



## Full wwPDB EM Validation Report ⓘ

Apr 27, 2026 – 11:14 am BST

PDB ID : 9T6H / pdb\_00009t6h  
EMDB ID : EMD-55615  
Title : Cryo-EM structure of the 70S ribosome from Francisella tularensis bound to antibiotics chloramphenicol and gentamicin  
Authors : Silhan, J.; Klima, M.; Boura, E.  
Deposited on : 2025-11-07  
Resolution : 2.40 Å(reported)  
Based on initial model : 9SDR

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:

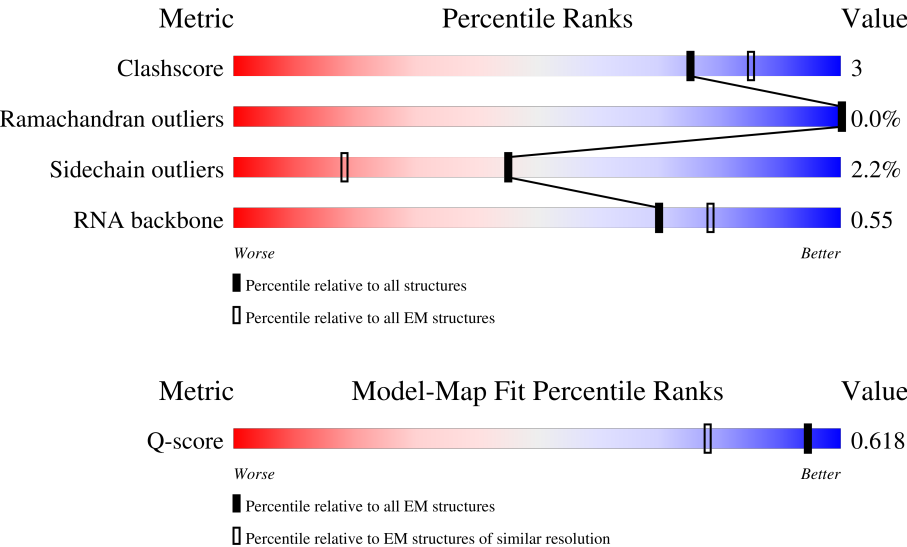
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.40 Å.

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



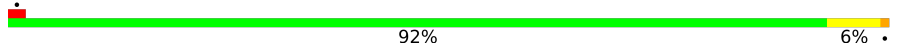
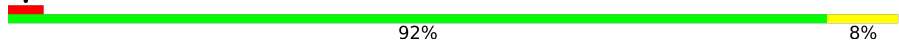



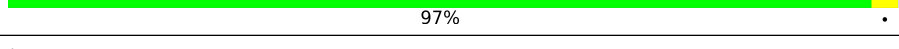
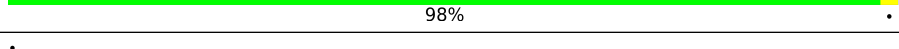
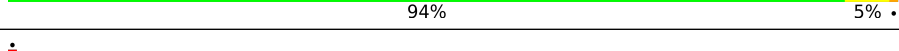
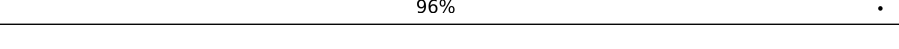
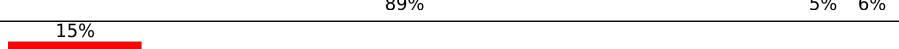
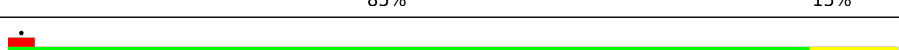
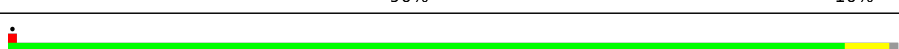
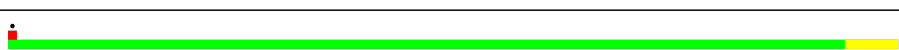
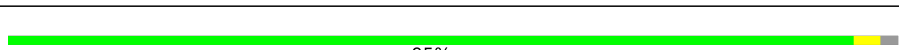
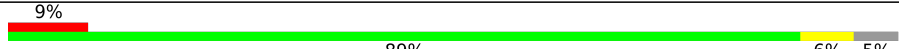



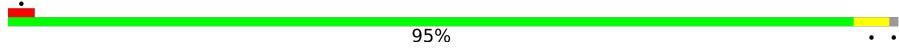
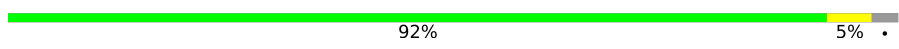
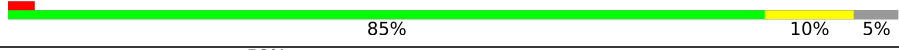
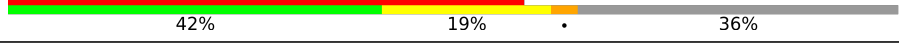



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 ( 1.90 - 2.90 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	2886	
2	B	115	
3	C	274	


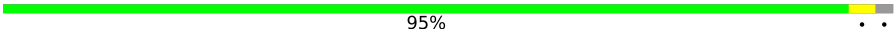









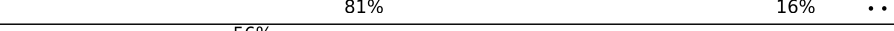


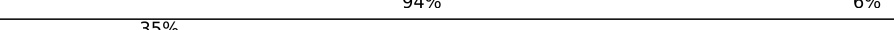



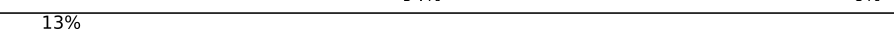
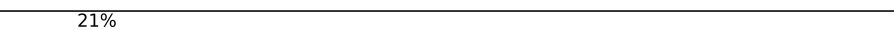

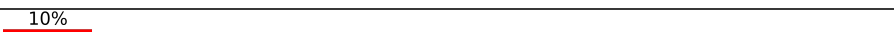



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	210	
5	E	207	
6	F	179	
7	G	178	
8	H	151	
9	I	142	
10	J	122	
11	K	143	
12	L	137	
13	M	145	
14	N	117	
15	O	115	
16	P	118	
17	Q	104	
18	R	111	
19	S	99	
20	T	105	
21	U	96	
22	V	84	
23	W	78	
24	X	66	
25	Y	61	
26	Z	72	
27	0	60	
28	1	51	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	2	44	
30	3	65	
31	4	37	
32	a	1528	
33	b	222	
34	c	209	
35	d	205	
36	e	166	
37	f	111	
38	g	157	
39	h	132	
40	i	129	
41	j	105	
42	k	129	
43	l	124	
44	m	118	
45	n	101	
46	o	88	
47	p	82	
48	q	83	
49	r	72	
50	s	92	
51	t	90	
52	u	65	
53	9	98	

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 135374 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2648	Total	C	N	O	P	0	0
			56859	25385	10454	18372	2648		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	115	Total	C	N	O	P	0	0
			2451	1097	445	794	115		

- Molecule 3 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	273	Total	C	N	O	S	0	0
			2126	1322	428	367	9		

- Molecule 4 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	209	Total	C	N	O	S	0	0
			1559	970	287	297	5		

- Molecule 5 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	207	Total	C	N	O	S	0	0
			1584	1000	281	297	6		

- Molecule 6 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	178	Total	C	N	O	S	0	0
			1398	893	244	256	5		

- Molecule 7 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	174	Total	C	N	O	S	0	0
			1307	826	230	250	1		

- Molecule 8 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	50	Total	C	N	O	S	0	0
			385	250	66	68	1		

- Molecule 9 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	142	Total	C	N	O	S	0	0
			1121	715	205	196	5		

- Molecule 10 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	122	Total	C	N	O	S	0	0
			928	579	178	167	4		

- Molecule 11 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	143	Total	C	N	O	S	0	0
			1061	666	200	192	3		

- Molecule 12 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	137	Total	C	N	O	S	0	0
			1106	701	218	183	4		

- Molecule 13 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	136	Total	C	N	O	S	0	0
			1110	700	215	190	5		

- Molecule 14 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	116	Total	C	N	O	S	0	0
			907	563	176	165	3		

- Molecule 15 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	115	Total	C	N	O	S	0	0
			936	591	178	163	4		

- Molecule 16 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	117	Total	C	N	O	S	0	0
			934	589	188	157			

- Molecule 17 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0
			812	517	148	143	4		

- Molecule 18 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	109	Total	C	N	O	S	0	0
			837	524	158	152	3		

- Molecule 19 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	94	Total	C	N	O	S	0	0
			753	480	138	135			

- Molecule 20 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	104	Total	C	N	O	S	0	0
			794	504	143	146	1		

- Molecule 21 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	94	Total	C	N	O	S	0	0
			754	479	137	137	1		

- Molecule 22 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	73	Total	C	N	O	S	0	0
			557	349	107	100	1		

- Molecule 23 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	77	Total	C	N	O	S	0	0
			619	386	126	105	2		

- Molecule 24 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	64	Total	C	N	O	S	0	0
			529	332	101	95	1		

- Molecule 25 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	58	Total	C	N	O	S	0	0
			456	289	85	80	2		

- Molecule 26 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	46	Total	C	N	O	S	0	0
			363	224	62	71	6		

- Molecule 27 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	55	Total	C	N	O	S	0	0
			441	267	91	82	1		

- Molecule 28 is a protein called Large ribosomal subunit protein bL33.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	49	Total	C	N	O	S	0	0
			411	263	75	70	3		

- Molecule 29 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	44	Total	C	N	O	S	0	0
			363	222	86	53	2		

- Molecule 30 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	64	Total	C	N	O	S	0	0
			505	313	106	82	4		

- Molecule 31 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	37	Total	C	N	O	S	0	0
			304	184	70	45	5		

- Molecule 32 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1437	Total	C	N	O	P	0	0
			30843	13761	5663	9982	1437		

- Molecule 33 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	222	Total	C	N	O	S	0	0
			1733	1106	301	316	10		

- Molecule 34 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	209	Total	C	N	O	S	0	0
			1638	1037	304	291	6		

- Molecule 35 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	205	Total	C	N	O	S	0	0
			1620	1003	309	300	8		

- Molecule 36 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	157	Total	C	N	O	S	0	0
			1155	721	214	215	5		

- Molecule 37 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	104	Total	C	N	O	S	0	0
			859	547	150	156	6		

- Molecule 38 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	154	Total	C	N	O	S	0	0
			1217	761	232	219	5		

- Molecule 39 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	131	Total	C	N	O	S	0	0
			1002	637	173	186	6		

- Molecule 40 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	127	Total	C	N	O	S	0	0
			1020	637	197	182	4		

- Molecule 41 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	100	Total	C	N	O	S	0	0
			799	507	145	146	1		

- Molecule 42 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	118	Total	C	N	O	S	0	0
			882	546	170	164	2		

- Molecule 43 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	123	Total	C	N	O	S	0	0
			963	594	201	166	2		

- Molecule 44 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	115	Total	C	N	O	S	0	0
			912	560	186	161	5		

- Molecule 45 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	100	Total	C	N	O	S	0	0
			814	514	157	139	4		

- Molecule 46 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	88	Total	C	N	O	S	0	0
			729	451	145	132	1		

- Molecule 47 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	82	Total	C	N	O	S	0	0
			639	406	123	108	2		

- Molecule 48 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	80	Total	C	N	O	S	0	0
			670	429	119	119	3		

- Molecule 49 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	67	Total	C	N	O	S	0	0
			544	347	99	96	2		

- Molecule 50 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	82	Total	C	N	O	S	0	0
			660	420	124	112	4		

- Molecule 51 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	89	Total	C	N	O	S	0	0
			704	439	142	121	2		

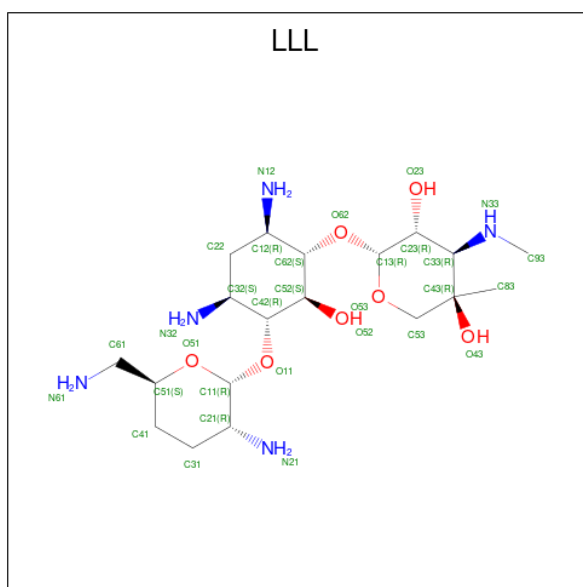
- Molecule 52 is a protein called Small ribosomal subunit protein bS21B.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	59	Total	C	N	O	S	0	0
			500	313	105	81	1		

- Molecule 53 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	9	96	Total	C	N	O	S	0	0
			765	479	135	147	4		

- Molecule 54 is (2R,3R,4R,5R)-2-((1S,2S,3R,4S,6R)-4,6-DIAMINO-3-((2R,3R,6S)-3-AMINO-6-(AMINOMETHYL)-TETRAHYDRO-2H-PYRAN-2-YLOXY)-2-HYDROXYCYCLOHEXYLOXY)-5-METHYL-4-(METHYLAMINO)-TETRAHYDRO-2H-PYRAN-3,5-DIOL (CCD ID: LLL) (formula: C<sub>19</sub>H<sub>39</sub>N<sub>5</sub>O<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
54	A	1	Total 31	C 19	N 5	O 7	0
54	A	1	Total 31	C 19	N 5	O 7	0
54	A	1	Total 31	C 19	N 5	O 7	0
54	A	1	Total 31	C 19	N 5	O 7	0
54	A	1	Total 31	C 19	N 5	O 7	0
54	a	1	Total 31	C 19	N 5	O 7	0
54	a	1	Total 31	C 19	N 5	O 7	0
54	a	1	Total 31	C 19	N 5	O 7	0
54	a	1	Total 31	C 19	N 5	O 7	0

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

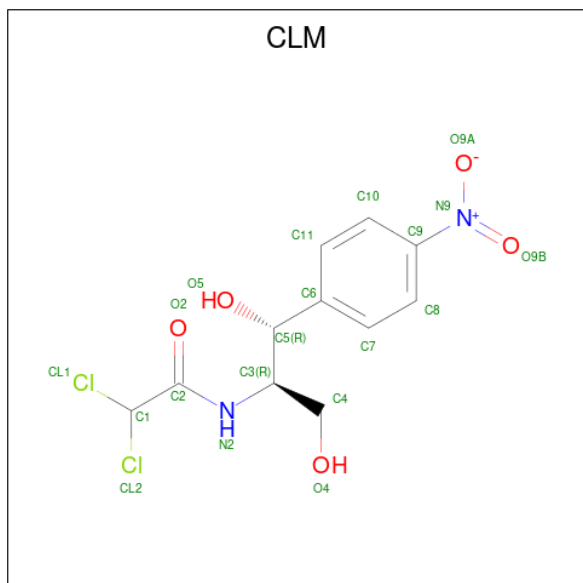
Mol	Chain	Residues	Atoms	AltConf
55	A	118	Total Mg 118 118	0
55	B	2	Total Mg 2 2	0
55	K	1	Total Mg 1 1	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
55	0	1	Total	Mg	0
			1	1	
55	a	14	Total	Mg	0
			14	14	

- Molecule 56 is CHLORAMPHENICOL (CCD ID: CLM) (formula:  $C_{11}H_{12}Cl_2N_2O_5$ ) (labeled as "Ligand of Interest" by depositor).

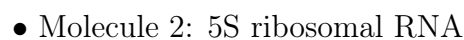


Mol	Chain	Residues	Atoms					AltConf
56	A	1	Total	C	Cl	N	O	0
			20	11	2	2	5	

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula:  $Zn$ ).

Mol	Chain	Residues	Atoms		AltConf
57	4	1	Total	Zn	0
			1	1	



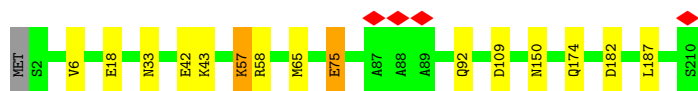


Chain C:  96%

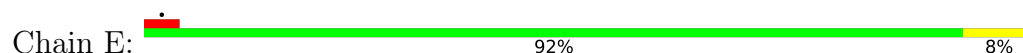




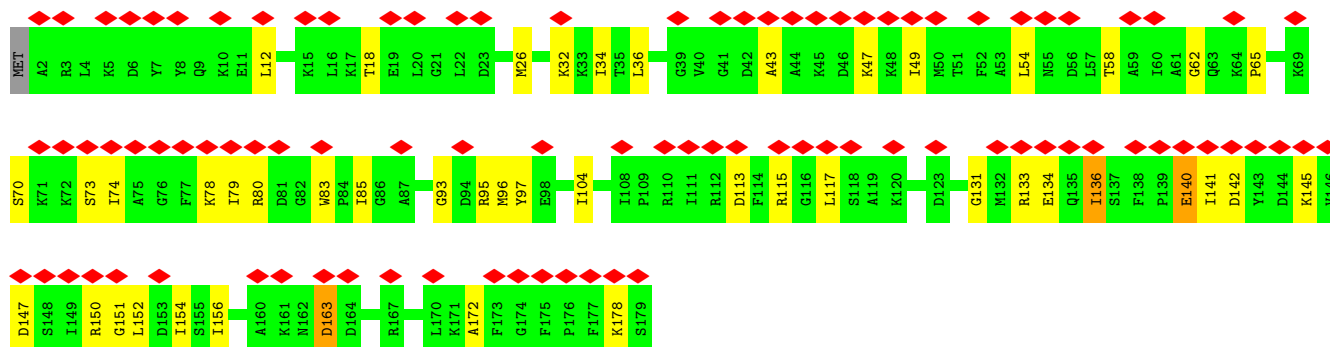
- Molecule 4: Large ribosomal subunit protein uL3



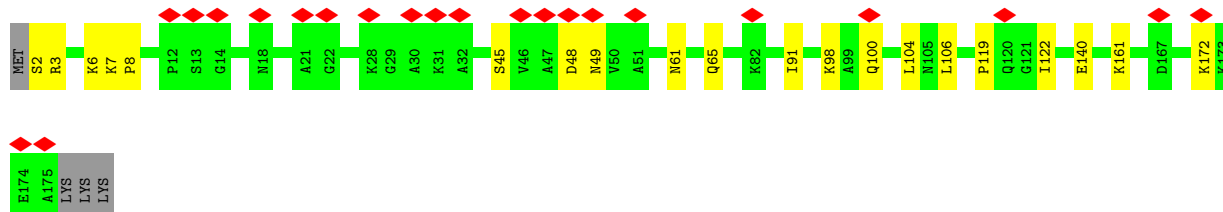
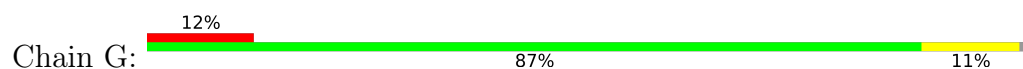
- Molecule 5: Large ribosomal subunit protein uL4



- Molecule 6: Large ribosomal subunit protein uL5



- Molecule 7: Large ribosomal subunit protein uL6



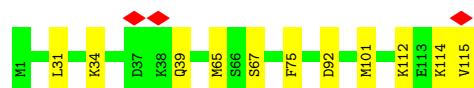
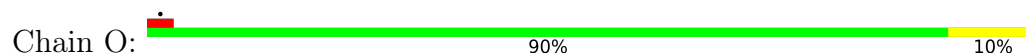
- Molecule 8: Large ribosomal subunit protein bL9



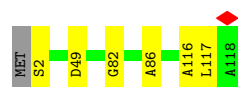




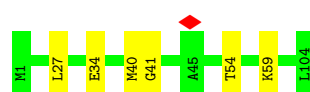
- Molecule 15: Large ribosomal subunit protein bL19



- Molecule 16: Large ribosomal subunit protein bL20



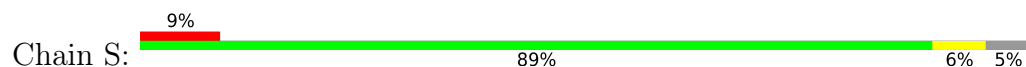
- Molecule 17: Large ribosomal subunit protein bL21



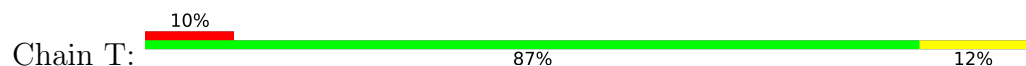
- Molecule 18: Large ribosomal subunit protein uL22



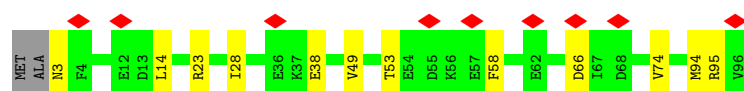
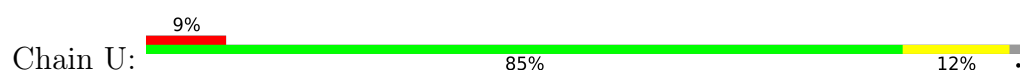
- Molecule 19: Large ribosomal subunit protein uL23



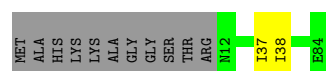
- Molecule 20: Large ribosomal subunit protein uL24



- Molecule 21: Large ribosomal subunit protein bL25



- Molecule 22: Large ribosomal subunit protein bL27



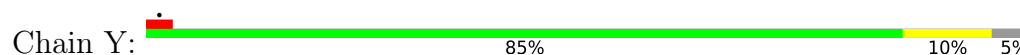
- Molecule 23: Large ribosomal subunit protein bL28



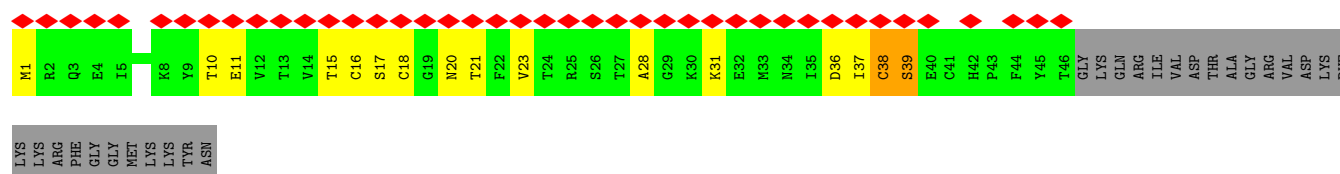
- Molecule 24: Large ribosomal subunit protein uL29



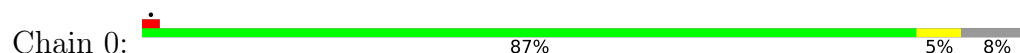
- Molecule 25: Large ribosomal subunit protein uL30

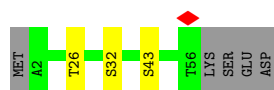


- Molecule 26: Large ribosomal subunit protein bL31

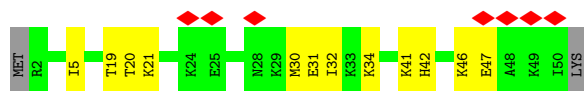
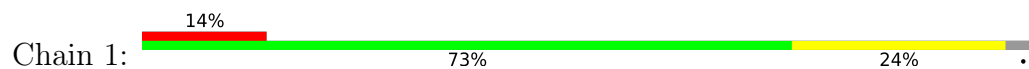


- Molecule 27: Large ribosomal subunit protein bL32





- Molecule 28: Large ribosomal subunit protein bL33



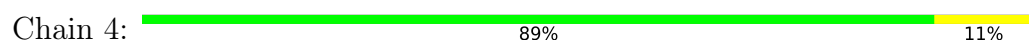
- Molecule 29: Large ribosomal subunit protein bL34



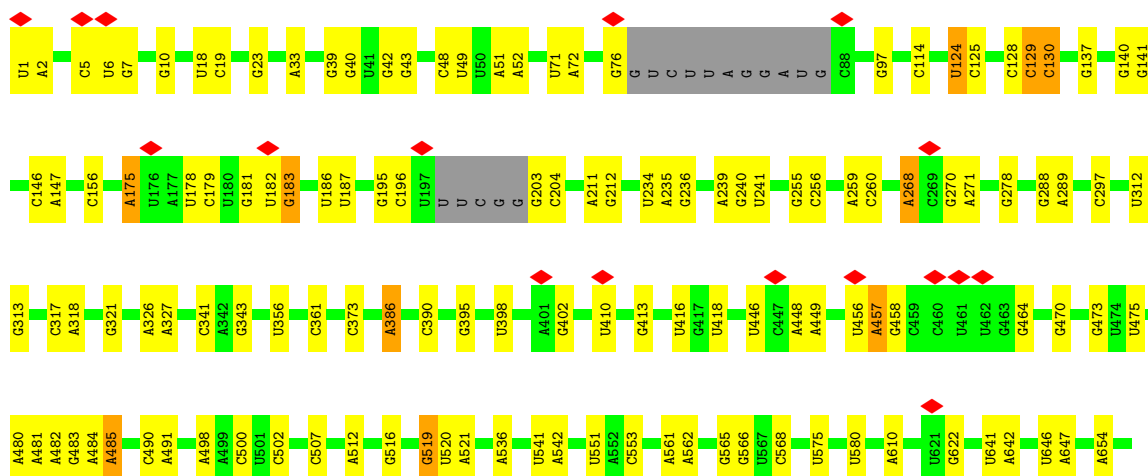
- Molecule 30: Large ribosomal subunit protein bL35

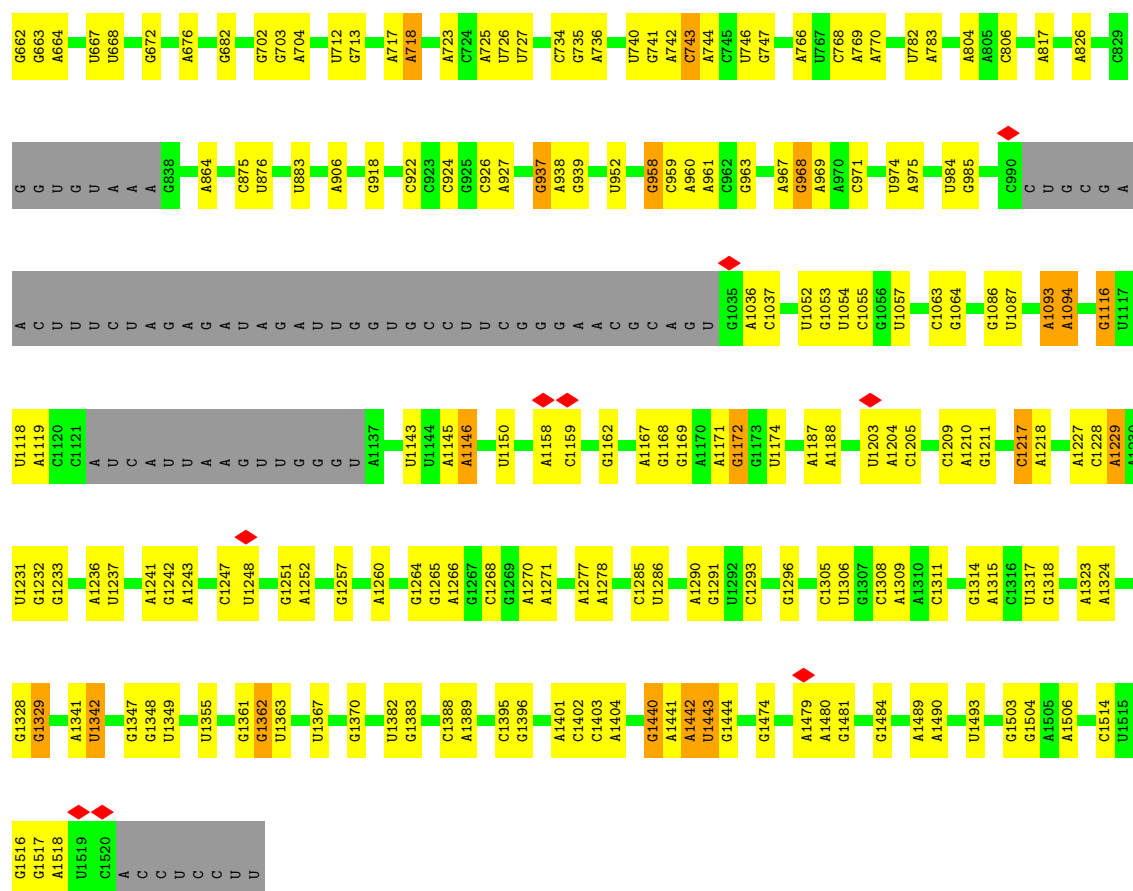


- Molecule 31: Large ribosomal subunit protein bL36

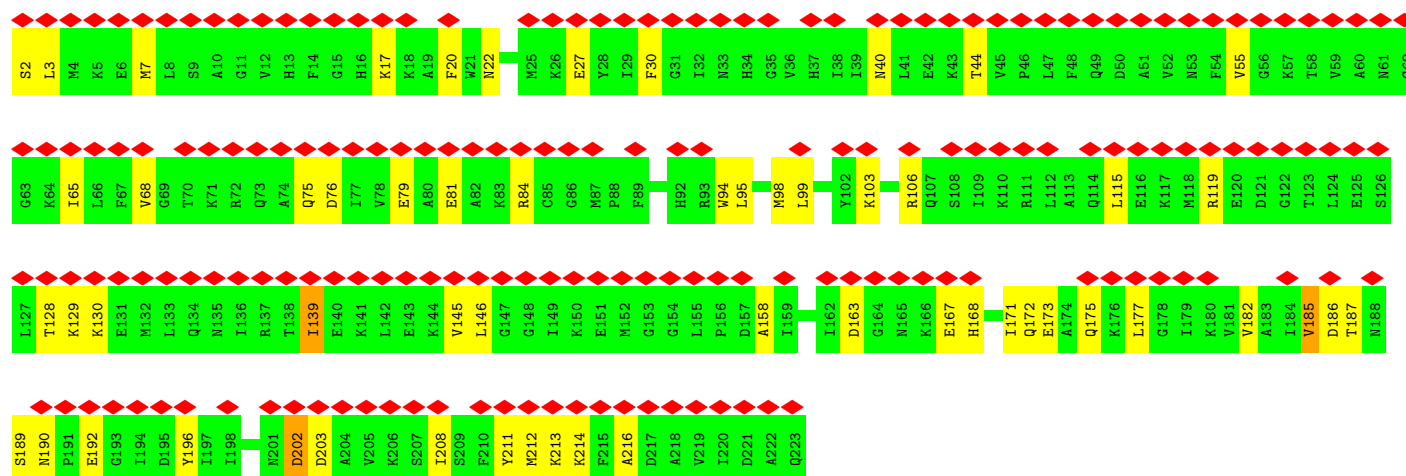
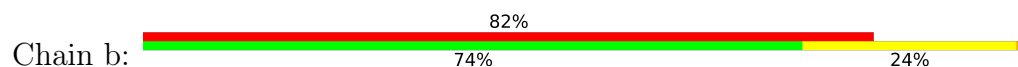


- Molecule 32: 16S ribosomal RNA

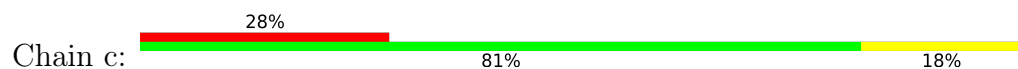


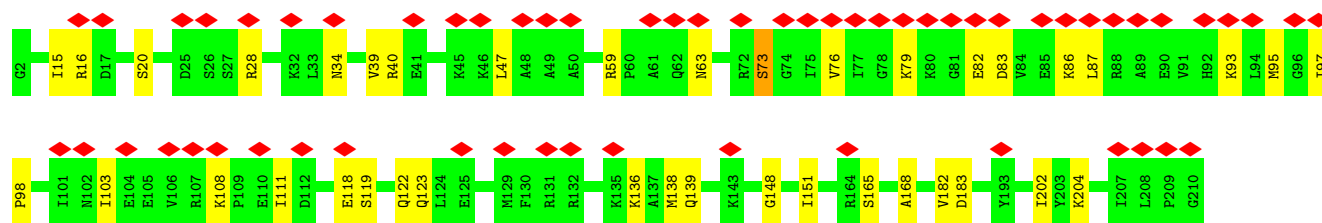


• Molecule 33: Small ribosomal subunit protein uS2

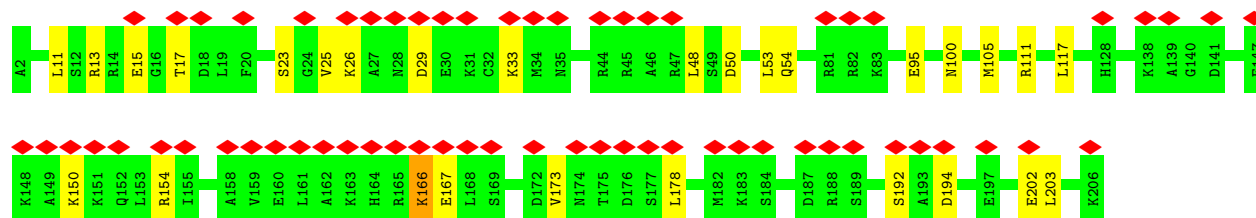
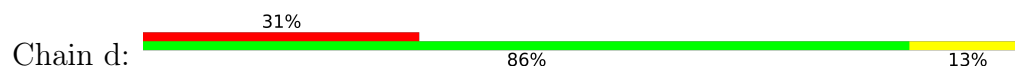


• Molecule 34: Small ribosomal subunit protein uS3

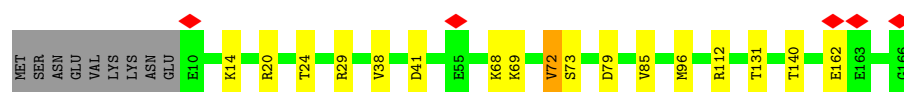
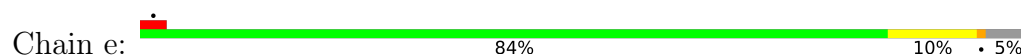




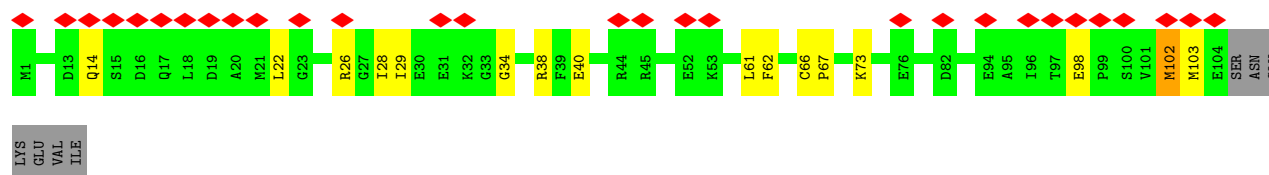
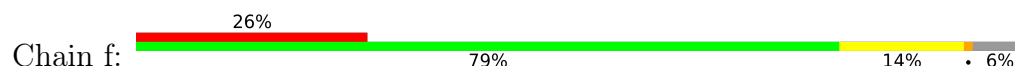
• Molecule 35: Small ribosomal subunit protein uS4



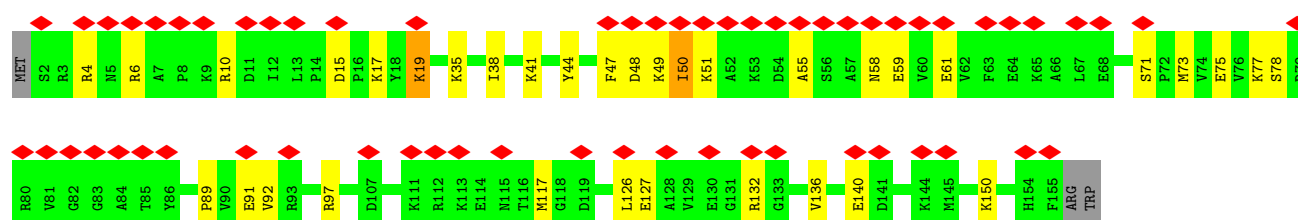
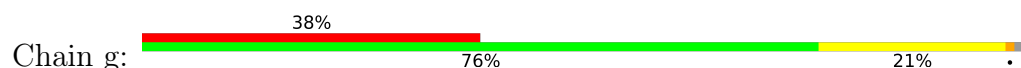
• Molecule 36: Small ribosomal subunit protein uS5




• Molecule 37: Small ribosomal subunit protein bS6



• Molecule 38: Small ribosomal subunit protein uS7




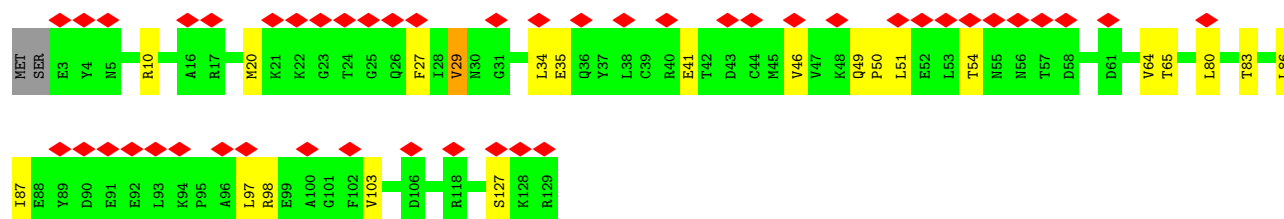
• Molecule 39: Small ribosomal subunit protein uS8

Chain h: 



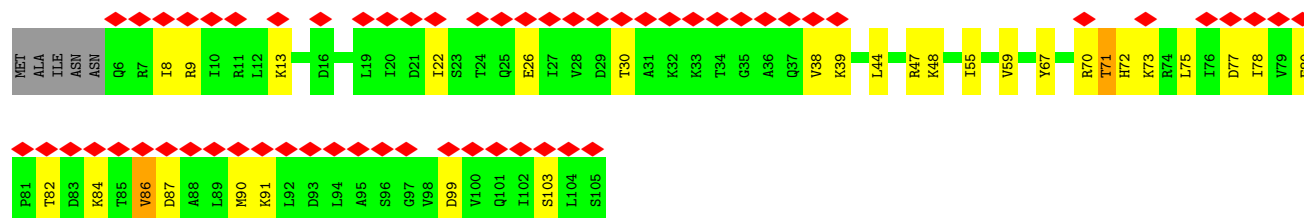
- Molecule 40: Small ribosomal subunit protein uS9

Chain i: 




- Molecule 41: Small ribosomal subunit protein uS10

Chain j: 



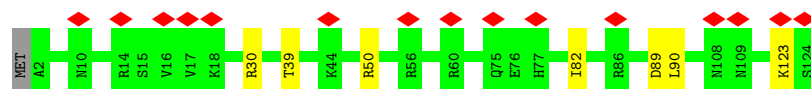
- Molecule 42: Small ribosomal subunit protein uS11

Chain k: 




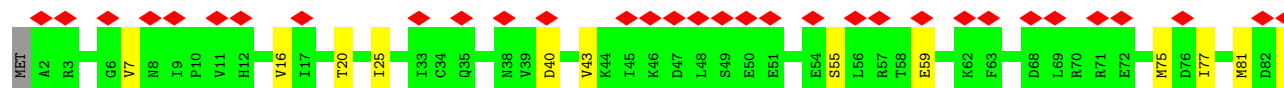
- Molecule 43: Small ribosomal subunit protein uS12

Chain l: 

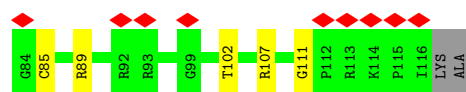


- Molecule 44: Small ribosomal subunit protein uS13

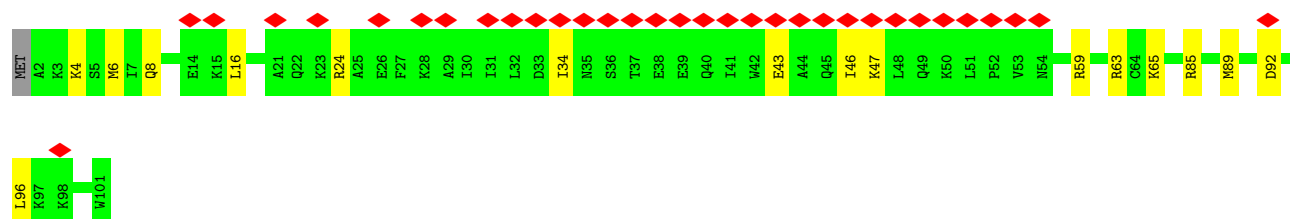
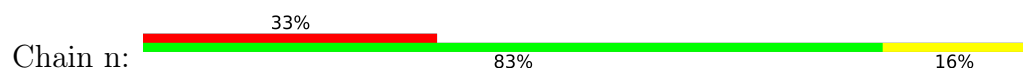
Chain m: 



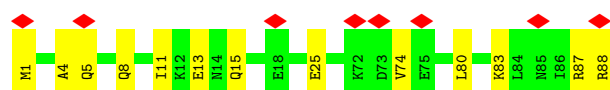
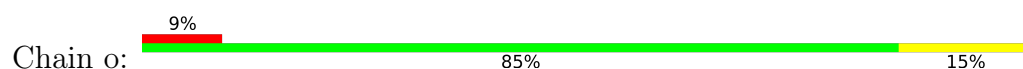




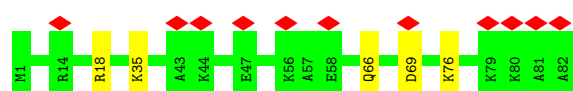
- Molecule 45: Small ribosomal subunit protein uS14



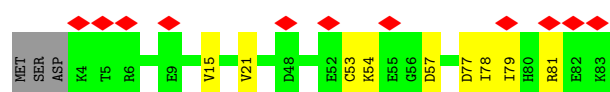
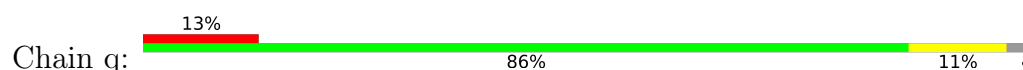
- Molecule 46: Small ribosomal subunit protein uS15



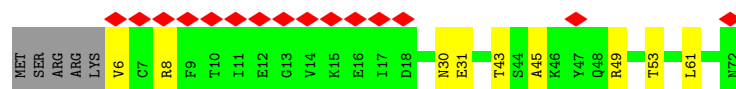
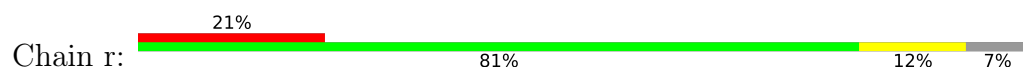
- Molecule 47: Small ribosomal subunit protein bS16



- Molecule 48: Small ribosomal subunit protein uS17

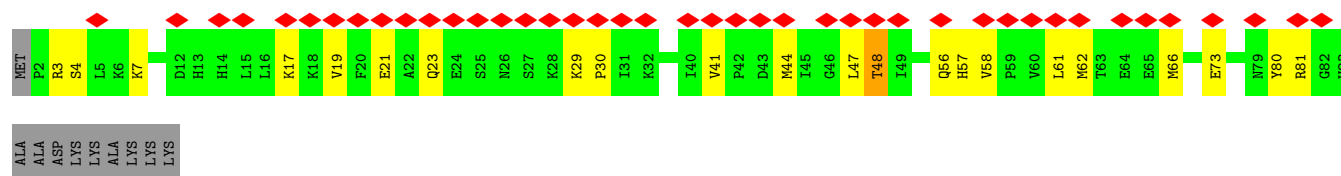


- Molecule 49: Small ribosomal subunit protein bS18

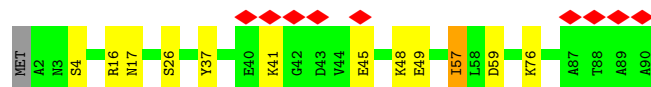
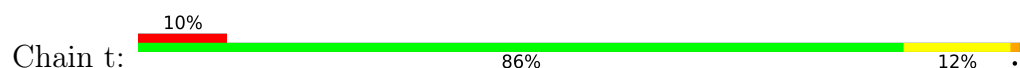


- Molecule 50: Small ribosomal subunit protein uS19

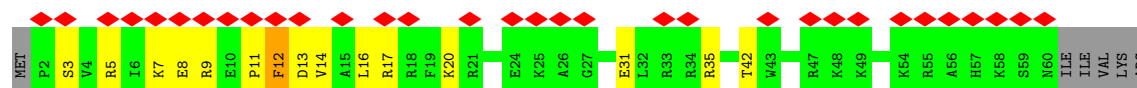




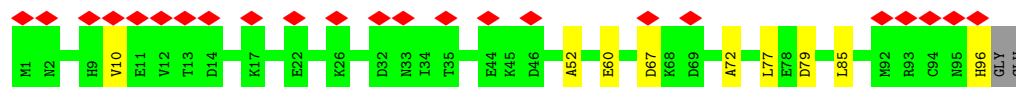
- Molecule 51: Small ribosomal subunit protein bS20



- Molecule 52: Small ribosomal subunit protein bS21B



- Molecule 53: Ribosome hibernation promoting factor



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	270000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.372	Depositor
Minimum map value	-0.133	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.05	Depositor
Map size ( $\text{\AA}$ )	456.0, 456.0, 456.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.76, 0.76, 0.76	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, MG, LLL, CLM, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.30	0/63667	0.42	0/99287
2	B	0.20	0/2742	0.32	0/4270
3	C	0.13	0/2162	0.34	0/2898
4	D	0.14	0/1584	0.35	0/2135
5	E	0.12	0/1603	0.32	0/2150
6	F	0.14	0/1419	0.38	0/1900
7	G	0.12	0/1326	0.31	0/1790
8	H	0.15	0/390	0.39	0/525
9	I	0.19	0/1146	0.36	0/1545
10	J	0.12	0/937	0.30	0/1254
11	K	0.14	0/1074	0.32	0/1428
12	L	0.13	0/1125	0.29	0/1501
13	M	0.16	0/1129	0.34	0/1505
14	N	0.18	0/918	0.43	0/1227
15	O	0.12	0/950	0.32	0/1265
16	P	0.20	0/946	0.33	0/1266
17	Q	0.13	0/822	0.32	0/1090
18	R	0.13	0/844	0.28	0/1132
19	S	0.13	0/764	0.33	0/1024
20	T	0.31	0/804	0.48	0/1076
21	U	0.13	0/765	0.35	0/1023
22	V	0.13	0/566	0.33	0/757
23	W	0.13	0/629	0.34	0/841
24	X	0.14	0/532	0.27	0/703
25	Y	0.14	0/461	0.33	0/616
26	Z	0.11	0/370	0.28	0/499
27	0	0.11	0/448	0.25	0/599
28	1	0.18	0/418	0.44	0/554
29	2	0.13	0/366	0.33	0/477
30	3	0.15	0/512	0.44	0/676
31	4	0.30	0/305	0.36	0/401
32	a	0.13	0/34539	0.29	0/53868

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	b	0.16	0/1761	0.43	0/2365
34	c	0.13	0/1663	0.34	0/2233
35	d	0.10	0/1639	0.24	0/2191
36	e	0.17	0/1169	0.37	0/1571
37	f	1.03	0/876	1.13	0/1177
38	g	0.13	0/1235	0.32	0/1652
39	h	0.15	0/1020	0.32	0/1369
40	i	0.36	0/1034	0.59	0/1380
41	j	0.16	0/809	0.45	0/1088
42	k	0.14	0/897	0.34	0/1214
43	l	0.13	0/978	0.33	0/1313
44	m	0.16	0/922	0.39	0/1235
45	n	0.15	0/826	0.36	0/1100
46	o	0.16	0/736	0.35	0/980
47	p	0.10	0/648	0.29	0/860
48	q	0.13	0/683	0.34	0/912
49	r	0.14	0/553	0.33	0/742
50	s	0.18	0/676	0.46	0/908
51	t	0.19	0/711	0.36	0/943
52	u	0.42	0/509	0.56	0/674
53	9	0.12	0/775	0.32	0/1041
All	All	0.24	0/146383	0.38	0/218230

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
37	f	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
37	f	26	ARG	Sidechain

## 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	A	56859	0	28548	170	0
2	B	2451	0	1242	13	0
3	C	2126	0	2242	6	0
4	D	1559	0	1570	13	0
5	E	1584	0	1660	10	0
6	F	1398	0	1461	36	0
7	G	1307	0	1365	12	0
8	H	385	0	408	5	0
9	I	1121	0	1170	1	0
10	J	928	0	993	2	0
11	K	1061	0	1134	4	0
12	L	1106	0	1177	4	0
13	M	1110	0	1155	3	0
14	N	907	0	943	9	0
15	O	936	0	985	6	0
16	P	934	0	991	3	0
17	Q	812	0	867	3	0
18	R	837	0	889	2	0
19	S	753	0	785	3	0
20	T	794	0	834	8	0
21	U	754	0	783	5	0
22	V	557	0	571	1	0
23	W	619	0	651	2	0
24	X	529	0	573	1	0
25	Y	456	0	488	4	0
26	Z	363	0	352	10	0
27	0	441	0	447	0	0
28	1	411	0	443	10	0
29	2	363	0	411	2	0
30	3	505	0	549	0	0
31	4	304	0	343	2	0
32	a	30843	0	15509	136	0
33	b	1733	0	1788	38	0
34	c	1638	0	1718	21	0
35	d	1620	0	1673	17	0
36	e	1155	0	1207	12	0
37	f	859	0	870	9	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	g	1217	0	1263	25	0
39	h	1002	0	1031	10	0
40	i	1020	0	1054	12	0
41	j	799	0	860	21	0
42	k	882	0	903	13	0
43	l	963	0	1025	4	0
44	m	912	0	967	10	0
45	n	814	0	867	11	0
46	o	729	0	769	8	0
47	p	639	0	686	4	0
48	q	670	0	699	6	0
49	r	544	0	565	4	0
50	s	660	0	680	18	0
51	t	704	0	762	7	0
52	u	500	0	532	12	0
53	9	765	0	776	5	0
54	A	155	0	195	2	0
54	a	124	0	156	5	0
55	0	1	0	0	0	0
55	A	118	0	0	0	0
55	B	2	0	0	0	0
55	K	1	0	0	0	0
55	a	14	0	0	0	0
56	A	20	0	11	1	0
57	4	1	0	0	0	0
All	All	135374	0	92596	698	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 3.

All (698) 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)
1:A:2187:A:O2'	1:A:2188:A:OP1	1.88	0.91
1:A:2294:U:H5''	6:F:131:GLY:HA3	1.53	0.89
1:A:2187:A:O2'	1:A:2188:A:P	2.31	0.88
6:F:136:ILE:HA	6:F:141:ILE:HD11	1.56	0.86
6:F:80:ARG:HB2	6:F:83:TRP:HE1	1.39	0.85
1:A:2298:A:O2'	1:A:2299:A:H5'	1.78	0.83
34:c:34:ASN:HD21	45:n:65:LYS:HG3	1.48	0.77
1:A:2193:U:O2'	1:A:2194:A:H2'	1.83	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:81:GLU:HG3	33:b:212:MET:HB3	1.68	0.76
37:f:28:ILE:HG23	37:f:73:LYS:HE3	1.68	0.75
42:k:36:ASP:OD1	42:k:37:ARG:N	2.22	0.73
3:C:240:THR:HG22	3:C:242:GLY:H	1.53	0.73
32:a:662:G:H2'	32:a:663:G:C8	2.23	0.72
41:j:67:TYR:HB3	45:n:96:LEU:HD11	1.72	0.72
32:a:181:G:O2'	32:a:183:G:N2	2.24	0.71
1:A:856:G:H2'	1:A:857:G:C8	2.27	0.70
32:a:130:C:OP1	47:p:66:GLN:NE2	2.25	0.69
42:k:52:PHE:HB3	42:k:56:ARG:HB2	1.74	0.69
26:Z:16:CYS:HB3	26:Z:20:ASN:HB2	1.73	0.69
1:A:1718:A:H2	1:A:1734:G:H21	1.41	0.68
32:a:97:G:OP1	51:t:16:ARG:NH1	2.27	0.68
1:A:2276:A:O2'	1:A:2277:A:H3'	1.92	0.68
2:B:75:U:OP1	21:U:23:ARG:NH2	2.27	0.68
19:S:5:GLU:OE2	19:S:5:GLU:N	2.27	0.67
32:a:416:U:OP1	35:d:13:ARG:NH2	2.28	0.67
40:i:35:GLU:OE1	40:i:35:GLU:N	2.29	0.66
1:A:1798:A:H2'	1:A:1799:A:C8	2.31	0.66
32:a:1252:A:N6	32:a:1265:G:O2'	2.29	0.65
32:a:1388:C:OP2	36:e:29:ARG:NH2	2.29	0.65
1:A:1428:A:H2'	1:A:1429:A:C8	2.32	0.65
32:a:1257:G:N2	32:a:1260:A:OP2	2.22	0.64
32:a:1118:U:OP1	41:j:9:ARG:NH2	2.30	0.64
28:l:41:LYS:HE3	28:l:42:HIS:H	1.62	0.64
32:a:1347:G:H2'	32:a:1348:G:C8	2.33	0.64
1:A:870:U:OP1	12:L:6:ARG:NH1	2.31	0.64
32:a:663:G:H2'	32:a:664:A:H8	1.63	0.63
6:F:80:ARG:HB2	6:F:83:TRP:NE1	2.11	0.63
44:m:75:MET:HA	44:m:75:MET:HE3	1.80	0.63
35:d:95:GLU:O	35:d:100:ASN:ND2	2.31	0.62
26:Z:16:CYS:SG	26:Z:17:SER:N	2.72	0.62
50:s:29:LYS:HA	50:s:29:LYS:HE2	1.81	0.62
1:A:2366:A:H2'	1:A:2367:A:C8	2.34	0.62
12:L:43:THR:HG22	12:L:94:VAL:HG12	1.82	0.62
32:a:826:A:H62	54:a:1616:LLL:H531	1.65	0.62
1:A:715:U:OP2	46:o:87:ARG:NH2	2.24	0.62
32:a:1171:A:OP2	40:i:98:ARG:NH2	2.32	0.62
37:f:102:MET:HA	37:f:102:MET:HE2	1.82	0.62
42:k:109:SER:HB3	52:u:5:ARG:HD3	1.82	0.62
51:t:37:TYR:O	51:t:41:LYS:HG2	2.00	0.62

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:U:H3	2:B:59:G:H1	1.47	0.61
36:e:162:GLU:H	36:e:162:GLU:CD	2.09	0.61
38:g:50:ILE:HD11	38:g:126:LEU:HD21	1.82	0.61
4:D:92:GLN:N	4:D:92:GLN:OE1	2.33	0.61
6:F:134:GLU:N	6:F:134:GLU:OE1	2.33	0.61
38:g:136:VAL:O	38:g:140:GLU:HG2	2.01	0.61
32:a:512:A:N6	43:l:89:ASP:OD2	2.32	0.61
42:k:103:LYS:HE3	42:k:103:LYS:HA	1.82	0.60
1:A:1465:A:H2'	1:A:1466:A:C8	2.37	0.60
32:a:958:G:N2	53:9:60:GLU:OE1	2.35	0.60
39:h:48:SER:OG	39:h:64:GLU:OE1	2.20	0.60
1:A:2187:A:HO2'	1:A:2188:A:P	2.17	0.60
32:a:457:A:H3'	32:a:458:G:H8	1.67	0.60
33:b:3:LEU:O	33:b:7:MET:HG2	2.00	0.60
42:k:46:THR:HG23	42:k:49:GLY:H	1.67	0.60
44:m:40:ASP:HB3	44:m:43:VAL:HG23	1.83	0.59
34:c:16:ARG:NH2	34:c:182:VAL:O	2.34	0.59
32:a:1209:C:H2'	32:a:1210:A:H8	1.67	0.59
49:r:6:VAL:O	49:r:8:ARG:NH1	2.36	0.59
1:A:1380:A:O2'	1:A:1391:U:O2	2.20	0.59
6:F:54:LEU:O	6:F:58:THR:HG23	2.02	0.59
7:G:91:ILE:HG22	7:G:161:LYS:HA	1.83	0.59
32:a:924:C:O3'	38:g:4:ARG:NH1	2.35	0.59
6:F:34:ILE:HG12	6:F:156:ILE:HG12	1.83	0.59
20:T:48:PRO:HB3	20:T:56:GLY:H	1.67	0.59
33:b:99:LEU:HB2	33:b:173:GLU:HG2	1.84	0.59
33:b:75:GLN:O	33:b:79:GLU:HG3	2.03	0.59
50:s:41:VAL:HG22	50:s:44:MET:HE2	1.85	0.59
32:a:938:A:H2'	32:a:939:G:C8	2.37	0.59
33:b:190:ASN:HD21	33:b:192:GLU:HG3	1.67	0.59
6:F:62:GLY:O	6:F:95:ARG:NH1	2.36	0.59
11:K:19:LEU:HB3	11:K:31:SER:HB2	1.85	0.59
32:a:326:A:H2'	32:a:327:A:C8	2.38	0.59
41:j:9:ARG:HD2	41:j:75:LEU:HD11	1.83	0.58
38:g:51:LYS:HD2	38:g:55:ALA:HA	1.84	0.58
46:o:11:ILE:O	46:o:15:GLN:HB3	2.02	0.58
1:A:272:U:O2'	1:A:352:G:N2	2.34	0.58
32:a:663:G:H2'	32:a:664:A:C8	2.38	0.58
1:A:6:A:H2'	1:A:7:A:C8	2.38	0.58
1:A:1853:G:H1'	1:A:1881:A:H61	1.67	0.58
32:a:39:G:H22	32:a:386:A:H5'	1.68	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:95:LEU:H	33:b:98:MET:HE2	1.69	0.58
1:A:413:C:H2'	1:A:414:A:H8	1.69	0.58
32:a:938:A:H2'	32:a:939:G:H8	1.67	0.58
33:b:171:ILE:HG22	33:b:175:GLN:NE2	2.19	0.58
43:l:50:ARG:HG3	43:l:90:LEU:HD21	1.86	0.58
1:A:2334:G:H4'	1:A:2335:A:H5''	1.86	0.57
14:N:104:LYS:O	14:N:108:GLU:HG3	2.05	0.57
32:a:922:C:H1'	54:a:1617:LLL:H531	1.86	0.57
46:o:13:GLU:OE2	46:o:83:LYS:NZ	2.32	0.57
32:a:1367:U:O4	38:g:10:ARG:NH1	2.38	0.57
41:j:90:MET:HE3	41:j:90:MET:HA	1.84	0.57
5:E:127:GLU:HG3	5:E:129:LYS:NZ	2.19	0.57
14:N:80:ASP:OD1	14:N:81:ARG:N	2.38	0.57
35:d:117:LEU:HD13	35:d:154:ARG:HH21	1.69	0.57
32:a:1209:C:H2'	32:a:1210:A:C8	2.40	0.57
40:i:83:THR:HG23	40:i:97:LEU:HD13	1.86	0.57
1:A:639:U:H2'	1:A:640:U:C6	2.40	0.57
40:i:41:GLU:CD	40:i:41:GLU:H	2.11	0.57
42:k:97:ILE:HG22	52:u:12:PHE:HZ	1.70	0.57
52:u:11:PRO:O	52:u:13:ASP:N	2.38	0.56
1:A:1001:A:H2'	1:A:1002:A:C8	2.41	0.56
13:M:123:ASP:N	13:M:123:ASP:OD1	2.39	0.56
41:j:47:ARG:HB3	41:j:71:THR:HG23	1.88	0.56
1:A:251:A:OP1	54:A:3023:LLL:N32	2.39	0.56
1:A:1524:G:O2'	1:A:1544:A:N6	2.38	0.56
32:a:140:G:H2'	32:a:141:G:C8	2.41	0.56
35:d:192:SER:OG	35:d:194:ASP:OD1	2.23	0.56
50:s:19:VAL:HG23	50:s:47:LEU:HD21	1.88	0.56
3:C:137:PRO:O	3:C:140:THR:OG1	2.24	0.56
41:j:9:ARG:HB2	41:j:103:SER:HB3	1.87	0.56
2:B:38:U:O4	26:Z:1:MET:N	2.31	0.56
32:a:1305:C:H2'	32:a:1306:U:C6	2.41	0.56
34:c:39:VAL:HG21	34:c:95:MET:HE2	1.88	0.55
35:d:29:ASP:N	35:d:29:ASP:OD1	2.35	0.55
35:d:202:GLU:OE1	36:e:112:ARG:NH2	2.34	0.55
6:F:79:ILE:HA	6:F:80:ARG:HH11	1.72	0.55
14:N:73:ILE:O	14:N:77:ILE:HG12	2.06	0.55
26:Z:11:GLU:O	26:Z:31:LYS:NZ	2.38	0.55
1:A:680:G:H2'	1:A:681:G:C8	2.40	0.55
8:H:14:VAL:HG12	8:H:15:LEU:H	1.72	0.55
32:a:1314:G:H2'	32:a:1315:A:C8	2.42	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:d:48:LEU:HD23	35:d:53:LEU:HD23	1.88	0.55
32:a:398:U:OP1	35:d:23:SER:OG	2.24	0.55
35:d:100:ASN:OD1	35:d:111:ARG:NH1	2.36	0.55
18:R:30:GLU:H	18:R:30:GLU:CD	2.14	0.55
40:i:20:MET:HE1	40:i:86:LEU:HD23	1.88	0.55
14:N:69:GLU:OE2	14:N:69:GLU:N	2.24	0.55
44:m:20:THR:HA	44:m:25:ILE:HG22	1.88	0.55
29:2:25:LEU:HD23	29:2:28:ARG:HH12	1.72	0.55
32:a:448:A:H2'	32:a:449:A:H8	1.71	0.54
37:f:22:LEU:HG	37:f:62:PHE:HZ	1.72	0.54
32:a:18:U:H2'	32:a:19:C:C6	2.42	0.54
1:A:2301:U:H5'	6:F:85:ILE:HD11	1.89	0.54
6:F:147:ASP:OD2	6:F:150:ARG:NH2	2.40	0.54
32:a:1218:A:OP1	50:s:80:TYR:OH	2.24	0.54
1:A:2773:U:O3'	4:D:43:LYS:NZ	2.40	0.54
32:a:968:G:OP2	32:a:1349:U:O2'	2.24	0.54
50:s:62:MET:HA	50:s:66:MET:HE2	1.90	0.54
1:A:848:A:H2'	1:A:849:A:C8	2.42	0.54
32:a:703:G:H2'	32:a:704:A:C8	2.43	0.54
32:a:1093:A:H4'	32:a:1094:A:O5'	2.07	0.54
13:M:28:LEU:HD23	13:M:48:VAL:HG21	1.89	0.54
32:a:717:A:H2'	32:a:718:A:C8	2.43	0.54
32:a:971:C:O2	45:n:59:ARG:NH1	2.41	0.54
34:c:108:LYS:HD3	34:c:111:ILE:HD11	1.90	0.54
46:o:5:GLN:N	46:o:5:GLN:OE1	2.41	0.54
1:A:6:A:H2'	1:A:7:A:H8	1.73	0.53
32:a:1217:C:H6	44:m:102:THR:HG23	1.72	0.53
32:a:1440:G:O2'	32:a:1441:A:H2'	2.07	0.53
41:j:8:ILE:HB	41:j:78:ILE:HG22	1.89	0.53
10:J:105:GLU:N	10:J:105:GLU:OE2	2.41	0.53
26:Z:38:CYS:SG	26:Z:39:SER:N	2.82	0.53
32:a:735:G:H2'	32:a:736:A:C8	2.43	0.53
21:U:49:VAL:O	21:U:53:THR:HG23	2.08	0.53
33:b:115:LEU:HB3	33:b:139:ILE:HD11	1.90	0.53
1:A:543:A:H2'	1:A:544:U:C6	2.44	0.53
1:A:1142:U:H4'	1:A:1143:A:O4'	2.09	0.53
1:A:2240:G:H3'	1:A:2241:G:H8	1.73	0.53
1:A:2635:U:OP2	1:A:2721:G:O2'	2.27	0.53
6:F:78:LYS:O	6:F:80:ARG:NH1	2.42	0.53
40:i:10:ARG:H	40:i:80:LEU:HD23	1.73	0.53
7:G:119:PRO:HG2	7:G:122:ILE:HD13	1.91	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1241:A:H2'	32:a:1242:G:C8	2.44	0.53
50:s:30:PRO:HA	50:s:48:THR:O	2.07	0.53
1:A:413:C:H2'	1:A:414:A:C8	2.43	0.53
1:A:1853:G:H1'	1:A:1881:A:N6	2.23	0.53
45:n:89:MET:HE2	45:n:89:MET:HA	1.90	0.53
47:p:69:ASP:OD1	47:p:69:ASP:N	2.42	0.53
2:B:101:A:H4'	21:U:94:MET:HE1	1.90	0.52
34:c:79:LYS:O	34:c:82:GLU:HG2	2.09	0.52
38:g:71:SER:HB2	38:g:97:ARG:HG3	1.91	0.52
1:A:295:A:H2'	1:A:296:A:H8	1.75	0.52
1:A:2187:A:H2'	1:A:2188:A:C8	2.43	0.52
7:G:48:ASP:OD1	7:G:49:ASN:N	2.42	0.52
32:a:1395:C:H2'	32:a:1396:G:C8	2.44	0.52
1:A:608:A:H2'	1:A:609:A:C8	2.44	0.52
33:b:182:VAL:HG22	33:b:196:TYR:HB2	1.92	0.52
34:c:47:LEU:HD11	34:c:87:LEU:HD11	1.91	0.52
1:A:2497:G:HO2'	1:A:2543:U:HO2'	1.55	0.52
32:a:1063:C:H2'	32:a:1064:G:H8	1.75	0.52
1:A:2227:G:N3	1:A:2227:G:H2'	2.25	0.52
33:b:2:SER:OG	33:b:3:LEU:N	2.43	0.52
38:g:17:LYS:O	38:g:19:LYS:NZ	2.42	0.52
32:a:1268:C:O2'	32:a:1270:A:H8	1.93	0.52
32:a:726:U:H2'	32:a:727:U:H6	1.75	0.52
32:a:1403:C:H2'	32:a:1404:A:C8	2.45	0.52
1:A:805:A:H5'	1:A:806:G:OP1	2.10	0.52
6:F:74:ILE:HD12	6:F:79:ILE:HD11	1.91	0.52
40:i:49:GLN:N	40:i:50:PRO:HD2	2.24	0.52
32:a:1442:A:H5'	32:a:1444:G:O4'	2.10	0.52
33:b:30:PHE:HB2	33:b:40:ASN:HD22	1.75	0.52
1:A:2536:A:H2'	1:A:2537:U:C6	2.45	0.51
25:Y:58:LYS:NZ	25:Y:60:GLU:OE2	2.38	0.51
38:g:48:ASP:OD1	38:g:49:LYS:N	2.43	0.51
1:A:668:A:H2'	1:A:670:A:H62	1.75	0.51
6:F:163:ASP:N	6:F:163:ASP:OD1	2.41	0.51
1:A:2187:A:O2'	1:A:2188:A:O5'	2.28	0.51
38:g:58:ASN:HB3	38:g:61:GLU:HG2	1.91	0.51
40:i:27:PHE:HB3	40:i:34:LEU:HD22	1.93	0.51
1:A:591:U:H2'	1:A:592:U:C6	2.46	0.51
5:E:138:PHE:O	5:E:142:ILE:HG23	2.10	0.51
32:a:481:A:H2'	32:a:482:A:C8	2.46	0.51
32:a:1370:G:OP1	38:g:6:ARG:NH2	2.44	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:c:97:ILE:HG13	34:c:98:PRO:HD2	1.91	0.51
52:u:31:GLU:OE1	52:u:35:ARG:NH1	2.42	0.51
2:B:52:G:H21	6:F:26:MET:HE1	1.75	0.51
41:j:86:VAL:O	41:j:90:MET:HG2	2.11	0.51
32:a:146:C:H2'	32:a:147:A:H8	1.76	0.51
35:d:166:LYS:HD2	35:d:167:GLU:H	1.76	0.51
51:t:59:ASP:OD1	51:t:76:LYS:NZ	2.41	0.51
44:m:55:SER:O	44:m:59:GLU:HG2	2.10	0.51
1:A:2348:C:H2'	1:A:2349:G:C8	2.46	0.51
1:A:2389:G:H1	1:A:2405:U:H3	1.59	0.51
1:A:1792:U:H2'	1:A:1793:C:H6	1.74	0.51
39:h:90:SER:OG	39:h:93:ASP:OD1	2.29	0.51
44:m:85:CYS:O	44:m:89:ARG:HG3	2.11	0.51
1:A:2:A:H2'	1:A:3:C:C6	2.47	0.50
32:a:42:G:H2'	32:a:43:G:H8	1.76	0.50
1:A:2294:U:C2	6:F:151:GLY:HA3	2.45	0.50
32:a:580:U:OP1	39:h:31:LYS:NZ	2.44	0.50
6:F:140:GLU:OE2	26:Z:28:ALA:N	2.42	0.50
1:A:295:A:H2'	1:A:296:A:C8	2.45	0.50
32:a:702:G:H2'	32:a:703:G:C8	2.46	0.50
33:b:84:ARG:HD2	33:b:84:ARG:C	2.36	0.50
39:h:115:ASP:N	39:h:115:ASP:OD1	2.45	0.50
42:k:93:ARG:O	42:k:97:ILE:HG13	2.11	0.50
1:A:1320:U:OP1	54:A:3021:LLL:N12	2.45	0.50
6:F:140:GLU:HA	6:F:140:GLU:OE1	2.11	0.50
1:A:1465:A:H2'	1:A:1466:A:H8	1.76	0.50
1:A:2206:A:C5	1:A:2207:U:H1'	2.47	0.50
38:g:59:GLU:CD	38:g:59:GLU:H	2.20	0.50
48:q:15:VAL:HG12	48:q:21:VAL:HG12	1.94	0.50
20:T:48:PRO:HD3	20:T:56:GLY:HA3	1.93	0.50
32:a:726:U:H2'	32:a:727:U:C6	2.47	0.50
32:a:1323:A:H2'	32:a:1324:A:C8	2.47	0.50
52:u:11:PRO:C	52:u:13:ASP:N	2.69	0.50
20:T:50:PRO:C	20:T:53:GLY:H	2.20	0.49
32:a:1308:C:OP1	45:n:24:ARG:NH1	2.45	0.49
1:A:2061:C:H5'	1:A:2240:G:H21	1.77	0.49
32:a:1169:G:N2	32:a:1172:G:OP2	2.38	0.49
34:c:83:ASP:OD1	34:c:83:ASP:N	2.41	0.49
1:A:2217:G:H2'	1:A:2218:U:C6	2.48	0.49
1:A:2738:A:OP1	7:G:2:SER:OG	2.28	0.49
5:E:63:PRO:HB2	5:E:64:TRP:CE3	2.48	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1165:A:H2'	1:A:1166:A:C8	2.47	0.49
54:a:1618:LLL:H322	54:a:1618:LLL:H51	1.78	0.49
1:A:1885:A:H2'	1:A:1886:A:C8	2.48	0.49
1:A:2289:U:H2'	1:A:2290:A:H8	1.77	0.49
5:E:126:GLU:HG2	5:E:127:GLU:OE2	2.12	0.49
17:Q:34:GLU:OE2	17:Q:59:LYS:HD2	2.12	0.49
15:O:114:LYS:HG3	15:O:115:VAL:HG23	1.94	0.49
21:U:3:ASN:HB2	21:U:58:PHE:HD1	1.77	0.49
38:g:15:ASP:OD1	38:g:44:TYR:OH	2.30	0.49
46:o:4:ALA:O	46:o:8:GLN:HG2	2.12	0.49
32:a:390:C:O2'	32:a:610:A:N3	2.44	0.49
32:a:541:U:C2	32:a:542:A:C8	3.01	0.49
32:a:1052:U:OP1	45:n:85:ARG:NH2	2.45	0.49
1:A:607:U:C5	1:A:620:G:C5	3.01	0.48
1:A:2298:A:C2'	1:A:2299:A:H5'	2.43	0.48
4:D:18:GLU:CD	4:D:18:GLU:H	2.21	0.48
18:R:59:GLU:HG3	18:R:66:VAL:HG23	1.95	0.48
4:D:58:ARG:NH1	4:D:75:GLU:OE1	2.36	0.48
15:O:92:ASP:OD2	15:O:112:LYS:NZ	2.47	0.48
32:a:1145:A:O2'	32:a:1146:A:OP1	2.28	0.48
1:A:785:G:H5'	1:A:786:G:OP1	2.14	0.48
32:a:641:U:O4	32:a:741:G:O2'	2.25	0.48
32:a:480:A:H2'	32:a:481:A:H8	1.78	0.48
1:A:1852:U:H2'	1:A:1853:G:O4'	2.14	0.48
40:i:29:VAL:HG12	40:i:64:VAL:HB	1.95	0.48
1:A:1792:U:H2'	1:A:1793:C:C6	2.48	0.48
1:A:2317:A:H2'	1:A:2318:A:C8	2.48	0.48
1:A:1525:A:H2'	1:A:1526:A:C8	2.49	0.48
1:A:2262:A:H2'	1:A:2263:A:C8	2.49	0.48
6:F:36:LEU:HB3	6:F:152:LEU:HD11	1.96	0.48
32:a:682:G:C4	53:9:96:HIS:HB2	2.49	0.48
32:a:1143:U:OP1	41:j:72:HIS:ND1	2.46	0.48
53:9:52:ALA:HB2	53:9:77:LEU:HD21	1.96	0.48
1:A:299:U:H2'	1:A:300:G:O4'	2.14	0.48
1:A:2409:C:O2	1:A:2409:C:H2'	2.14	0.48
42:k:35:THR:HG22	42:k:41:ALA:HA	1.96	0.48
1:A:213:G:H22	1:A:230:U:H4'	1.78	0.48
1:A:2748:G:N2	7:G:140:GLU:OE2	2.45	0.48
33:b:119:ARG:NE	33:b:119:ARG:O	2.47	0.48
37:f:66:CYS:HB2	37:f:67:PRO:HD2	1.96	0.48
5:E:127:GLU:HG3	5:E:129:LYS:HZ2	1.78	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:61:ASN:O	7:G:65:GLN:HG2	2.13	0.47
28:1:30:MET:H	28:1:47:GLU:HB2	1.79	0.47
32:a:1317:U:H2'	32:a:1318:G:H8	1.79	0.47
32:a:1227:A:H2'	32:a:1228:C:C6	2.49	0.47
1:A:593:U:H2'	1:A:594:U:C6	2.50	0.47
32:a:326:A:H2'	32:a:327:A:H8	1.78	0.47
32:a:1442:A:H5''	32:a:1443:U:H2'	1.96	0.47
32:a:1442:A:H4'	32:a:1443:U:O5'	2.12	0.47
36:e:14:LYS:HB2	36:e:38:VAL:HG23	1.95	0.47
36:e:72:VAL:HG12	36:e:73:SER:H	1.79	0.47
38:g:47:PHE:O	38:g:50:ILE:HG22	2.13	0.47
1:A:401:A:H2'	1:A:402:U:O4'	2.14	0.47
6:F:141:ILE:C	6:F:141:ILE:HD12	2.39	0.47
33:b:84:ARG:HH21	33:b:216:ALA:HB1	1.80	0.47
33:b:185:VAL:HG23	33:b:189:SER:HB2	1.96	0.47
1:A:1348:A:H2'	1:A:1349:A:C8	2.49	0.47
1:A:581:C:H2'	1:A:582:A:C8	2.49	0.47
28:1:19:THR:OG1	28:1:20:THR:N	2.48	0.47
50:s:17:LYS:O	50:s:21:GLU:HG3	2.15	0.47
1:A:282:A:H2'	1:A:283:U:C6	2.50	0.47
1:A:352:G:OP2	1:A:352:G:H8	1.97	0.47
6:F:36:LEU:HD22	6:F:154:ILE:HG12	1.97	0.47
14:N:76:GLU:OE2	14:N:113:HIS:ND1	2.48	0.47
16:P:86:ALA:HB2	16:P:116:ALA:HB2	1.96	0.47
25:Y:5:LYS:HE3	25:Y:5:LYS:HB3	1.83	0.47
38:g:150:LYS:O	38:g:150:LYS:NZ	2.33	0.47
1:A:722:A:H2'	1:A:723:A:C8	2.49	0.47
1:A:2632:G:H2'	1:A:2633:A:H8	1.80	0.47
33:b:139:ILE:HD12	33:b:139:ILE:HA	1.68	0.47
36:e:79:ASP:OD1	36:e:79:ASP:N	2.45	0.47
44:m:107:ARG:NH2	44:m:111:GLY:O	2.45	0.47
1:A:340:A:H2'	1:A:341:U:C6	2.50	0.47
1:A:1477:A:C2	1:A:1508:A:C5	3.03	0.47
26:Z:18:CYS:O	26:Z:20:ASN:ND2	2.44	0.47
33:b:65:ILE:HG13	33:b:158:ALA:HB3	1.96	0.47
17:Q:40:MET:HG2	17:Q:41:GLY:N	2.30	0.47
35:d:25:VAL:HG12	35:d:26:LYS:HG3	1.97	0.47
6:F:79:ILE:C	6:F:80:ARG:HD3	2.40	0.46
1:A:2:A:H2'	1:A:3:C:H6	1.80	0.46
1:A:580:U:H2'	1:A:581:C:C6	2.50	0.46
1:A:1165:A:H2'	1:A:1166:A:H8	1.80	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1544:A:H2'	1:A:1545:A:C8	2.51	0.46
32:a:42:G:H2'	32:a:43:G:C8	2.50	0.46
32:a:490:C:H2'	32:a:491:A:H8	1.79	0.46
4:D:42:GLU:OE1	4:D:42:GLU:N	2.40	0.46
32:a:211:A:H2'	32:a:212:G:H8	1.80	0.46
32:a:268:A:H5''	32:a:270:G:O4'	2.16	0.46
32:a:826:A:N6	54:a:1616:LLL:H531	2.29	0.46
41:j:26:GLU:O	41:j:30:THR:HG22	2.15	0.46
32:a:490:C:H2'	32:a:491:A:C8	2.50	0.46
32:a:937:G:C2	32:a:938:A:C8	3.04	0.46
34:c:136:LYS:HE2	34:c:136:LYS:HB2	1.75	0.46
50:s:73:GLU:H	50:s:73:GLU:CD	2.23	0.46
1:A:4:U:H2'	1:A:5:U:C6	2.50	0.46
6:F:80:ARG:O	6:F:83:TRP:HD1	1.97	0.46
32:a:1481:G:N7	54:a:1615:LLL:N32	2.63	0.46
35:d:11:LEU:O	35:d:15:GLU:HG2	2.16	0.46
42:k:94:ASP:OD1	42:k:94:ASP:N	2.49	0.46
17:Q:27:LEU:HA	17:Q:27:LEU:HD12	1.81	0.46
1:A:743:A:H2'	1:A:744:C:C6	2.51	0.46
19:S:13:ARG:NE	19:S:33:GLU:OE2	2.48	0.46
32:a:1:U:H3'	32:a:2:A:H8	1.79	0.46
48:q:53:CYS:C	48:q:54:LYS:HD3	2.40	0.46
1:A:581:C:H2'	1:A:582:A:H8	1.80	0.46
1:A:2441:C:H2'	1:A:2442:A:C8	2.50	0.46
5:E:15:SER:OG	5:E:16:LEU:N	2.48	0.46
6:F:133:ARG:HB2	6:F:134:GLU:OE1	2.16	0.46
32:a:1236:A:H2'	32:a:1237:U:C6	2.50	0.46
38:g:73:MET:HE1	38:g:97:ARG:HH11	1.80	0.46
6:F:43:ALA:HA	6:F:49:ILE:HD11	1.98	0.46
20:T:78:GLU:N	20:T:78:GLU:OE1	2.49	0.46
35:d:150:LYS:HE2	35:d:178:LEU:HB2	1.97	0.46
37:f:61:LEU:C	37:f:61:LEU:HD23	2.41	0.46
6:F:93:GLY:N	6:F:96:MET:HG2	2.31	0.46
32:a:1242:G:H2'	32:a:1243:A:C8	2.51	0.46
32:a:1309:A:H5''	50:s:3:ARG:HH12	1.81	0.46
33:b:168:HIS:O	33:b:172:GLN:HG2	2.16	0.46
1:A:186:A:H2'	1:A:187:C:C6	2.51	0.45
1:A:704:U:H2'	1:A:705:G:O4'	2.16	0.45
1:A:1403:U:H2'	1:A:1404:U:C6	2.52	0.45
2:B:11:A:N1	2:B:67:G:O2'	2.44	0.45
4:D:109:ASP:OD1	4:D:174:GLN:HA	2.17	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1:31:GLU:HG2	28:1:46:LYS:HD3	1.98	0.45
41:j:87:ASP:O	41:j:91:LYS:HE3	2.15	0.45
33:b:17:LYS:HB2	33:b:20:PHE:HD2	1.82	0.45
46:o:1:MET:HE2	46:o:1:MET:HB3	1.80	0.45
4:D:182:ASP:HB3	4:D:187:LEU:HB2	1.99	0.45
31:4:16:VAL:HG22	31:4:25:VAL:HG22	1.98	0.45
51:t:45:GLU:O	51:t:48:LYS:N	2.50	0.45
1:A:1311:U:H2'	1:A:1312:A:H8	1.81	0.45
1:A:2334:G:H1'	1:A:2371:G:H5'	1.99	0.45
1:A:2360:G:O3'	28:1:41:LYS:NZ	2.46	0.45
4:D:65:MET:HE3	4:D:65:MET:HA	1.97	0.45
32:a:1305:C:H2'	32:a:1306:U:H6	1.81	0.45
1:A:948:A:H2'	1:A:949:C:C6	2.51	0.45
1:A:2458:A:H4'	12:L:56:ARG:HD2	1.98	0.45
1:A:2461:G:H3'	1:A:2464:C:H42	1.82	0.45
47:p:76:LYS:HB3	47:p:76:LYS:HE3	1.71	0.45
1:A:1150:G:H2'	1:A:1151:C:C6	2.51	0.45
33:b:145:VAL:HG12	33:b:146:LEU:HG	1.99	0.45
39:h:80:VAL:HG23	39:h:129:GLY:HA2	1.99	0.45
41:j:44:LEU:HB3	41:j:73:LYS:HE2	1.97	0.45
1:A:2841:G:N2	1:A:2844:A:OP2	2.35	0.45
25:Y:19:LYS:HE2	25:Y:19:LYS:HB3	1.74	0.45
32:a:457:A:H3'	32:a:458:G:C8	2.49	0.45
7:G:2:SER:O	7:G:6:LYS:HG2	2.17	0.45
41:j:55:ILE:HG22	45:n:85:ARG:HD2	1.99	0.45
1:A:634:G:H2'	1:A:635:C:C6	2.52	0.45
33:b:214:LYS:HA	33:b:214:LYS:HD3	1.83	0.45
50:s:23:GLN:CD	50:s:47:LEU:HD11	2.42	0.45
1:A:910:A:H2'	1:A:913:C:H5	1.82	0.45
1:A:2187:A:H2'	1:A:2188:A:H8	1.82	0.45
28:1:31:GLU:HG2	28:1:46:LYS:CD	2.47	0.45
36:e:69:LYS:HD2	36:e:69:LYS:C	2.42	0.45
45:n:43:GLU:OE2	45:n:47:LYS:HE3	2.17	0.45
48:q:57:ASP:OD2	48:q:81:ARG:NH2	2.49	0.45
6:F:47:LYS:H	6:F:47:LYS:HD3	1.81	0.44
28:1:46:LYS:HD2	28:1:46:LYS:HA	1.75	0.44
32:a:1347:G:H2'	32:a:1348:G:H8	1.77	0.44
37:f:38:ARG:NH1	37:f:98:GLU:O	2.49	0.44
15:O:65:MET:HE3	15:O:65:MET:HB3	1.80	0.44
32:a:1054:U:H2'	32:a:1055:C:C6	2.52	0.44
48:q:57:ASP:N	48:q:57:ASP:OD1	2.51	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:96:MET:HE3	6:F:96:MET:HB2	1.88	0.44
32:a:575:U:O2'	39:h:4:GLN:OE1	2.26	0.44
34:c:28:ARG:H	34:c:28:ARG:HD2	1.82	0.44
1:A:2374:C:H2'	1:A:2375:U:C6	2.52	0.44
3:C:112:LYS:HB3	3:C:112:LYS:HE3	1.81	0.44
5:E:6:LYS:HD2	5:E:12:GLU:OE1	2.18	0.44
39:h:91:HIS:CE1	39:h:122:GLY:HA2	2.53	0.44
46:o:25:GLU:HG3	46:o:80:LEU:HD22	1.99	0.44
46:o:88:ARG:HG3	46:o:88:ARG:HH11	1.82	0.44
11:K:91:THR:H	11:K:94:THR:HB	1.81	0.44
25:Y:21:ASN:OD1	25:Y:21:ASN:N	2.49	0.44
32:a:740:U:H2'	32:a:741:G:O4'	2.18	0.44
37:f:14:GLN:OE1	37:f:14:GLN:N	2.50	0.44
5:E:131:GLU:OE1	5:E:131:GLU:N	2.48	0.44
9:I:31:GLU:HG3	9:I:32:VAL:N	2.30	0.44
14:N:98:LYS:HE3	14:N:98:LYS:HB3	1.71	0.44
20:T:25:LYS:NZ	20:T:37:GLU:HB2	2.33	0.44
40:i:87:ILE:HD11	40:i:97:LEU:HD12	1.99	0.44
52:u:14:VAL:O	52:u:17:ARG:HG2	2.18	0.44
1:A:2729:A:H2'	1:A:2730:A:C8	2.53	0.44
2:B:112:A:H2'	2:B:113:A:C8	2.52	0.44
14:N:69:GLU:O	14:N:73:ILE:HD13	2.18	0.44
32:a:288:G:H2'	32:a:289:A:C8	2.51	0.44
32:a:312:U:H2'	32:a:313:G:O4'	2.17	0.44
32:a:667:U:H2'	32:a:668:U:C6	2.53	0.44
33:b:40:ASN:O	33:b:44:THR:HG23	2.17	0.44
33:b:171:ILE:C	33:b:175:GLN:HE21	2.25	0.44
38:g:75:GLU:HG2	38:g:92:VAL:HG22	2.00	0.44
1:A:53:A:H2'	1:A:54:A:C8	2.52	0.44
4:D:42:GLU:H	4:D:42:GLU:CD	2.23	0.44
32:a:446:U:H3	32:a:464:G:H1	1.64	0.44
37:f:40:GLU:HB3	37:f:103:MET:HE3	2.00	0.44
1:A:1592:A:H2'	1:A:1593:A:C8	2.52	0.44
4:D:6:VAL:H	4:D:33:ASN:HD21	1.66	0.44
6:F:12:LEU:HD22	6:F:172:ALA:HB1	2.00	0.44
32:a:175:A:H62	32:a:187:U:H3	1.66	0.44
43:l:30:ARG:HD2	43:l:30:ARG:HA	1.76	0.44
1:A:533:U:O2'	16:P:49:ASP:OD2	2.30	0.43
1:A:1676:A:H2'	1:A:1677:A:H8	1.83	0.43
1:A:2204:A:H3'	1:A:2205:G:H8	1.82	0.43
35:d:54:GLN:HB3	35:d:203:LEU:HB2	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:j:48:LYS:HG2	41:j:70:ARG:HG2	2.00	0.43
49:r:61:LEU:HD23	49:r:61:LEU:HA	1.78	0.43
1:A:20:A:H2'	1:A:21:A:C8	2.53	0.43
14:N:115:LEU:HD23	14:N:115:LEU:HA	1.86	0.43
32:a:239:A:H1'	32:a:241:U:C5	2.53	0.43
34:c:59:ARG:HA	34:c:63:ASN:O	2.19	0.43
1:A:1427:G:H2'	1:A:1428:A:C8	2.53	0.43
16:P:82:GLY:HA2	16:P:117:LEU:HD13	1.99	0.43
32:a:742:A:H4'	32:a:743:C:O5'	2.18	0.43
32:a:1232:G:H2'	32:a:1233:G:H8	1.83	0.43
41:j:80:GLU:O	41:j:80:GLU:CD	2.61	0.43
1:A:848:A:H2'	1:A:849:A:H8	1.80	0.43
1:A:909:C:OP1	12:L:101:ARG:NH2	2.47	0.43
1:A:2240:G:H3'	1:A:2241:G:C8	2.51	0.43
1:A:2831:U:H2'	1:A:2832:G:O4'	2.19	0.43
32:a:875:C:O2'	32:a:876:U:H5'	2.18	0.43
36:e:20:ARG:HH11	36:e:20:ARG:HG2	1.83	0.43
44:m:77:ILE:O	44:m:81:MET:HG3	2.19	0.43
1:A:31:G:H2'	1:A:32:C:C6	2.53	0.43
1:A:2092:C:H2'	1:A:2093:U:C6	2.53	0.43
23:W:68:LEU:HD23	23:W:68:LEU:HA	1.82	0.43
33:b:84:ARG:HH21	33:b:216:ALA:CB	2.31	0.43
33:b:202:ASP:OD1	33:b:203:ASP:N	2.51	0.43
35:d:105:MET:HG2	35:d:173:VAL:HG22	1.99	0.43
52:u:7:LYS:NZ	52:u:9:ARG:HG3	2.33	0.43
1:A:2280:U:H2'	1:A:2281:G:C8	2.54	0.43
31:4:17:ILE:HD12	31:4:19:ARG:HG3	1.99	0.43
32:a:203:G:H2'	32:a:204:C:C6	2.54	0.43
32:a:1309:A:H5''	50:s:3:ARG:NH1	2.33	0.43
33:b:27:GLU:H	33:b:27:GLU:HG2	1.63	0.43
34:c:93:LYS:HE3	34:c:93:LYS:HB3	1.85	0.43
36:e:41:ASP:OD1	36:e:41:ASP:C	2.61	0.43
36:e:68:LYS:HE3	36:e:68:LYS:HB2	1.71	0.43
37:f:29:ILE:O	37:f:34:GLY:HA3	2.18	0.43
41:j:39:LYS:HA	41:j:39:LYS:HD3	1.74	0.43
1:A:640:U:H2'	1:A:641:U:C6	2.53	0.43
1:A:2235:G:H2'	1:A:2236:A:C8	2.53	0.43
1:A:2329:C:H2'	1:A:2330:G:C8	2.54	0.43
1:A:2793:A:H2'	1:A:2794:A:C8	2.54	0.43
6:F:96:MET:HG3	6:F:97:TYR:N	2.33	0.43
6:F:142:ASP:OD2	6:F:145:LYS:NZ	2.51	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1401:A:H2'	32:a:1402:C:C6	2.54	0.43
36:e:96:MET:HE1	36:e:140:THR:HG23	2.01	0.43
48:q:77:ASP:OD1	48:q:78:ILE:N	2.52	0.43
1:A:156:U:H2'	1:A:157:C:C6	2.53	0.43
3:C:67:ASP:OD2	3:C:103:ARG:NH1	2.51	0.43
32:a:1145:A:HO2'	32:a:1146:A:P	2.41	0.43
32:a:1382:U:H2'	32:a:1383:G:C8	2.53	0.43
33:b:103:LYS:O	33:b:106:ARG:HG2	2.19	0.43
41:j:9:ARG:HB2	41:j:103:SER:CB	2.49	0.43
1:A:2740:G:OP2	7:G:3:ARG:NH1	2.52	0.43
32:a:235:A:C2	32:a:271:A:C5	3.07	0.43
32:a:1229:A:H2	32:a:1232:G:N3	2.17	0.43
42:k:75:LEU:HD23	42:k:75:LEU:HA	1.83	0.43
6:F:54:LEU:HD13	6:F:65:PRO:HG2	1.99	0.43
7:G:98:LYS:HZ2	7:G:100:GLN:HG2	1.84	0.43
32:a:195:G:H2'	32:a:196:C:C6	2.54	0.43
32:a:1305:C:OP2	50:s:4:SER:OG	2.23	0.43
33:b:99:LEU:HB3	33:b:177:LEU:HD12	2.01	0.43
1:A:1680:A:H2'	1:A:1681:C:C6	2.54	0.42
1:A:2295:C:H3'	1:A:2296:G:H2'	2.01	0.42
2:B:7:G:C2	2:B:8:A:C8	3.06	0.42
11:K:132:LYS:O	11:K:136:GLU:HG3	2.19	0.42
20:T:3:ARG:O	20:T:94:ARG:NH1	2.51	0.42
24:X:17:GLN:O	24:X:21:VAL:HG23	2.19	0.42
28:1:32:ILE:HG23	28:1:34:LYS:HG3	2.00	0.42
40:i:51:LEU:HA	40:i:54:THR:HG22	2.01	0.42
53:9:85:LEU:HD23	53:9:85:LEU:HA	1.90	0.42
1:A:1649:G:H2'	1:A:1650:A:C8	2.54	0.42
6:F:80:ARG:HD3	6:F:80:ARG:N	2.34	0.42
32:a:448:A:H2'	32:a:449:A:C8	2.52	0.42
35:d:166:LYS:HB3	35:d:166:LYS:HE3	1.72	0.42
36:e:20:ARG:HG2	36:e:20:ARG:NH1	2.33	0.42
47:p:18:ARG:HG2	47:p:35:LYS:HE3	2.01	0.42
32:a:1116:G:O2'	32:a:1119:A:N6	2.52	0.42
33:b:190:ASN:ND2	33:b:192:GLU:HG3	2.33	0.42
38:g:35:LYS:HD3	38:g:38:ILE:HD12	2.01	0.42
50:s:23:GLN:OE1	50:s:23:GLN:HA	2.19	0.42
51:t:16:ARG:HG3	51:t:17:ASN:N	2.34	0.42
1:A:85:A:C2	1:A:104:A:C5	3.08	0.42
1:A:164:G:H2'	1:A:165:A:C8	2.54	0.42
1:A:1311:U:H2'	1:A:1312:A:C8	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:G:H2'	2:B:61:U:H6	1.85	0.42
7:G:104:LEU:HD23	7:G:106:LEU:HD21	2.01	0.42
8:H:1:MET:O	8:H:20:ASN:HA	2.19	0.42
1:A:1570:A:H2'	1:A:1571:A:C8	2.55	0.42
1:A:1676:A:H2'	1:A:1677:A:C8	2.54	0.42
1:A:1909:A:N6	32:a:1480:A:N3	2.68	0.42
1:A:2205:G:H2'	1:A:2206:A:C8	2.55	0.42
6:F:115:ARG:HB2	6:F:178:LYS:NZ	2.34	0.42
7:G:172:LYS:HE2	7:G:172:LYS:HB2	1.94	0.42
28:1:41:LYS:HE3	28:1:42:HIS:N	2.33	0.42
34:c:119:SER:O	34:c:123:GLN:HG3	2.19	0.42
38:g:50:ILE:HD12	38:g:50:ILE:HA	1.67	0.42
1:A:28:G:N2	1:A:511:G:H1'	2.35	0.42
1:A:1389:U:H2'	1:A:1390:A:O4'	2.20	0.42
8:H:47:PHE:O	8:H:50:GLN:HG3	2.20	0.42
33:b:213:LYS:HD2	33:b:213:LYS:HA	1.90	0.42
35:d:50:ASP:N	35:d:50:ASP:OD1	2.53	0.42
39:h:3:MET:HE2	39:h:3:MET:HB2	1.85	0.42
5:E:149:ASP:HB2	5:E:190:GLU:HB3	2.00	0.42
32:a:259:A:H2'	32:a:260:C:C6	2.54	0.42
34:c:15:ILE:HD13	34:c:15:ILE:HA	1.91	0.42
34:c:73:SER:O	34:c:76:VAL:HG12	2.20	0.42
38:g:150:LYS:HZ2	38:g:150:LYS:C	2.21	0.42
41:j:47:ARG:HB3	41:j:71:THR:CG2	2.49	0.42
50:s:48:THR:HB	50:s:61:LEU:HD12	2.02	0.42
1:A:2632:G:H2'	1:A:2633:A:C8	2.54	0.42
13:M:56:LYS:NZ	13:M:107:ARG:O	2.53	0.42
20:T:49:ASN:O	20:T:54:ILE:N	2.53	0.42
32:a:146:C:H2'	32:a:147:A:C8	2.55	0.42
32:a:1328:G:H5''	32:a:1329:G:OP1	2.19	0.42
34:c:20:SER:OG	34:c:40:ARG:NH2	2.53	0.42
32:a:186:U:H2'	32:a:187:U:C6	2.55	0.42
32:a:1210:A:H2'	32:a:1211:G:C8	2.55	0.42
33:b:171:ILE:HG22	33:b:175:GLN:HE21	1.82	0.42
41:j:13:LYS:HB2	41:j:99:ASP:HB3	2.02	0.42
42:k:116:LEU:HA	42:k:117:PRO:HD3	1.84	0.42
1:A:1413:G:N2	1:A:1579:A:N7	2.68	0.42
6:F:70:SER:HB3	6:F:85:ILE:HD13	2.02	0.42
32:a:1231:U:C5	38:g:117:MET:HG3	2.55	0.42
33:b:94:TRP:HA	33:b:98:MET:HE3	2.02	0.42
39:h:75:GLU:OE1	39:h:98:TYR:OH	2.28	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:m:85:CYS:HB2	50:s:73:GLU:HB3	2.02	0.42
48:q:54:LYS:HD3	48:q:54:LYS:N	2.35	0.42
2:B:27:A:H2'	2:B:28:C:O4'	2.20	0.41
15:O:34:LYS:NZ	15:O:39:GLN:HB2	2.35	0.41
22:V:37:ILE:HG22	22:V:38:ILE:HG13	2.02	0.41
32:a:483:G:O2'	32:a:485:A:H1'	2.20	0.41
1:A:1541:A:H2'	1:A:1542:C:C6	2.54	0.41
1:A:1786:C:H2'	1:A:1787:A:C5	2.55	0.41
1:A:2067:A:H2'	1:A:2068:C:C6	2.55	0.41
1:A:2774:C:OP1	4:D:43:LYS:NZ	2.49	0.41
14:N:79:ALA:O	14:N:83:LYS:HE2	2.19	0.41
32:a:1167:A:H2'	32:a:1168:G:C8	2.55	0.41
32:a:1285:C:H2'	32:a:1286:U:C6	2.55	0.41
32:a:1361:G:C2'	32:a:1362:G:H5'	2.50	0.41
38:g:127:GLU:OE1	38:g:132:ARG:NH2	2.54	0.41
42:k:106:LYS:NZ	52:u:8:GLU:OE1	2.53	0.41
1:A:2286:C:H3'	1:A:2287:G:H8	1.85	0.41
2:B:16:A:H2'	2:B:17:G:C8	2.54	0.41
4:D:57:LYS:HB3	4:D:57:LYS:HE2	1.77	0.41
32:a:717:A:H2'	32:a:718:A:H8	1.86	0.41
38:g:126:LEU:HD23	38:g:126:LEU:HA	1.75	0.41
41:j:59:VAL:HG23	41:j:59:VAL:O	2.20	0.41
53:9:67:ASP:OD2	53:9:72:ALA:HB3	2.20	0.41
1:A:1909:A:H62	32:a:1480:A:H2'	1.86	0.41
32:a:507:C:H5	32:a:519:G:H5'	1.86	0.41
32:a:1341:A:O2'	32:a:1342:U:OP1	2.34	0.41
51:t:57:ILE:H	51:t:57:ILE:HG13	1.61	0.41
1:A:2421:A:H2'	1:A:2422:A:C8	2.55	0.41
1:A:2651:A:O5'	1:A:2651:A:H8	2.03	0.41
20:T:50:PRO:HA	20:T:53:GLY:HA2	2.03	0.41
26:Z:15:THR:OG1	26:Z:21:THR:HG23	2.20	0.41
28:1:5:ILE:HD13	28:1:21:LYS:HB2	2.03	0.41
32:a:178:U:H2'	32:a:179:C:C6	2.55	0.41
32:a:974:U:H4'	32:a:975:A:O4'	2.21	0.41
49:r:45:ALA:O	49:r:49:ARG:HG3	2.20	0.41
1:A:607:U:N3	1:A:608:A:N7	2.69	0.41
1:A:1805:A:H2'	1:A:1806:A:C8	2.56	0.41
1:A:1897:A:OP2	3:C:255:LYS:HE3	2.21	0.41
1:A:2034:G:H2'	1:A:2035:U:O4'	2.21	0.41
1:A:2492:A:H1'	56:A:3019:CLM:O4	2.20	0.41
3:C:78:LYS:HB3	3:C:78:LYS:HE3	1.86	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:16:LEU:HD12	5:E:17:GLY:H	1.85	0.41
52:u:11:PRO:C	52:u:13:ASP:H	2.27	0.41
1:A:1525:A:H2'	1:A:1526:A:H8	1.85	0.41
1:A:2367:A:C5	1:A:2368:G:H1'	2.56	0.41
15:O:31:LEU:HD11	15:O:75:PHE:HE2	1.86	0.41
23:W:47:ILE:HD11	23:W:78:ILE:HG23	2.03	0.41
26:Z:10:THR:OG1	26:Z:11:GLU:N	2.52	0.41
33:b:22:ASN:HD22	33:b:190:ASN:HA	1.85	0.41
33:b:208:ILE:HA	33:b:211:TYR:HD2	1.85	0.41
40:i:51:LEU:HA	40:i:51:LEU:HD23	1.96	0.41
42:k:88:GLY:O	42:k:93:ARG:NH1	2.54	0.41
43:l:123:LYS:HD2	43:l:123:LYS:HA	1.92	0.41
45:n:6:MET:HE2	45:n:63:ARG:NH2	2.36	0.41
50:s:56:GLN:CD	50:s:57:HIS:H	2.29	0.41
1:A:265:G:H2'	1:A:265:G:N3	2.35	0.41
32:a:124:U:H2'	32:a:125:C:C6	2.55	0.41
32:a:768:C:H2'	32:a:769:A:O4'	2.21	0.41
33:b:163:ASP:O	33:b:167:GLU:HG2	2.21	0.41
34:c:118:GLU:O	34:c:122:GLN:HG3	2.21	0.41
34:c:148:GLY:O	34:c:202:ILE:HD12	2.21	0.41
51:t:45:GLU:N	51:t:45:GLU:OE1	2.54	0.41
52:u:16:LEU:O	52:u:20:LYS:HG3	2.21	0.41
1:A:265:G:H5''	1:A:266:G:H8	1.86	0.41
1:A:639:U:H2'	1:A:640:U:H6	1.83	0.41
1:A:1365:U:H2'	1:A:1366:G:O4'	2.21	0.41
1:A:1428:A:H2'	1:A:1429:A:H8	1.85	0.41
1:A:2329:C:H2'	1:A:2330:G:H8	1.86	0.41
2:B:12:U:OP2	2:B:68:C:O2'	2.38	0.41
11:K:68:SER:OG	11:K:71:LYS:HB2	2.20	0.41
21:U:74:VAL:HG12	21:U:95:ARG:HA	2.03	0.41
32:a:646:U:H2'	32:a:647:A:H8	1.86	0.41
38:g:41:LYS:HE2	38:g:41:LYS:HB2	1.94	0.41
41:j:84:LYS:HE2	41:j:84:LYS:HB2	1.88	0.41
44:m:81:MET:HE2	44:m:81:MET:HB3	1.82	0.41
52:u:11:PRO:O	52:u:12:PHE:C	2.63	0.41
1:A:1308:U:O2	1:A:1308:U:H2'	2.21	0.41
8:H:1:MET:HE3	8:H:23:PRO:HA	2.03	0.41
10:J:71:ARG:HD3	10:J:71:ARG:HA	1.95	0.41
15:O:101:MET:HE2	15:O:101:MET:HB3	1.96	0.41
32:a:662:G:H2'	32:a:663:G:H8	1.78	0.41
32:a:1503:G:N2	32:a:1506:A:OP2	2.53	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1514:C:OP2	52:u:42:THR:HG22	2.21	0.41
34:c:183:ASP:OD2	34:c:204:LYS:HE3	2.21	0.41
45:n:92:ASP:OD1	45:n:92:ASP:N	2.53	0.41
1:A:1681:C:H2'	1:A:1682:A:C8	2.57	0.40
1:A:2021:C:H2'	1:A:2022:U:C6	2.56	0.40
32:a:734:C:H2'	32:a:735:G:C8	2.56	0.40
32:a:746:U:H2'	32:a:747:G:O4'	2.21	0.40
38:g:19:LYS:HB2	38:g:19:LYS:HE2	1.88	0.40
39:h:18:LEU:HD22	39:h:72:PRO:HB3	2.02	0.40
1:A:2717:U:HO2'	1:A:2718:U:H6	1.69	0.40
32:a:725:A:H2'	32:a:726:U:C6	2.55	0.40
33:b:208:ILE:HA	33:b:211:TYR:CD2	2.56	0.40
49:r:30:ASN:HB2	49:r:31:GLU:OE2	2.21	0.40
50:s:3:ARG:HH21	50:s:7:LYS:HB3	1.86	0.40
50:s:81:ARG:HD2	50:s:81:ARG:HA	1.67	0.40
2:B:16:A:H2'	2:B:17:G:H8	1.85	0.40
4:D:42:GLU:N	4:D:42:GLU:CD	2.79	0.40
6:F:32:LYS:HE3	6:F:32:LYS:HB3	1.70	0.40
7:G:7:LYS:HA	7:G:8:PRO:HD3	1.97	0.40
8:H:7:GLU:OE2	8:H:8:LYS:N	2.55	0.40
19:S:66:LYS:H	19:S:77:THR:HG1	1.65	0.40
26:Z:36:ASP:OD1	26:Z:37:ILE:N	2.54	0.40
29:2:25:LEU:HD23	29:2:28:ARG:NH1	2.36	0.40
34:c:83:ASP:HA	34:c:86:LYS:HG2	2.02	0.40
45:n:4:LYS:O	45:n:8:GLN:HG2	2.21	0.40
1:A:1459:A:H2'	1:A:1460:G:C8	2.56	0.40
1:A:1798:A:H2'	1:A:1799:A:H8	1.84	0.40
33:b:186:ASP:OD1	33:b:187:THR:N	2.55	0.40
34:c:138:MET:HE1	34:c:168:ALA:C	2.47	0.40
38:g:89:PRO:HG3	38:g:150:LYS:HA	2.03	0.40
1:A:902:C:H2'	1:A:903:U:C6	2.56	0.40
1:A:2409:C:O2	1:A:2409:C:C2'	2.70	0.40
32:a:129:C:H2'	32:a:130:C:H6	1.87	0.40
33:b:129:LYS:HG3	33:b:130:LYS:N	2.36	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	
3	C	271/274 (99%)	265 (98%)	6 (2%)	0	100	100
4	D	207/210 (99%)	201 (97%)	5 (2%)	1 (0%)	24	37
5	E	205/207 (99%)	200 (98%)	5 (2%)	0	100	100
6	F	176/179 (98%)	173 (98%)	3 (2%)	0	100	100
7	G	172/178 (97%)	168 (98%)	4 (2%)	0	100	100
8	H	48/151 (32%)	45 (94%)	3 (6%)	0	100	100
9	I	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
10	J	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
11	K	141/143 (99%)	137 (97%)	4 (3%)	0	100	100
12	L	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
13	M	134/145 (92%)	132 (98%)	2 (2%)	0	100	100
14	N	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
15	O	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
16	P	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
17	Q	102/104 (98%)	102 (100%)	0	0	100	100
18	R	107/111 (96%)	105 (98%)	2 (2%)	0	100	100
19	S	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
20	T	102/105 (97%)	101 (99%)	1 (1%)	0	100	100
21	U	92/96 (96%)	88 (96%)	4 (4%)	0	100	100
22	V	71/84 (84%)	69 (97%)	2 (3%)	0	100	100
23	W	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
24	X	62/66 (94%)	61 (98%)	1 (2%)	0	100	100
25	Y	56/61 (92%)	55 (98%)	1 (2%)	0	100	100
26	Z	44/72 (61%)	43 (98%)	1 (2%)	0	100	100
27	0	53/60 (88%)	53 (100%)	0	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	1	47/51 (92%)	46 (98%)	1 (2%)	0	100	100
29	2	42/44 (96%)	42 (100%)	0	0	100	100
30	3	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	4	35/37 (95%)	35 (100%)	0	0	100	100
33	b	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
34	c	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
35	d	203/205 (99%)	202 (100%)	1 (0%)	0	100	100
36	e	155/166 (93%)	152 (98%)	3 (2%)	0	100	100
37	f	102/111 (92%)	102 (100%)	0	0	100	100
38	g	152/157 (97%)	144 (95%)	8 (5%)	0	100	100
39	h	129/132 (98%)	129 (100%)	0	0	100	100
40	i	125/129 (97%)	121 (97%)	4 (3%)	0	100	100
41	j	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
42	k	116/129 (90%)	111 (96%)	5 (4%)	0	100	100
43	l	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
44	m	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
45	n	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
46	o	86/88 (98%)	86 (100%)	0	0	100	100
47	p	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
48	q	78/83 (94%)	75 (96%)	3 (4%)	0	100	100
49	r	65/72 (90%)	65 (100%)	0	0	100	100
50	s	80/92 (87%)	79 (99%)	1 (1%)	0	100	100
51	t	87/90 (97%)	85 (98%)	2 (2%)	0	100	100
52	u	57/65 (88%)	54 (95%)	2 (4%)	1 (2%)	6	9
53	9	94/98 (96%)	89 (95%)	5 (5%)	0	100	100
All	All	5599/5949 (94%)	5468 (98%)	129 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
52	u	12	PHE
4	D	150	ASN

### 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	
3	C	226/227 (100%)	225 (100%)	1 (0%)	84	92
4	D	167/168 (99%)	165 (99%)	2 (1%)	63	81
5	E	171/171 (100%)	169 (99%)	2 (1%)	63	81
6	F	148/149 (99%)	140 (95%)	8 (5%)	20	35
7	G	140/144 (97%)	139 (99%)	1 (1%)	76	88
8	H	40/115 (35%)	40 (100%)	0	100	100
9	I	118/118 (100%)	116 (98%)	2 (2%)	53	74
10	J	99/99 (100%)	98 (99%)	1 (1%)	68	84
11	K	108/108 (100%)	107 (99%)	1 (1%)	70	85
12	L	112/112 (100%)	112 (100%)	0	100	100
13	M	115/122 (94%)	113 (98%)	2 (2%)	53	74
14	N	95/96 (99%)	91 (96%)	4 (4%)	26	45
15	O	101/101 (100%)	100 (99%)	1 (1%)	68	84
16	P	90/91 (99%)	89 (99%)	1 (1%)	65	82
17	Q	85/85 (100%)	84 (99%)	1 (1%)	63	81
18	R	90/92 (98%)	90 (100%)	0	100	100
19	S	81/84 (96%)	80 (99%)	1 (1%)	63	81
20	T	85/87 (98%)	83 (98%)	2 (2%)	43	65
21	U	81/82 (99%)	77 (95%)	4 (5%)	22	39
22	V	58/65 (89%)	58 (100%)	0	100	100
23	W	68/69 (99%)	68 (100%)	0	100	100
24	X	59/61 (97%)	58 (98%)	1 (2%)	53	74
25	Y	49/52 (94%)	48 (98%)	1 (2%)	48	70
26	Z	43/64 (67%)	40 (93%)	3 (7%)	14	24
27	0	51/56 (91%)	48 (94%)	3 (6%)	18	31
28	1	46/48 (96%)	46 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	2	36/36 (100%)	35 (97%)	1 (3%)	38	60
30	3	53/54 (98%)	51 (96%)	2 (4%)	29	49
31	4	35/35 (100%)	35 (100%)	0	100	100
33	b	186/186 (100%)	179 (96%)	7 (4%)	29	49
34	c	167/167 (100%)	162 (97%)	5 (3%)	36	58
35	d	172/172 (100%)	169 (98%)	3 (2%)	53	74
36	e	121/130 (93%)	117 (97%)	4 (3%)	33	55
37	f	93/100 (93%)	92 (99%)	1 (1%)	65	82
38	g	126/129 (98%)	121 (96%)	5 (4%)	28	47
39	h	109/110 (99%)	108 (99%)	1 (1%)	70	85
40	i	107/109 (98%)	102 (95%)	5 (5%)	23	41
41	j	91/95 (96%)	85 (93%)	6 (7%)	15	26
42	k	94/104 (90%)	92 (98%)	2 (2%)	47	69
43	l	106/107 (99%)	104 (98%)	2 (2%)	50	71
44	m	101/103 (98%)	98 (97%)	3 (3%)	36	58
45	n	85/86 (99%)	82 (96%)	3 (4%)	32	53
46	o	80/80 (100%)	79 (99%)	1 (1%)	61	80
47	p	62/62 (100%)	62 (100%)	0	100	100
48	q	75/78 (96%)	74 (99%)	1 (1%)	61	80
49	r	58/63 (92%)	56 (97%)	2 (3%)	32	54
50	s	74/81 (91%)	72 (97%)	2 (3%)	39	62
51	t	71/72 (99%)	67 (94%)	4 (6%)	19	33
52	u	52/58 (90%)	51 (98%)	1 (2%)	50	71
53	9	85/86 (99%)	83 (98%)	2 (2%)	43	65
All	All	4765/4969 (96%)	4660 (98%)	105 (2%)	45	67

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	3	GLU
4	D	57	LYS
4	D	75	GLU
5	E	69	THR
5	E	79	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	F	18	THR
6	F	73	SER
6	F	104	ILE
6	F	113	ASP
6	F	117	LEU
6	F	136	ILE
6	F	140	GLU
6	F	163	ASP
7	G	45	SER
9	I	64	VAL
9	I	142	ILE
10	J	120	GLU
11	K	68	SER
13	M	6	GLN
13	M	14	SER
14	N	28	VAL
14	N	36	TYR
14	N	45	SER
14	N	111	ARG
15	O	67	SER
16	P	2	SER
17	Q	54	THR
19	S	73	VAL
20	T	59	VAL
20	T	70	VAL
21	U	14	LEU
21	U	28	ILE
21	U	38	GLU
21	U	66	ASP
24	X	43	LYS
25	Y	49	MET
26	Z	23	VAL
26	Z	38	CYS
26	Z	39	SER
27	0	26	THR
27	0	32	SER
27	0	43	SER
29	2	26	SER
30	3	48	ASN
30	3	52	LYS
33	b	55	VAL
33	b	68	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
33	b	76	ASP
33	b	128	THR
33	b	139	ILE
33	b	185	VAL
33	b	202	ASP
34	c	73	SER
34	c	103	ILE
34	c	139	GLN
34	c	151	ILE
34	c	165	SER
35	d	17	THR
35	d	33	LYS
35	d	166	LYS
36	e	24	THR
36	e	72	VAL
36	e	85	VAL
36	e	131	THR
37	f	102	MET
38	g	19	LYS
38	g	50	ILE
38	g	77	LYS
38	g	78	SER
38	g	91	GLU
39	h	54	THR
40	i	29	VAL
40	i	46	VAL
40	i	65	THR
40	i	103	VAL
40	i	127	SER
41	j	22	ILE
41	j	38	VAL
41	j	71	THR
41	j	77	ASP
41	j	82	THR
41	j	86	VAL
42	k	58	SER
42	k	119	ASN
43	l	39	THR
43	l	82	ILE
44	m	7	VAL
44	m	16	VAL
44	m	83	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
45	n	16	LEU
45	n	34	ILE
45	n	46	ILE
46	o	74	VAL
48	q	79	ILE
49	r	43	THR
49	r	53	THR
50	s	48	THR
50	s	58	VAL
51	t	4	SER
51	t	26	SER
51	t	49	GLU
51	t	57	ILE
52	u	3	SER
53	9	10	VAL
53	9	79	ASP

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

Mol	Chain	Res	Type
3	C	144	ASN
3	C	164	GLN
3	C	245	HIS
4	D	47	ASN
4	D	50	GLN
4	D	141	HIS
6	F	9	GLN
6	F	24	ASN
7	G	105	ASN
9	I	141	ASN
12	L	57	HIS
12	L	96	GLN
13	M	31	HIS
13	M	75	GLN
15	O	3	ASN
16	P	102	ASN
18	R	23	GLN
19	S	27	ASN
19	S	39	ASN
20	T	49	ASN
23	W	36	HIS
27	0	19	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
28	1	15	HIS
30	3	49	GLN
30	3	61	GLN
33	b	175	GLN
33	b	190	ASN
34	c	6	ASN
34	c	34	ASN
40	i	49	GLN
42	k	119	ASN
43	l	112	HIS
46	o	14	ASN
46	o	15	GLN
46	o	61	GLN
51	t	20	HIS
53	9	29	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2636/2886 (91%)	334 (12%)	16 (0%)
2	B	114/115 (99%)	11 (9%)	0
32	a	1431/1528 (93%)	159 (11%)	0
All	All	4181/4529 (92%)	504 (12%)	16 (0%)

All (504) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	11	A
1	A	35	U
1	A	47	G
1	A	52	G
1	A	61	G
1	A	64	A
1	A	72	A
1	A	75	A
1	A	76	G
1	A	102	U
1	A	103	G
1	A	119	A
1	A	120	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	121	U
1	A	146	G
1	A	167	U
1	A	168	G
1	A	169	U
1	A	170	A
1	A	176	A
1	A	191	A
1	A	210	G
1	A	211	A
1	A	217	A
1	A	223	U
1	A	224	U
1	A	228	A
1	A	234	G
1	A	243	G
1	A	261	G
1	A	263	C
1	A	266	G
1	A	273	U
1	A	274	U
1	A	304	A
1	A	322	G
1	A	323	A
1	A	352	G
1	A	353	A
1	A	359	G
1	A	367	A
1	A	369	A
1	A	370	A
1	A	371	G
1	A	382	C
1	A	385	G
1	A	395	G
1	A	402	U
1	A	410	G
1	A	411	A
1	A	423	G
1	A	440	U
1	A	455	U
1	A	456	A
1	A	466	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	480	G
1	A	493	G
1	A	504	A
1	A	507	A
1	A	508	U
1	A	529	G
1	A	530	C
1	A	531	A
1	A	563	A
1	A	573	U
1	A	575	A
1	A	587	G
1	A	603	A
1	A	614	A
1	A	627	A
1	A	634	G
1	A	637	A
1	A	645	U
1	A	646	A
1	A	647	G
1	A	654	U
1	A	687	U
1	A	713	G
1	A	731	A
1	A	748	U
1	A	776	G
1	A	777	G
1	A	783	A
1	A	785	G
1	A	786	G
1	A	806	G
1	A	813	C
1	A	820	A
1	A	828	U
1	A	831	G
1	A	859	G
1	A	911	A
1	A	939	G
1	A	942	A
1	A	947	C
1	A	962	G
1	A	975	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	984	A
1	A	996	C
1	A	997	A
1	A	1006	C
1	A	1010	A
1	A	1013	U
1	A	1014	C
1	A	1023	G
1	A	1027	G
1	A	1034	A
1	A	1047	A
1	A	1048	G
1	A	1110	C
1	A	1111	G
1	A	1113	G
1	A	1115	C
1	A	1116	G
1	A	1133	U
1	A	1134	A
1	A	1136	C
1	A	1137	G
1	A	1143	A
1	A	1234	G
1	A	1246	G
1	A	1249	A
1	A	1252	G
1	A	1262	G
1	A	1267	G
1	A	1270	A
1	A	1284	C
1	A	1295	A
1	A	1296	A
1	A	1347	U
1	A	1360	A
1	A	1374	U
1	A	1378	A
1	A	1390	A
1	A	1391	U
1	A	1405	A
1	A	1422	A
1	A	1423	C
1	A	1447	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1449	A
1	A	1455	G
1	A	1463	G
1	A	1478	G
1	A	1489	C
1	A	1493	U
1	A	1506	U
1	A	1507	G
1	A	1513	A
1	A	1521	G
1	A	1522	A
1	A	1569	A
1	A	1578	U
1	A	1581	G
1	A	1597	A
1	A	1606	U
1	A	1607	A
1	A	1609	A
1	A	1617	U
1	A	1646	U
1	A	1672	G
1	A	1718	A
1	A	1754	U
1	A	1760	G
1	A	1769	A
1	A	1778	C
1	A	1796	C
1	A	1797	G
1	A	1812	A
1	A	1815	A
1	A	1825	A
1	A	1834	C
1	A	1862	A
1	A	1880	G
1	A	1902	G
1	A	1909	A
1	A	1910	C
1	A	1912	A
1	A	1925	G
1	A	1926	G
1	A	1934	A
1	A	1937	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1951	U
1	A	1959	U
1	A	1963	C
1	A	1966	A
1	A	1967	U
1	A	1968	G
1	A	1987	U
1	A	1989	U
1	A	1993	C
1	A	2002	C
1	A	2018	U
1	A	2019	C
1	A	2023	G
1	A	2027	A
1	A	2029	A
1	A	2032	C
1	A	2039	C
1	A	2051	C
1	A	2052	G
1	A	2055	C
1	A	2056	A
1	A	2057	G
1	A	2058	A
1	A	2059	C
1	A	2065	G
1	A	2078	A
1	A	2081	U
1	A	2089	G
1	A	2092	C
1	A	2188	A
1	A	2190	U
1	A	2194	A
1	A	2199	A
1	A	2200	G
1	A	2212	G
1	A	2213	G
1	A	2214	A
1	A	2215	C
1	A	2219	G
1	A	2223	G
1	A	2227	G
1	A	2239	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	2240	G
1	A	2248	U
1	A	2257	A
1	A	2259	A
1	A	2267	A
1	A	2268	G
1	A	2271	G
1	A	2272	U
1	A	2276	A
1	A	2278	G
1	A	2280	U
1	A	2293	G
1	A	2294	U
1	A	2296	G
1	A	2297	G
1	A	2300	A
1	A	2301	U
1	A	2303	G
1	A	2306	C
1	A	2308	A
1	A	2310	G
1	A	2311	A
1	A	2314	A
1	A	2316	A
1	A	2320	G
1	A	2322	A
1	A	2325	A
1	A	2334	G
1	A	2336	C
1	A	2339	C
1	A	2343	A
1	A	2345	U
1	A	2346	G
1	A	2350	G
1	A	2351	C
1	A	2364	G
1	A	2368	G
1	A	2372	G
1	A	2374	C
1	A	2395	A
1	A	2399	G
1	A	2403	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	2410	G
1	A	2411	C
1	A	2412	U
1	A	2413	C
1	A	2414	A
1	A	2416	C
1	A	2418	G
1	A	2419	A
1	A	2424	A
1	A	2430	U
1	A	2434	2MG
1	A	2437	A
1	A	2439	A
1	A	2447	A
1	A	2457	A
1	A	2458	A
1	A	2459	G
1	A	2465	A
1	A	2473	G
1	A	2477	G
1	A	2480	U
1	A	2481	U
1	A	2483	G
1	A	2487	C
1	A	2489	U
1	A	2491	G
1	A	2492	A
1	A	2494	G
1	A	2507	A
1	A	2518	G
1	A	2536	A
1	A	2555	A
1	A	2556	G
1	A	2591	A
1	A	2592	G
1	A	2598	U
1	A	2602	U
1	A	2618	U
1	A	2635	U
1	A	2678	U
1	A	2679	U
1	A	2703	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	2715	C
1	A	2722	A
1	A	2733	G
1	A	2737	A
1	A	2742	A
1	A	2746	A
1	A	2753	A
1	A	2754	A
1	A	2755	G
1	A	2767	A
1	A	2779	U
1	A	2790	A
1	A	2804	G
1	A	2805	A
1	A	2845	U
1	A	2848	A
1	A	2851	A
1	A	2856	U
1	A	2857	A
1	A	2864	C
1	A	2867	A
1	A	2868	U
1	A	2874	G
1	A	2875	A
1	A	2877	A
1	A	2879	A
2	B	11	A
2	B	12	U
2	B	22	G
2	B	34	C
2	B	40	C
2	B	51	A
2	B	64	C
2	B	87	G
2	B	89	C
2	B	102	G
2	B	106	A
32	a	5	C
32	a	6	U
32	a	7	G
32	a	10	G
32	a	23	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
32	a	33	A
32	a	40	G
32	a	48	C
32	a	49	U
32	a	51	A
32	a	52	A
32	a	71	U
32	a	72	A
32	a	76	G
32	a	114	C
32	a	124	U
32	a	128	C
32	a	129	C
32	a	130	C
32	a	137	G
32	a	156	C
32	a	175	A
32	a	182	U
32	a	183	G
32	a	234	U
32	a	236	G
32	a	240	G
32	a	255	G
32	a	256	C
32	a	268	A
32	a	278	G
32	a	297	C
32	a	317	C
32	a	318	A
32	a	321	G
32	a	341	C
32	a	343	G
32	a	356	U
32	a	361	C
32	a	373	C
32	a	386	A
32	a	395	G
32	a	402	G
32	a	410	U
32	a	413	G
32	a	418	U
32	a	456	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	a	457	A
32	a	470	G
32	a	473	G
32	a	475	U
32	a	484	A
32	a	485	A
32	a	498	A
32	a	500	C
32	a	502	C
32	a	516	G
32	a	519	G
32	a	520	U
32	a	521	A
32	a	536	A
32	a	551	U
32	a	553	C
32	a	561	A
32	a	562	A
32	a	565	G
32	a	566	G
32	a	568	C
32	a	622	G
32	a	642	A
32	a	654	A
32	a	672	G
32	a	676	A
32	a	712	U
32	a	713	G
32	a	718	A
32	a	723	A
32	a	743	C
32	a	744	A
32	a	766	A
32	a	770	A
32	a	782	U
32	a	783	A
32	a	804	A
32	a	806	C
32	a	817	A
32	a	864	A
32	a	883	U
32	a	906	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	a	918	G
32	a	926	C
32	a	927	A
32	a	937	G
32	a	952	U
32	a	958	G
32	a	959	C
32	a	960	A
32	a	961	A
32	a	963	G
32	a	967	A
32	a	968	G
32	a	969	A
32	a	984	U
32	a	985	G
32	a	1036	A
32	a	1037	C
32	a	1053	G
32	a	1057	U
32	a	1086	G
32	a	1087	U
32	a	1093	A
32	a	1094	A
32	a	1116	G
32	a	1146	A
32	a	1150	U
32	a	1158	A
32	a	1159	C
32	a	1162	G
32	a	1172	G
32	a	1174	U
32	a	1187	A
32	a	1188	A
32	a	1203	U
32	a	1204	A
32	a	1205	C
32	a	1217	C
32	a	1229	A
32	a	1247	C
32	a	1248	U
32	a	1251	G
32	a	1264	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	a	1266	A
32	a	1271	A
32	a	1277	A
32	a	1278	A
32	a	1290	A
32	a	1291	G
32	a	1293	C
32	a	1296	G
32	a	1311	C
32	a	1329	G
32	a	1342	U
32	a	1355	U
32	a	1362	G
32	a	1363	U
32	a	1389	A
32	a	1440	G
32	a	1442	A
32	a	1443	U
32	a	1474	G
32	a	1479	A
32	a	1484	G
32	a	1489	A
32	a	1490	A
32	a	1493	U
32	a	1504	G
32	a	1516	G
32	a	1517	G
32	a	1518	A

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	129	C
1	A	645	U
1	A	785	G
1	A	1116	G
1	A	1607	A
1	A	1814	U
1	A	2055	C
1	A	2187	A
1	A	2199	A
1	A	2271	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	2296	G
1	A	2300	A
1	A	2419	A
1	A	2457	A
1	A	2492	A
1	A	2745	U

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
1	2MG	A	2434	1	23,26,27	0.36	0	32,38,41	0.37	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
1	2MG	A	2434	1	-	2/9/27/28	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2434	2MG	C3'-C4'-C5'-O5'
1	A	2434	2MG	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 147 ligands modelled in this entry, 137 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
54	LLL	A	3024	-	29,33,33	0.37	0	34,49,49	0.51	0
54	LLL	A	3021	-	29,33,33	0.37	0	34,49,49	0.53	0
54	LLL	a	1617	-	29,33,33	0.35	0	34,49,49	0.46	0
54	LLL	A	3022	-	29,33,33	0.37	0	34,49,49	0.53	0
54	LLL	a	1618	-	29,33,33	0.66	0	34,49,49	1.30	3 (8%)
56	CLM	A	3019	-	19,20,20	0.26	0	23,27,27	0.50	0
54	LLL	A	2901	-	29,33,33	0.36	0	34,49,49	0.58	0
54	LLL	a	1615	-	29,33,33	0.37	0	34,49,49	0.50	0
54	LLL	A	3023	-	29,33,33	0.37	0	34,49,49	0.58	0
54	LLL	a	1616	-	29,33,33	0.36	0	34,49,49	0.49	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
54	LLL	A	3024	-	-	2/11/65/65	0/3/3/3
54	LLL	A	3021	-	-	1/11/65/65	0/3/3/3
54	LLL	a	1617	-	-	1/11/65/65	1/3/3/3
54	LLL	A	3022	-	-	3/11/65/65	0/3/3/3
54	LLL	a	1618	-	-	2/11/65/65	0/3/3/3
56	CLM	A	3019	-	-	0/20/22/22	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	LLL	A	2901	-	-	3/11/65/65	0/3/3/3
54	LLL	a	1615	-	-	2/11/65/65	0/3/3/3
54	LLL	A	3023	-	-	3/11/65/65	0/3/3/3
54	LLL	a	1616	-	-	1/11/65/65	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	a	1618	LLL	C53-O53-C13	3.99	117.95	111.53
54	a	1618	LLL	C11-O51-C51	2.91	116.36	113.13
54	a	1618	LLL	O53-C13-C23	2.64	114.09	110.04

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	A	2901	LLL	C41-C51-C61-N61
54	A	2901	LLL	O51-C51-C61-N61
54	A	2901	LLL	C23-C33-N33-C93
54	A	3021	LLL	C23-C33-N33-C93
54	A	3022	LLL	C41-C51-C61-N61
54	A	3022	LLL	O51-C51-C61-N61
54	A	3022	LLL	C23-C33-N33-C93
54	A	3023	LLL	C41-C51-C61-N61
54	A	3023	LLL	O51-C51-C61-N61
54	A	3023	LLL	C23-C33-N33-C93
54	A	3024	LLL	C23-C33-N33-C93
54	a	1615	LLL	C23-C33-N33-C93
54	a	1616	LLL	C23-C33-N33-C93
54	a	1617	LLL	C23-C33-N33-C93
54	a	1618	LLL	C23-C33-N33-C93
54	a	1615	LLL	O51-C51-C61-N61
54	a	1618	LLL	C52-C62-O62-C13
54	A	3024	LLL	O53-C13-O62-C62

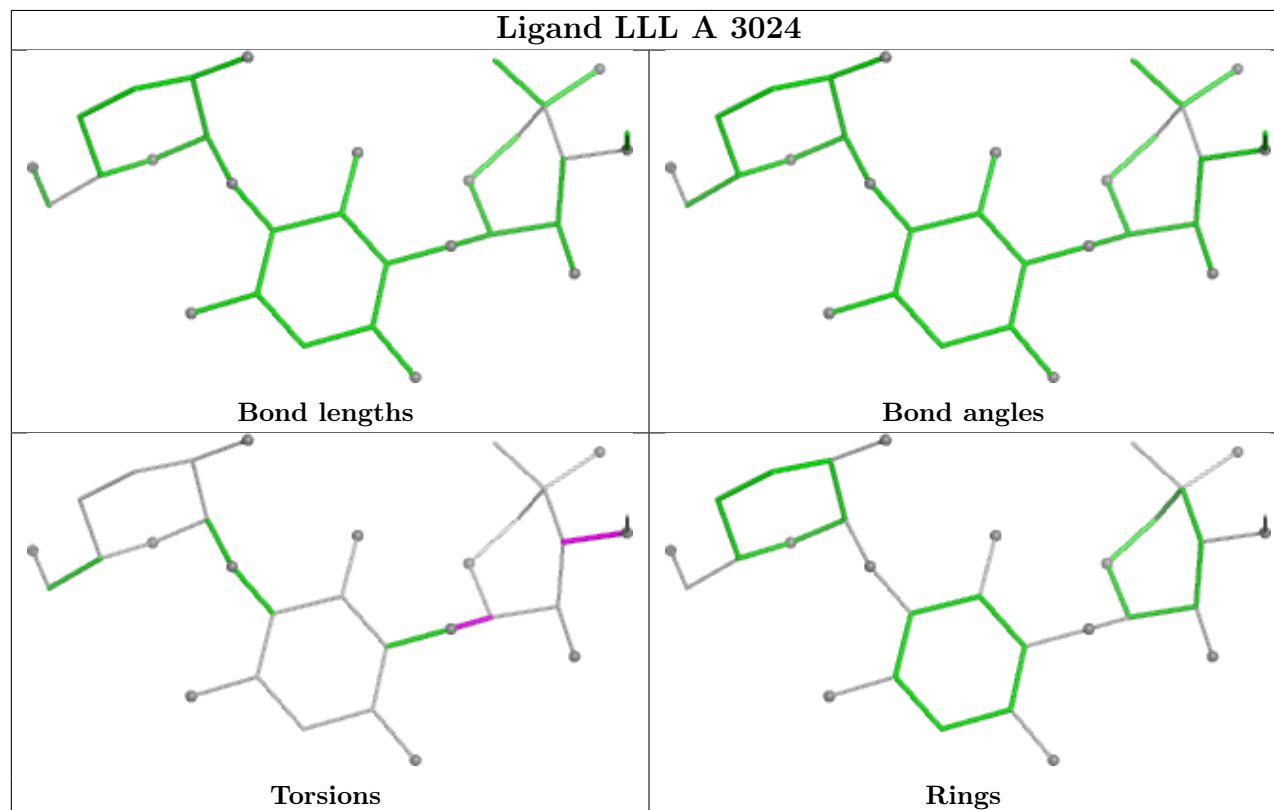
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	a	1617	LLL	C11-C21-C31-C41-C51-O51

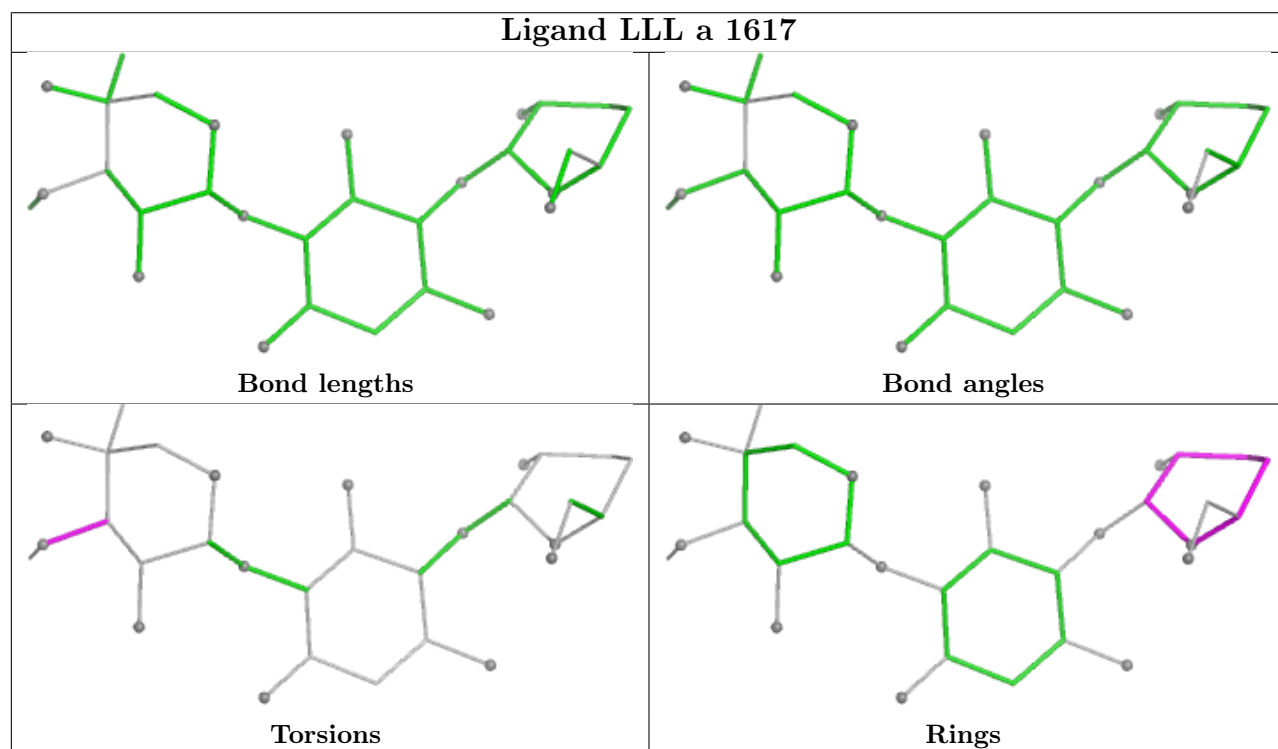
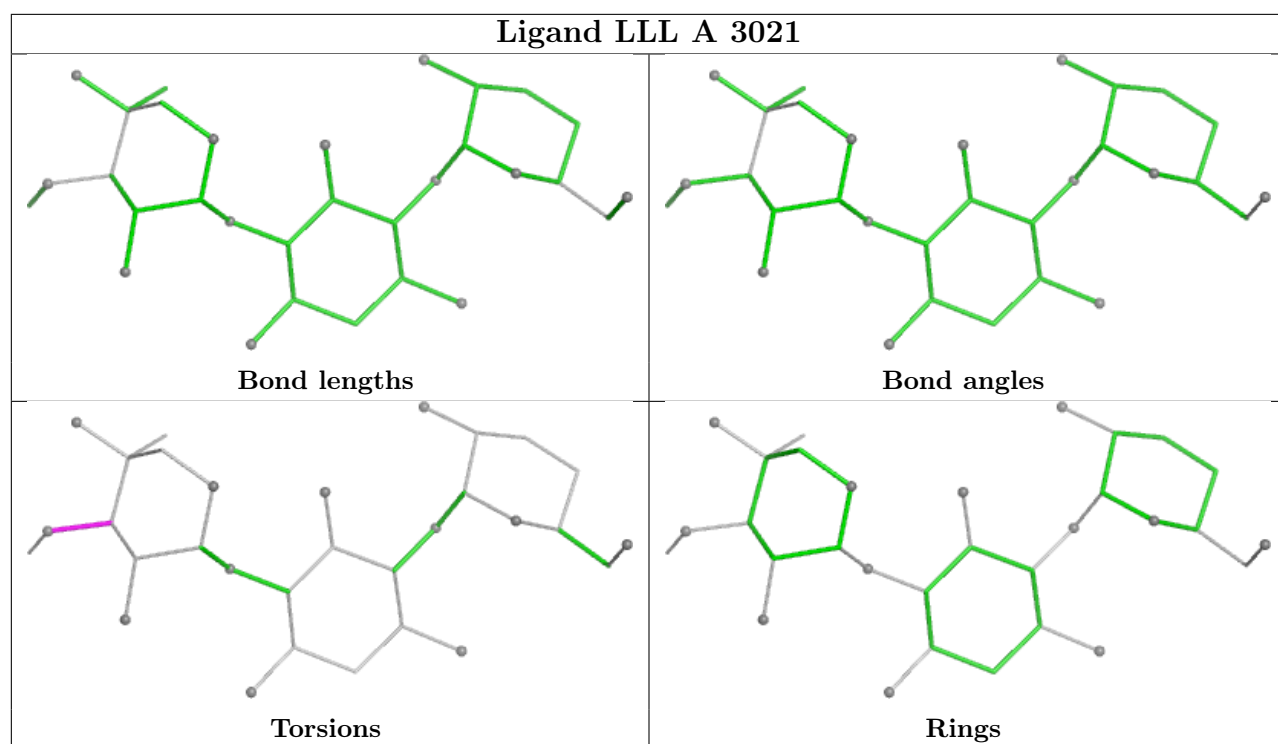
7 monomers are involved in 8 short contacts:

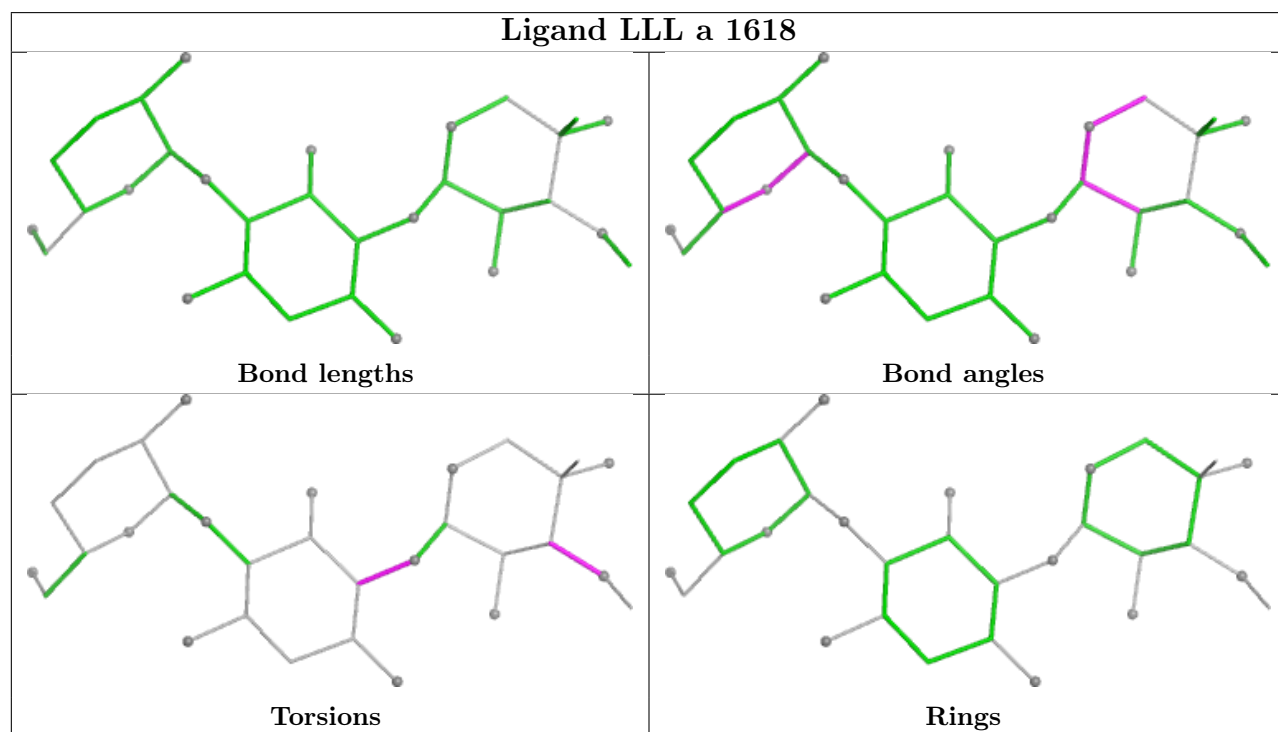
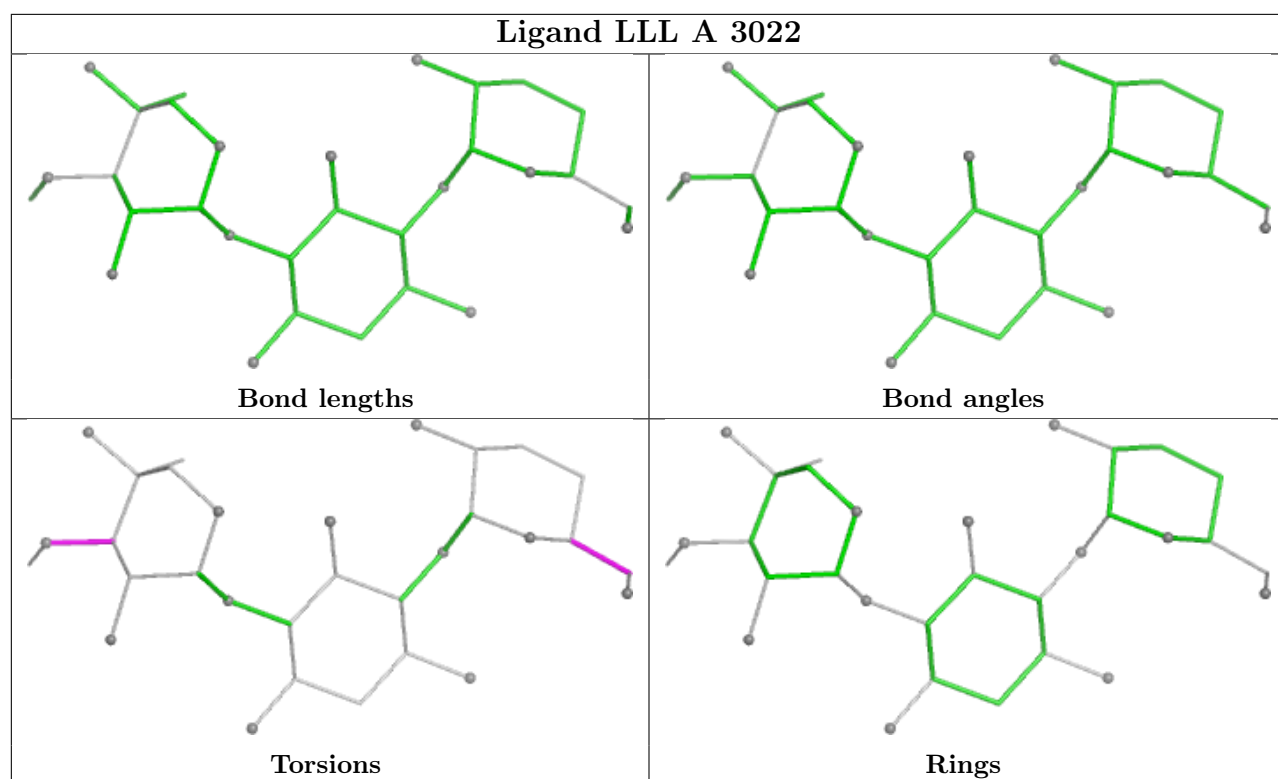
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	A	3021	LLL	1	0
54	a	1617	LLL	1	0
54	a	1618	LLL	1	0
56	A	3019	CLM	1	0
54	a	1615	LLL	1	0
54	A	3023	LLL	1	0
54	a	1616	LLL	2	0

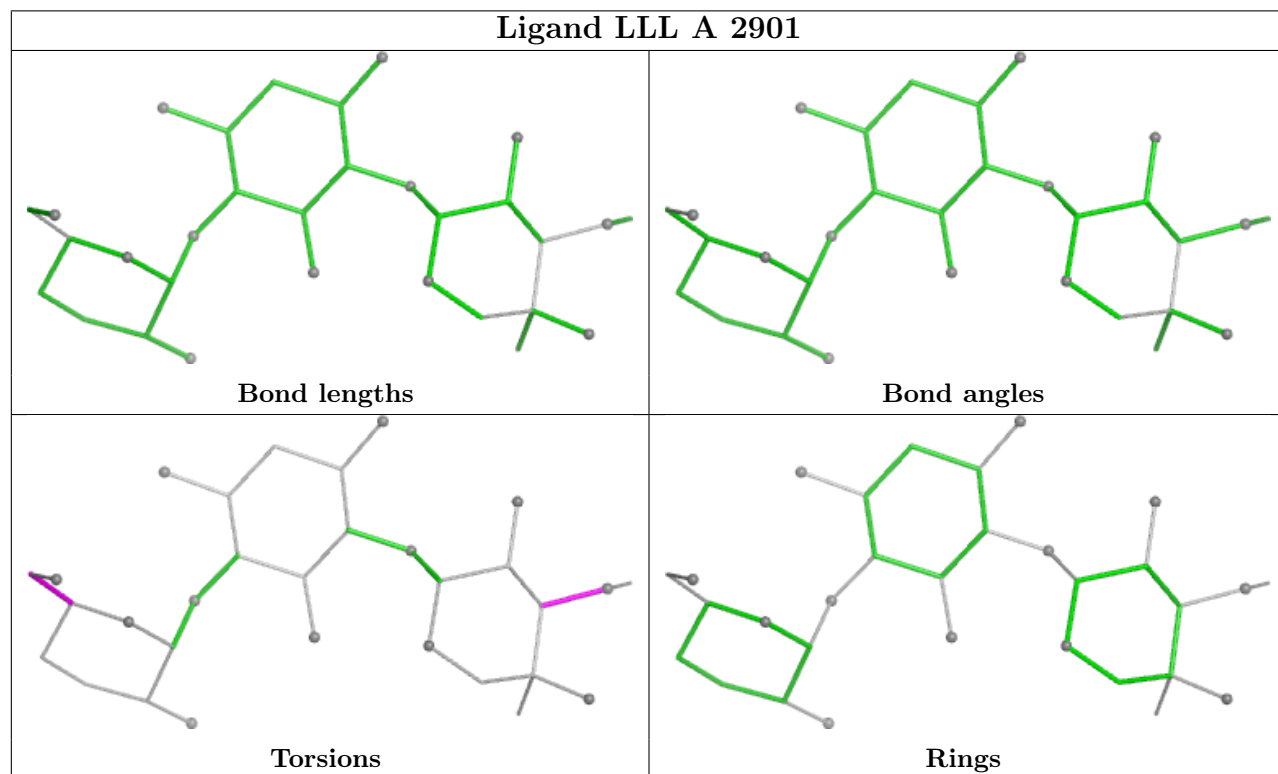
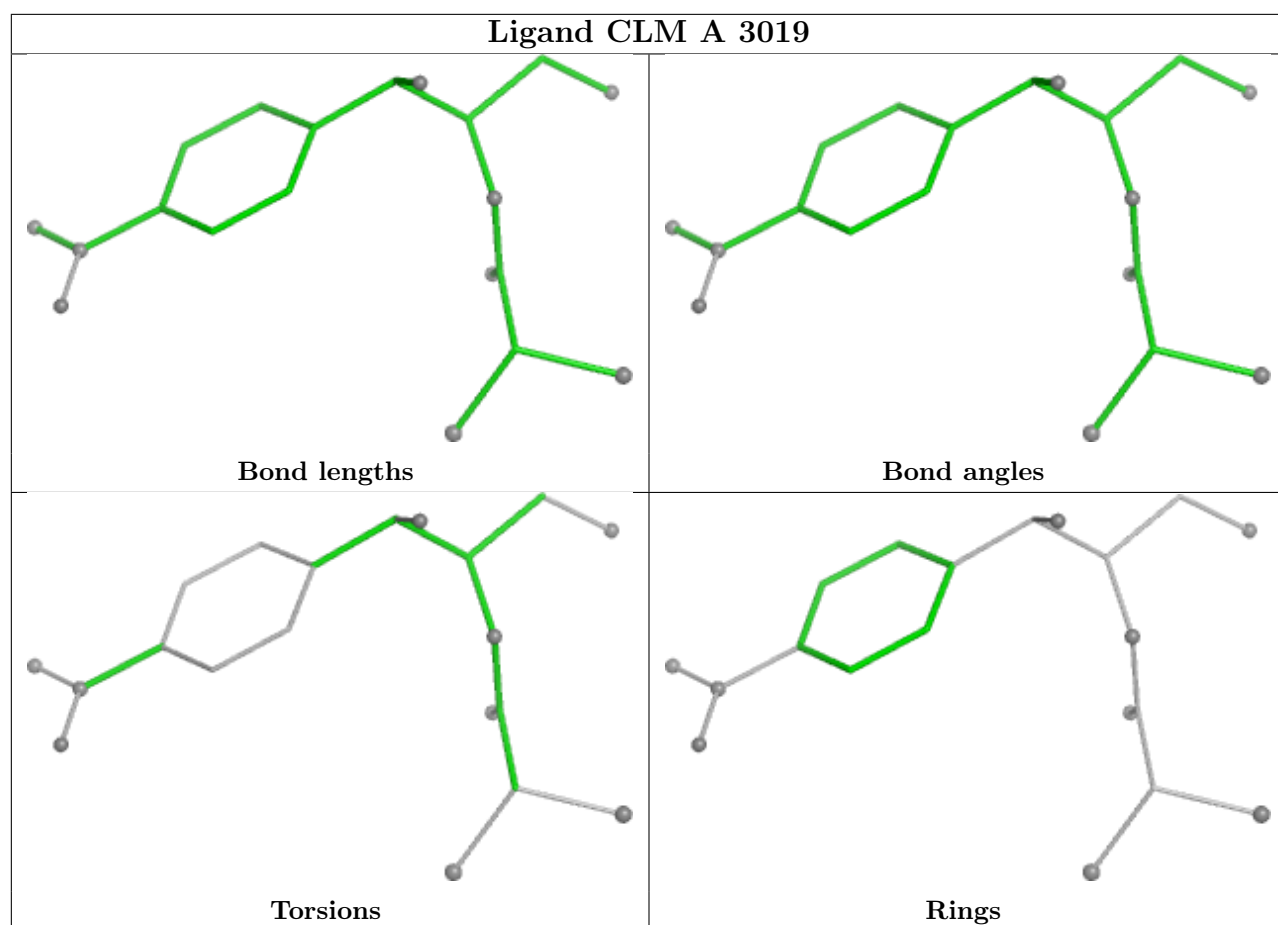
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



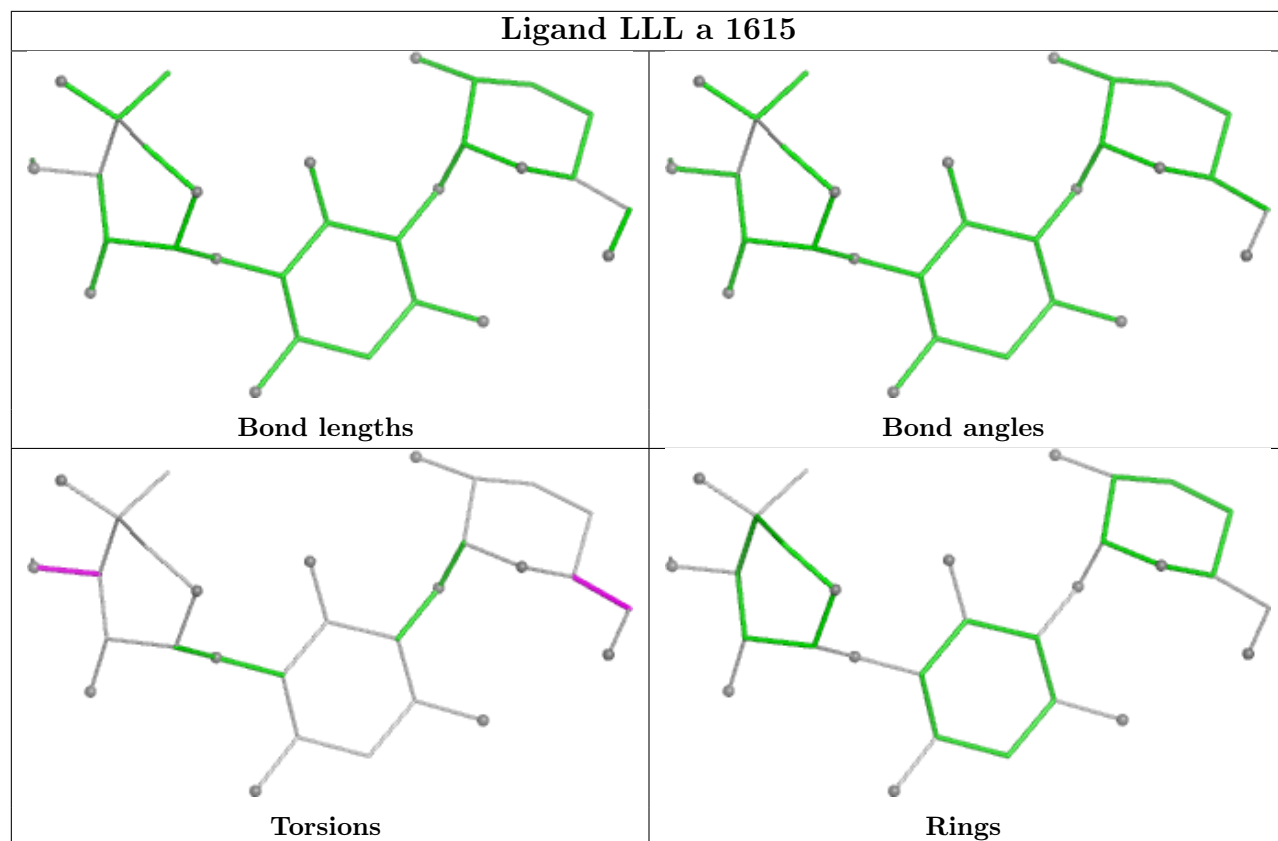




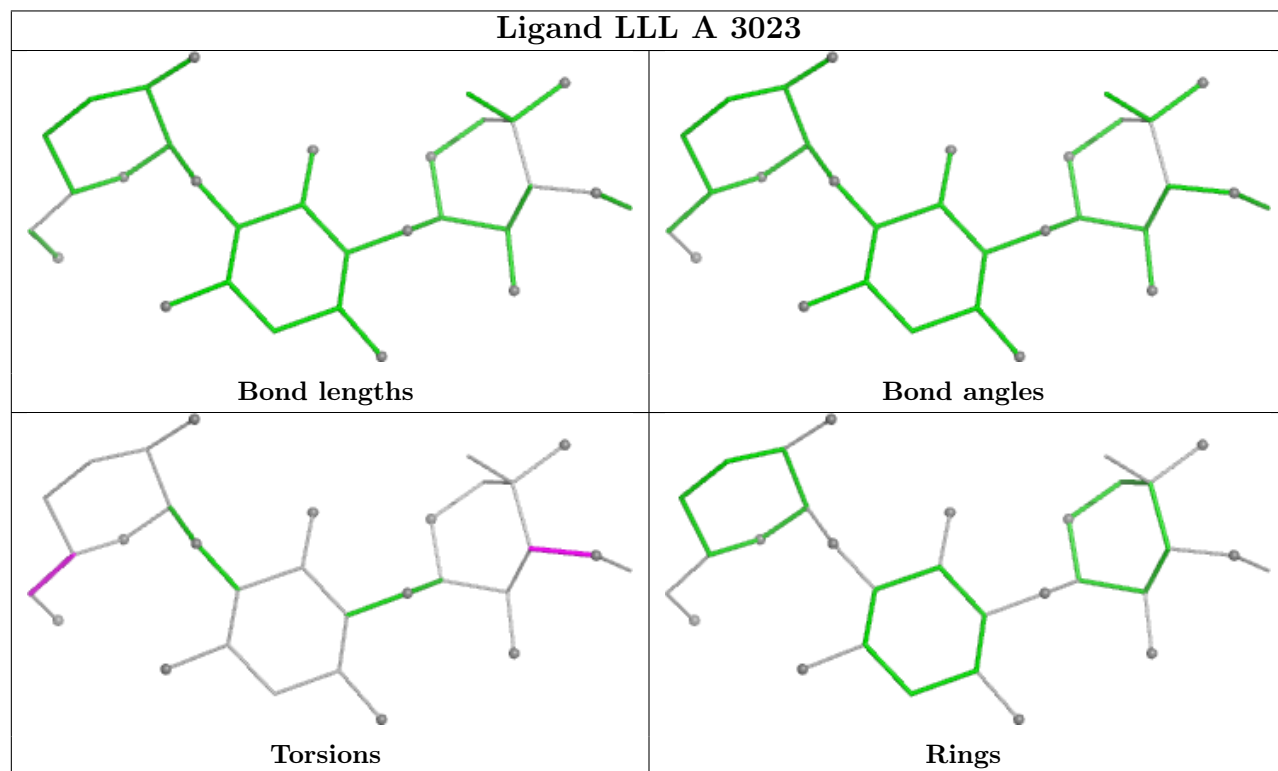


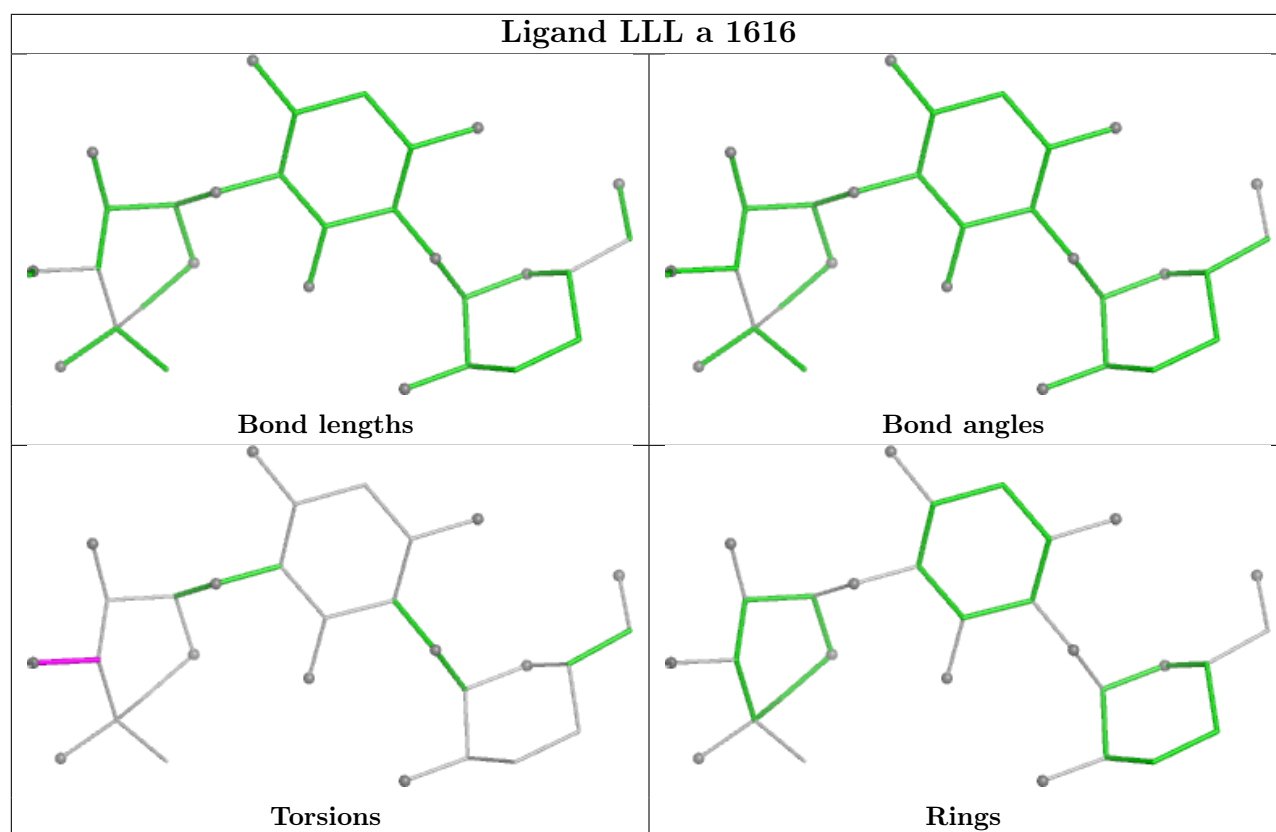


## Ligand LLL a 1615



## Ligand LLL A 3023





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

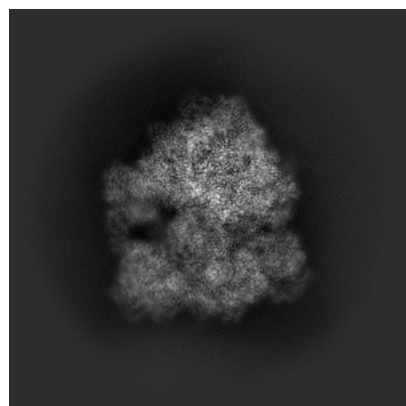
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55615. These allow visual inspection of the internal detail of the map and identification of artifacts.

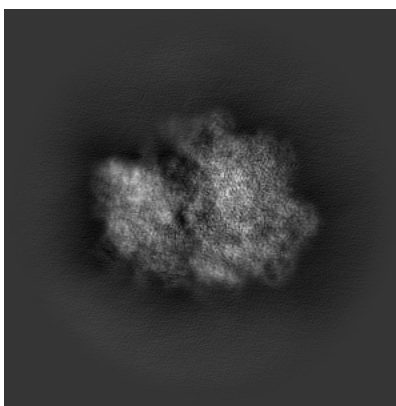
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

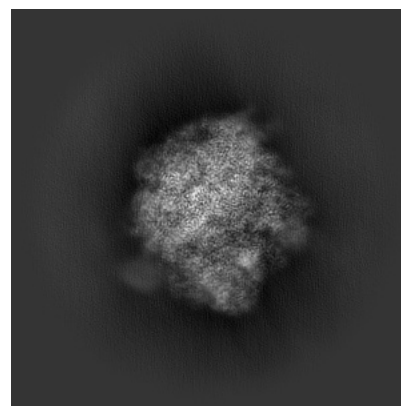
#### 6.1.1 Primary map



X

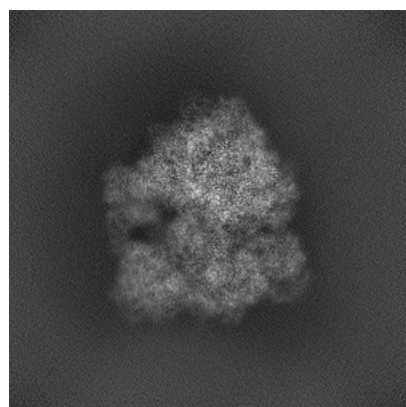


Y

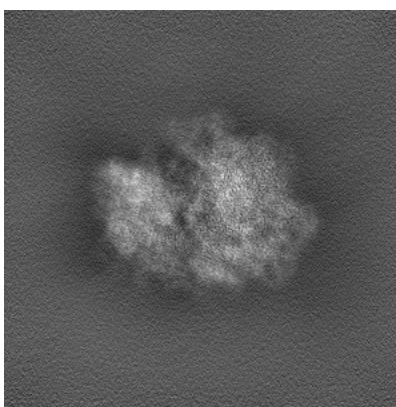


Z

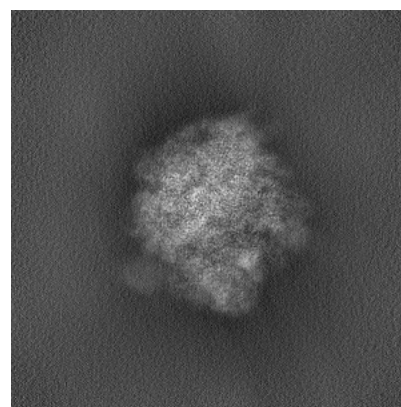
#### 6.1.2 Raw map



X



Y

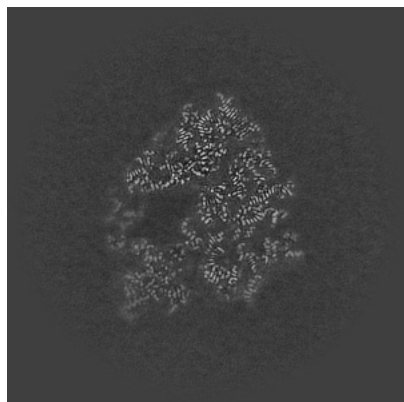


Z

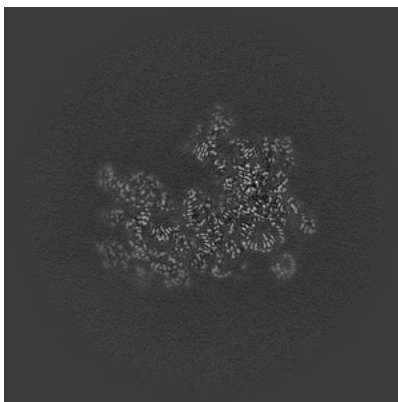
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

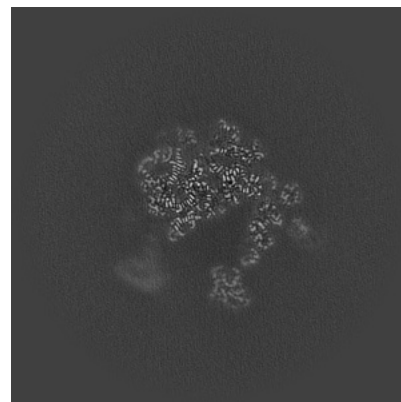
### 6.2.1 Primary map



X Index: 300

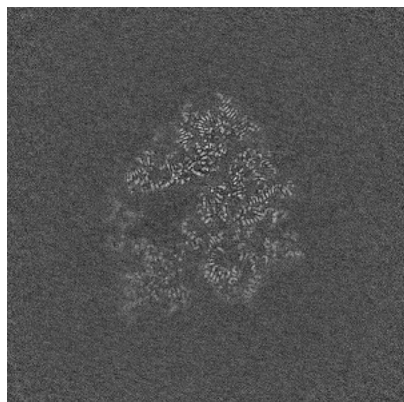


Y Index: 300

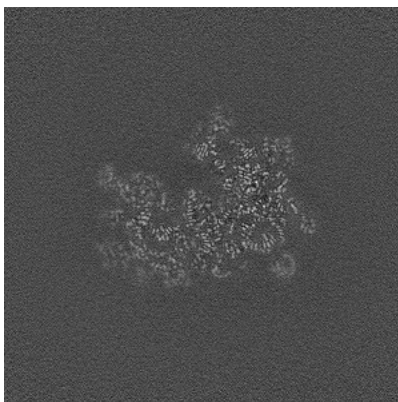


Z Index: 300

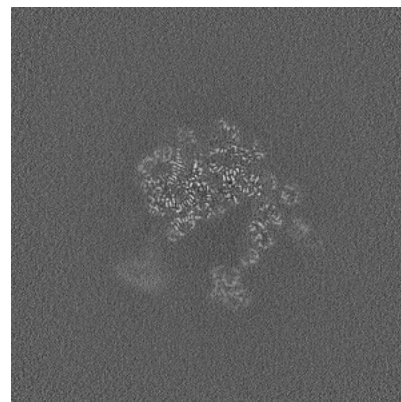
### 6.2.2 Raw map



X Index: 300



Y Index: 300



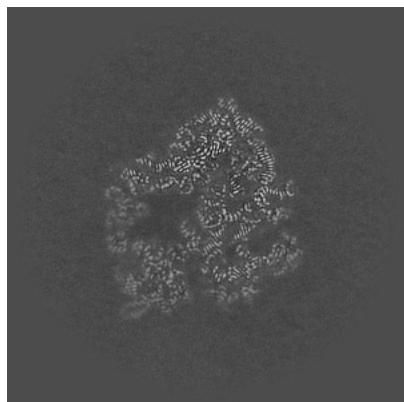
Z Index: 300

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

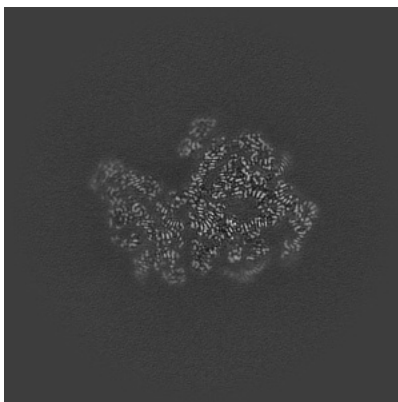


## 6.3 Largest variance slices [i](#)

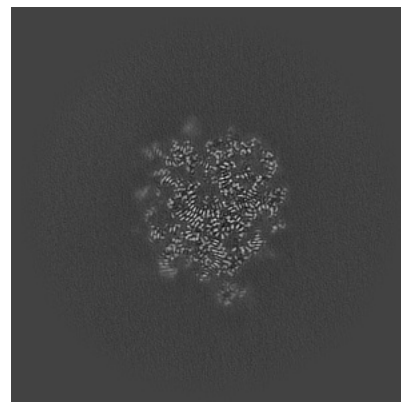
### 6.3.1 Primary map



X Index: 306

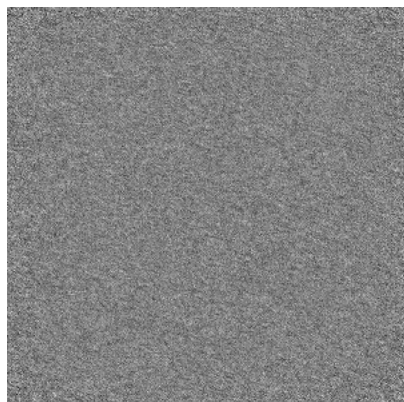


Y Index: 322

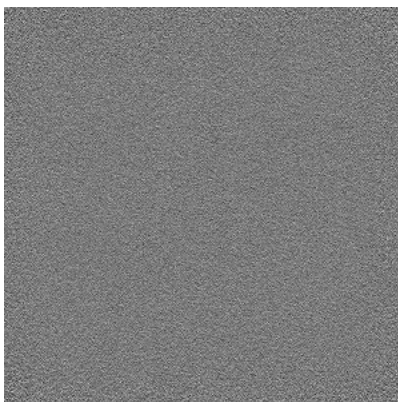


Z Index: 363

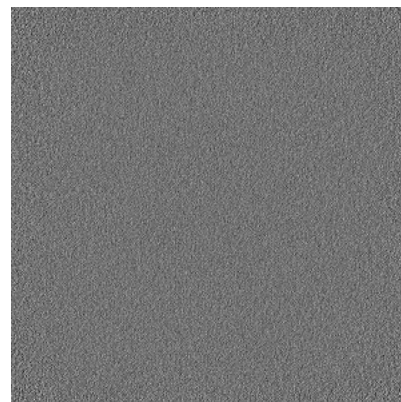
### 6.3.2 Raw map



X Index: 0



Y Index: 0



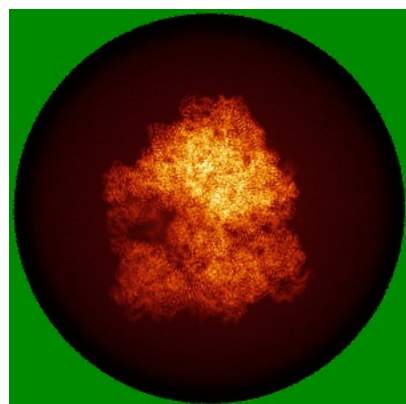
Z Index: 0

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

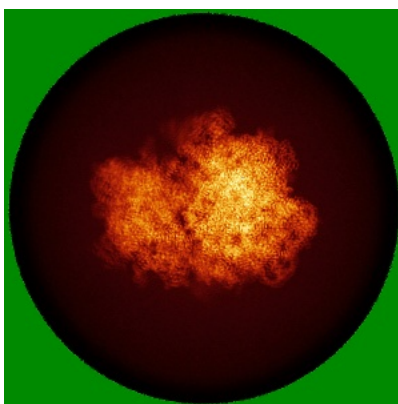


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

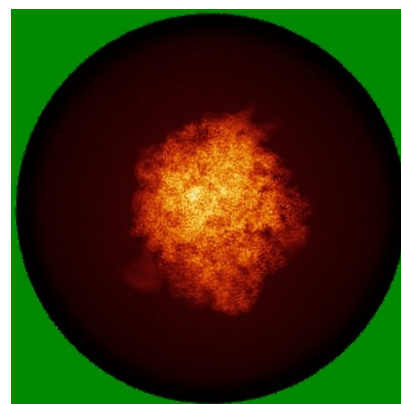
### 6.4.1 Primary map



X

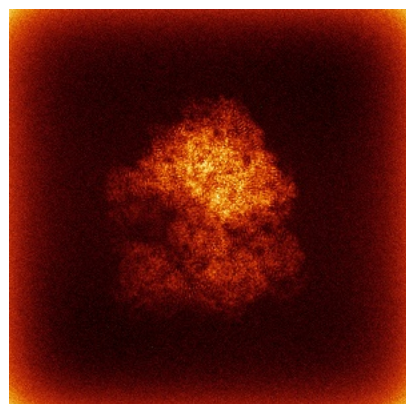


Y

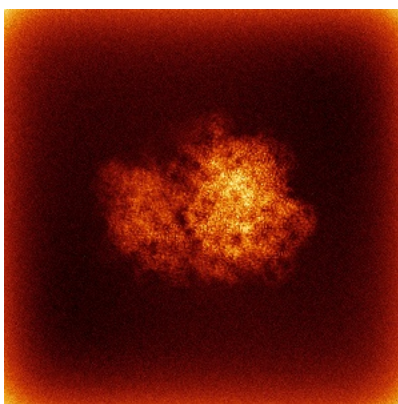


Z

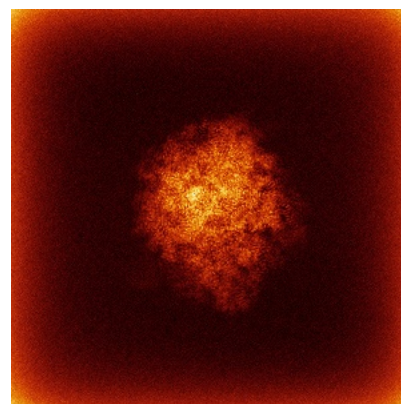
### 6.4.2 Raw map



X



Y



Z

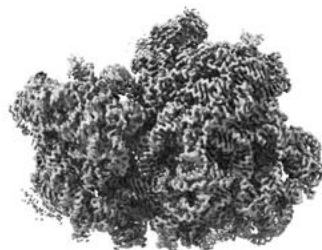
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



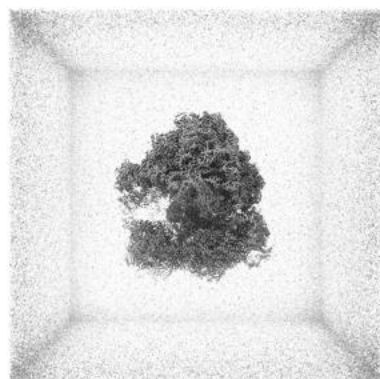
Y



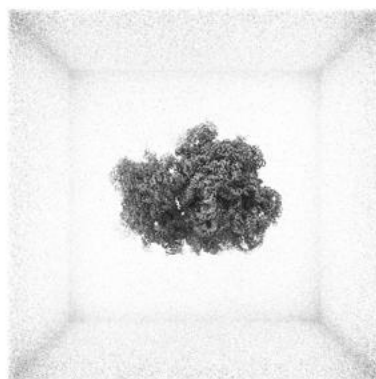
Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

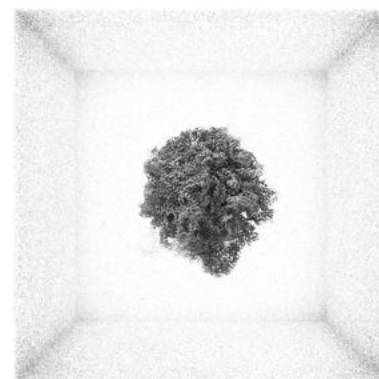
### 6.5.2 Raw map



X



Y



Z

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

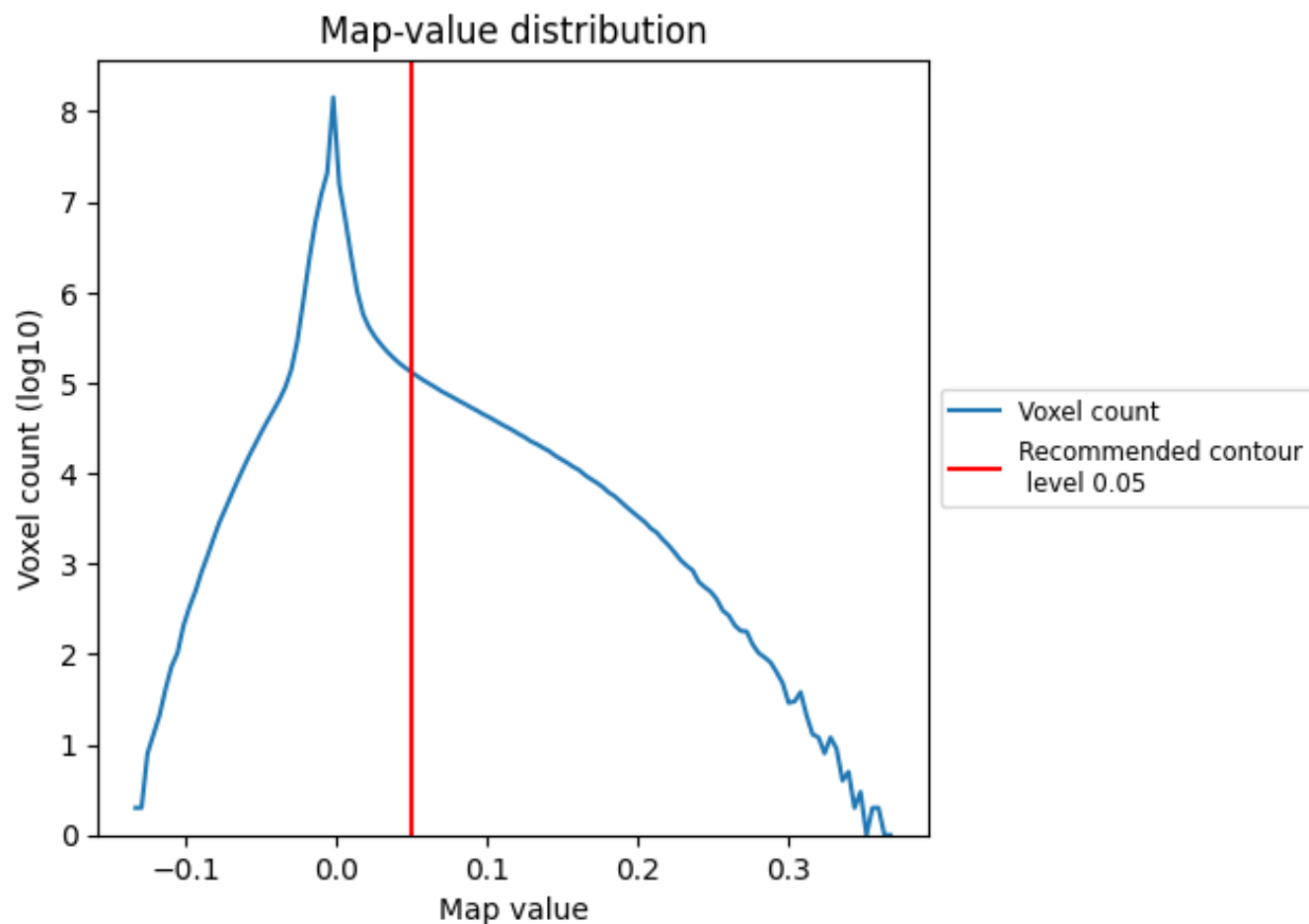
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

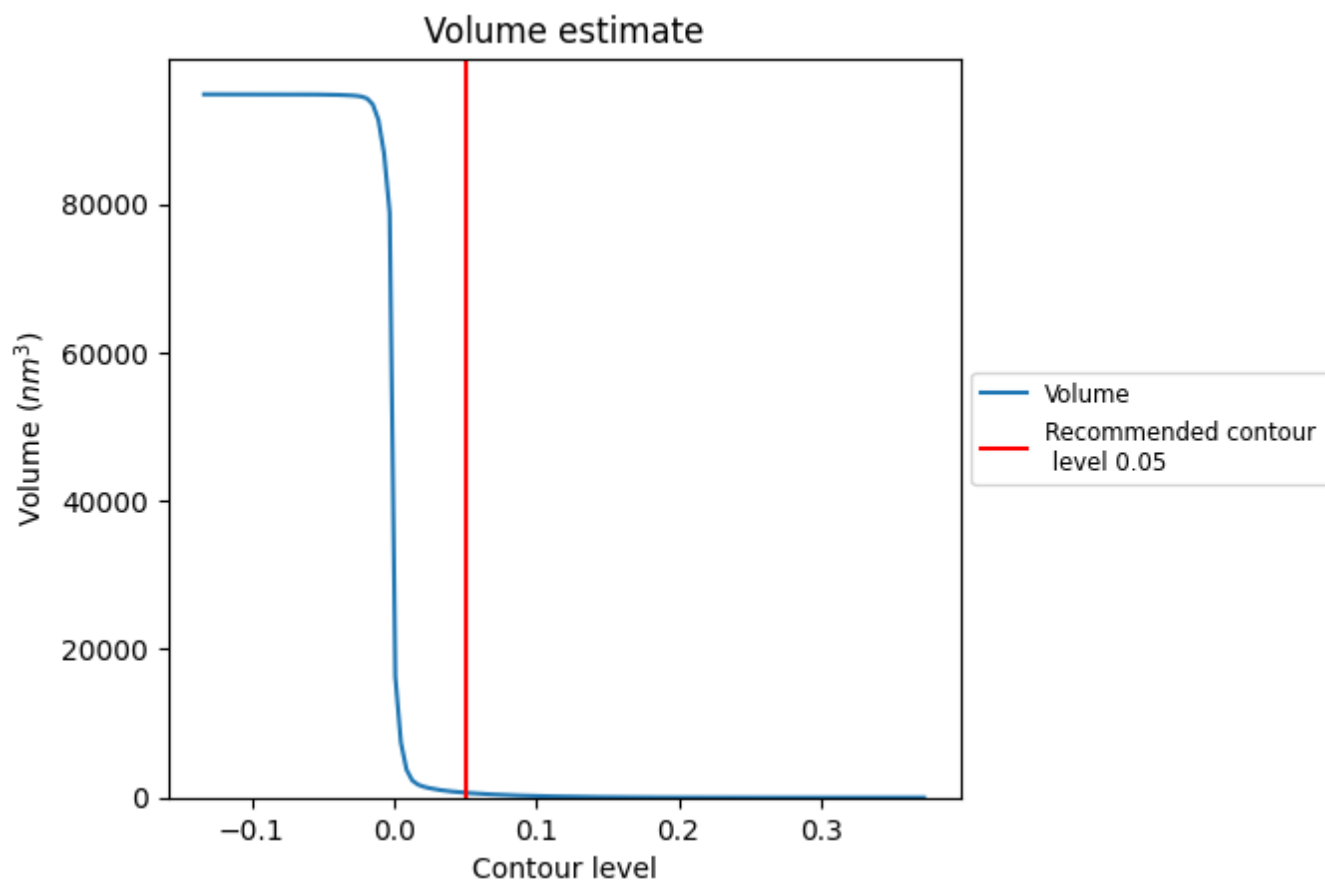
This section contains the results of statistical analysis of the map.

### 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.

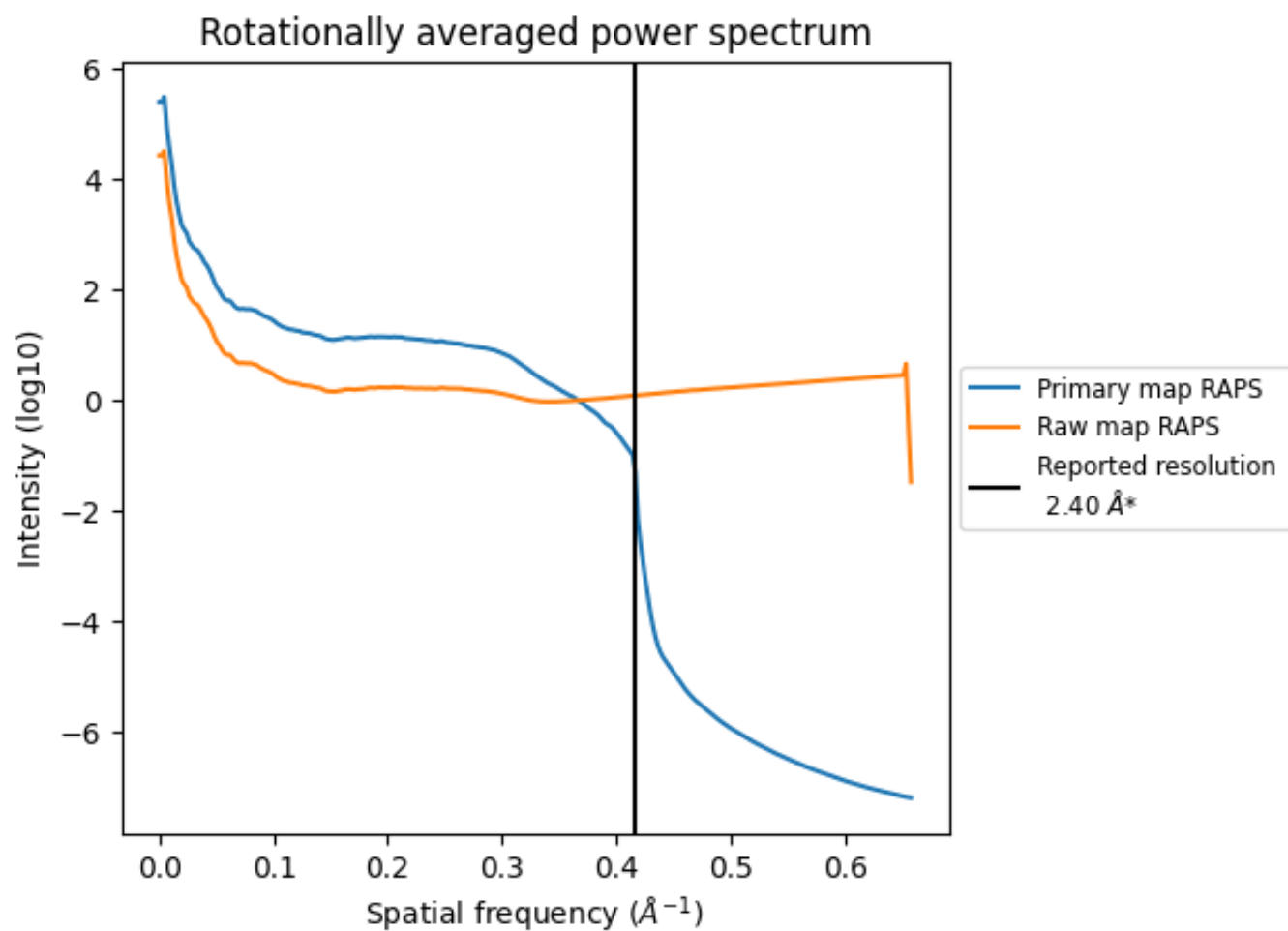
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 653  $\text{nm}^3$ ; this corresponds to an approximate mass of 590 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

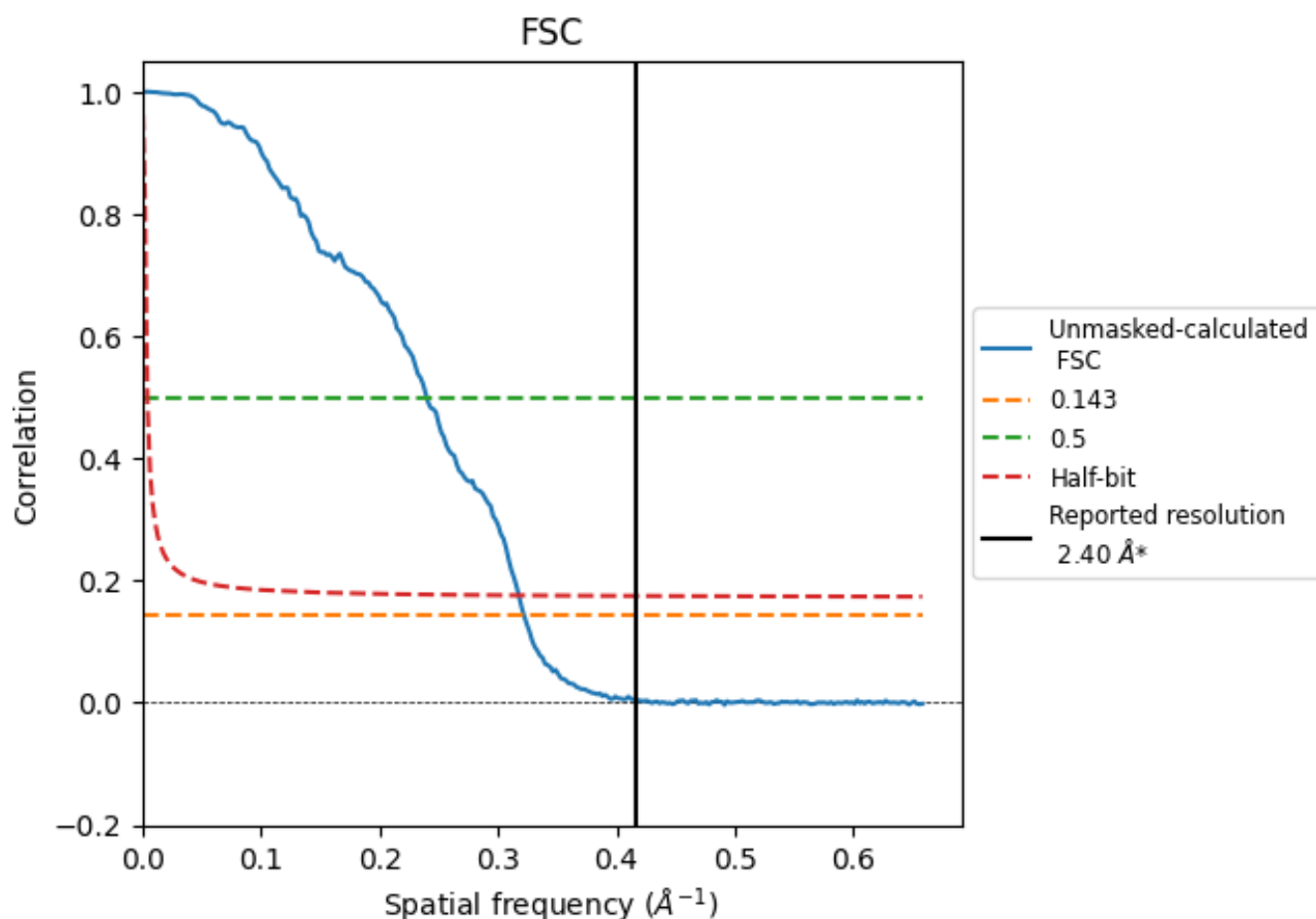


\*Reported resolution corresponds to spatial frequency of 0.417 Å<sup>-1</sup>

## 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  $0.417 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

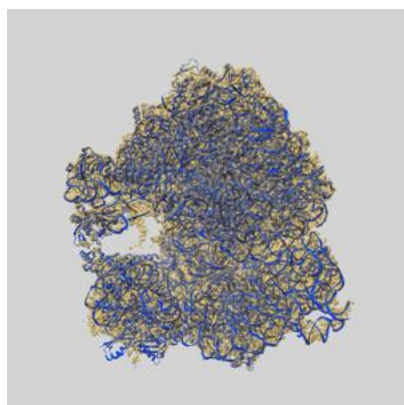
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.11	4.16	3.15

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.11 differs from the reported value 2.4 by more than 10 %

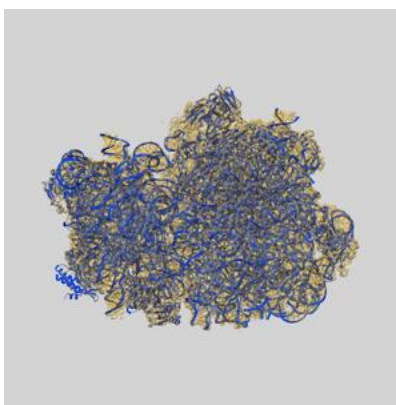
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55615 and PDB model 9T6H. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

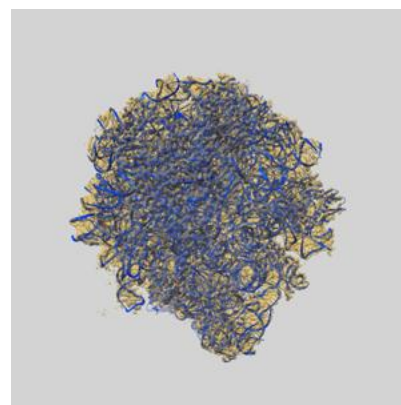
### 9.1 Map-model overlay [i](#)



X



Y

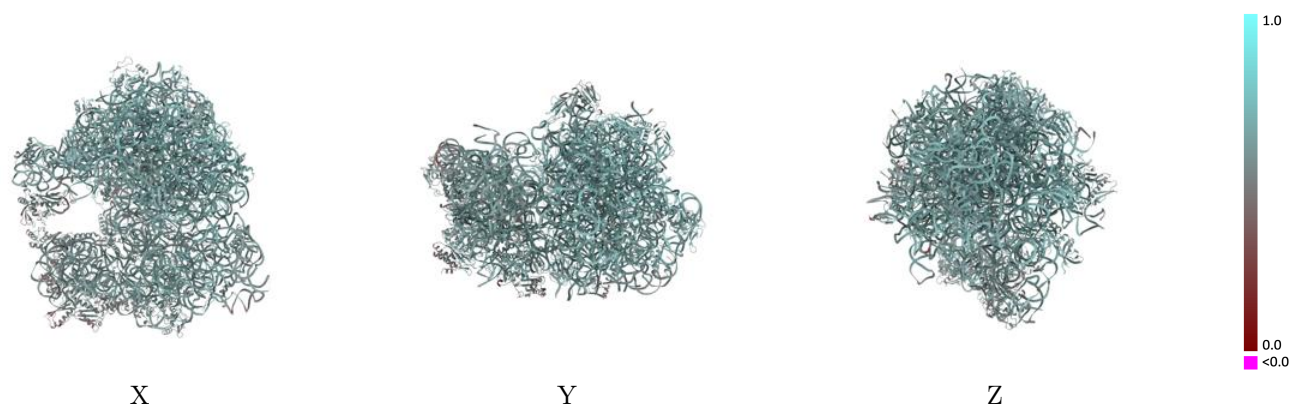


Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

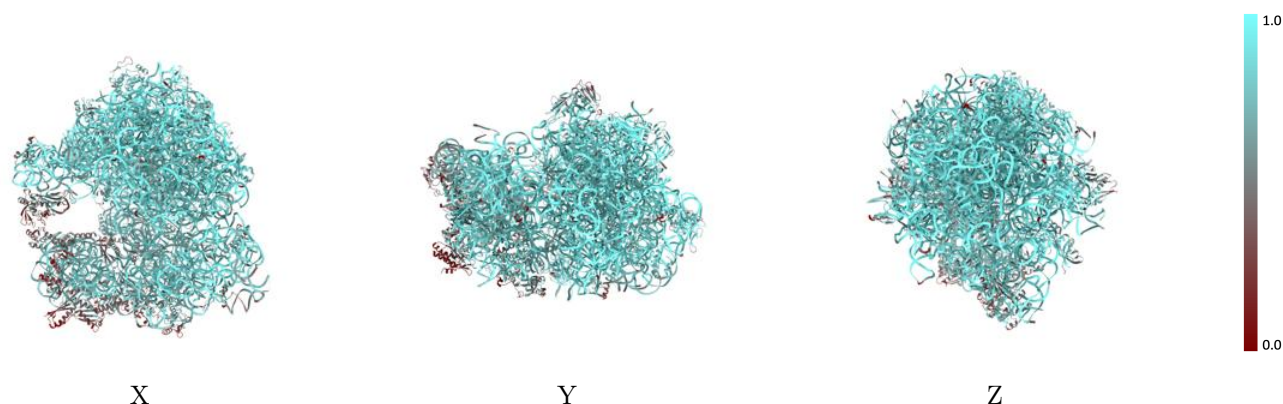


## 9.2 Q-score mapped to coordinate model [i](#)



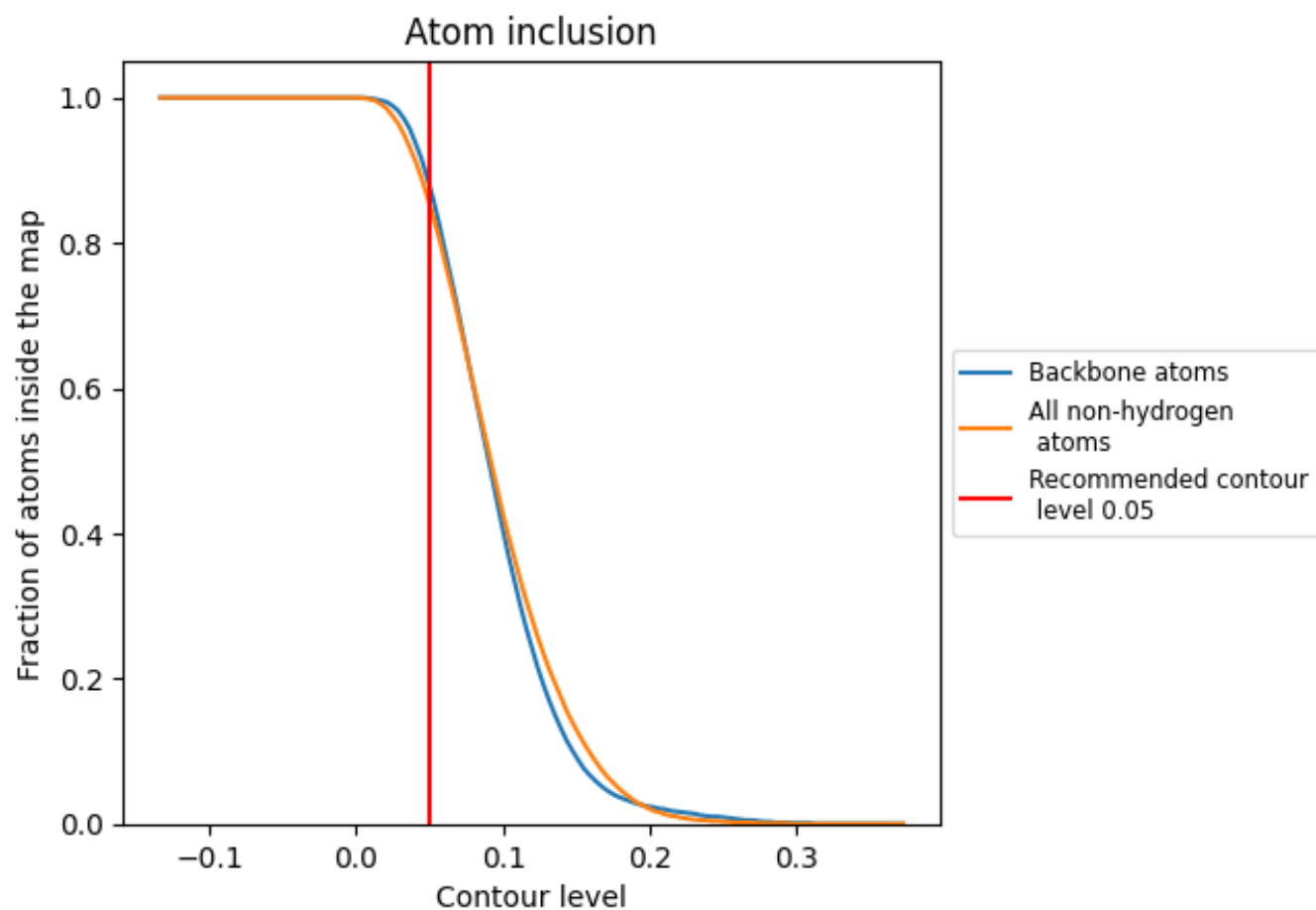
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 85% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8530	 0.6180
0	 0.8790	 0.6530
1	 0.6890	 0.6100
2	 0.9560	 0.6770
3	 0.8980	 0.6550
4	 0.9070	 0.6480
9	 0.5220	 0.5930
A	 0.9540	 0.6400
B	 0.8890	 0.5980
C	 0.9040	 0.6650
D	 0.9140	 0.6550
E	 0.8210	 0.6280
F	 0.3720	 0.5040
G	 0.6400	 0.5740
H	 0.6180	 0.5650
I	 0.9130	 0.6570
J	 0.8650	 0.6550
K	 0.8590	 0.6430
L	 0.8640	 0.6480
M	 0.9130	 0.6540
N	 0.6930	 0.5720
O	 0.8560	 0.6520
P	 0.9320	 0.6600
Q	 0.8700	 0.6490
R	 0.9180	 0.6630
S	 0.7560	 0.6230
T	 0.7560	 0.6120
U	 0.7480	 0.6120
V	 0.9010	 0.6540
W	 0.8670	 0.6490
X	 0.7800	 0.6040
Y	 0.8810	 0.6460
Z	 0.2040	 0.4700
a	 0.8920	 0.6090
b	 0.2120	 0.5060



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
c	 0.5360	 0.5510
d	 0.5320	 0.5640
e	 0.7530	 0.6130
f	 0.5280	 0.5050
g	 0.4470	 0.5290
h	 0.7960	 0.6240
i	 0.5020	 0.5460
j	 0.3660	 0.4990
k	 0.7290	 0.6000
l	 0.7030	 0.6150
m	 0.4630	 0.5440
n	 0.5300	 0.5510
o	 0.7190	 0.5980
p	 0.7060	 0.6010
q	 0.6680	 0.5910
r	 0.6100	 0.5690
s	 0.4090	 0.5340
t	 0.7100	 0.5860
u	 0.3870	 0.5350