C3'-O3'	5.41	121.11	113.00
7	A	1138	G	C4'-C3'-O3'	-5.40	104.90	113.00
7	A	2498	C	C3'-C2'-O2'	5.39	118.79	110.70
7	A	1970	A	C2'-C3'-O3'	5.38	117.58	109.50
39	h	976	G	C4'-C3'-O3'	-5.38	104.92	113.00
7	A	1757	A	C4'-C3'-O3'	-5.38	104.93	113.00
42	k	6	GLY	CA-C-N	5.37	126.55	119.84
42	k	6	GLY	C-N-CA	5.37	126.55	119.84
39	h	572	A	C4'-C3'-O3'	-5.35	104.97	113.00
7	A	1378	A	C1'-C2'-O2'	5.32	119.77	111.80
7	A	2871	U	C4'-C3'-O3'	-5.30	105.05	113.00
4	4	333	ILE	CB-CA-C	-5.28	102.63	111.29
7	A	1131	G	C4'-C3'-O3'	5.28	117.32	109.40
7	A	202	U	C4'-C3'-O3'	-5.21	105.19	113.00
39	h	1075	U	C3'-C2'-O2'	5.20	118.50	110.70
51	t	4	ILE	N-CA-C	5.20	117.26	109.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2158	A	C2'-C3'-O3'	5.20	117.29	109.50
7	A	2525	G	C3'-C2'-O2'	5.17	118.46	110.70
39	h	1279	G	N9-C1'-C2'	5.17	119.75	112.00
4	4	151	MET	N-CA-C	-5.15	99.82	110.80
7	A	2756	U	C2'-C3'-O3'	-5.11	101.83	109.50
39	h	820	U	C4'-C3'-O3'	5.11	117.06	109.40
7	A	1418	G	C2'-C3'-O3'	5.11	121.36	113.70
7	A	962	G	C3'-C2'-O2'	5.11	118.36	110.70
7	A	804	A	C3'-C2'-O2'	5.10	118.34	110.70
39	h	811	C	C4'-C3'-O3'	-5.09	105.36	113.00
7	A	1214	A	C3'-C2'-O2'	5.08	118.33	110.70
7	A	2571	U	C4'-C3'-O3'	-5.08	105.38	113.00
7	A	2057	G	C3'-C2'-O2'	5.07	118.31	110.70
7	A	1358	G	C3'-C2'-O2'	5.04	118.26	110.70
39	h	412	A	C4'-C3'-O3'	5.03	116.95	109.40
4	4	333	ILE	N-CA-C	5.02	119.78	109.34
7	A	2251	G	C3'-C2'-O2'	5.02	118.23	110.70
39	h	1403	C	C3'-C2'-O2'	5.02	118.23	110.70
7	A	1371	G	C3'-C2'-O2'	5.00	118.21	110.70
7	A	1240	U	C4'-C3'-O3'	-5.00	105.50	113.00
39	h	982	U	C2'-C3'-O3'	-5.00	102.00	109.50

There are no chirality outliers.

All (111) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	42	GLY	Peptide
2	2	55	ARG	Peptide
3	3	2	SER	Peptide
3	3	35	GLY	Peptide
3	3	36	LYS	Peptide
3	3	37	GLY	Peptide
4	4	168	GLU	Peptide
4	4	210	GLY	Peptide
4	4	219	SER	Peptide
4	4	273	GLN	Peptide
4	4	306	GLU	Peptide
4	4	353	LEU	Peptide
9	C	185	GLU	Peptide
9	C	232	HIS	Peptide
9	C	233	GLY	Peptide
9	C	242	LYS	Peptide

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Mol	Chain	Res	Type	Group
9	C	71	LYS	Peptide
9	C	86	ASN	Peptide
10	D	208	LYS	Peptide
10	D	30	GLU	Peptide
10	D	72	GLY	Peptide
11	E	54	GLY	Peptide
11	E	56	GLY	Peptide
11	E	72	SER	Peptide
12	F	125	ARG	Peptide
12	F	131	GLY	Peptide
12	F	177	PHE	Peptide
12	F	72	LYS	Peptide
13	G	125	CYS	Peptide
13	G	176	LYS	Peptide
13	G	2	SER	Peptide
13	G	47	ASP	Peptide
13	G	48	ASN	Peptide
13	G	95	ARG	Peptide
14	H	50	ARG	Peptide
15	I	128	THR	Peptide
15	I	132	TYR	Peptide
15	I	67	THR	Peptide
18	L	22	ILE	Peptide
19	M	45	GLY	Peptide
19	M	53	GLY	Peptide
20	N	105	MET	Peptide
20	N	59	ARG	Peptide
21	O	118	ARG	Peptide
22	P	55	GLU	Peptide
23	Q	15	GLN	Peptide
23	Q	35	GLY	Peptide
25	S	42	ALA	Peptide
25	S	65	ALA	Peptide
25	S	86	GLN	Peptide
26	T	4	ILE	Peptide
27	U	13	ALA	Peptide
27	U	69	ARG	Peptide
27	U	90	GLY	Peptide
28	V	83	VAL	Peptide
29	W	34	LYS	Peptide
31	Y	16	ASN	Peptide
31	Y	44	LYS	Peptide

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Mol	Chain	Res	Type	Group
32	Z	3	ALA	Peptide
35	c	10	LYS	Peptide
35	c	16	GLY	Peptide
36	d	38	GLY	Peptide
40	i	125	THR	Peptide
40	i	127	ASP	Peptide
40	i	129	LEU	Peptide
40	i	72	THR	Peptide
41	j	105	GLU	Peptide
41	j	154	SER	Peptide
41	j	185	ASN	Peptide
41	j	53	SER	Peptide
42	k	146	ARG	Peptide
42	k	174	ASP	Peptide
42	k	205	SER	Peptide
42	k	22	LYS	Peptide
43	l	160	SER	Peptide
44	m	54	LEU	Peptide
44	m	63	ASN	Peptide
45	n	123	GLU	Peptide
45	n	129	GLU	Peptide
45	n	4	ARG	Peptide
46	o	2	SER	Peptide
46	o	3	MET	Peptide
46	o	76	GLN	Peptide
46	o	98	GLY	Peptide
47	p	24	GLY	Peptide
47	p	26	GLY	Peptide
47	p	46	MET	Peptide
47	p	56	ASP	Peptide
47	p	57	MET	Peptide
48	q	19	ASP	Peptide
48	q	38	GLY	Peptide
48	q	43	PRO	Peptide
49	r	103	ALA	Peptide
49	r	118	HIS	Peptide
49	r	89	PRO	Peptide
49	r	92	GLY	Peptide
50	s	35	THR	Peptide
51	t	104	THR	Peptide
51	t	106	ALA	Peptide
51	t	112	PRO	Peptide

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Mol	Chain	Res	Type	Group
51	t	46	SER	Peptide
52	u	20	TYR	Peptide
52	u	33	ASP	Peptide
52	u	41	ARG	Peptide
53	v	16	GLY	Peptide
54	w	45	GLU	Peptide
54	w	47	GLU	Peptide
55	x	11	ARG	Peptide
56	y	21	ILE	Peptide
57	z	27	ASP	Peptide
57	z	8	GLY	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	1	670	0	719	3	0
2	2	465	0	491	4	0
3	3	369	0	381	3	0
4	4	2829	0	2734	38	0
5	5	1620	0	826	1	0
6	7	127	0	65	0	0
7	A	62240	0	31297	96	0
8	B	2569	0	1301	1	0
9	C	2082	0	2154	13	0
10	D	1565	0	1616	26	0
11	E	1552	0	1619	0	0
12	F	1410	0	1444	19	0
13	G	1323	0	1371	9	0
14	H	1101	0	1142	4	0
15	I	1023	0	1052	1	0
16	J	509	0	547	5	0
17	K	1129	0	1162	3	0
18	L	946	0	1023	2	0
19	M	1053	0	1129	24	0
20	N	1082	0	1170	7	0
21	O	993	0	1034	4	0
22	P	900	0	935	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	Q	917	0	962	2	0
24	R	947	0	1019	4	0
25	S	816	0	839	35	0
26	T	857	0	922	9	0
27	U	738	0	807	5	0
28	V	779	0	831	12	0
29	W	753	0	780	5	0
30	X	591	0	606	4	0
31	Y	625	0	652	8	0
32	Z	501	0	531	1	0
33	a	463	0	504	2	0
34	b	444	0	458	0	0
35	c	414	0	442	1	0
36	d	377	0	418	1	0
37	e	504	0	572	2	0
38	f	302	0	343	1	0
39	h	32917	0	16564	49	0
40	i	1753	0	1780	16	0
41	j	1624	0	1696	15	0
42	k	1643	0	1707	5	0
43	l	1144	0	1185	1	0
44	m	862	0	864	4	0
45	n	1181	0	1238	2	0
46	o	979	0	1031	6	0
47	p	1022	0	1070	4	0
48	q	795	0	836	7	0
49	r	877	0	885	21	0
50	s	955	0	1016	10	0
51	t	883	0	941	53	0
52	u	805	0	844	15	0
53	v	714	0	734	1	0
54	w	649	0	666	6	0
55	x	648	0	691	5	0
56	y	455	0	478	1	0
57	z	637	0	665	2	0
All	All	148128	0	100789	515	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 2.

All (515) 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)
25:S:37:GLU:CB	25:S:53:PHE:HE1	1.04	1.67
25:S:37:GLU:HB3	25:S:53:PHE:CE1	1.25	1.64
51:t:19:LEU:CD1	51:t:34:LEU:HD21	1.46	1.43
25:S:37:GLU:CB	25:S:53:PHE:CE1	1.88	1.39
7:A:1061:U:H1'	7:A:1070:A:C1'	1.54	1.34
50:s:42:PRO:CB	50:s:89:ASP:OD1	1.75	1.31
25:S:37:GLU:CG	25:S:53:PHE:CE1	2.13	1.31
12:F:112:ARG:HA	51:t:7:ILE:CD1	1.63	1.29
51:t:31:LYS:HE3	51:t:41:GLU:OE2	1.31	1.28
25:S:37:GLU:HG2	25:S:53:PHE:CE1	1.67	1.28
10:D:150:GLN:O	10:D:153:GLY:N	1.72	1.21
51:t:19:LEU:HD11	51:t:34:LEU:HD21	1.24	1.17
4:4:300:MET:HE3	4:4:300:MET:HA	1.24	1.13
50:s:42:PRO:HB3	50:s:89:ASP:OD1	1.38	1.13
25:S:52:PRO:HG2	25:S:53:PHE:HD2	1.10	1.12
51:t:31:LYS:CE	51:t:41:GLU:OE2	1.99	1.11
50:s:42:PRO:HB2	50:s:89:ASP:OD1	1.48	1.08
50:s:89:ASP:O	50:s:90:LEU:HB2	1.43	1.06
12:F:112:ARG:HA	51:t:7:ILE:HD12	1.14	1.06
51:t:19:LEU:CD1	51:t:34:LEU:CD2	2.33	1.06
4:4:239:LEU:CD1	4:4:288:MET:HE1	1.86	1.05
7:A:1061:U:H4'	7:A:1062:G:OP2	1.26	1.05
41:j:81:GLY:O	41:j:83:ASP:N	1.89	1.05
25:S:52:PRO:HG2	25:S:53:PHE:CD2	1.93	1.03
7:A:1061:U:C1'	7:A:1070:A:H1'	1.88	1.03
10:D:128:ARG:HH11	10:D:128:ARG:HB3	1.21	1.03
28:V:59:VAL:HG12	28:V:60:GLU:H	1.22	1.03
51:t:16:VAL:HG23	51:t:30:SER:OG	1.59	1.01
20:N:80:VAL:O	20:N:82:MET:N	1.94	1.00
7:A:1061:U:H1'	7:A:1070:A:H1'	0.99	0.99
17:K:43:GLU:OE1	17:K:43:GLU:N	2.00	0.95
49:r:86:VAL:HG21	49:r:97:ILE:HD11	1.49	0.94
4:4:239:LEU:HD11	4:4:288:MET:HE1	1.50	0.93
50:s:89:ASP:O	50:s:90:LEU:CB	2.16	0.93
7:A:1061:U:C4'	7:A:1062:G:OP2	2.18	0.91
12:F:112:ARG:HA	51:t:7:ILE:HD13	1.53	0.91
4:4:151:MET:HE3	4:4:353:LEU:HD21	1.52	0.90
51:t:4:ILE:O	51:t:6:GLY:N	2.05	0.90
4:4:300:MET:HA	4:4:300:MET:CE	2.03	0.89
51:t:19:LEU:HD12	51:t:34:LEU:HD21	1.54	0.89
25:S:37:GLU:CB	25:S:53:PHE:CD1	2.55	0.88
4:4:147:MET:CE	4:4:349:LEU:HD22	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2572:A:N7	10:D:150:GLN:NE2	2.21	0.88
51:t:31:LYS:HE3	51:t:41:GLU:CD	1.99	0.88
50:s:50:ARG:NE	50:s:89:ASP:OD2	2.07	0.86
10:D:128:ARG:HH11	10:D:128:ARG:CB	1.88	0.86
39:h:1147:C:O2	47:p:18:ARG:NH2	2.09	0.86
10:D:149:ASN:O	10:D:149:ASN:ND2	2.08	0.85
7:A:1061:U:C1'	7:A:1070:A:C1'	2.49	0.84
7:A:2683:C:O2	18:L:70:ARG:NH2	2.11	0.84
25:S:37:GLU:CG	25:S:53:PHE:HE1	1.69	0.84
28:V:58:ILE:O	28:V:59:VAL:O	1.93	0.84
25:S:37:GLU:HA	25:S:53:PHE:HD1	1.43	0.84
4:4:332:ARG:HH11	4:4:332:ARG:HG2	1.40	0.84
51:t:16:VAL:CG2	51:t:30:SER:OG	2.26	0.82
40:i:121:SER:O	40:i:125:THR:N	2.13	0.81
25:S:37:GLU:HG2	25:S:53:PHE:CD1	2.15	0.80
51:t:19:LEU:HD13	51:t:34:LEU:HD21	1.60	0.80
19:M:131:ALA:O	19:M:134:ALA:N	2.15	0.80
19:M:126:ARG:HH21	19:M:126:ARG:HG3	1.45	0.79
9:C:172:VAL:HG13	9:C:186:ALA:HB2	1.65	0.79
25:S:37:GLU:CG	25:S:53:PHE:CD1	2.65	0.79
4:4:333:ILE:HG22	4:4:334:LYS:N	1.97	0.78
4:4:239:LEU:HD13	4:4:288:MET:HE1	1.62	0.78
41:j:79:LYS:HB3	41:j:82:GLU:OE2	1.82	0.77
4:4:118:MET:HE3	4:4:361:LEU:HD13	1.67	0.77
52:u:65:ARG:HG3	52:u:78:GLY:O	1.84	0.77
7:A:1061:U:H1'	7:A:1070:A:O4'	1.85	0.76
10:D:150:GLN:O	10:D:153:GLY:CA	2.34	0.76
51:t:19:LEU:HD13	51:t:34:LEU:CD2	2.15	0.75
40:i:121:SER:O	40:i:125:THR:HA	1.87	0.75
7:A:1060:U:H4'	7:A:1061:U:O5'	1.86	0.75
4:4:118:MET:HE3	4:4:361:LEU:CD1	2.17	0.74
12:F:112:ARG:HB3	51:t:7:ILE:HG21	1.69	0.74
12:F:112:ARG:CA	51:t:7:ILE:HD12	2.08	0.72
19:M:126:ARG:HG3	19:M:126:ARG:NH2	2.00	0.72
7:A:12:U:H2'	7:A:12:U:O2	1.89	0.72
25:S:37:GLU:CA	25:S:53:PHE:CD1	2.73	0.72
12:F:112:ARG:CB	51:t:7:ILE:HG21	2.20	0.72
50:s:88:LYS:O	50:s:90:LEU:N	2.22	0.72
7:A:637:A:OP1	19:M:130:GLY:HA3	1.90	0.71
4:4:332:ARG:HG2	4:4:332:ARG:NH1	2.00	0.71
51:t:16:VAL:HG21	51:t:31:LYS:HG2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:112:ARG:CA	51:t:7:ILE:CD1	2.57	0.71
25:S:37:GLU:HA	25:S:53:PHE:CD1	2.23	0.70
19:M:123:ARG:O	19:M:125:LEU:CD1	2.39	0.70
7:A:1060:U:OP2	16:J:75:PRO:HA	1.93	0.69
51:t:7:ILE:O	51:t:8:ASN:ND2	2.26	0.68
13:G:121:ILE:HG22	13:G:122:THR:N	2.08	0.68
19:M:131:ALA:O	19:M:132:ARG:C	2.35	0.68
19:M:131:ALA:O	19:M:133:ALA:N	2.27	0.67
54:w:12:LYS:O	54:w:13:LYS:HB2	1.94	0.67
40:i:121:SER:O	40:i:122:GLN:C	2.37	0.67
10:D:148:GLN:O	10:D:149:ASN:CB	2.41	0.66
12:F:112:ARG:CA	51:t:7:ILE:HD13	2.24	0.66
7:A:1060:U:H4'	7:A:1061:U:C5'	2.25	0.66
25:S:50:GLY:C	25:S:52:PRO:O	2.38	0.66
4:4:147:MET:HE2	4:4:349:LEU:HD22	1.76	0.66
29:W:40:ILE:HD12	29:W:42:LEU:HD21	1.77	0.66
40:i:121:SER:O	40:i:125:THR:CA	2.43	0.65
40:i:121:SER:O	40:i:123:ASP:N	2.30	0.65
52:u:64:CYS:O	52:u:66:GLN:N	2.28	0.65
21:O:28:LEU:HD23	21:O:48:VAL:HG21	1.79	0.65
19:M:125:LEU:HD12	19:M:125:LEU:N	2.11	0.65
20:N:77:PRO:O	20:N:80:VAL:CG2	2.45	0.64
22:P:7:ARG:HD2	22:P:97:PHE:CZ	2.31	0.64
4:4:300:MET:HE3	4:4:300:MET:CA	2.15	0.64
49:r:86:VAL:CG2	49:r:97:ILE:HD11	2.26	0.64
7:A:125:A:OP2	36:d:19:ARG:NH2	2.30	0.64
25:S:37:GLU:HB3	25:S:53:PHE:HE1	0.51	0.63
25:S:37:GLU:CA	25:S:53:PHE:CE1	2.79	0.63
7:A:585:G:N7	24:R:6:ARG:NH1	2.47	0.63
25:S:50:GLY:HA3	25:S:52:PRO:O	1.99	0.63
12:F:143:TYR:C	12:F:145:LYS:H	2.07	0.62
28:V:59:VAL:CG1	28:V:60:GLU:H	2.06	0.62
7:A:499:U:OP1	28:V:43:LYS:NZ	2.31	0.62
10:D:150:GLN:O	10:D:152:PRO:C	2.40	0.62
10:D:148:GLN:O	10:D:149:ASN:HB3	1.99	0.62
17:K:43:GLU:H	17:K:43:GLU:CD	2.08	0.62
51:t:19:LEU:HD11	51:t:34:LEU:CD2	2.14	0.62
12:F:143:TYR:O	12:F:145:LYS:N	2.33	0.62
4:4:332:ARG:HB3	4:4:343:ARG:HD3	1.80	0.62
7:A:2202:U:O2'	7:A:2204:G:OP1	2.18	0.61
26:T:50:VAL:O	26:T:53:SER:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:P:7:ARG:HD2	22:P:97:PHE:CE1	2.35	0.61
19:M:126:ARG:HH21	19:M:126:ARG:CG	2.14	0.61
29:W:87:GLN:O	29:W:88:HIS:HB2	1.99	0.61
14:H:135:HIS:HD2	14:H:137:GLU:OE1	1.83	0.61
39:h:294:U:OP1	39:h:610:U:O2'	2.16	0.61
14:H:137:GLU:OE1	14:H:138:VAL:HG23	1.99	0.61
7:A:2223:G:OP1	9:C:171:TYR:OH	2.15	0.61
1:1:74:ARG:NH2	39:h:261:U:OP2	2.34	0.60
20:N:77:PRO:O	20:N:80:VAL:HG23	2.01	0.60
10:D:128:ARG:HH11	10:D:128:ARG:CG	2.14	0.60
28:V:59:VAL:HG12	28:V:60:GLU:N	2.02	0.60
49:r:97:ILE:HG22	49:r:97:ILE:O	2.01	0.60
28:V:58:ILE:O	28:V:58:ILE:HG22	2.02	0.60
27:U:11:LEU:HD22	27:U:32:LEU:HD13	1.82	0.60
19:M:123:ARG:O	19:M:125:LEU:HD12	2.02	0.60
10:D:148:GLN:O	10:D:149:ASN:ND2	2.34	0.59
52:u:64:CYS:HB2	52:u:80:SER:H	1.67	0.59
19:M:129:LYS:HZ3	19:M:129:LYS:HB3	1.67	0.59
25:S:51:VAL:HG23	25:S:51:VAL:O	2.02	0.59
4:4:333:ILE:CG2	4:4:334:LYS:N	2.66	0.59
21:O:24:MET:HE1	21:O:40:LYS:HD3	1.85	0.59
48:q:52:LEU:HD21	48:q:59:LYS:HD2	1.85	0.59
46:o:11:LEU:HD22	46:o:75:ILE:HD11	1.85	0.59
51:t:7:ILE:O	51:t:7:ILE:HG22	2.02	0.58
19:M:124:GLY:C	19:M:125:LEU:HD12	2.28	0.58
2:2:12:PHE:HZ	49:r:97:ILE:O	1.85	0.58
10:D:128:ARG:HB3	10:D:128:ARG:NH1	2.04	0.58
46:o:102:ALA:HB3	46:o:113:ASP:HB3	1.85	0.58
19:M:129:LYS:HB3	19:M:129:LYS:NZ	2.18	0.57
49:r:68:GLU:O	49:r:70:CYS:N	2.37	0.57
51:t:31:LYS:HE2	51:t:41:GLU:OE2	1.96	0.57
49:r:63:ALA:O	49:r:66:ALA:HB3	2.04	0.57
51:t:5:ALA:HB3	51:t:60:VAL:CG1	2.35	0.57
48:q:12:ALA:HB3	48:q:18:ILE:HD12	1.87	0.57
40:i:121:SER:OG	40:i:122:GLN:N	2.37	0.57
41:j:79:LYS:HE2	41:j:80:LYS:NZ	2.19	0.57
10:D:4:LEU:HD12	10:D:101:PHE:CE2	2.40	0.57
51:t:31:LYS:CE	51:t:41:GLU:CD	2.68	0.57
51:t:30:SER:O	51:t:33:ILE:N	2.36	0.57
7:A:1060:U:C4'	7:A:1061:U:H5''	2.35	0.57
14:H:135:HIS:CG	14:H:136:SER:N	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:77:ILE:HG22	19:M:78:ARG:O	2.05	0.56
25:S:53:PHE:CD2	25:S:53:PHE:N	2.73	0.56
41:j:34:ASP:OD2	52:u:65:ARG:NH1	2.38	0.56
44:m:26:THR:HG23	44:m:36:ILE:HD13	1.86	0.56
48:q:40:ILE:HD11	48:q:73:LEU:HD23	1.87	0.56
16:J:122:ILE:O	16:J:124:ALA:N	2.38	0.56
16:J:122:ILE:O	16:J:125:MET:N	2.38	0.56
19:M:23:ILE:HD12	25:S:84:ARG:NH1	2.21	0.56
31:Y:21:ALA:O	31:Y:22:LEU:HB2	2.05	0.56
51:t:4:ILE:HG22	51:t:5:ALA:N	2.21	0.56
49:r:61:PHE:O	49:r:64:GLN:HB2	2.05	0.56
16:J:122:ILE:O	16:J:123:GLU:C	2.49	0.56
7:A:910:A:H2'	7:A:911:A:C8	2.41	0.55
2:2:45:ARG:NH2	39:h:1526:G:OP1	2.39	0.55
41:j:40:ARG:NH1	41:j:55:ILE:O	2.40	0.55
28:V:58:ILE:C	28:V:59:VAL:O	2.50	0.55
54:w:13:LYS:O	54:w:14:ARG:HG2	2.07	0.55
51:t:6:GLY:O	51:t:7:ILE:HB	2.06	0.54
7:A:1059:G:H2'	7:A:1060:U:OP1	2.07	0.54
52:u:64:CYS:C	52:u:66:GLN:H	2.16	0.54
4:4:118:MET:CE	4:4:361:LEU:HD12	2.37	0.54
41:j:77:ILE:HA	41:j:84:VAL:HG23	1.90	0.54
41:j:79:LYS:HE2	41:j:80:LYS:HG2	1.89	0.54
51:t:29:ARG:O	51:t:32:ALA:HB3	2.07	0.54
26:T:29:VAL:HB	26:T:55:ILE:HD11	1.89	0.54
7:A:700:G:O2'	7:A:1632:A:N3	2.35	0.54
4:4:118:MET:CE	4:4:361:LEU:CD1	2.86	0.54
4:4:333:ILE:HG22	4:4:334:LYS:H	1.73	0.54
7:A:140:C:O4'	7:A:140:C:O2	2.25	0.54
13:G:24:ILE:HG21	13:G:72:LEU:HD21	1.90	0.54
49:r:68:GLU:C	49:r:70:CYS:H	2.15	0.54
7:A:1060:U:C4'	7:A:1061:U:C5'	2.85	0.53
25:S:48:LYS:HE3	25:S:103:ALA:HB1	1.90	0.53
28:V:44:LYS:HG3	28:V:45:HIS:N	2.23	0.53
22:P:99:TYR:O	22:P:100:HIS:HB2	2.09	0.53
7:A:84:A:N1	7:A:98:G:O2'	2.39	0.53
7:A:2053:G:OP1	10:D:149:ASN:HB2	2.08	0.53
41:j:81:GLY:C	41:j:83:ASP:N	2.63	0.53
51:t:33:ILE:O	51:t:35:ALA:N	2.42	0.53
7:A:1059:G:C2'	7:A:1060:U:OP1	2.57	0.53
7:A:1060:U:H4'	7:A:1061:U:H5''	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:74:ARG:NH1	39:h:263:A:OP2	2.42	0.53
7:A:1059:G:C2	7:A:1060:U:O4	2.62	0.53
7:A:1223:G:OP1	25:S:68:ARG:NH2	2.41	0.53
25:S:50:GLY:CA	25:S:52:PRO:O	2.57	0.53
39:h:523:A:N1	50:s:89:ASP:HB3	2.24	0.53
26:T:74:ILE:HG23	26:T:74:ILE:O	2.07	0.52
28:V:60:GLU:O	28:V:60:GLU:HG2	2.09	0.52
49:r:85:MET:HE3	49:r:113:VAL:HG11	1.91	0.52
48:q:10:LEU:CD2	48:q:98:VAL:HG12	2.40	0.52
51:t:29:ARG:O	51:t:30:SER:C	2.53	0.52
7:A:1817:G:OP1	9:C:87:ARG:NH2	2.43	0.52
39:h:769:G:H4'	39:h:1513:A:H4'	1.91	0.52
52:u:64:CYS:HB2	52:u:80:SER:N	2.25	0.52
19:M:129:LYS:NZ	19:M:129:LYS:CB	2.73	0.52
24:R:91:ASP:OD1	24:R:91:ASP:C	2.52	0.52
39:h:1218:C:H2'	39:h:1219:A:C8	2.44	0.52
47:p:21:ILE:HD13	47:p:63:LEU:HB3	1.91	0.52
7:A:1061:U:H2'	7:A:1061:U:O2	2.09	0.52
24:R:79:PHE:CZ	24:R:83:LEU:HD11	2.45	0.52
49:r:68:GLU:C	49:r:70:CYS:N	2.67	0.52
28:V:14:LEU:HD11	28:V:71:ALA:HB2	1.93	0.51
7:A:18:U:O3'	24:R:23:GLY:HA2	2.10	0.51
7:A:2602:A:C4'	7:A:2603:G:OP2	2.58	0.51
19:M:23:ILE:HD12	25:S:84:ARG:HH11	1.76	0.51
41:j:79:LYS:HE2	41:j:80:LYS:HZ3	1.75	0.51
4:4:148:LEU:O	4:4:149:GLU:C	2.52	0.51
39:h:1402:C:O2	39:h:1500:A:N1	2.43	0.51
42:k:9:LEU:HD13	42:k:32:CYS:HB3	1.93	0.51
44:m:36:ILE:HD11	44:m:39:LEU:HB2	1.92	0.51
23:Q:26:VAL:HG12	23:Q:28:VAL:HG23	1.93	0.51
13:G:121:ILE:CG2	13:G:122:THR:N	2.73	0.51
20:N:79:ALA:O	20:N:80:VAL:HG22	2.11	0.51
10:D:32:ASN:N	10:D:32:ASN:HD22	2.09	0.51
39:h:203:G:N2	39:h:215:C:C2	2.79	0.50
4:4:239:LEU:HD11	4:4:288:MET:CE	2.32	0.50
30:X:81:SER:O	30:X:82:ILE:HG12	2.12	0.50
39:h:945:G:C2	39:h:946:A:C8	2.99	0.50
10:D:148:GLN:O	10:D:149:ASN:CG	2.55	0.50
10:D:128:ARG:CG	10:D:128:ARG:NH1	2.73	0.50
10:D:187:LEU:C	10:D:188:LEU:HD23	2.37	0.50
25:S:68:ARG:N	25:S:93:PHE:CE2	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:q:57:VAL:HG13	48:q:58:ASN:N	2.27	0.49
10:D:48:ILE:HG23	10:D:84:LEU:HD11	1.94	0.49
51:t:7:ILE:C	51:t:8:ASN:HD22	2.20	0.49
4:4:300:MET:CE	4:4:300:MET:CA	2.86	0.49
31:Y:18:ARG:NH1	31:Y:22:LEU:O	2.44	0.49
4:4:310:MET:HG3	4:4:311:GLU:N	2.27	0.49
10:D:156:PHE:CE1	17:K:81:ILE:HD13	2.48	0.49
7:A:2052:A:O3'	10:D:149:ASN:HB3	2.13	0.49
12:F:143:TYR:C	12:F:145:LYS:N	2.67	0.49
37:e:62:LEU:HB3	37:e:65:ALA:HB2	1.94	0.49
39:h:979:C:O2	52:u:59:ARG:NH1	2.46	0.49
51:t:30:SER:O	51:t:32:ALA:N	2.46	0.49
52:u:21:PHE:HA	52:u:25:ALA:HB3	1.95	0.49
5:5:33:U:OP2	47:p:130:ARG:NH2	2.44	0.48
7:A:2626:C:H2'	7:A:2627:G:O4'	2.13	0.48
7:A:133:U:H2'	7:A:134:G:O4'	2.13	0.48
20:N:79:ALA:C	20:N:80:VAL:CG2	2.86	0.48
40:i:9:MET:CE	40:i:47:VAL:HG22	2.43	0.48
49:r:31:ILE:HG12	49:r:46:THR:HG22	1.95	0.48
7:A:381:G:OP1	31:Y:18:ARG:HD2	2.13	0.48
39:h:946:A:H2'	39:h:947:G:C8	2.49	0.48
52:u:42:TRP:C	52:u:44:ALA:H	2.21	0.48
45:n:69:VAL:HG23	45:n:100:ALA:HB1	1.96	0.48
46:o:27:MET:HE1	46:o:61:LEU:HD12	1.93	0.48
13:G:121:ILE:HG22	13:G:122:THR:H	1.79	0.48
15:I:82:ILE:HD12	15:I:84:TYR:CE2	2.48	0.48
25:S:53:PHE:HD2	25:S:53:PHE:H	1.62	0.48
26:T:75:PHE:N	26:T:75:PHE:CD2	2.81	0.48
35:c:17:THR:HG21	35:c:42:VAL:HB	1.95	0.48
7:A:565:C:H2'	7:A:566:U:O4'	2.13	0.48
9:C:29:PRO:HG2	9:C:34:LEU:HD11	1.95	0.48
19:M:112:LEU:HD22	19:M:130:GLY:O	2.13	0.48
41:j:79:LYS:HE2	41:j:80:LYS:CG	2.43	0.48
49:r:93:ARG:O	49:r:97:ILE:HG13	2.13	0.48
7:A:1969:A:O2'	7:A:1972:G:N3	2.46	0.48
13:G:35:ARG:NH1	13:G:71:LEU:HD13	2.29	0.48
51:t:3:ARG:HA	51:t:8:ASN:O	2.14	0.48
51:t:33:ILE:C	51:t:35:ALA:N	2.72	0.48
7:A:2511:U:OP1	10:D:128:ARG:HD2	2.14	0.47
39:h:5:U:O4'	39:h:5:U:O2	2.32	0.47
7:A:12:U:O2	7:A:12:U:C2'	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:t:8:ASN:OD1	51:t:66:GLU:OE2	2.32	0.47
27:U:3:ARG:O	27:U:5:GLU:N	2.48	0.47
4:4:199:HIS:CE1	4:4:323:ILE:HD11	2.49	0.47
22:P:51:ALA:HB3	22:P:78:VAL:HG13	1.96	0.47
51:t:16:VAL:CG2	51:t:31:LYS:HG2	2.42	0.47
12:F:25:VAL:O	12:F:28:VAL:HG12	2.14	0.47
26:T:51:LEU:C	26:T:53:SER:N	2.72	0.47
3:3:24:LEU:O	3:3:28:ARG:NH2	2.47	0.47
54:w:42:ILE:HG22	54:w:42:ILE:O	2.15	0.47
55:x:59:VAL:HG22	55:x:75:LEU:HD13	1.96	0.47
7:A:1060:U:O4'	7:A:1061:U:H5''	2.14	0.47
19:M:126:ARG:C	19:M:127:VAL:HG23	2.40	0.47
25:S:53:PHE:HD2	25:S:53:PHE:N	2.12	0.47
7:A:955:U:OP1	20:N:86:LYS:NZ	2.42	0.47
9:C:120:VAL:HG13	9:C:134:ASN:ND2	2.29	0.47
25:S:83:TYR:O	25:S:84:ARG:HB2	2.14	0.47
39:h:658:C:H1'	53:v:22:THR:HG21	1.97	0.47
51:t:7:ILE:C	51:t:8:ASN:ND2	2.73	0.47
7:A:310:A:H5''	28:V:15:THR:HG23	1.96	0.46
19:M:125:LEU:CD1	19:M:125:LEU:N	2.78	0.46
25:S:51:VAL:N	25:S:52:PRO:C	2.72	0.46
40:i:213:TYR:O	40:i:217:VAL:HG23	2.14	0.46
1:1:10:ARG:NH2	39:h:107:G:N7	2.62	0.46
12:F:111:ILE:C	51:t:7:ILE:HD13	2.41	0.46
4:4:332:ARG:HD2	4:4:333:ILE:N	2.30	0.46
7:A:1667:G:O2'	7:A:1991:U:O4	2.24	0.46
12:F:143:TYR:O	12:F:146:VAL:HG22	2.15	0.46
51:t:4:ILE:C	51:t:6:GLY:N	2.72	0.46
57:z:11:ILE:HD11	57:z:15:LEU:HD23	1.97	0.46
9:C:162:VAL:CG1	9:C:174:LEU:HD22	2.46	0.46
25:S:67:GLY:HA3	25:S:93:PHE:CZ	2.51	0.46
7:A:160:A:N3	7:A:2208:C:O2'	2.47	0.46
8:B:94:A:H2'	8:B:95:U:O4'	2.16	0.46
31:Y:13:VAL:CG2	31:Y:29:PHE:HB2	2.46	0.46
4:4:332:ARG:HH11	4:4:332:ARG:CG	2.17	0.46
7:A:981:A:N1	7:A:2027:G:O2'	2.44	0.46
49:r:23:ILE:HD11	49:r:86:VAL:HG13	1.97	0.46
4:4:188:ALA:O	4:4:189:TYR:C	2.58	0.45
39:h:580:C:H2'	39:h:581:G:O4'	2.16	0.45
49:r:65:VAL:HA	49:r:68:GLU:OE2	2.16	0.45
51:t:34:LEU:HD23	51:t:34:LEU:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:252:THR:OG1	9:C:253:LYS:N	2.49	0.45
25:S:26:ASP:O	25:S:27:ILE:HD13	2.16	0.45
44:m:11:HIS:CD2	44:m:54:LEU:HD11	2.51	0.45
4:4:332:ARG:O	4:4:333:ILE:HG12	2.15	0.45
40:i:185:ALA:HB3	40:i:196:VAL:HG11	1.98	0.45
51:t:33:ILE:C	51:t:35:ALA:H	2.25	0.45
7:A:380:G:H5'	31:Y:18:ARG:HG3	1.99	0.45
26:T:52:GLU:O	26:T:52:GLU:HG3	2.15	0.45
39:h:1316:G:N2	39:h:1318:A:H3'	2.30	0.45
7:A:323:C:C4	7:A:333:G:C8	3.05	0.45
10:D:150:GLN:H	10:D:150:GLN:HG2	1.49	0.45
39:h:393:A:OP2	54:w:12:LYS:NZ	2.48	0.45
39:h:1211:U:O2'	39:h:1212:U:OP2	2.21	0.45
46:o:126:ILE:HG22	46:o:127:CYS:HB3	1.98	0.45
49:r:49:GLY:C	49:r:69:ARG:HH12	2.25	0.45
51:t:30:SER:C	51:t:32:ALA:N	2.73	0.45
7:A:139:U:H2'	27:U:1:MET:HE1	1.98	0.45
7:A:861:A:C2	7:A:917:A:C4	3.05	0.45
39:h:868:C:H2'	39:h:869:G:O4'	2.15	0.45
40:i:119:THR:C	40:i:121:SER:N	2.72	0.45
2:2:12:PHE:CZ	49:r:97:ILE:O	2.69	0.45
10:D:149:ASN:ND2	10:D:149:ASN:C	2.73	0.45
39:h:951:G:OP2	51:t:101:ARG:NH2	2.49	0.45
52:u:21:PHE:CG	52:u:25:ALA:HB3	2.52	0.45
39:h:767:A:H2'	39:h:768:A:O4'	2.17	0.45
39:h:1391:U:H2'	39:h:1392:G:C8	2.52	0.45
25:S:52:PRO:HG2	25:S:53:PHE:H	1.82	0.45
7:A:1320:C:N3	7:A:1331:G:O6	2.50	0.44
40:i:187:VAL:HG21	40:i:199:VAL:HG23	1.99	0.44
41:j:14:ILE:HG22	41:j:15:VAL:HG13	1.99	0.44
7:A:2544:G:H2'	7:A:2545:G:O4'	2.18	0.44
39:h:208:U:O2	39:h:212:G:N2	2.50	0.44
9:C:171:TYR:CD2	9:C:171:TYR:N	2.85	0.44
20:N:33:LEU:HD12	20:N:129:THR:O	2.17	0.44
39:h:257:G:C2	39:h:270:A:C2	3.05	0.44
48:q:56:HIS:O	48:q:57:VAL:HG12	2.18	0.44
49:r:23:ILE:C	49:r:23:ILE:HD12	2.43	0.44
7:A:2194:U:O2	7:A:2194:U:O4'	2.35	0.44
12:F:74:VAL:CG2	12:F:79:ILE:HD11	2.48	0.44
12:F:112:ARG:CA	51:t:7:ILE:HG21	2.47	0.44
21:O:10:LEU:O	21:O:12:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:u:42:TRP:CD1	52:u:43:ASN:N	2.86	0.44
12:F:135:GLN:HG3	12:F:141:ILE:HG21	1.99	0.44
41:j:77:ILE:HG22	41:j:77:ILE:O	2.18	0.44
33:a:24:LEU:HD11	33:a:54:MET:SD	2.58	0.44
38:f:11:CYS:SG	38:f:33:HIS:ND1	2.84	0.44
41:j:21:THR:HG23	41:j:58:GLU:HB3	2.00	0.44
44:m:86:ARG:NH1	56:y:64:TYR:O	2.51	0.44
54:w:13:LYS:C	54:w:14:ARG:HG2	2.43	0.44
4:4:151:MET:CE	4:4:353:LEU:HD21	2.38	0.43
7:A:322:A:C5	7:A:340:A:C2	3.06	0.43
16:J:122:ILE:C	16:J:124:ALA:N	2.76	0.43
7:A:1425:G:H2'	7:A:1426:G:C8	2.53	0.43
7:A:1469:A:H2'	7:A:1470:A:C8	2.53	0.43
18:L:7:MET:HE1	18:L:44:LYS:HG3	2.01	0.43
31:Y:3:ARG:O	31:Y:12:PRO:HD3	2.17	0.43
4:4:148:LEU:O	4:4:151:MET:N	2.52	0.43
7:A:2585:U:O2	7:A:2585:U:O4'	2.36	0.43
21:O:38:LEU:HB3	21:O:39:PRO:HD3	1.99	0.43
32:Z:2:LYS:HE2	32:Z:6:LEU:HD11	2.00	0.43
40:i:119:THR:O	40:i:121:SER:N	2.51	0.43
55:x:53:CYS:SG	55:x:78:VAL:HG22	2.59	0.43
9:C:31:ALA:HB3	9:C:32:PRO:HD3	2.01	0.43
9:C:84:ASP:OD2	9:C:87:ARG:HD2	2.19	0.43
7:A:2053:G:OP1	10:D:149:ASN:CB	2.66	0.43
9:C:76:ALA:HB2	9:C:96:TYR:CD1	2.54	0.43
31:Y:13:VAL:HG22	31:Y:29:PHE:HB2	1.99	0.43
40:i:117:LEU:HA	40:i:120:GLN:HG2	2.01	0.43
48:q:65:TYR:HB3	52:u:96:LEU:HD11	1.99	0.43
55:x:9:GLN:O	55:x:25:ILE:HD12	2.18	0.43
27:U:1:MET:HE3	27:U:1:MET:HA	2.00	0.43
30:X:41[B]:ARG:HA	30:X:41[B]:ARG:HD3	1.39	0.43
39:h:61:G:H2'	39:h:62:U:O4'	2.19	0.43
39:h:496:A:H2'	39:h:496:A:N3	2.34	0.43
39:h:789:U:O2'	39:h:791:G:N7	2.50	0.43
4:4:148:LEU:O	4:4:151:MET:HB3	2.19	0.43
7:A:570:G:H2'	7:A:2030:A:N7	2.34	0.43
7:A:2504:U:O2	7:A:2504:U:O4'	2.34	0.43
13:G:4:VAL:HG12	13:G:69:ARG:HG2	2.01	0.43
7:A:141:G:N7	27:U:1:MET:HB3	2.34	0.43
19:M:23:ILE:CD1	25:S:84:ARG:HH11	2.32	0.43
30:X:49:ALA:H	30:X:81:SER:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:h:721:G:H4'	39:h:722:G:O4'	2.18	0.43
39:h:826:C:O2	46:o:16:ASN:ND2	2.52	0.43
49:r:50:SER:CB	49:r:69:ARG:NE	2.82	0.43
2:2:6:VAL:HG22	2:2:15:ALA:CB	2.49	0.42
7:A:819:A:C4	7:A:1189:A:C2	3.07	0.42
7:A:1266:G:O2'	7:A:2012:G:O6	2.29	0.42
7:A:2720:U:OP1	23:Q:53:ARG:NH2	2.52	0.42
39:h:404:G:N7	42:k:2:ALA:HB3	2.34	0.42
40:i:9:MET:HE3	40:i:47:VAL:HG22	2.01	0.42
42:k:131:ASN:O	42:k:131:ASN:CG	2.62	0.42
54:w:8:ARG:O	54:w:29:ASN:ND2	2.50	0.42
7:A:1357:C:H2'	7:A:1358:G:O4'	2.20	0.42
19:M:131:ALA:C	19:M:133:ALA:N	2.77	0.42
39:h:1130:A:OP1	47:p:18:ARG:NH1	2.53	0.42
12:F:112:ARG:HB3	51:t:7:ILE:CG2	2.46	0.42
43:l:161:VAL:HG12	43:l:162:GLU:H	1.84	0.42
49:r:64:GLN:O	49:r:67:ALA:N	2.52	0.42
7:A:1061:U:C1'	7:A:1070:A:O4'	2.50	0.42
7:A:2190:G:O2'	7:A:2191:A:OP1	2.34	0.42
7:A:2396:G:C2	7:A:2421:G:C2	3.07	0.42
25:S:81:LYS:HA	25:S:81:LYS:HD3	1.77	0.42
55:x:75:LEU:C	55:x:75:LEU:HD12	2.44	0.42
7:A:851:C:O2'	33:a:43:ALA:O	2.35	0.42
7:A:1494:A:H2'	7:A:1495:A:C8	2.54	0.42
7:A:2267:A:H5''	7:A:2268:A:H5'	2.02	0.42
7:A:2395:C:H2'	7:A:2396:G:O4'	2.20	0.42
29:W:4:ILE:HG22	29:W:5:ASN:O	2.20	0.42
42:k:93:LEU:O	42:k:136:GLN:NE2	2.53	0.42
7:A:1614:A:N1	26:T:93:ALA:HB2	2.34	0.42
4:4:333:ILE:CG2	4:4:334:LYS:H	2.31	0.42
9:C:6:CYS:SG	9:C:13:ARG:NH2	2.93	0.42
13:G:121:ILE:HD13	13:G:121:ILE:N	2.34	0.42
39:h:109:A:H2'	39:h:326:G:N2	2.35	0.42
39:h:947:G:OP1	51:t:107:ARG:HG3	2.20	0.42
39:h:1074:G:O2'	39:h:1101:A:N1	2.41	0.42
39:h:1322:C:P	57:z:78:ARG:HH22	2.43	0.42
14:H:137:GLU:O	14:H:138:VAL:C	2.60	0.42
29:W:4:ILE:HG12	29:W:50:MET:HE1	2.02	0.42
45:n:25:LYS:O	45:n:29:ILE:HD12	2.20	0.42
3:3:15:ALA:HB1	4:4:315:SER:HB3	2.02	0.42
7:A:748:G:C8	26:T:89:ALA:HB1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:811:U:H2'	19:M:21:ARG:HA	2.02	0.41
7:A:1009:A:N3	7:A:1153:C:O2'	2.50	0.41
39:h:112:G:HO2'	39:h:354:G:HO2'	1.68	0.41
7:A:1912:A:N1	39:h:1407:C:O2'	2.48	0.41
7:A:2511:U:O4	7:A:2575:C:N3	2.53	0.41
28:V:83:VAL:HG12	28:V:84:GLY:N	2.35	0.41
37:e:32:ILE:HG22	37:e:32:ILE:O	2.20	0.41
55:x:8:LEU:O	55:x:60:GLU:HG3	2.21	0.41
39:h:1060:U:OP1	52:u:85:ARG:NH2	2.53	0.41
51:t:16:VAL:HG23	51:t:30:SER:HG	1.76	0.41
3:3:15:ALA:HB2	4:4:311:GLU:HG3	2.02	0.41
4:4:147:MET:CE	4:4:349:LEU:CD2	2.89	0.41
7:A:263:G:O2'	7:A:429:A:N3	2.47	0.41
7:A:1488:C:O2	7:A:1502:A:C2	2.73	0.41
12:F:111:ILE:O	51:t:7:ILE:CD1	2.68	0.41
7:A:1380:G:N2	7:A:1570:A:N1	2.64	0.41
40:i:69:PHE:HB3	40:i:80:VAL:HG13	2.03	0.41
7:A:807:U:O2'	7:A:2060:A:N1	2.52	0.41
7:A:964:C:O2'	7:A:2273:A:N3	2.41	0.41
39:h:1251:A:H2'	39:h:1252:A:O4'	2.20	0.41
39:h:1356:G:H2'	39:h:1357:A:C8	2.56	0.41
40:i:57:LEU:HD13	40:i:217:VAL:HG13	2.02	0.41
7:A:2096:C:N3	7:A:2193:G:O6	2.54	0.41
13:G:35:ARG:HH11	13:G:71:LEU:HD13	1.86	0.41
13:G:121:ILE:CG2	13:G:122:THR:H	2.32	0.41
41:j:155:GLY:O	41:j:156:ARG:HB2	2.20	0.41
52:u:42:TRP:C	52:u:44:ALA:N	2.79	0.41
52:u:64:CYS:C	52:u:66:GLN:N	2.78	0.41
7:A:370:G:O2'	7:A:424:G:OP1	2.39	0.41
7:A:492:A:H2'	7:A:493:G:O4'	2.21	0.41
7:A:1209:U:O2'	7:A:1237:A:N1	2.47	0.41
7:A:2503:A:O2'	7:A:2505:G:OP2	2.37	0.41
9:C:239:ASN:OD1	9:C:239:ASN:N	2.54	0.41
26:T:51:LEU:C	26:T:53:SER:H	2.28	0.41
39:h:176:C:O4'	39:h:1447:A:C2	2.74	0.41
42:k:105:MET:HG2	42:k:171:LEU:HD13	2.01	0.41
49:r:50:SER:CB	49:r:69:ARG:HE	2.34	0.41
50:s:50:ARG:CZ	50:s:89:ASP:OD2	2.68	0.41
4:4:166:ILE:HD11	4:4:182:LYS:HB2	2.03	0.41
7:A:2259:U:C5	7:A:2427:C:N4	2.89	0.41
51:t:4:ILE:HG22	51:t:5:ALA:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:j:73:PRO:O	41:j:77:ILE:HG13	2.21	0.40
51:t:30:SER:C	51:t:32:ALA:H	2.29	0.40
7:A:1021:A:N3	7:A:1021:A:H3'	2.36	0.40
7:A:2514:U:H2'	7:A:2515:C:C6	2.56	0.40
30:X:41[B]:ARG:HD3	30:X:41[B]:ARG:HH11	1.78	0.40
39:h:501:C:OP1	50:s:114:ARG:NH2	2.53	0.40
39:h:1082:A:H2'	39:h:1083:U:O4'	2.21	0.40
4:4:118:MET:HE1	4:4:361:LEU:HD12	2.03	0.40
4:4:360:SER:O	4:4:364:GLY:N	2.52	0.40
29:W:28:ALA:HB1	29:W:89:ILE:O	2.22	0.40
39:h:1213:A:O2'	39:h:1215:G:N7	2.46	0.40
39:h:1287:A:H2'	39:h:1288:A:C8	2.56	0.40
39:h:1328:C:H2'	39:h:1329:A:O4'	2.22	0.40
7:A:1358:G:C8	7:A:1371:G:O6	2.74	0.40
10:D:149:ASN:HA	10:D:150:GLN:HA	1.82	0.40
31:Y:18:ARG:HE	31:Y:18:ARG:HB3	1.64	0.40
39:h:1512:U:H2'	39:h:1513:A:C8	2.56	0.40
49:r:20:VAL:N	49:r:35:THR:O	2.53	0.40
7:A:348:A:H2'	7:A:349:U:O4'	2.21	0.40
19:M:129:LYS:C	19:M:131:ALA:N	2.79	0.40
22:P:27:VAL:HG21	22:P:40:ILE:HD12	2.03	0.40
46:o:66:PHE:CD2	46:o:67:GLN:HG2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	84/86 (98%)	79 (94%)	4 (5%)	1 (1%)	10	38
2	2	54/70 (77%)	51 (94%)	3 (6%)	0	100	100
3	3	43/72 (60%)	32 (74%)	8 (19%)	3 (7%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	4	353/365 (97%)	316 (90%)	31 (9%)	6 (2%)	7	30
9	C	269/272 (99%)	245 (91%)	24 (9%)	0	100	100
10	D	207/209 (99%)	189 (91%)	16 (8%)	2 (1%)	12	43
11	E	199/201 (99%)	188 (94%)	10 (5%)	1 (0%)	24	59
12	F	175/178 (98%)	157 (90%)	15 (9%)	3 (2%)	7	30
13	G	174/176 (99%)	156 (90%)	18 (10%)	0	100	100
14	H	146/149 (98%)	131 (90%)	13 (9%)	2 (1%)	9	34
15	I	133/164 (81%)	116 (87%)	14 (10%)	3 (2%)	5	23
16	J	69/141 (49%)	61 (88%)	7 (10%)	1 (1%)	9	34
17	K	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
18	L	121/123 (98%)	108 (89%)	11 (9%)	2 (2%)	7	30
19	M	142/144 (99%)	127 (89%)	14 (10%)	1 (1%)	18	51
20	N	135/136 (99%)	125 (93%)	6 (4%)	4 (3%)	3	18
21	O	123/127 (97%)	110 (89%)	12 (10%)	1 (1%)	16	48
22	P	115/117 (98%)	112 (97%)	2 (2%)	1 (1%)	14	46
23	Q	112/114 (98%)	99 (88%)	13 (12%)	0	100	100
24	R	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
25	S	101/103 (98%)	93 (92%)	6 (6%)	2 (2%)	6	26
26	T	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
27	U	91/100 (91%)	83 (91%)	4 (4%)	4 (4%)	2	11
28	V	100/103 (97%)	88 (88%)	8 (8%)	4 (4%)	2	12
29	W	92/94 (98%)	83 (90%)	8 (9%)	1 (1%)	11	41
30	X	75/84 (89%)	66 (88%)	9 (12%)	0	100	100
31	Y	75/77 (97%)	66 (88%)	6 (8%)	3 (4%)	2	12
32	Z	60/63 (95%)	56 (93%)	4 (7%)	0	100	100
33	a	57/58 (98%)	52 (91%)	5 (9%)	0	100	100
34	b	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
35	c	49/54 (91%)	45 (92%)	4 (8%)	0	100	100
36	d	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
37	e	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
38	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	i	222/240 (92%)	196 (88%)	17 (8%)	9 (4%)	2	12
41	j	204/232 (88%)	176 (86%)	25 (12%)	3 (2%)	8	33
42	k	203/205 (99%)	193 (95%)	10 (5%)	0	100	100
43	l	153/166 (92%)	130 (85%)	20 (13%)	3 (2%)	6	26
44	m	104/135 (77%)	91 (88%)	11 (11%)	2 (2%)	6	28
45	n	149/178 (84%)	130 (87%)	16 (11%)	3 (2%)	6	26
46	o	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
47	p	125/129 (97%)	106 (85%)	14 (11%)	5 (4%)	2	12
48	q	97/103 (94%)	87 (90%)	8 (8%)	2 (2%)	5	25
49	r	115/128 (90%)	94 (82%)	17 (15%)	4 (4%)	3	15
50	s	121/123 (98%)	106 (88%)	13 (11%)	2 (2%)	7	30
51	t	112/117 (96%)	94 (84%)	12 (11%)	6 (5%)	1	8
52	u	98/100 (98%)	83 (85%)	10 (10%)	5 (5%)	1	9
53	v	86/88 (98%)	78 (91%)	8 (9%)	0	100	100
54	w	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	9	36
55	x	78/83 (94%)	73 (94%)	5 (6%)	0	100	100
56	y	53/74 (72%)	49 (92%)	3 (6%)	1 (2%)	6	28
57	z	77/91 (85%)	69 (90%)	7 (9%)	1 (1%)	9	36
All	All	6117/6556 (93%)	5506 (90%)	519 (8%)	92 (2%)	11	33

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	E	73	ILE
14	H	50	ARG
19	M	132	ARG
20	N	81	ARG
27	U	2	ILE
28	V	59	VAL
40	i	122	GLN
40	i	126	PHE
40	i	131	LYS
41	j	82	GLU
47	p	25	ASN
48	q	57	VAL
49	r	119	ASN

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Mol	Chain	Res	Type
50	s	90	LEU
51	t	5	ALA
51	t	30	SER
52	u	43	ASN
52	u	65	ARG
54	w	48	GLU
3	3	14	ASN
3	3	35	GLY
4	4	210	GLY
10	D	149	ASN
12	F	144	ASP
16	J	123	GLU
18	L	108	ARG
25	S	84	ARG
28	V	60	GLU
31	Y	3	ARG
31	Y	19	SER
40	i	21	ARG
40	i	98	GLY
41	j	156	ARG
43	l	16	ILE
47	p	30	ILE
47	p	53	GLU
47	p	123	ARG
49	r	69	ARG
50	s	89	ASP
51	t	31	LYS
51	t	34	LEU
52	u	20	TYR
52	u	40	ASP
1	1	69	LYS
3	3	26	ARG
18	L	75	SER
20	N	82	MET
21	O	100	CYS
27	U	4	GLU
27	U	25	GLU
40	i	120	GLN
40	i	130	THR
45	n	37	SER
51	t	105	ASN
56	y	43	ARG

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Mol	Chain	Res	Type
4	4	151	MET
10	D	129	THR
15	I	88	HIS
22	P	100	HIS
27	U	3	ARG
28	V	52	LEU
28	V	100	SER
40	i	95	ARG
47	p	92	GLU
4	4	120	SER
4	4	250	GLY
15	I	108	VAL
15	I	132	TYR
20	N	80	VAL
29	W	88	HIS
31	Y	22	LEU
44	m	56	LYS
45	n	57	SER
45	n	130	ASN
48	q	39	PRO
51	t	7	ILE
52	u	38	ASP
57	z	9	PRO
4	4	351	GLY
12	F	78	LYS
12	F	142	ASP
49	r	64	GLN
49	r	120	GLY
41	j	149	ILE
14	H	107	GLY
20	N	3	GLN
43	l	94	VAL
40	i	71	GLY
43	l	161	VAL
4	4	211	GLY
44	m	36	ILE
25	S	52	PRO

5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	65/65 (100%)	61 (94%)	4 (6%)	16	47
2	2	48/60 (80%)	45 (94%)	3 (6%)	16	46
3	3	38/59 (64%)	35 (92%)	3 (8%)	11	37
4	4	303/311 (97%)	278 (92%)	25 (8%)	10	35
9	C	216/217 (100%)	199 (92%)	17 (8%)	11	37
10	D	164/164 (100%)	151 (92%)	13 (8%)	11	37
11	E	165/165 (100%)	160 (97%)	5 (3%)	36	68
12	F	148/149 (99%)	140 (95%)	8 (5%)	20	52
13	G	137/137 (100%)	132 (96%)	5 (4%)	31	64
14	H	113/114 (99%)	106 (94%)	7 (6%)	16	47
15	I	103/122 (84%)	102 (99%)	1 (1%)	68	83
16	J	53/109 (49%)	51 (96%)	2 (4%)	29	62
17	K	116/116 (100%)	106 (91%)	10 (9%)	10	34
18	L	104/104 (100%)	96 (92%)	8 (8%)	12	38
19	M	103/103 (100%)	96 (93%)	7 (7%)	14	43
20	N	110/109 (101%)	108 (98%)	2 (2%)	51	76
21	O	102/103 (99%)	98 (96%)	4 (4%)	28	61
22	P	87/87 (100%)	86 (99%)	1 (1%)	65	82
23	Q	99/99 (100%)	92 (93%)	7 (7%)	13	42
24	R	89/89 (100%)	82 (92%)	7 (8%)	11	37
25	S	84/84 (100%)	77 (92%)	7 (8%)	10	35
26	T	93/93 (100%)	90 (97%)	3 (3%)	34	66
27	U	80/84 (95%)	74 (92%)	6 (8%)	12	39
28	V	83/84 (99%)	75 (90%)	8 (10%)	8	29
29	W	78/78 (100%)	77 (99%)	1 (1%)	61	80
30	X	58/62 (94%)	55 (95%)	3 (5%)	21	53
31	Y	67/67 (100%)	62 (92%)	5 (8%)	12	39
32	Z	54/55 (98%)	52 (96%)	2 (4%)	30	63
33	a	49/48 (102%)	45 (92%)	4 (8%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	b	47/47 (100%)	41 (87%)	6 (13%)	4	18
35	c	45/48 (94%)	40 (89%)	5 (11%)	6	23
36	d	38/38 (100%)	35 (92%)	3 (8%)	11	37
37	e	51/51 (100%)	48 (94%)	3 (6%)	18	49
38	f	34/34 (100%)	33 (97%)	1 (3%)	37	68
40	i	186/198 (94%)	176 (95%)	10 (5%)	20	52
41	j	170/189 (90%)	160 (94%)	10 (6%)	18	49
42	k	172/172 (100%)	164 (95%)	8 (5%)	23	56
43	l	118/125 (94%)	101 (86%)	17 (14%)	3	14
44	m	92/116 (79%)	83 (90%)	9 (10%)	7	29
45	n	124/146 (85%)	113 (91%)	11 (9%)	9	33
46	o	104/104 (100%)	95 (91%)	9 (9%)	9	34
47	p	105/106 (99%)	91 (87%)	14 (13%)	4	17
48	q	87/90 (97%)	79 (91%)	8 (9%)	8	31
49	r	90/98 (92%)	77 (86%)	13 (14%)	3	14
50	s	103/103 (100%)	93 (90%)	10 (10%)	8	29
51	t	92/95 (97%)	89 (97%)	3 (3%)	33	65
52	u	83/83 (100%)	75 (90%)	8 (10%)	8	29
53	v	76/76 (100%)	72 (95%)	4 (5%)	20	52
54	w	65/65 (100%)	60 (92%)	5 (8%)	12	38
55	x	74/77 (96%)	67 (90%)	7 (10%)	8	30
56	y	48/64 (75%)	47 (98%)	1 (2%)	47	74
57	z	70/78 (90%)	63 (90%)	7 (10%)	7	28
All	All	5083/5340 (95%)	4733 (93%)	350 (7%)	16	43

All (350) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	5	LYS
1	1	6	SER
1	1	57	ILE
1	1	69	LYS
2	2	4	ILE
2	2	43	THR

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Mol	Chain	Res	Type
2	2	54	LYS
3	3	10	GLN
3	3	20	LEU
3	3	26	ARG
4	4	25	LEU
4	4	73	MET
4	4	79	ASP
4	4	86	LEU
4	4	122	GLU
4	4	159	ARG
4	4	167	GLU
4	4	195	GLU
4	4	216	SER
4	4	240	ARG
4	4	259	SER
4	4	271	VAL
4	4	272	THR
4	4	277	ASP
4	4	297	GLU
4	4	298	LEU
4	4	299	GLU
4	4	300	MET
4	4	303	LYS
4	4	310	MET
4	4	313	ASN
4	4	316	ASP
4	4	332	ARG
4	4	336	LEU
4	4	355	GLN
9	C	10	SER
9	C	24	LEU
9	C	59	LYS
9	C	88	SER
9	C	111	LYS
9	C	130	LEU
9	C	140	THR
9	C	182	ARG
9	C	192	LEU
9	C	202	LEU
9	C	236	GLU
9	C	239	ASN
9	C	245	VAL

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Mol	Chain	Res	Type
9	C	251	GLN
9	C	252	THR
9	C	262	ARG
9	C	264	ASP
10	D	32	ASN
10	D	56	LYS
10	D	62	LYS
10	D	77	ARG
10	D	100	LEU
10	D	105	LYS
10	D	128	ARG
10	D	131	ASP
10	D	149	ASN
10	D	150	GLN
10	D	154	LYS
10	D	157	LYS
10	D	193	VAL
11	E	75	SER
11	E	96	VAL
11	E	125	SER
11	E	163	ASN
11	E	173	THR
12	F	14	LYS
12	F	26	MET
12	F	35	THR
12	F	74	VAL
12	F	77	PHE
12	F	129	SER
12	F	135	GLN
12	F	144	ASP
13	G	11	VAL
13	G	29	LYS
13	G	36	THR
13	G	87	LEU
13	G	103	ILE
14	H	21	VAL
14	H	48	GLU
14	H	53	GLU
14	H	54	LEU
14	H	87	GLU
14	H	121	VAL
14	H	137	GLU

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Mol	Chain	Res	Type
15	I	71	CYS
16	J	117	MET
16	J	123	GLU
17	K	12	LYS
17	K	24	THR
17	K	39	LYS
17	K	40	HIS
17	K	43	GLU
17	K	50	THR
17	K	90	GLU
17	K	101	ILE
17	K	124	VAL
17	K	142	ILE
18	L	8	LEU
18	L	17	ARG
18	L	41	ILE
18	L	58	LEU
18	L	70	ARG
18	L	80	ASP
18	L	105	ARG
18	L	110	GLU
19	M	7	SER
19	M	14	LYS
19	M	25	SER
19	M	46	VAL
19	M	68	SER
19	M	116	VAL
19	M	126	ARG
20	N	6	ARG
20	N	80	VAL
21	O	6	SER
21	O	43	GLU
21	O	47	VAL
21	O	117	ASP
22	P	38	GLN
23	Q	30	VAL
23	Q	37	LYS
23	Q	63	LYS
23	Q	65	SER
23	Q	85	SER
23	Q	87	LYS
23	Q	115	ASN

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Mol	Chain	Res	Type
24	R	6	ARG
24	R	19	LYS
24	R	40	ILE
24	R	53	ARG
24	R	56	GLN
24	R	84	LYS
24	R	91	ASP
25	S	6	GLN
25	S	25	LEU
25	S	38	VAL
25	S	45	GLU
25	S	53	PHE
25	S	55	ASP
25	S	64	VAL
26	T	28	LYS
26	T	52	GLU
26	T	108	SER
27	U	1	MET
27	U	10	VAL
27	U	16	VAL
27	U	27	SER
27	U	60	THR
27	U	81	LYS
28	V	30	SER
28	V	46	GLN
28	V	61	LYS
28	V	68	SER
28	V	72	ILE
28	V	77	THR
28	V	81	ASP
28	V	89	ASP
29	W	25	LYS
30	X	20	ARG
30	X	70	GLU
30	X	81	SER
31	Y	2	SER
31	Y	14	THR
31	Y	18	ARG
31	Y	28	ARG
31	Y	43	GLU
32	Z	16	THR
32	Z	23	ARG

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Mol	Chain	Res	Type
33	a	4	THR
33	a	21	LYS
33	a	37	GLU
33	a	58	GLU
34	b	6	ASN
34	b	9	THR
34	b	29	SER
34	b	39	LEU
34	b	40	ARG
34	b	52	ARG
35	c	6	ARG
35	c	10	LYS
35	c	12	VAL
35	c	23	THR
35	c	51	GLU
36	d	19	ARG
36	d	44	VAL
36	d	46	LYS
37	e	38	THR
37	e	51	SER
37	e	54	ASP
38	f	20	ASP
40	i	26	LYS
40	i	31	ILE
40	i	94	HIS
40	i	112	LYS
40	i	126	PHE
40	i	129	LEU
40	i	161	LEU
40	i	167	ASP
40	i	188	ASP
40	i	223	GLU
41	j	33	LEU
41	j	39	VAL
41	j	58	GLU
41	j	88	ARG
41	j	103	ILE
41	j	111	LEU
41	j	149	ILE
41	j	150	LYS
41	j	151	VAL
41	j	165	THR

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Mol	Chain	Res	Type
42	k	3	ARG
42	k	95	GLU
42	k	100	ASN
42	k	131	ASN
42	k	143	VAL
42	k	179	GLU
42	k	197	GLU
42	k	206	LYS
43	l	12	GLN
43	l	19	ASN
43	l	22	SER
43	l	26	LYS
43	l	32	SER
43	l	46	VAL
43	l	69	ARG
43	l	73	ASN
43	l	74	VAL
43	l	103	THR
43	l	106	ILE
43	l	111	MET
43	l	123	VAL
43	l	130	SER
43	l	137	VAL
43	l	161	VAL
43	l	163	GLU
44	m	36	ILE
44	m	38	ARG
44	m	68	GLN
44	m	69	GLU
44	m	71	ILE
44	m	89	VAL
44	m	92	THR
44	m	96	VAL
44	m	102	MET
45	n	23	LEU
45	n	25	LYS
45	n	30	LEU
45	n	37	SER
45	n	38	THR
45	n	68	ASN
45	n	72	THR
45	n	78	ARG

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Mol	Chain	Res	Type
45	n	90	GLU
45	n	109	ARG
45	n	144	MET
46	o	3	MET
46	o	15	ARG
46	o	31	LYS
46	o	41	LYS
46	o	51	VAL
46	o	58	GLU
46	o	60	GLU
46	o	80	ARG
46	o	101	ILE
47	p	12	ARG
47	p	14	SER
47	p	18	ARG
47	p	43	THR
47	p	53	GLU
47	p	57	MET
47	p	61	LEU
47	p	62	ASP
47	p	63	LEU
47	p	65	ILE
47	p	89	GLU
47	p	98	LEU
47	p	114	LYS
47	p	129	LYS
48	q	17	LEU
48	q	54	SER
48	q	57	VAL
48	q	63	ASP
48	q	71	LEU
48	q	80	THR
48	q	90	LEU
48	q	102	LEU
49	r	23	ILE
49	r	26	SER
49	r	33	THR
49	r	64	GLN
49	r	69	ARG
49	r	82	LEU
49	r	95	SER
49	r	96	THR

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Mol	Chain	Res	Type
49	r	108	THR
49	r	111	THR
49	r	121	CYS
49	r	125	LYS
49	r	129	VAL
50	s	24	LEU
50	s	33	VAL
50	s	34	CYS
50	s	52	VAL
50	s	79	VAL
50	s	88	LYS
50	s	89	ASP
50	s	97	THR
50	s	102	LEU
50	s	104	CYS
51	t	17	ILE
51	t	34	LEU
51	t	54	ASP
52	u	12	LYS
52	u	19	LYS
52	u	26	GLU
52	u	59	ARG
52	u	64	CYS
52	u	65	ARG
52	u	97	LYS
52	u	100	SER
53	v	5	THR
53	v	13	SER
53	v	18	ASP
53	v	61	SER
54	w	12	LYS
54	w	20	VAL
54	w	36	VAL
54	w	70	ARG
54	w	78	VAL
55	x	9	GLN
55	x	16	LYS
55	x	29	VAL
55	x	33	ILE
55	x	53	CYS
55	x	75	LEU
55	x	80	GLU

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Mol	Chain	Res	Type
56	y	66	SER
57	z	5	LEU
57	z	7	LYS
57	z	27	ASP
57	z	38	SER
57	z	39	THR
57	z	63	THR
57	z	81	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	82	GLN
3	3	5	GLN
3	3	27	GLN
3	3	32	ASN
4	4	38	ASN
4	4	199	HIS
4	4	214	HIS
4	4	252	GLN
4	4	255	ASN
4	4	265	HIS
4	4	280	GLN
4	4	290	GLN
4	4	304	ASN
9	C	70	ASN
9	C	134	ASN
9	C	251	GLN
9	C	260	ASN
10	D	42	ASN
10	D	149	ASN
10	D	150	GLN
11	E	94	GLN
12	F	37	ASN
13	G	48	ASN
13	G	88	GLN
14	H	2	GLN
14	H	20	ASN
14	H	66	ASN
14	H	135	HIS
15	I	88	HIS
18	L	90	ASN

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Mol	Chain	Res	Type
19	M	35	HIS
20	N	3	GLN
20	N	13	HIS
21	O	9	GLN
21	O	107	ASN
22	P	19	GLN
22	P	104	GLN
23	Q	12	GLN
23	Q	77	HIS
23	Q	115	ASN
24	R	44	GLN
24	R	72	ASN
25	S	12	HIS
26	T	9	HIS
27	U	91	GLN
27	U	92	ASN
28	V	54	GLN
29	W	44	HIS
29	W	75	GLN
30	X	57	HIS
30	X	76	ASN
32	Z	31	GLN
32	Z	36	GLN
33	a	20	HIS
36	d	26	ASN
37	e	28	ASN
40	i	15	HIS
40	i	94	HIS
40	i	146	ASN
40	i	227	GLN
41	j	6	HIS
41	j	69	HIS
43	l	83	HIS
43	l	97	GLN
44	m	11	HIS
44	m	94	HIS
45	n	86	GLN
45	n	148	ASN
46	o	38	ASN
46	o	67	GLN
47	p	110	GLN
50	s	6	GLN

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Mol	Chain	Res	Type
50	s	72	HIS
51	t	8	ASN
51	t	12	HIS
53	v	20	ASN
54	w	9	HIS
54	w	59	HIS
54	w	63	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
39	h	1533/1534 (99%)	293 (19%)	0
5	5	75/76 (98%)	20 (26%)	2 (2%)
6	7	5/6 (83%)	3 (60%)	1 (20%)
7	A	2892/2903 (99%)	541 (18%)	62 (2%)
8	B	119/120 (99%)	17 (14%)	0
All	All	4624/4639 (99%)	874 (18%)	65 (1%)

All (874) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	5	9	G
5	5	14	A
5	5	17(A)	U
5	5	18	G
5	5	19	G
5	5	20	U
5	5	22	G
5	5	25	C
5	5	30	G
5	5	31	G
5	5	44	A
5	5	47	U
5	5	48	C
5	5	53	G
5	5	62	C
5	5	64	G
5	5	69	C
5	5	73	A
5	5	74	C
5	5	76	A

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Mol	Chain	Res	Type
6	7	14	C
6	7	15	U
6	7	16	A
7	A	4	U
7	A	10	A
7	A	34	U
7	A	35	G
7	A	46	G
7	A	49	A
7	A	58	G
7	A	63	A
7	A	66	C
7	A	71	A
7	A	74	A
7	A	75	G
7	A	84	A
7	A	88	G
7	A	89	A
7	A	96	C
7	A	101	A
7	A	102	U
7	A	118	A
7	A	119	A
7	A	120	U
7	A	125	A
7	A	126	A
7	A	131	A
7	A	134	G
7	A	137	U
7	A	139	U
7	A	140	C
7	A	142	A
7	A	163	C
7	A	165	A
7	A	167	A
7	A	171	U
7	A	181	A
7	A	186	G
7	A	196	A
7	A	197	A
7	A	199	A
7	A	200	U

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Mol	Chain	Res	Type
7	A	216	A
7	A	221	A
7	A	222	A
7	A	248	G
7	A	264	C
7	A	266	G
7	A	272	A
7	A	276	U
7	A	280	U
7	A	282	A
7	A	284	U
7	A	290	U
7	A	302	C
7	A	310	A
7	A	311	A
7	A	329	G
7	A	330	A
7	A	332	A
7	A	362	A
7	A	367	G
7	A	372	G
7	A	386	G
7	A	387	U
7	A	399	U
7	A	403	U
7	A	411	G
7	A	412	A
7	A	424	G
7	A	429	A
7	A	451	U
7	A	455	C
7	A	456	C
7	A	467	G
7	A	473	G
7	A	479	A
7	A	480	A
7	A	481	G
7	A	491	G
7	A	501	A
7	A	503	A
7	A	504	A
7	A	505	A

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Mol	Chain	Res	Type
7	A	508	A
7	A	509	C
7	A	510	C
7	A	512	G
7	A	513	A
7	A	529	A
7	A	530	G
7	A	531	C
7	A	532	A
7	A	533	G
7	A	538	A
7	A	544	C
7	A	546	U
7	A	547	A
7	A	548	G
7	A	549	G
7	A	550	C
7	A	555	G
7	A	556	A
7	A	559	G
7	A	563	A
7	A	573	U
7	A	575	A
7	A	602	A
7	A	603	A
7	A	613	A
7	A	614	A
7	A	615	U
7	A	620	G
7	A	621	A
7	A	627	A
7	A	637	A
7	A	645	C
7	A	646	U
7	A	647	G
7	A	653	U
7	A	654	A
7	A	655	A
7	A	670	A
7	A	686	U
7	A	722	A
7	A	726	G

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Mol	Chain	Res	Type
7	A	730	A
7	A	738	G
7	A	746	U
7	A	747	U
7	A	764	A
7	A	765	C
7	A	775	G
7	A	776	G
7	A	782	A
7	A	784	G
7	A	785	G
7	A	789	A
7	A	790	U
7	A	792	A
7	A	805	G
7	A	812	C
7	A	827	U
7	A	828	U
7	A	835	C
7	A	845	A
7	A	846	U
7	A	858	G
7	A	859	G
7	A	866	A
7	A	869	G
7	A	876	C
7	A	877	A
7	A	878	A
7	A	880	G
7	A	881	G
7	A	882	G
7	A	883	G
7	A	885	C
7	A	896	A
7	A	898	C
7	A	910	A
7	A	914	G
7	A	915	C
7	A	931	U
7	A	933	A
7	A	934	U
7	A	945	A

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Mol	Chain	Res	Type
7	A	946	C
7	A	961	C
7	A	974	G
7	A	983	A
7	A	984	A
7	A	985	C
7	A	996	A
7	A	999	U
7	A	1002	G
7	A	1005	C
7	A	1012	U
7	A	1013	C
7	A	1022	G
7	A	1025	G
7	A	1026	G
7	A	1033	U
7	A	1057	A
7	A	1059	G
7	A	1060	U
7	A	1061	U
7	A	1062	G
7	A	1070	A
7	A	1073	A
7	A	1078	U
7	A	1079	C
7	A	1082	U
7	A	1084	A
7	A	1087	G
7	A	1088	A
7	A	1090	A
7	A	1091	G
7	A	1098	A
7	A	1111	A
7	A	1112	G
7	A	1119	U
7	A	1128	G
7	A	1129	A
7	A	1132	U
7	A	1133	A
7	A	1134	A
7	A	1135	C
7	A	1136	G

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Mol	Chain	Res	Type
7	A	1137	G
7	A	1142	A
7	A	1172	C
7	A	1173	U
7	A	1175	A
7	A	1176	U
7	A	1206	G
7	A	1210	G
7	A	1238	G
7	A	1253	A
7	A	1256	G
7	A	1268	A
7	A	1271	G
7	A	1272	A
7	A	1275	A
7	A	1287	A
7	A	1289	C
7	A	1301	A
7	A	1310	G
7	A	1313	U
7	A	1321	A
7	A	1327	A
7	A	1330	C
7	A	1345	C
7	A	1347	A
7	A	1352	U
7	A	1365	A
7	A	1371	G
7	A	1379	U
7	A	1383	A
7	A	1394	U
7	A	1395	A
7	A	1401	G
7	A	1416	G
7	A	1417	C
7	A	1419	A
7	A	1424	G
7	A	1427	A
7	A	1428	C
7	A	1435	G
7	A	1449	G
7	A	1451	C

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Mol	Chain	Res	Type
7	A	1452	G
7	A	1453	A
7	A	1455	G
7	A	1460	U
7	A	1478	G
7	A	1482	G
7	A	1490	A
7	A	1491	G
7	A	1493	C
7	A	1494	A
7	A	1495	A
7	A	1497	U
7	A	1498	C
7	A	1504	A
7	A	1507	C
7	A	1510	G
7	A	1515	A
7	A	1523	U
7	A	1524	G
7	A	1529	G
7	A	1530	G
7	A	1532	A
7	A	1533	C
7	A	1535	A
7	A	1537	G
7	A	1540	G
7	A	1557	C
7	A	1569	A
7	A	1578	U
7	A	1584	U
7	A	1585	C
7	A	1593	A
7	A	1607	C
7	A	1608	A
7	A	1609	A
7	A	1610	A
7	A	1618	A
7	A	1630	A
7	A	1634	A
7	A	1639	C
7	A	1647	U
7	A	1648	U

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Mol	Chain	Res	Type
7	A	1649	G
7	A	1674	G
7	A	1686	C
7	A	1715	G
7	A	1725	U
7	A	1729	U
7	A	1730	C
7	A	1732	C
7	A	1735	A
7	A	1738	G
7	A	1750	G
7	A	1758	U
7	A	1764	C
7	A	1773	A
7	A	1782	U
7	A	1791	A
7	A	1800	C
7	A	1802	A
7	A	1808	A
7	A	1809	A
7	A	1811	G
7	A	1816	C
7	A	1829	A
7	A	1847	A
7	A	1848	A
7	A	1869	G
7	A	1870	C
7	A	1871	A
7	A	1872	A
7	A	1873	G
7	A	1882	U
7	A	1891	G
7	A	1896	G
7	A	1905	C
7	A	1906	G
7	A	1910	G
7	A	1927	A
7	A	1929	G
7	A	1930	G
7	A	1934	C
7	A	1938	A
7	A	1939	U

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Mol	Chain	Res	Type
7	A	1955	U
7	A	1965	C
7	A	1967	C
7	A	1970	A
7	A	1971	U
7	A	1972	G
7	A	1975	G
7	A	1991	U
7	A	1993	U
7	A	1997	C
7	A	2020	A
7	A	2023	C
7	A	2026	U
7	A	2027	G
7	A	2030	A
7	A	2031	A
7	A	2033	A
7	A	2043	C
7	A	2051	A
7	A	2052	A
7	A	2055	C
7	A	2056	G
7	A	2059	A
7	A	2060	A
7	A	2061	G
7	A	2062	A
7	A	2063	C
7	A	2069	G
7	A	2077	A
7	A	2080	A
7	A	2093	G
7	A	2102	G
7	A	2105	U
7	A	2108	A
7	A	2109	U
7	A	2110	G
7	A	2111	U
7	A	2112	G
7	A	2113	U
7	A	2115	G
7	A	2116	G
7	A	2118	U

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Mol	Chain	Res	Type
7	A	2119	A
7	A	2120	G
7	A	2122	U
7	A	2126	A
7	A	2127	G
7	A	2128	G
7	A	2130	U
7	A	2131	U
7	A	2132	U
7	A	2133	G
7	A	2134	A
7	A	2136	G
7	A	2145	C
7	A	2146	C
7	A	2148	G
7	A	2149	U
7	A	2151	U
7	A	2154	A
7	A	2159	G
7	A	2161	C
7	A	2162	G
7	A	2163	A
7	A	2164	C
7	A	2165	C
7	A	2167	U
7	A	2168	G
7	A	2169	A
7	A	2170	A
7	A	2171	A
7	A	2172	U
7	A	2178	C
7	A	2179	C
7	A	2181	U
7	A	2186	G
7	A	2187	U
7	A	2188	U
7	A	2189	U
7	A	2190	G
7	A	2191	A
7	A	2192	U
7	A	2193	G
7	A	2194	U

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Mol	Chain	Res	Type
7	A	2198	A
7	A	2204	G
7	A	2211	A
7	A	2212	A
7	A	2214	C
7	A	2221	G
7	A	2225	A
7	A	2238	G
7	A	2239	G
7	A	2268	A
7	A	2278	A
7	A	2279	G
7	A	2282	G
7	A	2283	C
7	A	2286	G
7	A	2287	A
7	A	2297	A
7	A	2305	U
7	A	2308	G
7	A	2311	A
7	A	2312	U
7	A	2321	U
7	A	2322	A
7	A	2325	G
7	A	2327	A
7	A	2333	A
7	A	2335	A
7	A	2340	A
7	A	2347	C
7	A	2350	C
7	A	2357	G
7	A	2377	A
7	A	2383	G
7	A	2385	C
7	A	2399	G
7	A	2402	U
7	A	2406	A
7	A	2419	U
7	A	2425	A
7	A	2431	U
7	A	2435	A
7	A	2436	G

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Mol	Chain	Res	Type
7	A	2441	U
7	A	2445	G
7	A	2447	G
7	A	2448	A
7	A	2449	U
7	A	2459	A
7	A	2473	U
7	A	2474	U
7	A	2475	C
7	A	2476	A
7	A	2491	U
7	A	2492	U
7	A	2493	U
7	A	2494	G
7	A	2498	C
7	A	2499	C
7	A	2502	G
7	A	2503	A
7	A	2505	G
7	A	2518	A
7	A	2520	C
7	A	2525	G
7	A	2529	G
7	A	2530	A
7	A	2542	A
7	A	2547	A
7	A	2566	A
7	A	2567	G
7	A	2573	C
7	A	2574	G
7	A	2585	U
7	A	2602	A
7	A	2603	G
7	A	2606	C
7	A	2608	G
7	A	2609	U
7	A	2613	U
7	A	2615	U
7	A	2624	G
7	A	2629	U
7	A	2639	A
7	A	2661	G

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Mol	Chain	Res	Type
7	A	2663	G
7	A	2668	G
7	A	2682	A
7	A	2689	U
7	A	2690	U
7	A	2705	A
7	A	2714	G
7	A	2716	C
7	A	2720	U
7	A	2725	A
7	A	2726	A
7	A	2733	A
7	A	2744	G
7	A	2748	A
7	A	2757	A
7	A	2762	C
7	A	2778	A
7	A	2779	U
7	A	2791	G
7	A	2800	A
7	A	2809	A
7	A	2818	U
7	A	2820	A
7	A	2821	A
7	A	2825	G
7	A	2843	G
7	A	2850	A
7	A	2859	G
7	A	2861	U
7	A	2867	G
7	A	2873	A
7	A	2874	C
7	A	2879	A
7	A	2880	C
7	A	2884	U
7	A	2885	G
7	A	2886	A
7	A	2891	U
7	A	2899	A
7	A	2901	C
8	B	9	G
8	B	12	C

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Mol	Chain	Res	Type
8	B	13	G
8	B	18	G
8	B	24	G
8	B	25	U
8	B	26	C
8	B	35	C
8	B	42	C
8	B	44	G
8	B	56	G
8	B	66	A
8	B	69	G
8	B	89	U
8	B	90	C
8	B	109	A
8	B	112	G
39	h	4	U
39	h	5	U
39	h	9	G
39	h	19	A
39	h	22	G
39	h	28	A
39	h	32	A
39	h	39	G
39	h	47	C
39	h	48	C
39	h	50	A
39	h	51	A
39	h	52	C
39	h	70	U
39	h	71	A
39	h	72	A
39	h	74	A
39	h	75	G
39	h	76	G
39	h	77	A
39	h	79	G
39	h	80	A
39	h	81	A
39	h	82	G
39	h	83	C
39	h	84	U
39	h	85	U

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Mol	Chain	Res	Type
39	h	86	G
39	h	87	C
39	h	89	U
39	h	90	C
39	h	91	U
39	h	95	C
39	h	97	G
39	h	108	G
39	h	119	A
39	h	120	A
39	h	121	U
39	h	122	G
39	h	130	A
39	h	131	A
39	h	141	G
39	h	149	A
39	h	150	U
39	h	151	A
39	h	161	A
39	h	164	G
39	h	189	A
39	h	197	A
39	h	198	G
39	h	201	G
39	h	205	A
39	h	206	C
39	h	209	U
39	h	210	C
39	h	212	G
39	h	220	G
39	h	226	G
39	h	240	G
39	h	245	U
39	h	247	G
39	h	248	C
39	h	251	G
39	h	252	U
39	h	258	G
39	h	266	G
39	h	267	C
39	h	271	C
39	h	289	G

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Mol	Chain	Res	Type
39	h	300	A
39	h	321	A
39	h	328	C
39	h	329	A
39	h	330	C
39	h	332	G
39	h	341	C
39	h	345	C
39	h	352	C
39	h	354	G
39	h	367	U
39	h	372	C
39	h	373	A
39	h	384	G
39	h	393	A
39	h	406	G
39	h	411	A
39	h	412	A
39	h	413	G
39	h	414	A
39	h	421	U
39	h	422	C
39	h	423	G
39	h	424	G
39	h	429	U
39	h	430	A
39	h	436	C
39	h	439	U
39	h	446	G
39	h	454	G
39	h	458	U
39	h	462	G
39	h	467	U
39	h	468	A
39	h	469	C
39	h	474	G
39	h	481	G
39	h	482	A
39	h	486	U
39	h	505	G
39	h	511	C
39	h	518	C

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Mol	Chain	Res	Type
39	h	521	G
39	h	526	C
39	h	527	G
39	h	533	A
39	h	541	G
39	h	547	A
39	h	559	A
39	h	562	U
39	h	564	C
39	h	572	A
39	h	573	A
39	h	576	C
39	h	577	G
39	h	579	A
39	h	583	A
39	h	596	A
39	h	628	G
39	h	633	G
39	h	641	U
39	h	642	A
39	h	653	U
39	h	665	A
39	h	671	G
39	h	682	G
39	h	705	G
39	h	723	U
39	h	724	G
39	h	733	G
39	h	734	G
39	h	748	G
39	h	751	U
39	h	755	G
39	h	760	G
39	h	763	G
39	h	777	A
39	h	793	U
39	h	794	A
39	h	802	A
39	h	815	A
39	h	817	C
39	h	828	U
39	h	829	G

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Mol	Chain	Res	Type
39	h	832	G
39	h	836	G
39	h	840	C
39	h	841	C
39	h	842	U
39	h	843	U
39	h	845	A
39	h	846	G
39	h	847	G
39	h	851	G
39	h	884	U
39	h	885	G
39	h	891	U
39	h	902	G
39	h	914	A
39	h	926	G
39	h	927	G
39	h	934	C
39	h	935	A
39	h	948	C
39	h	960	U
39	h	966	G
39	h	968	A
39	h	969	A
39	h	972	C
39	h	975	A
39	h	976	G
39	h	977	A
39	h	978	A
39	h	992	U
39	h	993	G
39	h	1004	A
39	h	1006	G
39	h	1009	U
39	h	1016	A
39	h	1018	G
39	h	1019	A
39	h	1024	G
39	h	1025	U
39	h	1028	C
39	h	1030	U
39	h	1031	C

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Mol	Chain	Res	Type
39	h	1032	G
39	h	1033	G
39	h	1035	A
39	h	1039	G
39	h	1046	A
39	h	1053	G
39	h	1055	A
39	h	1065	U
39	h	1074	G
39	h	1085	U
39	h	1086	U
39	h	1094	G
39	h	1095	U
39	h	1099	G
39	h	1101	A
39	h	1124	G
39	h	1133	G
39	h	1135	U
39	h	1137	C
39	h	1139	G
39	h	1140	C
39	h	1141	C
39	h	1142	G
39	h	1143	G
39	h	1152	A
39	h	1158	C
39	h	1159	U
39	h	1160	G
39	h	1168	U
39	h	1169	A
39	h	1171	A
39	h	1184	G
39	h	1187	G
39	h	1196	A
39	h	1197	A
39	h	1212	U
39	h	1213	A
39	h	1225	A
39	h	1226	C
39	h	1227	A
39	h	1238	A
39	h	1239	A

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Mol	Chain	Res	Type
39	h	1240	U
39	h	1241	G
39	h	1246	A
39	h	1248	A
39	h	1256	A
39	h	1257	A
39	h	1260	G
39	h	1261	A
39	h	1280	A
39	h	1286	U
39	h	1287	A
39	h	1294	G
39	h	1300	G
39	h	1301	U
39	h	1302	C
39	h	1305	G
39	h	1317	C
39	h	1318	A
39	h	1319	A
39	h	1320	C
39	h	1322	C
39	h	1323	G
39	h	1338	G
39	h	1340	A
39	h	1346	A
39	h	1353	G
39	h	1363	A
39	h	1368	A
39	h	1370	G
39	h	1379	G
39	h	1397	C
39	h	1402	C
39	h	1406	U
39	h	1415	G
39	h	1419	G
39	h	1429	A
39	h	1433	A
39	h	1438	G
39	h	1441	A
39	h	1442	G
39	h	1446	A
39	h	1452	C

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Mol	Chain	Res	Type
39	h	1454	G
39	h	1475	G
39	h	1487	G
39	h	1491	G
39	h	1494	G
39	h	1497	G
39	h	1503	A
39	h	1505	G
39	h	1506	U
39	h	1511	G
39	h	1517	G
39	h	1529	G
39	h	1530	G
39	h	1533	C

All (65) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	5	14	A
5	5	16	C
6	7	15	U
7	A	125	A
7	A	139	U
7	A	196	A
7	A	199	A
7	A	215	G
7	A	249	C
7	A	301	G
7	A	310	A
7	A	446	G
7	A	455	C
7	A	503	A
7	A	512	G
7	A	532	A
7	A	555	G
7	A	620	G
7	A	746	U
7	A	764	A
7	A	784	G
7	A	827	U
7	A	858	G
7	A	871	U

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Mol	Chain	Res	Type
7	A	961	C
7	A	983	A
7	A	984	A
7	A	1061	U
7	A	1070	A
7	A	1089	A
7	A	1128	G
7	A	1141	U
7	A	1142	A
7	A	1286	A
7	A	1288	G
7	A	1320	C
7	A	1451	C
7	A	1490	A
7	A	1494	A
7	A	1497	U
7	A	1607	C
7	A	1608	A
7	A	1647	U
7	A	1818	U
7	A	1900	A
7	A	1918	A
7	A	1938	A
7	A	2030	A
7	A	2062	A
7	A	2127	G
7	A	2158	A
7	A	2191	A
7	A	2282	G
7	A	2296	U
7	A	2311	A
7	A	2326	C
7	A	2406	A
7	A	2468	A
7	A	2491	U
7	A	2498	C
7	A	2529	G
7	A	2573	C
7	A	2602	A
7	A	2609	U
7	A	2873	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

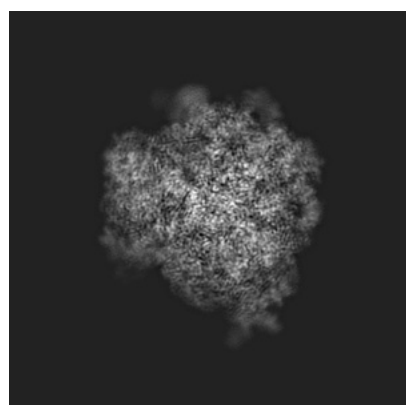
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6667. These allow visual inspection of the internal detail of the map and identification of artifacts.

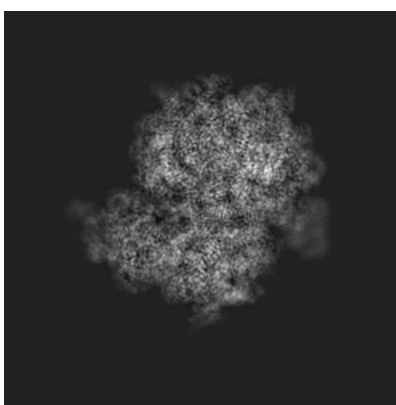
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

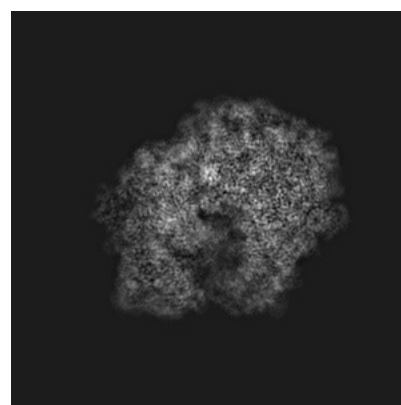
6.1.1 Primary map



X



Y

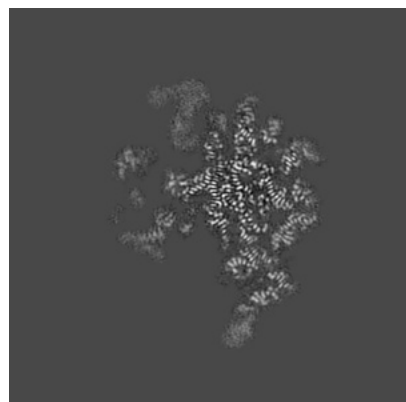


Z

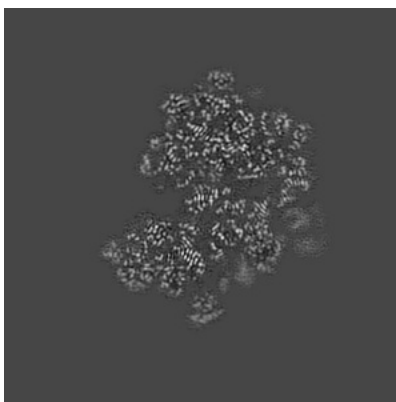
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

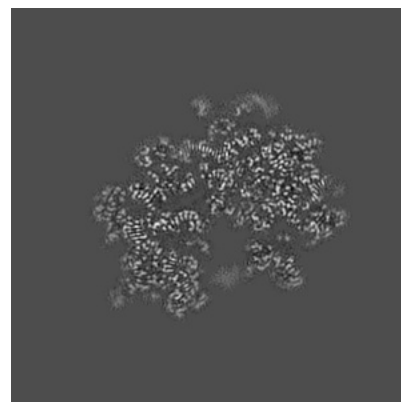
6.2.1 Primary map



X Index: 180



Y Index: 180

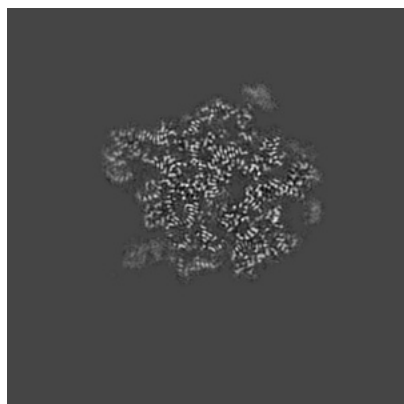


Z Index: 180

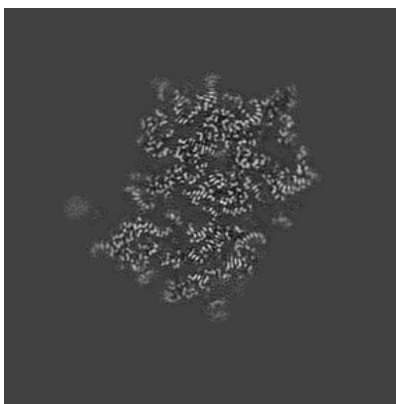
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

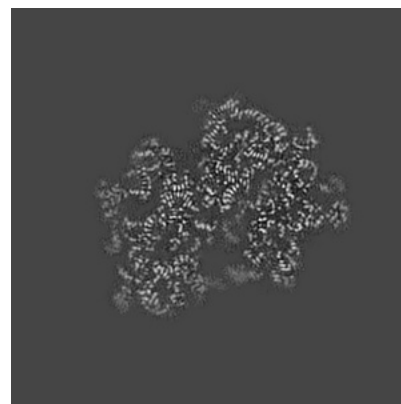
6.3.1 Primary map



X Index: 222



Y Index: 200

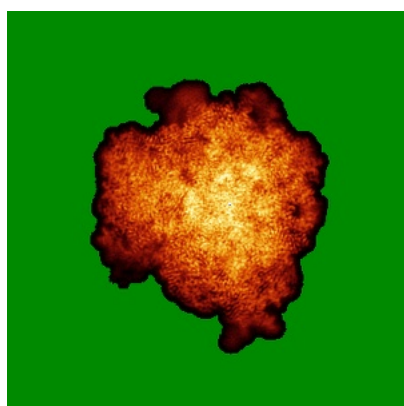


Z Index: 191

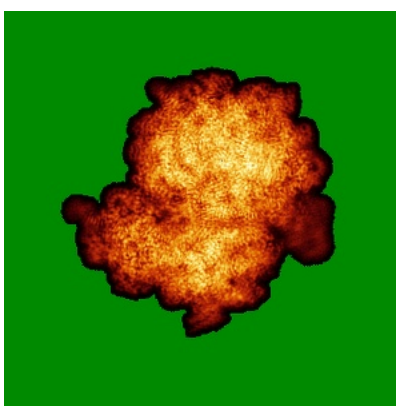
The images above show the largest variance slices of the map in three orthogonal directions.

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

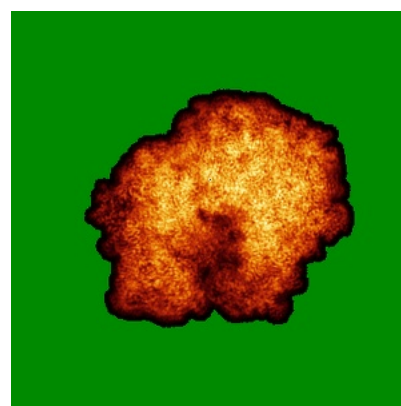
6.4.1 Primary map



X



Y

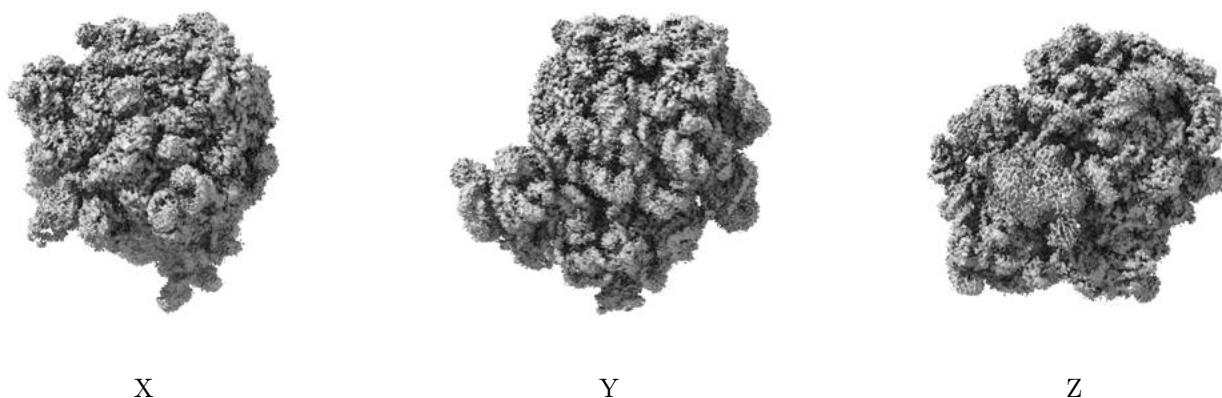


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

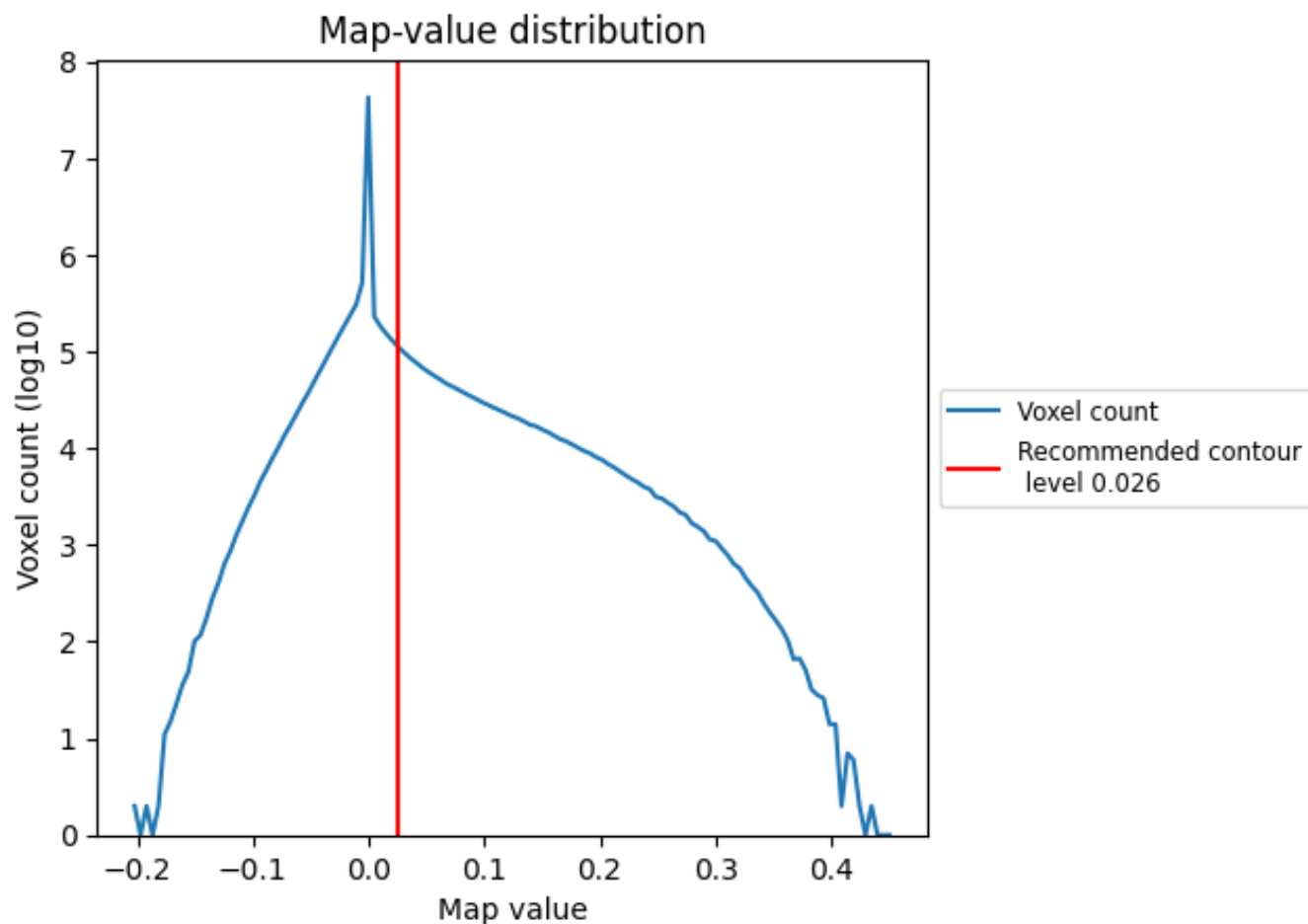
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

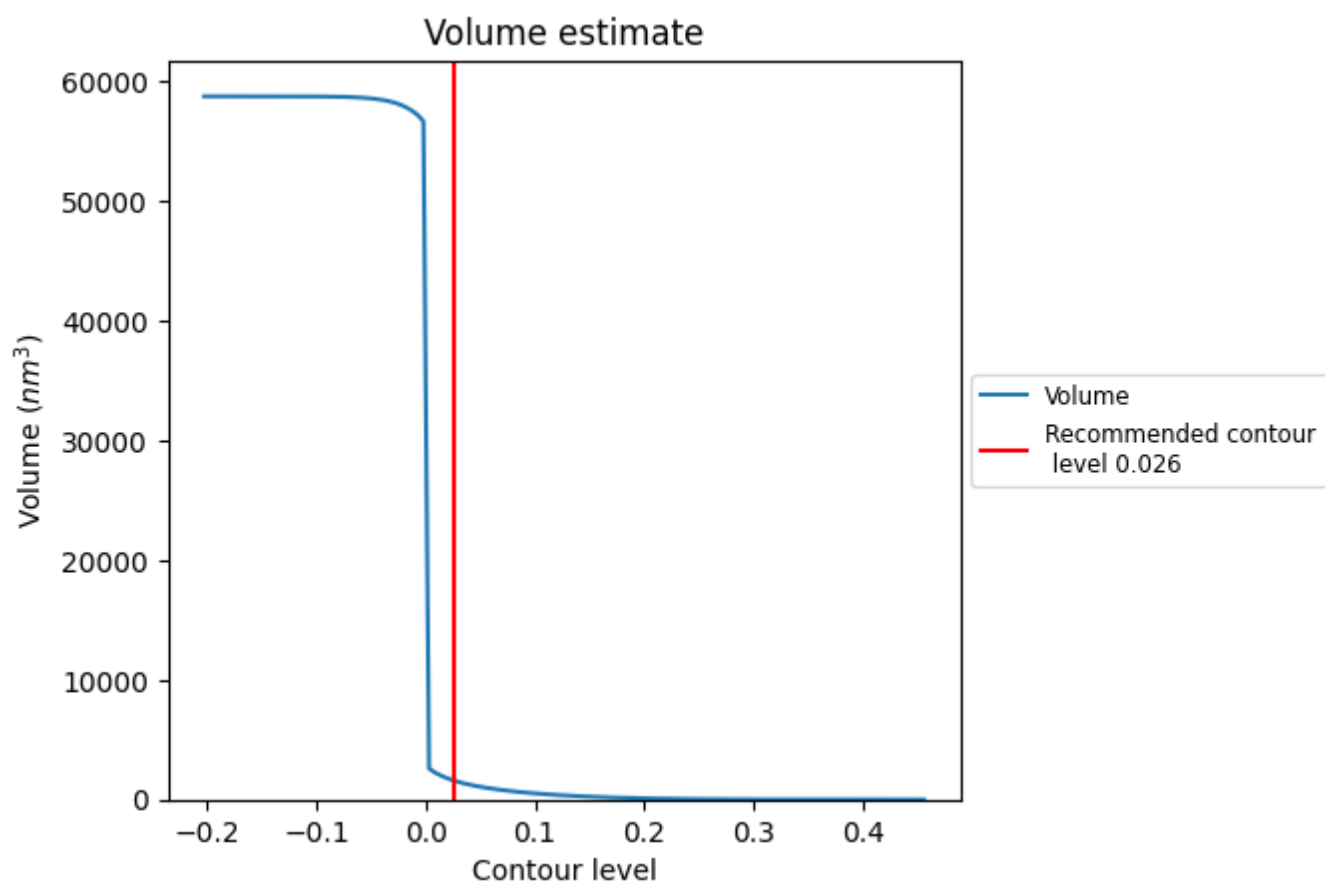
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

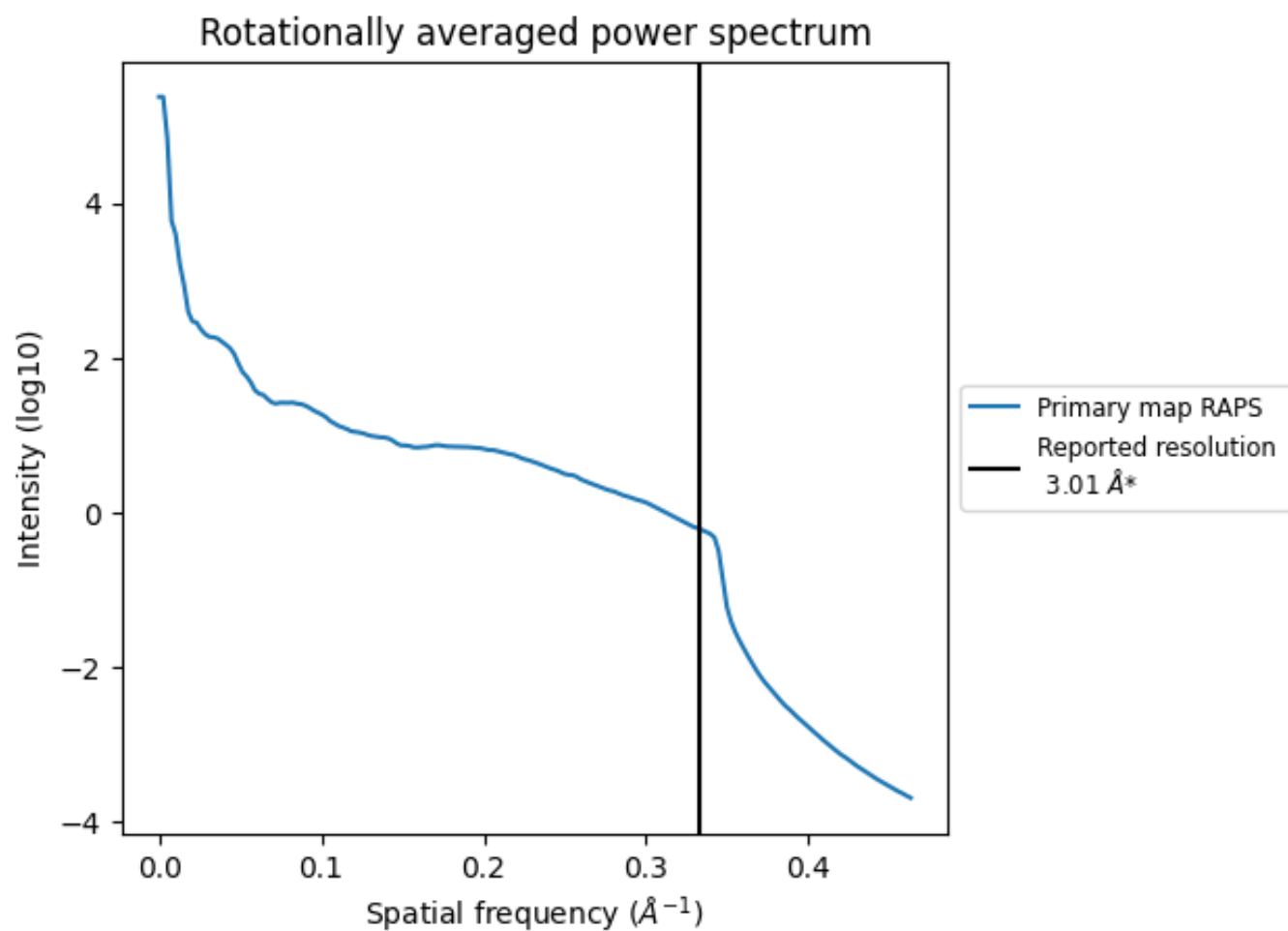
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1587 nm^3 ; this corresponds to an approximate mass of 1434 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.332 Å⁻¹

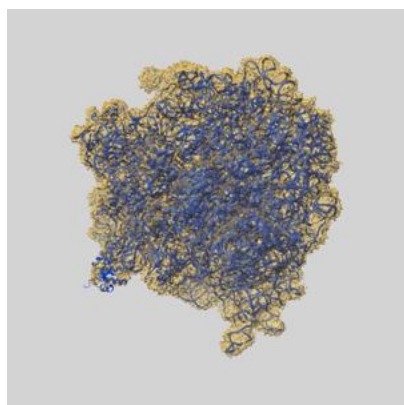
8 Fourier-Shell correlation

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

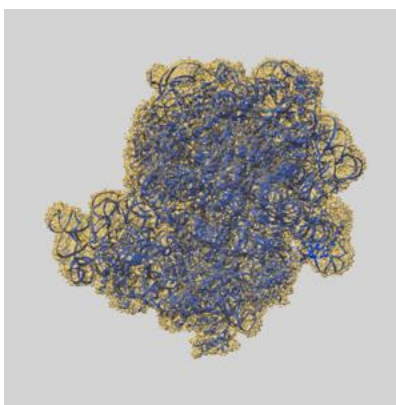
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6667 and PDB model 5H5U. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

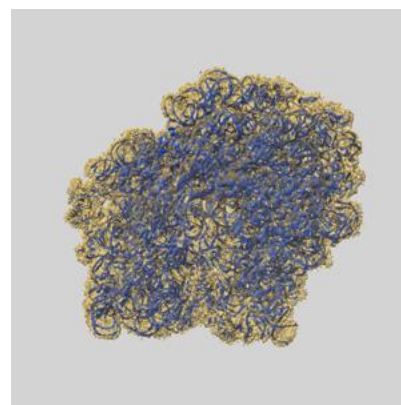
9.1 Map-model overlay [i](#)



X



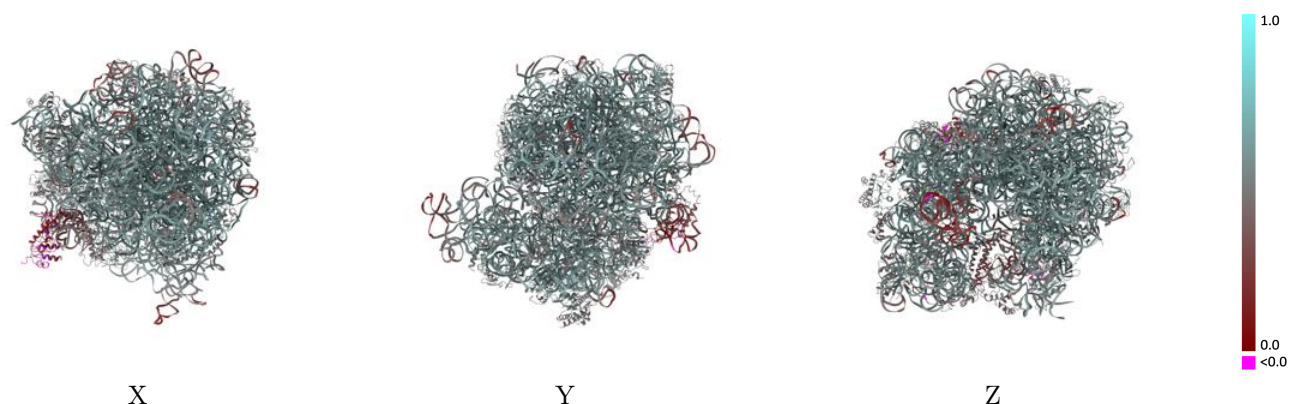
Y



Z

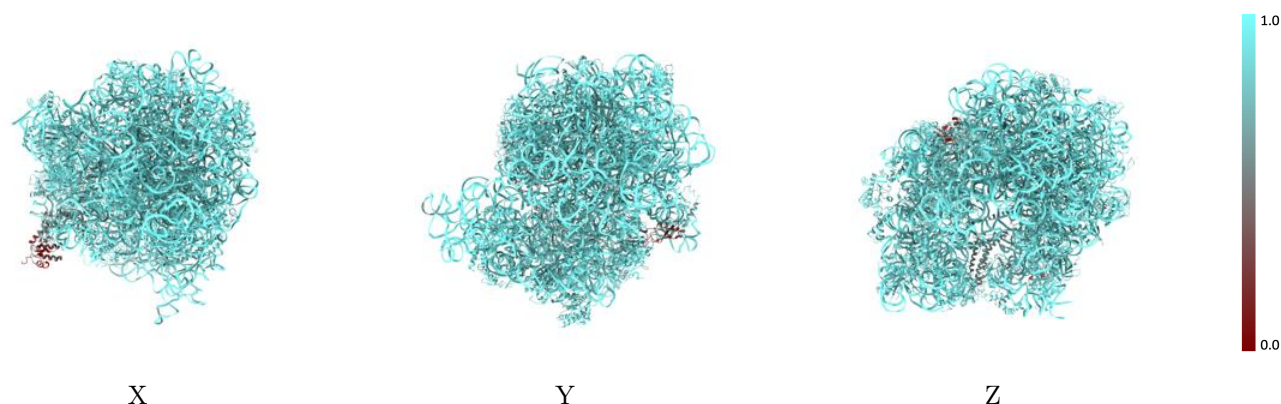
The images above show the 3D surface view of the map at the recommended contour level 0.026 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



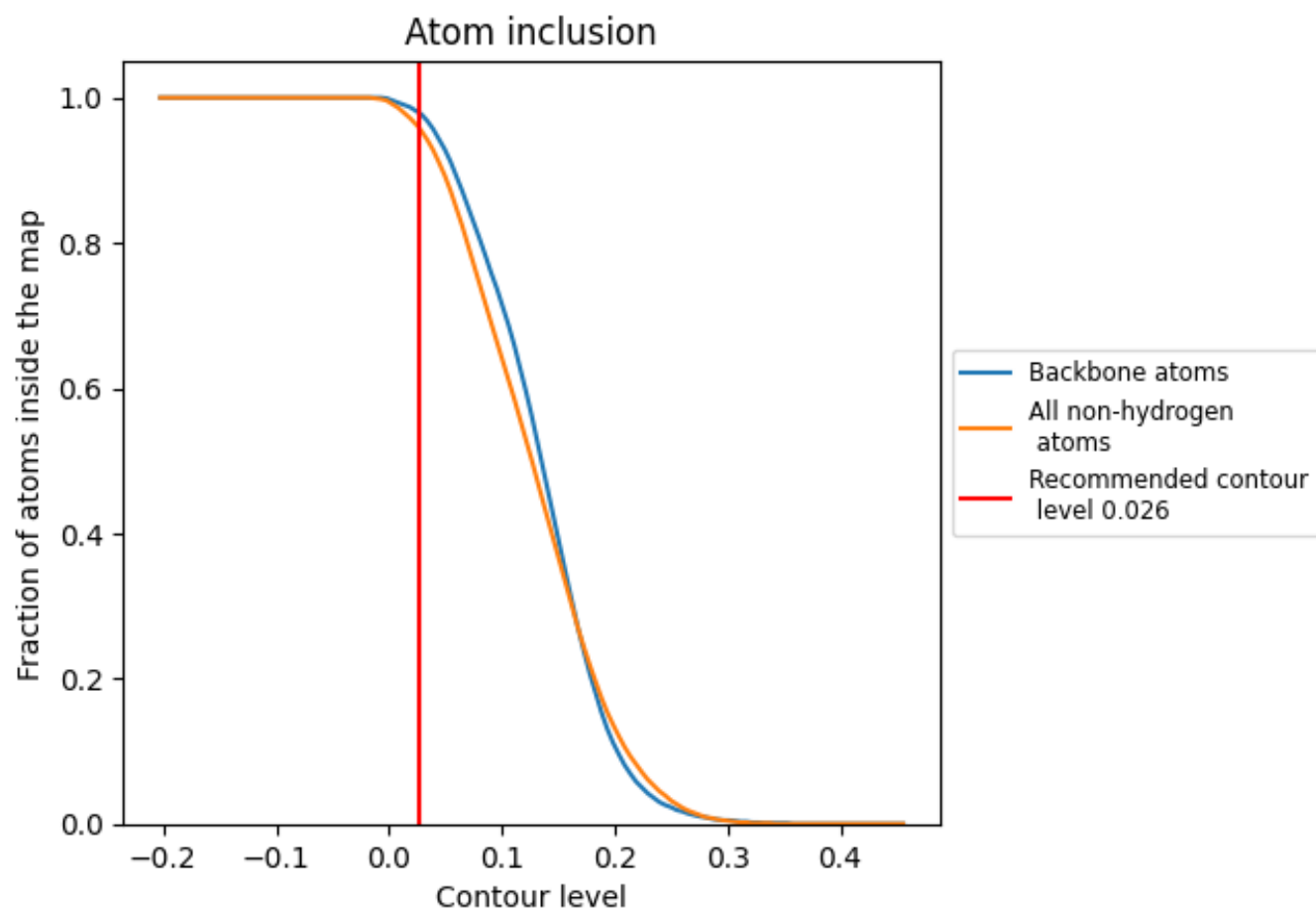
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.026).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9600	 0.5380
1	 0.9500	 0.5340
2	 0.8650	 0.4780
3	 0.9280	 0.5630
4	 0.7590	 0.4140
5	 0.9690	 0.5080
7	 0.9450	 0.5010
A	 0.9900	 0.5540
B	 0.9970	 0.5480
C	 0.9490	 0.5760
D	 0.9490	 0.5650
E	 0.9180	 0.5210
F	 0.9100	 0.4490
G	 0.9310	 0.4730
H	 0.5520	 0.3180
I	 0.2920	 0.1140
J	 0.6080	 0.2110
K	 0.9420	 0.5560
L	 0.9350	 0.5560
M	 0.9400	 0.5520
N	 0.9440	 0.5670
O	 0.9340	 0.5600
P	 0.9400	 0.5130
Q	 0.9230	 0.5450
R	 0.9670	 0.5710
S	 0.9350	 0.5390
T	 0.9370	 0.5590
U	 0.9320	 0.5310
V	 0.9470	 0.5100
W	 0.9350	 0.5250
X	 0.9450	 0.5750
Y	 0.9370	 0.5140
Z	 0.9280	 0.5000
a	 0.9270	 0.5480
b	 0.9420	 0.5590



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Chain	Atom inclusion	Q-score
c	 0.9240	 0.5430
d	 0.9470	 0.5780
e	 0.9550	 0.5850
f	 0.9380	 0.5540
h	 0.9940	 0.5600
i	 0.9200	 0.4840
j	 0.9350	 0.5260
k	 0.8860	 0.5080
l	 0.9500	 0.5460
m	 0.9170	 0.4940
n	 0.8980	 0.4740
o	 0.9470	 0.5590
p	 0.9350	 0.5120
q	 0.8900	 0.4800
r	 0.9450	 0.5310
s	 0.9360	 0.5660
t	 0.9260	 0.4920
u	 0.9110	 0.5210
v	 0.9360	 0.5250
w	 0.9490	 0.5500
x	 0.9130	 0.4990
y	 0.9360	 0.5340
z	 0.9440	 0.4940