



## Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 03:36 PM UTC

PDB ID : 9FY1 / pdb\_00009fy1  
EMDB ID : EMD-50855  
Title : Structure of CliM-stalled Bacillus subtilis 70S ribosome with release factor bound in the A-site  
Authors : Gersteuer, F.; Wilson, D.N.  
Deposited on : 2024-07-02  
Resolution : 2.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

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

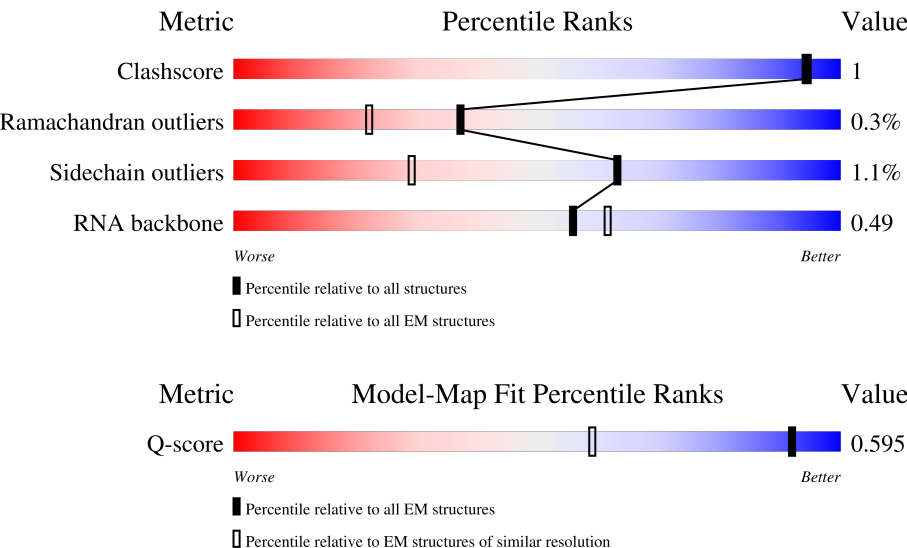


# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.30 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	4254 ( 1.80 - 2.80 )



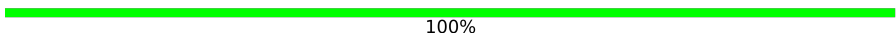








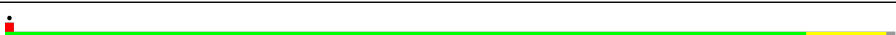

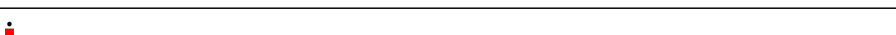
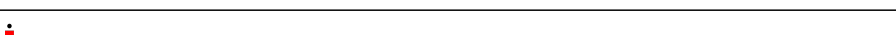
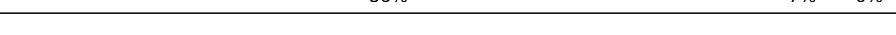

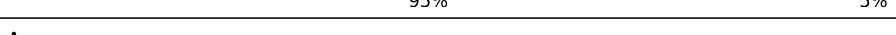


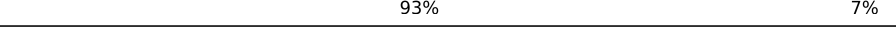

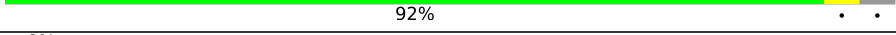
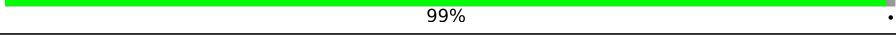

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey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

Mol	Chain	Length	Quality of chain
1	0	59	
2	1	49	
3	2	44	

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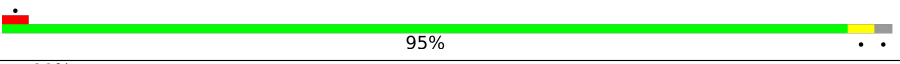
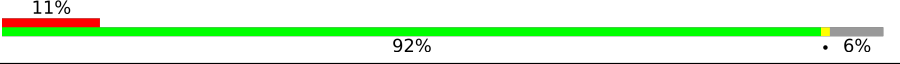
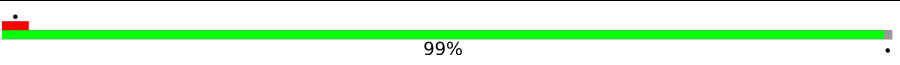
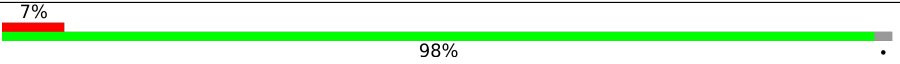
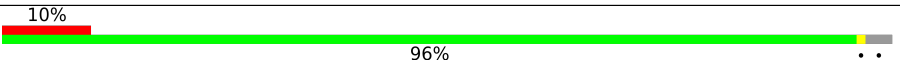
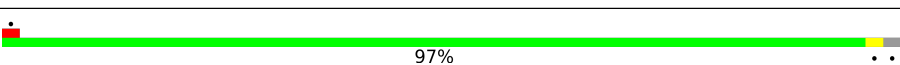
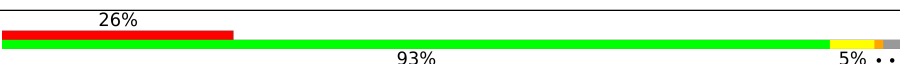
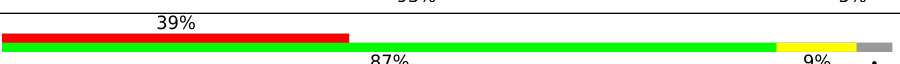
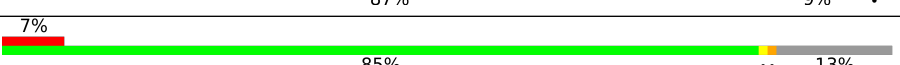
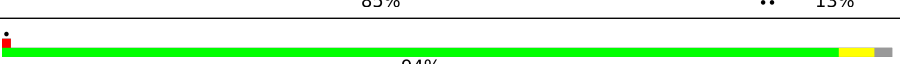
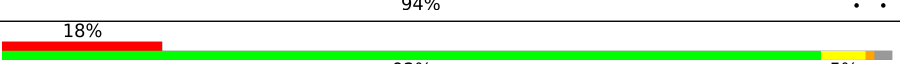
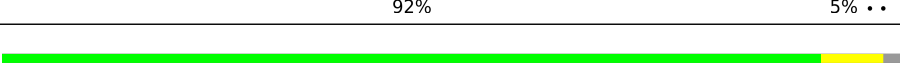
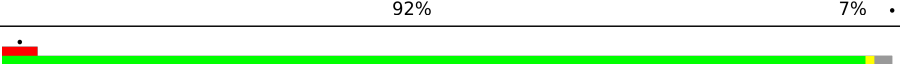
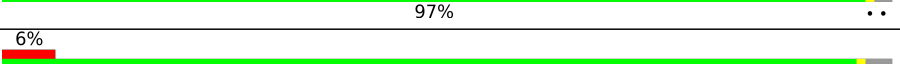
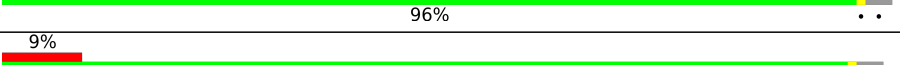
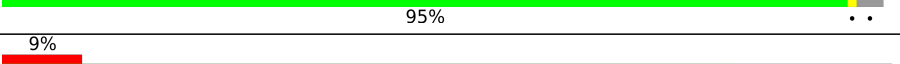

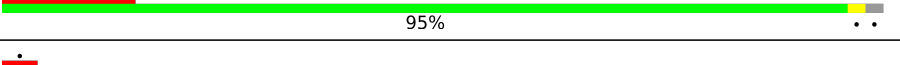

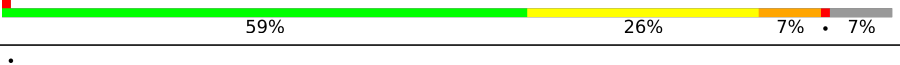
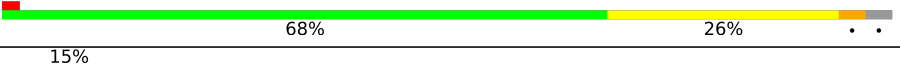


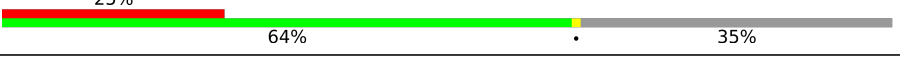

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Mol	Chain	Length	Quality of chain
4	3	66	
5	4	37	
6	5	38	
7	6	66	
8	7	9	
9	B	112	
10	C	277	
11	D	209	
12	E	207	
13	F	179	
14	G	179	
15	J	145	
16	K	122	
17	L	146	
18	M	144	
19	N	120	
20	O	120	
21	P	115	
22	Q	119	
23	R	102	
24	S	113	
25	T	95	
26	U	103	
27	X	62	
28	Y	66	

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Mol	Chain	Length	Quality of chain
29	Z	59	
30	c	218	
31	e	166	
32	f	95	
33	g	156	
34	h	132	
35	i	130	
36	j	102	
37	k	131	
38	l	138	
39	m	121	
40	n	61	
41	o	89	
42	p	90	
43	q	87	
44	r	79	
45	t	88	
46	v	76	
47	A	2928	
48	a	1554	
49	b	246	
50	s	92	
51	8	366	
52	W	94	
53	d	200	



## 2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 138648 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 Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	55	Total	C	N	O	S	0	0
			432	267	87	72	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	11	VAL	MET	conflict	UNP O34687

- Molecule 2 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	48	Total	C	N	O	S	0	0
			403	245	81	74	3		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	44	Total	C	N	O	S	0	0
			368	222	89	55	2		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

- Molecule 6 is a protein called Nascent Chain CliM.



Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	38	Total	C	N	O	S	0	0
			346	232	56	57	1		

- Molecule 7 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	46	Total	C	N	O	S	0	0
			356	222	63	66	5		

- Molecule 8 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	9	Total	C	N	O	P	0	0
			187	84	27	67	9		

- Molecule 9 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

- Molecule 10 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	273	Total	C	N	O	S	0	0
			2093	1301	412	374	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	216	VAL	ILE	conflict	UNP P42919

- Molecule 11 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	207	Total	C	N	O	S	0	0
			1575	988	290	292	5		

- Molecule 12 is a protein called 50S ribosomal protein L4.



Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	206	Total	C	N	O	S	0	0
			1567	983	290	292	2		

- Molecule 13 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	178	Total	C	N	O	S	0	0
			1405	893	245	260	7		

- Molecule 14 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

- Molecule 15 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	144	Total	C	N	O	S	0	0
			1142	720	211	206	5		

- Molecule 16 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	122	Total	C	N	O	S	0	0
			921	571	173	173	4		

- Molecule 17 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	146	Total	C	N	O	S	0	0
			1082	671	207	202	2		

- Molecule 18 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	135	Total	C	N	O	S	0	0
			1076	690	205	176	5		

- Molecule 19 is a protein called 50S ribosomal protein L17.



Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	119	Total	C	N	O	S	0	0
			954	583	186	181	4		

- Molecule 20 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	120	Total	C	N	O	S	0	0
			913	564	176	172	1		

- Molecule 21 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	114	Total	C	N	O	S	0	0
			937	595	184	158			

- Molecule 22 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	118	Total	C	N	O	S	0	0
			950	597	191	158	4		

- Molecule 23 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	102	Total	C	N	O	S	0	0
			795	506	140	148	1		

- Molecule 24 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	110	Total	C	N	O	S	0	0
			850	530	165	151	4		

- Molecule 25 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	91	Total	C	N	O	S	0	0
			733	458	135	137	3		

- Molecule 26 is a protein called 50S ribosomal protein L24.



Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	102	Total	C	N	O	S	0	0
			770	482	143	141	4		

- Molecule 27 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	61	Total	C	N	O	S	0	0
			467	288	98	79	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	33	VAL	LEU	conflict	UNP P37807

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	66	Total	C	N	O	S	0	0
			540	334	104	100	2		

- Molecule 29 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	58	Total	C	N	O	S	0	0
			456	281	89	85	1		

- Molecule 30 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	204	Total	C	N	O	S	0	0
			1608	1004	302	299	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	148	ILE	VAL	conflict	UNP P21465

- Molecule 31 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	164	Total	C	N	O	S	0	0
			1219	767	225	225	2		



- Molecule 32 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	93	Total	C	N	O	S	0	0
			765	482	136	145	2		

- Molecule 33 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	151	Total	C	N	O	S	0	0
			1199	751	225	217	6		

- Molecule 34 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	130	Total	C	N	O	S	0	0
			1030	650	190	187	3		

- Molecule 35 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	128	Total	C	N	O	S	0	0
			997	618	198	180	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	72	PHE	LEU	conflict	UNP P21470

- Molecule 36 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	98	Total	C	N	O	S	0	0
			788	497	144	145	2		

- Molecule 37 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	114	Total	C	N	O	S	0	0
			839	515	165	157	2		

- Molecule 38 is a protein called Small ribosomal subunit protein uS12.



Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	135	Total	C	N	O	S	0	0
			1045	648	210	185	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	2	ALA	PRO	conflict	UNP P21472

- Molecule 39 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	118	Total	C	N	O	S	0	0
			943	579	194	170			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	33	ILE	VAL	conflict	UNP P20282

- Molecule 40 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	60	Total	C	N	O	S	0	0
			498	317	98	78	5		

- Molecule 41 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	87	Total	C	N	O	S	0	0
			730	448	149	132	1		

- Molecule 42 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	p	87	Total	C	N	O	S	0	0
			691	439	127	123	2		

- Molecule 43 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	q	84	Total	C	N	O	S	0	0
			693	438	128	125	2		



- Molecule 44 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	r	65	Total	C	N	O	S	0	0
			522	334	97	89	2		

- Molecule 45 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	t	86	Total	C	N	O	S	0	0
			658	402	134	121	1		

- Molecule 46 is a RNA chain called P-site tRNA-Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	v	76	Total	C	N	O	P	0	0
			1622	723	290	533	76		

- Molecule 47 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	A	2729	Total	C	N	O	P	0	0
			58630	26158	10860	18885	2727		

- Molecule 48 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	a	1509	Total	C	N	O	P	0	0
			32391	14444	5959	10479	1509		

- Molecule 49 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	b	195	Total	C	N	O	S	0	0
			1564	996	277	285	6		

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	83	Total	C	N	O	S	0	0
			668	429	122	115	2		

- Molecule 51 is a protein called Peptide chain release factor 2.



Mol	Chain	Residues	Atoms					AltConf	Trace
51	8	237	Total	C	N	O	S	0	0
			1450	871	284	292	3		

- Molecule 52 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	W	82	Total	C	N	O	0	0
			629	390	123	116		

- Molecule 53 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	d	199	Total	C	N	O	S	0	0
			1604	1013	298	291	2		

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).


Mol	Chain	Residues	Atoms		AltConf
54	0	1	Total	Zn	0
			1	1	
54	4	1	Total	Zn	0
			1	1	
54	6	1	Total	Zn	0
			1	1	
54	n	1	Total	Zn	0
			1	1	

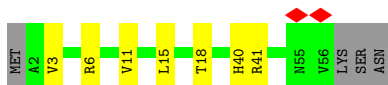


### 3 Residue-property plots [i](#)

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

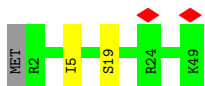
- Molecule 1: Large ribosomal subunit protein bL32

Chain 0:  81% 12% 7%



- Molecule 2: 50S ribosomal protein L33 1

Chain 1:  94% . .




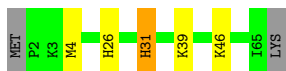
- Molecule 3: 50S ribosomal protein L34

Chain 2:  98% .

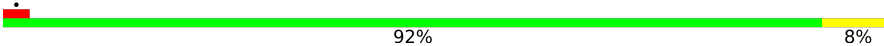


- Molecule 4: 50S ribosomal protein L35

Chain 3:  89% 6% . .



- Molecule 5: 50S ribosomal protein L36

Chain 4:  92% 8%



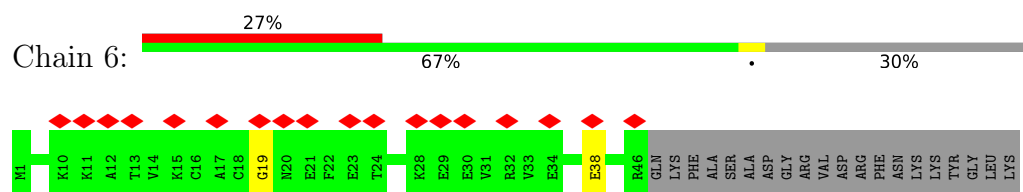
- Molecule 6: Nascent Chain ClIM



Chain 5:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: 50S ribosomal protein L31



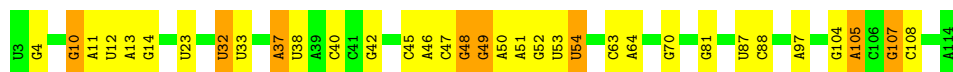
- Molecule 8: mRNA

Chain 7:  44% 56%



- Molecule 9: 5S rRNA

Chain B:  70% 23% 7%




- Molecule 10: Large ribosomal subunit protein uL2

Chain C:  92% 5% ..



- Molecule 11: 50S ribosomal protein L3

Chain D:  90% 9% .



- Molecule 12: 50S ribosomal protein L4

Chain E:  95% .



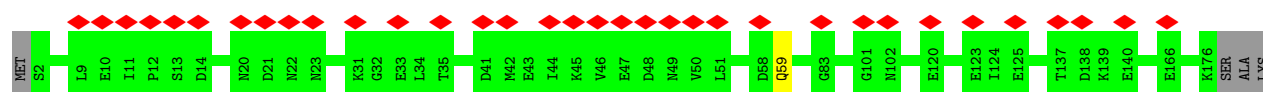
- Molecule 13: 50S ribosomal protein L5

Chain F:  8% 96% ..





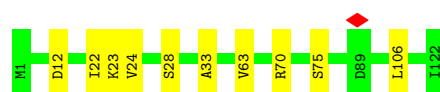
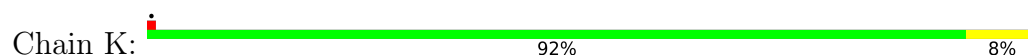
- Molecule 14: Large ribosomal subunit protein uL6



- Molecule 15: 50S ribosomal protein L13



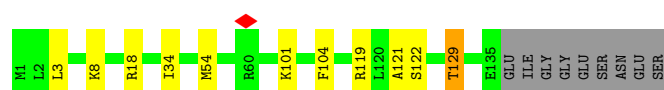
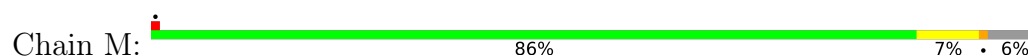
- Molecule 16: 50S ribosomal protein L14



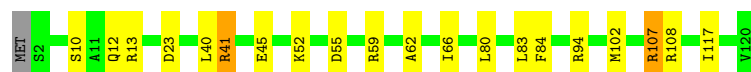
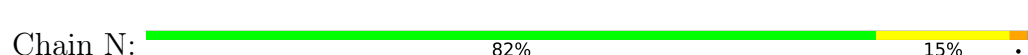
- Molecule 17: 50S ribosomal protein L15



- Molecule 18: 50S ribosomal protein L16

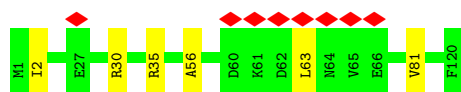


- Molecule 19: 50S ribosomal protein L17

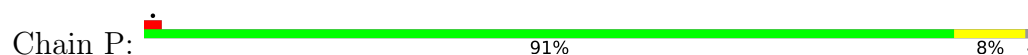


- Molecule 20: 50S ribosomal protein L18

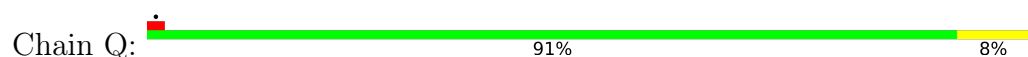




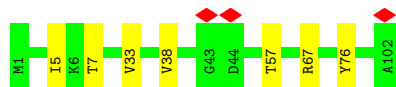
- Molecule 21: 50S ribosomal protein L19



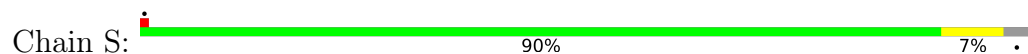
- Molecule 22: Large ribosomal subunit protein bL20



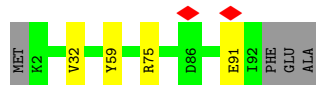
- Molecule 23: 50S ribosomal protein L21



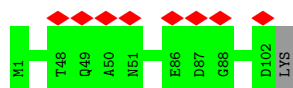
- Molecule 24: 50S ribosomal protein L22



- Molecule 25: Large ribosomal subunit protein uL23

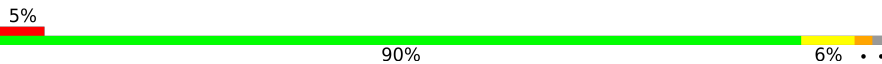


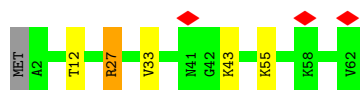
- Molecule 26: 50S ribosomal protein L24





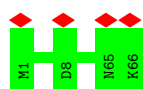
- Molecule 27: Large ribosomal subunit protein bL28

Chain X:  5% 90% 6% ..



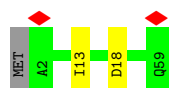
- Molecule 28: 50S ribosomal protein L29

Chain Y:  6% 100%

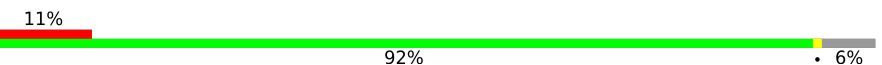


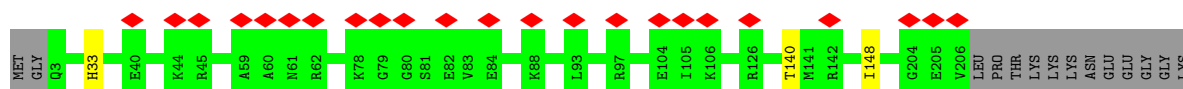
- Molecule 29: Large ribosomal subunit protein uL30

Chain Z:  95% ..



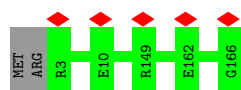
- Molecule 30: Small ribosomal subunit protein uS3

Chain c:  11% 92% 6% ..



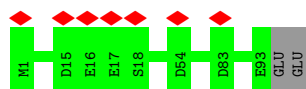
- Molecule 31: 30S ribosomal protein S5

Chain e:  99% .



- Molecule 32: 30S ribosomal protein S6

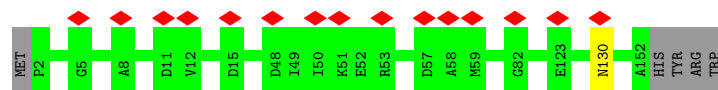
Chain f:  7% 98% .



- Molecule 33: Small ribosomal subunit protein uS7

Chain g:  10% 96% ..

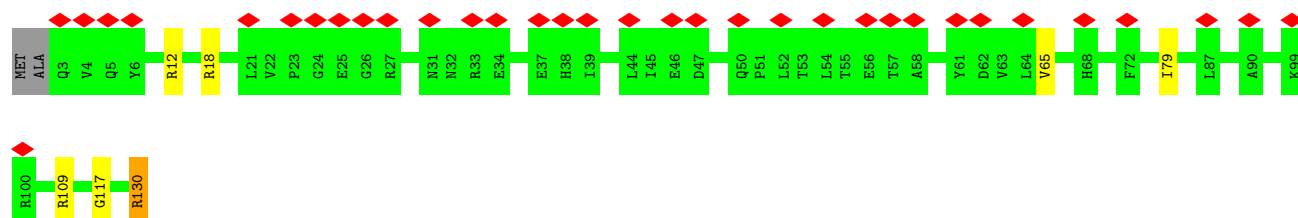




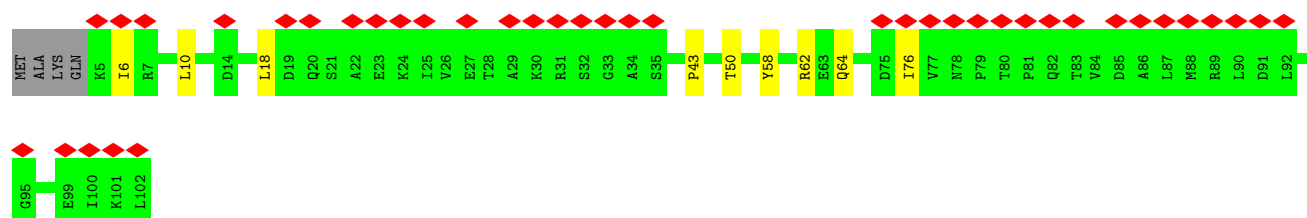
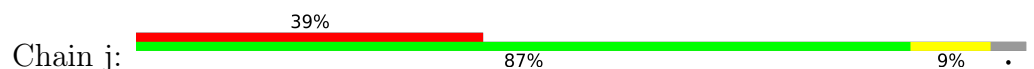
- Molecule 34: 30S ribosomal protein S8



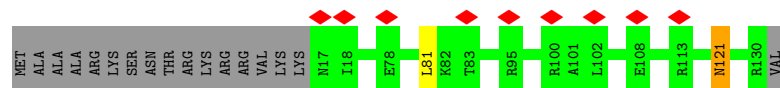
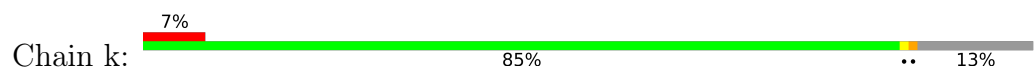
- Molecule 35: Small ribosomal subunit protein uS9



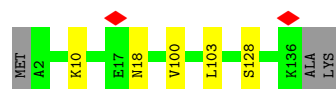
- Molecule 36: 30S ribosomal protein S10



- Molecule 37: 30S ribosomal protein S11

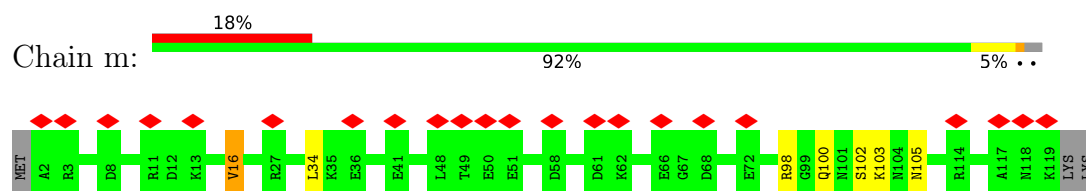


- Molecule 38: Small ribosomal subunit protein uS12

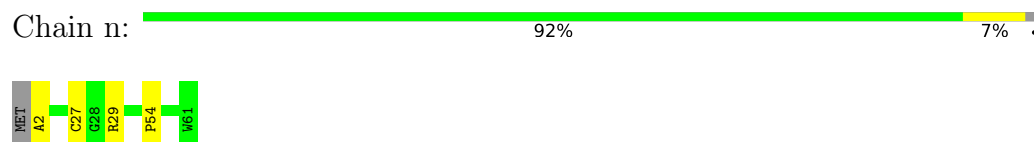


- Molecule 39: Small ribosomal subunit protein uS13

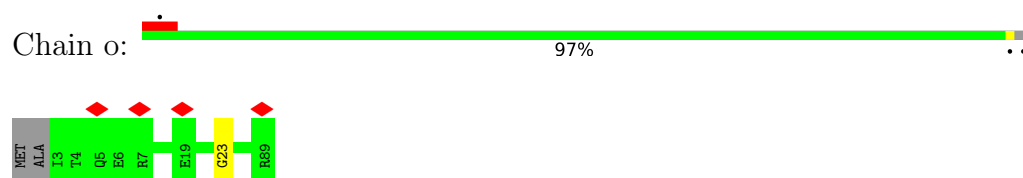




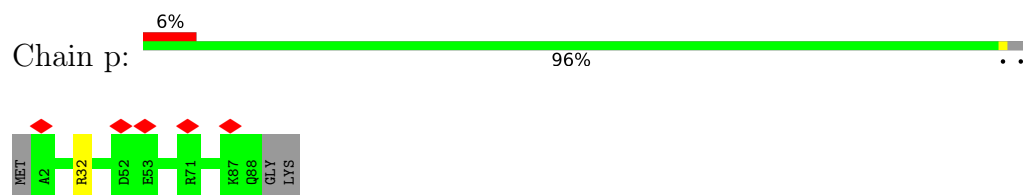
- Molecule 40: 30S ribosomal protein S14



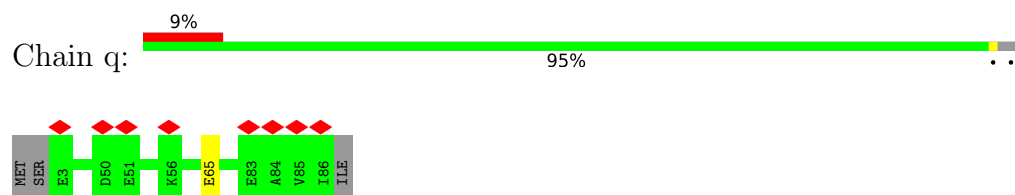
- Molecule 41: 30S ribosomal protein S15



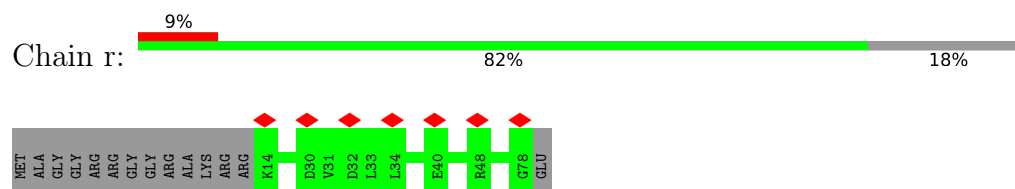
- Molecule 42: 30S ribosomal protein S16



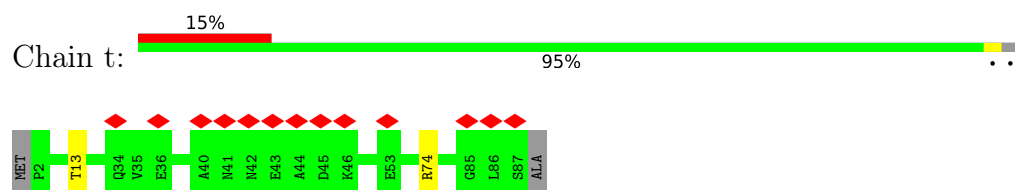
- Molecule 43: 30S ribosomal protein S17



- Molecule 44: 30S ribosomal protein S18

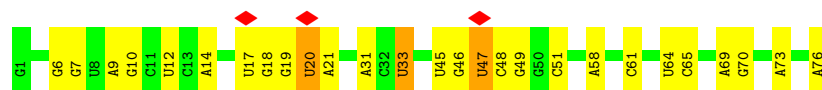


- Molecule 45: 30S ribosomal protein S20

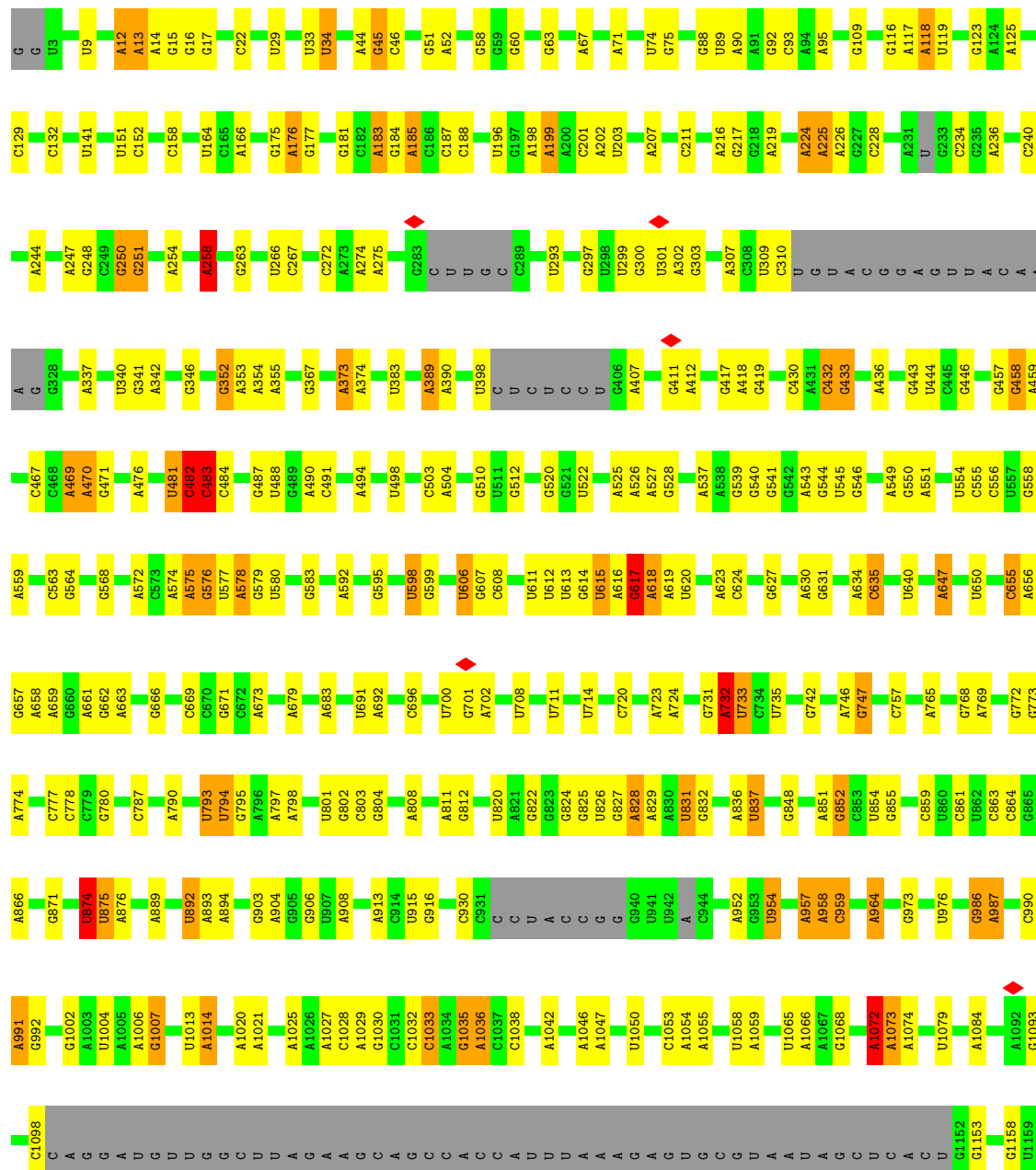




Chain v:  64% 32%



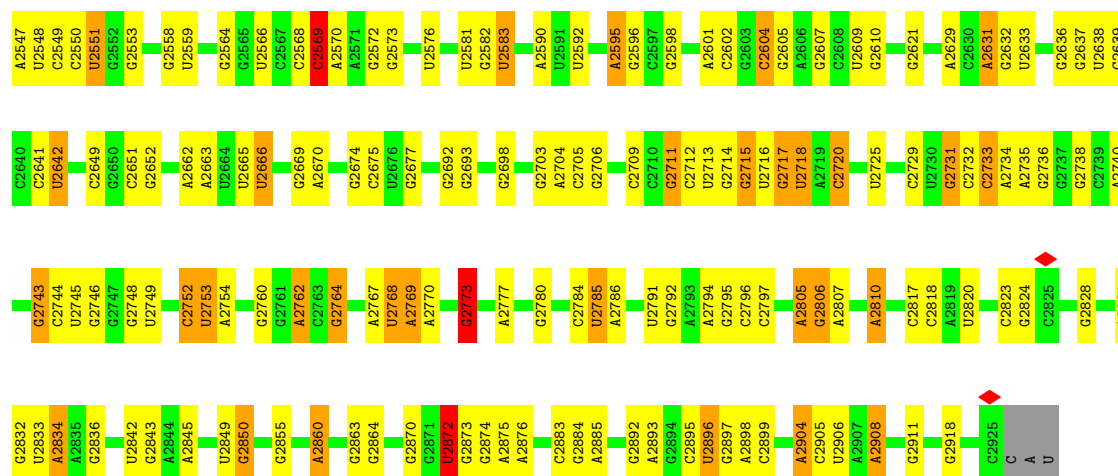
Chain A:  59% 26% 7% 7%





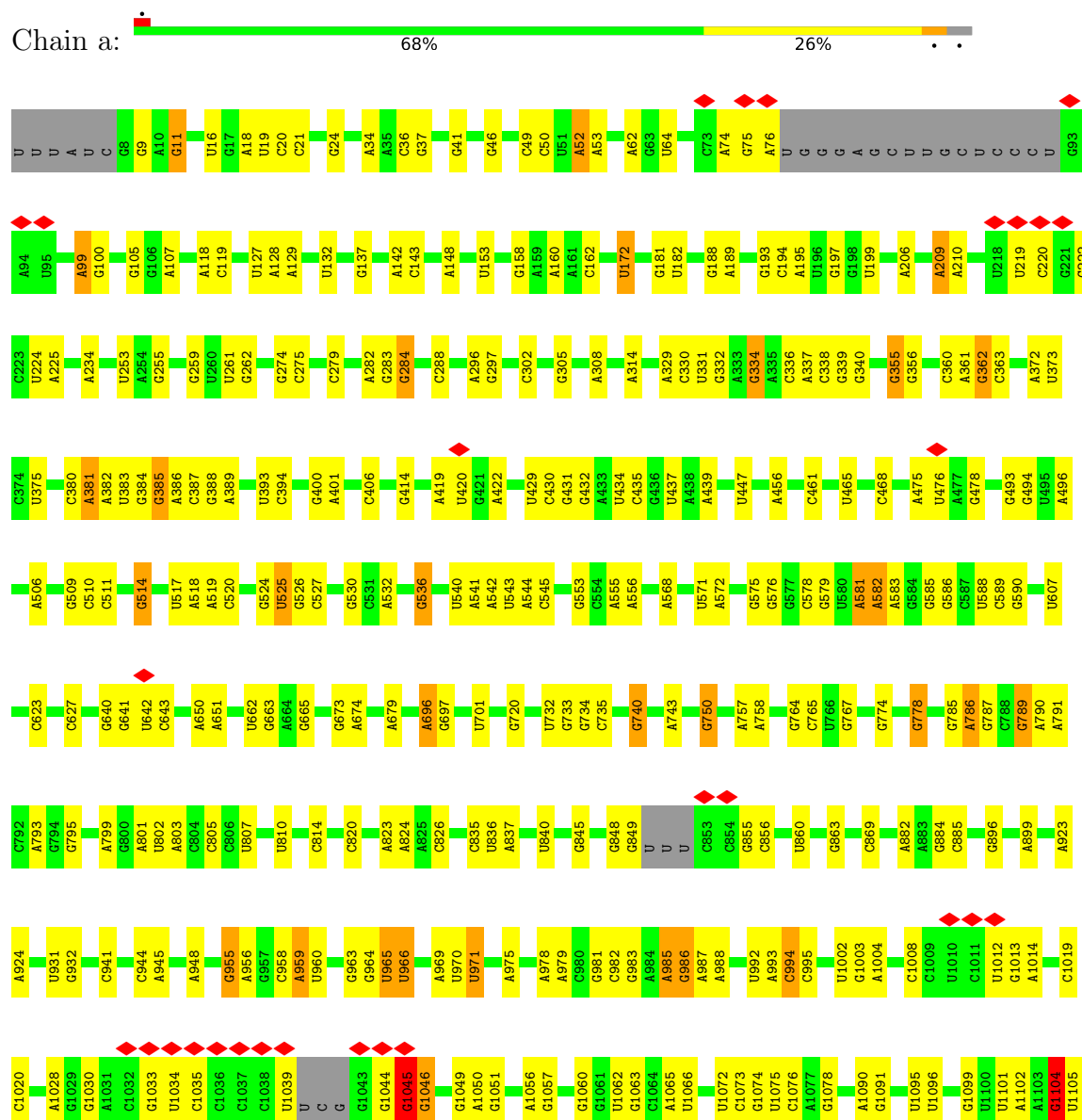




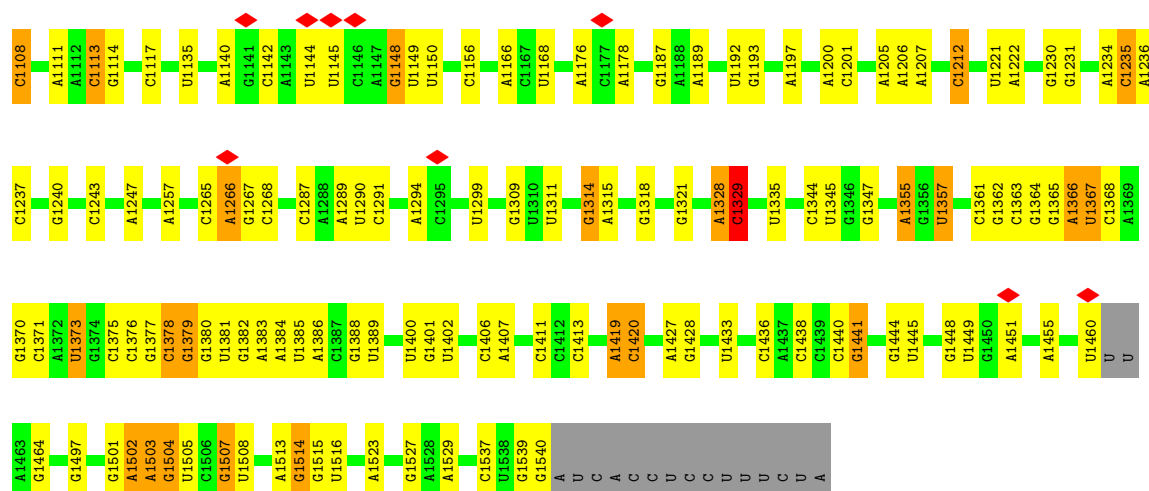


# Molecule 48: 16S rRNA

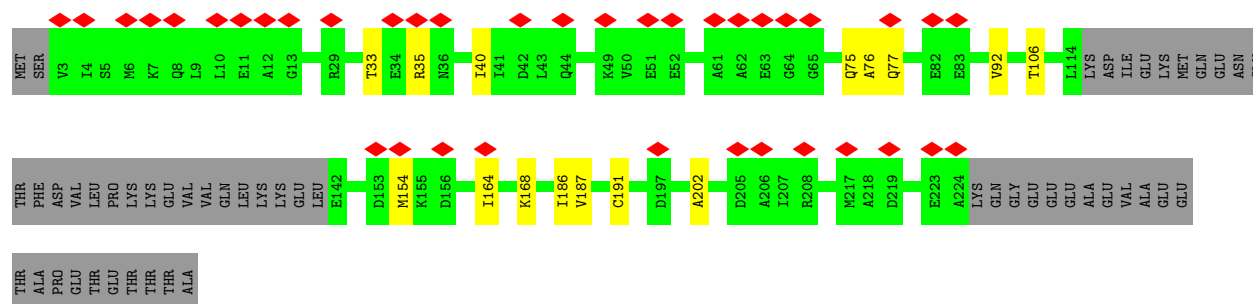
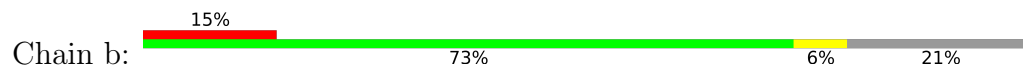
Chain a:



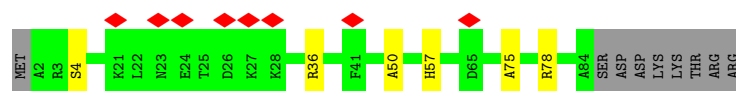
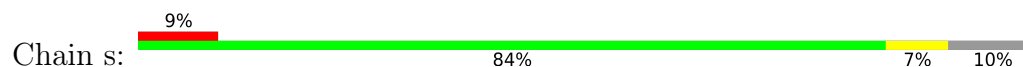




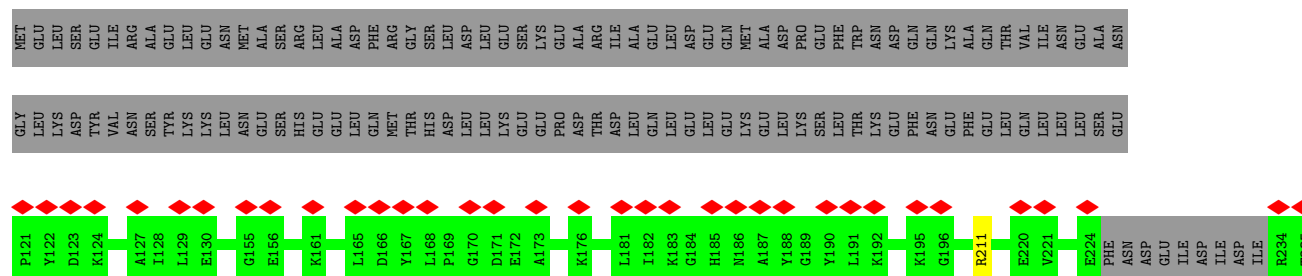
• Molecule 49: 30S ribosomal protein S2



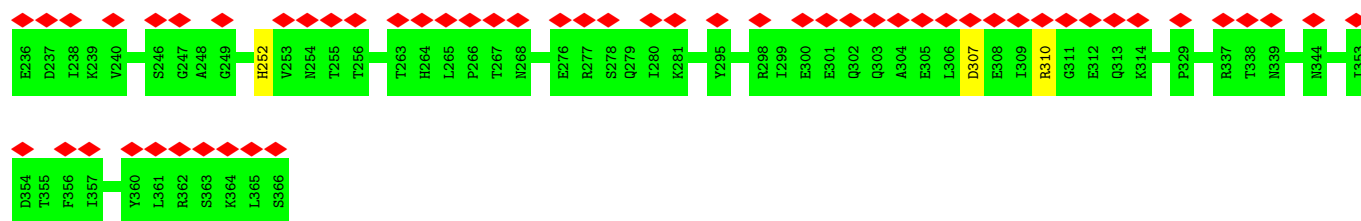
• Molecule 50: 30S ribosomal protein S19



• Molecule 51: Peptide chain release factor 2

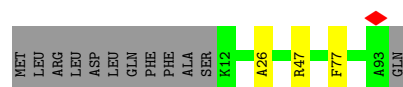






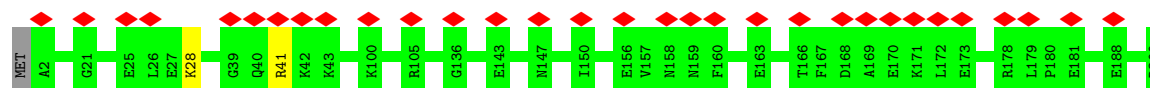
- Molecule 52: Large ribosomal subunit protein bL27

Chain W: 84% 13%



- Molecule 53: 30S ribosomal protein S4

Chain d: 16% 98%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	348223	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.14	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	319.104, 319.104, 319.104	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83100003, 0.83100003, 0.83100003	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PSU, OMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	0	0.61	0/439	1.17	1/584 (0.2%)
2	1	0.51	0/408	0.95	0/541
3	2	0.68	0/371	1.13	0/483
4	3	0.65	0/519	1.11	0/680
5	4	0.54	0/300	1.03	0/393
6	5	0.48	0/356	0.99	0/481
7	6	0.53	0/363	1.01	0/485
8	7	0.60	0/207	1.18	0/319
9	B	0.56	0/2675	1.10	18/4170 (0.4%)
10	C	0.63	1/2130 (0.0%)	1.05	1/2858 (0.0%)
11	D	0.63	0/1597	1.11	2/2140 (0.1%)
12	E	0.55	0/1586	1.02	1/2139 (0.0%)
13	F	0.50	0/1424	1.04	0/1910
14	G	0.53	0/1360	0.99	0/1832
15	J	0.61	0/1165	1.06	0/1566
16	K	0.57	0/928	1.07	2/1245 (0.2%)
17	L	0.55	0/1094	1.01	0/1457
18	M	0.54	0/1099	0.99	0/1468
19	N	0.61	0/961	1.20	2/1284 (0.2%)
20	O	0.52	0/922	0.98	0/1236
21	P	0.54	0/950	1.10	0/1269
22	Q	0.65	0/962	1.08	0/1277
23	R	0.53	0/806	0.95	0/1080
24	S	0.59	0/859	1.11	1/1156 (0.1%)
25	T	0.52	0/739	1.01	1/985 (0.1%)
26	U	0.53	0/780	0.95	0/1043
27	X	0.58	0/471	1.09	1/626 (0.2%)
28	Y	0.46	0/541	0.98	0/718
29	Z	0.52	0/458	1.01	1/613 (0.2%)
30	c	0.50	0/1630	0.99	1/2193 (0.0%)
31	e	0.52	0/1231	1.00	0/1655
32	f	0.47	0/776	0.96	0/1043



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	g	0.51	0/1215	1.08	0/1629
34	h	0.50	0/1042	0.95	0/1397
35	i	0.56	0/1011	1.04	0/1356
36	j	0.54	0/800	1.09	1/1077 (0.1%)
37	k	0.56	0/853	1.00	0/1154
38	l	0.52	0/1061	0.93	0/1424
39	m	0.52	0/949	1.06	0/1268
40	n	0.50	0/508	1.01	0/672
41	o	0.48	0/738	1.03	0/985
42	p	0.49	0/704	0.99	0/945
43	q	0.49	0/701	0.95	0/936
44	r	0.48	0/530	1.06	0/710
45	t	0.49	0/661	1.22	0/882
46	v	0.58	0/1812	1.09	9/2823 (0.3%)
47	A	0.57	0/65622	1.26	613/102356 (0.6%)
48	a	0.56	0/36267	1.09	189/56571 (0.3%)
49	b	0.49	0/1586	1.08	0/2130
50	s	0.52	0/685	1.05	0/920
51	8	0.61	0/1461	1.03	0/1993
52	W	0.54	0/637	1.00	0/846
53	d	0.52	0/1635	1.05	0/2196
All	All	0.56	1/150585 (0.0%)	1.16	844/225199 (0.4%)

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	0	0	2
3	2	0	1
5	4	0	1
10	C	0	6
11	D	0	1
12	E	0	2
17	L	0	1
18	M	0	1
19	N	0	2
20	O	0	2
21	P	0	3
22	Q	0	1
23	R	0	2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
24	S	0	2
34	h	0	1
35	i	0	2
36	j	0	1
45	t	0	1
47	A	0	4
50	s	0	1
51	8	0	1
52	W	0	2
53	d	0	1
All	All	0	41

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	53	HIS	CG-CD2	-5.19	1.30	1.35

All (844) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	732	A	O3'-P-O5'	-18.22	76.67	104.00
47	A	2904	A	C2'-C3'-O3'	15.95	133.43	109.50
47	A	2753	U	C1'-C2'-O2'	-14.57	86.55	108.40
47	A	1244	A	O3'-P-O5'	14.43	125.64	104.00
47	A	490	A	O3'-P-O5'	-13.04	84.45	104.00
47	A	1375	A	O3'-P-O5'	-12.52	85.22	104.00
47	A	617	G	O3'-P-O5'	-12.24	85.63	104.00
48	a	963	G	O3'-P-O5'	-11.91	86.14	104.00
47	A	2753	U	C3'-C2'-O2'	11.87	128.51	110.70
47	A	1606	A	O3'-P-O5'	-11.66	86.50	104.00
47	A	2468	A	C2'-C3'-O3'	11.65	126.98	109.50
47	A	2748	G	O3'-P-O5'	-11.52	86.71	104.00
47	A	2025	C	O3'-P-O5'	-11.52	86.72	104.00
48	a	899	A	O3'-P-O5'	-11.44	86.85	104.00
47	A	354	A	O3'-P-O5'	-11.33	87.00	104.00
47	A	2805	A	C2'-C3'-O3'	10.98	125.97	109.50
47	A	207	A	O3'-P-O5'	-10.98	87.53	104.00
48	a	387	C	O3'-P-O5'	-10.97	87.54	104.00
47	A	482	C	C4'-C3'-O3'	10.95	125.83	109.40
47	A	444	U	O3'-P-O5'	-10.88	87.68	104.00
47	A	481	U	O3'-P-O5'	10.68	120.03	104.00
48	a	1207	A	O3'-P-O5'	-10.62	88.07	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	2720	C	O3'-P-O5'	-10.58	88.13	104.00
47	A	2415	U	O3'-P-O5'	-10.55	88.17	104.00
47	A	2382	G	O3'-P-O5'	-10.49	88.27	104.00
47	A	1770	C	O3'-P-O5'	-10.34	88.50	104.00
47	A	196	U	O3'-P-O5'	-10.27	88.59	104.00
48	a	1090	A	O3'-P-O5'	-10.23	88.65	104.00
47	A	2636	G	O3'-P-O5'	-10.22	88.67	104.00
47	A	2754	A	O3'-P-O5'	-10.12	88.82	104.00
47	A	1966	A	O3'-P-O5'	-10.12	88.82	104.00
47	A	1004	U	O3'-P-O5'	-9.90	89.14	104.00
47	A	2746	G	C1'-C2'-O2'	9.89	123.23	108.40
47	A	29	U	O3'-P-O5'	-9.82	89.26	104.00
47	A	2506	C	O3'-P-O5'	-9.68	89.48	104.00
47	A	1181	C	C4'-C3'-O3'	-9.66	98.50	113.00
9	B	54	U	O3'-P-O5'	-9.62	89.57	104.00
48	a	1419	A	O3'-P-O5'	-9.60	89.60	104.00
47	A	2746	G	O3'-P-O5'	-9.59	89.61	104.00
47	A	723	A	O3'-P-O5'	-9.52	89.72	104.00
48	a	789	G	O3'-P-O5'	-9.51	89.73	104.00
47	A	915	U	O3'-P-O5'	-9.50	89.74	104.00
48	a	785	G	O3'-P-O5'	-9.50	89.75	104.00
47	A	2665	U	C4'-C3'-O3'	-9.48	98.78	113.00
47	A	2121	U	O3'-P-O5'	-9.43	89.85	104.00
47	A	2079	C	O3'-P-O5'	-9.39	89.91	104.00
47	A	1417	A	C2'-C3'-O3'	9.37	123.56	109.50
47	A	2753	U	O3'-P-O5'	-9.35	89.97	104.00
48	a	20	C	O3'-P-O5'	-9.34	89.99	104.00
47	A	2704	A	O3'-P-O5'	-9.31	90.04	104.00
47	A	1759	U	C4'-C3'-O3'	9.27	123.30	109.40
47	A	1515	C	O3'-P-O5'	-9.24	90.14	104.00
47	A	1167	C	O3'-P-O5'	-9.21	90.19	104.00
47	A	828	A	O3'-P-O5'	-9.20	90.19	104.00
47	A	986	G	O3'-P-O5'	9.19	117.78	104.00
47	A	1751	U	O3'-P-O5'	-9.16	90.26	104.00
48	a	986	G	O3'-P-O5'	-9.15	90.27	104.00
47	A	118	A	O3'-P-O5'	-9.14	90.28	104.00
48	a	786	A	O3'-P-O5'	-9.14	90.28	104.00
47	A	1998	A	O3'-P-O5'	-9.13	90.30	104.00
48	a	994	C	O3'-P-O5'	-9.11	90.33	104.00
9	B	14	G	O3'-P-O5'	-9.09	90.37	104.00
47	A	2340	A	O3'-P-O5'	-9.04	90.43	104.00
47	A	211	C	O3'-P-O5'	-9.03	90.45	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	1398	A	O3'-P-O5'	-9.00	90.50	104.00
47	A	2770	A	O3'-P-O5'	-8.97	90.54	104.00
47	A	1560	U	O3'-P-O5'	-8.91	90.63	104.00
47	A	1182	G	O3'-P-O5'	-8.88	90.69	104.00
47	A	373	A	O3'-P-O5'	-8.87	90.70	104.00
48	a	793	A	O3'-P-O5'	-8.87	90.70	104.00
47	A	2334	U	O3'-P-O5'	-8.84	90.74	104.00
47	A	1055	A	O3'-P-O5'	-8.84	90.74	104.00
47	A	2424	C	O3'-P-O5'	-8.83	90.76	104.00
47	A	2745	U	O3'-P-O5'	-8.78	90.82	104.00
47	A	2908	A	O3'-P-O5'	-8.78	90.83	104.00
47	A	1613	C	O3'-P-O5'	-8.78	90.83	104.00
47	A	1911	C	O3'-P-O5'	-8.78	90.83	104.00
47	A	543	A	O3'-P-O5'	-8.73	90.91	104.00
47	A	274	A	O3'-P-O5'	-8.72	90.92	104.00
47	A	2605	G	O3'-P-O5'	-8.68	90.98	104.00
47	A	457	G	C2'-C3'-O3'	-8.66	100.71	113.70
47	A	1690	G	O3'-P-O5'	-8.52	91.22	104.00
47	A	669	C	O3'-P-O5'	-8.49	91.26	104.00
47	A	1939	G	O3'-P-O5'	-8.47	91.30	104.00
47	A	2860	A	O3'-P-O5'	-8.46	91.31	104.00
47	A	2439	G	O3'-P-O5'	-8.46	91.31	104.00
47	A	2435	C	O3'-P-O5'	-8.45	91.33	104.00
47	A	16	G	O3'-P-O5'	-8.41	91.39	104.00
48	a	283	G	O3'-P-O5'	-8.36	91.46	104.00
48	a	261	U	O3'-P-O5'	-8.33	91.50	104.00
47	A	2831	A	O3'-P-O5'	-8.28	91.59	104.00
47	A	1776	A	O3'-P-O5'	-8.27	91.59	104.00
47	A	958	A	O3'-P-O5'	-8.25	91.62	104.00
47	A	2665	U	O3'-P-O5'	-8.25	91.63	104.00
47	A	129	C	O3'-P-O5'	-8.24	91.65	104.00
47	A	1690	G	C2'-C3'-O3'	-8.22	101.37	113.70
47	A	2057	U	O3'-P-O5'	-8.18	91.73	104.00
47	A	1277	A	O3'-P-O5'	-8.18	91.74	104.00
47	A	1369	C	O3'-P-O5'	-8.12	91.82	104.00
48	a	1508	U	O3'-P-O5'	-8.10	91.85	104.00
47	A	2717	G	C1'-C2'-O2'	8.07	120.51	108.40
27	X	27	ARG	CB-CA-C	-8.00	95.05	111.22
47	A	1516	A	O3'-P-O5'	-7.99	92.02	104.00
48	a	544	A	O3'-P-O5'	-7.98	92.03	104.00
47	A	1884	G	O3'-P-O5'	-7.97	92.05	104.00
47	A	1715	C	C3'-C2'-O2'	7.93	122.59	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	1339	A	C2'-C3'-O3'	7.92	121.38	109.50
48	a	1370	G	O3'-P-O5'	-7.91	92.13	104.00
47	A	1014	A	O3'-P-O5'	-7.91	92.14	104.00
47	A	2550	C	C4'-C3'-O3'	-7.89	101.16	113.00
47	A	2677	G	O3'-P-O5'	-7.88	92.18	104.00
48	a	1363	C	O3'-P-O5'	-7.87	92.19	104.00
48	a	1383	A	O3'-P-O5'	-7.87	92.20	104.00
48	a	840	U	O3'-P-O5'	-7.85	92.22	104.00
47	A	613	U	C4'-C3'-O3'	-7.83	101.26	113.00
47	A	2032	A	O3'-P-O5'	-7.81	92.28	104.00
48	a	296	A	O3'-P-O5'	-7.81	92.29	104.00
48	a	385	G	O3'-P-O5'	-7.80	92.30	104.00
47	A	2842	U	C3'-C2'-O2'	7.77	122.36	110.70
47	A	2711	G	O3'-P-O5'	-7.74	92.39	104.00
47	A	572	A	C4'-C3'-O3'	-7.74	101.40	113.00
47	A	2553	G	O3'-P-O5'	-7.71	92.43	104.00
47	A	225	A	O3'-P-O5'	-7.71	92.43	104.00
47	A	1374	C	O3'-P-O5'	-7.69	92.47	104.00
47	A	342	A	O3'-P-O5'	-7.68	92.48	104.00
47	A	1945	A	C4'-C3'-O3'	7.67	120.90	109.40
47	A	1959	G	O3'-P-O5'	-7.66	92.51	104.00
9	B	37	A	C2'-C3'-O3'	7.66	125.19	113.70
47	A	2473	G	O3'-P-O5'	-7.65	92.53	104.00
47	A	266	U	O3'-P-O5'	-7.61	92.59	104.00
47	A	2569	C	C2'-C3'-O3'	7.59	125.08	113.70
47	A	863	C	O3'-P-O5'	-7.58	92.63	104.00
47	A	801	U	O3'-P-O5'	-7.58	92.63	104.00
47	A	2669	G	O3'-P-O5'	-7.54	92.70	104.00
47	A	14	A	O3'-P-O5'	-7.52	92.72	104.00
47	A	2290	C	O3'-P-O5'	-7.52	92.72	104.00
48	a	896	G	O3'-P-O5'	-7.51	92.73	104.00
47	A	2000	A	O3'-P-O5'	-7.51	92.73	104.00
9	B	48	G	C2'-C3'-O3'	7.50	124.95	113.70
47	A	1934	C	O3'-P-O5'	-7.50	92.75	104.00
47	A	2347	G	O3'-P-O5'	-7.48	92.79	104.00
47	A	2365	A	O3'-P-O5'	-7.47	92.80	104.00
48	a	118	A	O3'-P-O5'	-7.46	92.80	104.00
47	A	2796	C	O3'-P-O5'	-7.46	92.81	104.00
48	a	982	C	C4'-C3'-O3'	-7.46	101.81	113.00
48	a	536	G	O3'-P-O5'	-7.44	92.84	104.00
48	a	1148	G	C2'-C3'-O3'	7.44	120.65	109.50
47	A	1305	A	O3'-P-O5'	-7.43	92.86	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	2302	A	C4'-C3'-O3'	-7.42	101.86	113.00
47	A	1893	U	O3'-P-O5'	-7.42	92.87	104.00
47	A	539	G	O3'-P-O5'	-7.41	92.89	104.00
47	A	2740	A	C4'-C3'-O3'	-7.41	101.89	113.00
48	a	355	G	O3'-P-O5'	-7.39	92.91	104.00
47	A	635	C	O3'-P-O5'	-7.39	92.92	104.00
47	A	1307	U	C4'-C3'-O3'	-7.38	101.92	113.00
47	A	746	A	O3'-P-O5'	-7.38	92.94	104.00
47	A	1364	C	O3'-P-O5'	-7.37	92.95	104.00
47	A	747	G	O3'-P-O5'	-7.35	92.97	104.00
47	A	540	G	C4'-C3'-O3'	-7.34	101.98	113.00
9	B	45	C	O3'-P-O5'	-7.34	92.99	104.00
47	A	1682	C	O3'-P-O5'	-7.33	93.00	104.00
48	a	372	A	C4'-C3'-O3'	7.33	124.00	113.00
47	A	1498	U	O3'-P-O5'	-7.31	93.04	104.00
47	A	2078	A	O3'-P-O5'	-7.30	93.04	104.00
47	A	583	G	C4'-C3'-O3'	-7.30	102.06	113.00
47	A	2592	U	C4'-C3'-O3'	-7.29	102.06	113.00
47	A	1654	A	C1'-C2'-O2'	-7.29	100.87	111.80
47	A	1054	A	O3'-P-O5'	-7.28	93.08	104.00
46	v	45	U	O3'-P-O5'	-7.27	93.10	104.00
47	A	1250	G	C4'-C3'-O3'	7.26	120.29	109.40
47	A	2610	G	O3'-P-O5'	-7.26	93.11	104.00
47	A	1244	A	C2'-C3'-O3'	7.24	124.56	113.70
47	A	615	U	O3'-P-O5'	-7.23	93.15	104.00
48	a	1091	G	O3'-P-O5'	-7.23	93.16	104.00
48	a	1384	A	O3'-P-O5'	-7.23	93.16	104.00
47	A	583	G	O3'-P-O5'	-7.20	93.21	104.00
47	A	1816	A	C4'-C3'-O3'	-7.19	102.21	113.00
47	A	1255	G	O3'-P-O5'	-7.19	93.21	104.00
47	A	12	A	O3'-P-O5'	-7.18	93.22	104.00
48	a	386	A	O3'-P-O5'	-7.16	93.25	104.00
47	A	1486	G	O3'-P-O5'	-7.16	93.27	104.00
48	a	555	A	O3'-P-O5'	-7.14	93.30	104.00
47	A	2054	C	C4'-C3'-O3'	-7.13	102.31	113.00
47	A	1876	A	O3'-P-O5'	-7.11	93.33	104.00
46	v	47	U	C2'-C3'-O3'	7.11	120.16	109.50
47	A	2478	U	C1'-C2'-O2'	-7.10	101.15	111.80
47	A	2834	A	O3'-P-O5'	-7.08	93.39	104.00
48	a	1436	C	O3'-P-O5'	-7.07	93.39	104.00
48	a	735	C	O3'-P-O5'	-7.07	93.40	104.00
47	A	228	C	C3'-C2'-O2'	7.05	121.27	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	1256	C	O3'-P-O5'	-7.04	93.44	104.00
48	a	1329	C	O3'-P-O5'	-7.04	93.44	104.00
47	A	836	A	O3'-P-O5'	-7.03	93.45	104.00
48	a	1113	C	O3'-P-O5'	-7.03	93.46	104.00
47	A	2740	A	O3'-P-O5'	-7.02	93.47	104.00
48	a	1117	C	O3'-P-O5'	-7.02	93.47	104.00
47	A	228	C	C2'-C3'-O3'	7.02	124.23	113.70
47	A	874	U	C2'-C3'-O3'	-7.02	103.17	113.70
47	A	1188	A	O3'-P-O5'	-7.01	93.48	104.00
48	a	356	G	O3'-P-O5'	-7.01	93.49	104.00
48	a	696	A	O3'-P-O5'	-7.00	93.51	104.00
47	A	2037	C	O3'-P-O5'	-6.99	93.52	104.00
48	a	127	U	O3'-P-O5'	-6.98	93.53	104.00
48	a	884	G	O3'-P-O5'	-6.97	93.54	104.00
48	a	1504	G	O3'-P-O5'	-6.96	93.56	104.00
47	A	1171	G	C4'-C3'-O3'	-6.95	102.58	113.00
48	a	400	G	O3'-P-O5'	-6.93	93.61	104.00
47	A	2581	U	O3'-P-O5'	-6.93	93.61	104.00
47	A	2768	U	C2'-C3'-O3'	-6.91	103.34	113.70
47	A	201	C	O3'-P-O5'	-6.89	93.66	104.00
47	A	2904	A	C4'-C3'-O3'	-6.89	99.07	109.40
47	A	2308	G	O3'-P-O5'	-6.88	93.68	104.00
48	a	509	G	O3'-P-O5'	-6.88	93.69	104.00
47	A	254	A	O3'-P-O5'	-6.86	93.71	104.00
48	a	837	A	O3'-P-O5'	-6.85	93.72	104.00
47	A	123	G	O3'-P-O5'	-6.85	93.73	104.00
9	B	81	G	O3'-P-O5'	-6.85	93.73	104.00
47	A	546	G	O3'-P-O5'	-6.84	93.74	104.00
47	A	2639	C	C4'-C3'-O3'	-6.83	99.15	109.40
47	A	1973	U	O3'-P-O5'	-6.82	93.77	104.00
47	A	2253	G	O3'-P-O5'	-6.82	93.77	104.00
48	a	795	G	O3'-P-O5'	-6.81	93.78	104.00
47	A	1313	A	O3'-P-O5'	-6.80	93.79	104.00
48	a	679	A	O3'-P-O5'	-6.79	93.81	104.00
47	A	1750	G	O3'-P-O5'	-6.79	93.82	104.00
47	A	512	G	O3'-P-O5'	-6.77	93.84	104.00
47	A	1310	C	O3'-P-O5'	-6.76	93.85	104.00
47	A	2874	G	O3'-P-O5'	-6.76	93.86	104.00
48	a	525	U	O3'-P-O5'	-6.75	93.87	104.00
48	a	1502	A	O3'-P-O5'	-6.75	93.87	104.00
47	A	1013	U	O3'-P-O5'	-6.73	93.90	104.00
47	A	1941	A	O3'-P-O5'	-6.73	93.91	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	1228	G	C4'-C3'-O3'	-6.72	102.91	113.00
47	A	2665	U	C2'-C3'-O3'	6.71	123.77	113.70
47	A	2753	U	C4'-C3'-O3'	-6.71	102.94	113.00
47	A	228	C	C1'-C2'-O2'	-6.70	98.36	108.40
47	A	2855	G	C3'-C2'-O2'	6.70	120.75	110.70
47	A	1704	U	O3'-P-O5'	-6.70	93.96	104.00
48	a	1230	G	C2'-C3'-O3'	-6.70	103.66	113.70
47	A	624	C	C4'-C3'-O3'	-6.69	102.97	113.00
47	A	1275	G	C4'-C3'-O3'	-6.68	102.98	113.00
47	A	598	U	C4'-C3'-O3'	-6.67	103.00	113.00
47	A	1941	A	C2'-C3'-O3'	6.66	119.50	109.50
47	A	2551	U	O3'-P-O5'	-6.66	94.01	104.00
47	A	2713	U	O3'-P-O5'	-6.65	94.02	104.00
48	a	882	A	O3'-P-O5'	-6.64	94.03	104.00
47	A	1265	A	O3'-P-O5'	-6.64	94.04	104.00
47	A	2715	G	C4'-C3'-C2'	-6.64	95.96	102.60
48	a	982	C	O3'-P-O5'	-6.63	94.05	104.00
47	A	217	G	O3'-P-O5'	-6.63	94.06	104.00
47	A	2753	U	C2'-C3'-O3'	6.63	123.64	113.70
47	A	525	A	O3'-P-O5'	-6.63	94.06	104.00
47	A	1810	G	O3'-P-O5'	-6.62	94.07	104.00
47	A	2760	G	O3'-P-O5'	-6.61	94.09	104.00
47	A	2296	A	C4'-C3'-O3'	-6.61	103.09	113.00
19	N	23	ASP	CA-CB-CG	6.60	119.20	112.60
36	j	43	PRO	N-CA-C	6.60	121.44	111.14
47	A	1674	G	O3'-P-O5'	-6.60	94.10	104.00
47	A	1383	U	O3'-P-O5'	-6.60	94.11	104.00
47	A	803	C	O3'-P-O5'	-6.59	94.11	104.00
47	A	2569	C	C4'-C3'-C2'	-6.59	96.01	102.60
47	A	1301	U	O3'-P-O5'	-6.58	94.12	104.00
47	A	1678	G	C4'-C3'-O3'	-6.58	103.14	113.00
47	A	2485	C	O3'-P-O5'	-6.57	94.15	104.00
48	a	588	U	O3'-P-O5'	-6.56	94.16	104.00
47	A	837	U	O3'-P-O5'	-6.56	94.16	104.00
48	a	992	U	O3'-P-O5'	-6.56	94.16	104.00
48	a	284	G	O3'-P-O5'	-6.56	94.17	104.00
48	a	1411	C	C3'-C2'-O2'	6.55	120.53	110.70
47	A	1448	U	O3'-P-O5'	-6.53	94.20	104.00
11	D	150	ASP	CA-CB-CG	6.53	119.13	112.60
47	A	2109	G	O3'-P-O5'	-6.53	94.21	104.00
47	A	2604	C	C4'-C3'-O3'	-6.52	103.21	113.00
48	a	807	U	O3'-P-O5'	-6.52	94.22	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	a	965	U	C2'-C3'-O3'	6.52	123.48	113.70
48	a	988	A	O3'-P-O5'	-6.52	94.23	104.00
48	a	305	G	O3'-P-O5'	-6.51	94.23	104.00
48	a	434	U	O3'-P-O5'	-6.51	94.23	104.00
47	A	1258	A	O3'-P-O5'	-6.51	94.24	104.00
9	B	42	G	O3'-P-O5'	-6.50	94.25	104.00
47	A	13	A	O3'-P-O5'	-6.50	94.25	104.00
47	A	2566	U	C4'-C3'-O3'	-6.50	103.25	113.00
47	A	1316	A	O3'-P-O5'	-6.49	94.27	104.00
47	A	188	C	O3'-P-O5'	-6.49	94.27	104.00
47	A	1699	A	O3'-P-O5'	-6.48	94.28	104.00
47	A	1999	A	O3'-P-O5'	-6.47	94.29	104.00
47	A	2520	U	C4'-C3'-O3'	-6.47	103.29	113.00
48	a	960	U	O3'-P-O5'	-6.46	94.31	104.00
47	A	1822	G	C4'-C3'-O3'	-6.46	103.32	113.00
47	A	1257	G	O3'-P-O5'	-6.46	94.32	104.00
47	A	228	C	C4'-C3'-O3'	-6.45	103.33	113.00
47	A	575	A	O3'-P-O5'	-6.45	94.33	104.00
47	A	1415	C	O3'-P-O5'	-6.44	94.34	104.00
47	A	2849	U	C4'-C3'-O3'	-6.43	103.36	113.00
47	A	297	G	O3'-P-O5'	-6.42	94.36	104.00
47	A	2117	A	O3'-P-O5'	-6.42	94.37	104.00
47	A	733	U	O5'-P-OP1	6.41	127.24	108.00
48	a	995	C	O3'-P-O5'	-6.41	94.38	104.00
47	A	2414	C	O3'-P-O5'	-6.41	94.39	104.00
48	a	1427	A	O3'-P-O5'	-6.40	94.39	104.00
47	A	889	A	O3'-P-O5'	-6.39	94.41	104.00
47	A	352	G	O3'-P-O5'	-6.39	94.41	104.00
47	A	2805	A	O3'-P-O5'	6.39	113.59	104.00
47	A	1388	A	P-O5'-C5'	-6.39	111.32	120.90
47	A	540	G	O3'-P-O5'	-6.39	94.42	104.00
47	A	772	G	C4'-C3'-O3'	-6.38	103.42	113.00
48	a	701	U	O3'-P-O5'	-6.38	94.42	104.00
47	A	2705	C	O3'-P-O5'	-6.38	94.43	104.00
47	A	470	A	O3'-P-O5'	-6.38	94.43	104.00
47	A	2649	C	O3'-P-O5'	-6.37	94.44	104.00
47	A	1301	U	C4'-C3'-O3'	-6.37	103.44	113.00
47	A	2850	G	O3'-P-O5'	6.36	113.54	104.00
47	A	2531	G	O5'-C5'-C4'	-6.36	101.96	111.50
48	a	210	A	O3'-P-O5'	-6.35	94.47	104.00
47	A	2629	A	O3'-P-O5'	-6.35	94.47	104.00
46	v	70	G	O3'-P-O5'	-6.34	94.50	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	a	579	G	C4'-C3'-O3'	-6.34	103.50	113.00
47	A	1530	G	C2'-C3'-O3'	6.33	123.19	113.70
47	A	564	G	C4'-C3'-O3'	-6.33	103.51	113.00
47	A	1771	C	O3'-P-O5'	-6.31	94.53	104.00
47	A	2078	A	C4'-C3'-O3'	-6.31	103.53	113.00
47	A	2843	G	C3'-C2'-O2'	6.31	120.16	110.70
47	A	875	U	C4'-C3'-O3'	-6.30	103.55	113.00
48	a	607	U	O3'-P-O5'	-6.30	94.55	104.00
47	A	2052	A	C4'-C3'-O3'	-6.29	103.57	113.00
47	A	1988	G	O3'-P-O5'	-6.28	94.58	104.00
48	a	206	A	O3'-P-O5'	-6.28	94.58	104.00
48	a	581	A	O3'-P-O5'	-6.27	94.59	104.00
47	A	469	A	O3'-P-O5'	-6.26	94.61	104.00
47	A	1481	G	O3'-P-O5'	-6.24	94.64	104.00
47	A	1055	A	C4'-C3'-O3'	-6.24	103.64	113.00
47	A	1543	U	O3'-P-O5'	-6.23	94.65	104.00
48	a	394	C	O3'-P-O5'	-6.23	94.65	104.00
1	0	40	HIS	CA-CB-CG	6.23	120.03	113.80
47	A	1072	A	C4'-C3'-O3'	6.23	118.74	109.40
47	A	2663	A	C4'-C3'-O3'	-6.23	103.66	113.00
47	A	251	G	O3'-P-O5'	-6.22	94.67	104.00
47	A	1179	A	O3'-P-O5'	-6.22	94.67	104.00
47	A	2548	U	O3'-P-O5'	-6.22	94.67	104.00
47	A	1337	C	O3'-P-O5'	-6.21	94.68	104.00
46	v	64	U	O3'-P-O5'	-6.21	94.68	104.00
47	A	2264	G	O3'-P-O5'	-6.21	94.69	104.00
47	A	367	G	O3'-P-O5'	-6.21	94.69	104.00
48	a	1266	A	C2'-C3'-O3'	6.21	118.81	109.50
47	A	2670	A	O3'-P-O5'	-6.20	94.70	104.00
47	A	794	U	O3'-P-O5'	-6.20	94.70	104.00
47	A	720	C	O3'-P-O5'	-6.19	94.71	104.00
48	a	836	U	O3'-P-O5'	-6.19	94.72	104.00
47	A	1841	G	C4'-C3'-O3'	-6.19	103.72	113.00
47	A	2662	A	O3'-P-O5'	-6.19	94.72	104.00
47	A	2377	U	C1'-C2'-O2'	6.18	117.67	108.40
47	A	2059	A	C3'-C2'-O2'	-6.18	105.33	114.60
47	A	383	U	O3'-P-O5'	-6.18	94.73	104.00
47	A	1525	G	C2'-C3'-O3'	6.17	122.96	113.70
47	A	1886	G	C4'-C3'-O3'	6.17	118.65	109.40
48	a	400	G	C4'-C3'-O3'	-6.17	103.75	113.00
47	A	1332	U	O3'-P-O5'	-6.16	94.76	104.00
47	A	991	A	O5'-P-OP1	-6.16	89.53	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	1789	A	O3'-P-O5'	-6.16	94.76	104.00
47	A	458	G	C1'-C2'-O2'	-6.15	102.57	111.80
48	a	363	C	C4'-C3'-O3'	-6.15	103.78	113.00
48	a	583	A	C4'-C3'-O3'	-6.15	103.78	113.00
47	A	1184	G	C2'-C3'-O3'	-6.14	104.48	113.70
47	A	1480	A	O3'-P-O5'	-6.13	94.80	104.00
47	A	1757	G	C1'-O4'-C4'	-6.13	103.57	109.70
47	A	1168	G	O3'-P-O5'	-6.13	94.80	104.00
48	a	965	U	C4'-C3'-C2'	-6.12	96.48	102.60
47	A	768	G	O3'-P-O5'	-6.12	94.83	104.00
48	a	1201	C	O3'-P-O5'	-6.12	94.83	104.00
47	A	52	A	O3'-P-O5'	-6.11	94.83	104.00
47	A	176	A	O3'-P-O5'	-6.11	94.83	104.00
47	A	627	G	O3'-P-O5'	-6.11	94.83	104.00
47	A	2842	U	O3'-P-O5'	-6.11	94.83	104.00
47	A	826	U	O3'-P-O5'	6.11	113.16	104.00
47	A	1047	A	O3'-P-O5'	-6.10	94.85	104.00
47	A	2248	G	O3'-P-O5'	-6.09	94.86	104.00
47	A	724	A	C4'-C3'-O3'	-6.07	103.90	113.00
47	A	2549	C	O3'-P-O5'	-6.06	94.91	104.00
47	A	2863	G	O3'-P-O5'	-6.05	94.92	104.00
47	A	2237	C	O3'-P-O5'	-6.05	94.92	104.00
47	A	1981	A	O3'-P-O5'	-6.05	94.93	104.00
47	A	2438	G	O3'-P-O5'	-6.04	94.94	104.00
48	a	805	C	O3'-P-O5'	-6.04	94.95	104.00
47	A	798	A	O3'-P-O5'	-6.03	94.95	104.00
48	a	734	G	O3'-P-O5'	-6.03	94.95	104.00
48	a	966	U	O3'-P-O5'	-6.03	94.96	104.00
47	A	2583	U	O5'-P-OP1	-6.02	89.94	108.00
47	A	198	A	C4'-C3'-O3'	-6.01	103.98	113.00
47	A	1204	C	O3'-P-O5'	-6.01	94.99	104.00
47	A	22	C	O3'-P-O5'	-6.00	95.00	104.00
47	A	2332	G	O3'-P-O5'	-6.00	95.00	104.00
47	A	1682	C	C1'-C2'-O2'	6.00	117.39	108.40
47	A	2495	C	C4'-C3'-O3'	-6.00	104.00	113.00
47	A	831	U	C2'-C3'-O3'	-5.99	104.71	113.70
48	a	1501	G	O3'-P-O5'	-5.99	95.01	104.00
48	a	1062	U	O3'-P-O5'	-5.99	95.02	104.00
47	A	1073	A	C4'-C3'-O3'	-5.97	104.04	113.00
48	a	1243	C	O3'-P-O5'	-5.97	95.05	104.00
9	B	37	A	C4'-C3'-C2'	-5.96	96.64	102.60
47	A	1188	A	C4'-C3'-O3'	5.96	118.35	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	a	1200	A	O3'-P-O5'	-5.96	95.05	104.00
48	a	1057	G	O3'-P-O5'	-5.96	95.06	104.00
47	A	34	U	C2'-C3'-O3'	5.96	118.43	109.50
47	A	1842	C	O3'-P-O5'	-5.95	95.07	104.00
47	A	2229	C	O3'-P-O5'	-5.94	95.09	104.00
48	a	823	A	C4'-C3'-O3'	-5.94	104.09	113.00
47	A	1645	C	O3'-P-O5'	-5.94	95.09	104.00
47	A	1236	G	O3'-P-O5'	-5.93	95.10	104.00
47	A	2054	C	O3'-P-O5'	-5.93	95.10	104.00
47	A	2030	A	O3'-P-O5'	-5.93	95.11	104.00
48	a	641	G	C2'-C3'-O3'	5.92	118.38	109.50
47	A	1427	G	C3'-C2'-O2'	5.92	119.58	110.70
47	A	1203	G	O5'-P-OP1	-5.91	90.26	108.00
48	a	1503	A	C4'-C3'-O3'	5.91	118.27	109.40
47	A	2287	C	C3'-C2'-O2'	-5.90	105.75	114.60
47	A	1359	G	O3'-P-O5'	-5.89	95.16	104.00
47	A	1375	A	C4'-C3'-O3'	-5.89	104.16	113.00
48	a	860	U	O3'-P-O5'	-5.89	95.16	104.00
47	A	527	A	O3'-P-O5'	-5.89	95.17	104.00
47	A	1285	G	O3'-P-O5'	-5.89	95.17	104.00
47	A	2053	C	C2'-C3'-O3'	5.88	122.52	113.70
47	A	606	U	O3'-P-O5'	-5.87	95.19	104.00
47	A	1230	A	C4'-C3'-O3'	-5.87	104.19	113.00
47	A	1627	A	O3'-P-O5'	-5.87	95.19	104.00
9	B	10	G	O3'-P-O5'	-5.87	95.20	104.00
47	A	1631	A	C4'-C3'-O3'	5.86	118.19	109.40
47	A	2693	G	O3'-P-O5'	-5.86	95.21	104.00
48	a	1368	C	O3'-P-O5'	-5.86	95.22	104.00
47	A	1774	A	O3'-P-O5'	-5.85	95.22	104.00
47	A	1178	U	C2'-C3'-O3'	5.85	118.28	109.50
47	A	1200	G	O3'-P-O5'	-5.85	95.22	104.00
48	a	1063	G	O3'-P-O5'	-5.85	95.22	104.00
47	A	1186	C	C4'-C3'-O3'	-5.85	104.23	113.00
47	A	2033	G	C2'-C3'-O3'	5.85	122.47	113.70
48	a	1268	C	O3'-P-O5'	-5.84	95.24	104.00
47	A	2797	C	O3'-P-O5'	-5.83	95.25	104.00
47	A	1183	G	C4'-C3'-C2'	-5.83	96.77	102.60
48	a	1514	G	O3'-P-O5'	-5.83	95.25	104.00
48	a	553	G	O3'-P-O5'	-5.83	95.26	104.00
47	A	708	U	C2'-C3'-O3'	-5.83	104.96	113.70
47	A	2760	G	C4'-C3'-O3'	-5.83	104.26	113.00
47	A	2876	A	C2'-C3'-O3'	-5.82	104.96	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	696	C	C4'-C3'-O3'	-5.81	104.28	113.00
47	A	389	A	O3'-P-O5'	-5.81	95.28	104.00
47	A	541	G	O3'-P-O5'	-5.81	95.28	104.00
48	a	955	G	O3'-P-O5'	-5.81	95.29	104.00
9	B	107	G	C4'-C3'-O3'	5.80	118.11	109.40
48	a	334	G	O3'-P-O5'	-5.80	95.29	104.00
47	A	1601	A	O3'-P-O5'	-5.80	95.30	104.00
47	A	1244	A	O4'-C4'-C3'	-5.80	98.20	104.00
47	A	58	G	O3'-P-O5'	-5.80	95.31	104.00
47	A	1616	G	O3'-P-O5'	-5.80	95.31	104.00
48	a	923	A	O3'-P-O5'	-5.80	95.31	104.00
47	A	1565	U	C2'-C3'-O3'	5.79	122.39	113.70
47	A	2073	C	C3'-C2'-O2'	5.79	119.38	110.70
47	A	714	U	O3'-P-O5'	-5.78	95.33	104.00
47	A	1350	U	O3'-P-O5'	-5.78	95.33	104.00
47	A	2674	G	O3'-P-O5'	5.78	112.67	104.00
48	a	64	U	O3'-P-O5'	-5.78	95.33	104.00
48	a	1438	C	O3'-P-O5'	-5.78	95.33	104.00
48	a	623	C	O3'-P-O5'	-5.78	95.34	104.00
48	a	381	A	O3'-P-O5'	-5.77	95.34	104.00
47	A	185	A	O3'-P-O5'	-5.77	95.35	104.00
47	A	679	A	C2'-C3'-O3'	-5.77	105.05	113.70
48	a	302	C	O3'-P-O5'	-5.77	95.35	104.00
47	A	417	G	O3'-P-O5'	-5.76	95.35	104.00
47	A	2063	U	C4'-C3'-O3'	-5.75	104.37	113.00
48	a	339	G	O3'-P-O5'	-5.75	95.38	104.00
48	a	362	G	C4'-C3'-O3'	-5.75	104.38	113.00
48	a	330	C	O3'-P-O5'	-5.74	95.39	104.00
47	A	2762	A	O3'-P-O5'	-5.74	95.39	104.00
47	A	2791	U	O3'-P-O5'	-5.74	95.39	104.00
48	a	1357	U	O3'-P-O5'	-5.74	95.39	104.00
47	A	563	C	O3'-P-O5'	-5.74	95.39	104.00
47	A	1804	U	C3'-C2'-O2'	5.74	119.31	110.70
47	A	2872	U	O3'-P-O5'	-5.74	95.40	104.00
47	A	483	C	O3'-P-O5'	-5.73	95.40	104.00
47	A	1050	U	C4'-C3'-O3'	-5.73	104.40	113.00
47	A	2896	U	C4'-C3'-O3'	-5.72	104.42	113.00
47	A	187	C	O3'-P-O5'	-5.72	95.42	104.00
48	a	1104	G	O3'-P-O5'	-5.71	95.43	104.00
47	A	1940	U	O3'-P-O5'	-5.71	95.43	104.00
48	a	540	U	O3'-P-O5'	-5.71	95.44	104.00
48	a	948	A	O3'-P-O5'	-5.71	95.44	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	1863	U	O3'-P-O5'	-5.70	95.45	104.00
47	A	2736	G	O3'-P-O5'	-5.70	95.45	104.00
47	A	1246	G	O4'-C4'-C3'	-5.70	98.30	104.00
47	A	2576	U	C2'-C3'-O3'	-5.70	105.15	113.70
47	A	747	G	C4'-C3'-O3'	-5.69	104.46	113.00
47	A	1358	G	O3'-P-O5'	-5.69	95.46	104.00
47	A	1340	A	O3'-P-O5'	-5.69	95.47	104.00
47	A	1751	U	C2'-C3'-O3'	5.68	118.03	109.50
47	A	1709	A	C4'-C3'-O3'	-5.68	104.48	113.00
47	A	263	G	O3'-P-O5'	-5.67	95.49	104.00
47	A	1406	A	O3'-P-O5'	-5.67	95.49	104.00
47	A	2703	G	C3'-C2'-O2'	5.67	119.21	110.70
47	A	1642	G	C4'-C3'-O3'	-5.67	104.49	113.00
47	A	2601	A	O3'-P-O5'	-5.67	95.50	104.00
9	B	49	G	C2'-C3'-O3'	5.67	122.20	113.70
47	A	432	C	O3'-P-O5'	-5.67	95.50	104.00
47	A	2631	A	C1'-O4'-C4'	-5.67	104.03	109.70
47	A	2642	U	O3'-P-O5'	-5.67	95.50	104.00
47	A	1501	U	O3'-P-O5'	5.66	112.49	104.00
47	A	436	A	O3'-P-O5'	-5.66	95.52	104.00
47	A	1035	G	O3'-P-O5'	-5.65	95.52	104.00
47	A	1366	C	C4'-C3'-O3'	-5.65	104.52	113.00
47	A	2504	C	O3'-P-O5'	-5.65	95.52	104.00
47	A	2425	G	O3'-P-O5'	-5.65	95.52	104.00
47	A	2649	C	C3'-C2'-O2'	5.65	119.18	110.70
48	a	767	G	C4'-C3'-O3'	-5.65	104.53	113.00
48	a	1507	G	C4'-C3'-O3'	-5.64	104.54	113.00
48	a	582	A	O3'-P-O5'	-5.64	95.54	104.00
47	A	1877	A	O3'-P-O5'	-5.64	95.55	104.00
9	B	105	A	O3'-P-O5'	-5.62	95.56	104.00
47	A	1711	G	O4'-C4'-C3'	-5.62	98.38	104.00
47	A	778	C	O3'-P-O5'	-5.62	95.57	104.00
47	A	2729	C	O3'-P-O5'	-5.62	95.57	104.00
48	a	384	G	O3'-P-O5'	-5.62	95.57	104.00
48	a	1101	U	O3'-P-O5'	-5.62	95.57	104.00
48	a	1389	U	O3'-P-O5'	-5.62	95.58	104.00
47	A	2598	G	O3'-P-O5'	-5.61	95.58	104.00
47	A	731	G	C4'-C3'-O3'	-5.61	104.59	113.00
47	A	2311	G	O3'-P-O5'	-5.61	95.59	104.00
47	A	1255	G	C1'-C2'-O2'	5.61	116.81	108.40
47	A	1036	A	O3'-P-O5'	-5.60	95.59	104.00
47	A	1751	U	C4'-C3'-O3'	5.60	117.80	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	2292	C	O3'-P-O5'	-5.60	95.60	104.00
47	A	1197	A	O3'-P-O5'	-5.60	95.60	104.00
47	A	476	A	O3'-P-O5'	-5.60	95.61	104.00
47	A	1027	A	C2'-C3'-O3'	-5.60	105.31	113.70
48	a	885	C	O3'-P-O5'	-5.59	95.61	104.00
48	a	720	G	O3'-P-O5'	-5.59	95.61	104.00
48	a	1378	C	O3'-P-O5'	-5.59	95.61	104.00
47	A	1694	G	O5'-C5'-C4'	-5.59	103.11	111.50
48	a	532	A	O3'-P-O5'	-5.58	95.62	104.00
47	A	808	A	C4'-C3'-O3'	-5.58	104.63	113.00
48	a	848	G	C2'-C3'-O3'	5.58	122.07	113.70
48	a	519	A	O3'-P-O5'	-5.58	95.64	104.00
47	A	757	C	O3'-P-O5'	-5.57	95.64	104.00
47	A	95	A	O3'-P-O5'	-5.57	95.64	104.00
47	A	481	U	C2'-C3'-O3'	5.57	117.86	109.50
47	A	2486	U	C4'-C3'-O3'	-5.57	104.65	113.00
48	a	19	U	O3'-P-O5'	-5.57	95.65	104.00
47	A	794	U	C4'-C3'-O3'	-5.57	104.65	113.00
47	A	240	C	C3'-C2'-O2'	5.56	119.05	110.70
9	B	32	U	O3'-P-O5'	-5.56	95.66	104.00
47	A	2267	G	O3'-P-O5'	-5.56	95.66	104.00
47	A	2550	C	C2'-C3'-O3'	5.56	122.04	113.70
47	A	1397	G	O3'-P-O5'	-5.55	95.67	104.00
47	A	1769	G	O3'-P-O5'	-5.55	95.67	104.00
47	A	2752	C	C4'-C3'-C2'	-5.55	97.05	102.60
29	Z	18	ASP	CA-CB-CG	5.55	118.15	112.60
47	A	559	A	O3'-P-O5'	-5.54	95.69	104.00
47	A	1701	C	C2'-C3'-O3'	5.54	122.01	113.70
47	A	2641	C	C4'-C3'-O3'	-5.54	104.69	113.00
47	A	824	G	O3'-P-O5'	5.54	112.31	104.00
47	A	1863	U	C4'-C3'-O3'	-5.54	104.69	113.00
48	a	1091	G	C4'-C3'-O3'	-5.54	104.69	113.00
47	A	2459	A	C1'-O4'-C4'	-5.54	104.16	109.70
47	A	2743	G	O3'-P-O5'	-5.54	95.70	104.00
47	A	2849	U	O3'-P-O5'	-5.54	95.70	104.00
47	A	2042	A	C3'-C2'-O2'	-5.53	102.41	110.70
47	A	2860	A	C2'-C3'-O3'	5.53	117.79	109.50
48	a	1364	G	O3'-P-O5'	-5.52	95.72	104.00
48	a	1448	G	O3'-P-O5'	-5.52	95.72	104.00
47	A	1379	U	C2'-C3'-O3'	-5.52	101.22	109.50
48	a	983	G	C4'-C3'-O3'	-5.51	104.74	113.00
47	A	2582	G	C1'-C2'-O2'	5.51	116.66	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	2524	G	O3'-P-O5'	-5.51	95.74	104.00
48	a	1361	C	O3'-P-O5'	-5.50	95.74	104.00
47	A	1279	C	O3'-P-O5'	-5.50	95.74	104.00
47	A	1755	C	O3'-P-O5'	-5.50	95.75	104.00
47	A	482	C	C4'-C3'-C2'	-5.50	97.10	102.60
47	A	116	G	O3'-P-O5'	-5.50	95.76	104.00
47	A	2003	C	O3'-P-O5'	-5.49	95.76	104.00
47	A	2725	U	C1'-C2'-O2'	-5.49	100.17	108.40
47	A	650	U	C3'-C2'-O2'	5.49	118.93	110.70
48	a	814	C	C4'-C3'-O3'	-5.49	104.77	113.00
47	A	1437	C	O3'-P-O5'	-5.48	95.78	104.00
47	A	2045	U	O3'-P-O5'	5.48	112.22	104.00
47	A	1888	A	O3'-P-O5'	-5.48	95.78	104.00
48	a	1433	U	O3'-P-O5'	-5.48	95.78	104.00
47	A	2773	G	O3'-P-O5'	-5.48	95.78	104.00
48	a	1240	G	O3'-P-O5'	-5.48	95.78	104.00
47	A	2506	C	C4'-C3'-O3'	-5.48	104.79	113.00
47	A	2342	C	O3'-P-O5'	-5.47	95.79	104.00
47	A	795	G	C4'-C3'-O3'	-5.47	104.80	113.00
48	a	172	U	O3'-P-O5'	-5.47	95.80	104.00
9	B	70	G	O3'-P-O5'	-5.47	95.80	104.00
47	A	2418	G	C4'-C3'-O3'	-5.47	104.80	113.00
47	A	1339	A	P-O3'-C3'	5.46	128.40	120.20
47	A	2225	C	O3'-P-O5'	-5.46	95.81	104.00
48	a	36	C	O3'-P-O5'	-5.46	95.81	104.00
9	B	46	A	C4'-C3'-O3'	-5.46	104.82	113.00
48	a	1065	A	O3'-P-O5'	-5.46	95.82	104.00
47	A	1600	G	O3'-P-O5'	-5.45	95.82	104.00
48	a	1413	C	O3'-P-O5'	-5.45	95.82	104.00
47	A	1653	A	C2'-C3'-O3'	5.45	117.67	109.50
47	A	2415	U	C4'-C3'-O3'	-5.45	104.83	113.00
47	A	1999	A	C2'-C3'-O3'	5.45	117.67	109.50
47	A	2769	A	C3'-C2'-O2'	5.44	118.86	110.70
47	A	1065	U	C4'-C3'-O3'	-5.44	104.84	113.00
47	A	2458	G	C4'-C3'-O3'	-5.44	104.84	113.00
47	A	655	C	O3'-P-O5'	-5.44	95.84	104.00
47	A	774	A	O3'-P-O5'	-5.44	95.84	104.00
47	A	1006	A	O3'-P-O5'	5.44	112.16	104.00
48	a	1373	U	O3'-P-O5'	-5.44	95.84	104.00
47	A	793	U	O3'-P-O5'	-5.44	95.84	104.00
47	A	851	A	O3'-P-O5'	-5.44	95.84	104.00
47	A	1651	G	C2'-C3'-O3'	-5.44	105.55	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	1613	C	C2'-C3'-O3'	5.43	117.65	109.50
47	A	2725	U	C3'-C2'-O2'	5.43	118.85	110.70
47	A	1740	G	O3'-P-O5'	-5.43	95.85	104.00
47	A	620	U	C4'-C3'-O3'	-5.43	104.86	113.00
47	A	2457	G	O3'-P-O5'	-5.43	95.86	104.00
47	A	2027	A	C4'-C3'-C2'	-5.43	97.17	102.60
47	A	2714	G	C3'-C2'-O2'	5.43	118.84	110.70
47	A	1294	A	C4'-C3'-O3'	-5.42	104.86	113.00
47	A	1306	G	C2'-C3'-O3'	5.42	117.64	109.50
47	A	1385	G	O3'-P-O5'	-5.42	95.86	104.00
9	B	47	C	O3'-P-O5'	-5.42	95.87	104.00
48	a	393	U	O3'-P-O5'	-5.42	95.87	104.00
47	A	787	C	O3'-P-O5'	-5.42	95.87	104.00
47	A	2754	A	P-O3'-C3'	5.42	128.33	120.20
47	A	1516	A	C4'-C3'-O3'	-5.42	104.88	113.00
47	A	612	U	C3'-C2'-O2'	5.41	118.82	110.70
47	A	1935	G	O3'-P-O5'	-5.41	95.88	104.00
48	a	282	A	O3'-P-O5'	-5.41	95.88	104.00
48	a	308	A	O3'-P-O5'	-5.41	95.88	104.00
47	A	747	G	C2'-C3'-O3'	5.41	121.81	113.70
47	A	1173	A	O3'-P-O5'	-5.40	95.90	104.00
47	A	2666	U	C4'-C3'-O3'	-5.40	104.90	113.00
47	A	2870	G	O3'-P-O5'	5.40	112.09	104.00
48	a	518	A	O3'-P-O5'	-5.39	95.91	104.00
47	A	640	U	O3'-P-O5'	-5.39	95.91	104.00
47	A	711	U	O3'-P-O5'	-5.39	95.92	104.00
47	A	2354	G	O3'-P-O5'	-5.38	95.93	104.00
47	A	2530	C	O3'-P-O5'	-5.38	95.93	104.00
46	v	31	A	O3'-P-O5'	-5.38	95.94	104.00
47	A	123	G	C4'-C3'-O3'	-5.38	104.93	113.00
47	A	2413	G	O3'-P-O5'	-5.38	95.93	104.00
47	A	987	A	C2'-C3'-O3'	-5.37	105.64	113.70
47	A	1266	A	O3'-P-O5'	-5.37	95.94	104.00
47	A	2050	G	C4'-C3'-O3'	5.37	117.46	109.40
47	A	1033	C	C3'-C2'-O2'	5.37	118.75	110.70
48	a	1212	C	O3'-P-O5'	-5.37	95.95	104.00
47	A	1200	G	C4'-C3'-O3'	-5.37	104.95	113.00
47	A	2519	G	O3'-P-O5'	-5.37	95.95	104.00
47	A	2015	G	O3'-P-O5'	-5.36	95.96	104.00
47	A	2099	G	C4'-C3'-C2'	-5.36	97.24	102.60
48	a	1197	A	O3'-P-O5'	-5.36	95.97	104.00
24	S	83	LYS	CB-CA-C	5.35	118.86	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	574	A	C4'-C3'-O3'	-5.35	104.97	113.00
47	A	831	U	O3'-P-O5'	-5.35	95.97	104.00
47	A	2001	G	O5'-C5'-C4'	-5.35	103.47	111.50
47	A	2764	G	C1'-C2'-O2'	5.35	116.43	108.40
47	A	2745	U	C4'-C3'-O3'	-5.35	104.98	113.00
47	A	2749	U	C1'-C2'-O2'	5.35	116.42	108.40
48	a	52	A	O3'-P-O5'	-5.35	95.98	104.00
47	A	1007	G	C1'-C2'-O2'	-5.34	103.78	111.80
48	a	1192	U	C4'-C3'-O3'	-5.34	104.98	113.00
47	A	125	A	C4'-C3'-O3'	-5.34	104.99	113.00
47	A	1788	A	O3'-P-O5'	-5.34	95.99	104.00
47	A	2468	A	P-O3'-C3'	5.34	128.21	120.20
48	a	799	A	O3'-P-O5'	-5.34	95.99	104.00
47	A	1819	C	C4'-C3'-O3'	-5.34	104.99	113.00
47	A	1315	G	C4'-C3'-O3'	-5.33	105.00	113.00
47	A	2085	G	O3'-P-O5'	-5.33	96.00	104.00
47	A	2744	C	O3'-P-O5'	-5.33	96.00	104.00
47	A	1542	A	C4'-C3'-O3'	5.33	121.00	113.00
47	A	871	G	C3'-C2'-O2'	5.33	118.69	110.70
47	A	1189	A	C3'-C2'-O2'	-5.33	106.61	114.60
47	A	2412	G	O3'-P-O5'	-5.33	96.01	104.00
47	A	1235	A	O3'-P-O5'	-5.32	96.02	104.00
47	A	2058	G	O3'-P-O5'	-5.32	96.02	104.00
48	a	385	G	C4'-C3'-O3'	-5.32	105.02	113.00
48	a	981	G	O3'-P-O5'	-5.32	96.02	104.00
47	A	623	A	C4'-C3'-O3'	-5.31	105.04	113.00
16	K	12	ASP	CA-CB-CG	5.30	117.91	112.60
47	A	88	G	C4'-C3'-O3'	-5.30	105.05	113.00
47	A	2334	U	C4'-C3'-O3'	-5.30	105.05	113.00
48	a	640	G	O3'-P-O5'	-5.30	96.05	104.00
47	A	2543	U	O3'-P-O5'	-5.30	96.06	104.00
47	A	2605	G	C2'-C3'-O3'	-5.30	105.75	113.70
48	a	785	G	C4'-C3'-O3'	-5.29	105.06	113.00
47	A	303	G	O3'-P-O5'	-5.29	96.06	104.00
47	A	861	C	C2'-C3'-O3'	-5.29	105.77	113.70
47	A	1366	C	C2'-C3'-O3'	5.29	121.63	113.70
47	A	1386	G	C4'-C3'-C2'	-5.29	97.31	102.60
47	A	1675	A	C1'-C2'-O2'	5.28	116.32	108.40
48	a	1537	C	O3'-P-O5'	-5.28	96.08	104.00
47	A	1260	A	O3'-P-O5'	-5.28	96.09	104.00
47	A	258	A	C2'-C3'-O3'	-5.27	105.79	113.70
47	A	2904	A	P-O3'-C3'	5.27	128.11	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	825	G	C4'-C3'-O3'	-5.27	105.09	113.00
47	A	2016	G	C4'-C3'-O3'	-5.27	105.10	113.00
47	A	2810	A	O3'-P-O5'	-5.27	96.10	104.00
48	a	279	C	O3'-P-O5'	-5.26	96.10	104.00
48	a	959	A	O3'-P-O5'	-5.26	96.10	104.00
47	A	141	U	O3'-P-O5'	-5.26	96.11	104.00
47	A	1829	C	C1'-C2'-O2'	-5.26	103.91	111.80
47	A	2832	G	O3'-P-O5'	-5.26	96.11	104.00
10	C	238	ARG	CG-CD-NE	-5.25	100.44	112.00
47	A	1949	C	C3'-C2'-O2'	5.25	118.58	110.70
47	A	2087	A	C2'-C3'-O3'	-5.25	105.82	113.70
48	a	820	C	C4'-C3'-O3'	-5.25	105.12	113.00
47	A	1180	C	O3'-P-O5'	-5.25	96.13	104.00
47	A	2291	U	C1'-C2'-O2'	5.25	116.27	108.40
47	A	827	G	C2'-C3'-O3'	-5.24	105.83	113.70
48	a	801	A	C3'-C2'-C1'	-5.24	96.26	101.50
47	A	1294	A	O3'-P-O5'	-5.24	96.14	104.00
47	A	2704	A	C3'-C2'-O2'	5.24	118.56	110.70
48	a	524	G	O3'-P-O5'	-5.24	96.14	104.00
48	a	572	A	O3'-P-O5'	-5.24	96.14	104.00
47	A	802	G	O3'-P-O5'	-5.24	96.15	104.00
48	a	774	G	O3'-P-O5'	-5.24	96.15	104.00
47	A	132	C	O3'-P-O5'	-5.23	96.15	104.00
48	a	931	U	C2'-C3'-O3'	-5.23	105.85	113.70
47	A	1804	U	C1'-C2'-O2'	-5.23	100.56	108.40
47	A	780	G	O3'-P-O5'	-5.22	96.17	104.00
47	A	2051	U	O3'-P-O5'	-5.22	96.17	104.00
48	a	361	A	O3'-P-O5'	-5.22	96.17	104.00
48	a	778	G	C4'-C3'-O3'	-5.22	105.17	113.00
47	A	2531	G	C4'-C3'-O3'	-5.22	105.17	113.00
47	A	1002	G	C4'-C3'-O3'	-5.21	105.18	113.00
48	a	1235	C	O3'-P-O5'	-5.21	96.18	104.00
47	A	2048	U	C3'-C2'-O2'	5.21	118.51	110.70
16	K	70	ARG	CB-CA-C	5.20	118.39	109.80
47	A	1695	A	O3'-P-O5'	-5.20	96.19	104.00
9	B	47	C	C4'-C3'-O3'	-5.20	105.20	113.00
19	N	55	ASP	CA-CB-CG	5.20	117.80	112.60
47	A	9	U	C4'-C3'-O3'	-5.20	105.20	113.00
47	A	1385	G	C3'-C2'-O2'	5.20	118.50	110.70
47	A	2362	A	O3'-P-O5'	-5.20	96.20	104.00
47	A	373	A	C2'-C3'-O3'	5.20	117.29	109.50
48	a	1045	G	O3'-P-O5'	5.19	111.79	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	2333	G	C4'-C3'-O3'	-5.19	105.21	113.00
47	A	2738	G	O3'-P-O5'	-5.19	96.21	104.00
47	A	1288	G	O3'-P-O5'	-5.19	96.22	104.00
47	A	2061	G	O3'-P-O5'	-5.19	96.22	104.00
47	A	1649	C	C4'-C3'-O3'	-5.18	105.22	113.00
47	A	1777	G	O3'-P-O5'	-5.18	96.22	104.00
48	a	1335	U	O3'-P-O5'	-5.18	96.22	104.00
47	A	1182	G	P-O5'-C5'	-5.18	113.14	120.90
46	v	33	U	O3'-P-O5'	-5.17	96.25	104.00
46	v	73	A	O3'-P-O5'	-5.17	96.25	104.00
47	A	2049	A	O3'-P-O5'	-5.17	96.25	104.00
47	A	2353	U	C4'-C3'-O3'	-5.17	105.25	113.00
47	A	1677	A	O3'-P-O5'	-5.16	96.25	104.00
48	a	530	G	O3'-P-O5'	-5.16	96.25	104.00
11	D	139	TYR	N-CA-CB	-5.16	102.46	110.87
47	A	1379	U	O3'-P-O5'	-5.16	96.26	104.00
47	A	617	G	OP2-P-O3'	5.16	123.47	108.00
47	A	228	C	C4'-C3'-C2'	-5.15	97.45	102.60
47	A	2296	A	N9-C1'-C2'	5.15	119.73	112.00
47	A	228	C	O3'-P-O5'	-5.15	96.28	104.00
47	A	526	A	O3'-P-O5'	-5.15	96.28	104.00
9	B	52	G	O3'-P-O5'	-5.15	96.28	104.00
46	v	20	U	C2'-C3'-O3'	5.15	117.22	109.50
47	A	342	A	C4'-C3'-O3'	-5.15	105.28	113.00
47	A	797	A	C4'-C3'-O3'	-5.14	105.28	113.00
48	a	1102	A	O3'-P-O5'	-5.14	96.28	104.00
47	A	1703	C	C4'-C3'-O3'	-5.14	105.29	113.00
47	A	2400	G	O3'-P-O5'	-5.14	96.28	104.00
47	A	484	C	O3'-P-O5'	-5.14	96.29	104.00
47	A	2652	G	O5'-C5'-C4'	-5.14	103.79	111.50
47	A	959	C	O3'-P-O5'	5.14	111.71	104.00
48	a	11	G	O3'-P-O5'	-5.14	96.29	104.00
48	a	1406	C	C2'-C3'-O3'	5.13	117.20	109.50
48	a	750	G	O3'-P-O5'	-5.13	96.30	104.00
48	a	740	G	O3'-P-O5'	-5.13	96.31	104.00
47	A	612	U	C1'-C2'-O2'	-5.13	100.71	108.40
47	A	1246	G	C4'-C3'-C2'	-5.13	97.47	102.60
48	a	1420	C	O3'-P-O5'	-5.13	96.31	104.00
47	A	244	A	O3'-P-O5'	-5.12	96.31	104.00
47	A	1416	G	O3'-P-O5'	-5.12	96.31	104.00
47	A	2711	G	C1'-C2'-O2'	5.12	116.09	108.40
48	a	1096	U	O3'-P-O5'	-5.12	96.31	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	a	262	G	O3'-P-O5'	-5.12	96.32	104.00
48	a	576	G	O3'-P-O5'	-5.12	96.33	104.00
47	A	2261	C	C3'-C2'-O2'	5.12	118.37	110.70
47	A	2609	U	C4'-C3'-O3'	-5.12	105.33	113.00
47	A	544	G	O3'-P-O5'	-5.11	96.33	104.00
47	A	1534	A	O3'-P-O5'	-5.11	96.33	104.00
47	A	2569	C	O4'-C4'-C3'	-5.11	98.89	104.00
47	A	2731	G	O3'-P-O5'	-5.11	96.34	104.00
47	A	258	A	O5'-P-OP1	-5.11	92.68	108.00
47	A	545	U	C4'-C3'-O3'	-5.11	105.34	113.00
47	A	2770	A	C3'-C2'-O2'	5.11	118.36	110.70
47	A	1481	G	C4'-C3'-O3'	-5.10	105.35	113.00
47	A	267	C	O3'-P-O5'	-5.10	96.35	104.00
47	A	2053	C	C4'-C3'-O3'	-5.10	105.35	113.00
48	a	578	C	O3'-P-O5'	-5.10	96.35	104.00
25	T	75	ARG	CB-CA-C	5.10	118.36	109.65
47	A	1387	G	C3'-C2'-O2'	5.09	118.34	110.70
47	A	116	G	C4'-C3'-O3'	-5.09	105.36	113.00
47	A	1055	A	C2'-C3'-O3'	5.09	121.34	113.70
47	A	1352	U	O4'-C4'-C3'	-5.09	98.91	104.00
47	A	2072	C	O5'-P-OP2	-5.09	92.72	108.00
47	A	773	G	O3'-P-O5'	-5.09	96.36	104.00
12	E	90	PHE	CB-CA-C	-5.09	104.66	111.89
47	A	158	C	O3'-P-O5'	-5.09	96.37	104.00
30	c	33	HIS	CA-CB-CG	-5.09	108.71	113.80
47	A	1757	G	O4'-C1'-C2'	-5.09	100.71	105.80
47	A	611	U	C4'-C3'-O3'	-5.08	105.38	113.00
48	a	193	G	O3'-P-O5'	-5.08	96.38	104.00
47	A	795	G	C1'-O4'-C4'	-5.08	104.83	109.90
48	a	511	C	O3'-P-O5'	-5.07	96.39	104.00
48	a	1294	A	O3'-P-O5'	-5.07	96.40	104.00
47	A	1398	A	C4'-C3'-O3'	-5.07	105.40	113.00
48	a	1402	U	O3'-P-O5'	-5.07	96.40	104.00
47	A	1782	G	C3'-C2'-O2'	5.06	118.30	110.70
47	A	2397	C	O3'-P-O5'	-5.06	96.41	104.00
47	A	2735	A	C1'-C2'-O2'	5.06	115.99	108.40
48	a	142	A	O3'-P-O5'	-5.06	96.42	104.00
47	A	224	A	O3'-P-O5'	-5.05	96.42	104.00
48	a	1441	G	O3'-P-O5'	-5.05	96.42	104.00
48	a	575	G	O3'-P-O5'	-5.05	96.42	104.00
47	A	2514	G	O3'-P-O5'	-5.05	96.43	104.00
48	a	650	A	O3'-P-O5'	-5.05	96.43	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	a	1328	A	C2'-C3'-O3'	5.04	117.07	109.50
47	A	1771	C	C4'-C3'-O3'	-5.04	105.44	113.00
47	A	44	A	O3'-P-O5'	-5.04	96.44	104.00
47	A	250	G	C4'-C3'-O3'	-5.04	105.44	113.00
47	A	1305	A	C3'-C2'-O2'	-5.04	107.04	114.60
47	A	1807	U	C4'-C3'-O3'	-5.03	105.46	113.00
47	A	1340	A	C2'-C3'-O3'	5.02	117.03	109.50
47	A	1475	G	O3'-P-O5'	-5.02	96.47	104.00
47	A	1514	C	O4'-C4'-C3'	-5.02	98.98	104.00
47	A	2117	A	C3'-C2'-O2'	5.02	118.23	110.70
48	a	209	A	O3'-P-O5'	-5.02	96.47	104.00
47	A	443	G	O3'-P-O5'	-5.02	96.47	104.00
47	A	1047	A	C3'-C2'-O2'	5.02	118.22	110.70
48	a	971	U	C4'-C3'-C2'	-5.02	97.58	102.60
47	A	2259	G	O3'-P-O5'	5.01	111.52	104.00
48	a	765	C	O3'-P-O5'	-5.01	96.48	104.00
48	a	132	U	O3'-P-O5'	-5.01	96.48	104.00
47	A	2805	A	P-O3'-C3'	5.01	127.71	120.20
47	A	522	U	O3'-P-O5'	-5.00	96.49	104.00
47	A	578	A	O5'-C5'-C4'	-5.00	104.20	111.70
47	A	1969	U	O3'-P-O5'	-5.00	96.49	104.00
46	v	12	U	O3'-P-O5'	-5.00	96.50	104.00
47	A	51	G	O3'-P-O5'	-5.00	96.50	104.00
47	A	1526	G	O3'-P-O5'	-5.00	96.50	104.00

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	41	ARG	Sidechain
1	0	6	ARG	Sidechain
3	2	36	ARG	Sidechain
5	4	19	ARG	Sidechain
51	8	211	ARG	Sidechain
47	A	2066	A	Sidechain
47	A	2546	C	Sidechain
47	A	510	G	Sidechain
47	A	558	G	Sidechain
10	C	13	ARG	Sidechain
10	C	14	ARG	Sidechain
10	C	156	ARG	Sidechain
10	C	238	ARG	Sidechain

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Mol	Chain	Res	Type	Group
10	C	243	ARG	Sidechain
10	C	43	ARG	Sidechain
11	D	57	ARG	Sidechain
12	E	168	ARG	Sidechain
12	E	41	ARG	Sidechain
17	L	60	ARG	Sidechain
18	M	18	ARG	Sidechain
19	N	107	ARG	Sidechain
19	N	108	ARG	Sidechain
20	O	30	ARG	Sidechain
20	O	35	ARG	Sidechain
21	P	104	ARG	Sidechain
21	P	51	ARG	Sidechain
21	P	94	ARG	Sidechain
22	Q	51	ARG	Sidechain
23	R	67	ARG	Sidechain
23	R	7	THR	Peptide
24	S	11	ARG	Sidechain
24	S	8	ARG	Sidechain
52	W	47	ARG	Sidechain
52	W	77	PHE	Peptide
53	d	41	ARG	Sidechain
34	h	21	ARG	Sidechain
35	i	12	ARG	Sidechain
35	i	130	ARG	Sidechain
36	j	62	ARG	Sidechain
50	s	78	ARG	Sidechain
45	t	74	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	432	0	450	4	0
2	1	403	0	414	0	0
3	2	368	0	410	0	0
4	3	512	0	564	3	0
5	4	297	0	339	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	5	346	0	345	0	0
7	6	356	0	346	0	0
8	7	187	0	94	0	0
9	B	2392	0	1213	1	0
10	C	2093	0	2179	9	0
11	D	1575	0	1642	10	0
12	E	1567	0	1652	2	0
13	F	1405	0	1467	3	0
14	G	1342	0	1388	0	0
15	J	1142	0	1182	9	0
16	K	921	0	977	6	0
17	L	1082	0	1132	2	0
18	M	1076	0	1145	5	0
19	N	954	0	983	9	0
20	O	913	0	947	1	0
21	P	937	0	1008	2	0
22	Q	950	0	1018	5	0
23	R	795	0	838	2	0
24	S	850	0	911	3	0
25	T	733	0	781	1	0
26	U	770	0	825	0	0
27	X	467	0	512	2	0
28	Y	540	0	581	0	0
29	Z	456	0	491	1	0
30	c	1608	0	1646	1	0
31	e	1219	0	1300	0	0
32	f	765	0	765	0	0
33	g	1199	0	1256	0	0
34	h	1030	0	1086	1	0
35	i	997	0	1033	5	0
36	j	788	0	832	3	0
37	k	839	0	851	0	0
38	l	1045	0	1104	2	0
39	m	943	0	1008	4	0
40	n	498	0	529	2	0
41	o	730	0	759	0	0
42	p	691	0	718	0	0
43	q	693	0	734	0	0
44	r	522	0	558	0	0
45	t	658	0	715	0	0
46	v	1622	0	820	1	0
47	A	58630	0	29517	162	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	a	32391	0	16310	52	0
49	b	1564	0	1625	3	0
50	s	668	0	682	3	0
51	8	1450	0	1038	1	0
52	W	629	0	644	1	0
53	d	1604	0	1638	0	0
54	0	1	0	0	0	0
54	4	1	0	0	0	0
54	6	1	0	0	0	0
54	n	1	0	0	0	0
All	All	138648	0	93002	273	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 1.

All (273) 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)
47:A:2027:A:O2'	47:A:2753:U:O2'	2.02	0.72
1:0:15:LEU:O	1:0:18:THR:HG23	1.90	0.70
47:A:2569:C:O2'	47:A:2769:A:N3	2.30	0.63
10:C:150:LYS:NZ	47:A:1830:G:OP2	2.31	0.63
47:A:1066:A:N1	47:A:1187:U:O2'	2.30	0.62
47:A:2229:C:O2	47:A:2255:C:N4	2.33	0.61
47:A:656:A:H2	47:A:662:G:H22	1.48	0.61
48:a:1380:G:C6	48:a:1381:U:C4	2.89	0.61
47:A:892:U:HO2'	47:A:894:A:H2	1.47	0.59
47:A:2715:G:C5	47:A:2716:U:C4	2.91	0.58
15:J:38:ARG:NH1	47:A:1053:C:OP1	2.36	0.58
4:3:39:LYS:NZ	47:A:2394:G:N7	2.52	0.58
18:M:34:ILE:HD11	18:M:129:THR:HG21	1.86	0.58
35:i:117:GLY:N	48:a:1376:C:OP1	2.35	0.57
48:a:778:G:H4'	48:a:1523:A:H4'	1.87	0.57
38:l:100:VAL:HG11	38:l:103:LEU:HD12	1.87	0.57
47:A:1074:A:N3	47:A:2515:G:O2'	2.32	0.57
47:A:2767:A:C2	47:A:2768:U:H1'	2.40	0.57
38:l:128:SER:OG	48:a:37:G:N3	2.38	0.56
47:A:1028:C:O2	47:A:1028:C:O5'	2.24	0.56
47:A:2752:C:C4	47:A:2753:U:C5	2.93	0.56
48:a:1444:G:H2'	48:a:1445:U:C6	2.40	0.56
47:A:747:G:O2'	47:A:1677:A:N3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:A:2231:C:O2'	47:A:2233:C:OP1	2.24	0.55
11:D:191:ASN:OD1	11:D:191:ASN:N	2.40	0.55
48:a:514:G:H5''	48:a:543:U:H2'	1.88	0.55
16:K:23:LYS:NZ	47:A:2590:A:N3	2.52	0.55
17:L:17:ASN:HD21	17:L:27:ASN:HD22	1.54	0.54
48:a:985:A:N1	48:a:1375:C:O2'	2.39	0.54
10:C:63:ARG:NH2	47:A:1616:G:OP2	2.41	0.54
50:s:36:ARG:NH2	50:s:75:ALA:O	2.40	0.54
11:D:191:ASN:HD22	47:A:2709:C:H1'	1.72	0.54
47:A:614:G:H2'	47:A:2059:A:N7	2.22	0.54
47:A:2733:C:C4	47:A:2734:A:C5	2.96	0.54
48:a:1072:U:H2'	48:a:1073:C:C6	2.42	0.54
16:K:63:VAL:HG12	16:K:106:LEU:HD11	1.90	0.53
47:A:790:A:O2'	47:A:1704:U:OP1	2.26	0.53
47:A:2752:C:N4	47:A:2753:U:C4	2.77	0.53
4:3:31:HIS:HE1	47:A:2421:A:OP2	1.91	0.53
47:A:1542:A:O2'	47:A:1544:C:N4	2.42	0.52
47:A:2055:U:H2'	47:A:2056:G:O4'	2.10	0.52
18:M:101:LYS:NZ	47:A:954:U:O3'	2.43	0.52
48:a:1329:C:O2	50:s:36:ARG:NH1	2.43	0.52
47:A:2467:U:O3'	47:A:2468:A:H3'	2.10	0.52
15:J:111:PRO:O	15:J:116:GLY:HA3	2.09	0.51
48:a:969:A:C2	48:a:1231:G:O4'	2.63	0.51
15:J:54:HIS:HA	15:J:122:LYS:HB3	1.93	0.51
47:A:1825:U:H2'	47:A:1826:C:C6	2.44	0.51
19:N:66:ILE:CD1	19:N:83:LEU:HD22	2.41	0.51
47:A:1968:U:OP1	47:A:2633:U:O2'	2.29	0.51
47:A:2715:G:C6	47:A:2716:U:N3	2.78	0.51
39:m:16:VAL:HG13	39:m:34:LEU:HD12	1.92	0.51
48:a:1379:G:C2	48:a:1380:G:C8	2.99	0.51
48:a:1380:G:C5	48:a:1381:U:C5	2.99	0.51
47:A:1245:G:C5'	47:A:1245:G:N3	2.74	0.51
35:i:130:ARG:NH2	46:v:33:U:OP2	2.43	0.50
47:A:2009:G:O2'	47:A:2011:U:OP2	2.28	0.50
10:C:142:HIS:CE1	10:C:191:SER:OG	2.64	0.50
47:A:1995:A:N3	47:A:2621:G:O2'	2.43	0.50
47:A:647:A:N1	47:A:671:G:O2'	2.39	0.50
47:A:1072:A:OP2	47:A:1180:C:O2'	2.26	0.50
47:A:2806:G:OP2	47:A:2810:A:O2'	2.23	0.50
48:a:1107:C:H2'	48:a:1108:C:C6	2.46	0.50
19:N:41:ARG:NH1	47:A:2906:U:O2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:m:105:ASN:ND2	48:a:959:A:N7	2.61	0.49
47:A:482:C:O2'	47:A:483:C:O5'	2.30	0.49
47:A:903:G:H2'	47:A:904:A:C8	2.46	0.49
18:M:54:MET:HE2	18:M:121:ALA:CB	2.42	0.49
48:a:1106:C:H2'	48:a:1107:C:O4'	2.12	0.49
19:N:10:SER:HA	19:N:13:ARG:NH2	2.28	0.49
47:A:1527:C:H3'	47:A:1528:U:H5''	1.95	0.49
47:A:1961:A:H2'	47:A:1962:G:O4'	2.13	0.49
48:a:1355:A:C8	48:a:1357:U:C2	3.01	0.49
47:A:1759:U:HO2'	47:A:1760:A:H8	1.59	0.49
11:D:153:ARG:HA	47:A:2081:G:N3	2.28	0.48
23:R:76:TYR:OH	47:A:608:C:OP1	2.28	0.48
47:A:576:G:N3	47:A:576:G:H2'	2.28	0.48
47:A:1367:G:H2'	47:A:1369:C:C5	2.48	0.48
47:A:1779:G:N3	47:A:2885:A:H2	2.11	0.48
47:A:1379:U:C5	47:A:1648:A:C8	3.00	0.48
18:M:54:MET:HE1	18:M:104:PHE:CG	2.48	0.48
48:a:1078:G:N7	48:a:1104:G:O2'	2.44	0.48
36:j:10:LEU:HB3	36:j:18:LEU:HD11	1.94	0.48
47:A:199:A:O2'	47:A:852:G:O6	2.18	0.48
47:A:1425:C:O2'	47:A:1516:A:N3	2.44	0.48
35:i:65:VAL:HG11	35:i:79:ILE:HG12	1.95	0.48
36:j:6:ILE:HB	36:j:76:ILE:HB	1.96	0.48
47:A:662:G:O5'	47:A:662:G:C8	2.67	0.48
15:J:36:ILE:HD11	15:J:141:TYR:CZ	2.49	0.48
21:P:86:VAL:HG11	21:P:89:TYR:CE1	2.49	0.48
48:a:589:C:H2'	48:a:590:G:O4'	2.14	0.48
27:X:12:THR:HG21	47:A:1404:A:OP1	2.14	0.48
16:K:24:VAL:HG13	16:K:33:ALA:HB2	1.96	0.47
47:A:1941:A:N7	48:a:1505:U:H1'	2.29	0.47
48:a:673:G:H22	48:a:750:G:H1	1.62	0.47
30:c:140:THR:HG21	30:c:148:ILE:HD12	1.95	0.47
47:A:655:C:H42	47:A:663:A:H61	1.63	0.47
49:b:35:ARG:HB2	49:b:40:ILE:HD11	1.95	0.47
47:A:45:G:H21	47:A:183:A:H61	1.61	0.47
35:i:18:ARG:NH1	48:a:1156:C:O2	2.48	0.47
19:N:45:GLU:OE2	47:A:2864:G:O2'	2.30	0.47
47:A:598:U:H2'	47:A:599:G:O4'	2.15	0.47
47:A:1033:C:O2'	47:A:1046:A:N3	2.47	0.47
20:O:56:ALA:HB3	20:O:81:VAL:HB	1.95	0.47
47:A:662:G:O5'	47:A:662:G:H8	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:A:1411:U:O2'	47:A:2241:A:H8	1.97	0.47
48:a:1366:A:H2'	48:a:1367:U:C6	2.49	0.47
13:F:131:GLY:HA3	47:A:2334:U:H5''	1.97	0.47
19:N:12:GLN:HG2	47:A:1314:A:N7	2.29	0.47
47:A:1883:A:H2'	47:A:1884:G:O4'	2.15	0.47
47:A:1426:A:H2'	47:A:1427:G:O4'	2.15	0.46
48:a:224:U:H2'	48:a:225:A:C8	2.50	0.46
50:s:50:ALA:HB1	50:s:57:HIS:HB3	1.97	0.46
47:A:2715:G:C6	47:A:2716:U:C4	3.04	0.46
47:A:2817:C:O2'	47:A:2834:A:N3	2.41	0.46
47:A:656:A:H2	47:A:662:G:N2	2.14	0.46
15:J:45:TYR:CD2	22:Q:63:THR:HG21	2.50	0.46
22:Q:31:LEU:HB2	22:Q:34:VAL:HG22	1.98	0.46
24:S:42:ALA:HB2	47:A:2039:G:H5''	1.97	0.46
15:J:38:ARG:NH1	47:A:1053:C:H5''	2.30	0.46
47:A:1807:U:H2'	47:A:1813:A:N6	2.31	0.46
24:S:82:LEU:HB2	24:S:98:LYS:HB2	1.98	0.46
10:C:210:ARG:NE	47:A:1614:A:OP1	2.49	0.46
10:C:243:ARG:HH22	47:A:2268:G:P	2.39	0.45
47:A:494:A:O2'	47:A:520:G:N7	2.40	0.45
47:A:617:G:O2'	47:A:618:A:H3'	2.16	0.45
29:Z:13:ILE:HD11	47:A:1035:G:C8	2.52	0.45
47:A:1755:C:O2'	47:A:2883:C:N3	2.49	0.45
47:A:2092:C:O2	47:A:2479:A:N1	2.49	0.45
48:a:1365:G:H2'	48:a:1366:A:C8	2.52	0.45
11:D:63:LYS:N	11:D:64:PRO:CD	2.79	0.45
47:A:1363:G:C6	47:A:1367:G:C6	3.04	0.45
47:A:1788:A:O2'	47:A:2743:G:H1'	2.16	0.45
1:O:3:VAL:HG12	47:A:2044:A:C2	2.52	0.45
10:C:145:GLU:HB2	10:C:188:CYS:HB3	1.98	0.45
12:E:46:GLN:NE2	47:A:488:U:O2'	2.50	0.45
47:A:2768:U:C5	47:A:2792:G:C5	3.04	0.45
48:a:331:U:H2'	48:a:332:G:O4'	2.15	0.45
19:N:40:LEU:HD23	19:N:117:ILE:HG21	1.99	0.45
47:A:2094:C:H4'	47:A:2280:OMG:HM22	1.99	0.45
48:a:955:G:C2	48:a:956:A:C8	3.05	0.45
1:O:11:VAL:HG22	47:A:17:G:H5''	1.99	0.45
27:X:55:LYS:HE2	47:A:446:G:OP2	2.17	0.45
47:A:957:A:H2'	47:A:958:A:C8	2.51	0.45
48:a:1187:G:N2	48:a:1189:A:H3'	2.31	0.45
5:4:5:PRO:HD2	47:A:2495:C:OP1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:A:352:G:H2'	47:A:353:A:C8	2.51	0.45
47:A:1653:A:O2'	47:A:1655:A:OP2	2.31	0.45
47:A:2084:C:H2'	47:A:2533:U:H4'	1.99	0.45
47:A:2604:C:O2'	47:A:2607:G:N7	2.49	0.45
48:a:1380:G:C5	48:a:1381:U:C4	3.05	0.45
40:n:2:ALA:N	48:a:1212:C:OP1	2.50	0.44
47:A:1066:A:C2	47:A:1187:U:C2	3.06	0.44
47:A:1322:G:O2'	47:A:1324:G:N7	2.46	0.44
47:A:2121:U:H4'	47:A:2122:G:O5'	2.17	0.44
11:D:126:HIS:ND1	11:D:159:LEU:HD13	2.33	0.44
16:K:28:SER:OG	47:A:2595:A:N1	2.41	0.44
47:A:2785:U:O2	47:A:2785:U:O5'	2.34	0.44
13:F:106:VAL:O	13:F:109:PRO:O	2.36	0.44
47:A:908:A:C2	47:A:964:A:C4	3.06	0.44
47:A:1485:A:H2	47:A:1600:G:H21	1.65	0.44
22:Q:58:ARG:HA	22:Q:61:TRP:CE3	2.53	0.44
47:A:340:U:H2'	47:A:341:G:O4'	2.17	0.44
47:A:1308:A:C2	47:A:2042:A:C4	3.06	0.44
48:a:332:G:N2	48:a:334:G:H3'	2.33	0.44
48:a:1234:A:H2'	48:a:1234:A:N3	2.33	0.44
49:b:186:ILE:HG23	49:b:202:ALA:HB3	2.00	0.44
47:A:876:A:N7	47:A:2277:C:H5'	2.33	0.44
47:A:2300:G:OP1	52:W:26:ALA:HB1	2.17	0.44
47:A:2360:G:O2'	47:A:2365:A:N1	2.41	0.44
47:A:247:A:C2	47:A:258:A:C4	3.06	0.43
47:A:1308:A:H2'	47:A:1309:G:O4'	2.18	0.43
48:a:107:A:C6	48:a:334:G:C6	3.06	0.43
4:3:26:HIS:HD2	4:3:46:LYS:O	2.01	0.43
15:J:38:ARG:HH11	47:A:1053:C:H5''	1.83	0.43
19:N:52:LYS:NZ	19:N:94:ARG:O	2.51	0.43
48:a:1440:C:H2'	48:a:1441:G:O4'	2.18	0.43
47:A:732:A:H1'	47:A:735:U:O4	2.18	0.43
47:A:1754:U:C2	47:A:1779:G:N2	2.87	0.43
1:0:18:THR:HG22	47:A:15:G:H4'	2.01	0.43
48:a:1400:U:H2'	48:a:1401:G:C8	2.53	0.43
48:a:1381:U:C4	48:a:1382:G:C4	3.07	0.43
39:m:98:ARG:NH2	48:a:1318:G:N7	2.66	0.43
47:A:482:C:O2'	47:A:483:C:P	2.77	0.43
47:A:892:U:O2'	47:A:894:A:H2	2.02	0.43
48:a:789:G:N2	48:a:810:U:C5	2.86	0.43
17:L:55:MET:HE3	47:A:2458:G:N7	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:A:2540:U:O4	47:A:2604:C:N3	2.51	0.43
48:a:382:A:C6	48:a:383:U:C4	3.07	0.43
48:a:790:A:H5'	48:a:791:A:OP2	2.18	0.43
11:D:62:ASN:HB2	47:A:2836:G:H5''	2.01	0.43
16:K:75:SER:OG	21:P:72:ARG:NH2	2.52	0.43
47:A:661:A:H3'	47:A:662:G:H8	1.84	0.43
47:A:1304:G:C6	47:A:1305:A:N6	2.87	0.43
47:A:2872:U:H2'	47:A:2873:G:O4'	2.19	0.43
47:A:2884:G:C6	47:A:2885:A:N6	2.86	0.43
13:F:66:VAL:N	13:F:88:LYS:O	2.52	0.42
23:R:5:ILE:HG22	23:R:38:VAL:HG22	2.01	0.42
47:A:2439:G:C2	47:A:2440:A:H1'	2.54	0.42
47:A:1377:G:O2'	47:A:1432:A:N1	2.44	0.42
47:A:1945:A:O2'	47:A:1946:U:P	2.77	0.42
47:A:2096:G:O2'	47:A:2098:G:H5'	2.19	0.42
48:a:62:A:N1	48:a:105:G:O2'	2.44	0.42
18:M:119:ARG:O	18:M:122:SER:OG	2.33	0.42
47:A:634:A:H2'	47:A:635:C:O4'	2.19	0.42
47:A:2767:A:N1	47:A:2768:U:C2	2.87	0.42
49:b:187:VAL:HG13	49:b:191:CYS:HB2	2.00	0.42
47:A:874:U:H2'	47:A:2097:U:C2	2.55	0.42
48:a:1377:G:C6	48:a:1378:C:C5	3.08	0.42
47:A:1363:G:N1	47:A:1367:G:C6	2.86	0.42
47:A:1713:A:O2'	47:A:1719:G:N7	2.42	0.42
47:A:2399:G:C6	47:A:2400:G:C6	3.07	0.42
5:4:6:SER:OG	47:A:2496:C:OP1	2.34	0.42
24:S:29:VAL:HB	24:S:55:ILE:HD11	2.01	0.42
47:A:661:A:H3'	47:A:662:G:C8	2.54	0.42
47:A:2321:U:H2'	47:A:2322:C:O4'	2.19	0.42
47:A:2438:G:C6	47:A:2439:G:C5	3.07	0.42
48:a:1514:G:H4'	48:a:1515:G:C4	2.55	0.42
47:A:151:U:H2'	47:A:152:C:O4'	2.19	0.42
47:A:1887:G:O2'	47:A:1912:G:N2	2.52	0.42
10:C:140:VAL:HG13	10:C:161:SER:HB2	2.01	0.42
47:A:854:U:O2'	47:A:2089:A:N1	2.52	0.41
47:A:2343:A:H2'	47:A:2344:U:C6	2.55	0.41
48:a:1045:G:H3'	48:a:1046:G:H5''	2.00	0.41
10:C:119:GLY:HA2	10:C:189:ARG:HH12	1.84	0.41
11:D:160:LEU:HB3	11:D:161:PRO:CD	2.49	0.41
15:J:93:MET:O	15:J:97:TYR:C	2.64	0.41
47:A:1021:A:H1'	47:A:1036:A:C2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:A:2435:C:H6	47:A:2435:C:H5'	1.84	0.41
48:a:456:A:C5	48:a:496:A:C2	3.09	0.41
35:i:109:ARG:NH1	48:a:1355:A:N3	2.68	0.41
47:A:1752:G:C2	47:A:1753:C:C2	3.08	0.41
47:A:1933:G:O2'	47:A:1957:A:N1	2.52	0.41
47:A:575:A:C2	47:A:2052:A:C8	3.08	0.41
11:D:187:LEU:N	11:D:187:LEU:HD12	2.35	0.41
16:K:22:ILE:HG23	47:A:1981:A:C2	2.56	0.41
36:j:50:THR:HG23	36:j:64:GLN:HG2	2.02	0.41
47:A:469:A:C6	47:A:470:A:C6	3.08	0.41
47:A:2320:U:H2'	47:A:2321:U:C6	2.56	0.41
47:A:2733:C:N4	47:A:2734:A:C6	2.89	0.41
48:a:16:U:O2'	48:a:18:A:N7	2.47	0.41
10:C:150:LYS:NZ	47:A:2233:C:OP2	2.50	0.41
47:A:2651:C:O2'	47:A:2850:G:N7	2.52	0.41
47:A:2895:C:C4	47:A:2896:U:C4	3.09	0.41
48:a:1314:G:O2'	48:a:1315:A:H8	2.04	0.41
39:m:102:SER:O	39:m:103:LYS:C	2.63	0.41
47:A:1387:G:H2'	47:A:1388:A:H5''	2.02	0.41
19:N:62:ALA:HB3	19:N:80:LEU:HD11	2.03	0.41
11:D:108:VAL:HG11	11:D:176:ILE:HD11	2.03	0.41
12:E:51:VAL:HG21	12:E:91:GLY:HA3	2.02	0.41
19:N:59:ARG:HA	19:N:84:PHE:CZ	2.56	0.41
22:Q:72:ASN:ND2	22:Q:107:ASN:OD1	2.49	0.41
25:T:59:TYR:OH	47:A:1379:U:OP2	2.29	0.41
48:a:1381:U:H2'	48:a:1382:G:O4'	2.21	0.41
47:A:2572:G:H21	47:A:2675:C:H5''	1.86	0.41
51:8:307:ASP:HA	51:8:310:ARG:HB3	2.03	0.41
9:B:104:G:H2'	9:B:105:A:O4'	2.20	0.40
22:Q:49:ASP:OD2	47:A:580:U:O2'	2.39	0.40
47:A:250:G:H4'	47:A:433:G:C5	2.56	0.40
47:A:732:A:O2'	47:A:820:U:O4	2.37	0.40
47:A:1444:C:H2'	47:A:1445:A:C8	2.56	0.40
47:A:2716:U:H2'	47:A:2717:G:O4'	2.20	0.40
48:a:99:A:C5	48:a:100:G:C8	3.09	0.40
48:a:1385:U:H2'	48:a:1386:A:C8	2.55	0.40
48:a:1113:C:H2'	48:a:1114:G:O4'	2.22	0.40
34:h:16:ASN:ND2	48:a:835:C:O2	2.55	0.40
47:A:482:C:O2'	47:A:483:C:O4'	2.39	0.40
47:A:2572:G:H2'	47:A:2573:G:O4'	2.21	0.40
40:n:27:CYS:SG	40:n:29:ARG:HB2	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:A:2731:G:C2	47:A:2732:C:C6	3.10	0.40
11:D:24:PRO:HB3	47:A:2711:G:C2	2.57	0.40
15:J:105:ALA:O	15:J:109:MET:HG3	2.21	0.40
47:A:2773:G:N7	47:A:2784:C:H1'	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	53/59 (90%)	48 (91%)	5 (9%)	0	100	100
2	1	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
3	2	42/44 (96%)	42 (100%)	0	0	100	100
4	3	62/66 (94%)	62 (100%)	0	0	100	100
5	4	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
6	5	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	6	44/66 (67%)	41 (93%)	2 (4%)	1 (2%)	5	4
10	C	271/277 (98%)	259 (96%)	12 (4%)	0	100	100
11	D	205/209 (98%)	194 (95%)	10 (5%)	1 (0%)	24	31
12	E	204/207 (99%)	198 (97%)	6 (3%)	0	100	100
13	F	176/179 (98%)	154 (88%)	20 (11%)	2 (1%)	11	13
14	G	173/179 (97%)	150 (87%)	23 (13%)	0	100	100
15	J	142/145 (98%)	138 (97%)	4 (3%)	0	100	100
16	K	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
17	L	144/146 (99%)	139 (96%)	4 (3%)	1 (1%)	18	23
18	M	133/144 (92%)	128 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	N	117/120 (98%)	108 (92%)	9 (8%)	0	100	100
20	O	118/120 (98%)	109 (92%)	8 (7%)	1 (1%)	16	20
21	P	112/115 (97%)	109 (97%)	2 (2%)	1 (1%)	14	17
22	Q	116/119 (98%)	113 (97%)	3 (3%)	0	100	100
23	R	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
24	S	108/113 (96%)	104 (96%)	4 (4%)	0	100	100
25	T	89/95 (94%)	87 (98%)	2 (2%)	0	100	100
26	U	100/103 (97%)	96 (96%)	4 (4%)	0	100	100
27	X	59/62 (95%)	57 (97%)	2 (3%)	0	100	100
28	Y	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
29	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
30	c	202/218 (93%)	181 (90%)	21 (10%)	0	100	100
31	e	162/166 (98%)	156 (96%)	6 (4%)	0	100	100
32	f	91/95 (96%)	90 (99%)	1 (1%)	0	100	100
33	g	149/156 (96%)	138 (93%)	10 (7%)	1 (1%)	18	23
34	h	128/132 (97%)	124 (97%)	4 (3%)	0	100	100
35	i	126/130 (97%)	112 (89%)	14 (11%)	0	100	100
36	j	96/102 (94%)	86 (90%)	9 (9%)	1 (1%)	12	15
37	k	112/131 (86%)	107 (96%)	4 (4%)	1 (1%)	14	17
38	l	133/138 (96%)	128 (96%)	5 (4%)	0	100	100
39	m	116/121 (96%)	111 (96%)	5 (4%)	0	100	100
40	n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
41	o	85/89 (96%)	81 (95%)	3 (4%)	1 (1%)	10	12
42	p	85/90 (94%)	81 (95%)	3 (4%)	1 (1%)	10	12
43	q	82/87 (94%)	80 (98%)	2 (2%)	0	100	100
44	r	63/79 (80%)	59 (94%)	4 (6%)	0	100	100
45	t	84/88 (96%)	80 (95%)	4 (5%)	0	100	100
49	b	191/246 (78%)	178 (93%)	10 (5%)	3 (2%)	7	7
50	s	81/92 (88%)	76 (94%)	4 (5%)	1 (1%)	10	12
51	8	233/366 (64%)	215 (92%)	17 (7%)	1 (0%)	30	38
52	W	80/94 (85%)	78 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	d	197/200 (98%)	188 (95%)	8 (4%)	1 (0%)	24	31
All	All	5479/5922 (92%)	5179 (94%)	282 (5%)	18 (0%)	37	46

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
51	8	252	HIS
49	b	76	ALA
13	F	3	ARG
13	F	110	ARG
20	O	2	ILE
33	g	130	ASN
37	k	121	ASN
42	p	32	ARG
49	b	106	THR
11	D	54	ASP
17	L	29	LYS
53	d	28	LYS
36	j	58	TYR
50	s	4	SER
21	P	28	VAL
49	b	154	MET
41	o	23	GLY
7	6	19	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	49/53 (92%)	49 (100%)	0	100	100
2	1	46/47 (98%)	44 (96%)	2 (4%)	26	39
3	2	39/39 (100%)	39 (100%)	0	100	100
4	3	54/56 (96%)	52 (96%)	2 (4%)	30	45
5	4	35/35 (100%)	35 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	5	38/38 (100%)	38 (100%)	0	100	100
7	6	39/55 (71%)	38 (97%)	1 (3%)	40	59
10	C	221/225 (98%)	218 (99%)	3 (1%)	59	76
11	D	168/170 (99%)	165 (98%)	3 (2%)	51	70
12	E	169/170 (99%)	166 (98%)	3 (2%)	51	70
13	F	153/154 (99%)	153 (100%)	0	100	100
14	G	148/151 (98%)	147 (99%)	1 (1%)	76	87
15	J	122/123 (99%)	121 (99%)	1 (1%)	73	86
16	K	101/101 (100%)	101 (100%)	0	100	100
17	L	110/110 (100%)	109 (99%)	1 (1%)	70	84
18	M	109/116 (94%)	106 (97%)	3 (3%)	38	56
19	N	99/100 (99%)	96 (97%)	3 (3%)	36	53
20	O	93/93 (100%)	92 (99%)	1 (1%)	65	81
21	P	99/100 (99%)	97 (98%)	2 (2%)	48	67
22	Q	97/98 (99%)	96 (99%)	1 (1%)	68	82
23	R	84/84 (100%)	82 (98%)	2 (2%)	43	62
24	S	91/93 (98%)	91 (100%)	0	100	100
25	T	82/85 (96%)	80 (98%)	2 (2%)	43	62
26	U	86/87 (99%)	86 (100%)	0	100	100
27	X	49/50 (98%)	46 (94%)	3 (6%)	17	24
28	Y	57/57 (100%)	57 (100%)	0	100	100
29	Z	52/53 (98%)	52 (100%)	0	100	100
30	c	167/178 (94%)	167 (100%)	0	100	100
31	e	128/130 (98%)	128 (100%)	0	100	100
32	f	82/84 (98%)	82 (100%)	0	100	100
33	g	127/132 (96%)	127 (100%)	0	100	100
34	h	110/112 (98%)	110 (100%)	0	100	100
35	i	101/102 (99%)	101 (100%)	0	100	100
36	j	89/92 (97%)	89 (100%)	0	100	100
37	k	86/100 (86%)	84 (98%)	2 (2%)	44	63
38	l	113/115 (98%)	111 (98%)	2 (2%)	51	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	m	101/104 (97%)	99 (98%)	2 (2%)	48	67
40	n	53/54 (98%)	52 (98%)	1 (2%)	50	69
41	o	82/83 (99%)	82 (100%)	0	100	100
42	p	74/76 (97%)	74 (100%)	0	100	100
43	q	77/80 (96%)	76 (99%)	1 (1%)	61	77
44	r	56/64 (88%)	56 (100%)	0	100	100
45	t	69/70 (99%)	68 (99%)	1 (1%)	59	76
49	b	167/212 (79%)	161 (96%)	6 (4%)	31	47
50	s	72/81 (89%)	72 (100%)	0	100	100
51	8	80/323 (25%)	80 (100%)	0	100	100
52	W	63/74 (85%)	63 (100%)	0	100	100
53	d	172/173 (99%)	172 (100%)	0	100	100
All	All	4559/4982 (92%)	4510 (99%)	49 (1%)	63	81

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	5	ILE
2	1	19	SER
4	3	4	MET
4	3	31	HIS
7	6	38	GLU
10	C	63	ARG
10	C	182	ARG
10	C	191	SER
11	D	49	ILE
11	D	61	SER
11	D	191	ASN
12	E	32	VAL
12	E	66	ARG
12	E	126	LEU
14	G	59	GLN
15	J	29	LEU
17	L	59	GLN
18	M	3	LEU
18	M	8	LYS
18	M	129	THR
19	N	41	ARG

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Mol	Chain	Res	Type
19	N	102	MET
19	N	107	ARG
20	O	63	LEU
21	P	5	ILE
21	P	21	ARG
22	Q	2	PRO
23	R	33	VAL
23	R	57	THR
25	T	32	VAL
25	T	91	GLU
27	X	27	ARG
27	X	33	VAL
27	X	43	LYS
37	k	81	LEU
37	k	121	ASN
38	l	10	LYS
38	l	18	ASN
39	m	16	VAL
39	m	100	GLN
40	n	54	PRO
43	q	65	GLU
45	t	13	THR
49	b	33	THR
49	b	75	GLN
49	b	77	GLN
49	b	92	VAL
49	b	164	ILE
49	b	168	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	40	HIS
4	3	26	HIS
4	3	31	HIS
4	3	35	ASN
4	3	60	GLN
7	6	8	ASN
10	C	61	GLN
10	C	199	GLN
11	D	14	GLN
11	D	172	GLN

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Mol	Chain	Res	Type
12	E	9	GLN
12	E	46	GLN
13	F	2	ASN
13	F	46	ASN
14	G	22	ASN
15	J	54	HIS
16	K	4	GLN
17	L	17	ASN
17	L	114	ASN
20	O	64	ASN
21	P	41	GLN
25	T	58	ASN
26	U	53	GLN
26	U	59	GLN
27	X	17	ASN
27	X	23	ASN
28	Y	31	GLN
30	c	99	HIS
30	c	135	GLN
30	c	146	GLN
32	f	61	GLN
32	f	64	ASN
33	g	148	ASN
35	i	3	GLN
35	i	5	GLN
35	i	81	HIS
35	i	126	GLN
37	k	42	ASN
40	n	52	GLN
41	o	5	GLN
41	o	72	ASN
43	q	54	GLN
44	r	21	ASN
45	t	3	ASN
49	b	75	GLN
53	d	36	HIS
53	d	115	ASN
53	d	158	ASN

### 5.3.3 RNA ⓘ



Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	v	75/76 (98%)	20 (26%)	0
47	A	2716/2928 (92%)	457 (16%)	91 (3%)
48	a	1504/1554 (96%)	252 (16%)	0
8	7	8/9 (88%)	5 (62%)	1 (12%)
9	B	111/112 (99%)	24 (21%)	5 (4%)
All	All	4414/4679 (94%)	758 (17%)	97 (2%)

All (758) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	404	U
8	7	405	G
8	7	408	U
8	7	409	U
8	7	411	A
9	B	4	G
9	B	10	G
9	B	11	A
9	B	12	U
9	B	13	A
9	B	23	U
9	B	32	U
9	B	33	U
9	B	37	A
9	B	38	U
9	B	40	C
9	B	48	G
9	B	49	G
9	B	50	A
9	B	51	A
9	B	53	U
9	B	54	U
9	B	63	C
9	B	64	A
9	B	87	U
9	B	88	C
9	B	97	A
9	B	107	G
9	B	108	C
46	v	6	G
46	v	7	G
46	v	9	A
46	v	10	G

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Mol	Chain	Res	Type
46	v	14	A
46	v	17	U
46	v	18	G
46	v	19	G
46	v	20	U
46	v	21	A
46	v	46	G
46	v	47	U
46	v	48	C
46	v	49	G
46	v	51	C
46	v	58	A
46	v	61	C
46	v	65	C
46	v	69	A
46	v	76	A
47	A	12	A
47	A	13	A
47	A	34	U
47	A	45	G
47	A	46	C
47	A	60	G
47	A	63	G
47	A	71	A
47	A	74	U
47	A	75	G
47	A	89	U
47	A	90	A
47	A	93	C
47	A	109	G
47	A	117	A
47	A	118	A
47	A	119	U
47	A	164	U
47	A	166	A
47	A	175	G
47	A	176	A
47	A	177	G
47	A	183	A
47	A	184	G
47	A	185	A
47	A	199	A

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Mol	Chain	Res	Type
47	A	202	A
47	A	203	U
47	A	216	A
47	A	219	A
47	A	224	A
47	A	225	A
47	A	226	A
47	A	234	C
47	A	236	A
47	A	248	G
47	A	251	G
47	A	258	A
47	A	272	C
47	A	275	A
47	A	293	U
47	A	299	U
47	A	300	G
47	A	301	U
47	A	302	A
47	A	307	A
47	A	309	U
47	A	310	C
47	A	346	G
47	A	355	A
47	A	373	A
47	A	374	A
47	A	389	A
47	A	390	A
47	A	398	U
47	A	407	A
47	A	411	G
47	A	412	A
47	A	418	A
47	A	419	G
47	A	430	C
47	A	432	C
47	A	433	G
47	A	458	G
47	A	459	A
47	A	467	C
47	A	471	G
47	A	482	C

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Mol	Chain	Res	Type
47	A	483	C
47	A	487	G
47	A	491	C
47	A	498	U
47	A	503	C
47	A	504	A
47	A	528	G
47	A	537	A
47	A	549	A
47	A	550	G
47	A	551	A
47	A	554	U
47	A	555	C
47	A	556	C
47	A	568	G
47	A	576	G
47	A	577	U
47	A	578	A
47	A	579	G
47	A	592	A
47	A	595	G
47	A	606	U
47	A	607	G
47	A	615	U
47	A	616	A
47	A	617	G
47	A	618	A
47	A	619	A
47	A	630	A
47	A	631	G
47	A	647	A
47	A	657	G
47	A	658	A
47	A	659	A
47	A	666	G
47	A	673	A
47	A	683	A
47	A	691	U
47	A	692	A
47	A	700	U
47	A	701	G
47	A	702	A

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Mol	Chain	Res	Type
47	A	732	A
47	A	733	U
47	A	765	A
47	A	769	A
47	A	777	C
47	A	793	U
47	A	794	U
47	A	804	G
47	A	811	A
47	A	812	G
47	A	822	G
47	A	829	A
47	A	831	U
47	A	832	G
47	A	837	U
47	A	852	G
47	A	859	C
47	A	864	C
47	A	866	A
47	A	874	U
47	A	875	U
47	A	892	U
47	A	893	A
47	A	906	G
47	A	913	A
47	A	916	G
47	A	930	C
47	A	952	A
47	A	954	U
47	A	957	A
47	A	959	C
47	A	964	A
47	A	973	G
47	A	976	U
47	A	987	A
47	A	990	C
47	A	991	A
47	A	992	G
47	A	1007	G
47	A	1014	A
47	A	1020	A
47	A	1029	A

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Mol	Chain	Res	Type
47	A	1032	C
47	A	1038	C
47	A	1042	A
47	A	1058	U
47	A	1059	A
47	A	1068	G
47	A	1072	A
47	A	1073	A
47	A	1079	U
47	A	1084	A
47	A	1093	G
47	A	1098	C
47	A	1153	G
47	A	1158	G
47	A	1160	G
47	A	1174	A
47	A	1179	A
47	A	1180	C
47	A	1181	C
47	A	1182	G
47	A	1188	A
47	A	1189	A
47	A	1190	A
47	A	1197	A
47	A	1203	G
47	A	1204	C
47	A	1244	A
47	A	1245	G
47	A	1246	G
47	A	1247	G
47	A	1250	G
47	A	1251	U
47	A	1258	A
47	A	1278	G
47	A	1290	G
47	A	1293	A
47	A	1296	G
47	A	1311	G
47	A	1312	A
47	A	1315	G
47	A	1319	G
47	A	1338	G

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Mol	Chain	Res	Type
47	A	1339	A
47	A	1340	A
47	A	1341	U
47	A	1342	G
47	A	1344	C
47	A	1346	A
47	A	1360	A
47	A	1375	A
47	A	1377	G
47	A	1388	A
47	A	1389	C
47	A	1391	U
47	A	1404	A
47	A	1412	A
47	A	1414	G
47	A	1418	U
47	A	1423	A
47	A	1435	U
47	A	1450	C
47	A	1461	A
47	A	1465	A
47	A	1473	A
47	A	1474	C
47	A	1489	U
47	A	1490	A
47	A	1498	U
47	A	1499	A
47	A	1500	U
47	A	1501	U
47	A	1502	G
47	A	1505	U
47	A	1506	A
47	A	1514	C
47	A	1516	A
47	A	1525	G
47	A	1526	G
47	A	1527	C
47	A	1528	U
47	A	1529	G
47	A	1531	G
47	A	1536	A
47	A	1539	C

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Mol	Chain	Res	Type
47	A	1540	A
47	A	1542	A
47	A	1543	U
47	A	1544	C
47	A	1556	A
47	A	1557	G
47	A	1558	G
47	A	1559	C
47	A	1560	U
47	A	1561	G
47	A	1566	G
47	A	1590	C
47	A	1595	U
47	A	1596	U
47	A	1607	C
47	A	1617	A
47	A	1626	U
47	A	1630	G
47	A	1631	A
47	A	1632	G
47	A	1640	G
47	A	1653	A
47	A	1654	A
47	A	1655	A
47	A	1661	A
47	A	1691	A
47	A	1692	U
47	A	1693	C
47	A	1698	G
47	A	1719	G
47	A	1752	G
47	A	1757	G
47	A	1758	U
47	A	1759	U
47	A	1760	A
47	A	1768	A
47	A	1770	C
47	A	1771	C
47	A	1776	A
47	A	1777	G
47	A	1779	G
47	A	1788	A

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Mol	Chain	Res	Type
47	A	1791	A
47	A	1792	G
47	A	1793	G
47	A	1802	A
47	A	1805	G
47	A	1811	C
47	A	1829	C
47	A	1831	A
47	A	1845	A
47	A	1858	A
47	A	1867	C
47	A	1876	A
47	A	1877	A
47	A	1886	G
47	A	1887	G
47	A	1898	G
47	A	1899	U
47	A	1900	A
47	A	1901	A
47	A	1902	G
47	A	1911	C
47	A	1912	G
47	A	1934	C
47	A	1935	G
47	A	1936	G
47	A	1940	U
47	A	1941	A
47	A	1942	A
47	A	1943	C
47	A	1944	U
47	A	1945	A
47	A	1946	U
47	A	1958	G
47	A	1959	G
47	A	1966	A
47	A	1967	A
47	A	1984	U
47	A	1992	C
47	A	1996	C
47	A	1999	A
47	A	2000	A
47	A	2001	G

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Mol	Chain	Res	Type
47	A	2020	U
47	A	2022	U
47	A	2026	A
47	A	2050	G
47	A	2052	A
47	A	2055	U
47	A	2060	A
47	A	2061	G
47	A	2062	A
47	A	2072	C
47	A	2080	A
47	A	2081	G
47	A	2084	C
47	A	2085	G
47	A	2089	A
47	A	2090	G
47	A	2091	A
47	A	2098	G
47	A	2122	G
47	A	2124	A
47	A	2128	U
47	A	2129	G
47	A	2131	U
47	A	2219	G
47	A	2227	A
47	A	2232	G
47	A	2233	C
47	A	2240	U
47	A	2241	A
47	A	2254	A
47	A	2267	G
47	A	2268	G
47	A	2296	A
47	A	2308	G
47	A	2312	C
47	A	2315	A
47	A	2316	A
47	A	2318	G
47	A	2334	U
47	A	2335	U
47	A	2336	G
47	A	2337	G

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Mol	Chain	Res	Type
47	A	2338	A
47	A	2341	U
47	A	2342	C
47	A	2348	C
47	A	2349	A
47	A	2350	G
47	A	2351	A
47	A	2354	G
47	A	2356	A
47	A	2360	G
47	A	2362	A
47	A	2363	C
47	A	2364	A
47	A	2376	C
47	A	2379	C
47	A	2383	A
47	A	2408	G
47	A	2412	G
47	A	2414	C
47	A	2416	U
47	A	2418	G
47	A	2431	U
47	A	2432	C
47	A	2435	C
47	A	2440	A
47	A	2453	C
47	A	2454	A
47	A	2458	G
47	A	2459	A
47	A	2464	A
47	A	2468	A
47	A	2469	C
47	A	2470	C
47	A	2477	A
47	A	2503	C
47	A	2505	A
47	A	2507	A
47	A	2531	G
47	A	2534	G
47	A	2535	U
47	A	2547	A
47	A	2551	U

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Mol	Chain	Res	Type
47	A	2558	G
47	A	2559	U
47	A	2564	G
47	A	2568	C
47	A	2569	C
47	A	2570	A
47	A	2583	U
47	A	2595	A
47	A	2596	G
47	A	2602	C
47	A	2631	A
47	A	2632	G
47	A	2637	G
47	A	2638	U
47	A	2642	U
47	A	2666	U
47	A	2692	G
47	A	2698	G
47	A	2706	G
47	A	2712	C
47	A	2718	PSU
47	A	2720	C
47	A	2733	C
47	A	2762	A
47	A	2764	G
47	A	2773	G
47	A	2777	A
47	A	2780	G
47	A	2786	A
47	A	2794	A
47	A	2795	G
47	A	2806	G
47	A	2807	A
47	A	2818	C
47	A	2820	U
47	A	2823	C
47	A	2824	G
47	A	2828	G
47	A	2833	U
47	A	2845	A
47	A	2860	A
47	A	2872	U

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Mol	Chain	Res	Type
47	A	2875	A
47	A	2892	G
47	A	2893	A
47	A	2897	G
47	A	2898	A
47	A	2899	C
47	A	2904	A
47	A	2905	C
47	A	2908	A
47	A	2911	G
47	A	2918	G
48	a	9	G
48	a	11	G
48	a	21	C
48	a	24	G
48	a	34	A
48	a	41	G
48	a	46	G
48	a	49	C
48	a	50	C
48	a	52	A
48	a	53	A
48	a	74	A
48	a	75	G
48	a	76	A
48	a	99	A
48	a	119	C
48	a	128	A
48	a	129	A
48	a	137	G
48	a	143	C
48	a	148	A
48	a	153	U
48	a	158	G
48	a	160	A
48	a	162	C
48	a	172	U
48	a	181	G
48	a	182	U
48	a	188	G
48	a	189	A
48	a	194	C

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Mol	Chain	Res	Type
48	a	195	A
48	a	197	G
48	a	199	U
48	a	209	A
48	a	219	U
48	a	220	C
48	a	222	G
48	a	234	A
48	a	253	U
48	a	255	G
48	a	259	G
48	a	274	G
48	a	275	C
48	a	284	G
48	a	288	C
48	a	297	G
48	a	314	A
48	a	329	A
48	a	336	C
48	a	337	A
48	a	338	C
48	a	340	G
48	a	355	G
48	a	360	C
48	a	362	G
48	a	373	U
48	a	375	U
48	a	380	C
48	a	381	A
48	a	385	G
48	a	388	G
48	a	389	A
48	a	401	A
48	a	406	C
48	a	414	G
48	a	419	A
48	a	420	U
48	a	422	A
48	a	429	U
48	a	430	C
48	a	431	G
48	a	432	G

*Continued on next page...*



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Mol	Chain	Res	Type
48	a	435	C
48	a	437	U
48	a	439	A
48	a	447	U
48	a	461	C
48	a	465	U
48	a	468	C
48	a	475	A
48	a	476	U
48	a	478	G
48	a	493	G
48	a	494	G
48	a	506	A
48	a	510	C
48	a	514	G
48	a	517	U
48	a	520	C
48	a	525	U
48	a	526	G
48	a	527	C
48	a	536	G
48	a	541	A
48	a	542	A
48	a	545	C
48	a	556	A
48	a	568	A
48	a	571	U
48	a	581	A
48	a	582	A
48	a	585	G
48	a	586	G
48	a	627	C
48	a	642	U
48	a	643	C
48	a	651	A
48	a	662	U
48	a	663	G
48	a	665	G
48	a	674	A
48	a	696	A
48	a	697	G
48	a	732	U

*Continued on next page...*



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Mol	Chain	Res	Type
48	a	733	G
48	a	740	G
48	a	743	A
48	a	757	A
48	a	758	A
48	a	764	G
48	a	786	A
48	a	787	G
48	a	802	U
48	a	803	A
48	a	824	A
48	a	826	C
48	a	845	G
48	a	849	G
48	a	855	G
48	a	856	C
48	a	863	G
48	a	869	C
48	a	924	A
48	a	932	G
48	a	941	C
48	a	944	C
48	a	945	A
48	a	958	C
48	a	964	G
48	a	965	U
48	a	966	U
48	a	970	U
48	a	971	U
48	a	975	A
48	a	978	A
48	a	979	A
48	a	985	A
48	a	986	G
48	a	987	A
48	a	993	A
48	a	994	C
48	a	1002	U
48	a	1003	G
48	a	1004	A
48	a	1008	C
48	a	1012	U

*Continued on next page...*



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Mol	Chain	Res	Type
48	a	1013	G
48	a	1014	A
48	a	1019	C
48	a	1020	C
48	a	1028	A
48	a	1030	G
48	a	1033	G
48	a	1034	U
48	a	1035	C
48	a	1039	U
48	a	1044	G
48	a	1045	G
48	a	1046	G
48	a	1049	G
48	a	1050	A
48	a	1051	G
48	a	1056	A
48	a	1060	G
48	a	1066	U
48	a	1074	G
48	a	1075	U
48	a	1076	C
48	a	1095	U
48	a	1099	G
48	a	1104	G
48	a	1105	U
48	a	1108	C
48	a	1111	A
48	a	1135	U
48	a	1140	A
48	a	1142	C
48	a	1144	U
48	a	1145	U
48	a	1148	G
48	a	1149	U
48	a	1150	U
48	a	1166	A
48	a	1168	U
48	a	1176	A
48	a	1178	A
48	a	1193	G
48	a	1205	A

*Continued on next page...*



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Mol	Chain	Res	Type
48	a	1206	A
48	a	1221	U
48	a	1222	A
48	a	1235	C
48	a	1236	A
48	a	1237	C
48	a	1247	A
48	a	1257	A
48	a	1265	C
48	a	1266	A
48	a	1267	G
48	a	1287	C
48	a	1289	A
48	a	1290	U
48	a	1291	C
48	a	1299	U
48	a	1309	G
48	a	1311	U
48	a	1314	G
48	a	1321	G
48	a	1328	A
48	a	1329	C
48	a	1344	C
48	a	1345	U
48	a	1347	G
48	a	1355	A
48	a	1362	G
48	a	1366	A
48	a	1367	U
48	a	1371	C
48	a	1373	U
48	a	1379	G
48	a	1388	G
48	a	1407	A
48	a	1419	A
48	a	1420	C
48	a	1428	G
48	a	1449	U
48	a	1451	A
48	a	1455	A
48	a	1460	U
48	a	1464	G

*Continued on next page...*



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Mol	Chain	Res	Type
48	a	1497	G
48	a	1502	A
48	a	1503	A
48	a	1504	G
48	a	1507	G
48	a	1513	A
48	a	1516	U
48	a	1527	G
48	a	1529	A
48	a	1539	G
48	a	1540	G

All (97) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	7	408	U
9	B	32	U
9	B	37	A
9	B	48	G
9	B	49	G
9	B	63	C
47	A	12	A
47	A	33	U
47	A	67	A
47	A	75	G
47	A	92	G
47	A	176	A
47	A	181	G
47	A	184	G
47	A	202	A
47	A	299	U
47	A	300	G
47	A	337	A
47	A	389	A
47	A	411	G
47	A	458	G
47	A	481	U
47	A	482	C
47	A	549	A
47	A	592	A
47	A	615	U
47	A	691	U

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Mol	Chain	Res	Type
47	A	701	G
47	A	732	A
47	A	742	G
47	A	793	U
47	A	811	A
47	A	828	A
47	A	831	U
47	A	848	G
47	A	852	G
47	A	855	G
47	A	916	G
47	A	986	G
47	A	990	C
47	A	1025	A
47	A	1030	G
47	A	1179	A
47	A	1187	U
47	A	1188	A
47	A	1203	G
47	A	1244	A
47	A	1246	G
47	A	1250	G
47	A	1266	A
47	A	1278	G
47	A	1339	A
47	A	1341	U
47	A	1344	C
47	A	1480	A
47	A	1485	A
47	A	1498	U
47	A	1505	U
47	A	1514	C
47	A	1525	G
47	A	1527	C
47	A	1530	G
47	A	1535	U
47	A	1536	A
47	A	1543	U
47	A	1558	G
47	A	1565	U
47	A	1631	A
47	A	1653	A

*Continued on next page...*



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Mol	Chain	Res	Type
47	A	1654	A
47	A	1691	A
47	A	1692	U
47	A	1751	U
47	A	1757	G
47	A	1791	A
47	A	1876	A
47	A	1941	A
47	A	2080	A
47	A	2127	U
47	A	2241	A
47	A	2254	A
47	A	2315	A
47	A	2316	A
47	A	2337	G
47	A	2349	A
47	A	2375	A
47	A	2451	C
47	A	2459	A
47	A	2468	A
47	A	2558	G
47	A	2569	C
47	A	2631	A
47	A	2785	U
47	A	2805	A
47	A	2892	G
47	A	2898	A
47	A	2904	A

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

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

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



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
47	PSU	A	2718	47	18,21,22	0.97	1 (5%)	21,30,33	0.83	0
47	OMG	A	2280	47,46	23,26,27	0.39	0	32,38,41	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PSU	A	2718	47	-	1/7/25/26	0/2/2/2
47	OMG	A	2280	47,46	-	0/9/27/28	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	2718	PSU	C6-C5	3.35	1.39	1.35

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	A	2718	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	A	2280	OMG	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.



There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



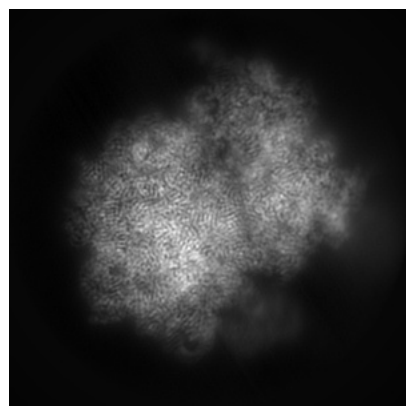
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50855. These allow visual inspection of the internal detail of the map and identification of artifacts.

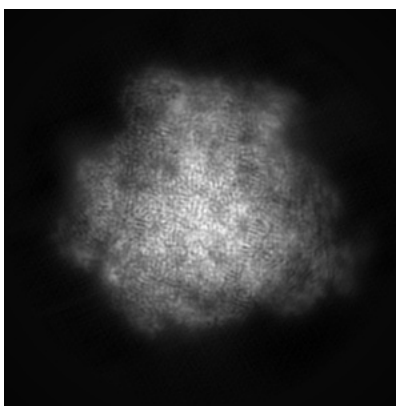
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

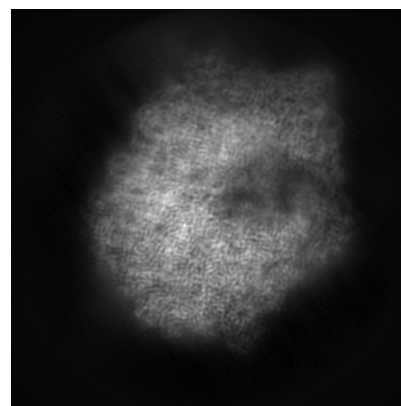
#### 6.1.1 Primary map



X

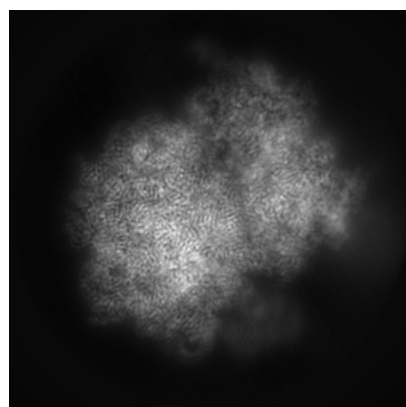


Y

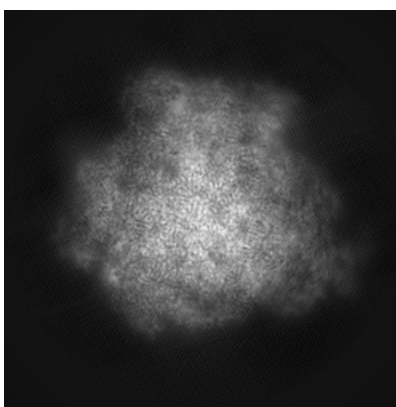


Z

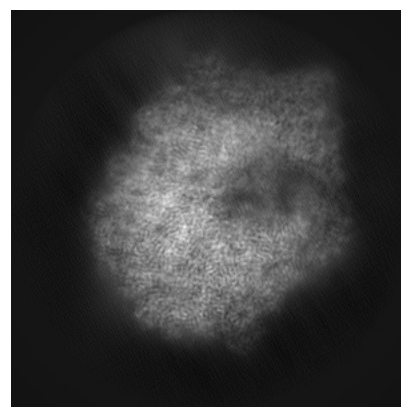
#### 6.1.2 Raw map



X



Y



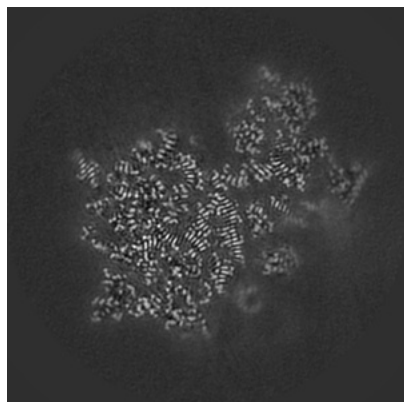
Z

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

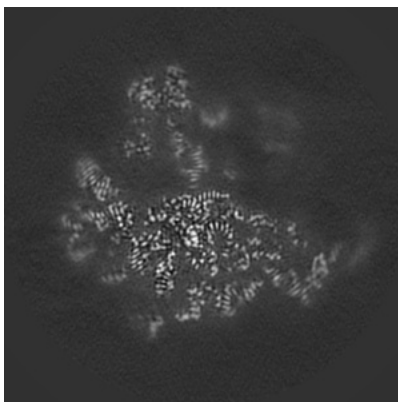


## 6.2 Central slices [i](#)

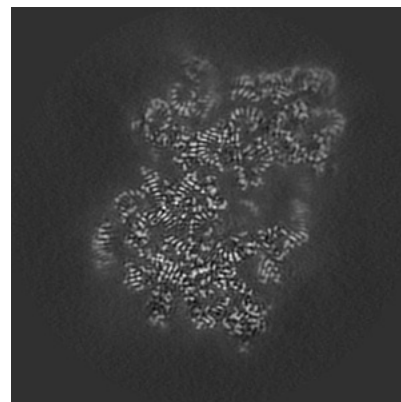
### 6.2.1 Primary map



X Index: 192

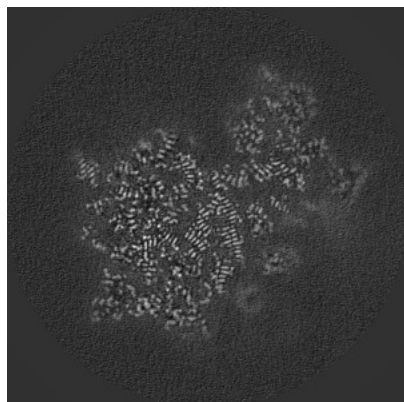


Y Index: 192

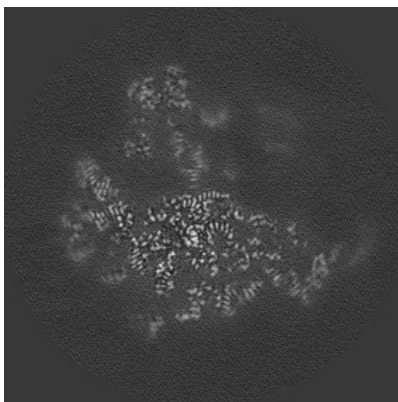


Z Index: 192

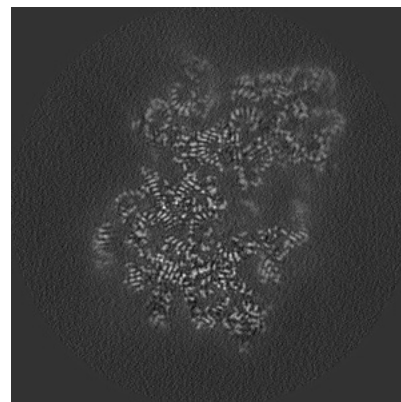
### 6.2.2 Raw map



X Index: 192



Y Index: 192



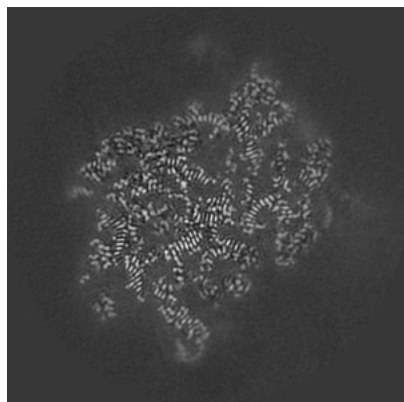
Z Index: 192

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

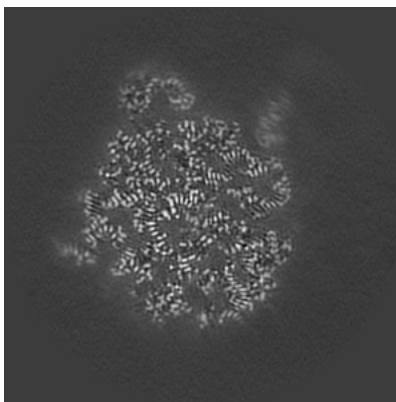


## 6.3 Largest variance slices [i](#)

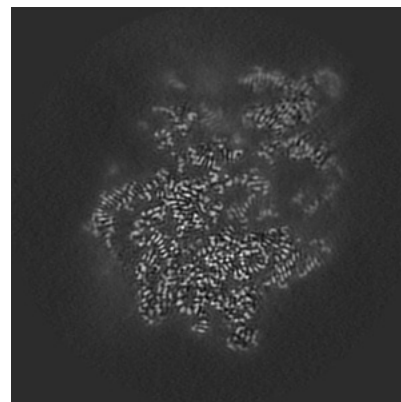
### 6.3.1 Primary map



X Index: 164

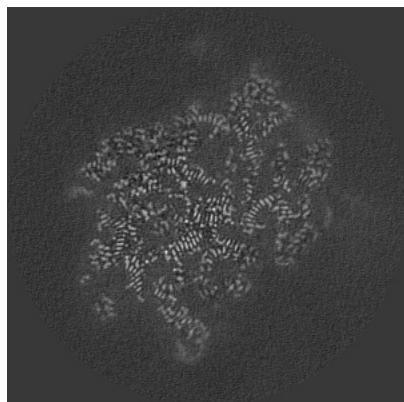


Y Index: 157

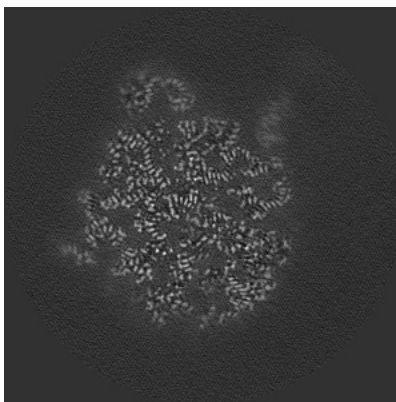


Z Index: 178

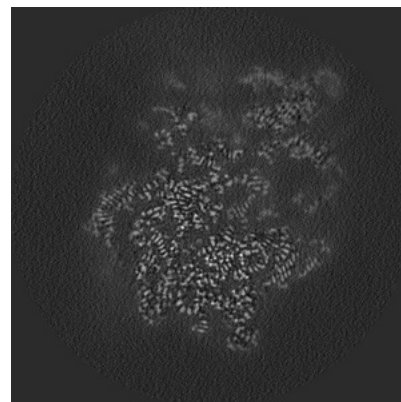
### 6.3.2 Raw map



X Index: 164



Y Index: 156



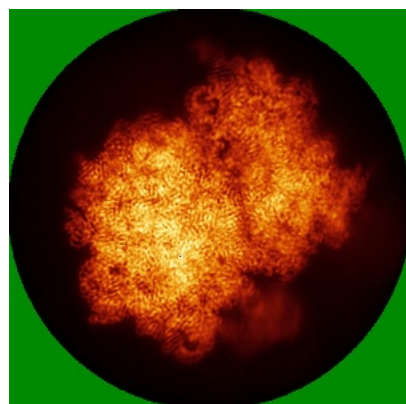
Z Index: 178

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

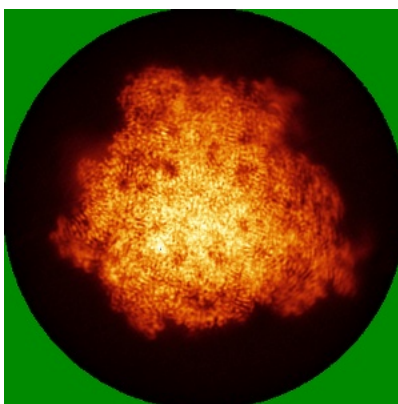


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

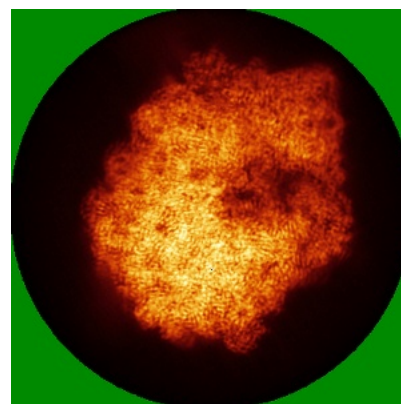
### 6.4.1 Primary map



X

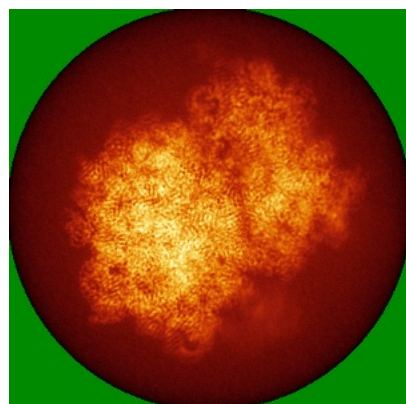


Y

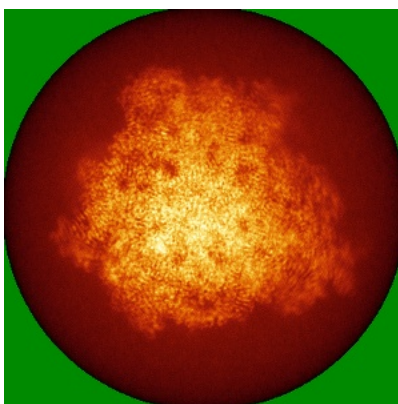


Z

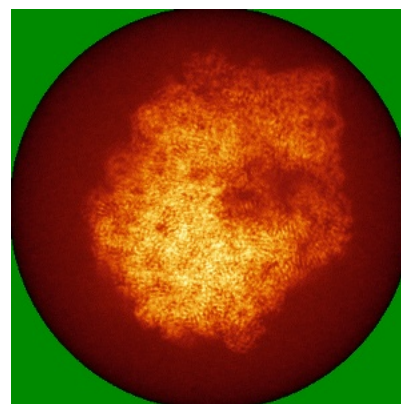
### 6.4.2 Raw map



X



Y



Z

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



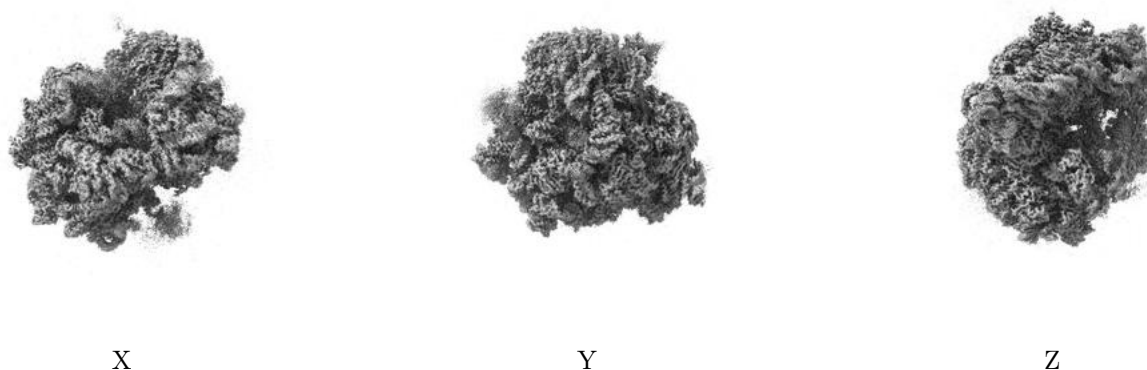
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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



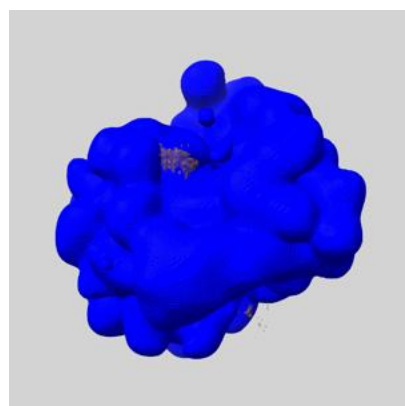
## 6.6 Mask visualisation [i](#)

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

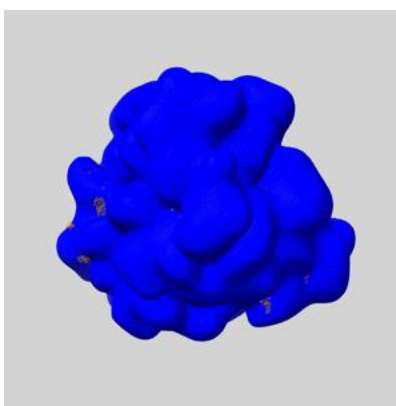
A mask typically either:

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

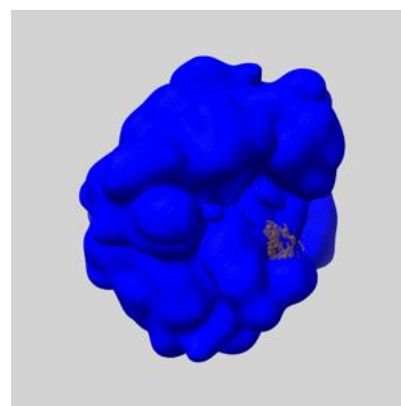
### 6.6.1 emd\_50855\_msk\_1.map [i](#)



X



Y



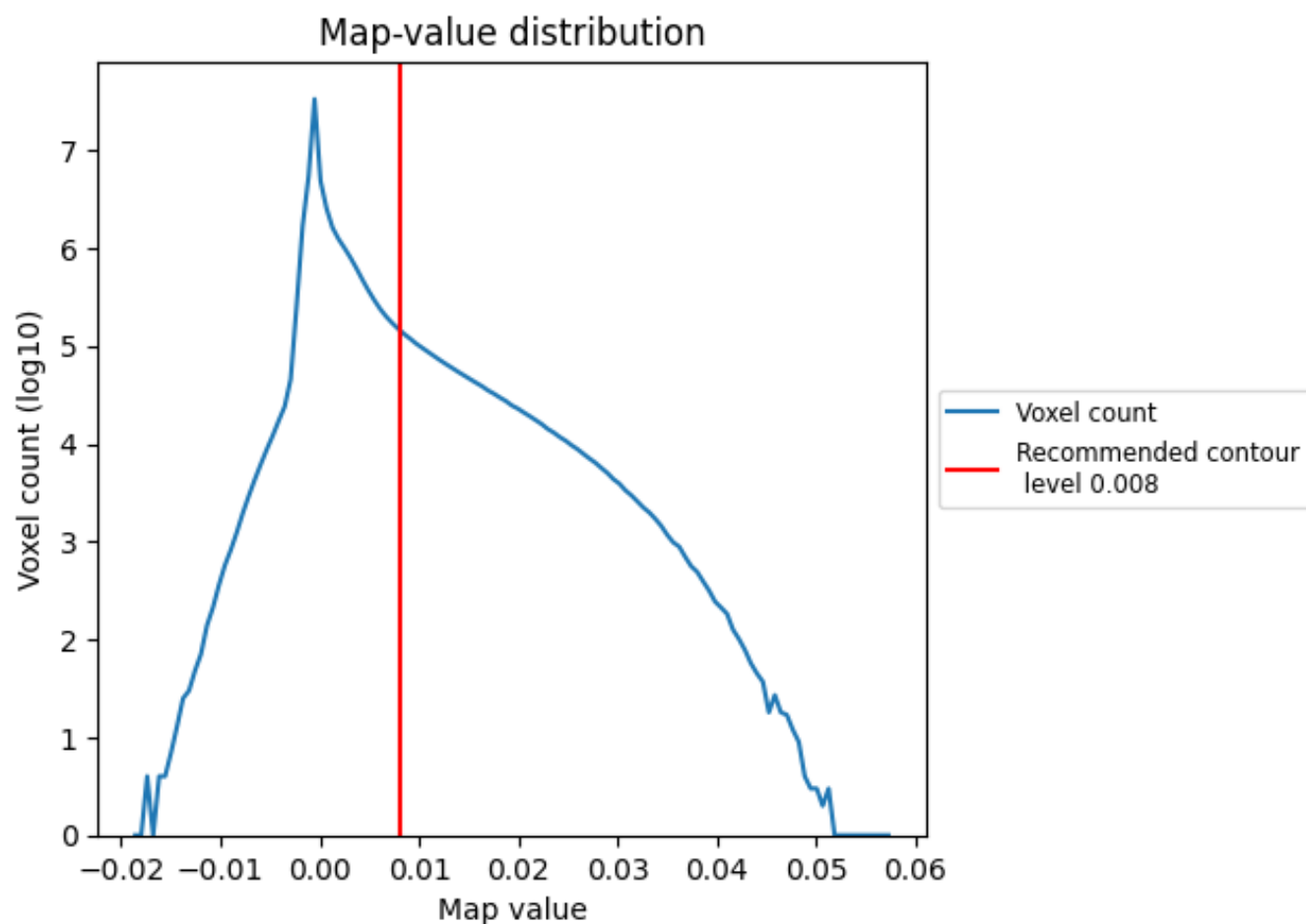
Z



## 7 Map analysis [i](#)

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

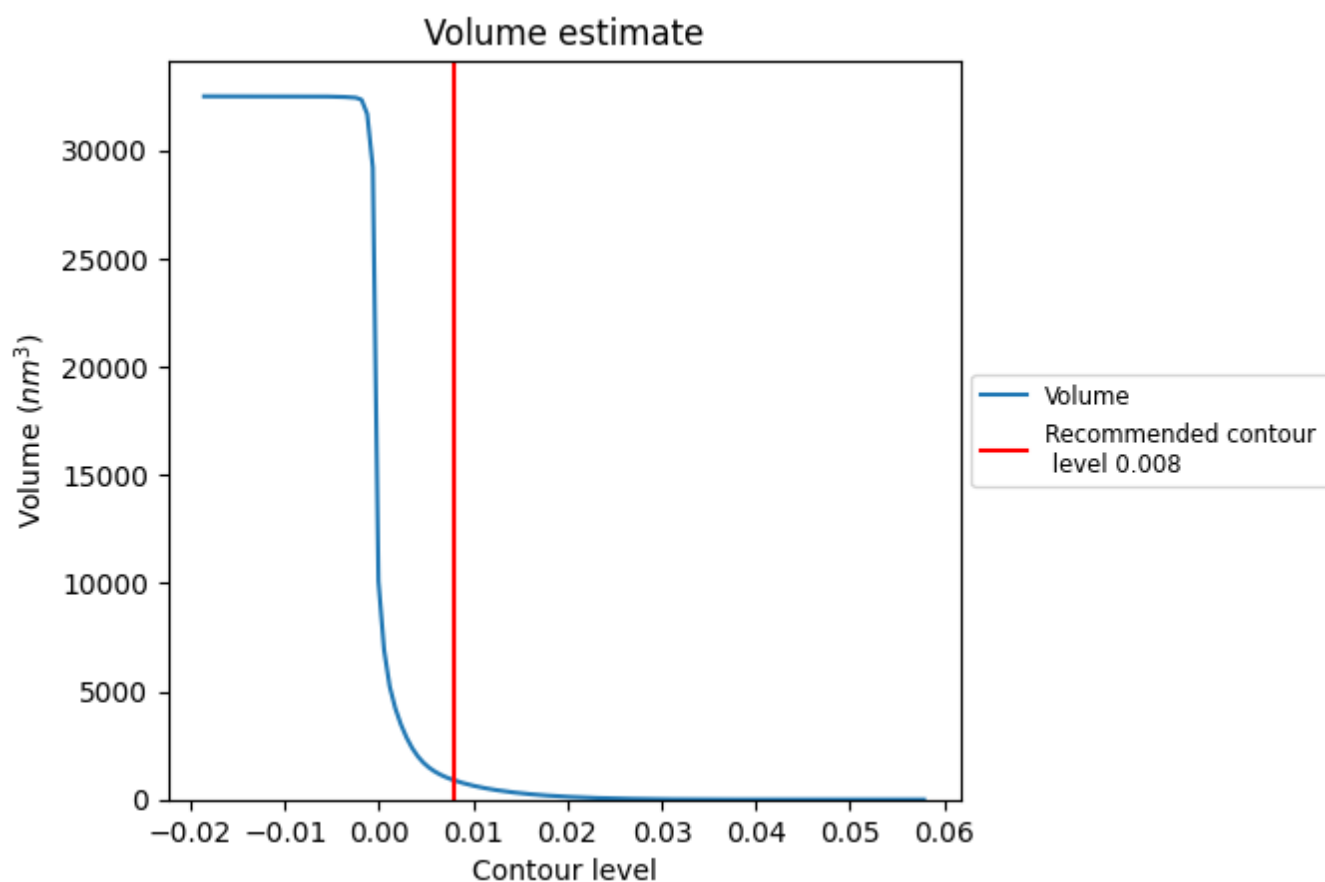
### 7.1 Map-value distribution [i](#)



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



## 7.2 Volume estimate [i](#)

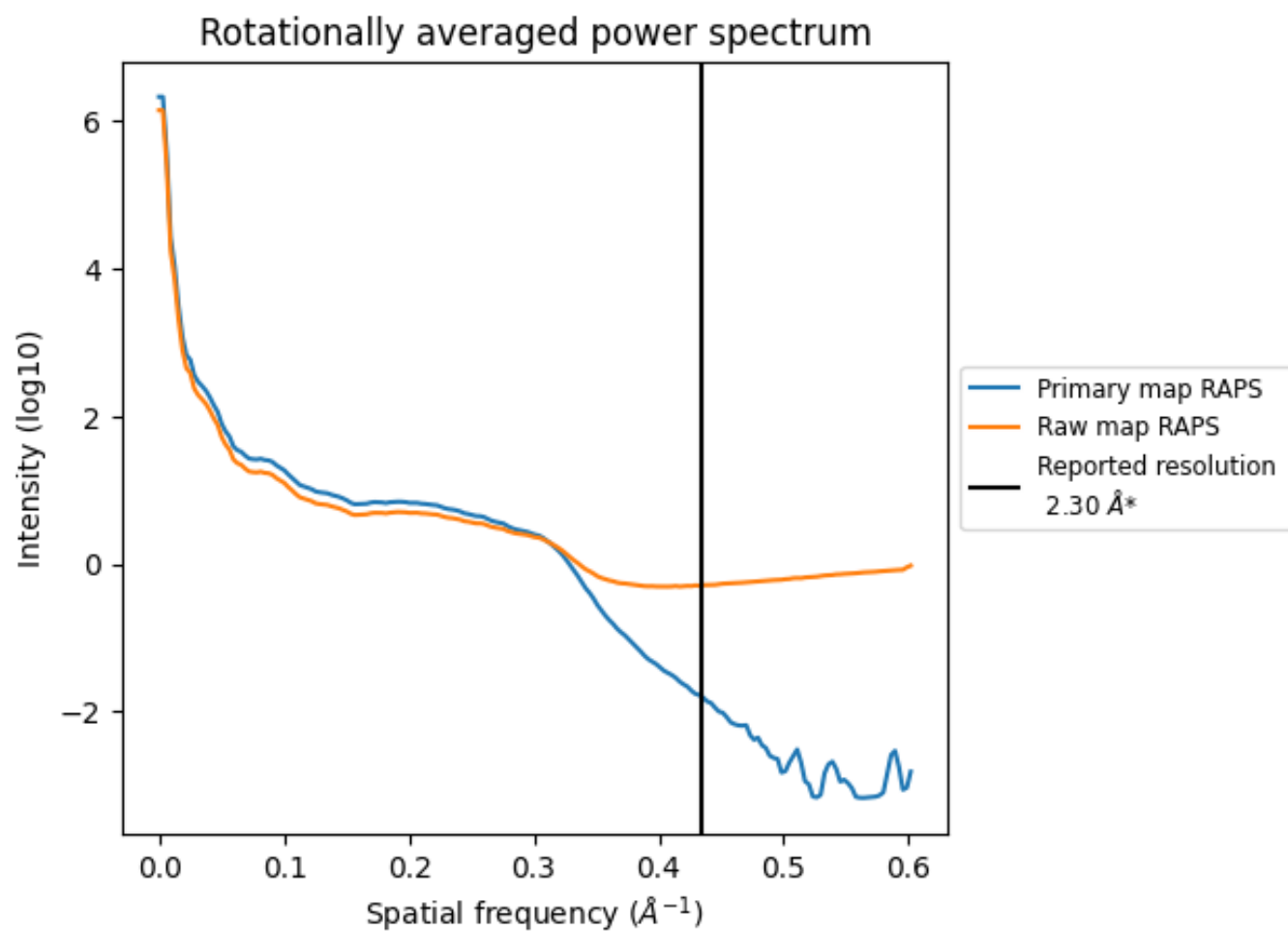


The volume at the recommended contour level is 887 nm<sup>3</sup>; this corresponds to an approximate mass of 801 kDa.

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 ⓘ



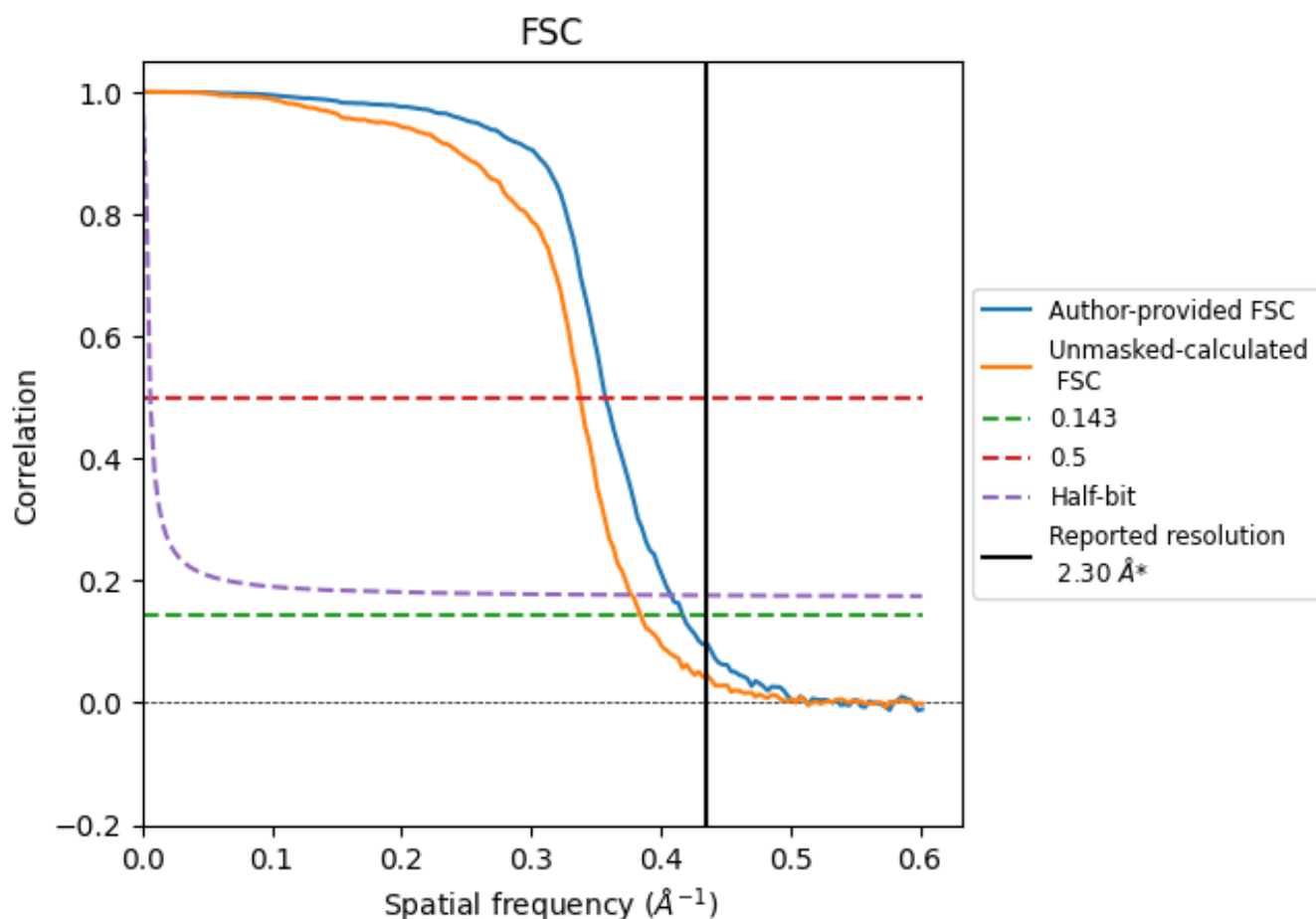
\*Reported resolution corresponds to spatial frequency of 0.435 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.435  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.40	2.80	2.45
Unmasked-calculated*	2.60	2.96	2.65

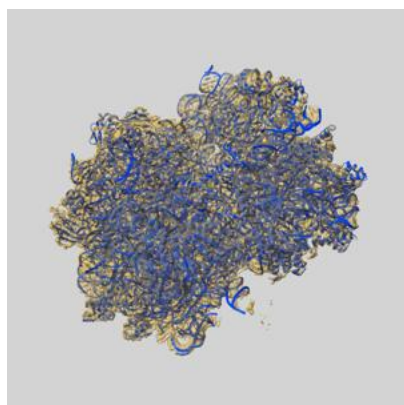
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.60 differs from the reported value 2.3 by more than 10 %



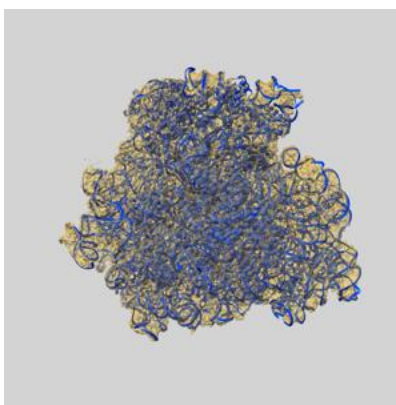
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50855 and PDB model 9FY1. Per-residue inclusion information can be found in section [3](#) on page [14](#).

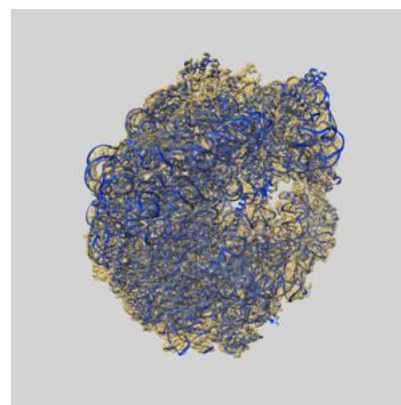
### 9.1 Map-model overlay [i](#)



X



Y

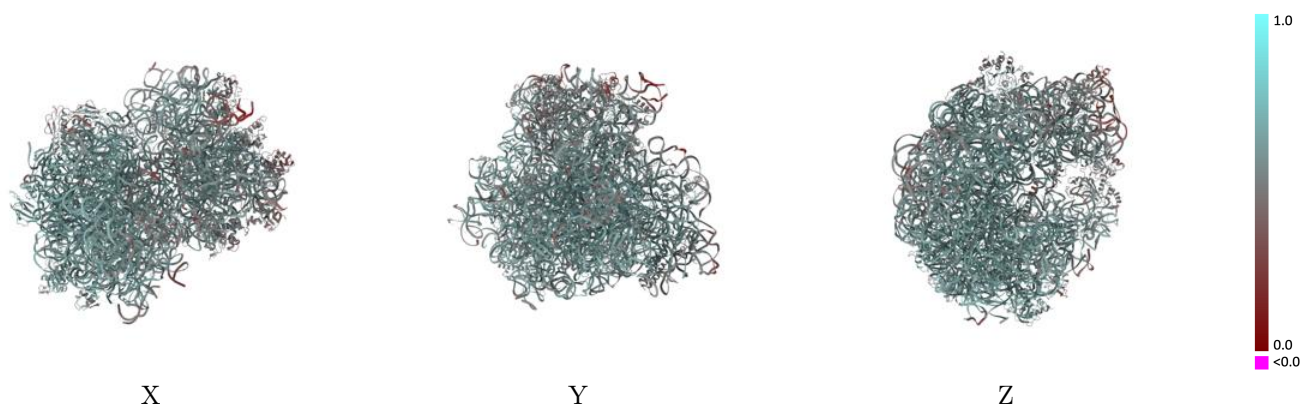


Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 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.

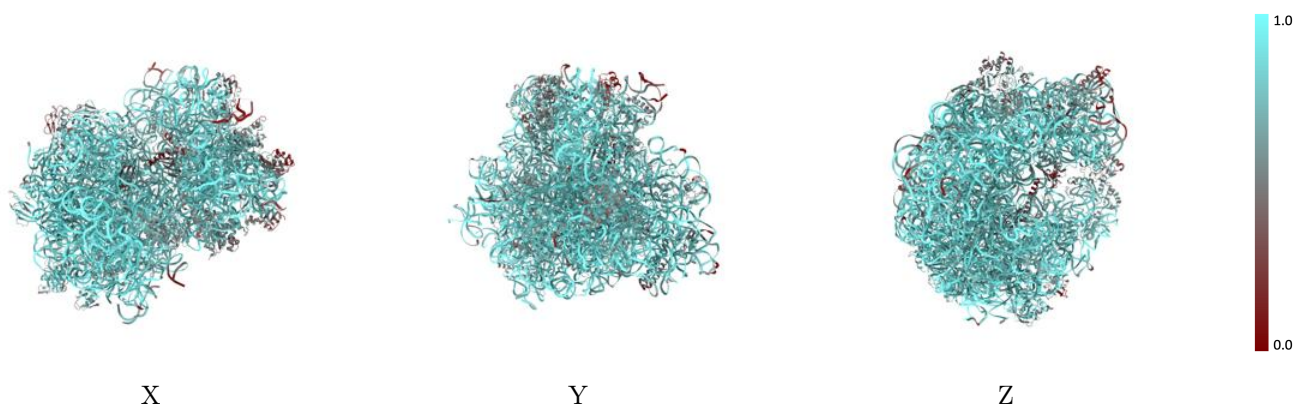


## 9.2 Q-score mapped to coordinate model [i](#)



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.

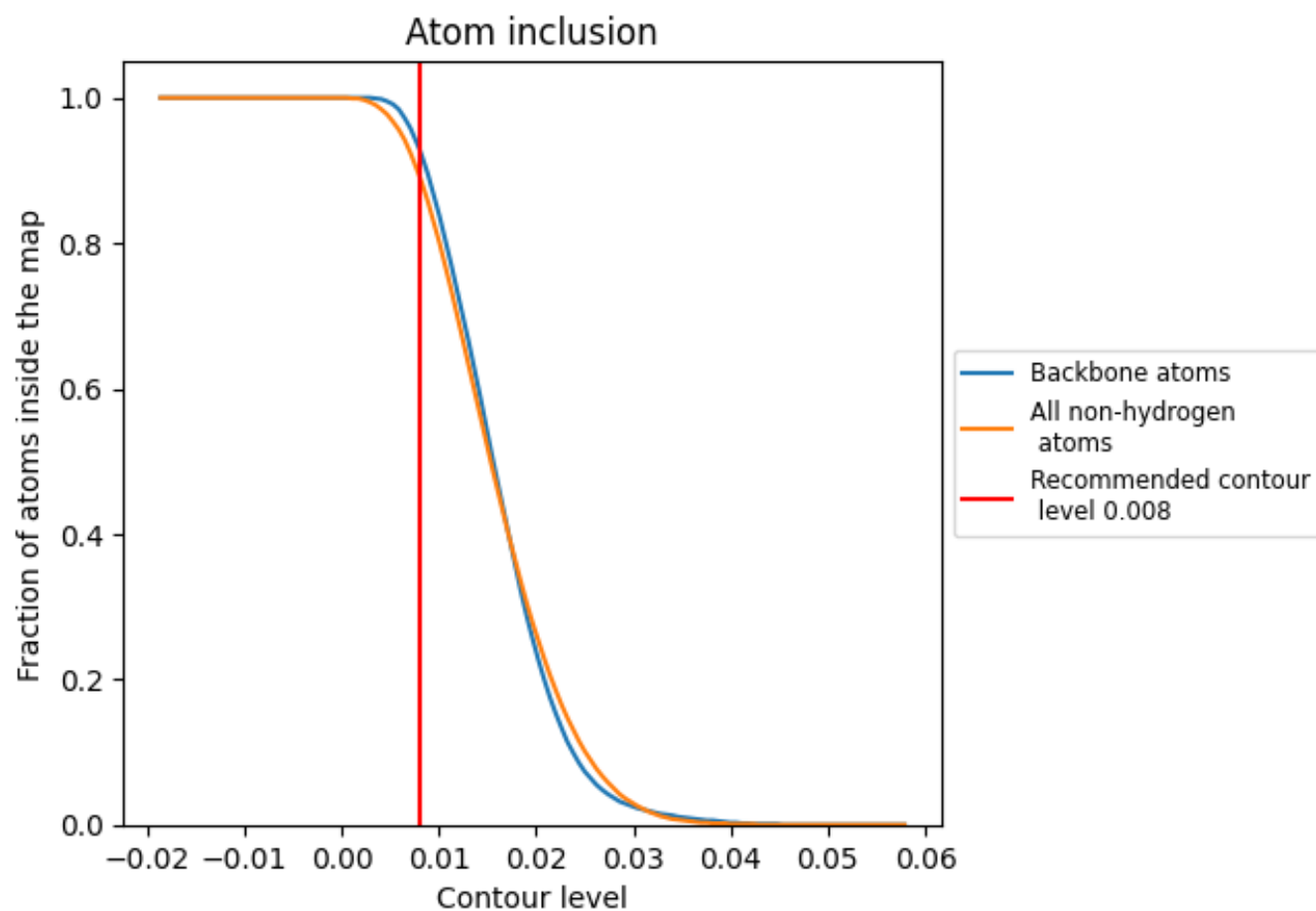
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.008).



## 9.4 Atom inclusion ⓘ









































































At the recommended contour level, 93% of all backbone atoms, 89% 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 (0.008) and Q-score for the entire model and for each chain.







































Chain	Atom inclusion	Q-score
All	 0.8930	 0.5950
0	 0.8880	 0.6020
1	 0.8070	 0.6000
2	 0.9770	 0.6690
3	 0.9500	 0.6490
4	 0.8940	 0.6160
5	 0.8680	 0.6270
6	 0.5140	 0.4370
7	 0.9360	 0.5910
8	 0.5060	 0.5370
A	 0.9710	 0.6270
B	 0.9400	 0.5760
C	 0.9310	 0.6390
D	 0.8820	 0.6220
E	 0.8390	 0.6140
F	 0.6410	 0.4920
G	 0.5850	 0.4990
J	 0.8890	 0.6150
K	 0.8960	 0.6240
L	 0.8380	 0.6110
M	 0.9060	 0.6230
N	 0.8830	 0.6070
O	 0.7080	 0.5410
P	 0.8430	 0.5980
Q	 0.9050	 0.6360
R	 0.8240	 0.6200
S	 0.8970	 0.6260
T	 0.8360	 0.5930
U	 0.7510	 0.5850
W	 0.9110	 0.6320
X	 0.7900	 0.5810
Y	 0.7420	 0.5590
Z	 0.8660	 0.6090
a	 0.9200	 0.5730
b	 0.5910	 0.5130



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Chain	Atom inclusion	Q-score
c	 0.6790	 0.5210
d	 0.6420	 0.5290
e	 0.7830	 0.5840
f	 0.6900	 0.5600
g	 0.6290	 0.4910
h	 0.8150	 0.5910
i	 0.5930	 0.4750
j	 0.5310	 0.4480
k	 0.6990	 0.5370
l	 0.8360	 0.6060
m	 0.6570	 0.5030
n	 0.8380	 0.5700
o	 0.8140	 0.5810
p	 0.7420	 0.5510
q	 0.7320	 0.5540
r	 0.7290	 0.5630
s	 0.6960	 0.5060
t	 0.6520	 0.5060
v	 0.9240	 0.5720