



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 03:48 AM JST

PDB ID : 7D6Z  
EMDB ID : EMD-30598  
Title : Molecular model of the cryo-EM structure of 70S ribosome in complex with peptide deformylase and trigger factor  
Authors : Akbar, S.; Bhakta, S.; Sengupta, J.  
Deposited on : 2020-10-02  
Resolution : 3.40 Å(reported)

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

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

---

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

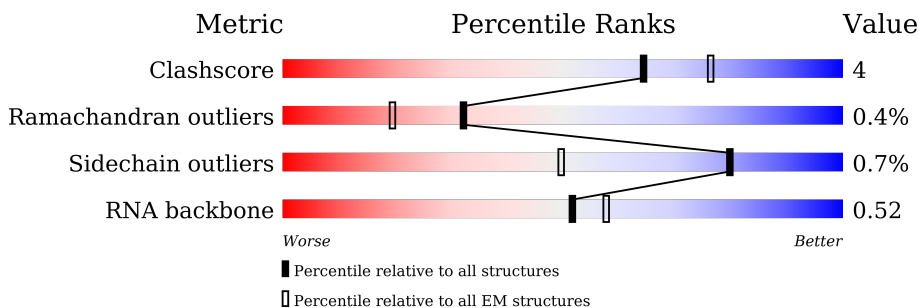
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 Å.

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
























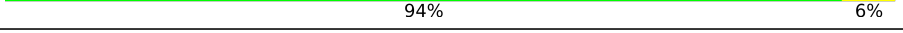



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	0	87	
2	1	71	
3	2	73	
4	3	77	
5	4	76	
6	6	70	
7	A	2903	

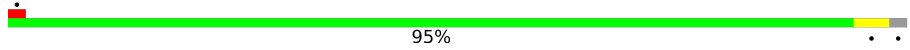

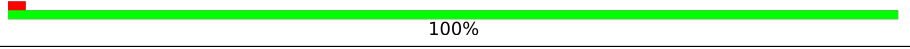
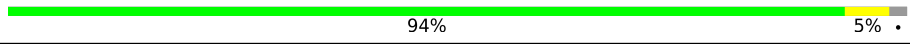
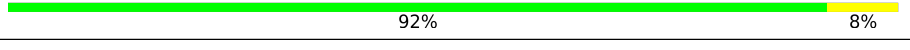

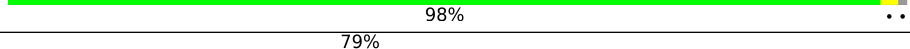
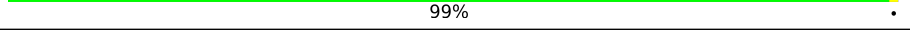
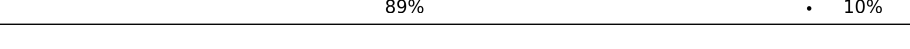
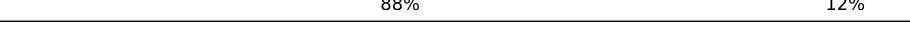
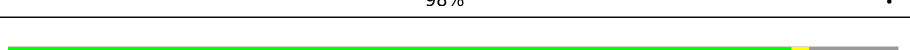

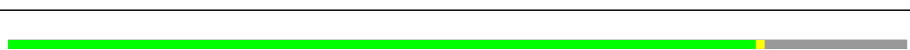
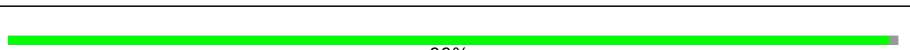
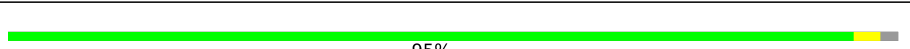
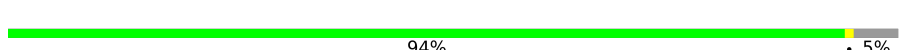

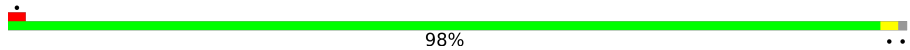
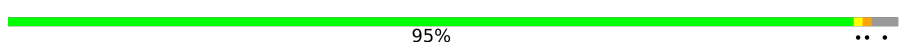
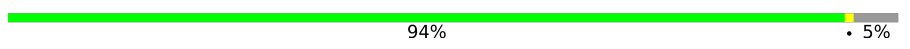
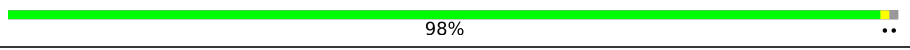
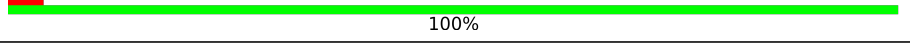



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	B	118	 79%19%.
9	C	273	 83%16%.
10	D	209	 90%10%
11	E	201	 89%11%
12	F	179	 84%15%.
13	G	177	 84%14%..
14	H	149	 27%5%68%
15	I	142	 20%73%26%..
16	J	142	 92%8%
17	K	123	 87%12%.
18	L	144	 85%12%..
19	M	136	 87%11%.
20	N	127	 87%6%6%
21	O	117	 80%18%..
22	P	115	 83%16%.
23	Q	118	 91%8%.
24	R	103	 88%12%
25	S	110	 92%8%
26	T	59	 88%10%.
27	U	104	 82%15%..
28	V	94	 94%6%
29	W	85	 82%6%12%
30	X	78	 85%14%.
31	Y	63	 75%25%.
32	Z	100	 73%23%.

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	a	57	
34	b	55	
35	c	46	
36	d	65	
37	e	38	
38	f	1539	
39	g	169	
40	h	118	
41	i	241	
42	j	233	
43	k	206	
44	l	167	
45	m	135	
46	n	179	
47	o	130	
48	p	130	
49	q	103	
50	r	129	
51	s	124	
52	t	118	
53	u	101	
54	v	89	
55	w	82	
56	x	84	
57	y	75	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
58	z	92	<div><div></div><div>86%</div><div>14%</div></div>

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 148863 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 3 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	65	Total	C	N	O	P	0	0
			1392	621	258	449	64		

- Molecule 4 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	70	Total	C	N	O	P	0	0
			1496	665	267	494	70		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	66	Total	C	N	O	P	0	0
			1406	629	255	457	65		

- Molecule 6 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	2903	Total	C	N	O	P	0	0
			62317	27801	11467	20147	2902		

- Molecule 8 is a RNA chain called 5S ribosomal rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	47	Total	C	N	O	S	0	0
			359	233	62	63	1		

- Molecule 15 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 16 is a protein called 50S ribosomal protein L13.

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

- Molecule 17 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 18 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 19 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 20 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 21 is a protein called 50S ribosomal protein L18.



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

- Molecule 22 is a protein called 50S ribosomal protein L19.

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

- Molecule 23 is a protein called 50S ribosomal protein L20.

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

- Molecule 24 is a protein called 50S ribosomal protein L21.

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

- Molecule 25 is a protein called 50S ribosomal protein L22.

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

- Molecule 26 is a protein called 50S ribosomal protein L30.

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

- Molecule 27 is a protein called 50S ribosomal protein L24.

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

- Molecule 28 is a protein called 50S ribosomal protein L25.

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

- Molecule 29 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 30 is a protein called 50S ribosomal protein L28.

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

- Molecule 31 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 32 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	96	Total	C	N	O	S	0	0
			764	484	142	136	2		

- Molecule 33 is a protein called 50S ribosomal protein L32.

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

- Molecule 34 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	b	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 35 is a protein called 50S ribosomal protein L34.

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

- Molecule 36 is a protein called 50S ribosomal protein L35.

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

- Molecule 37 is a protein called 50S ribosomal protein L36.

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

- Molecule 38 is a RNA chain called 16S ribosomal rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	1539	Total	C	N	O	P	0	0
			33015	14725	6052	10699	1539		

- Molecule 39 is a protein called Peptide deformylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	168	Total	C	N	O	S	0	0
			1346	844	241	255	6		

- Molecule 40 is a protein called Trigger factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	118	Total	C	N	O	S	0	0
			919	583	157	176	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	0	HIS	-	expression tag	UNP P0A850

- Molecule 41 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 42 is a protein called 30S ribosomal protein S3.

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

- Molecule 43 is a protein called 30S ribosomal protein S4.

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

- Molecule 44 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 45 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 46 is a protein called 30S ribosomal protein S7.

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

- Molecule 47 is a protein called 30S ribosomal protein S8.

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

- Molecule 48 is a protein called 30S ribosomal protein S9.

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

- Molecule 49 is a protein called 30S ribosomal protein S10.

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

- Molecule 50 is a protein called 30S ribosomal protein S11.

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

- Molecule 51 is a protein called 30S ribosomal protein S12.

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

- Molecule 52 is a protein called 30S ribosomal protein S13.

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

- Molecule 53 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 54 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	v	88	Total	C	N	O	S	0	0
			710	437	143	129	1		

- Molecule 55 is a protein called 30S ribosomal protein S16.

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

- Molecule 56 is a protein called 30S ribosomal protein S17.

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

- Molecule 57 is a protein called 30S ribosomal protein S18.

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


- Molecule 58 is a protein called 30S ribosomal protein S19.

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

### 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: 30S ribosomal protein S20

Chain 0: 



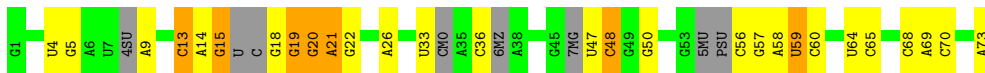
- Molecule 2: 30S ribosomal protein S21

Chain 1: 



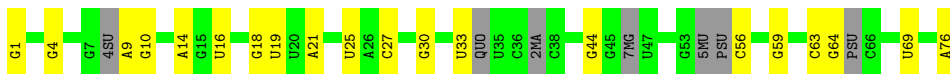
- Molecule 3: E-site tRNA

Chain 2: 



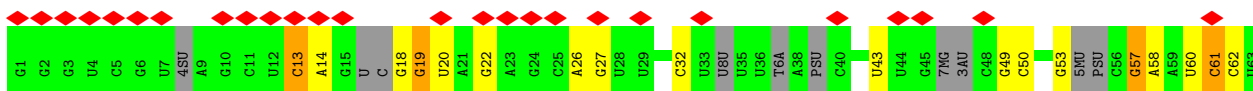
- Molecule 4: P-site tRNA

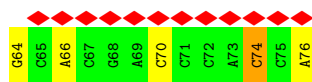
Chain 3: 



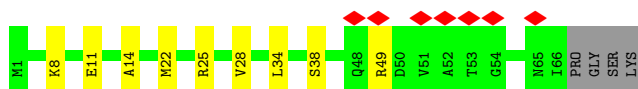
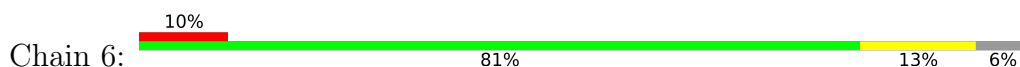
- Molecule 5: A-site tRNA

Chain 4: 

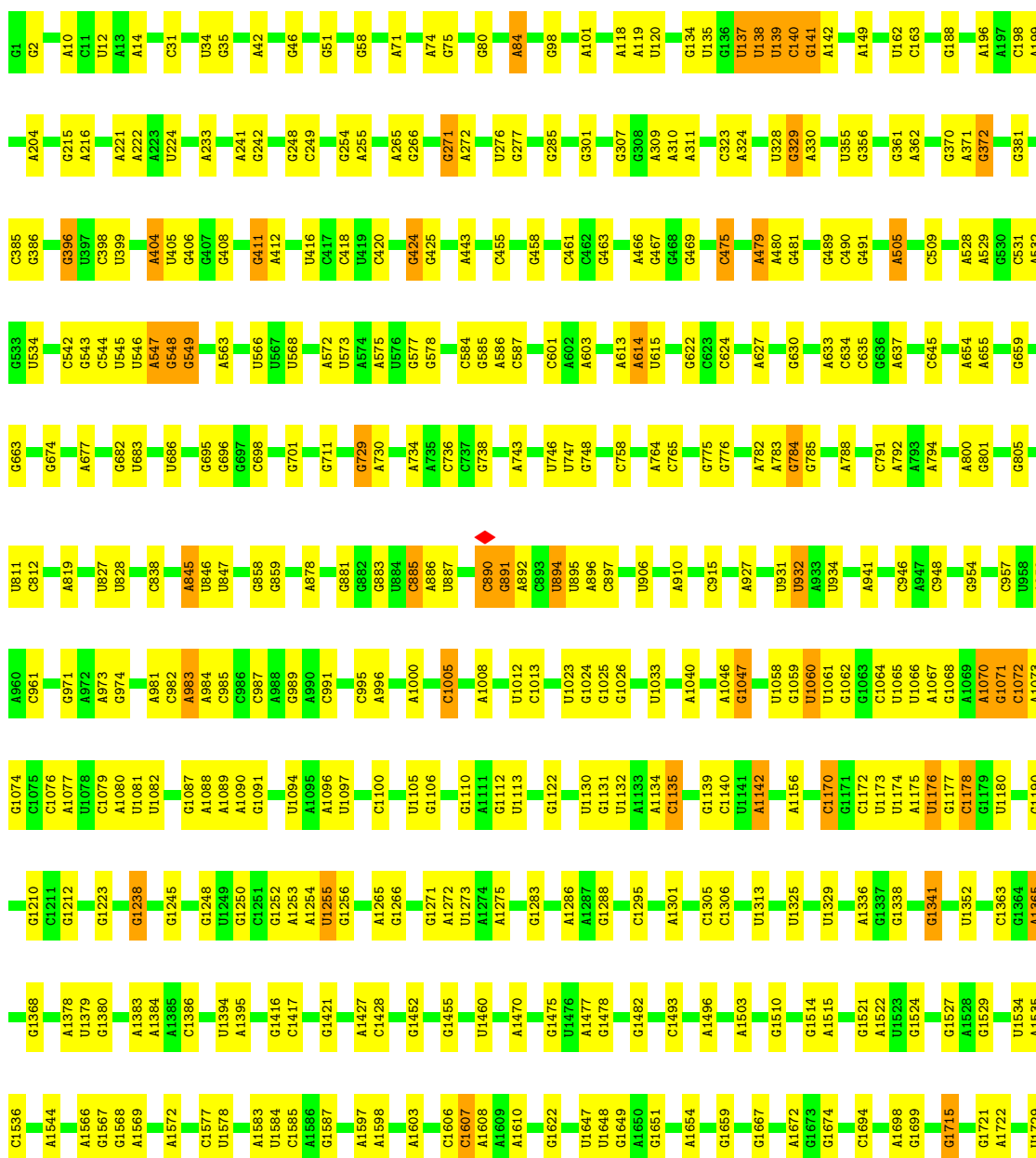
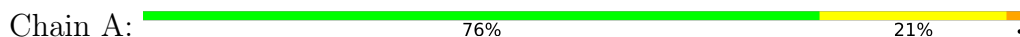




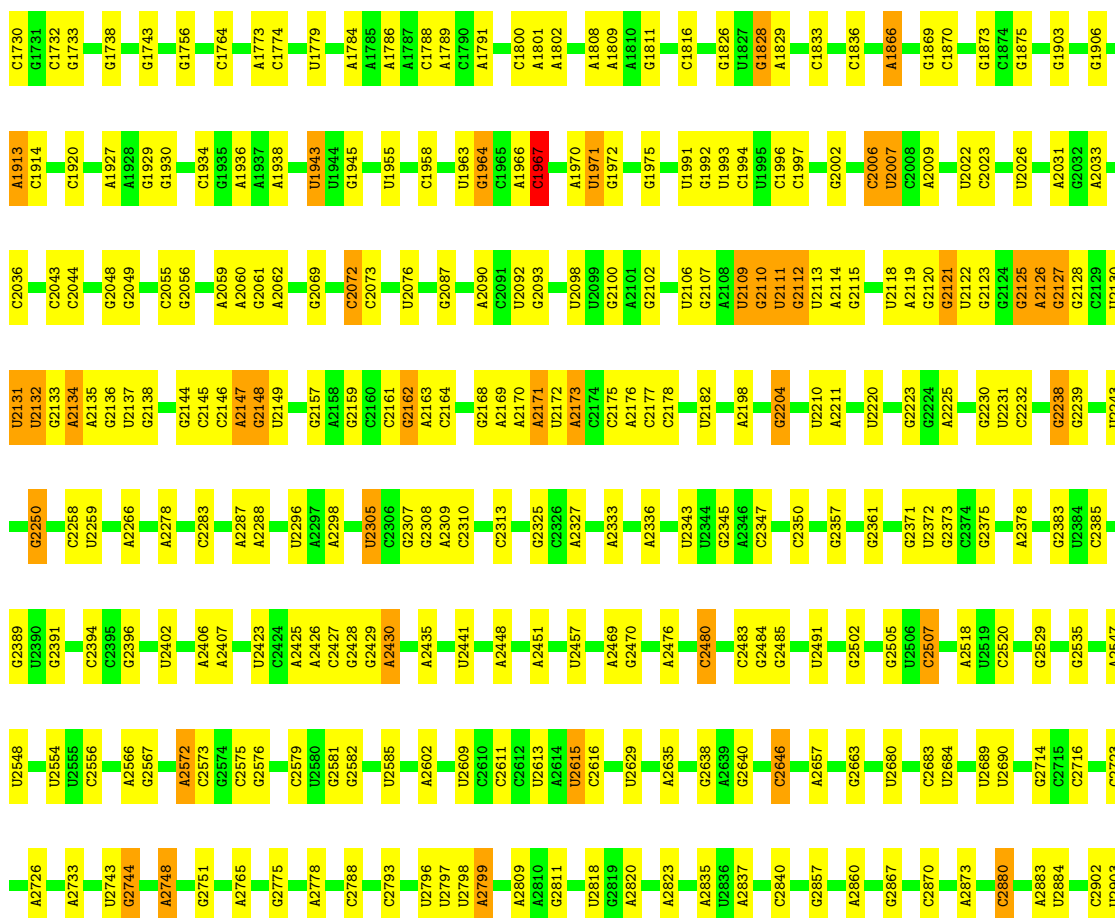
• Molecule 6: 50S ribosomal protein L31



• Molecule 7: 23S ribosomal rRNA

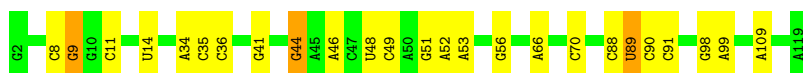






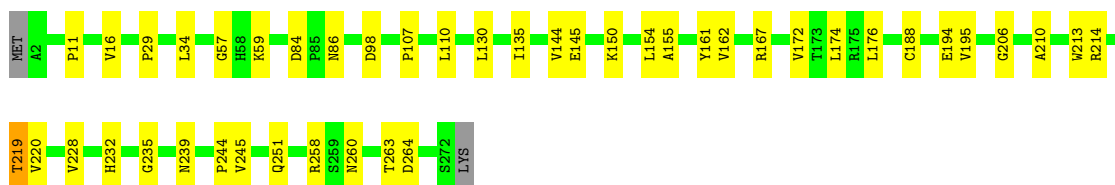
- Molecule 8: 5S ribosomal rRNA

Chain B: 79% 19% .



- Molecule 9: 50S ribosomal protein L2

Chain C: 83% 16% .




- Molecule 10: 50S ribosomal protein L3

Chain D: 90% 10%






Chain K:  87% 12%




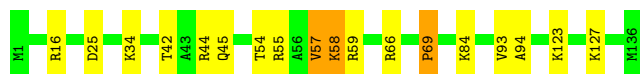
- Molecule 18: 50S ribosomal protein L15

Chain L:  85% 12%



- Molecule 19: 50S ribosomal protein L16

Chain M:  87% 11%




- Molecule 20: 50S ribosomal protein L17

Chain N:  87% 6% 6%




- Molecule 21: 50S ribosomal protein L18

Chain O:  80% 18%



- Molecule 22: 50S ribosomal protein L19

Chain P:  83% 16%




- Molecule 23: 50S ribosomal protein L20

Chain Q:  91% 8%



- Molecule 24: 50S ribosomal protein L21

Chain R:  88% 12%




- Molecule 25: 50S ribosomal protein L22

Chain S:  92% 8%




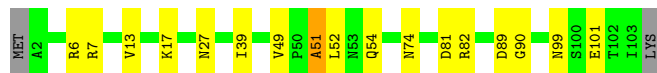
- Molecule 26: 50S ribosomal protein L30

Chain T:  88% 10% .



- Molecule 27: 50S ribosomal protein L24

Chain U:  82% 15% ..




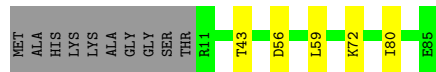
- Molecule 28: 50S ribosomal protein L25

Chain V:  94% 6%




- Molecule 29: 50S ribosomal protein L27

Chain W:  82% 6% 12%

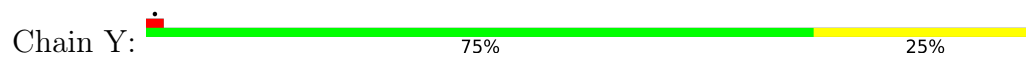


- Molecule 30: 50S ribosomal protein L28

Chain X:  85% 14% .



- Molecule 31: 50S ribosomal protein L29



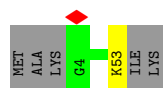
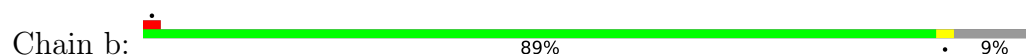
- Molecule 32: 50S ribosomal protein L23



- Molecule 33: 50S ribosomal protein L32



- Molecule 34: 50S ribosomal protein L33



- Molecule 35: 50S ribosomal protein L34



- Molecule 36: 50S ribosomal protein L35

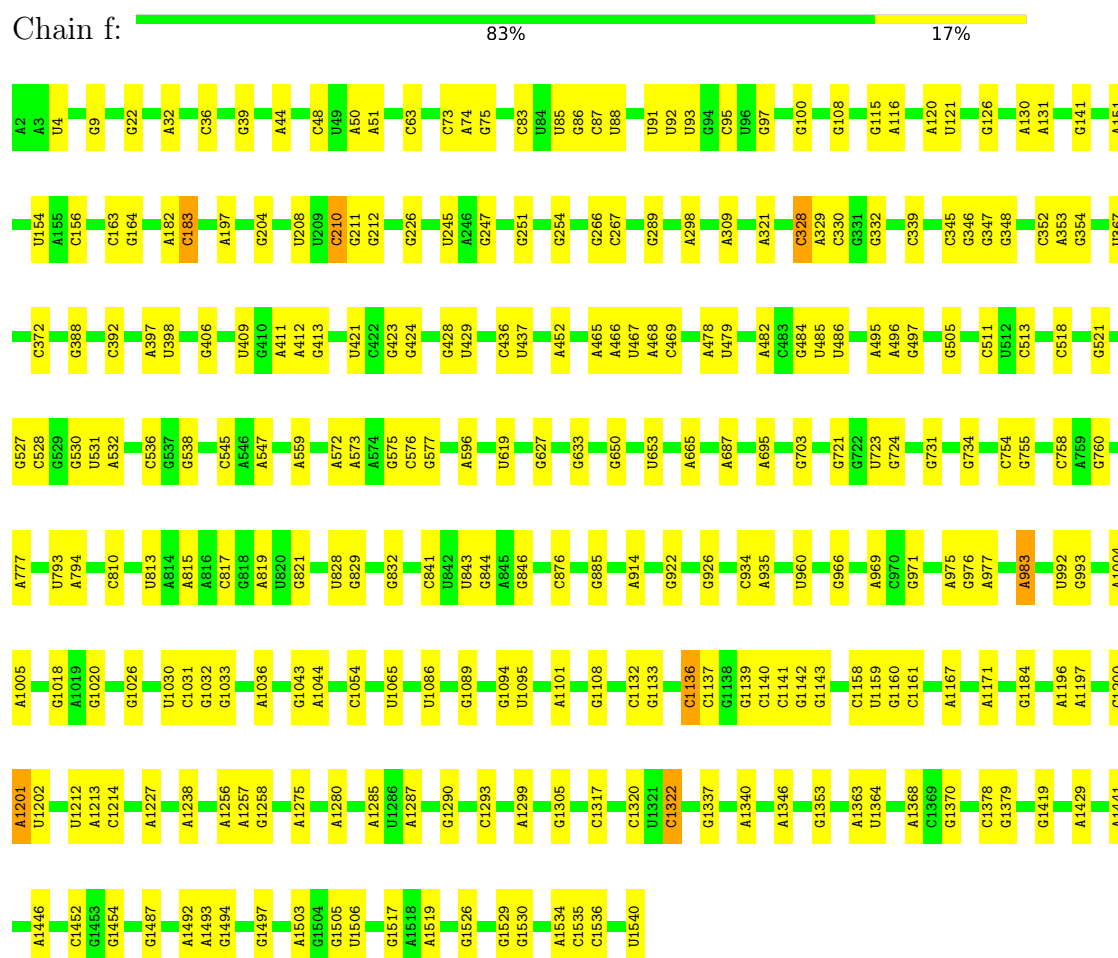


- Molecule 37: 50S ribosomal protein L36



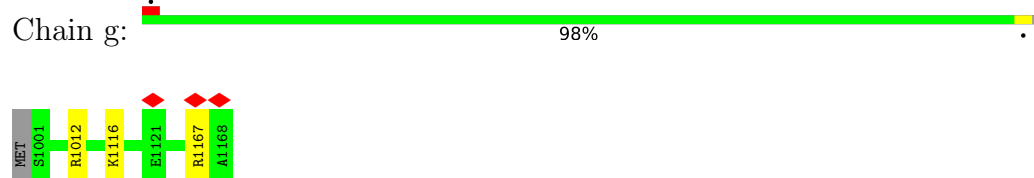
- Molecule 38: 16S ribosomal rRNA

Chain f:



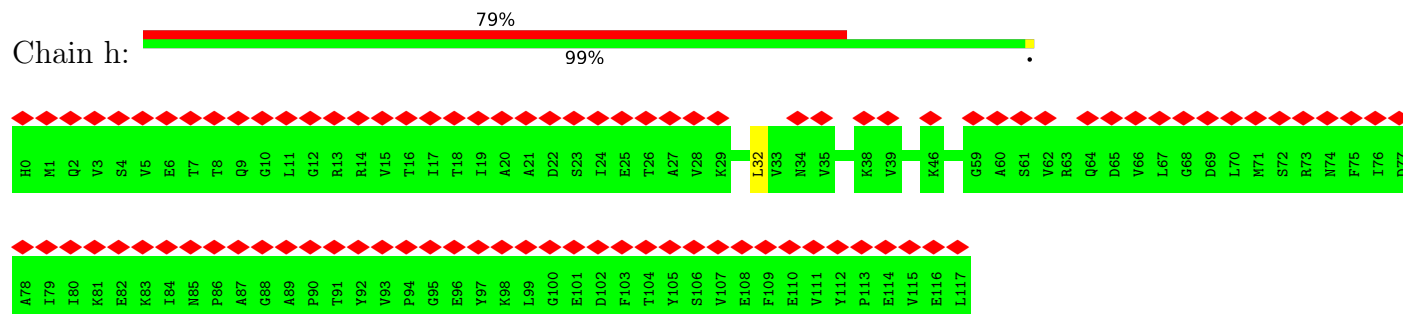
- Molecule 39: Peptide deformylase

Chain g:



- Molecule 40: Trigger factor

Chain h:



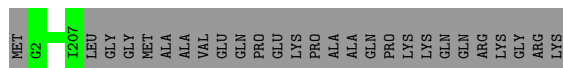
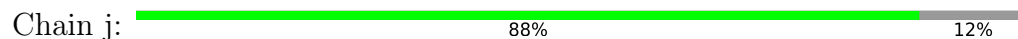
- Molecule 41: 30S ribosomal protein S2

Chain i:





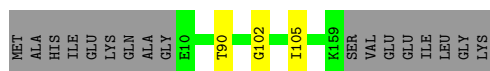
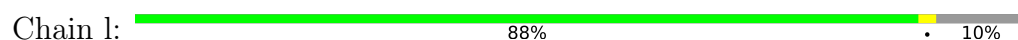
- Molecule 42: 30S ribosomal protein S3



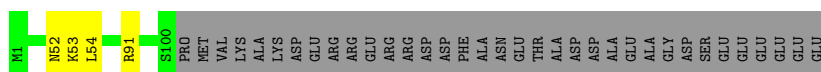
- Molecule 43: 30S ribosomal protein S4



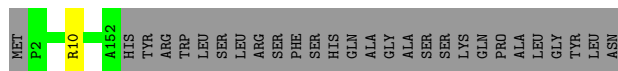
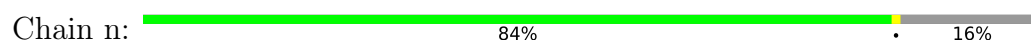
- Molecule 44: 30S ribosomal protein S5



- Molecule 45: 30S ribosomal protein S6, fully modified isoform



- Molecule 46: 30S ribosomal protein S7



- Molecule 47: 30S ribosomal protein S8



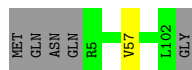
- Molecule 48: 30S ribosomal protein S9





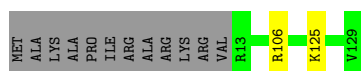
- Molecule 49: 30S ribosomal protein S10

Chain q: 94% • 5%



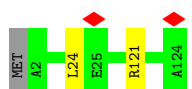
- Molecule 50: 30S ribosomal protein S11

Chain r: 89% • 9%



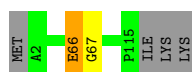
- Molecule 51: 30S ribosomal protein S12

Chain s: 98% ••



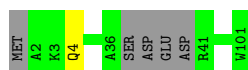
- Molecule 52: 30S ribosomal protein S13

Chain t: 95% ••



- Molecule 53: 30S ribosomal protein S14

Chain u: 94% • 5%



- Molecule 54: 30S ribosomal protein S15

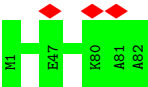
Chain v: 98% ••



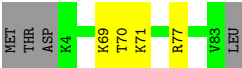
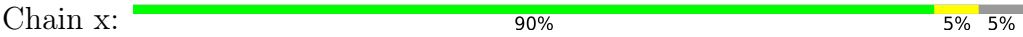
- Molecule 55: 30S ribosomal protein S16

Chain w: 100%

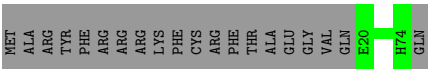




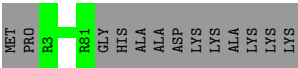
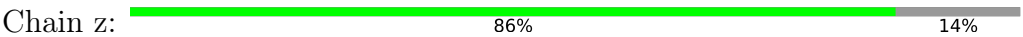
• Molecule 56: 30S ribosomal protein S17



• Molecule 57: 30S ribosomal protein S18



• Molecule 58: 30S ribosomal protein S19



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	194157	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	32.57	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	25.576	Depositor
Minimum map value	-14.991	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	441.6, 441.6, 441.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	0	0.27	0/671	0.50	0/888
2	1	0.35	0/430	0.74	2/570 (0.4%)
3	2	0.28	0/1551	0.89	1/2404 (0.0%)
4	3	0.49	1/1664 (0.1%)	0.89	0/2577
5	4	0.26	0/1565	0.92	1/2421 (0.0%)
6	6	0.28	0/531	0.51	0/709
7	A	0.87	2/69796 (0.0%)	0.95	77/108888 (0.1%)
8	B	0.66	0/2828	0.89	1/4410 (0.0%)
9	C	0.50	0/2121	0.61	1/2852 (0.0%)
10	D	0.48	0/1586	0.57	0/2134
11	E	0.44	0/1571	0.53	0/2113
12	F	0.32	0/1434	0.52	0/1926
13	G	0.35	0/1343	0.52	0/1816
14	H	0.36	0/364	0.69	0/490
15	I	0.28	0/1046	0.60	1/1410 (0.1%)
16	J	0.46	0/1152	0.51	0/1551
17	K	0.46	0/947	0.63	0/1268
18	L	0.44	0/1054	0.65	1/1403 (0.1%)
19	M	0.43	0/1093	0.57	0/1460
20	N	0.44	0/973	0.62	0/1301
21	O	0.37	0/902	0.50	0/1209
22	P	0.45	0/929	0.56	1/1242 (0.1%)
23	Q	0.53	0/960	0.52	0/1278
24	R	0.46	0/829	0.57	0/1107
25	S	0.42	0/864	0.52	0/1156
26	T	0.40	0/453	0.58	0/605
27	U	0.42	0/787	0.57	0/1051
28	V	0.38	0/766	0.50	0/1025
29	W	0.45	0/576	0.51	0/762
30	X	0.45	0/635	0.49	0/848
31	Y	0.36	0/510	0.51	0/677
32	Z	0.39	0/771	0.63	0/1031
33	a	0.43	0/450	0.62	0/599
34	b	0.35	0/416	0.53	0/554

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	c	0.46	0/380	0.56	0/498
36	d	0.44	0/513	0.66	0/676
37	e	0.45	0/303	0.59	0/397
38	f	0.59	0/36966	0.89	28/57666 (0.0%)
39	g	0.28	0/1361	0.58	0/1830
40	h	0.28	0/933	0.57	1/1261 (0.1%)
41	i	0.32	0/1735	0.56	0/2338
42	j	0.32	0/1651	0.52	0/2225
43	k	0.32	0/1665	0.58	0/2227
44	l	0.39	0/1118	0.63	0/1504
45	m	0.34	0/835	0.65	1/1128 (0.1%)
46	n	0.29	0/1195	0.48	0/1602
47	o	0.36	0/989	0.50	0/1326
48	p	0.31	0/1034	0.57	0/1375
49	q	0.31	0/796	0.58	0/1077
50	r	0.35	0/893	0.55	0/1205
51	s	0.36	0/969	0.60	0/1300
52	t	0.30	0/892	0.56	0/1193
53	u	0.30	0/785	0.52	0/1043
54	v	0.32	0/718	0.53	0/959
55	w	0.29	0/659	0.56	0/884
56	x	0.32	0/657	0.67	0/881
57	y	0.34	0/462	0.51	0/621
58	z	0.30	0/652	0.52	0/877
All	All	0.68	3/161729 (0.0%)	0.85	116/241828 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	D	0	1
12	F	0	1
13	G	0	2
17	K	0	1
18	L	0	1
19	M	0	2
20	N	0	1
27	U	0	2
33	a	0	1
36	d	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
37	e	0	1
41	i	0	1
43	k	0	1
44	l	0	2
45	m	0	2
48	p	0	1
51	s	0	1
52	t	0	1
56	x	0	2
All	All	0	25

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	1	G	OP3-P	-10.68	1.48	1.61
7	A	1142	A	N9-C4	-5.69	1.34	1.37
7	A	528	A	N9-C4	-5.29	1.34	1.37

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	f	328	C	N1-C2-O2	9.60	124.66	118.90
45	m	54	LEU	CA-CB-CG	9.20	136.46	115.30
38	f	328	C	C2-N1-C1'	8.62	128.28	118.80
7	A	12	U	N3-C2-O2	-8.44	116.30	122.20
38	f	328	C	N3-C2-O2	-8.14	116.20	121.90
38	f	1322	C	C2-N1-C1'	7.72	127.29	118.80
7	A	475	C	C6-N1-C2	-7.56	117.28	120.30
38	f	1322	C	N1-C2-O2	7.52	123.41	118.90
38	f	1158	C	C2-N1-C1'	7.40	126.94	118.80
38	f	754	C	C2-N1-C1'	7.29	126.81	118.80
7	A	1313	U	C2-N1-C1'	7.28	126.43	117.70
7	A	12	U	N1-C2-O2	7.25	127.88	122.80
38	f	328	C	C6-N1-C2	-7.19	117.42	120.30
7	A	475	C	C5-C6-N1	7.12	124.56	121.00
7	A	1913	A	P-O3'-C3'	7.09	128.21	119.70
38	f	1158	C	N1-C2-O2	7.03	123.12	118.90
7	A	2616	C	C6-N1-C2	-7.03	117.49	120.30
38	f	1322	C	N3-C2-O2	-7.01	116.99	121.90
15	I	11	LEU	CA-CB-CG	6.92	131.22	115.30
38	f	983	A	C2-N3-C4	6.88	114.04	110.60
7	A	1788	C	C6-N1-C2	-6.84	117.56	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	f	754	C	N1-C2-O2	6.84	123.00	118.90
7	A	1788	C	C5-C6-N1	6.69	124.34	121.00
7	A	2870	C	C6-N1-C2	-6.62	117.65	120.30
7	A	271	G	P-O3'-C3'	6.59	127.61	119.70
38	f	1201	A	P-O3'-C3'	6.55	127.56	119.70
22	P	114	LEU	CA-CB-CG	6.53	130.33	115.30
7	A	2723	C	C5-C6-N1	6.50	124.25	121.00
7	A	12	U	C2-N1-C1'	6.50	125.50	117.70
7	A	404	A	P-O3'-C3'	6.47	127.47	119.70
7	A	528	A	N7-C8-N9	6.47	117.03	113.80
7	A	1313	U	N3-C2-O2	-6.45	117.68	122.20
7	A	2723	C	C6-N1-C2	-6.43	117.73	120.30
7	A	2616	C	C5-C6-N1	6.37	124.19	121.00
7	A	1313	U	N1-C2-O2	6.36	127.25	122.80
7	A	528	A	C5-N7-C8	-6.35	100.73	103.90
7	A	528	A	C8-N9-C4	-6.34	103.26	105.80
7	A	915	C	N1-C2-O2	6.28	122.67	118.90
7	A	1135	C	N1-C2-O2	6.19	122.61	118.90
38	f	115	G	P-O3'-C3'	6.14	127.06	119.70
7	A	1958	C	C6-N1-C2	-6.04	117.89	120.30
7	A	2884	U	N3-C2-O2	-6.01	117.99	122.20
2	1	16	LEU	CA-CB-CG	6.00	129.10	115.30
7	A	1994	C	C6-N1-C2	-5.99	117.90	120.30
7	A	1967	C	N1-C2-O2	5.96	122.47	118.90
7	A	1920	C	C5-C6-N1	5.92	123.96	121.00
7	A	634	C	C5-C6-N1	5.88	123.94	121.00
7	A	545	U	C2-N1-C1'	5.84	124.71	117.70
7	A	2430	A	C2-N3-C4	5.84	113.52	110.60
7	A	890	C	P-O3'-C3'	5.82	126.68	119.70
7	A	2006	C	C5-C6-N1	5.73	123.86	121.00
38	f	183	C	N1-C2-O2	5.73	122.34	118.90
7	A	890	C	OP2-P-O3'	5.72	117.80	105.20
7	A	2026	U	C5-C6-N1	5.71	125.55	122.70
38	f	754	C	N3-C2-O2	-5.71	117.91	121.90
7	A	624	C	C6-N1-C2	-5.69	118.02	120.30
7	A	461	C	C6-N1-C2	-5.68	118.03	120.30
38	f	536	C	C6-N1-C2	-5.68	118.03	120.30
7	A	1005	C	C6-N1-C2	-5.67	118.03	120.30
7	A	601	C	C6-N1-C2	-5.65	118.04	120.30
7	A	2884	U	C2-N1-C1'	5.64	124.46	117.70
7	A	885	C	P-O3'-C3'	5.62	126.45	119.70
38	f	983	A	N3-C4-N9	5.62	131.90	127.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	f	1158	C	N3-C2-O2	-5.56	118.01	121.90
7	A	1836	C	C5-C6-N1	5.53	123.77	121.00
38	f	328	C	C6-N1-C1'	-5.50	114.20	120.80
38	f	1322	C	C6-N1-C1'	-5.43	114.28	120.80
7	A	1135	C	C2-N1-C1'	5.43	124.77	118.80
7	A	1295	C	C6-N1-C2	-5.40	118.14	120.30
7	A	461	C	C5-C6-N1	5.40	123.70	121.00
7	A	729	G	C4-N9-C1'	5.37	133.47	126.50
7	A	758	C	C6-N1-C2	-5.36	118.15	120.30
7	A	2751	G	C4-N9-C1'	5.32	133.41	126.50
38	f	36	C	N1-C2-O2	5.31	122.08	118.90
9	C	130	LEU	CA-CB-CG	5.30	127.50	115.30
7	A	418	C	C6-N1-C2	-5.30	118.18	120.30
7	A	635	C	C6-N1-C2	-5.29	118.19	120.30
7	A	323	C	N1-C2-O2	5.28	122.06	118.90
7	A	634	C	C6-N1-C2	-5.27	118.19	120.30
7	A	1774	C	C6-N1-C2	-5.25	118.20	120.30
7	A	2006	C	C6-N1-C2	-5.25	118.20	120.30
38	f	528	C	C6-N1-C2	-5.25	118.20	120.30
7	A	2073	C	C6-N1-C2	-5.24	118.20	120.30
38	f	328	C	C5-C6-N1	5.23	123.61	121.00
7	A	271	G	OP1-P-O3'	5.22	116.69	105.20
7	A	2250	G	C5-N7-C8	-5.22	101.69	104.30
7	A	2880	C	N1-C2-O2	5.21	122.03	118.90
38	f	1136	C	N1-C2-O2	5.21	122.02	118.90
7	A	915	C	C2-N1-C1'	5.18	124.50	118.80
3	2	33	U	C2-N1-C1'	5.18	123.92	117.70
7	A	2250	G	C4-C5-N7	5.18	112.87	110.80
38	f	210	C	C2-N1-C1'	5.17	124.49	118.80
40	h	32	LEU	CA-CB-CG	5.17	127.20	115.30
7	A	838	C	C6-N1-C2	-5.15	118.24	120.30
7	A	915	C	N3-C2-O2	-5.15	118.30	121.90
7	A	1920	C	C6-N1-C2	-5.12	118.25	120.30
7	A	2615	U	N1-C2-O2	5.12	126.38	122.80
7	A	2646	C	C6-N1-C2	-5.12	118.25	120.30
8	B	89	U	C2-N1-C1'	5.12	123.84	117.70
7	A	2072	C	C6-N1-C2	-5.12	118.25	120.30
7	A	736	C	C6-N1-C2	-5.11	118.25	120.30
5	4	13	C	P-O3'-C3'	5.10	125.83	119.70
7	A	1836	C	C6-N1-C2	-5.10	118.26	120.30
7	A	2884	U	N1-C2-O2	5.10	126.37	122.80
7	A	1958	C	C5-C6-N1	5.10	123.55	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	f	1158	C	C6-N1-C1'	-5.08	114.70	120.80
7	A	2007	U	C5-C6-N1	5.08	125.24	122.70
38	f	36	C	C6-N1-C2	-5.07	118.27	120.30
2	1	37	PHE	C-N-CA	5.06	134.36	121.70
7	A	545	U	N3-C2-O2	-5.06	118.66	122.20
7	A	2870	C	C5-C6-N1	5.06	123.53	121.00
18	L	29	LYS	C-N-CA	5.05	134.32	121.70
7	A	2480	C	C5-C6-N1	5.05	123.52	121.00
7	A	2232	C	C6-N1-C2	-5.04	118.28	120.30
7	A	891	G	N1-C6-O6	5.01	122.90	119.90
7	A	2072	C	C5-C6-N1	5.00	123.50	121.00

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	D	151	THR	Peptide
12	F	174	ASP	Peptide
13	G	46	ALA	Peptide
13	G	47	ASP	Peptide
17	K	92	GLU	Peptide
18	L	55	MET	Peptide
19	M	57	VAL	Peptide
19	M	58	LYS	Peptide
20	N	2	ARG	Peptide
27	U	6	ARG	Peptide
27	U	89	ASP	Peptide
33	a	54	VAL	Peptide
36	d	31	HIS	Peptide
37	e	20	ASP	Peptide
41	i	34	ALA	Peptide
43	k	28	ILE	Peptide
44	l	102	GLY	Peptide
44	l	105	ILE	Peptide
45	m	52	ASN	Peptide
45	m	53	LYS	Peptide
48	p	55	VAL	Peptide
51	s	24	LEU	Peptide
52	t	66	GLU	Peptide
56	x	69	LYS	Peptide
56	x	70	THR	Peptide



## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	665	0	714	9	0
2	1	425	0	449	7	0
3	2	1392	0	714	16	0
4	3	1496	0	764	7	0
5	4	1406	0	722	6	0
6	6	522	0	522	6	0
7	A	62317	0	31345	179	0
8	B	2529	0	1281	11	0
9	C	2082	0	2154	26	0
10	D	1565	0	1616	14	0
11	E	1552	0	1619	15	0
12	F	1410	0	1444	18	0
13	G	1323	0	1371	17	0
14	H	359	0	381	5	0
15	I	1032	0	1085	25	0
16	J	1129	0	1162	7	0
17	K	938	0	1012	9	0
18	L	1045	0	1117	17	0
19	M	1074	0	1157	13	0
20	N	960	0	1000	5	0
21	O	892	0	923	17	0
22	P	917	0	962	10	0
23	Q	947	0	1019	8	0
24	R	816	0	839	9	0
25	S	857	0	922	5	0
26	T	449	0	488	4	0
27	U	779	0	831	8	0
28	V	753	0	780	4	0
29	W	569	0	581	4	0
30	X	625	0	652	8	0
31	Y	509	0	543	18	0
32	Z	764	0	829	26	0
33	a	444	0	458	0	0
34	b	409	0	440	0	0
35	c	377	0	418	0	0
36	d	504	0	572	0	0
37	e	302	0	343	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	f	33015	0	16617	0	0
39	g	1346	0	1391	0	0
40	h	919	0	938	0	0
41	i	1704	0	1732	0	0
42	j	1624	0	1696	0	0
43	k	1643	0	1707	0	0
44	l	1105	0	1148	0	0
45	m	817	0	808	0	0
46	n	1181	0	1238	0	0
47	o	979	0	1031	0	0
48	p	1022	0	1070	0	0
49	q	786	0	828	0	0
50	r	877	0	887	0	0
51	s	955	0	1016	0	0
52	t	883	0	941	0	0
53	u	774	0	824	0	0
54	v	710	0	728	0	0
55	w	649	0	666	0	0
56	x	648	0	691	0	0
57	y	455	0	478	0	0
58	z	637	0	665	0	0
All	All	148863	0	100329	435	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 4.

All (435) 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)
31:Y:21:LEU:CD1	32:Z:5:GLU:OE2	1.82	1.28
31:Y:21:LEU:HD13	32:Z:5:GLU:OE2	1.33	1.25
31:Y:21:LEU:HD11	32:Z:5:GLU:OE2	1.70	0.91
31:Y:33:ALA:CB	32:Z:13:ALA:HB1	2.03	0.88
31:Y:33:ALA:HB2	32:Z:13:ALA:CB	2.18	0.74
31:Y:33:ALA:HB1	32:Z:13:ALA:HB1	1.71	0.71
7:A:1071:G:H22	7:A:1090:A:H62	1.37	0.71
7:A:1047:G:HO2'	7:A:1110:G:H1	1.37	0.70
7:A:1341:G:H21	32:Z:59:ASN:HD22	1.39	0.69
31:Y:33:ALA:HB2	32:Z:13:ALA:HB1	1.74	0.66
7:A:1059:G:H21	15:I:128:SER:HA	1.61	0.65
23:Q:44:GLN:HE21	24:R:77:PHE:HB3	1.62	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:110:THR:HG21	10:D:169:ARG:HH11	1.62	0.64
7:A:2336:A:H61	29:W:43:THR:HG21	1.63	0.64
16:J:62:VAL:HG11	16:J:101:ILE:HD11	1.80	0.63
3:2:5:G:N2	3:2:68:C:N3	2.45	0.63
18:L:74:THR:HG22	18:L:107:PHE:HB2	1.80	0.63
5:4:19:G:H1	5:4:57:G:H21	1.46	0.62
7:A:2126:A:H62	7:A:2171:A:H5''	1.64	0.62
7:A:1365:A:OP1	30:X:3:ARG:NH2	2.34	0.61
3:2:4:U:H3	3:2:70:C:H42	1.45	0.61
11:E:5:LEU:HD12	11:E:10:SER:HB2	1.82	0.61
32:Z:24:MET:HG2	32:Z:93:LEU:HD21	1.83	0.60
2:1:41:PRO:HA	2:1:44:GLU:HB3	1.82	0.60
30:X:19:SER:OG	30:X:20:HIS:N	2.35	0.60
7:A:1607:C:N4	7:A:1622:G:OP2	2.35	0.60
2:1:10:GLU:HG2	2:1:11:PRO:HD3	1.82	0.59
3:2:20:G:O2'	3:2:48:C:N4	2.35	0.59
4:3:56:C:N3	12:F:80:ARG:NH2	2.51	0.59
22:P:63:LYS:HE3	22:P:65:SER:HB2	1.84	0.59
15:I:37:GLU:HA	15:I:41:ALA:HB3	1.82	0.59
32:Z:3:ARG:NE	32:Z:3:ARG:O	2.36	0.59
7:A:2121:G:N2	7:A:2176:A:N1	2.50	0.59
13:G:86:LYS:HG2	13:G:132:VAL:HG22	1.85	0.58
25:S:59:GLU:HB2	25:S:66:ILE:HD11	1.85	0.58
9:C:29:PRO:HG2	9:C:34:LEU:HD11	1.85	0.58
7:A:2204:G:H4'	9:C:150:LYS:HD3	1.85	0.58
7:A:2109:U:O2	7:A:2110:G:N2	2.37	0.58
9:C:235:GLY:O	9:C:239:ASN:ND2	2.36	0.58
31:Y:33:ALA:HB2	32:Z:13:ALA:HB2	1.86	0.58
8:B:9:G:HO2'	21:O:45:SER:HG	1.49	0.57
9:C:258:ARG:NH1	9:C:264:ASP:OD1	2.37	0.57
13:G:104:ASN:ND2	13:G:114:ASP:OD1	2.38	0.57
7:A:883:G:N2	7:A:894:U:O2'	2.37	0.57
7:A:2296:U:O4	21:O:9:ARG:NH2	2.36	0.57
7:A:2484:G:OP1	19:M:44:ARG:NH2	2.36	0.57
19:M:69:PRO:HA	19:M:94:ALA:HB2	1.86	0.57
7:A:698:C:O2'	7:A:734:A:N6	2.38	0.57
7:A:2744:G:H21	13:G:143:GLN:HE22	1.53	0.57
7:A:370:G:O2'	7:A:424:G:OP1	2.22	0.57
26:T:6:LYS:HG2	26:T:37:GLU:HB3	1.87	0.57
7:A:1173:U:O2	7:A:1176:U:N3	2.38	0.57
7:A:2483:C:N3	19:M:123:LYS:NZ	2.53	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2796:U:H3	7:A:2799:A:H61	1.53	0.56
31:Y:26:PHE:CZ	32:Z:50:LEU:HD23	2.40	0.56
18:L:91:ASP:OD1	18:L:91:ASP:N	2.38	0.56
20:N:22:ARG:HG3	20:N:70:THR:HA	1.87	0.56
21:O:31:THR:O	21:O:102:ARG:NH1	2.38	0.56
3:2:56:C:O2	7:A:2112:G:N2	2.38	0.56
7:A:1791:A:N6	7:A:1828:G:O2'	2.39	0.56
7:A:1936:A:H2	7:A:1943:U:H3	1.52	0.56
7:A:2305:U:H5''	12:F:131:GLY:HA3	1.87	0.56
7:A:2857:G:N2	7:A:2860:A:OP2	2.36	0.56
9:C:161:TYR:HB3	9:C:194:GLU:HB2	1.87	0.56
22:P:2:SER:OG	22:P:3:ASN:N	2.38	0.56
16:J:125:TYR:OH	16:J:132:HIS:NE2	2.35	0.56
7:A:682:G:O6	7:A:794:A:N6	2.38	0.56
24:R:46:GLU:OE2	24:R:48:LYS:NZ	2.39	0.56
5:4:18:G:O6	5:4:61:C:N4	2.39	0.55
5:4:76:A:HO3'	7:A:2451:A:HO2'	1.54	0.55
12:F:2:ALA:N	12:F:94:GLU:OE2	2.39	0.55
7:A:729:G:N2	9:C:11:PRO:O	2.39	0.55
15:I:123:GLU:O	15:I:127:ARG:NH1	2.39	0.55
32:Z:6:ARG:NH2	32:Z:37:ASP:OD1	2.39	0.55
7:A:2134:A:O2'	7:A:2159:G:N3	2.39	0.55
7:A:2575:C:OP1	10:D:149:ASN:ND2	2.40	0.55
7:A:301:G:OP2	27:U:82:ARG:NH1	2.39	0.55
15:I:81:LYS:HA	15:I:136:MET:HE1	1.87	0.55
11:E:6:LYS:HG3	11:E:119:ILE:HG23	1.87	0.55
7:A:1170:C:N3	7:A:1178:C:N4	2.55	0.54
28:V:77:VAL:HG23	28:V:89:ILE:HG12	1.88	0.54
9:C:210:ALA:O	9:C:214:ARG:NH1	2.40	0.54
11:E:176:ASP:N	11:E:176:ASP:OD1	2.37	0.54
30:X:12:PRO:HB3	30:X:30:LEU:HD23	1.88	0.54
7:A:1336:A:OP2	32:Z:68:LYS:NZ	2.38	0.54
9:C:135:ILE:O	9:C:167:ARG:NH1	2.40	0.54
7:A:1341:G:H21	32:Z:59:ASN:ND2	2.04	0.54
7:A:2092:U:OP2	14:H:27:ARG:NH2	2.40	0.54
32:Z:7:LEU:HD12	32:Z:46:ALA:HA	1.89	0.54
3:2:4:U:O4	3:2:69:A:N6	2.41	0.54
17:K:70:ARG:HG2	17:K:76:VAL:HG12	1.90	0.54
32:Z:61:LEU:HD21	32:Z:82:LYS:HD2	1.90	0.54
7:A:138:U:H4'	7:A:140:C:H42	1.73	0.53
7:A:138:U:H5'	32:Z:1:MET:CE	2.37	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:987:C:O2'	7:A:1000:A:N3	2.39	0.53
7:A:2298:A:OP1	12:F:71:ARG:NH2	2.40	0.53
11:E:153:LEU:HD11	11:E:158:PHE:HB2	1.90	0.53
31:Y:49:ASP:OD1	31:Y:52:ARG:NH2	2.41	0.53
9:C:16:VAL:HG22	9:C:206:GLY:HA3	1.90	0.53
13:G:121:ILE:HD12	13:G:141:ILE:HG22	1.89	0.53
7:A:505:A:HO2'	7:A:509:C:HO2'	1.55	0.53
22:P:51:ARG:NH1	22:P:56:HIS:O	2.42	0.53
7:A:2006:C:O2'	7:A:2823:A:N3	2.41	0.53
17:K:63:VAL:HG12	17:K:107:LEU:HD11	1.89	0.53
15:I:80:LEU:HD22	15:I:84:ALA:HB2	1.90	0.53
27:U:74:ASN:ND2	27:U:81:ASP:OD2	2.42	0.53
7:A:2840:C:H5''	20:N:53:THR:HG21	1.89	0.53
27:U:51:ALA:O	27:U:54:GLN:NE2	2.42	0.53
7:A:572:A:OP2	24:R:80:ARG:NH2	2.42	0.53
7:A:2122:U:H3	7:A:2177:C:H1'	1.73	0.53
7:A:2635:A:O2'	10:D:49:GLN:NE2	2.42	0.53
28:V:51:GLN:OE1	28:V:57:TYR:OH	2.27	0.53
7:A:981:A:OP2	7:A:982:C:N4	2.42	0.53
7:A:2485:G:OP1	19:M:45:GLN:NE2	2.39	0.53
12:F:34:ILE:HG12	12:F:156:ILE:HG12	1.90	0.53
7:A:2638:G:O2'	7:A:2775:G:N2	2.41	0.52
7:A:443:A:N6	11:E:36:ALA:O	2.41	0.52
4:3:63:C:H2'	4:3:64:G:H8	1.75	0.52
7:A:309:A:N3	7:A:329:G:O2'	2.41	0.52
7:A:1826:G:O2'	7:A:1971:U:OP2	2.27	0.52
22:P:106:LYS:O	22:P:109:ARG:NH2	2.37	0.52
30:X:2:SER:OG	30:X:3:ARG:N	2.41	0.52
4:3:27:C:O2	4:3:44:G:N2	2.42	0.52
15:I:78:VAL:O	15:I:82:LYS:NZ	2.43	0.52
19:M:55:ARG:O	19:M:55:ARG:NH2	2.42	0.52
26:T:41:THR:HG23	26:T:43:ALA:H	1.74	0.52
2:1:7:ARG:NH1	2:1:8:GLU:O	2.43	0.52
7:A:2743:U:O2'	13:G:153:ARG:NH1	2.43	0.52
16:J:11:VAL:HG21	16:J:50:THR:HG22	1.92	0.52
7:A:1252:G:H22	23:Q:37:GLN:HE21	1.57	0.52
7:A:396:G:OP2	30:X:10:LYS:NZ	2.42	0.51
7:A:2144:G:O2'	7:A:2147:A:N6	2.42	0.51
7:A:971:G:O2'	7:A:983:A:N3	2.43	0.51
9:C:219:THR:O	9:C:219:THR:OG1	2.25	0.51
3:2:18:G:O2'	3:2:57:G:O6	2.28	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2788:C:O2'	7:A:2809:A:N3	2.37	0.51
7:A:585:G:N7	23:Q:6:ARG:NH1	2.58	0.51
7:A:1113:U:H5'	13:G:3:ARG:HH12	1.75	0.51
11:E:41:GLN:NE2	11:E:43:THR:OG1	2.42	0.51
13:G:80:THR:OG1	13:G:81:GLU:OE1	2.28	0.51
1:O:49:LYS:O	1:O:49:LYS:NZ	2.37	0.51
7:A:1245:G:OP1	18:L:13:LYS:NZ	2.43	0.51
7:A:1527:G:N1	7:A:1544:A:OP2	2.38	0.51
13:G:84:THR:HG22	13:G:134:LYS:HG2	1.93	0.51
5:4:74:C:N4	7:A:2507:C:O2'	2.43	0.51
7:A:1866:A:N6	7:A:1875:G:O2'	2.44	0.51
21:O:8:ILE:O	21:O:12:THR:OG1	2.27	0.51
8:B:11:C:OP1	29:W:72:LYS:NZ	2.41	0.50
14:H:24:GLY:O	14:H:28:ASN:ND2	2.42	0.50
7:A:1667:G:N2	7:A:1992:G:OP2	2.41	0.50
7:A:2680:U:H5'	10:D:194:PRO:HA	1.92	0.50
9:C:145:GLU:HB2	9:C:188:CYS:HB3	1.93	0.50
10:D:39:ASP:N	10:D:39:ASP:OD1	2.44	0.50
7:A:2576:G:O2'	7:A:2579:C:OP2	2.27	0.50
7:A:1070:A:H1'	15:I:10:LYS:HD2	1.94	0.50
8:B:98:G:H1	28:V:14:LYS:HB3	1.77	0.50
7:A:411:G:OP2	7:A:2406:A:O2'	2.29	0.50
7:A:547:A:H8	7:A:548:G:H5'	1.76	0.50
18:L:17:LYS:HE3	18:L:27:LEU:HD21	1.94	0.50
22:P:22:PRO:HD3	22:P:50:ILE:HD12	1.92	0.50
32:Z:62:VAL:HG22	32:Z:81:LYS:HG3	1.93	0.50
6:6:14:ALA:HB3	6:6:22:MET:HG3	1.94	0.50
7:A:2144:G:N2	7:A:2148:G:O6	2.45	0.50
24:R:55:ASP:OD1	24:R:55:ASP:N	2.44	0.50
7:A:568:U:O4	24:R:81:LYS:NZ	2.44	0.50
1:O:80:THR:O	1:O:84:ASN:ND2	2.45	0.49
32:Z:19:LYS:NZ	32:Z:84:TYR:OH	2.44	0.49
3:2:13:C:N4	3:2:48:C:O2	2.45	0.49
9:C:260:ASN:ND2	9:C:263:THR:OG1	2.39	0.49
7:A:1394:U:H4'	7:A:1603:A:H4'	1.93	0.49
7:A:2123:G:O6	7:A:2125:G:N2	2.45	0.49
12:F:162:SER:OG	12:F:163:ASP:N	2.45	0.49
7:A:1223:G:OP1	24:R:68:ARG:NH2	2.45	0.49
9:C:107:PRO:HA	9:C:195:VAL:HA	1.94	0.49
21:O:28:VAL:HG11	21:O:103:VAL:HG13	1.95	0.49
7:A:2130:U:H1'	7:A:2159:G:H1	1.77	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:25:ASP:N	19:M:25:ASP:OD1	2.44	0.49
21:O:16:ARG:NH2	21:O:19:GLN:OE1	2.46	0.49
15:I:88:SER:OG	15:I:89:GLY:N	2.45	0.49
19:M:54:THR:HA	19:M:57:VAL:HG12	1.94	0.49
7:A:788:A:OP1	7:A:791:C:N4	2.40	0.49
7:A:1072:C:N4	7:A:1091:G:O6	2.45	0.49
19:M:42:THR:HG22	19:M:93:VAL:HG12	1.95	0.49
23:Q:26:GLY:O	23:Q:30:ARG:NH1	2.44	0.49
3:2:21:A:N6	3:2:47:U:OP2	2.46	0.49
12:F:15:LYS:NZ	12:F:19:GLU:OE2	2.42	0.49
6:6:34:LEU:HD23	12:F:110:ARG:HD2	1.95	0.48
7:A:659:G:O2'	11:E:95:LYS:O	2.30	0.48
7:A:1779:U:OP2	7:A:1784:A:N6	2.45	0.48
7:A:1597:A:H5''	7:A:1598:A:H5'	1.95	0.48
7:A:577:G:O2'	7:A:1254:A:OP1	2.31	0.48
16:J:37:ARG:NH2	16:J:44:TYR:OH	2.41	0.48
24:R:32:THR:HA	24:R:62:GLU:HA	1.95	0.48
31:Y:30:MET:SD	32:Z:14:PRO:HD3	2.54	0.48
27:U:99:ASN:ND2	27:U:101:GLU:OE2	2.47	0.48
7:A:2683:C:OP1	22:P:51:ARG:NH2	2.39	0.48
11:E:127:GLU:O	11:E:156:ASN:ND2	2.46	0.48
15:I:90:SER:OG	15:I:91:GLY:N	2.46	0.48
17:K:30:ARG:NH2	17:K:37:ASP:OD2	2.47	0.48
32:Z:3:ARG:O	32:Z:5:GLU:N	2.45	0.48
4:3:4:G:H1	4:3:69:U:H3	1.60	0.48
27:U:27:ASN:N	27:U:27:ASN:OD1	2.46	0.48
7:A:396:G:N2	7:A:2231:U:O2'	2.47	0.47
7:A:2137:U:H2'	7:A:2138:G:H8	1.78	0.47
7:A:2250:G:OP1	19:M:84:LYS:NZ	2.47	0.47
7:A:2581:G:N2	7:A:2581:G:OP2	2.47	0.47
7:A:2657:A:O2'	13:G:160:LYS:NZ	2.47	0.47
11:E:58:LYS:NZ	11:E:70:SER:O	2.46	0.47
13:G:152:ARG:HA	13:G:152:ARG:HD3	1.74	0.47
15:I:83:ALA:HB3	15:I:105:GLN:HG3	1.96	0.47
18:L:78:ARG:NH2	18:L:80:SER:OG	2.47	0.47
21:O:31:THR:OG1	21:O:34:HIS:O	2.32	0.47
4:3:10:G:H1	4:3:25:U:H3	1.62	0.47
9:C:232:HIS:HE2	9:C:244:PRO:HA	1.79	0.47
12:F:61:SER:HB2	12:F:91:LEU:HD21	1.95	0.47
5:4:58:A:O2'	5:4:60:U:OP2	2.30	0.47
7:A:1070:A:N7	7:A:1096:A:O2'	2.41	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1105:U:H2'	7:A:1106:G:H8	1.80	0.47
7:A:906:U:O2'	19:M:66:ARG:NH2	2.47	0.47
7:A:1568:G:H4'	9:C:59:LYS:HG2	1.96	0.47
7:A:2131:U:H5'	7:A:2132:U:H5''	1.96	0.47
15:I:28:LEU:HD13	15:I:38:PHE:HZ	1.79	0.47
8:B:34:A:N6	8:B:44:G:O2'	2.47	0.47
9:C:107:PRO:HD2	9:C:110:LEU:HD22	1.96	0.47
9:C:245:VAL:HG12	9:C:251:GLN:HA	1.96	0.47
14:H:40:THR:OG1	14:H:43:ASN:ND2	2.47	0.47
7:A:630:G:N2	7:A:633:A:OP2	2.44	0.47
7:A:1715:G:O2'	7:A:1743:G:O6	2.27	0.47
7:A:2125:G:H2'	7:A:2173:A:H61	1.80	0.47
13:G:86:LYS:NZ	13:G:130:GLU:OE2	2.42	0.47
15:I:92:LYS:HB3	15:I:95:LYS:HD2	1.96	0.47
4:3:16:U:O4'	4:3:59:G:N2	2.48	0.47
3:2:47:U:O2'	3:2:50:G:OP1	2.29	0.47
7:A:784:G:C6	9:C:228:VAL:HG21	2.49	0.47
12:F:8:TYR:HB2	12:F:173:PHE:HZ	1.80	0.47
2:1:24:GLU:HB2	2:1:27:GLY:H	1.79	0.46
23:Q:50:ARG:O	23:Q:54:LYS:NZ	2.46	0.46
7:A:1077:A:H1'	15:I:93:PRO:HG2	1.97	0.46
7:A:2394:C:H5''	18:L:63:LYS:HE2	1.97	0.46
17:K:43:ILE:HD12	17:K:56:ASP:HB2	1.98	0.46
3:2:19:G:N3	3:2:57:G:N2	2.54	0.46
7:A:948:C:O2	7:A:984:A:O2'	2.29	0.46
3:2:19:G:H1	7:A:2112:G:H2'	1.81	0.46
3:2:20:G:N2	3:2:22:G:O4'	2.49	0.46
3:2:50:G:N2	3:2:64:U:O2'	2.43	0.46
9:C:167:ARG:HG3	9:C:172:VAL:HG22	1.97	0.46
15:I:76:ALA:HA	15:I:79:LEU:HB2	1.98	0.46
7:A:58:G:OP1	32:Z:78:SER:HB2	2.16	0.46
7:A:463:G:N2	7:A:466:A:OP2	2.43	0.46
7:A:1082:U:H1'	15:I:118:THR:HB	1.98	0.46
10:D:77:ARG:NH1	10:D:200:ASP:OD1	2.48	0.46
7:A:2798:U:H4'	7:A:2799:A:H5'	1.97	0.46
31:Y:13:GLU:HA	31:Y:16:THR:HG22	1.98	0.46
31:Y:20:ASN:HB3	31:Y:50:VAL:HG12	1.97	0.46
4:3:9:A:O2'	4:3:10:G:N7	2.49	0.46
7:A:381:G:OP1	30:X:18:ARG:NH1	2.48	0.46
7:A:663:G:H5''	18:L:17:LYS:HD3	1.97	0.46
7:A:1080:A:O2'	15:I:127:ARG:NE	2.49	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2313:C:H5''	12:F:88:LYS:HD2	1.97	0.46
18:L:108:ALA:HB3	18:L:125:LEU:HG	1.98	0.46
20:N:106:ASP:N	20:N:106:ASP:OD1	2.49	0.46
1:O:48:GLN:OE1	1:O:52:ASN:ND2	2.49	0.46
6:6:11:GLU:HA	6:6:25:ARG:HA	1.97	0.46
7:A:1081:U:O5'	15:I:127:ARG:NH2	2.49	0.46
8:B:8:C:O3'	21:O:25:ARG:NH1	2.49	0.46
12:F:6:ASP:OD1	12:F:6:ASP:N	2.48	0.46
32:Z:28:ASN:ND2	32:Z:88:LYS:O	2.49	0.46
7:A:1964:G:O2'	7:A:1967:C:OP2	2.29	0.45
7:A:2114:A:H62	7:A:2115:G:H21	1.64	0.45
8:B:36:C:N4	8:B:49:C:O2	2.49	0.45
29:W:56:ASP:OD1	29:W:56:ASP:N	2.44	0.45
31:Y:11:VAL:O	31:Y:15:ASN:ND2	2.49	0.45
7:A:84:A:N1	7:A:98:G:O2'	2.41	0.45
7:A:811:U:H2'	18:L:21:ARG:HA	1.98	0.45
7:A:1288:G:OP2	7:A:1288:G:N2	2.44	0.45
7:A:743:A:O2'	7:A:1659:G:OP1	2.34	0.45
7:A:2106:U:H2'	7:A:2107:G:H8	1.81	0.45
7:A:2258:C:O2'	7:A:2427:C:OP2	2.35	0.45
7:A:2009:A:OP1	25:S:41:LYS:NZ	2.50	0.45
7:A:2127:G:N2	7:A:2162:G:O5'	2.50	0.45
7:A:475:C:O2	7:A:479:A:N6	2.47	0.45
9:C:98:ASP:OD1	9:C:98:ASP:N	2.40	0.45
10:D:45:TYR:OH	10:D:81:GLU:OE2	2.35	0.45
22:P:64:ILE:HA	22:P:69:GLY:HA2	1.99	0.45
25:S:59:GLU:HA	25:S:64:ALA:HA	1.98	0.45
7:A:1721:G:HO2'	7:A:1722:A:H8	1.63	0.45
1:O:59:ASP:OD2	1:O:76:LYS:NZ	2.43	0.45
7:A:578:G:OP1	7:A:1255:U:O2'	2.28	0.45
9:C:144:VAL:HG11	9:C:174:LEU:HD21	1.99	0.45
7:A:959:A:N3	7:A:2457:U:O2'	2.44	0.44
7:A:1306:C:H41	7:A:1606:C:H2'	1.83	0.44
7:A:1945:G:N2	7:A:1963:U:O4	2.50	0.44
13:G:45:HIS:HA	13:G:50:LEU:HD23	1.98	0.44
7:A:372:G:H2'	30:X:58:VAL:HG12	1.99	0.44
1:O:85:LYS:HB2	1:O:85:LYS:HE2	1.75	0.44
7:A:2076:U:OP2	7:A:2238:G:N2	2.46	0.44
7:A:2111:U:O3'	7:A:2118:U:O2'	2.35	0.44
7:A:2375:G:N2	7:A:2378:A:OP2	2.45	0.44
8:B:46:A:H5''	21:O:3:LYS:HE2	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:48:ASN:N	13:G:48:ASN:OD1	2.51	0.44
18:L:78:ARG:HB3	18:L:113:ALA:HB3	1.99	0.44
7:A:458:G:O2'	7:A:469:G:O6	2.28	0.44
7:A:534:U:O2'	23:Q:45:TYR:O	2.35	0.44
7:A:566:U:H5''	18:L:29:LYS:HE3	1.99	0.44
7:A:1064:C:N4	7:A:1070:A:OP2	2.50	0.44
12:F:29:PRO:HB2	12:F:169:LEU:HD22	1.99	0.44
14:H:21:VAL:HG21	14:H:26:ALA:HB2	1.99	0.44
3:2:15:G:H2'	3:2:59:U:H3	1.83	0.44
7:A:587:C:OP2	18:L:21:ARG:NH2	2.50	0.44
7:A:1475:G:O2'	7:A:1514:G:O6	2.30	0.44
7:A:1477:A:N6	7:A:1514:G:O2'	2.50	0.44
8:B:48:U:H4'	21:O:100:HIS:HD2	1.81	0.44
11:E:88:ARG:HA	11:E:88:ARG:HD3	1.72	0.44
15:I:32:GLY:O	15:I:65:ARG:NH2	2.47	0.44
15:I:46:THR:HB	15:I:51:LYS:HE3	1.99	0.44
7:A:2:G:N2	7:A:2902:C:O2'	2.51	0.44
12:F:57:LEU:O	12:F:61:SER:OG	2.31	0.44
15:I:79:LEU:HD22	15:I:105:GLN:HE22	1.83	0.44
26:T:40:ASP:OD1	26:T:45:ARG:NE	2.48	0.44
7:A:1105:U:H2'	7:A:1106:G:C8	2.53	0.44
18:L:19:LEU:HG	18:L:27:LEU:HD23	1.99	0.44
6:6:8:LYS:HA	6:6:8:LYS:HD2	1.87	0.43
13:G:89:LEU:HD23	13:G:94:TYR:HB3	2.00	0.43
30:X:16:ASN:HD22	30:X:24:ALA:HB1	1.82	0.43
7:A:932:U:O2'	7:A:934:U:O4	2.35	0.43
7:A:1060:U:H4'	15:I:77:ALA:HB2	2.00	0.43
8:B:14:U:OP2	8:B:70:C:O2'	2.35	0.43
15:I:78:VAL:HA	15:I:81:LYS:HB2	1.99	0.43
17:K:21:CYS:HA	17:K:41:ILE:HG22	2.00	0.43
3:2:20:G:N2	3:2:21:A:O2'	2.51	0.43
7:A:398:C:OP1	7:A:2090:A:O2'	2.33	0.43
17:K:76:VAL:HG22	22:P:73:VAL:HG22	1.99	0.43
6:6:38:SER:HB3	12:F:105:THR:HA	2.01	0.43
7:A:1789:A:H5'	9:C:220:VAL:HG22	2.00	0.43
13:G:115:HIS:HE1	13:G:144:VAL:HG13	1.84	0.43
5:4:27:G:H1	5:4:43:U:H3	1.65	0.43
7:A:954:G:OP2	19:M:16:ARG:NH1	2.52	0.43
11:E:24:ASN:HB3	11:E:27:LEU:HB3	2.00	0.43
15:I:8:TYR:HE2	15:I:10:LYS:HE3	1.83	0.43
25:S:109:ASP:OD1	25:S:109:ASP:N	2.50	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:57:GLY:HA2	9:C:213:TRP:HA	2.00	0.43
9:C:155:ALA:HB2	9:C:162:VAL:HG23	2.00	0.43
10:D:130:GLN:NE2	10:D:139:SER:OG	2.52	0.43
6:6:28:VAL:HG22	12:F:140:GLU:HA	2.00	0.43
7:A:2343:U:O2'	7:A:2373:G:O2'	2.35	0.43
17:K:18:ARG:HB3	17:K:45:GLU:HB2	2.00	0.43
29:W:59:LEU:HD12	29:W:80:ILE:HD12	2.00	0.43
7:A:1140:C:H5'	16:J:26:GLY:HA3	2.01	0.43
7:A:1378:A:O2'	7:A:1380:G:OP2	2.37	0.43
7:A:2579:C:O2'	10:D:136:ASN:OD1	2.37	0.43
16:J:141:ASP:OD1	16:J:141:ASP:N	2.44	0.43
2:1:23:CYS:SG	2:1:24:GLU:N	2.89	0.42
2:1:24:GLU:H	2:1:24:GLU:HG3	1.67	0.42
7:A:31:C:O2'	7:A:1238:G:OP1	2.36	0.42
10:D:199:SER:OG	10:D:200:ASP:N	2.52	0.42
18:L:105:ILE:HD12	18:L:105:ILE:HA	3.05	0.42
31:Y:12:GLU:HA	31:Y:15:ASN:HD21	1.84	0.42
31:Y:21:LEU:HD13	32:Z:5:GLU:CD	2.24	0.42
7:A:1363:C:O2'	7:A:1809:A:N3	2.48	0.42
7:A:2748:A:H1'	13:G:67:THR:HG22	2.01	0.42
24:R:49:ILE:HB	24:R:52:PRO:HA	2.01	0.42
7:A:746:U:O2'	7:A:2611:C:O2'	2.34	0.42
7:A:1283:G:N1	7:A:1286:A:OP2	2.52	0.42
15:I:43:ASN:ND2	15:I:47:ASP:OD2	2.53	0.42
21:O:95:SER:O	21:O:95:SER:OG	2.30	0.42
21:O:27:VAL:HG21	21:O:40:ILE:HD12	2.00	0.42
26:T:6:LYS:HB3	26:T:6:LYS:HE2	1.83	0.42
15:I:100:LYS:HA	15:I:100:LYS:HD3	1.84	0.42
21:O:67:ASN:OD1	21:O:70:ALA:N	2.48	0.42
23:Q:15:LYS:HB3	23:Q:15:LYS:HE2	1.81	0.42
7:A:138:U:H5'	32:Z:1:MET:HE2	2.00	0.42
20:N:117:ASP:OD1	20:N:117:ASP:N	2.47	0.42
7:A:137:U:O4	7:A:140:C:O2'	2.36	0.42
7:A:845:A:N6	7:A:847:U:O2	2.52	0.42
7:A:1047:G:O2'	7:A:1110:G:N1	2.43	0.42
7:A:2684:U:O4'	17:K:70:ARG:NH1	2.52	0.42
8:B:52:A:N7	21:O:64:TYR:OH	2.48	0.42
9:C:154:LEU:HD13	9:C:176:LEU:HD21	2.00	0.42
1:0:35:VAL:HG21	1:0:54:MET:HG2	2.02	0.42
7:A:1470:A:N6	7:A:1521:G:O2'	2.53	0.42
1:0:48:GLN:HE22	1:0:83:ILE:HD12	1.85	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:674:G:H1'	11:E:69:ARG:HD3	2.01	0.42
21:O:34:HIS:HB3	21:O:53:THR:HB	2.01	0.42
25:S:69:LEU:HG	25:S:107:VAL:HG22	2.02	0.42
28:V:40:ILE:HD13	28:V:40:ILE:HA	1.91	0.42
7:A:811:U:O4	18:L:21:ARG:NH1	2.53	0.41
7:A:1248:G:OP1	11:E:44:ARG:NH1	2.53	0.41
13:G:56:ASP:OD1	13:G:56:ASP:N	2.46	0.41
7:A:881:G:N1	7:A:895:U:O2	2.48	0.41
20:N:28:LEU:HD23	20:N:48:VAL:HG11	2.02	0.41
7:A:1417:C:O2'	7:A:1587:G:O2'	2.30	0.41
7:A:2175:C:H2'	7:A:2176:A:C8	2.56	0.41
7:A:2547:A:H2'	7:A:2548:U:C6	2.56	0.41
9:C:84:ASP:OD1	9:C:86:ASN:ND2	2.52	0.41
18:L:81:ASP:OD1	18:L:81:ASP:N	2.52	0.41
21:O:89:ASP:OD1	21:O:89:ASP:N	2.46	0.41
22:P:104:THR:OG1	22:P:105:GLY:N	2.53	0.41
7:A:659:G:N2	11:E:30:GLN:OE1	2.48	0.41
22:P:10:GLN:HA	22:P:13:MET:HG3	2.01	0.41
1:O:48:GLN:O	1:O:52:ASN:ND2	2.39	0.41
7:A:139:U:O2'	7:A:141:G:N2	2.47	0.41
19:M:127:LYS:HE3	19:M:127:LYS:HB2	1.83	0.41
7:A:2572:A:P	10:D:151:THR:HG1	2.43	0.41
10:D:197:THR:O	10:D:197:THR:OG1	2.37	0.41
3:2:9:A:N6	3:2:22:G:OP2	2.45	0.41
7:A:1058:U:H2'	7:A:1059:G:H8	1.85	0.41
12:F:133:ARG:HA	12:F:133:ARG:HD3	1.87	0.41
18:L:92:LEU:HD12	18:L:92:LEU:HA	1.91	0.41
7:A:548:G:H4'	7:A:549:G:C4	2.56	0.41
10:D:88:GLU:HB3	10:D:90:PHE:HE1	1.86	0.41
16:J:4:PHE:O	23:Q:64:ARG:NH2	2.45	0.41
27:U:49:VAL:O	27:U:54:GLN:NE2	2.41	0.41
12:F:44:ILE:H	12:F:44:ILE:HG13	1.75	0.41
14:H:27:ARG:HH21	14:H:27:ARG:HD2	1.76	0.41
2:1:17:ARG:HE	2:1:20:LYS:HE2	1.85	0.40
7:A:242:G:O2'	7:A:254:G:O6	2.37	0.40
7:A:613:A:H5''	7:A:614:A:H8	1.86	0.40
8:B:9:G:O2'	21:O:45:SER:OG	2.30	0.40
31:Y:37:LEU:HD12	31:Y:37:LEU:HA	1.95	0.40
7:A:224:U:OP2	7:A:408:G:N2	2.44	0.40
7:A:1496:A:N3	7:A:1577:C:O2'	2.43	0.40
27:U:17:LYS:HE3	27:U:17:LYS:HB3	1.86	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:48:ILE:HG23	10:D:84:LEU:HD21	2.03	0.40
17:K:17:ARG:HB3	17:K:45:GLU:HB3	2.03	0.40
1:0:46:ALA:HA	1:0:49:LYS:HB3	2.02	0.40
7:A:355:U:H2'	7:A:356:G:H8	1.86	0.40
7:A:1654:A:N1	7:A:2048:G:O2'	2.54	0.40
7:A:1992:G:N2	7:A:1996:C:O2'	2.46	0.40
11:E:148:ILE:HB	11:E:169:VAL:HG22	2.03	0.40
24:R:29:THR:O	24:R:29:THR:OG1	2.36	0.40
7:A:307:G:N2	7:A:310:A:OP2	2.51	0.40
7:A:1417:C:HO2'	7:A:1587:G:HO2'	1.66	0.40
19:M:34:LYS:HE3	19:M:34:LYS:HB2	1.95	0.40
27:U:13:VAL:HG21	27:U:39:ILE:HG21	2.02	0.40
31:Y:25:GLN:HE22	31:Y:47:ARG:HG2	1.86	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	83/87 (95%)	77 (93%)	5 (6%)	1 (1%)	11	35
2	1	49/71 (69%)	34 (69%)	15 (31%)	0	100	100
6	6	64/70 (91%)	55 (86%)	9 (14%)	0	100	100
9	C	269/273 (98%)	241 (90%)	28 (10%)	0	100	100
10	D	207/209 (99%)	194 (94%)	12 (6%)	1 (0%)	25	54
11	E	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
12	F	175/179 (98%)	159 (91%)	16 (9%)	0	100	100
13	G	174/177 (98%)	160 (92%)	12 (7%)	2 (1%)	12	37
14	H	45/149 (30%)	35 (78%)	10 (22%)	0	100	100
15	I	139/142 (98%)	112 (81%)	27 (19%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	J	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
17	K	120/123 (98%)	101 (84%)	18 (15%)	1 (1%)	16	44
18	L	141/144 (98%)	122 (86%)	18 (13%)	1 (1%)	19	47
19	M	134/136 (98%)	123 (92%)	8 (6%)	3 (2%)	5	24
20	N	118/127 (93%)	103 (87%)	14 (12%)	1 (1%)	16	44
21	O	114/117 (97%)	106 (93%)	8 (7%)	0	100	100
22	P	112/115 (97%)	99 (88%)	13 (12%)	0	100	100
23	Q	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
24	R	101/103 (98%)	92 (91%)	9 (9%)	0	100	100
25	S	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
26	T	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
27	U	100/104 (96%)	85 (85%)	12 (12%)	3 (3%)	3	19
28	V	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
29	W	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
30	X	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
31	Y	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
32	Z	94/100 (94%)	82 (87%)	12 (13%)	0	100	100
33	a	54/57 (95%)	49 (91%)	4 (7%)	1 (2%)	6	26
34	b	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
35	c	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
36	d	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	3	18
37	e	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	4	20
39	g	166/169 (98%)	158 (95%)	8 (5%)	0	100	100
40	h	116/118 (98%)	105 (90%)	11 (10%)	0	100	100
41	i	216/241 (90%)	185 (86%)	31 (14%)	0	100	100
42	j	204/233 (88%)	181 (89%)	23 (11%)	0	100	100
43	k	203/206 (98%)	167 (82%)	36 (18%)	0	100	100
44	l	148/167 (89%)	119 (80%)	29 (20%)	0	100	100
45	m	98/135 (73%)	85 (87%)	13 (13%)	0	100	100
46	n	149/179 (83%)	141 (95%)	8 (5%)	0	100	100
47	o	127/130 (98%)	122 (96%)	5 (4%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	p	125/130 (96%)	106 (85%)	18 (14%)	1 (1%)	16	44
49	q	96/103 (93%)	82 (85%)	13 (14%)	1 (1%)	13	39
50	r	115/129 (89%)	99 (86%)	16 (14%)	0	100	100
51	s	121/124 (98%)	100 (83%)	21 (17%)	0	100	100
52	t	112/118 (95%)	103 (92%)	7 (6%)	2 (2%)	7	27
53	u	92/101 (91%)	78 (85%)	13 (14%)	1 (1%)	12	37
54	v	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	11	35
55	w	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
56	x	78/84 (93%)	67 (86%)	10 (13%)	1 (1%)	10	33
57	y	53/75 (71%)	48 (91%)	5 (9%)	0	100	100
58	z	77/92 (84%)	70 (91%)	7 (9%)	0	100	100
All	All	5864/6342 (92%)	5255 (90%)	585 (10%)	24 (0%)	32	60

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	G	48	ASN
18	L	82	LEU
36	d	32	ILE
52	t	67	GLY
1	0	69	LYS
13	G	47	ASP
19	M	59	ARG
27	U	90	GLY
36	d	33	LEU
37	e	21	GLY
54	v	47	LYS
56	x	71	LYS
10	D	152	PRO
52	t	66	GLU
33	a	55	ILE
19	M	58	LYS
20	N	3	HIS
53	u	4	GLN
17	K	93	GLN
27	U	51	ALA
27	U	52	LEU
48	p	54	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
49	q	57	VAL
19	M	69	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	65/66 (98%)	65 (100%)	0	100	100
2	1	44/61 (72%)	43 (98%)	1 (2%)	45	67
6	6	59/62 (95%)	58 (98%)	1 (2%)	56	74
9	C	216/218 (99%)	215 (100%)	1 (0%)	86	91
10	D	164/164 (100%)	164 (100%)	0	100	100
11	E	165/165 (100%)	165 (100%)	0	100	100
12	F	148/150 (99%)	147 (99%)	1 (1%)	81	88
13	G	137/138 (99%)	137 (100%)	0	100	100
14	H	38/114 (33%)	38 (100%)	0	100	100
15	I	109/110 (99%)	106 (97%)	3 (3%)	38	62
16	J	116/116 (100%)	116 (100%)	0	100	100
17	K	103/104 (99%)	103 (100%)	0	100	100
18	L	102/103 (99%)	101 (99%)	1 (1%)	73	83
19	M	109/109 (100%)	109 (100%)	0	100	100
20	N	100/103 (97%)	99 (99%)	1 (1%)	73	83
21	O	86/87 (99%)	85 (99%)	1 (1%)	67	80
22	P	99/100 (99%)	99 (100%)	0	100	100
23	Q	89/90 (99%)	89 (100%)	0	100	100
24	R	84/84 (100%)	84 (100%)	0	100	100
25	S	93/93 (100%)	91 (98%)	2 (2%)	47	68
26	T	48/49 (98%)	48 (100%)	0	100	100
27	U	83/85 (98%)	82 (99%)	1 (1%)	67	80

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	V	78/78 (100%)	78 (100%)	0	100	100
29	W	56/63 (89%)	56 (100%)	0	100	100
30	X	67/68 (98%)	67 (100%)	0	100	100
31	Y	55/55 (100%)	55 (100%)	0	100	100
32	Z	83/84 (99%)	83 (100%)	0	100	100
33	a	47/48 (98%)	47 (100%)	0	100	100
34	b	45/49 (92%)	44 (98%)	1 (2%)	47	68
35	c	38/38 (100%)	38 (100%)	0	100	100
36	d	51/52 (98%)	51 (100%)	0	100	100
37	e	34/34 (100%)	33 (97%)	1 (3%)	37	61
39	g	148/149 (99%)	145 (98%)	3 (2%)	50	70
40	h	100/100 (100%)	100 (100%)	0	100	100
41	i	180/199 (90%)	177 (98%)	3 (2%)	56	74
42	j	170/190 (90%)	170 (100%)	0	100	100
43	k	172/173 (99%)	169 (98%)	3 (2%)	56	74
44	l	113/126 (90%)	112 (99%)	1 (1%)	75	86
45	m	87/116 (75%)	86 (99%)	1 (1%)	70	81
46	n	124/147 (84%)	123 (99%)	1 (1%)	79	87
47	o	104/105 (99%)	104 (100%)	0	100	100
48	p	105/107 (98%)	103 (98%)	2 (2%)	52	71
49	q	86/90 (96%)	86 (100%)	0	100	100
50	r	90/99 (91%)	88 (98%)	2 (2%)	47	68
51	s	103/104 (99%)	102 (99%)	1 (1%)	73	83
52	t	92/96 (96%)	92 (100%)	0	100	100
53	u	79/84 (94%)	79 (100%)	0	100	100
54	v	75/77 (97%)	75 (100%)	0	100	100
55	w	65/65 (100%)	65 (100%)	0	100	100
56	x	74/78 (95%)	73 (99%)	1 (1%)	62	77
57	y	48/65 (74%)	48 (100%)	0	100	100
58	z	70/79 (89%)	70 (100%)	0	100	100
All	All	4896/5189 (94%)	4863 (99%)	33 (1%)	80	88

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	7	ARG
6	6	49	ARG
9	C	219	THR
12	F	14	LYS
15	I	40	LYS
15	I	127	ARG
15	I	134	ARG
18	L	91	ASP
20	N	2	ARG
21	O	9	ARG
25	S	11	ARG
25	S	92	ARG
27	U	7	ARG
34	b	53	LYS
37	e	36	ARG
39	g	1012	ARG
39	g	1116	LYS
39	g	1167	ARG
41	i	14	VAL
41	i	47	VAL
41	i	63	ARG
43	k	128	ARG
43	k	184	ARG
43	k	188	ARG
44	l	90	THR
45	m	91	ARG
46	n	10	ARG
48	p	12	ARG
48	p	45	ARG
50	r	106	ARG
50	r	125	LYS
51	s	121	ARG
56	x	77	ARG

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	48	GLN
1	0	52	ASN
1	0	75	HIS
6	6	61	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
9	C	260	ASN
10	D	32	ASN
10	D	49	GLN
11	E	41	GLN
12	F	5	HIS
13	G	104	ASN
13	G	115	HIS
13	G	143	GLN
14	H	43	ASN
15	I	6	GLN
15	I	19	ASN
15	I	34	ASN
15	I	43	ASN
16	J	40	HIS
17	K	88	ASN
21	O	38	GLN
21	O	116	GLN
23	Q	37	GLN
23	Q	44	GLN
23	Q	71	GLN
27	U	45	HIS
27	U	74	ASN
30	X	16	ASN
31	Y	15	ASN
31	Y	25	GLN
31	Y	27	ASN
32	Z	59	ASN
32	Z	70	HIS
33	a	42	HIS
35	c	13	ASN
39	g	1131	GLN
41	i	89	GLN
43	k	136	GLN
46	n	28	ASN
47	o	18	GLN
48	p	75	GLN
50	r	109	ASN
51	s	5	ASN
51	s	75	GLN
54	v	20	ASN
54	v	46	HIS
55	w	63	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
56	x	31	HIS
57	y	52	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	2	58/73 (79%)	13 (22%)	1 (1%)
38	f	1538/1539 (99%)	262 (17%)	0
4	3	63/77 (81%)	7 (11%)	0
5	4	58/76 (76%)	17 (29%)	1 (1%)
7	A	2902/2903 (99%)	477 (16%)	7 (0%)
8	B	117/118 (99%)	14 (11%)	0
All	All	4736/4786 (98%)	790 (16%)	9 (0%)

All (790) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	2	13	C
3	2	14	A
3	2	15	G
3	2	19	G
3	2	20	G
3	2	21	A
3	2	26	A
3	2	36	C
3	2	48	C
3	2	59	U
3	2	60	C
3	2	65	C
3	2	73	A
4	3	14	A
4	3	18	G
4	3	19	U
4	3	21	A
4	3	30	G
4	3	33	U
4	3	76	A
5	4	13	C
5	4	14	A
5	4	19	G
5	4	20	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	4	22	G
5	4	26	A
5	4	32	C
5	4	49	G
5	4	50	C
5	4	53	G
5	4	57	G
5	4	61	C
5	4	62	C
5	4	64	G
5	4	66	A
5	4	70	C
5	4	74	C
7	A	10	A
7	A	14	A
7	A	34	U
7	A	35	G
7	A	42	A
7	A	46	G
7	A	51	G
7	A	71	A
7	A	74	A
7	A	75	G
7	A	80	G
7	A	84	A
7	A	101	A
7	A	118	A
7	A	119	A
7	A	120	U
7	A	134	G
7	A	135	U
7	A	137	U
7	A	138	U
7	A	139	U
7	A	140	C
7	A	141	G
7	A	142	A
7	A	149	A
7	A	162	U
7	A	163	C
7	A	188	G
7	A	196	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	A	198	C
7	A	199	A
7	A	204	A
7	A	215	G
7	A	216	A
7	A	221	A
7	A	222	A
7	A	233	A
7	A	241	A
7	A	248	G
7	A	249	C
7	A	255	A
7	A	265	A
7	A	266	G
7	A	271	G
7	A	272	A
7	A	276	U
7	A	277	G
7	A	285	G
7	A	311	A
7	A	324	A
7	A	328	U
7	A	329	G
7	A	330	A
7	A	361	G
7	A	362	A
7	A	371	A
7	A	372	G
7	A	385	C
7	A	386	G
7	A	396	G
7	A	399	U
7	A	405	U
7	A	406	G
7	A	411	G
7	A	412	A
7	A	416	U
7	A	420	C
7	A	424	G
7	A	425	G
7	A	455	C
7	A	467	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	A	480	A
7	A	481	G
7	A	489	G
7	A	490	C
7	A	491	G
7	A	505	A
7	A	529	A
7	A	531	C
7	A	532	A
7	A	542	C
7	A	543	G
7	A	544	C
7	A	546	U
7	A	547	A
7	A	548	G
7	A	549	G
7	A	563	A
7	A	573	U
7	A	575	A
7	A	584	C
7	A	586	A
7	A	603	A
7	A	614	A
7	A	615	U
7	A	622	G
7	A	627	A
7	A	637	A
7	A	645	C
7	A	654	A
7	A	655	A
7	A	677	A
7	A	683	U
7	A	686	U
7	A	695	G
7	A	696	G
7	A	701	G
7	A	711	G
7	A	730	A
7	A	738	G
7	A	747	U
7	A	748	G
7	A	764	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	A	765	C
7	A	775	G
7	A	776	G
7	A	782	A
7	A	783	A
7	A	784	G
7	A	785	G
7	A	792	A
7	A	800	A
7	A	801	G
7	A	805	G
7	A	812	C
7	A	819	A
7	A	827	U
7	A	828	U
7	A	845	A
7	A	846	U
7	A	858	G
7	A	859	G
7	A	878	A
7	A	885	C
7	A	886	A
7	A	887	U
7	A	890	C
7	A	891	G
7	A	892	A
7	A	894	U
7	A	896	A
7	A	897	C
7	A	910	A
7	A	927	A
7	A	931	U
7	A	932	U
7	A	941	A
7	A	946	C
7	A	957	C
7	A	961	C
7	A	973	A
7	A	974	G
7	A	983	A
7	A	985	C
7	A	989	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
7	A	991	C
7	A	995	C
7	A	996	A
7	A	1005	C
7	A	1008	A
7	A	1012	U
7	A	1013	C
7	A	1023	U
7	A	1024	G
7	A	1025	G
7	A	1026	G
7	A	1033	U
7	A	1040	A
7	A	1046	A
7	A	1047	G
7	A	1060	U
7	A	1061	U
7	A	1062	G
7	A	1065	U
7	A	1066	U
7	A	1067	A
7	A	1068	G
7	A	1070	A
7	A	1071	G
7	A	1072	C
7	A	1073	A
7	A	1074	G
7	A	1076	C
7	A	1079	C
7	A	1087	G
7	A	1088	A
7	A	1089	A
7	A	1094	U
7	A	1097	U
7	A	1100	C
7	A	1112	G
7	A	1122	G
7	A	1130	U
7	A	1131	G
7	A	1132	U
7	A	1134	A
7	A	1135	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	A	1139	G
7	A	1142	A
7	A	1156	A
7	A	1170	C
7	A	1172	C
7	A	1174	U
7	A	1175	A
7	A	1176	U
7	A	1177	G
7	A	1178	C
7	A	1180	U
7	A	1190	G
7	A	1210	G
7	A	1212	G
7	A	1238	G
7	A	1250	G
7	A	1253	A
7	A	1255	U
7	A	1256	G
7	A	1265	A
7	A	1266	G
7	A	1271	G
7	A	1272	A
7	A	1273	U
7	A	1275	A
7	A	1301	A
7	A	1305	C
7	A	1325	U
7	A	1329	U
7	A	1338	G
7	A	1341	G
7	A	1352	U
7	A	1365	A
7	A	1368	G
7	A	1379	U
7	A	1383	A
7	A	1384	A
7	A	1386	C
7	A	1395	A
7	A	1416	G
7	A	1421	G
7	A	1427	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	A	1428	C
7	A	1452	G
7	A	1455	G
7	A	1460	U
7	A	1478	G
7	A	1482	G
7	A	1493	C
7	A	1503	A
7	A	1510	G
7	A	1515	A
7	A	1522	A
7	A	1524	G
7	A	1529	G
7	A	1534	U
7	A	1535	A
7	A	1536	C
7	A	1566	A
7	A	1567	G
7	A	1569	A
7	A	1572	A
7	A	1578	U
7	A	1583	A
7	A	1584	U
7	A	1585	C
7	A	1607	C
7	A	1608	A
7	A	1610	A
7	A	1647	U
7	A	1648	U
7	A	1649	G
7	A	1651	G
7	A	1672	A
7	A	1674	G
7	A	1694	C
7	A	1698	A
7	A	1699	G
7	A	1715	G
7	A	1729	U
7	A	1730	C
7	A	1732	C
7	A	1733	G
7	A	1738	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	A	1756	G
7	A	1764	C
7	A	1773	A
7	A	1786	A
7	A	1800	C
7	A	1801	A
7	A	1802	A
7	A	1808	A
7	A	1811	G
7	A	1816	C
7	A	1828	G
7	A	1829	A
7	A	1833	C
7	A	1866	A
7	A	1869	G
7	A	1870	C
7	A	1873	G
7	A	1903	G
7	A	1906	G
7	A	1913	A
7	A	1914	C
7	A	1927	A
7	A	1929	G
7	A	1930	G
7	A	1934	C
7	A	1938	A
7	A	1943	U
7	A	1955	U
7	A	1964	G
7	A	1966	A
7	A	1967	C
7	A	1970	A
7	A	1971	U
7	A	1972	G
7	A	1975	G
7	A	1991	U
7	A	1993	U
7	A	1997	C
7	A	2002	G
7	A	2007	U
7	A	2022	U
7	A	2023	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	A	2031	A
7	A	2033	A
7	A	2036	C
7	A	2043	C
7	A	2044	C
7	A	2049	G
7	A	2055	C
7	A	2056	G
7	A	2059	A
7	A	2060	A
7	A	2061	G
7	A	2062	A
7	A	2069	G
7	A	2072	C
7	A	2087	G
7	A	2093	G
7	A	2098	U
7	A	2100	G
7	A	2102	G
7	A	2109	U
7	A	2110	G
7	A	2111	U
7	A	2112	G
7	A	2113	U
7	A	2119	A
7	A	2120	G
7	A	2121	G
7	A	2125	G
7	A	2126	A
7	A	2127	G
7	A	2128	G
7	A	2131	U
7	A	2132	U
7	A	2133	G
7	A	2134	A
7	A	2135	A
7	A	2136	G
7	A	2145	C
7	A	2146	C
7	A	2147	A
7	A	2148	G
7	A	2149	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	A	2157	G
7	A	2161	C
7	A	2162	G
7	A	2163	A
7	A	2164	C
7	A	2168	G
7	A	2169	A
7	A	2170	A
7	A	2171	A
7	A	2172	U
7	A	2173	A
7	A	2178	C
7	A	2182	U
7	A	2198	A
7	A	2204	G
7	A	2210	U
7	A	2211	A
7	A	2220	U
7	A	2223	G
7	A	2225	A
7	A	2230	G
7	A	2238	G
7	A	2239	G
7	A	2243	U
7	A	2259	U
7	A	2266	A
7	A	2278	A
7	A	2283	C
7	A	2287	A
7	A	2288	A
7	A	2305	U
7	A	2307	G
7	A	2308	G
7	A	2309	A
7	A	2310	C
7	A	2325	G
7	A	2327	A
7	A	2333	A
7	A	2345	G
7	A	2347	C
7	A	2350	C
7	A	2357	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	A	2361	G
7	A	2371	G
7	A	2372	U
7	A	2383	G
7	A	2385	C
7	A	2389	G
7	A	2391	G
7	A	2396	G
7	A	2402	U
7	A	2407	A
7	A	2423	U
7	A	2425	A
7	A	2426	A
7	A	2428	G
7	A	2429	G
7	A	2430	A
7	A	2435	A
7	A	2441	U
7	A	2448	A
7	A	2469	A
7	A	2470	G
7	A	2476	A
7	A	2480	C
7	A	2491	U
7	A	2502	G
7	A	2505	G
7	A	2507	C
7	A	2518	A
7	A	2520	C
7	A	2529	G
7	A	2535	G
7	A	2554	U
7	A	2556	C
7	A	2566	A
7	A	2567	G
7	A	2572	A
7	A	2573	C
7	A	2582	G
7	A	2585	U
7	A	2602	A
7	A	2609	U
7	A	2613	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	A	2615	U
7	A	2629	U
7	A	2640	G
7	A	2646	C
7	A	2663	G
7	A	2689	U
7	A	2690	U
7	A	2714	G
7	A	2716	C
7	A	2726	A
7	A	2733	A
7	A	2744	G
7	A	2748	A
7	A	2765	A
7	A	2778	A
7	A	2793	C
7	A	2797	U
7	A	2799	A
7	A	2811	G
7	A	2818	U
7	A	2820	A
7	A	2835	A
7	A	2837	A
7	A	2867	G
7	A	2873	A
7	A	2880	C
7	A	2883	A
7	A	2903	U
8	B	9	G
8	B	35	C
8	B	41	G
8	B	44	G
8	B	51	G
8	B	53	A
8	B	56	G
8	B	66	A
8	B	88	C
8	B	89	U
8	B	90	C
8	B	91	C
8	B	99	A
8	B	109	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
38	f	4	U
38	f	9	G
38	f	22	G
38	f	32	A
38	f	39	G
38	f	44	A
38	f	48	C
38	f	50	A
38	f	51	A
38	f	63	C
38	f	73	C
38	f	74	A
38	f	75	G
38	f	83	C
38	f	85	U
38	f	86	G
38	f	87	C
38	f	88	U
38	f	91	U
38	f	92	U
38	f	93	U
38	f	95	C
38	f	97	G
38	f	100	G
38	f	108	G
38	f	116	A
38	f	120	A
38	f	121	U
38	f	126	G
38	f	130	A
38	f	131	A
38	f	141	G
38	f	151	A
38	f	154	U
38	f	156	C
38	f	163	C
38	f	164	G
38	f	182	A
38	f	183	C
38	f	197	A
38	f	204	G
38	f	208	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
38	f	210	C
38	f	211	G
38	f	212	G
38	f	226	G
38	f	245	U
38	f	247	G
38	f	251	G
38	f	254	G
38	f	266	G
38	f	267	C
38	f	289	G
38	f	298	A
38	f	309	A
38	f	321	A
38	f	328	C
38	f	329	A
38	f	330	C
38	f	332	G
38	f	339	C
38	f	345	C
38	f	346	G
38	f	347	G
38	f	348	G
38	f	352	C
38	f	353	A
38	f	354	G
38	f	367	U
38	f	372	C
38	f	388	G
38	f	392	C
38	f	397	A
38	f	398	U
38	f	406	G
38	f	409	U
38	f	411	A
38	f	412	A
38	f	413	G
38	f	421	U
38	f	423	G
38	f	424	G
38	f	428	G
38	f	429	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
38	f	436	C
38	f	437	U
38	f	452	A
38	f	465	A
38	f	466	A
38	f	467	U
38	f	468	A
38	f	469	C
38	f	478	A
38	f	479	U
38	f	482	A
38	f	484	G
38	f	485	U
38	f	486	U
38	f	495	A
38	f	496	A
38	f	497	G
38	f	505	G
38	f	511	C
38	f	513	C
38	f	518	C
38	f	521	G
38	f	527	G
38	f	530	G
38	f	531	U
38	f	532	A
38	f	538	G
38	f	545	C
38	f	547	A
38	f	559	A
38	f	572	A
38	f	573	A
38	f	575	G
38	f	576	C
38	f	577	G
38	f	596	A
38	f	619	U
38	f	627	G
38	f	633	G
38	f	650	G
38	f	653	U
38	f	665	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
38	f	687	A
38	f	695	A
38	f	703	G
38	f	721	G
38	f	723	U
38	f	724	G
38	f	731	G
38	f	734	G
38	f	755	G
38	f	758	C
38	f	760	G
38	f	777	A
38	f	793	U
38	f	794	A
38	f	810	C
38	f	813	U
38	f	815	A
38	f	817	C
38	f	819	A
38	f	821	G
38	f	828	U
38	f	829	G
38	f	832	G
38	f	841	C
38	f	843	U
38	f	844	G
38	f	846	G
38	f	876	C
38	f	885	G
38	f	914	A
38	f	922	G
38	f	926	G
38	f	934	C
38	f	935	A
38	f	960	U
38	f	966	G
38	f	969	A
38	f	971	G
38	f	975	A
38	f	976	G
38	f	977	A
38	f	983	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
38	f	992	U
38	f	993	G
38	f	1004	A
38	f	1005	A
38	f	1018	G
38	f	1020	G
38	f	1026	G
38	f	1030	U
38	f	1031	C
38	f	1032	G
38	f	1033	G
38	f	1036	A
38	f	1043	G
38	f	1044	A
38	f	1054	C
38	f	1065	U
38	f	1086	U
38	f	1089	G
38	f	1094	G
38	f	1095	U
38	f	1101	A
38	f	1108	G
38	f	1132	C
38	f	1133	G
38	f	1136	C
38	f	1137	C
38	f	1139	G
38	f	1140	C
38	f	1141	C
38	f	1142	G
38	f	1143	G
38	f	1159	U
38	f	1160	G
38	f	1161	C
38	f	1167	A
38	f	1171	A
38	f	1184	G
38	f	1196	A
38	f	1197	A
38	f	1200	C
38	f	1201	A
38	f	1202	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
38	f	1212	U
38	f	1213	A
38	f	1214	C
38	f	1227	A
38	f	1238	A
38	f	1256	A
38	f	1257	A
38	f	1258	G
38	f	1275	A
38	f	1280	A
38	f	1285	A
38	f	1287	A
38	f	1290	G
38	f	1293	C
38	f	1299	A
38	f	1305	G
38	f	1317	C
38	f	1320	C
38	f	1322	C
38	f	1337	G
38	f	1340	A
38	f	1346	A
38	f	1353	G
38	f	1363	A
38	f	1364	U
38	f	1368	A
38	f	1370	G
38	f	1378	C
38	f	1379	G
38	f	1419	G
38	f	1429	A
38	f	1441	A
38	f	1446	A
38	f	1452	C
38	f	1454	G
38	f	1487	G
38	f	1492	A
38	f	1493	A
38	f	1494	G
38	f	1497	G
38	f	1503	A
38	f	1505	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
38	f	1506	U
38	f	1517	G
38	f	1519	A
38	f	1526	G
38	f	1529	G
38	f	1530	G
38	f	1534	A
38	f	1535	C
38	f	1536	C
38	f	1540	U

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	2	58	A
5	4	13	C
7	A	271	G
7	A	404	A
7	A	479	A
7	A	885	C
7	A	1913	A
7	A	2146	C
7	A	2428	G

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



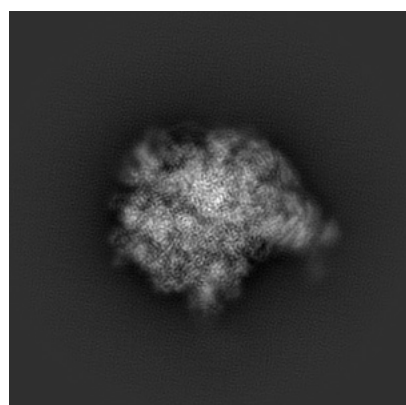
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30598. These allow visual inspection of the internal detail of the map and identification of artifacts.

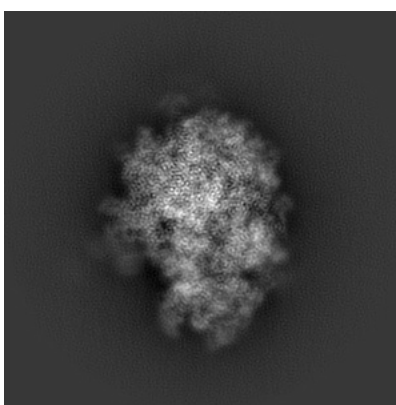
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

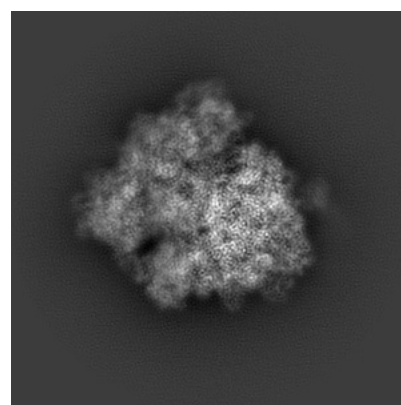
#### 6.1.1 Primary map



X



Y

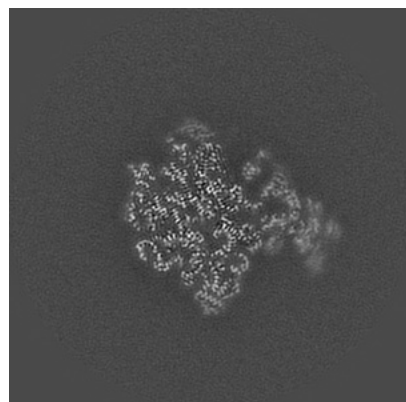


Z

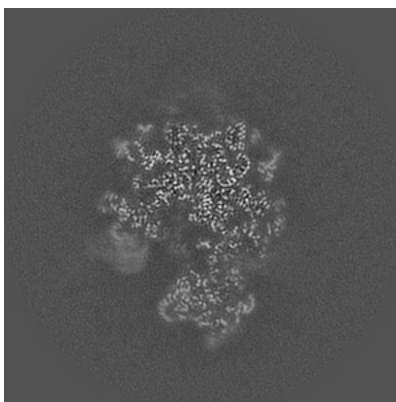
The images above show the map projected in three orthogonal directions.

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

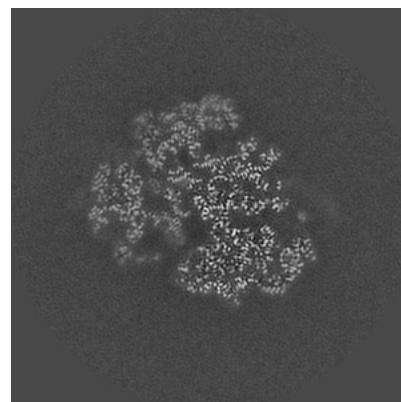
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

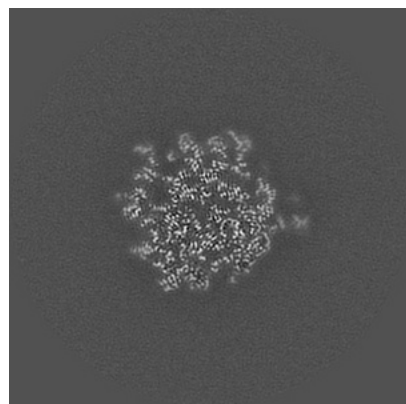


Z Index: 160

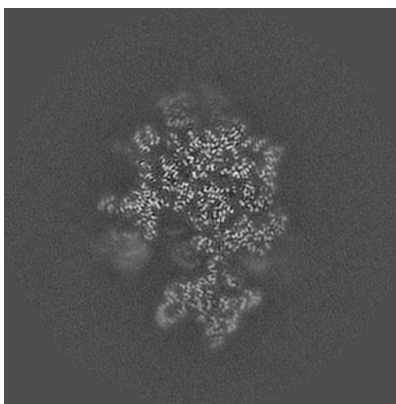
The images above show central slices of the map in three orthogonal directions.

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

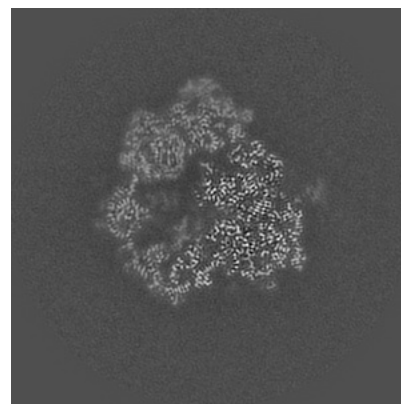
### 6.3.1 Primary map



X Index: 186



Y Index: 165

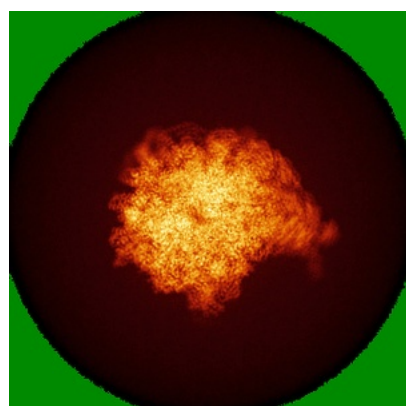


Z Index: 146

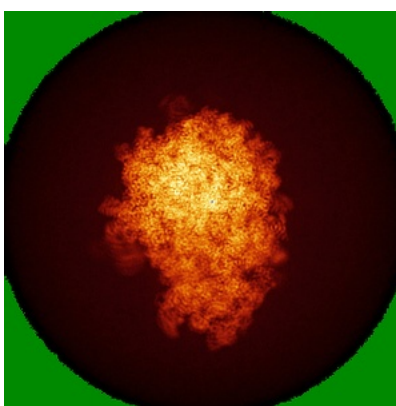
The images above show the largest variance slices of the map in three orthogonal directions.

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

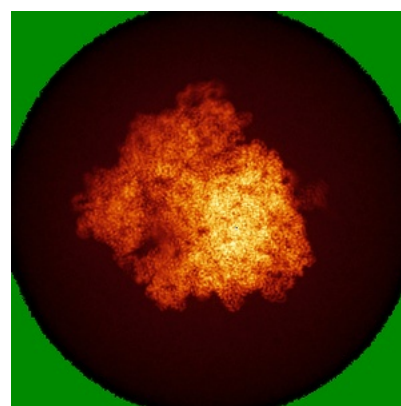
### 6.4.1 Primary map



X



Y

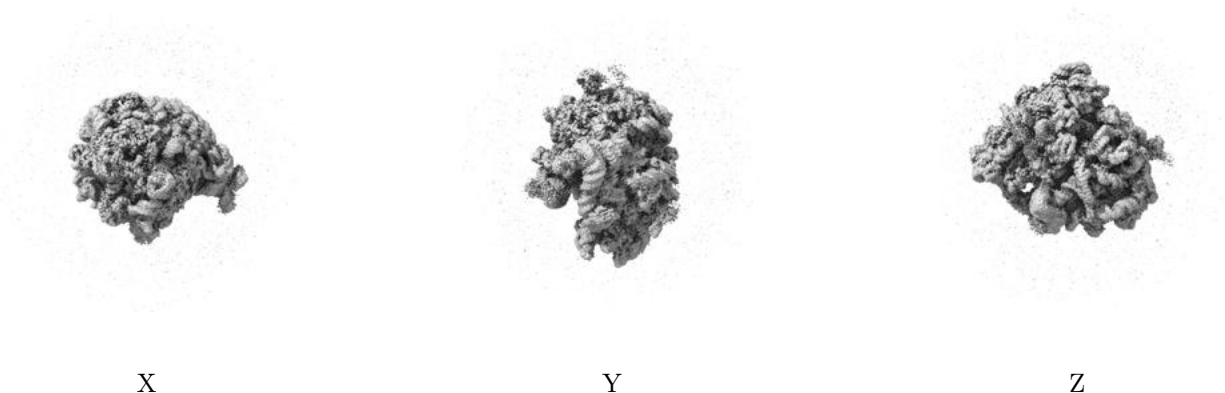


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

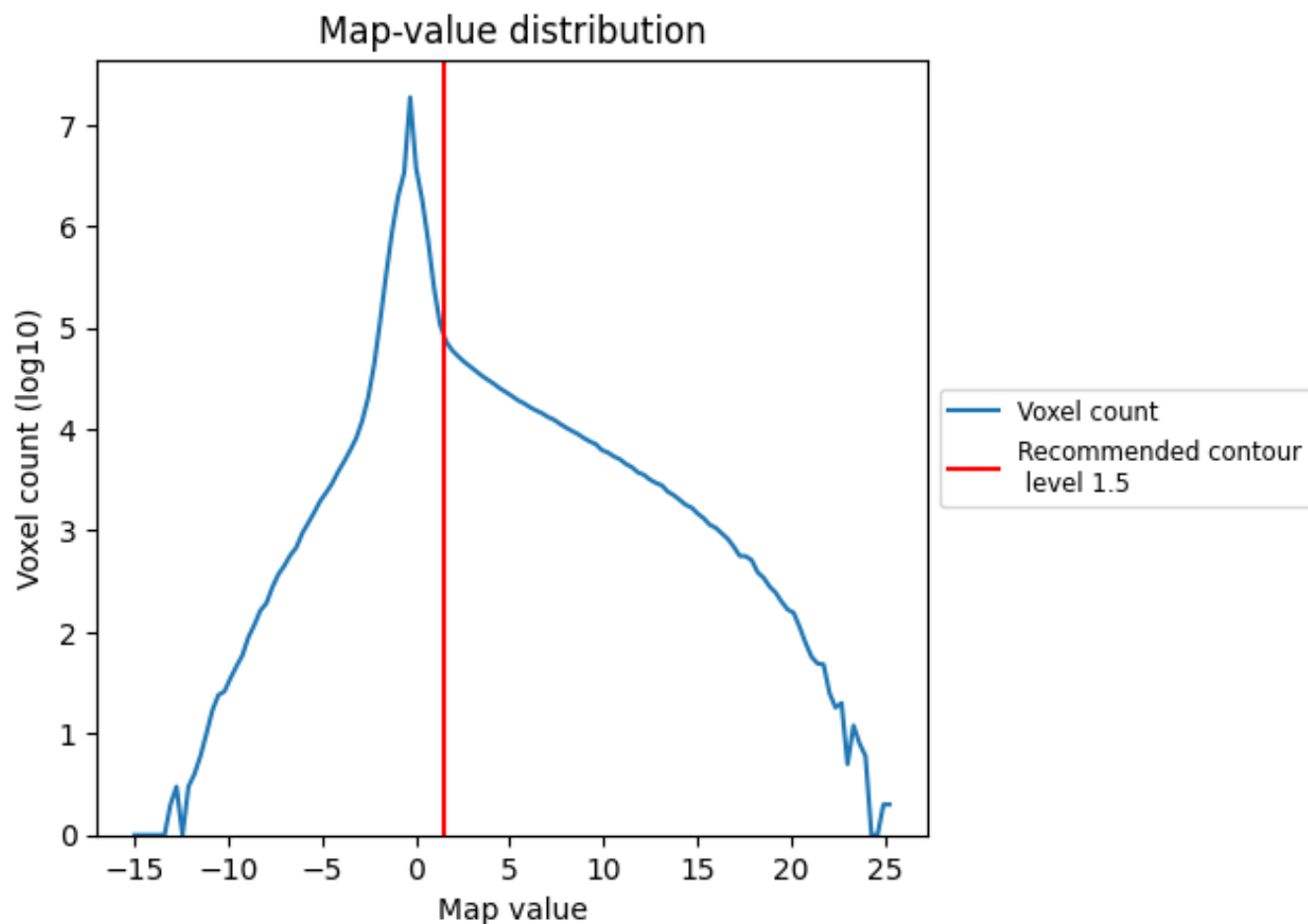
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

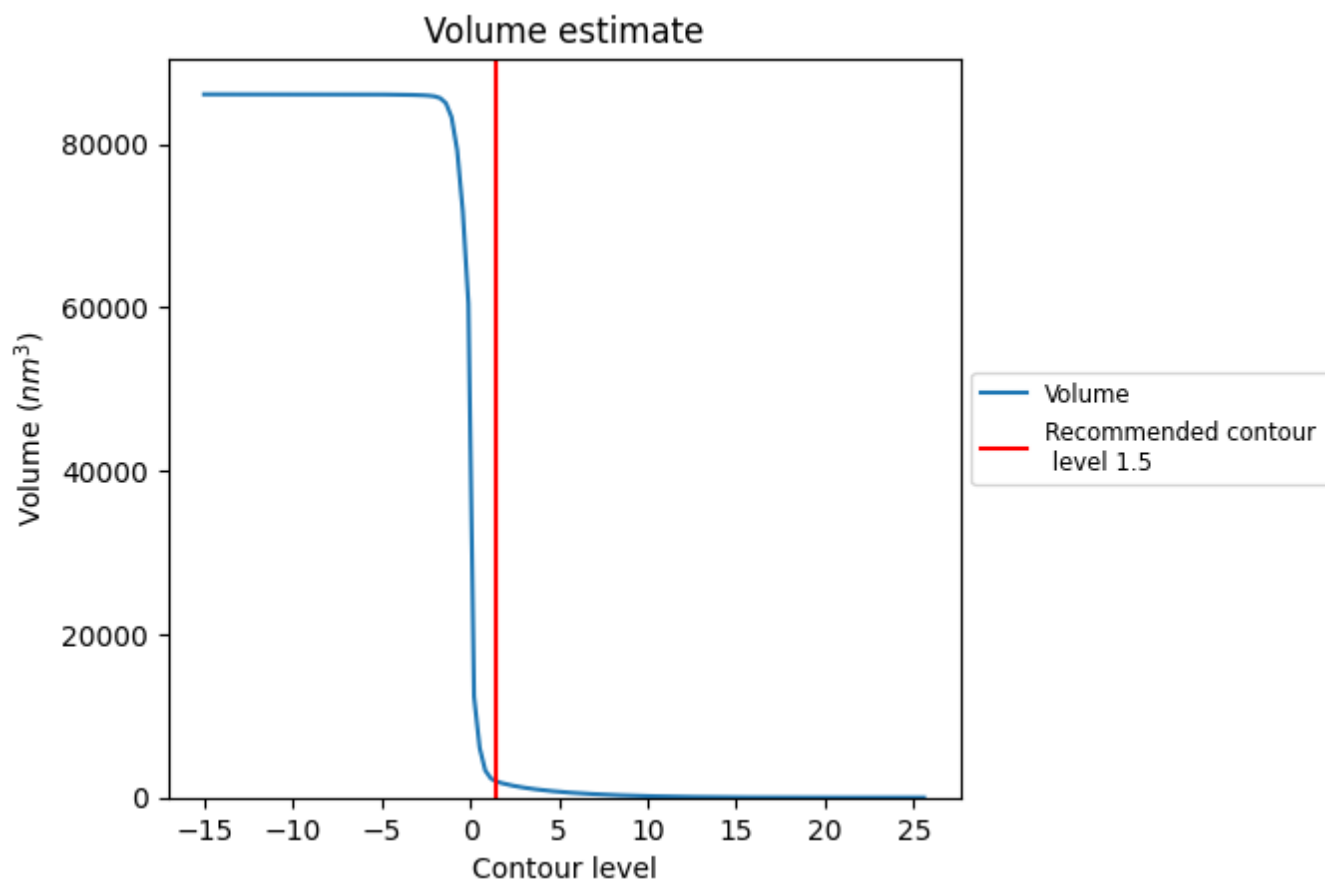
This section contains the results of statistical analysis of the map.

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



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

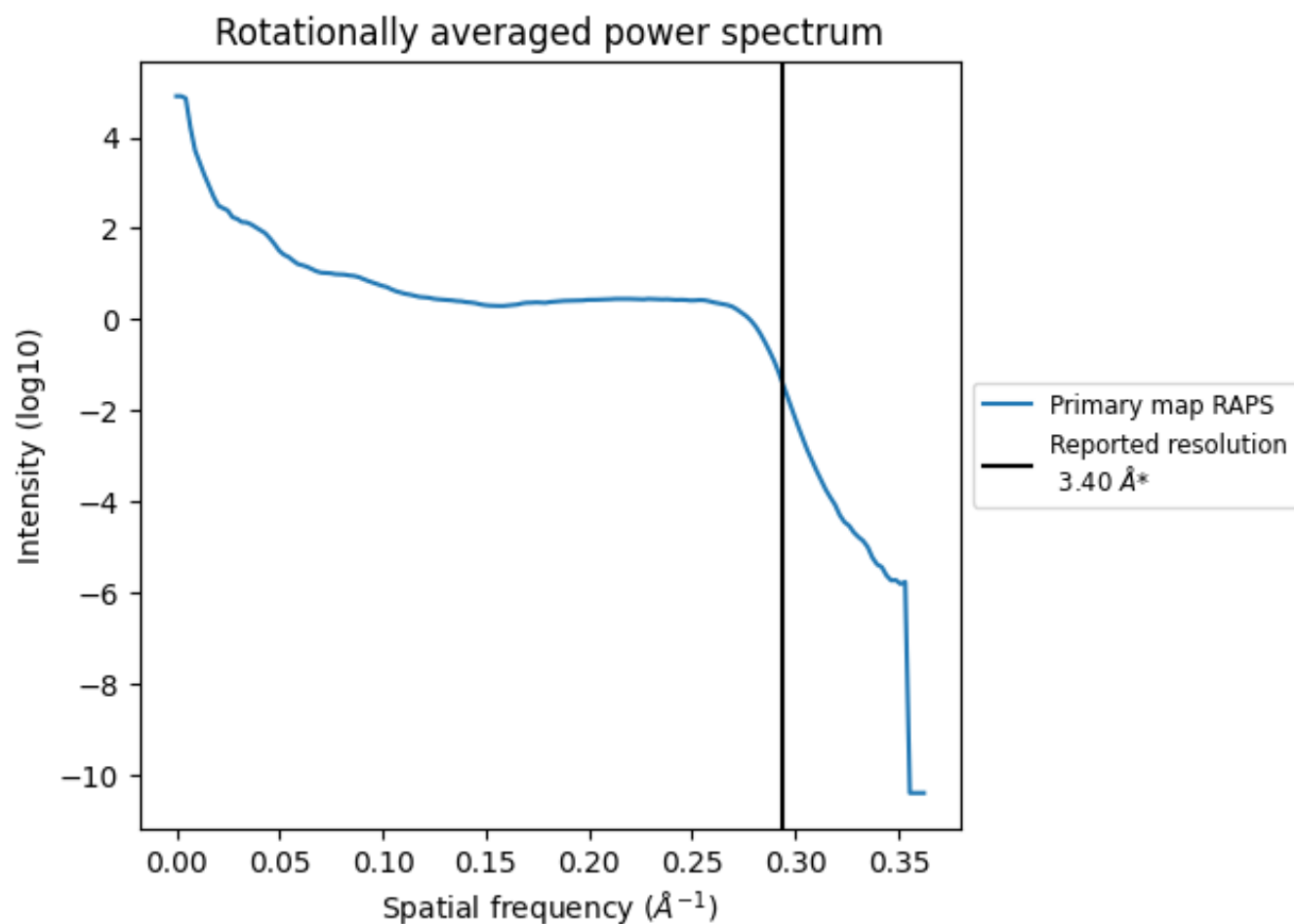
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1962 nm<sup>3</sup>; this corresponds to an approximate mass of 1772 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 ⓘ

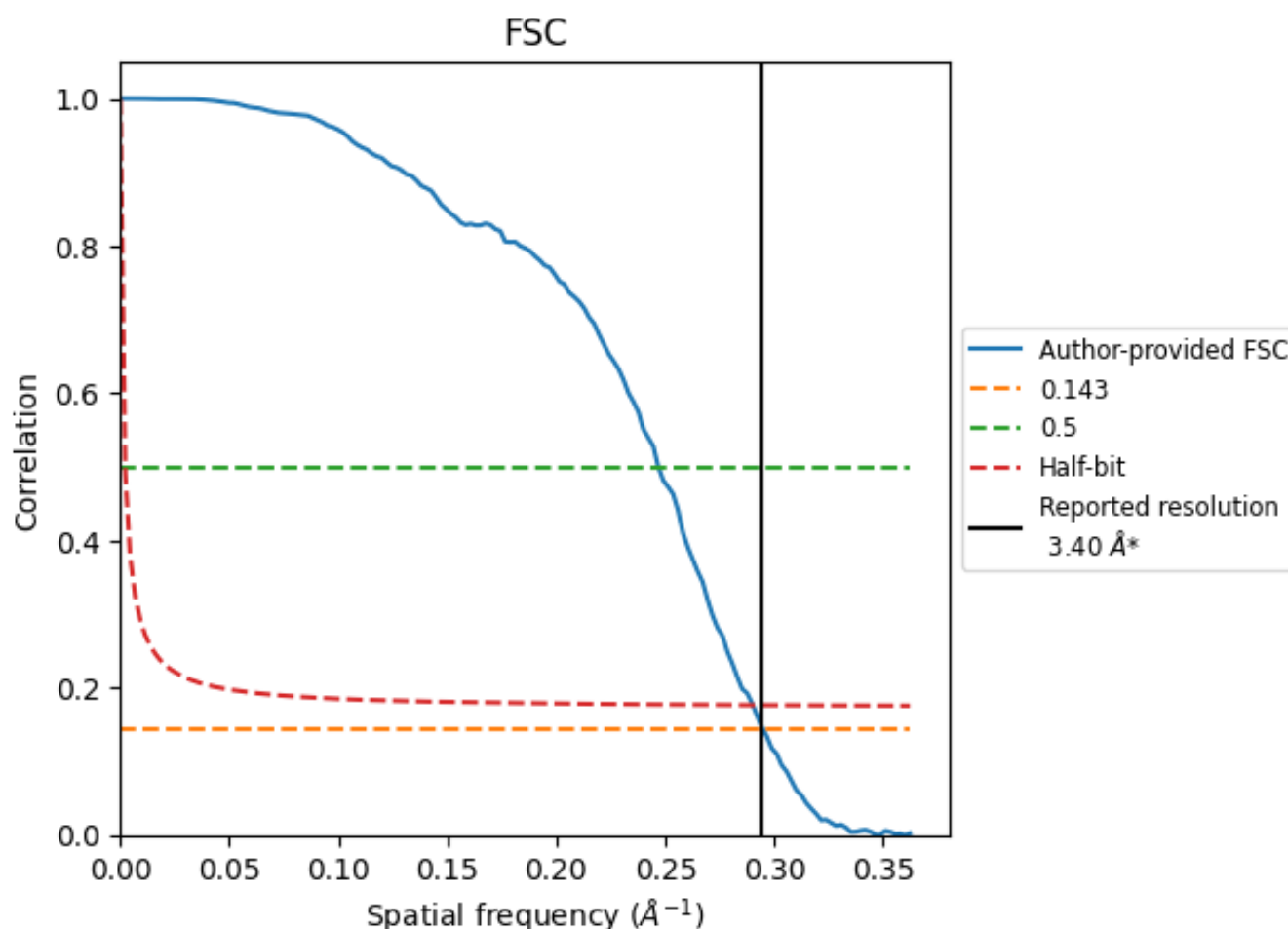


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 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 0.294  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	4.05	3.45
Unmasked-calculated*	-	-	-

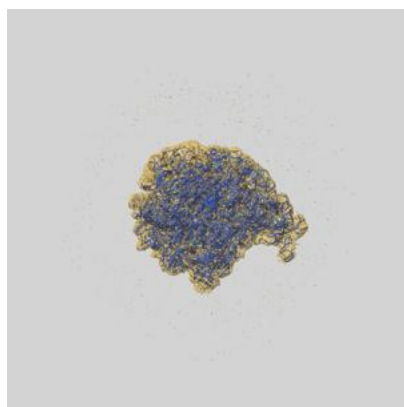
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



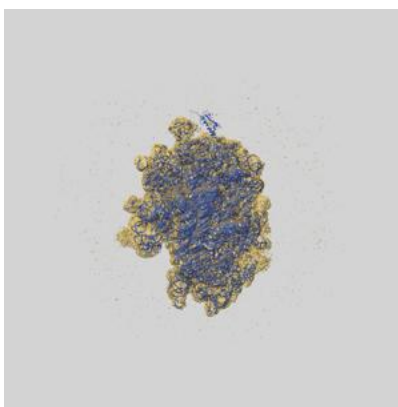
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30598 and PDB model 7D6Z. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

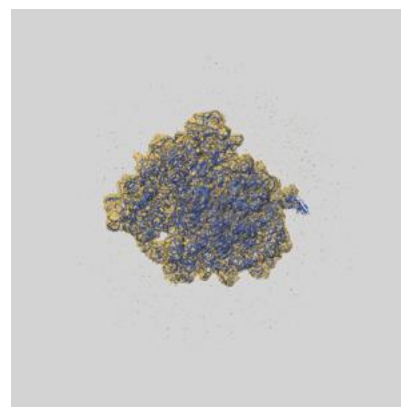
### 9.1 Map-model overlay [i](#)



X



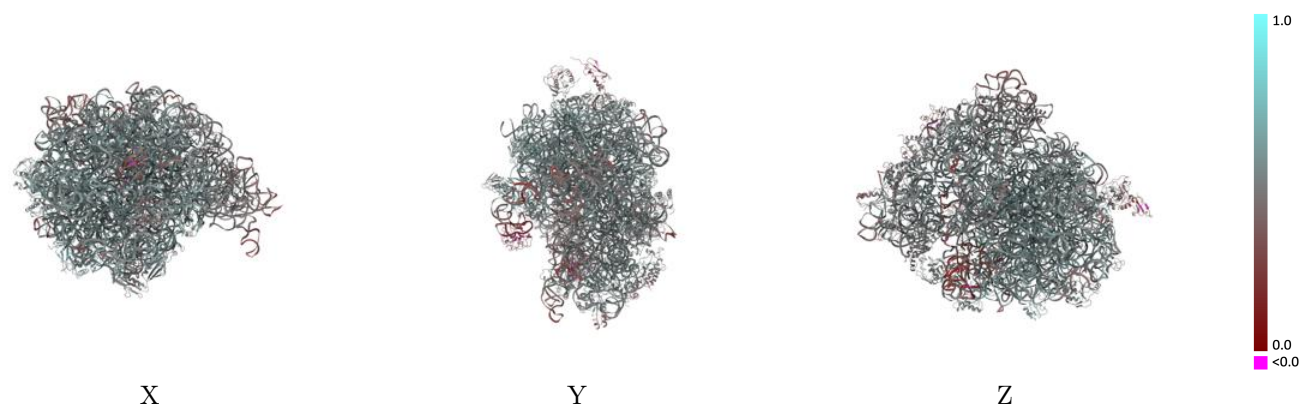
Y



Z

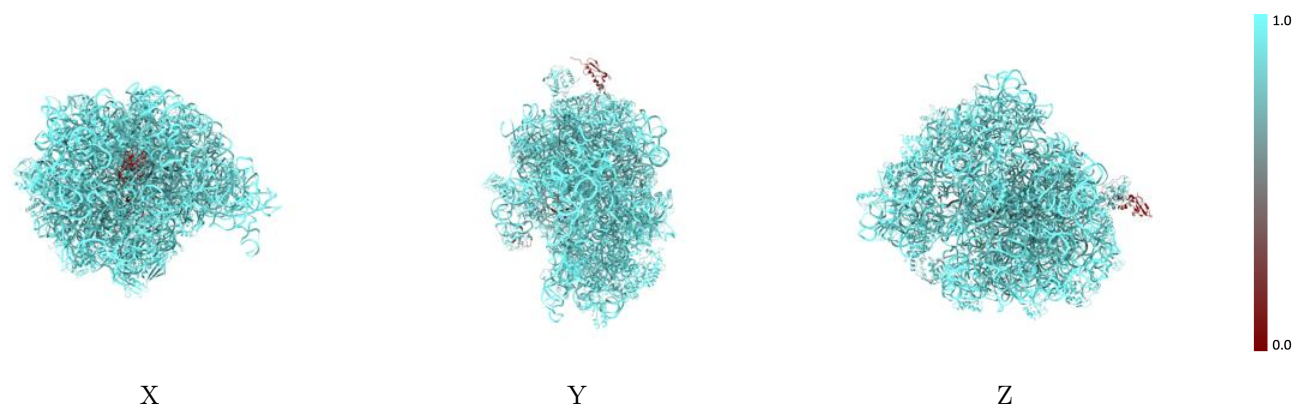
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



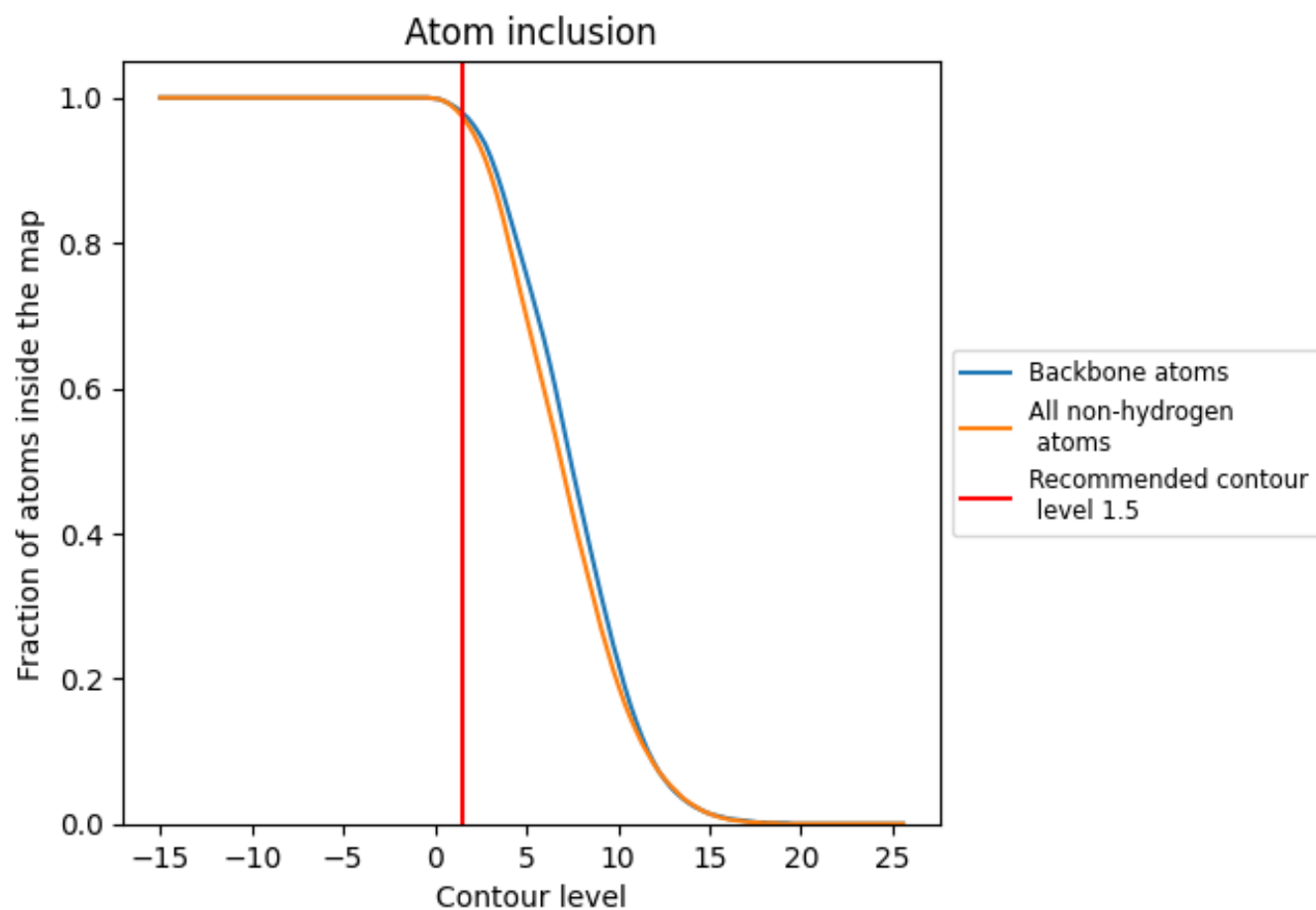
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9740	 0.5050
0	 0.9680	 0.4600
1	 0.8500	 0.4020
2	 0.9540	 0.3200
3	 0.9630	 0.4720
4	 0.3710	 0.3900
6	 0.7260	 0.4510
A	 0.9960	 0.5210
B	 0.9980	 0.5200
C	 0.9820	 0.5700
D	 0.9810	 0.5600
E	 0.9880	 0.5520
F	 0.9760	 0.4950
G	 0.9820	 0.5180
H	 0.9690	 0.5040
I	 0.7500	 0.2130
J	 0.9840	 0.5670
K	 0.9760	 0.5520
L	 0.9790	 0.5560
M	 0.9840	 0.5660
N	 0.9910	 0.5640
O	 0.9910	 0.5330
P	 0.9730	 0.5540
Q	 0.9920	 0.5660
R	 0.9750	 0.5520
S	 0.9640	 0.5570
T	 0.9790	 0.5520
U	 0.9820	 0.5290
V	 0.9840	 0.5490
W	 0.9820	 0.5760
X	 0.9850	 0.5640
Y	 0.9560	 0.5140
Z	 0.9610	 0.5170
a	 0.9670	 0.5610
b	 0.9100	 0.5480



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
c	 0.9750	 0.5740
d	 0.9820	 0.5840
e	 0.9900	 0.5670
f	 0.9970	 0.4880
g	 0.8380	 0.4190
h	 0.2200	 0.3370
i	 0.9670	 0.4670
j	 0.9730	 0.5140
k	 0.9420	 0.3810
l	 0.9730	 0.5250
m	 0.9640	 0.4830
n	 0.9730	 0.4870
o	 0.9720	 0.5260
p	 0.9700	 0.4720
q	 0.9760	 0.4610
r	 0.9770	 0.5160
s	 0.9450	 0.4750
t	 0.9790	 0.4810
u	 0.9740	 0.4900
v	 0.9750	 0.5080
w	 0.9410	 0.4790
x	 0.9590	 0.4680
y	 0.9860	 0.5290
z	 0.9740	 0.5000