



## Full wwPDB EM Validation Report ⓘ

Sep 17, 2024 – 03:23 pm BST

PDB ID : 7ZTA  
EMDB ID : EMD-14956  
Title : Structure of an Escherichia coli 70S ribosome stalled by Tetracenomycin X during translation of an MAAAPQK(C) peptide  
Authors : Leroy, E.C.; Perry, T.N.; Renault, T.T.; Innis, C.A.  
Deposited on : 2022-05-09  
Resolution : 2.70 Å(reported)  
Based on initial model : 6TC3

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev112  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.2

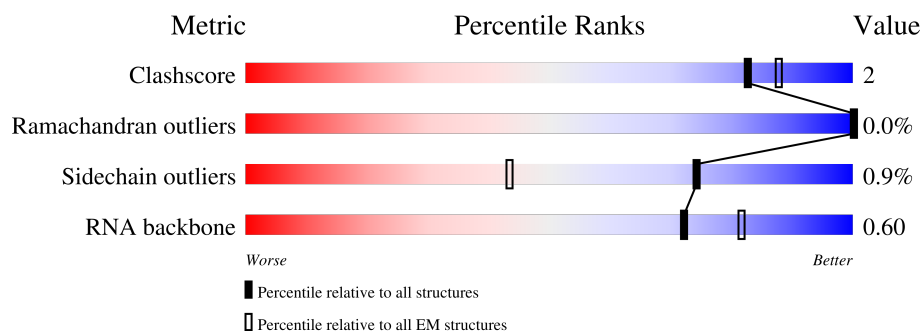
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*


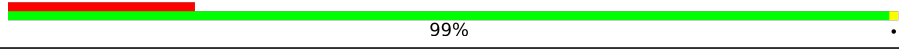
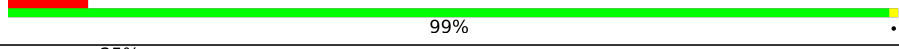
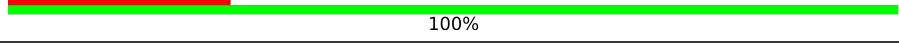
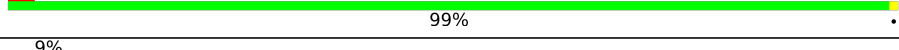
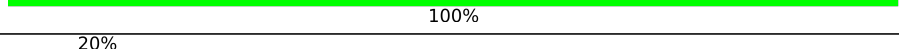
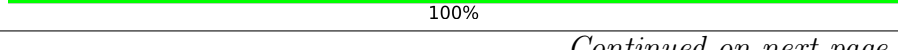
The reported resolution of this entry is 2.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	16S1	1534	
2	S021	224	
3	S031	206	
4	S041	205	
5	S051	155	
6	S061	106	
7	S071	151	

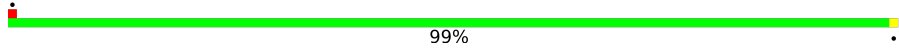
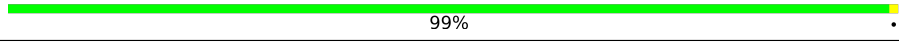
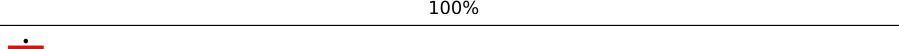
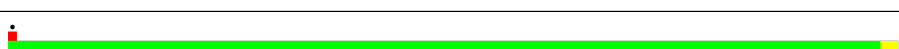

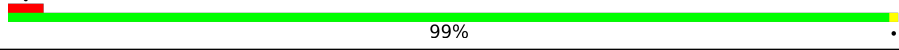
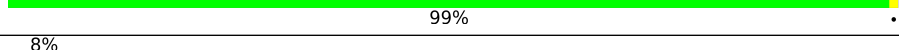
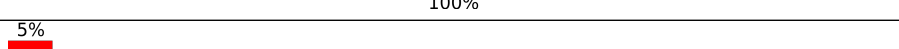

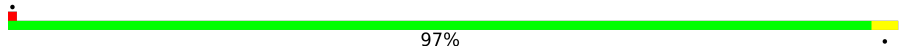
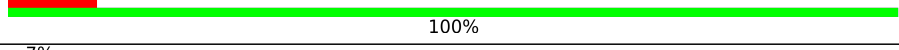
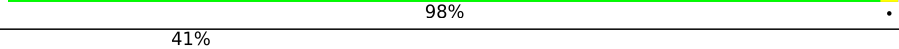
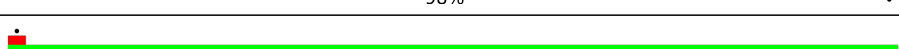
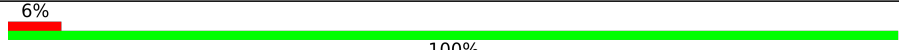
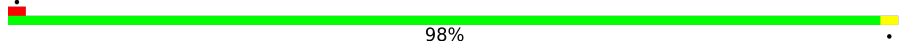
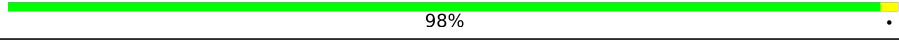
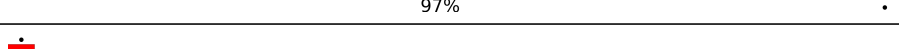







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Mol	Chain	Length	Quality of chain
8	S081	129	6% 100%
9	S091	127	8% 98%
10	S101	99	29% 99%
11	S111	117	9% 99%
12	S121	123	9% 99%
13	S131	114	18% 97%
14	S141	101	8% 100%
15	S151	88	5% 100%
16	S161	82	18% 100%
17	S171	80	16% 99%
18	S181	65	5% 100%
19	S191	83	13% 99%
20	S201	86	10% 99%
21	S211	56	29% 100%
22	23S1	2903	5% 90% 9%
23	05S1	120	92% 8%
24	L021	271	100%
25	L031	209	98%
26	L041	201	8% 99%
27	L051	177	14% 100%
28	L061	176	14% 99%
29	L091	149	81% 97%
30	L131	142	100%
31	L141	123	100%
32	L151	144	99%

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Mol	Chain	Length	Quality of chain
33	L161	136	 99%
34	L171	118	 99%
35	L181	117	 100%
36	L191	114	 100%
37	L201	117	 98%
38	L211	103	 100%
39	L221	110	 99%
40	L231	93	 99%
41	L241	102	 100%
42	L251	94	 100%
43	L271	84	 100%
44	L281	77	 97%
45	L291	62	 100%
46	L301	58	 98%
47	L311	66	 98%
48	L321	56	 100%
49	L331	51	 100%
50	L341	46	 98%
51	L351	64	 98%
52	L361	38	 97%
53	ATR1	74	 64%34%
54	PTR1	76	 80%11%5%
55	PQK1	7	 71%29%
56	ETR1	75	 72%21%7%
57	MRN1	14	86%14%

## 2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 148592 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	16S1	1534	Total	C	N	O	P	0	0
			32930	14694	6041	10661	1534		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S021	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S031	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S041	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S051	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S061	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S071	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S081	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S091	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S101	99	Total	C	N	O	S	0	0
			796	498	152	145	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S111	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S121	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S131	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S141	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S141	35	ALA	-	insertion	UNP P0AG59

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S151	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S161	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S171	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S181	65	Total	C	N	O	S	0	0
			536	339	100	96	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S191	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S201	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S211	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	23S1	2903	Total	C	N	O	P	0	0
			62334	27815	11467	20149	2903		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	05S1	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	L021	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L031	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	L041	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
27	L051	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	L061	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	L091	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	L131	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L141	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	L151	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L161	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	L171	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L181	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	L191	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
37	L201	117	Total	C	N	O	0	0
			947	604	192	151		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	L211	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	L221	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	L231	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
41	L241	102	Total	C	N	O		
			780	492	146	142	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	L251	94	Total	C	N	O	S		
			753	479	137	134	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	L271	84	Total	C	N	O	S		
			634	391	129	113	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	L281	77	Total	C	N	O	S		
			625	388	129	106	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	L291	62	Total	C	N	O	S		
			501	308	98	94	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	L301	58	Total	C	N	O	S		
			449	281	87	79	2	0	0

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	L311	66	Total	C	N	O	S		
			522	323	99	94	6	0	0

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	L321	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	L331	51	Total	C	N	O		0	0
			414	266	76	72			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	L341	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	L351	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	L361	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 53 is a RNA chain called tRNA-Cys.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	ATR1	72	Total	C	N	O	P S	0	0
			1540	692	276	499	71 2		

- Molecule 54 is a RNA chain called tRNA-Lys.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	PTR1	73	Total	C	N	O	P S	0	0
			1569	703	277	515	73 1		

- Molecule 55 is a protein called MAAAPQK nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	PQK1	5	Total	C	N	O	0	0
			35	22	7	6		

- Molecule 56 is a RNA chain called tRNA-Gln.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	ETR1	72	Total	C	N	O	P	S	0	0
			1537	688	274	502	72	1		

- Molecule 57 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	MRN1	14	Total	C	N	O	P	0	0
			303	135	58	96	14		

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	16S1	76	Total	Mg	0
			76	76	
58	23S1	209	Total	Mg	0
			209	209	
58	05S1	1	Total	Mg	0
			1	1	
58	L021	1	Total	Mg	0
			1	1	
58	L031	1	Total	Mg	0
			1	1	
58	L041	1	Total	Mg	0
			1	1	

- Molecule 59 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
59	16S1	31	Total	K	0
			31	31	
59	S131	1	Total	K	0
			1	1	
59	23S1	81	Total	K	0
			81	81	
59	05S1	1	Total	K	0
			1	1	

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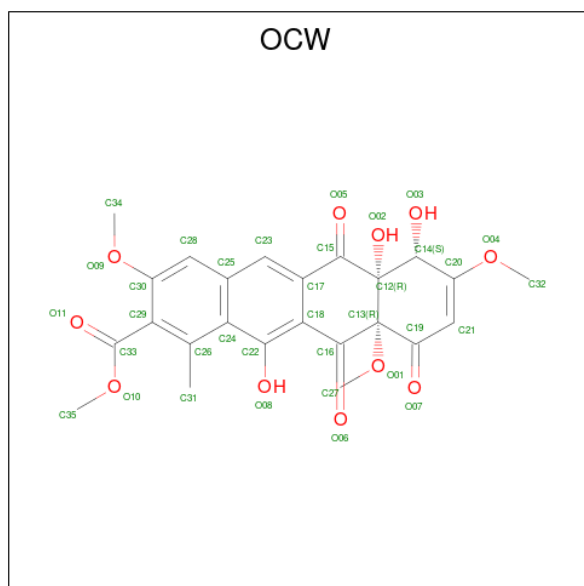
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Mol	Chain	Residues	Atoms		AltConf
59	L021	1	Total	K	0
			1	1	

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

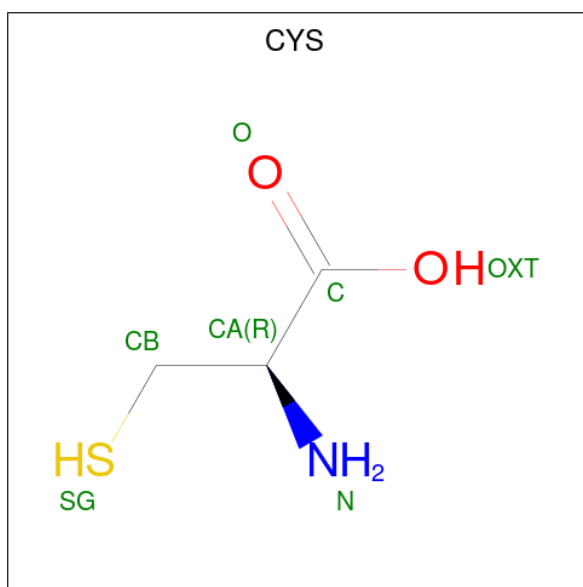
Mol	Chain	Residues	Atoms		AltConf
60	S021	1	Total	Zn	0
			1	1	
60	L311	1	Total	Zn	0
			1	1	
60	L361	1	Total	Zn	0
			1	1	

- Molecule 61 is Tetracenomycin X (three-letter code: OCW) (formula: C<sub>24</sub>H<sub>22</sub>O<sub>11</sub>) (labeled as "Ligand of Interest" by depositor).



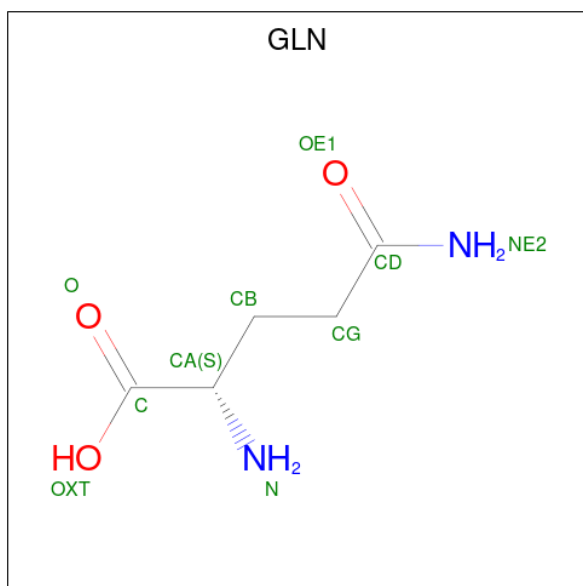
Mol	Chain	Residues	Atoms		AltConf
61	23S1	1	Total	C O	0
			35	24 11	

- Molecule 62 is CYSTEINE (three-letter code: CYS) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>S).



Mol	Chain	Residues	Atoms					AltConf
62	ATR1	1	Total	C	N	O	S	0
			6	3	1	1	1	

- Molecule 63 is GLUTAMINE (three-letter code: GLN) (formula:  $C_5H_{10}N_2O_3$ ).



Mol	Chain	Residues	Atoms					AltConf
63	ETR1	1	Total	C	N	O		0
			9	5	2	2		

- Molecule 64 is water.

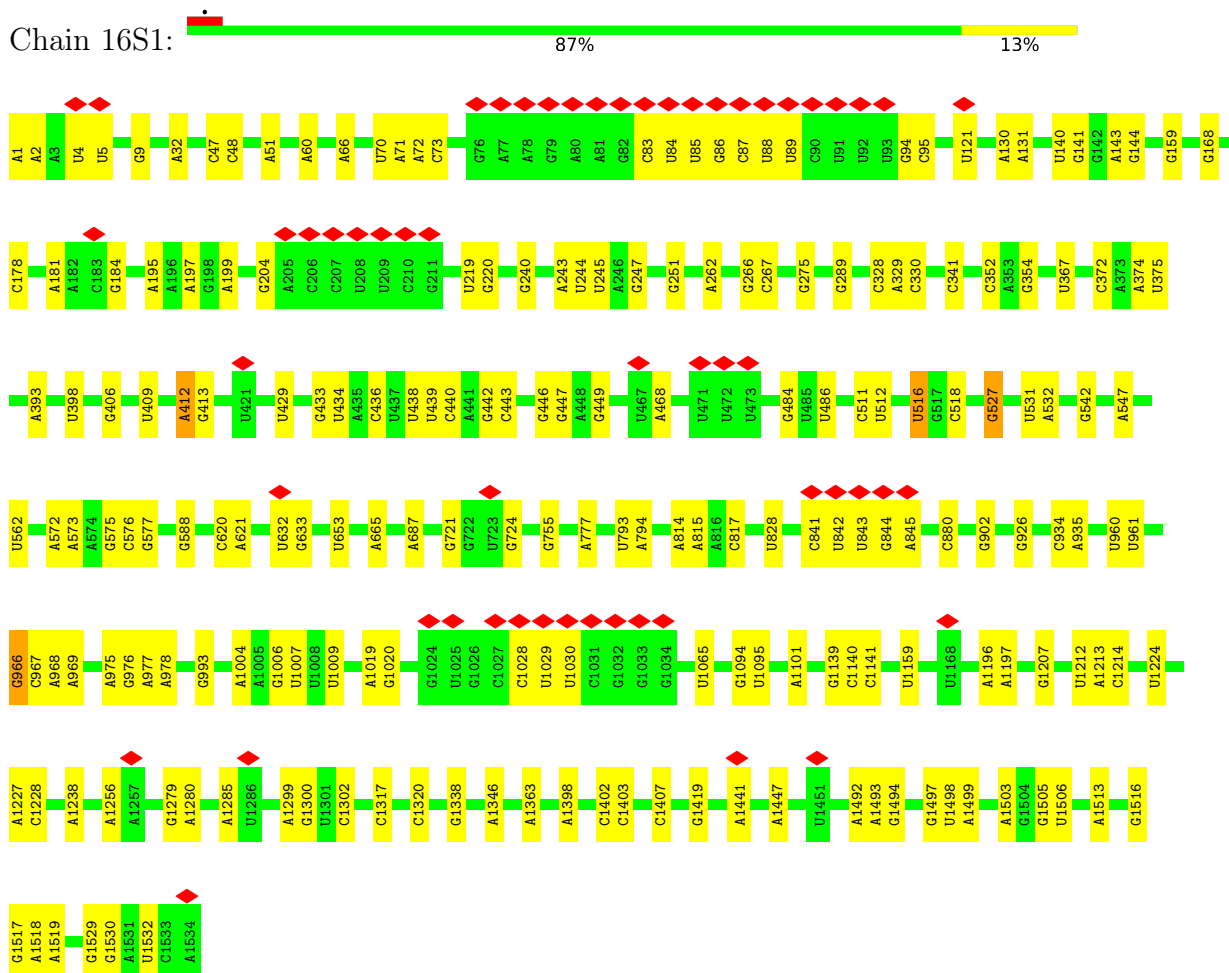
Mol	Chain	Residues	Atoms		AltConf
64	16S1	147	Total 147	O 147	0
64	S111	1	Total 1	O 1	0
64	S141	2	Total 2	O 2	0
64	23S1	604	Total 604	O 604	0
64	05S1	5	Total 5	O 5	0
64	L021	7	Total 7	O 7	0
64	L031	4	Total 4	O 4	0
64	L131	1	Total 1	O 1	0
64	L171	4	Total 4	O 4	0



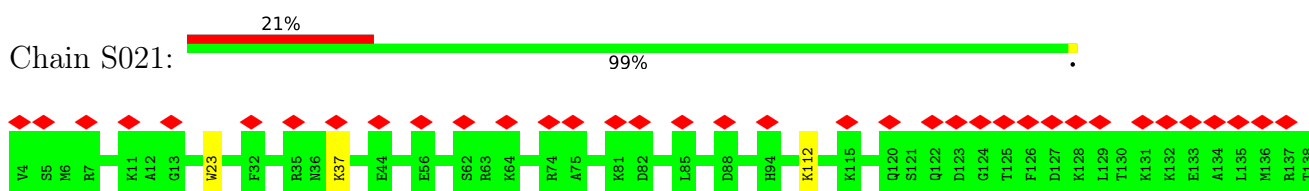
### 3 Residue-property plots

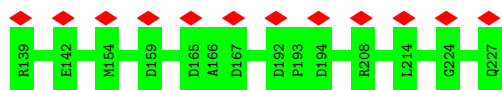
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: 16S ribosomal RNA

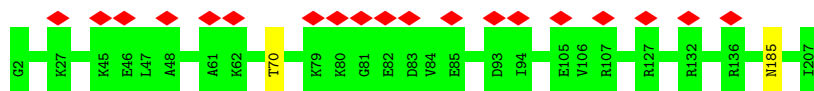


#### • Molecule 2: 30S ribosomal protein S2

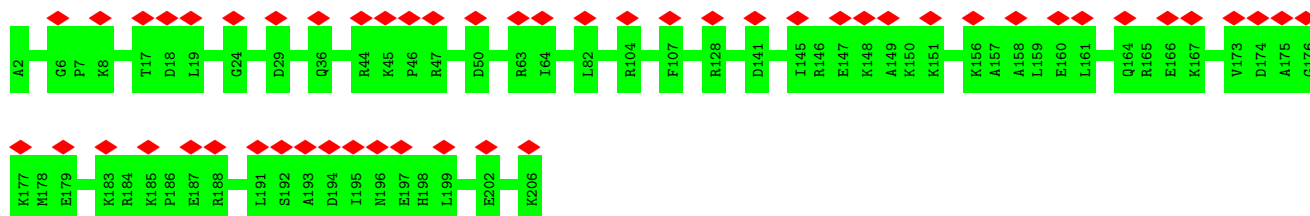




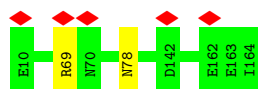
- Molecule 3: 30S ribosomal protein S3



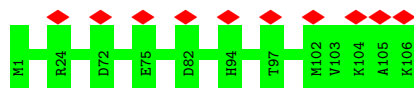
- Molecule 4: 30S ribosomal protein S4



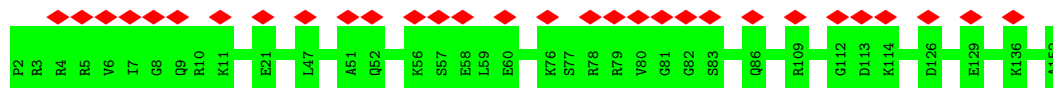
- Molecule 5: 30S ribosomal protein S5



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

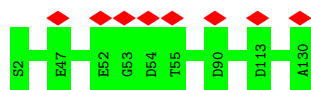


- Molecule 7: 30S ribosomal protein S7

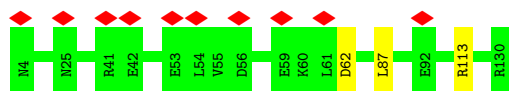


- Molecule 8: 30S ribosomal protein S8

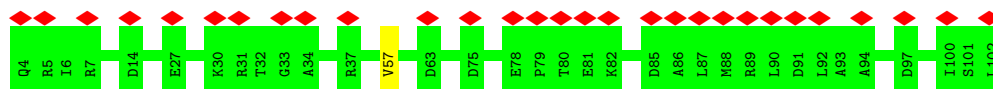




- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10



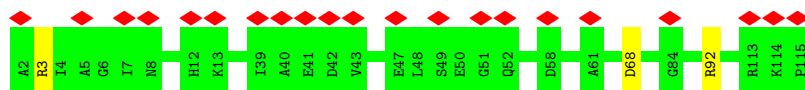
- Molecule 11: 30S ribosomal protein S11



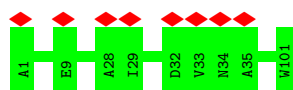
- Molecule 12: 30S ribosomal protein S12



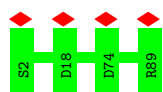
- Molecule 13: 30S ribosomal protein S13



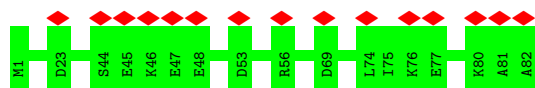
- Molecule 14: 30S ribosomal protein S14



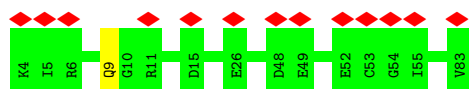
- Molecule 15: 30S ribosomal protein S15



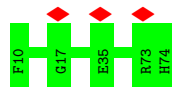
- Molecule 16: 30S ribosomal protein S16



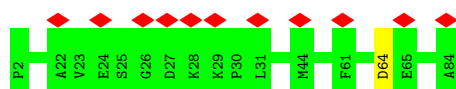
- Molecule 17: 30S ribosomal protein S17



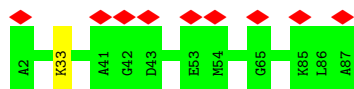
- Molecule 18: 30S ribosomal protein S18



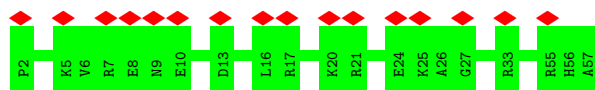
- Molecule 19: 30S ribosomal protein S19



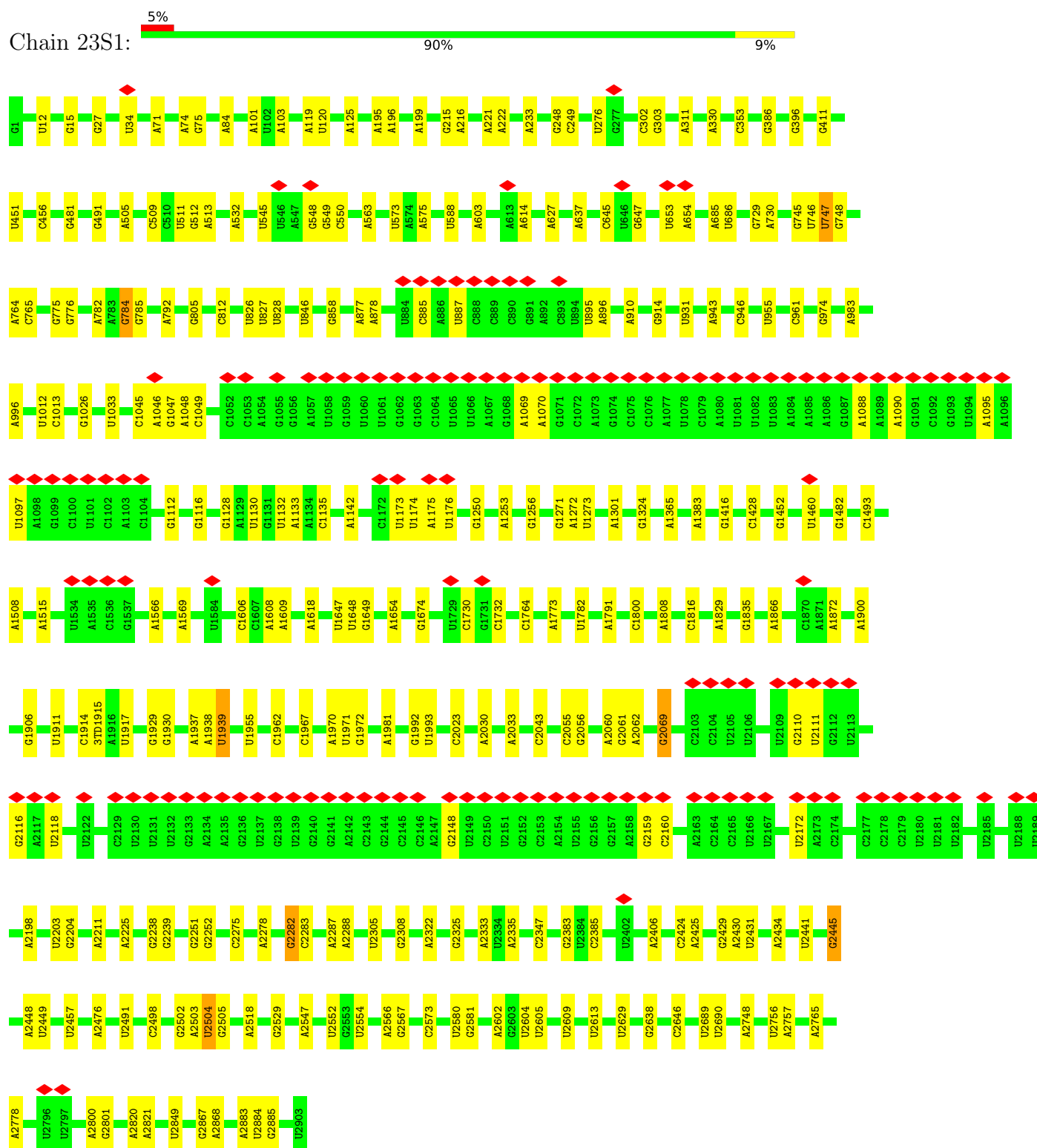
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21

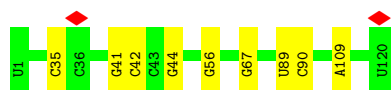


- Molecule 22: 23S ribosomal RNA

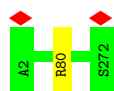


- Molecule 23: 5S ribosomal RNA

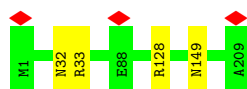




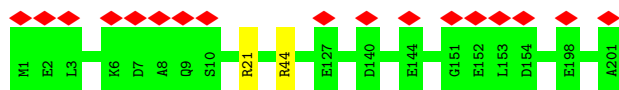
- Molecule 24: 50S ribosomal protein L2



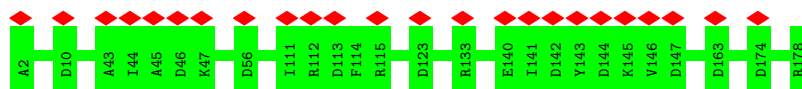
- Molecule 25: 50S ribosomal protein L3



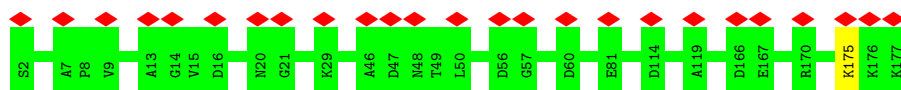
- Molecule 26: 50S ribosomal protein L4



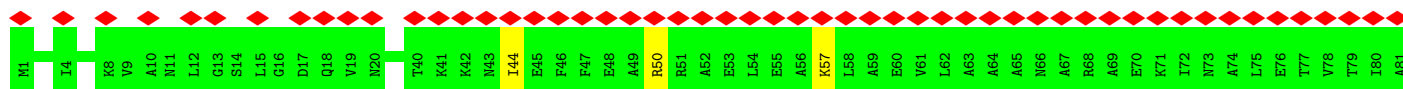
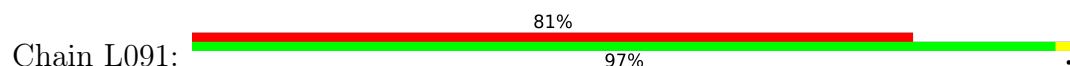
- Molecule 27: 50S ribosomal protein L5

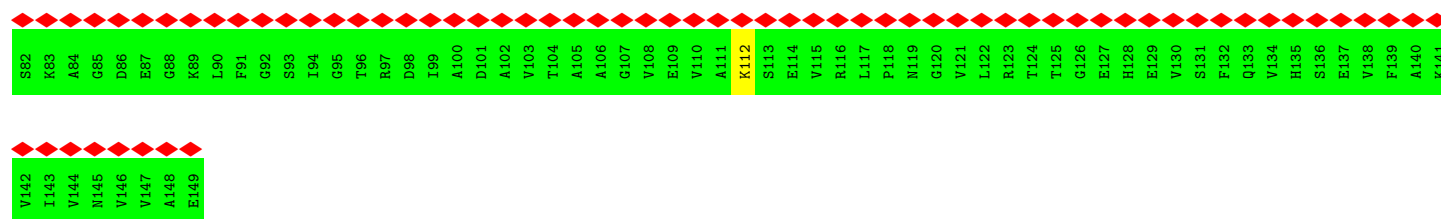


- Molecule 28: 50S ribosomal protein L6



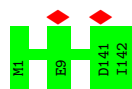
- Molecule 29: 50S ribosomal protein L9





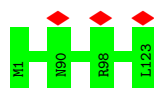
- Molecule 30: 50S ribosomal protein L13

Chain L131:  100%



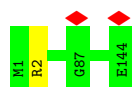
- Molecule 31: 50S ribosomal protein L14

Chain L141:  100%



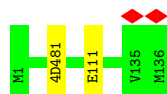
- Molecule 32: 50S ribosomal protein L15

Chain L151:  99%



- Molecule 33: 50S ribosomal protein L16

Chain L161:  99%



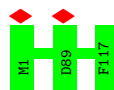
- Molecule 34: 50S ribosomal protein L17

Chain L171:  99%

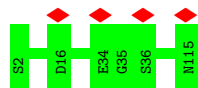


- Molecule 35: 50S ribosomal protein L18

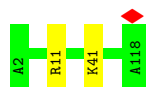
Chain L181:  100%



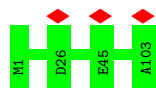
- Molecule 36: 50S ribosomal protein L19



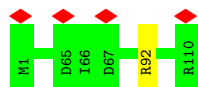
- Molecule 37: 50S ribosomal protein L20



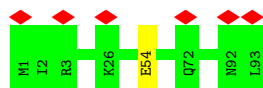
- Molecule 38: 50S ribosomal protein L21



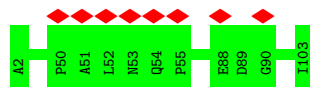
- Molecule 39: 50S ribosomal protein L22



- Molecule 40: 50S ribosomal protein L23

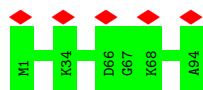


- Molecule 41: 50S ribosomal protein L24

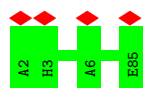


- Molecule 42: 50S ribosomal protein L25





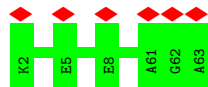
- Molecule 43: 50S ribosomal protein L27



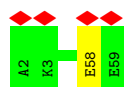
- Molecule 44: 50S ribosomal protein L28



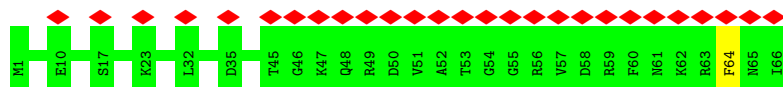
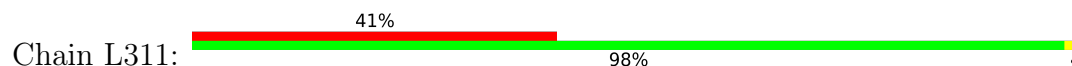
- Molecule 45: 50S ribosomal protein L29



- Molecule 46: 50S ribosomal protein L30



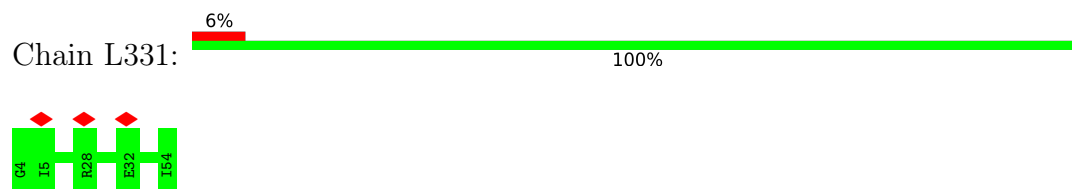
- Molecule 47: 50S ribosomal protein L31



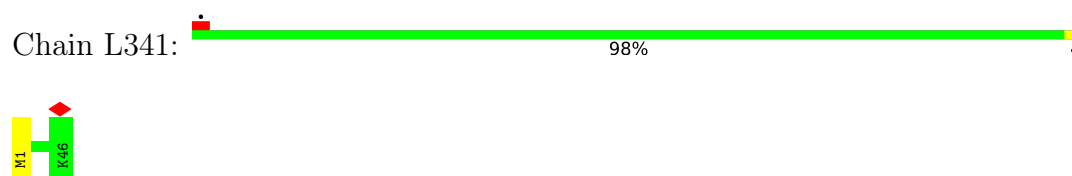
- Molecule 48: 50S ribosomal protein L32



- Molecule 49: 50S ribosomal protein L33



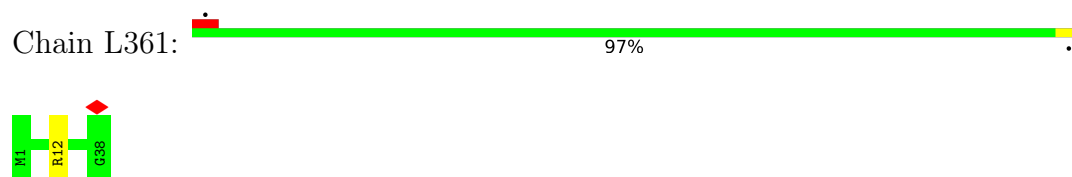
- Molecule 50: 50S ribosomal protein L34



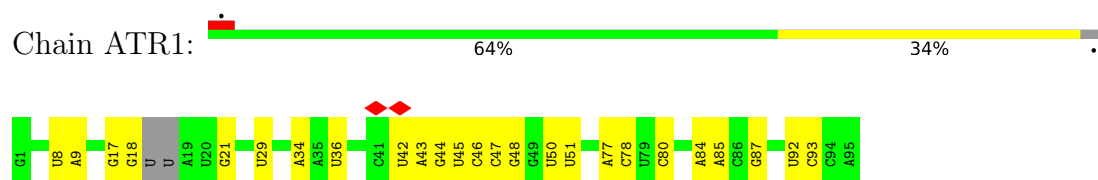
- Molecule 51: 50S ribosomal protein L35



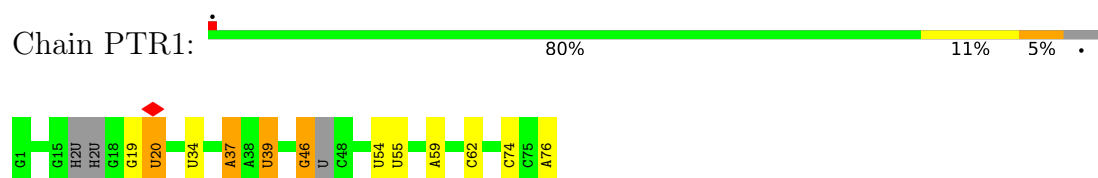
- Molecule 52: 50S ribosomal protein L36



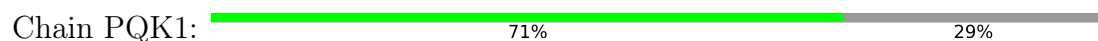
- Molecule 53: tRNA-Cys



- Molecule 54: tRNA-Lys

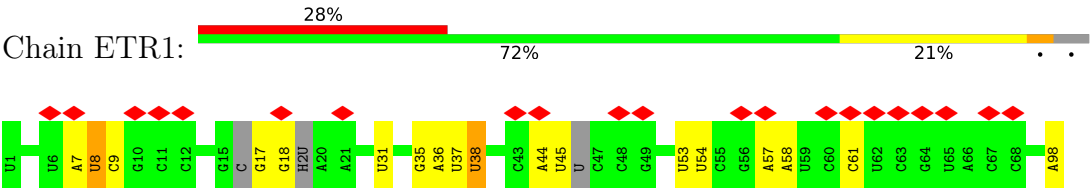


- Molecule 55: MAAAPQK nascent peptide

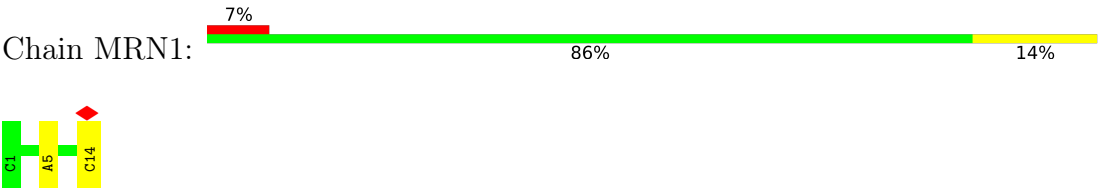




• Molecule 56: tRNA-Gln



• Molecule 57: mRNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	86672	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	35.71	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	26.007	Depositor
Minimum map value	-12.528	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.8	Depositor
Map size ( $\text{\AA}$ )	369.24, 369.24, 369.24	wwPDB
Map dimensions	408, 408, 408	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.905, 0.905, 0.905	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, D2T, 4SU, H2U, MG, PSU, 3TD, OCW, ZN, 4D4, MIA, 5MU, T6A, MA6, 2MA, U8U, 6MZ, K, 1MG, 2MG, 4OC, OMG, UR3, OMC, 5MC, MEQ, G7M

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	16S1	0.70	0/36593	0.89	3/57081 (0.0%)
2	S021	0.28	0/1784	0.52	0/2403
3	S031	0.31	0/1652	0.55	0/2225
4	S041	0.29	0/1665	0.57	0/2227
5	S051	0.34	0/1157	0.58	0/1557
6	S061	0.33	0/881	0.54	0/1189
7	S071	0.28	0/1196	0.58	0/1602
8	S081	0.32	0/989	0.55	0/1326
9	S091	0.31	0/1034	0.62	0/1375
10	S101	0.29	0/806	0.60	0/1089
11	S111	0.33	0/893	0.60	0/1205
12	S121	0.33	0/960	0.62	0/1286
13	S131	0.29	0/893	0.61	0/1193
14	S141	0.29	0/811	0.60	0/1081
15	S151	0.32	0/722	0.59	0/964
16	S161	0.30	0/659	0.58	0/884
17	S171	0.31	0/658	0.54	0/881
18	S181	0.35	0/545	0.58	0/731
19	S191	0.29	0/680	0.55	0/915
20	S201	0.28	0/676	0.51	0/895
21	S211	0.32	0/472	0.61	0/627
22	23S1	0.96	0/69239	0.91	6/108014 (0.0%)
23	05S1	0.75	0/2872	0.82	0/4478
24	L021	0.42	0/2122	0.62	0/2852
25	L031	0.40	0/1576	0.56	0/2119
26	L041	0.37	0/1571	0.53	0/2113
27	L051	0.32	0/1435	0.54	0/1926
28	L061	0.31	0/1343	0.53	0/1816
29	L091	0.27	0/1121	0.49	0/1515
30	L131	0.41	0/1152	0.54	0/1551
31	L141	0.38	0/955	0.60	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	L151	0.37	0/1062	0.62	0/1413
33	L161	0.40	0/1081	0.58	0/1443
34	L171	0.41	0/958	0.62	0/1281
35	L181	0.34	0/910	0.58	0/1219
36	L191	0.40	0/929	0.59	0/1242
37	L201	0.48	0/960	0.61	0/1278
38	L211	0.41	0/829	0.56	0/1107
39	L221	0.35	0/864	0.56	0/1156
40	L231	0.36	0/745	0.53	0/994
41	L241	0.33	0/788	0.52	0/1051
42	L251	0.35	0/766	0.51	0/1025
43	L271	0.40	0/642	0.58	0/848
44	L281	0.38	0/635	0.62	0/848
45	L291	0.29	0/502	0.53	0/667
46	L301	0.35	0/453	0.60	0/605
47	L311	0.29	0/531	0.54	0/709
48	L321	0.41	0/450	0.62	0/599
49	L331	0.37	0/421	0.55	0/561
50	L341	0.40	0/380	0.76	0/498
51	L351	0.38	0/513	0.60	0/676
52	L361	0.40	0/303	0.60	0/397
53	ATR1	0.62	0/1575	0.99	0/2450
54	PTR1	0.63	0/1572	0.91	0/2441
55	PQK1	0.32	0/35	0.43	0/46
56	ETR1	0.48	0/1527	1.01	0/2374
57	MRN1	0.64	0/339	0.83	0/527
All	All	0.75	0/158882	0.83	9/237854 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	784	G	O5'-P-OP2	8.06	120.37	110.70
1	16S1	412	A	O4'-C1'-N9	6.83	113.66	108.20
22	23S1	195	A	N9-C4-C5	6.21	108.28	105.80
22	23S1	2638	G	O4'-C1'-N9	5.36	112.48	108.20
1	16S1	60	A	C8-N9-C4	-5.27	103.69	105.80
1	16S1	880	C	N1-C2-O2	-5.06	115.86	118.90
22	23S1	27	G	O4'-C1'-N9	5.05	112.24	108.20
22	23S1	1324	G	O4'-C1'-N9	5.04	112.23	108.20
22	23S1	2282	G	O4'-C1'-N9	5.04	112.23	108.20

There are no chirality outliers.

There are no planarity outliers.

## 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	16S1	32930	0	0	0	0
2	S021	1753	0	0	0	0
3	S031	1625	0	0	0	0
4	S041	1643	0	0	0	0
5	S051	1144	0	0	0	0
6	S061	862	0	0	0	0
7	S071	1182	0	0	0	0
8	S081	979	0	0	0	0
9	S091	1022	0	0	0	0
10	S101	796	0	0	0	0
11	S111	877	0	0	0	0
12	S121	957	0	0	0	0
13	S131	884	0	0	0	0
14	S141	799	0	0	0	0
15	S151	714	0	0	0	0
16	S161	649	0	0	0	0
17	S171	649	0	0	0	0
18	S181	536	0	0	0	0
19	S191	663	0	0	0	0
20	S201	670	0	0	0	0
21	S211	465	0	0	0	0
22	23S1	62334	0	0	0	0
23	05S1	2569	0	0	0	0
24	L021	2083	0	0	0	0
25	L031	1566	0	0	0	0
26	L041	1552	0	0	0	0
27	L051	1411	0	0	0	0
28	L061	1323	0	0	0	0
29	L091	1110	0	0	0	0
30	L131	1129	0	0	0	0
31	L141	946	0	0	0	0
32	L151	1053	0	0	0	0
33	L161	1075	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	L171	945	0	0	0	0
35	L181	900	0	0	0	0
36	L191	917	0	0	0	0
37	L201	947	0	0	0	0
38	L211	816	0	0	0	0
39	L221	857	0	0	0	0
40	L231	739	0	0	0	0
41	L241	780	0	0	0	0
42	L251	753	0	0	0	0
43	L271	634	0	0	0	0
44	L281	625	0	0	0	0
45	L291	501	0	0	0	0
46	L301	449	0	0	0	0
47	L311	522	0	0	0	0
48	L321	444	0	0	0	0
49	L331	414	0	0	0	0
50	L341	377	0	0	0	0
51	L351	504	0	0	0	0
52	L361	302	0	0	0	0
53	ATR1	1540	0	0	0	0
54	PTR1	1569	0	0	0	0
55	PQK1	35	0	0	0	0
56	ETR1	1537	0	0	0	0
57	MRN1	303	0	0	0	0
58	05S1	1	0	0	0	0
58	16S1	76	0	0	0	0
58	23S1	209	0	0	0	0
58	L021	1	0	0	0	0
58	L031	1	0	0	0	0
58	L041	1	0	0	0	0
59	05S1	1	0	0	0	0
59	16S1	31	0	0	0	0
59	23S1	81	0	0	0	0
59	L021	1	0	0	0	0
59	S131	1	0	0	0	0
60	L311	1	0	0	0	0
60	L361	1	0	0	0	0
60	S021	1	0	0	0	0
61	23S1	35	0	0	0	0
62	ATR1	6	0	0	0	0
63	ETR1	9	0	0	0	0
64	05S1	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	16S1	147	0	0	0	0
64	23S1	604	0	0	0	0
64	L021	7	0	0	0	0
64	L031	4	0	0	0	0
64	L131	1	0	0	0	0
64	L171	4	0	0	0	0
64	S111	1	0	0	0	0
64	S141	2	0	0	0	0
All	All	148592	0	0	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S021	222/224 (99%)	217 (98%)	5 (2%)	0	100	100
3	S031	204/206 (99%)	202 (99%)	2 (1%)	0	100	100
4	S041	203/205 (99%)	201 (99%)	2 (1%)	0	100	100
5	S051	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
6	S061	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
7	S071	149/151 (99%)	146 (98%)	3 (2%)	0	100	100
8	S081	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
9	S091	125/127 (98%)	119 (95%)	6 (5%)	0	100	100
10	S101	97/99 (98%)	96 (99%)	0	1 (1%)	13	33
11	S111	115/117 (98%)	111 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	S121	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
13	S131	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
14	S141	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
15	S151	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
16	S161	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
17	S171	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
18	S181	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
19	S191	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
20	S201	84/86 (98%)	84 (100%)	0	0	100	100
21	S211	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
24	L021	269/271 (99%)	259 (96%)	10 (4%)	0	100	100
25	L031	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	25	49
26	L041	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
27	L051	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
28	L061	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
29	L091	147/149 (99%)	141 (96%)	6 (4%)	0	100	100
30	L131	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
31	L141	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
32	L151	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
33	L161	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
34	L171	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
35	L181	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
36	L191	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
37	L201	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
38	L211	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
39	L221	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
40	L231	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
41	L241	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
42	L251	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
43	L271	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
44	L281	75/77 (97%)	74 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	L291	60/62 (97%)	60 (100%)	0	0	100	100
46	L301	56/58 (97%)	56 (100%)	0	0	100	100
47	L311	64/66 (97%)	62 (97%)	2 (3%)	0	100	100
48	L321	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
49	L331	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
50	L341	44/46 (96%)	44 (100%)	0	0	100	100
51	L351	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
52	L361	36/38 (95%)	36 (100%)	0	0	100	100
55	PQK1	3/7 (43%)	3 (100%)	0	0	100	100
All	All	5597/5702 (98%)	5466 (98%)	129 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	L031	149	ASN
10	S101	57	VAL

### 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	
2	S021	186/186 (100%)	183 (98%)	3 (2%)	58	82
3	S031	170/170 (100%)	168 (99%)	2 (1%)	67	86
4	S041	172/172 (100%)	172 (100%)	0	100	100
5	S051	118/118 (100%)	116 (98%)	2 (2%)	56	81
6	S061	92/92 (100%)	92 (100%)	0	100	100
7	S071	124/124 (100%)	124 (100%)	0	100	100
8	S081	104/104 (100%)	104 (100%)	0	100	100
9	S091	105/105 (100%)	102 (97%)	3 (3%)	37	67
10	S101	87/87 (100%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	S111	90/90 (100%)	89 (99%)	1 (1%)	70	87
12	S121	102/102 (100%)	102 (100%)	0	100	100
13	S131	92/92 (100%)	89 (97%)	3 (3%)	33	62
14	S141	79/83 (95%)	79 (100%)	0	100	100
15	S151	76/76 (100%)	76 (100%)	0	100	100
16	S161	65/65 (100%)	65 (100%)	0	100	100
17	S171	74/74 (100%)	73 (99%)	1 (1%)	62	84
18	S181	56/56 (100%)	56 (100%)	0	100	100
19	S191	72/72 (100%)	71 (99%)	1 (1%)	62	84
20	S201	65/65 (100%)	64 (98%)	1 (2%)	60	83
21	S211	48/48 (100%)	48 (100%)	0	100	100
24	L021	216/216 (100%)	215 (100%)	1 (0%)	86	95
25	L031	163/163 (100%)	160 (98%)	3 (2%)	54	80
26	L041	165/165 (100%)	163 (99%)	2 (1%)	67	86
27	L051	148/148 (100%)	148 (100%)	0	100	100
28	L061	137/137 (100%)	136 (99%)	1 (1%)	81	93
29	L091	114/114 (100%)	110 (96%)	4 (4%)	31	60
30	L131	116/116 (100%)	116 (100%)	0	100	100
31	L141	104/104 (100%)	104 (100%)	0	100	100
32	L151	103/103 (100%)	102 (99%)	1 (1%)	73	89
33	L161	108/108 (100%)	107 (99%)	1 (1%)	75	90
34	L171	98/98 (100%)	97 (99%)	1 (1%)	73	89
35	L181	87/87 (100%)	87 (100%)	0	100	100
36	L191	99/99 (100%)	99 (100%)	0	100	100
37	L201	89/89 (100%)	87 (98%)	2 (2%)	47	76
38	L211	84/84 (100%)	84 (100%)	0	100	100
39	L221	93/93 (100%)	92 (99%)	1 (1%)	70	87
40	L231	80/80 (100%)	79 (99%)	1 (1%)	65	85
41	L241	83/83 (100%)	83 (100%)	0	100	100
42	L251	78/78 (100%)	78 (100%)	0	100	100
43	L271	62/62 (100%)	62 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	L281	67/67 (100%)	65 (97%)	2 (3%)	36	65
45	L291	54/54 (100%)	54 (100%)	0	100	100
46	L301	48/48 (100%)	47 (98%)	1 (2%)	48	76
47	L311	59/59 (100%)	58 (98%)	1 (2%)	56	81
48	L321	47/47 (100%)	47 (100%)	0	100	100
49	L331	45/46 (98%)	45 (100%)	0	100	100
50	L341	38/38 (100%)	37 (97%)	1 (3%)	41	70
51	L351	51/51 (100%)	50 (98%)	1 (2%)	50	78
52	L361	34/34 (100%)	33 (97%)	1 (3%)	37	67
55	PQK1	3/4 (75%)	3 (100%)	0	100	100
All	All	4650/4656 (100%)	4608 (99%)	42 (1%)	74	90

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S021	23	TRP
2	S021	37	LYS
2	S021	112	LYS
3	S031	70	THR
3	S031	185	ASN
5	S051	69	ARG
5	S051	78	ASN
9	S091	62	ASP
9	S091	87	LEU
9	S091	113	ARG
11	S111	119	ASN
13	S131	3	ARG
13	S131	68	ASP
13	S131	92	ARG
17	S171	9	GLN
19	S191	64	ASP
20	S201	33	LYS
24	L021	80	ARG
25	L031	32	ASN
25	L031	33	ARG
25	L031	128	ARG
26	L041	21	ARG
26	L041	44	ARG

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Mol	Chain	Res	Type
28	L061	175	LYS
29	L091	44	ILE
29	L091	50	ARG
29	L091	57	LYS
29	L091	112	LYS
32	L151	2	ARG
33	L161	111	GLU
34	L171	2	ARG
37	L201	11	ARG
37	L201	41	LYS
39	L221	92	ARG
40	L231	54	GLU
44	L281	27	ARG
44	L281	72	ARG
46	L301	58	GLU
47	L311	64	PHE
50	L341	1	MET
51	L351	31	HIS
52	L361	12	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16S1	1531/1534 (99%)	184 (12%)	15 (0%)
22	23S1	2898/2903 (99%)	250 (8%)	24 (0%)
23	05S1	119/120 (99%)	9 (7%)	1 (0%)
53	ATR1	69/74 (93%)	19 (27%)	3 (4%)
54	PTR1	69/76 (90%)	9 (13%)	2 (2%)
56	ETR1	67/75 (89%)	11 (16%)	2 (2%)
57	MRN1	13/14 (92%)	2 (15%)	0
All	All	4766/4796 (99%)	484 (10%)	47 (0%)

All (484) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16S1	2	A
1	16S1	4	U
1	16S1	5	U

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Mol	Chain	Res	Type
1	16S1	9	G
1	16S1	32	A
1	16S1	47	C
1	16S1	48	C
1	16S1	51	A
1	16S1	66	A
1	16S1	70	U
1	16S1	71	A
1	16S1	72	A
1	16S1	73	C
1	16S1	83	C
1	16S1	84	U
1	16S1	85	U
1	16S1	86	G
1	16S1	87	C
1	16S1	88	U
1	16S1	89	U
1	16S1	94	G
1	16S1	95	C
1	16S1	121	U
1	16S1	130	A
1	16S1	131	A
1	16S1	140	U
1	16S1	141	G
1	16S1	143	A
1	16S1	144	G
1	16S1	159	G
1	16S1	168	G
1	16S1	178	C
1	16S1	181	A
1	16S1	184	G
1	16S1	195	A
1	16S1	197	A
1	16S1	199	A
1	16S1	204	G
1	16S1	219	U
1	16S1	220	G
1	16S1	240	G
1	16S1	244	U
1	16S1	245	U
1	16S1	247	G
1	16S1	251	G

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Mol	Chain	Res	Type
1	16S1	262	A
1	16S1	266	G
1	16S1	267	C
1	16S1	275	G
1	16S1	289	G
1	16S1	328	C
1	16S1	329	A
1	16S1	330	C
1	16S1	341	C
1	16S1	352	C
1	16S1	354	G
1	16S1	367	U
1	16S1	372	C
1	16S1	374	A
1	16S1	375	U
1	16S1	393	A
1	16S1	398	U
1	16S1	406	G
1	16S1	409	U
1	16S1	412	A
1	16S1	413	G
1	16S1	429	U
1	16S1	433	G
1	16S1	434	U
1	16S1	436	C
1	16S1	438	U
1	16S1	439	U
1	16S1	440	C
1	16S1	442	G
1	16S1	443	C
1	16S1	447	G
1	16S1	449	G
1	16S1	468	A
1	16S1	484	G
1	16S1	486	U
1	16S1	511	C
1	16S1	512	U
1	16S1	516	PSU
1	16S1	518	C
1	16S1	527	G7M
1	16S1	531	U
1	16S1	532	A

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Mol	Chain	Res	Type
1	16S1	542	G
1	16S1	547	A
1	16S1	562	U
1	16S1	572	A
1	16S1	573	A
1	16S1	576	C
1	16S1	577	G
1	16S1	588	G
1	16S1	620	C
1	16S1	621	A
1	16S1	632	U
1	16S1	633	G
1	16S1	653	U
1	16S1	665	A
1	16S1	687	A
1	16S1	721	G
1	16S1	724	G
1	16S1	755	G
1	16S1	777	A
1	16S1	793	U
1	16S1	794	A
1	16S1	814	A
1	16S1	815	A
1	16S1	817	C
1	16S1	828	U
1	16S1	841	C
1	16S1	842	U
1	16S1	843	U
1	16S1	844	G
1	16S1	845	A
1	16S1	902	G
1	16S1	926	G
1	16S1	934	C
1	16S1	935	A
1	16S1	960	U
1	16S1	961	U
1	16S1	966	2MG
1	16S1	968	A
1	16S1	969	A
1	16S1	975	A
1	16S1	976	G
1	16S1	977	A

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Mol	Chain	Res	Type
1	16S1	978	A
1	16S1	993	G
1	16S1	1004	A
1	16S1	1007	U
1	16S1	1009	U
1	16S1	1019	A
1	16S1	1020	G
1	16S1	1028	C
1	16S1	1029	U
1	16S1	1030	U
1	16S1	1065	U
1	16S1	1094	G
1	16S1	1095	U
1	16S1	1101	A
1	16S1	1139	G
1	16S1	1140	C
1	16S1	1141	C
1	16S1	1159	U
1	16S1	1196	A
1	16S1	1197	A
1	16S1	1212	U
1	16S1	1213	A
1	16S1	1214	C
1	16S1	1227	A
1	16S1	1228	C
1	16S1	1238	A
1	16S1	1256	A
1	16S1	1279	G
1	16S1	1280	A
1	16S1	1285	A
1	16S1	1299	A
1	16S1	1300	G
1	16S1	1302	C
1	16S1	1317	C
1	16S1	1320	C
1	16S1	1338	G
1	16S1	1346	A
1	16S1	1363	A
1	16S1	1398	A
1	16S1	1403	C
1	16S1	1419	G
1	16S1	1441	A

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Mol	Chain	Res	Type
1	16S1	1447	A
1	16S1	1492	A
1	16S1	1494	G
1	16S1	1497	G
1	16S1	1499	A
1	16S1	1503	A
1	16S1	1505	G
1	16S1	1506	U
1	16S1	1513	A
1	16S1	1517	G
1	16S1	1529	G
1	16S1	1530	G
1	16S1	1532	U
22	23S1	12	U
22	23S1	15	G
22	23S1	34	U
22	23S1	71	A
22	23S1	74	A
22	23S1	75	G
22	23S1	84	A
22	23S1	101	A
22	23S1	103	A
22	23S1	119	A
22	23S1	120	U
22	23S1	196	A
22	23S1	199	A
22	23S1	215	G
22	23S1	216	A
22	23S1	221	A
22	23S1	222	A
22	23S1	233	A
22	23S1	248	G
22	23S1	276	U
22	23S1	302	C
22	23S1	303	G
22	23S1	311	A
22	23S1	330	A
22	23S1	353	C
22	23S1	386	G
22	23S1	396	G
22	23S1	411	G
22	23S1	451	U

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Mol	Chain	Res	Type
22	23S1	456	C
22	23S1	481	G
22	23S1	491	G
22	23S1	505	A
22	23S1	509	C
22	23S1	511	U
22	23S1	512	G
22	23S1	513	A
22	23S1	532	A
22	23S1	545	U
22	23S1	549	G
22	23S1	550	C
22	23S1	563	A
22	23S1	573	U
22	23S1	575	A
22	23S1	588	U
22	23S1	603	A
22	23S1	614	A
22	23S1	627	A
22	23S1	637	A
22	23S1	645	C
22	23S1	647	G
22	23S1	653	U
22	23S1	654	A
22	23S1	685	A
22	23S1	686	U
22	23S1	729	G
22	23S1	730	A
22	23S1	747	5MU
22	23S1	748	G
22	23S1	764	A
22	23S1	765	C
22	23S1	775	G
22	23S1	776	G
22	23S1	782	A
22	23S1	784	G
22	23S1	785	G
22	23S1	792	A
22	23S1	805	G
22	23S1	812	C
22	23S1	826	U
22	23S1	827	U

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Mol	Chain	Res	Type
22	23S1	828	U
22	23S1	846	U
22	23S1	858	G
22	23S1	877	A
22	23S1	878	A
22	23S1	885	C
22	23S1	887	U
22	23S1	896	A
22	23S1	910	A
22	23S1	914	G
22	23S1	931	U
22	23S1	943	A
22	23S1	946	C
22	23S1	961	C
22	23S1	974	G
22	23S1	983	A
22	23S1	996	A
22	23S1	1012	U
22	23S1	1013	C
22	23S1	1026	G
22	23S1	1033	U
22	23S1	1045	C
22	23S1	1046	A
22	23S1	1047	G
22	23S1	1048	A
22	23S1	1049	C
22	23S1	1069	A
22	23S1	1070	A
22	23S1	1088	A
22	23S1	1090	A
22	23S1	1095	A
22	23S1	1097	U
22	23S1	1112	G
22	23S1	1116	G
22	23S1	1130	U
22	23S1	1132	U
22	23S1	1133	A
22	23S1	1135	C
22	23S1	1142	A
22	23S1	1173	U
22	23S1	1174	U
22	23S1	1175	A

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Mol	Chain	Res	Type
22	23S1	1176	U
22	23S1	1250	G
22	23S1	1253	A
22	23S1	1256	G
22	23S1	1271	G
22	23S1	1272	A
22	23S1	1273	U
22	23S1	1301	A
22	23S1	1365	A
22	23S1	1383	A
22	23S1	1416	G
22	23S1	1428	C
22	23S1	1452	G
22	23S1	1460	U
22	23S1	1482	G
22	23S1	1493	C
22	23S1	1508	A
22	23S1	1515	A
22	23S1	1566	A
22	23S1	1569	A
22	23S1	1606	C
22	23S1	1608	A
22	23S1	1609	A
22	23S1	1647	U
22	23S1	1648	U
22	23S1	1649	G
22	23S1	1654	A
22	23S1	1674	G
22	23S1	1730	C
22	23S1	1732	C
22	23S1	1764	C
22	23S1	1773	A
22	23S1	1782	U
22	23S1	1791	A
22	23S1	1800	C
22	23S1	1808	A
22	23S1	1816	C
22	23S1	1829	A
22	23S1	1866	A
22	23S1	1872	A
22	23S1	1906	G
22	23S1	1914	C

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Mol	Chain	Res	Type
22	23S1	1929	G
22	23S1	1930	G
22	23S1	1937	A
22	23S1	1938	A
22	23S1	1939	5MU
22	23S1	1955	U
22	23S1	1967	C
22	23S1	1970	A
22	23S1	1971	U
22	23S1	1972	G
22	23S1	1981	A
22	23S1	1992	G
22	23S1	1993	U
22	23S1	2023	C
22	23S1	2033	A
22	23S1	2043	C
22	23S1	2055	C
22	23S1	2056	G
22	23S1	2060	A
22	23S1	2061	G
22	23S1	2062	A
22	23S1	2069	G7M
22	23S1	2110	G
22	23S1	2111	U
22	23S1	2116	G
22	23S1	2118	U
22	23S1	2148	G
22	23S1	2159	G
22	23S1	2160	C
22	23S1	2172	U
22	23S1	2198	A
22	23S1	2203	U
22	23S1	2204	G
22	23S1	2211	A
22	23S1	2225	A
22	23S1	2238	G
22	23S1	2239	G
22	23S1	2252	G
22	23S1	2278	A
22	23S1	2283	C
22	23S1	2287	A
22	23S1	2288	A

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Mol	Chain	Res	Type
22	23S1	2305	U
22	23S1	2308	G
22	23S1	2322	A
22	23S1	2325	G
22	23S1	2333	A
22	23S1	2335	A
22	23S1	2347	C
22	23S1	2383	G
22	23S1	2385	C
22	23S1	2406	A
22	23S1	2424	C
22	23S1	2425	A
22	23S1	2429	G
22	23S1	2430	A
22	23S1	2431	U
22	23S1	2434	A
22	23S1	2441	U
22	23S1	2445	2MG
22	23S1	2448	A
22	23S1	2476	A
22	23S1	2491	U
22	23S1	2502	G
22	23S1	2504	PSU
22	23S1	2505	G
22	23S1	2518	A
22	23S1	2529	G
22	23S1	2547	A
22	23S1	2554	U
22	23S1	2566	A
22	23S1	2567	G
22	23S1	2573	C
22	23S1	2581	G
22	23S1	2602	A
22	23S1	2609	U
22	23S1	2613	U
22	23S1	2629	U
22	23S1	2646	C
22	23S1	2689	U
22	23S1	2690	U
22	23S1	2748	A
22	23S1	2757	A
22	23S1	2765	A

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Mol	Chain	Res	Type
22	23S1	2778	A
22	23S1	2800	A
22	23S1	2801	G
22	23S1	2820	A
22	23S1	2821	A
22	23S1	2849	U
22	23S1	2867	G
22	23S1	2868	A
22	23S1	2883	A
22	23S1	2884	U
22	23S1	2885	G
23	05S1	35	C
23	05S1	41	G
23	05S1	42	C
23	05S1	44	G
23	05S1	56	G
23	05S1	67	G
23	05S1	89	U
23	05S1	90	C
23	05S1	109	A
53	ATR1	9	A
53	ATR1	17	G
53	ATR1	18	G
53	ATR1	21	G
53	ATR1	42	U
53	ATR1	43	A
53	ATR1	44	G
53	ATR1	45	U
53	ATR1	46	C
53	ATR1	47	C
53	ATR1	48	G
53	ATR1	77	A
53	ATR1	78	C
53	ATR1	80	C
53	ATR1	84	A
53	ATR1	85	A
53	ATR1	87	G
53	ATR1	92	U
53	ATR1	93	C
54	PTR1	19	G
54	PTR1	20	H2U
54	PTR1	37	T6A

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Mol	Chain	Res	Type
54	PTR1	39	PSU
54	PTR1	46	G7M
54	PTR1	59	A
54	PTR1	62	C
54	PTR1	74	C
54	PTR1	76	A
56	ETR1	7	A
56	ETR1	8	4SU
56	ETR1	9	C
56	ETR1	18	G
56	ETR1	35	G
56	ETR1	38	PSU
56	ETR1	45	U
56	ETR1	57	A
56	ETR1	58	A
56	ETR1	61	C
56	ETR1	98	A
57	MRN1	5	A
57	MRN1	14	C

All (47) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	16S1	1	A
1	16S1	70	U
1	16S1	85	U
1	16S1	195	A
1	16S1	243	A
1	16S1	328	C
1	16S1	438	U
1	16S1	442	G
1	16S1	446	G
1	16S1	575	G
1	16S1	793	U
1	16S1	844	G
1	16S1	1006	G
1	16S1	1224	U
1	16S1	1493	A
22	23S1	125	A
22	23S1	199	A
22	23S1	249	C
22	23S1	548	G

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Mol	Chain	Res	Type
22	23S1	685	A
22	23S1	764	A
22	23S1	784	G
22	23S1	827	U
22	23S1	895	U
22	23S1	1047	G
22	23S1	1069	A
22	23S1	1128	G
22	23S1	1142	A
22	23S1	1175	A
22	23S1	1608	A
22	23S1	1647	U
22	23S1	1900	A
22	23S1	2110	G
22	23S1	2275	C
22	23S1	2282	G
22	23S1	2430	A
22	23S1	2581	G
22	23S1	2756	U
22	23S1	2867	G
23	05S1	41	G
53	ATR1	42	U
53	ATR1	46	C
53	ATR1	84	A
54	PTR1	19	G
54	PTR1	59	A
56	ETR1	44	A
56	ETR1	57	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
53	MIA	ATR1	34	53	24,31,32	2.53	4 (16%)	26,44,47	2.54	8 (30%)
1	2MG	16S1	966	1	18,26,27	2.14	6 (33%)	16,38,41	1.41	3 (18%)
1	MA6	16S1	1518	1	18,26,27	1.27	2 (11%)	19,38,41	2.00	2 (10%)
1	UR3	16S1	1498	1	19,22,23	2.93	8 (42%)	26,32,35	1.32	2 (7%)
22	PSU	23S1	955	22	18,21,22	3.96	6 (33%)	22,30,33	2.83	6 (27%)
54	T6A	PTR1	37	54	27,34,35	2.23	6 (22%)	29,49,52	2.09	5 (17%)
54	U8U	PTR1	34	54,57	19,24,25	2.46	6 (31%)	23,34,37	1.27	4 (17%)
22	2MA	23S1	2503	22,59,58	17,25,26	2.35	5 (29%)	17,37,40	1.39	4 (23%)
22	1MG	23S1	745	22	18,26,27	2.41	5 (27%)	19,39,42	1.41	3 (15%)
1	4OC	16S1	1402	1,58	20,23,24	2.95	8 (40%)	26,32,35	0.88	1 (3%)
33	4D4	L161	81	33	9,11,12	2.48	3 (33%)	8,13,15	0.86	0
22	OMG	23S1	2251	22,59,54	18,26,27	2.34	8 (44%)	19,38,41	1.53	4 (21%)
53	PSU	ATR1	36	53	18,21,22	4.15	6 (33%)	22,30,33	2.70	5 (22%)
22	PSU	23S1	746	22,58	18,21,22	4.00	8 (44%)	22,30,33	2.53	5 (22%)
56	4SU	ETR1	8	56	18,21,22	3.64	8 (44%)	26,30,33	2.29	4 (15%)
1	PSU	16S1	516	1,58	18,21,22	4.16	8 (44%)	22,30,33	2.43	5 (22%)
1	5MC	16S1	967	1	18,22,23	3.45	7 (38%)	26,32,35	1.03	1 (3%)
1	2MG	16S1	1516	1	18,26,27	2.06	6 (33%)	16,38,41	1.46	4 (25%)
22	PSU	23S1	2580	22,59	18,21,22	3.90	7 (38%)	22,30,33	2.77	6 (27%)
54	H2U	PTR1	20	54	18,21,22	1.16	2 (11%)	21,30,33	0.98	2 (9%)
53	PSU	ATR1	29	53	18,21,22	4.19	6 (33%)	22,30,33	2.74	6 (27%)
54	PSU	PTR1	55	54	18,21,22	4.21	6 (33%)	22,30,33	2.59	5 (22%)
56	2MA	ETR1	36	56	17,25,26	2.47	4 (23%)	17,37,40	1.14	2 (11%)
1	G7M	16S1	527	1	20,26,27	2.15	7 (35%)	17,39,42	1.17	2 (11%)
12	D2T	S121	89	12	7,9,10	1.01	0	6,11,13	2.83	3 (50%)
22	5MU	23S1	747	22	19,22,23	4.52	7 (36%)	28,32,35	3.92	10 (35%)
56	5MU	ETR1	53	56	19,22,23	3.72	6 (31%)	28,32,35	4.39	10 (35%)
22	2MG	23S1	2445	22	18,26,27	1.97	6 (33%)	16,38,41	1.51	4 (25%)
53	5MU	ATR1	50	53	19,22,23	3.65	7 (36%)	28,32,35	4.56	10 (35%)
25	MEQ	L031	150	25	8,9,10	0.92	0	5,10,12	0.74	0
22	PSU	23S1	1917	22	18,21,22	4.11	6 (33%)	22,30,33	2.71	5 (22%)
56	PSU	ETR1	38	56	18,21,22	4.28	7 (38%)	22,30,33	2.56	5 (22%)
53	PSU	ATR1	51	53	18,21,22	4.19	7 (38%)	22,30,33	2.72	5 (22%)
22	OMU	23S1	2552	22	19,22,23	2.69	7 (36%)	26,31,34	1.86	6 (23%)
56	OMU	ETR1	31	56	19,22,23	3.00	8 (42%)	26,31,34	1.72	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	G7M	23S1	2069	22,59	20,26,27	2.11	7 (35%)	17,39,42	1.19	1 (5%)
22	PSU	23S1	2604	22	18,21,22	3.89	6 (33%)	22,30,33	2.81	5 (22%)
54	5MU	PTR1	54	54	19,22,23	4.70	7 (36%)	28,32,35	3.63	9 (32%)
22	PSU	23S1	2457	22	18,21,22	3.87	7 (38%)	22,30,33	2.89	5 (22%)
54	PSU	PTR1	39	54	18,21,22	4.13	7 (38%)	22,30,33	2.62	5 (22%)
56	OMG	ETR1	17	56	18,26,27	2.36	7 (38%)	19,38,41	1.79	5 (26%)
22	5MU	23S1	1939	22,59	19,22,23	4.64	7 (36%)	28,32,35	3.65	10 (35%)
22	3TD	23S1	1915	22	19,22,23	3.82	6 (31%)	21,32,35	1.80	3 (14%)
1	MA6	16S1	1519	1	18,26,27	1.29	2 (11%)	19,38,41	2.26	2 (10%)
22	5MC	23S1	1962	22,59	18,22,23	3.21	7 (38%)	26,32,35	0.99	2 (7%)
1	2MG	16S1	1207	1,59	18,26,27	2.06	6 (33%)	16,38,41	1.45	3 (18%)
22	6MZ	23S1	1618	22	18,25,26	1.43	3 (16%)	16,36,39	2.08	4 (25%)
22	H2U	23S1	2449	22	18,21,22	0.78	0	21,30,33	0.95	2 (9%)
1	5MC	16S1	1407	1	18,22,23	3.30	7 (38%)	26,32,35	0.95	1 (3%)
22	2MG	23S1	1835	22	18,26,27	1.98	6 (33%)	16,38,41	1.49	4 (25%)
22	PSU	23S1	1911	22	18,21,22	4.09	6 (33%)	22,30,33	2.71	5 (22%)
22	PSU	23S1	2504	22,59	18,21,22	3.90	6 (33%)	22,30,33	2.64	5 (22%)
54	G7M	PTR1	46	54	20,26,27	2.25	7 (35%)	17,39,42	1.08	1 (5%)
22	OMC	23S1	2498	22,58	19,22,23	2.74	7 (36%)	26,31,34	0.84	0
22	PSU	23S1	2605	22	18,21,22	3.94	6 (33%)	22,30,33	2.77	6 (27%)
53	4SU	ATR1	8	53	18,21,22	3.51	8 (44%)	26,30,33	2.20	5 (19%)
56	PSU	ETR1	37	56	18,21,22	4.23	7 (38%)	22,30,33	2.66	5 (22%)
22	6MZ	23S1	2030	22	18,25,26	1.46	3 (16%)	16,36,39	2.16	4 (25%)
56	PSU	ETR1	54	56	18,21,22	4.40	7 (38%)	22,30,33	2.65	5 (22%)

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
53	MIA	ATR1	34	53	-	2/11/33/34	0/3/3/3
1	2MG	16S1	966	1	-	2/5/27/28	0/3/3/3
1	MA6	16S1	1518	1	-	1/7/29/30	0/3/3/3
1	UR3	16S1	1498	1	-	1/7/25/26	0/2/2/2
22	PSU	23S1	955	22	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	T6A	PTR1	37	54	-	4/19/41/42	0/3/3/3
54	U8U	PTR1	34	54,57	-	0/9/28/29	0/2/2/2
22	2MA	23S1	2503	22,59,58	-	2/3/25/26	0/3/3/3
22	1MG	23S1	745	22	-	0/3/25/26	0/3/3/3
1	4OC	16S1	1402	1,58	-	2/9/29/30	0/2/2/2
33	4D4	L161	81	33	-	2/11/12/14	-
22	OMG	23S1	2251	22,59,54	-	0/5/27/28	0/3/3/3
53	PSU	ATR1	36	53	-	0/7/25/26	0/2/2/2
22	PSU	23S1	746	22,58	-	1/7/25/26	0/2/2/2
56	4SU	ETR1	8	56	-	0/7/25/26	0/2/2/2
1	PSU	16S1	516	1,58	-	0/7/25/26	0/2/2/2
1	5MC	16S1	967	1	-	0/7/25/26	0/2/2/2
1	2MG	16S1	1516	1	-	0/5/27/28	0/3/3/3
22	PSU	23S1	2580	22,59	-	1/7/25/26	0/2/2/2
54	H2U	PTR1	20	54	-	7/7/38/39	0/2/2/2
53	PSU	ATR1	29	53	-	0/7/25/26	0/2/2/2
54	PSU	PTR1	55	54	-	0/7/25/26	0/2/2/2
56	2MA	ETR1	36	56	-	0/3/25/26	0/3/3/3
1	G7M	16S1	527	1	-	2/3/25/26	0/3/3/3
12	D2T	S121	89	12	-	2/7/12/14	-
22	5MU	23S1	747	22	-	0/7/25/26	0/2/2/2
56	5MU	ETR1	53	56	-	0/7/25/26	0/2/2/2
22	2MG	23S1	2445	22	-	2/5/27/28	0/3/3/3
53	5MU	ATR1	50	53	-	0/7/25/26	0/2/2/2
25	MEQ	L031	150	25	-	2/8/9/11	-
22	PSU	23S1	1917	22	-	0/7/25/26	0/2/2/2
56	PSU	ETR1	38	56	-	2/7/25/26	0/2/2/2
53	PSU	ATR1	51	53	-	0/7/25/26	0/2/2/2
22	OMU	23S1	2552	22	-	0/9/27/28	0/2/2/2
56	OMU	ETR1	31	56	-	2/9/27/28	0/2/2/2
22	G7M	23S1	2069	22,59	-	3/3/25/26	0/3/3/3
22	PSU	23S1	2604	22	-	0/7/25/26	0/2/2/2
54	5MU	PTR1	54	54	-	0/7/25/26	0/2/2/2
22	PSU	23S1	2457	22	-	1/7/25/26	0/2/2/2
54	PSU	PTR1	39	54	-	2/7/25/26	0/2/2/2
56	OMG	ETR1	17	56	-	2/5/27/28	0/3/3/3
22	5MU	23S1	1939	22,59	-	2/7/25/26	0/2/2/2
22	3TD	23S1	1915	22	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	16S1	1519	1	-	2/7/29/30	0/3/3/3
22	5MC	23S1	1962	22,59	-	2/7/25/26	0/2/2/2
1	2MG	16S1	1207	1,59	-	0/5/27/28	0/3/3/3
22	6MZ	23S1	1618	22	-	0/5/27/28	0/3/3/3
22	H2U	23S1	2449	22	-	0/7/38/39	0/2/2/2
1	5MC	16S1	1407	1	-	0/7/25/26	0/2/2/2
22	2MG	23S1	1835	22	-	0/5/27/28	0/3/3/3
22	PSU	23S1	1911	22	-	0/7/25/26	0/2/2/2
22	PSU	23S1	2504	22,59	-	2/7/25/26	0/2/2/2
54	G7M	PTR1	46	54	-	1/3/25/26	0/3/3/3
22	OMC	23S1	2498	22,58	-	0/9/27/28	0/2/2/2
22	PSU	23S1	2605	22	-	0/7/25/26	0/2/2/2
53	4SU	ATR1	8	53	-	0/7/25/26	0/2/2/2
56	PSU	ETR1	37	56	-	0/7/25/26	0/2/2/2
22	6MZ	23S1	2030	22	-	2/5/27/28	0/3/3/3
56	PSU	ETR1	54	56	-	0/7/25/26	0/2/2/2

All (345) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	ETR1	54	PSU	C6-C5	12.15	1.49	1.35
56	ETR1	38	PSU	C6-C5	11.73	1.49	1.35
22	23S1	1915	3TD	C6-C5	11.73	1.49	1.35
56	ETR1	37	PSU	C6-C5	11.43	1.48	1.35
53	ATR1	36	PSU	C6-C5	11.43	1.48	1.35
54	PTR1	55	PSU	C6-C5	11.42	1.48	1.35
53	ATR1	29	PSU	C6-C5	11.40	1.48	1.35
54	PTR1	39	PSU	C6-C5	11.35	1.48	1.35
53	ATR1	51	PSU	C6-C5	11.27	1.48	1.35
22	23S1	1917	PSU	C6-C5	11.26	1.48	1.35
22	23S1	1911	PSU	C6-C5	11.20	1.48	1.35
1	16S1	516	PSU	C6-C5	11.04	1.48	1.35
22	23S1	955	PSU	C6-C5	10.89	1.48	1.35
22	23S1	746	PSU	C6-C5	10.86	1.48	1.35
22	23S1	2605	PSU	C6-C5	10.84	1.47	1.35
56	ETR1	53	5MU	C2-N1	10.84	1.55	1.38
22	23S1	2504	PSU	C6-C5	10.77	1.47	1.35
54	PTR1	54	5MU	C2-N1	10.71	1.55	1.38
22	23S1	2457	PSU	C6-C5	10.64	1.47	1.35
22	23S1	2580	PSU	C6-C5	10.62	1.47	1.35
22	23S1	2604	PSU	C6-C5	10.61	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	ATR1	50	5MU	C2-N1	10.23	1.54	1.38
54	PTR1	54	5MU	C6-N1	10.19	1.55	1.38
22	23S1	1939	5MU	C2-N1	10.18	1.54	1.38
22	23S1	1939	5MU	C6-N1	10.01	1.55	1.38
22	23S1	747	5MU	C2-N1	9.75	1.54	1.38
54	PTR1	54	5MU	C4-C5	9.61	1.60	1.44
22	23S1	747	5MU	C6-N1	9.55	1.54	1.38
22	23S1	747	5MU	C4-C5	9.49	1.60	1.44
56	ETR1	54	PSU	C2-N1	9.45	1.49	1.36
56	ETR1	38	PSU	C2-N1	9.40	1.49	1.36
56	ETR1	37	PSU	C2-N1	9.36	1.49	1.36
22	23S1	1939	5MU	C4-C5	9.33	1.60	1.44
53	ATR1	51	PSU	C2-N1	9.26	1.49	1.36
54	PTR1	55	PSU	C2-N1	9.15	1.49	1.36
53	ATR1	29	PSU	C2-N1	9.11	1.49	1.36
53	ATR1	36	PSU	C2-N1	8.98	1.48	1.36
22	23S1	1911	PSU	C2-N1	8.97	1.48	1.36
54	PTR1	39	PSU	C2-N1	8.92	1.48	1.36
1	16S1	516	PSU	C2-N1	8.92	1.48	1.36
22	23S1	1917	PSU	C2-N1	8.85	1.48	1.36
1	16S1	967	5MC	C6-C5	8.78	1.49	1.34
22	23S1	955	PSU	C2-N1	8.75	1.48	1.36
22	23S1	746	PSU	C2-N1	8.74	1.48	1.36
1	16S1	1407	5MC	C6-C5	8.68	1.48	1.34
22	23S1	2605	PSU	C2-N1	8.58	1.48	1.36
22	23S1	1915	3TD	C2-N1	8.47	1.48	1.37
22	23S1	2457	PSU	C2-N1	8.46	1.48	1.36
22	23S1	2504	PSU	C2-N1	8.38	1.48	1.36
22	23S1	2604	PSU	C2-N1	8.34	1.48	1.36
22	23S1	2580	PSU	C2-N1	8.27	1.47	1.36
22	23S1	747	5MU	C4-N3	-8.25	1.23	1.38
22	23S1	1939	5MU	C4-N3	-8.21	1.23	1.38
22	23S1	1962	5MC	C6-C5	8.06	1.47	1.34
1	16S1	1498	UR3	C2-N1	7.95	1.49	1.38
54	PTR1	54	5MU	C4-N3	-7.87	1.24	1.38
56	ETR1	36	2MA	C2-N3	7.69	1.47	1.31
56	ETR1	8	4SU	C4-N3	7.50	1.45	1.37
53	ATR1	34	MIA	C13-C14	7.45	1.53	1.32
53	ATR1	8	4SU	C4-N3	7.34	1.45	1.37
56	ETR1	53	5MU	C6-N1	7.19	1.50	1.38
56	ETR1	54	PSU	C2-N3	7.14	1.49	1.37
54	PTR1	37	T6A	C10-N11	7.03	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	ETR1	53	5MU	C2-N3	7.01	1.50	1.38
53	ATR1	51	PSU	C2-N3	7.01	1.49	1.37
56	ETR1	31	OMU	C2-N1	7.00	1.49	1.38
56	ETR1	37	PSU	C2-N3	7.00	1.49	1.37
22	23S1	2503	2MA	C2-N3	6.99	1.46	1.31
54	PTR1	55	PSU	C2-N3	6.96	1.49	1.37
53	ATR1	29	PSU	C2-N3	6.95	1.49	1.37
1	16S1	516	PSU	C2-N3	6.93	1.49	1.37
53	ATR1	50	5MU	C6-N1	6.90	1.49	1.38
56	ETR1	8	4SU	C2-N1	6.88	1.49	1.38
53	ATR1	50	5MU	C2-N3	6.84	1.50	1.38
56	ETR1	38	PSU	C2-N3	6.84	1.49	1.37
56	ETR1	31	OMU	C2-N3	6.78	1.50	1.38
22	23S1	1917	PSU	C2-N3	6.76	1.49	1.37
53	ATR1	36	PSU	C2-N3	6.70	1.49	1.37
22	23S1	2604	PSU	C2-N3	6.63	1.48	1.37
56	ETR1	8	4SU	C2-N3	6.58	1.49	1.38
53	ATR1	34	MIA	C2-S10	6.57	1.81	1.75
22	23S1	1911	PSU	C2-N3	6.50	1.48	1.37
54	PTR1	39	PSU	C2-N3	6.50	1.48	1.37
53	ATR1	8	4SU	C2-N3	6.47	1.49	1.38
1	16S1	1402	4OC	C4-N3	6.44	1.44	1.32
22	23S1	746	PSU	C2-N3	6.39	1.48	1.37
22	23S1	2580	PSU	C2-N3	6.37	1.48	1.37
53	ATR1	8	4SU	C2-N1	6.30	1.48	1.38
22	23S1	2605	PSU	C2-N3	6.30	1.48	1.37
1	16S1	967	5MC	C4-N3	6.29	1.44	1.34
22	23S1	2504	PSU	C2-N3	6.24	1.48	1.37
22	23S1	955	PSU	C2-N3	6.14	1.48	1.37
22	23S1	2457	PSU	C2-N3	6.06	1.47	1.37
1	16S1	1402	4OC	C6-C5	6.06	1.49	1.35
1	16S1	967	5MC	C2-N3	5.92	1.48	1.36
22	23S1	2552	OMU	C2-N3	5.92	1.48	1.38
22	23S1	2552	OMU	C2-N1	5.90	1.47	1.38
54	PTR1	37	T6A	C6-N6	5.88	1.46	1.36
53	ATR1	34	MIA	C6-N6	5.84	1.45	1.34
22	23S1	1962	5MC	C4-N3	5.83	1.44	1.34
22	23S1	745	1MG	C2-N3	5.77	1.45	1.34
33	L161	81	4D4	CZ-NE	5.71	1.44	1.33
22	23S1	2498	OMC	C2-N3	5.71	1.47	1.36
56	ETR1	8	4SU	C6-C5	5.70	1.48	1.35
1	16S1	1407	5MC	C4-N3	5.68	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	ETR1	17	OMG	C4-N3	5.67	1.51	1.37
22	23S1	1962	5MC	C2-N3	5.67	1.47	1.36
56	ETR1	31	OMU	C6-C5	5.64	1.48	1.35
53	ATR1	50	5MU	C6-C5	-5.61	1.25	1.34
1	16S1	1407	5MC	C2-N3	5.58	1.47	1.36
1	16S1	1402	4OC	C2-N3	5.58	1.47	1.36
22	23S1	2498	OMC	C6-C5	5.56	1.48	1.35
53	ATR1	8	4SU	C6-C5	5.55	1.48	1.35
1	16S1	1498	UR3	C6-C5	5.54	1.47	1.35
22	23S1	1939	5MU	C6-C5	5.53	1.43	1.34
54	PTR1	54	5MU	C6-C5	5.42	1.43	1.34
54	PTR1	34	U8U	C6-C5	5.26	1.49	1.34
56	ETR1	53	5MU	C6-C5	-5.24	1.26	1.34
56	ETR1	17	OMG	C2-N3	5.23	1.45	1.33
54	PTR1	34	U8U	C2-N3	5.21	1.49	1.37
22	23S1	2552	OMU	C6-C5	5.20	1.47	1.35
56	ETR1	54	PSU	C6-N1	5.16	1.44	1.36
56	ETR1	38	PSU	C6-N1	5.04	1.44	1.36
54	PTR1	55	PSU	C6-N1	5.04	1.44	1.36
22	23S1	1915	3TD	C6-N1	5.01	1.44	1.36
54	PTR1	46	G7M	C2-N2	4.99	1.46	1.34
22	23S1	747	5MU	C6-C5	4.93	1.42	1.34
56	ETR1	37	PSU	C6-N1	4.92	1.44	1.36
1	16S1	516	PSU	C6-N1	4.92	1.44	1.36
53	ATR1	51	PSU	C6-N1	4.84	1.44	1.36
1	16S1	966	2MG	C4-N3	4.83	1.49	1.37
54	PTR1	39	PSU	C6-N1	4.82	1.44	1.36
22	23S1	1911	PSU	C6-N1	4.81	1.44	1.36
56	ETR1	8	4SU	C5-C4	4.81	1.48	1.42
53	ATR1	29	PSU	C6-N1	4.81	1.44	1.36
1	16S1	966	2MG	C2-N1	4.78	1.44	1.36
53	ATR1	36	PSU	C6-N1	4.77	1.44	1.36
1	16S1	1207	2MG	C4-N3	4.74	1.48	1.37
22	23S1	1917	PSU	C6-N1	4.74	1.44	1.36
22	23S1	2251	OMG	C2-N3	4.71	1.44	1.33
56	ETR1	36	2MA	C4-N3	4.67	1.48	1.37
1	16S1	527	G7M	C2-N2	4.65	1.45	1.34
22	23S1	745	1MG	C4-N3	4.62	1.48	1.37
56	ETR1	8	4SU	C4-S4	-4.61	1.59	1.68
22	23S1	745	1MG	C2-N2	4.57	1.42	1.34
22	23S1	2069	G7M	C2-N2	4.57	1.45	1.34
22	23S1	955	PSU	C6-N1	4.52	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	ATR1	8	4SU	C4-S4	-4.52	1.59	1.68
22	23S1	2498	OMC	C4-N3	4.51	1.43	1.34
1	16S1	1516	2MG	C2-N1	4.49	1.43	1.36
22	23S1	2251	OMG	C4-N3	4.48	1.48	1.37
53	ATR1	8	4SU	C5-C4	4.46	1.48	1.42
22	23S1	2504	PSU	C6-N1	4.44	1.43	1.36
1	16S1	1207	2MG	C2-N1	4.44	1.43	1.36
22	23S1	2605	PSU	C6-N1	4.43	1.43	1.36
22	23S1	1835	2MG	C4-N3	4.42	1.48	1.37
1	16S1	1498	UR3	C2-N3	4.41	1.47	1.39
22	23S1	2580	PSU	C6-N1	4.40	1.43	1.36
1	16S1	1516	2MG	C4-N3	4.39	1.48	1.37
54	PTR1	46	G7M	C4-N3	4.38	1.48	1.37
22	23S1	2498	OMC	C4-N4	4.37	1.44	1.33
22	23S1	746	PSU	C6-N1	4.35	1.43	1.36
1	16S1	1498	UR3	O4-C4	-4.35	1.14	1.23
54	PTR1	34	U8U	C2-S2	-4.34	1.61	1.67
22	23S1	2503	2MA	C4-N3	4.34	1.47	1.37
22	23S1	1915	3TD	C2-N3	4.34	1.48	1.38
1	16S1	1402	4OC	C4-N4	4.30	1.44	1.35
22	23S1	2445	2MG	C4-N3	4.26	1.47	1.37
22	23S1	2457	PSU	C6-N1	4.26	1.43	1.36
1	16S1	967	5MC	C4-N4	4.25	1.45	1.34
22	23S1	2604	PSU	C6-N1	4.25	1.43	1.36
1	16S1	967	5MC	C6-N1	4.22	1.45	1.38
22	23S1	2251	OMG	C2-N2	4.22	1.44	1.34
54	PTR1	46	G7M	C2-N3	4.16	1.43	1.33
22	23S1	1962	5MC	C4-N4	4.11	1.44	1.34
1	16S1	516	PSU	C4-N3	4.08	1.46	1.38
54	PTR1	34	U8U	C6-N1	4.07	1.45	1.38
56	ETR1	17	OMG	C2-N2	4.06	1.43	1.34
1	16S1	1407	5MC	C4-N4	4.05	1.44	1.34
1	16S1	1407	5MC	C6-N1	4.05	1.45	1.38
56	ETR1	54	PSU	C4-N3	4.00	1.46	1.38
22	23S1	2445	2MG	C2-N1	4.00	1.43	1.36
1	16S1	527	G7M	C4-N3	3.99	1.47	1.37
54	PTR1	55	PSU	C4-N3	3.98	1.46	1.38
22	23S1	1835	2MG	C2-N1	3.97	1.43	1.36
1	16S1	967	5MC	C2-N1	3.97	1.48	1.40
22	23S1	2069	G7M	C4-N3	3.94	1.46	1.37
22	23S1	2498	OMC	C2-N1	3.91	1.48	1.40
56	ETR1	31	OMU	C4-N3	3.88	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1962	5MC	C6-N1	3.87	1.44	1.38
54	PTR1	34	U8U	C4-N3	3.84	1.46	1.38
56	ETR1	38	PSU	C4-N3	3.83	1.46	1.38
56	ETR1	37	PSU	C4-N3	3.81	1.45	1.38
53	ATR1	29	PSU	C4-N3	3.79	1.45	1.38
54	PTR1	37	T6A	C10-N6	3.76	1.45	1.37
1	16S1	1402	4OC	C5-C4	3.73	1.48	1.40
54	PTR1	39	PSU	C4-N3	3.70	1.45	1.38
53	ATR1	36	PSU	C4-N3	3.69	1.45	1.38
22	23S1	2069	G7M	O6-C6	-3.67	1.15	1.23
53	ATR1	51	PSU	C4-N3	3.66	1.45	1.38
1	16S1	527	G7M	C2-N3	3.62	1.42	1.33
22	23S1	1917	PSU	C4-N3	3.59	1.45	1.38
22	23S1	2069	G7M	C2-N3	3.58	1.41	1.33
1	16S1	1407	5MC	C2-N1	3.55	1.47	1.40
22	23S1	746	PSU	C4-N3	3.50	1.45	1.38
1	16S1	966	2MG	C6-N1	3.49	1.43	1.37
22	23S1	1911	PSU	C4-N3	3.48	1.45	1.38
22	23S1	2445	2MG	C5-C4	-3.46	1.34	1.43
1	16S1	1402	4OC	C2-N1	3.45	1.47	1.40
22	23S1	2604	PSU	C4-N3	3.39	1.45	1.38
22	23S1	2504	PSU	C4-N3	3.34	1.45	1.38
22	23S1	2552	OMU	O4-C4	-3.34	1.18	1.24
22	23S1	1962	5MC	C2-N1	3.31	1.47	1.40
22	23S1	745	1MG	C5-C4	-3.31	1.34	1.43
1	16S1	527	G7M	O6-C6	-3.30	1.16	1.23
22	23S1	2552	OMU	C4-N3	3.28	1.44	1.38
22	23S1	1618	6MZ	C2-N3	3.28	1.37	1.32
22	23S1	1835	2MG	C5-C4	-3.27	1.34	1.43
22	23S1	2605	PSU	C4-N3	3.26	1.44	1.38
1	16S1	1516	2MG	C6-N1	3.26	1.42	1.37
22	23S1	2498	OMC	O2-C2	-3.24	1.17	1.23
22	23S1	2580	PSU	C4-N3	3.24	1.44	1.38
54	PTR1	20	H2U	C2-N3	3.24	1.43	1.38
54	PTR1	46	G7M	O6-C6	-3.23	1.16	1.23
1	16S1	1516	2MG	C5-C4	-3.21	1.34	1.43
22	23S1	955	PSU	C4-N3	3.20	1.44	1.38
1	16S1	1402	4OC	O2-C2	-3.19	1.17	1.23
22	23S1	2251	OMG	C5-C4	-3.18	1.35	1.43
54	PTR1	20	H2U	C2-N1	3.17	1.40	1.35
22	23S1	2457	PSU	C4-N3	3.16	1.44	1.38
22	23S1	2030	6MZ	C2-N3	3.11	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	1207	2MG	C6-N1	3.11	1.42	1.37
33	L161	81	4D4	CZ-NH2	3.10	1.44	1.32
56	ETR1	31	OMU	O4-C4	-3.09	1.18	1.24
22	23S1	747	5MU	O2-C2	-3.07	1.17	1.23
22	23S1	1939	5MU	O4-C4	-3.06	1.17	1.23
22	23S1	1835	2MG	C6-N1	3.05	1.42	1.37
1	16S1	1407	5MC	O2-C2	-3.04	1.18	1.23
22	23S1	1962	5MC	O2-C2	-3.04	1.18	1.23
1	16S1	1519	MA6	C5-C4	-3.02	1.32	1.40
1	16S1	1518	MA6	C5-C4	-2.94	1.33	1.40
22	23S1	1939	5MU	O2-C2	-2.92	1.17	1.23
22	23S1	747	5MU	O4-C4	-2.91	1.18	1.23
53	ATR1	34	MIA	C5-C4	-2.90	1.33	1.40
1	16S1	1498	UR3	O2-C2	-2.89	1.17	1.22
1	16S1	966	2MG	C5-C4	-2.89	1.35	1.43
22	23S1	2552	OMU	O2-C2	-2.89	1.17	1.23
22	23S1	2251	OMG	C6-N1	2.88	1.42	1.37
1	16S1	1402	4OC	C6-N1	2.86	1.44	1.38
1	16S1	967	5MC	O2-C2	-2.86	1.18	1.23
53	ATR1	50	5MU	O4-C4	-2.84	1.18	1.23
1	16S1	1207	2MG	C5-C4	-2.84	1.35	1.43
54	PTR1	54	5MU	O4-C4	-2.84	1.18	1.23
54	PTR1	46	G7M	C2-N1	2.84	1.44	1.37
1	16S1	527	G7M	C2-N1	2.83	1.44	1.37
1	16S1	527	G7M	C6-N1	2.83	1.42	1.37
56	ETR1	8	4SU	C6-N1	2.82	1.44	1.38
1	16S1	1207	2MG	C5-C6	2.77	1.53	1.47
54	PTR1	46	G7M	C6-N1	2.75	1.42	1.37
22	23S1	2030	6MZ	C5-C4	-2.73	1.33	1.40
22	23S1	2445	2MG	C6-N1	2.73	1.41	1.37
1	16S1	1498	UR3	C5-C4	2.73	1.50	1.43
22	23S1	2030	6MZ	C9-N6	2.73	1.49	1.45
56	ETR1	36	2MA	C2-N1	2.73	1.45	1.36
22	23S1	2251	OMG	O6-C6	-2.71	1.17	1.23
1	16S1	966	2MG	C5-C6	2.71	1.52	1.47
22	23S1	1618	6MZ	C9-N6	2.71	1.49	1.45
22	23S1	2445	2MG	O6-C6	-2.70	1.17	1.23
22	23S1	2503	2MA	C2-N1	2.69	1.44	1.36
22	23S1	745	1MG	O6-C6	-2.69	1.17	1.22
56	ETR1	31	OMU	C6-N1	2.68	1.44	1.38
22	23S1	2498	OMC	C6-N1	2.68	1.44	1.38
54	PTR1	37	T6A	C2-N3	2.67	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	1516	2MG	C5-C6	2.66	1.52	1.47
22	23S1	746	PSU	O4'-C1'	-2.63	1.40	1.43
22	23S1	1618	6MZ	C5-C4	-2.62	1.34	1.40
53	ATR1	50	5MU	O2-C2	-2.62	1.18	1.23
56	ETR1	17	OMG	C5-C4	-2.59	1.36	1.43
22	23S1	1835	2MG	O6-C6	-2.59	1.18	1.23
22	23S1	2503	2MA	C5-C4	-2.59	1.36	1.43
1	16S1	516	PSU	O4'-C1'	-2.59	1.40	1.43
54	PTR1	54	5MU	O2-C2	-2.58	1.18	1.23
22	23S1	1915	3TD	O2-C2	-2.56	1.18	1.23
53	ATR1	8	4SU	O2-C2	-2.53	1.18	1.23
53	ATR1	8	4SU	C6-N1	2.53	1.44	1.38
1	16S1	1516	2MG	O6-C6	-2.50	1.18	1.23
33	L161	81	4D4	CZ-NH1	-2.47	1.24	1.34
22	23S1	2580	PSU	O4-C4	-2.47	1.18	1.23
56	ETR1	53	5MU	O4-C4	-2.46	1.18	1.23
1	16S1	1207	2MG	O6-C6	-2.45	1.18	1.23
56	ETR1	8	4SU	O2-C2	-2.42	1.18	1.23
22	23S1	955	PSU	O4-C4	-2.42	1.19	1.23
22	23S1	2069	G7M	C2-N1	2.41	1.43	1.37
22	23S1	1835	2MG	C5-C6	2.40	1.52	1.47
22	23S1	2605	PSU	O4-C4	-2.39	1.19	1.23
1	16S1	1498	UR3	C6-N1	2.39	1.43	1.38
22	23S1	2503	2MA	C6-N1	2.39	1.43	1.38
22	23S1	2580	PSU	O4'-C1'	-2.38	1.40	1.43
54	PTR1	34	U8U	O4-C4	-2.38	1.19	1.23
22	23S1	2457	PSU	O4-C4	-2.37	1.19	1.23
56	ETR1	17	OMG	C5-C6	2.36	1.52	1.47
56	ETR1	31	OMU	O2-C2	-2.35	1.18	1.23
22	23S1	746	PSU	O4-C4	-2.35	1.19	1.23
22	23S1	2604	PSU	O4-C4	-2.35	1.19	1.23
1	16S1	1498	UR3	C3U-N3	-2.35	1.42	1.47
1	16S1	966	2MG	O6-C6	-2.34	1.18	1.23
54	PTR1	39	PSU	O4-C4	-2.32	1.19	1.23
53	ATR1	50	5MU	C4-C5	-2.32	1.40	1.44
22	23S1	1917	PSU	O4-C4	-2.31	1.19	1.23
1	16S1	516	PSU	C1'-C5	2.30	1.55	1.50
56	ETR1	36	2MA	C6-N1	2.29	1.43	1.38
56	ETR1	17	OMG	C6-N1	2.28	1.41	1.37
22	23S1	2504	PSU	O4-C4	-2.27	1.19	1.23
1	16S1	1519	MA6	C4-N3	-2.27	1.32	1.35
56	ETR1	54	PSU	C1'-C5	2.26	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	PTR1	46	G7M	C5-C6	2.25	1.51	1.45
53	ATR1	36	PSU	O4-C4	-2.24	1.19	1.23
56	ETR1	53	5MU	O2-C2	-2.24	1.18	1.23
22	23S1	2552	OMU	C6-N1	2.24	1.43	1.38
22	23S1	2251	OMG	C5-C6	2.23	1.51	1.47
56	ETR1	38	PSU	C1'-C5	2.23	1.55	1.50
22	23S1	1915	3TD	O4-C4	-2.23	1.18	1.23
54	PTR1	39	PSU	C1'-C5	2.23	1.55	1.50
22	23S1	2251	OMG	C2-N1	2.22	1.43	1.37
56	ETR1	17	OMG	O6-C6	-2.22	1.18	1.23
53	ATR1	29	PSU	O4-C4	-2.22	1.19	1.23
22	23S1	1911	PSU	O4-C4	-2.20	1.19	1.23
22	23S1	2457	PSU	O4'-C1'	-2.19	1.40	1.43
22	23S1	2069	G7M	C6-N1	2.18	1.41	1.37
56	ETR1	31	OMU	C5-C4	2.18	1.48	1.43
22	23S1	2445	2MG	C5-C6	2.18	1.51	1.47
53	ATR1	51	PSU	O4-C4	-2.17	1.19	1.23
1	16S1	516	PSU	O4-C4	-2.16	1.19	1.23
22	23S1	746	PSU	C1'-C5	2.12	1.55	1.50
1	16S1	527	G7M	C5-C6	2.11	1.50	1.45
54	PTR1	37	T6A	C4-N3	-2.10	1.32	1.35
56	ETR1	37	PSU	O4-C4	-2.10	1.19	1.23
22	23S1	2069	G7M	C5-C4	-2.09	1.34	1.39
1	16S1	1518	MA6	C4-N3	-2.08	1.32	1.35
56	ETR1	38	PSU	O4-C4	-2.07	1.19	1.23
54	PTR1	55	PSU	O4-C4	-2.04	1.19	1.23
53	ATR1	51	PSU	C1'-C5	2.03	1.54	1.50
56	ETR1	54	PSU	O4-C4	-2.02	1.19	1.23
56	ETR1	37	PSU	C1'-C5	2.02	1.54	1.50
54	PTR1	37	T6A	C5-N7	-2.01	1.32	1.39

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	PTR1	54	5MU	C5-C4-N3	12.90	126.32	115.31
22	23S1	747	5MU	C5-C4-N3	12.62	126.08	115.31
22	23S1	1939	5MU	C5-C4-N3	12.51	125.98	115.31
53	ATR1	50	5MU	C4-N3-C2	-11.84	112.02	127.35
53	ATR1	50	5MU	C5-C4-N3	11.54	125.17	115.31
56	ETR1	53	5MU	C4-N3-C2	-11.48	112.48	127.35
56	ETR1	53	5MU	C5-C4-N3	11.38	125.02	115.31
22	23S1	747	5MU	C5-C6-N1	-10.72	112.31	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	ATR1	50	5MU	C6-N1-C2	-10.30	110.87	121.30
56	ETR1	53	5MU	C6-N1-C2	-9.69	111.48	121.30
22	23S1	1939	5MU	C5-C6-N1	-9.10	113.97	123.34
54	PTR1	54	5MU	C5-C6-N1	-8.80	114.29	123.34
56	ETR1	8	4SU	C4-N3-C2	-7.94	119.63	127.34
53	ATR1	50	5MU	C6-C5-C4	7.72	124.49	118.03
22	23S1	2457	PSU	N1-C2-N3	7.72	123.88	115.13
53	ATR1	8	4SU	C4-N3-C2	-7.69	119.86	127.34
56	ETR1	53	5MU	C6-C5-C4	7.63	124.41	118.03
22	23S1	955	PSU	N1-C2-N3	7.61	123.75	115.13
22	23S1	2580	PSU	N1-C2-N3	7.34	123.44	115.13
22	23S1	2604	PSU	N1-C2-N3	7.33	123.44	115.13
22	23S1	2605	PSU	N1-C2-N3	7.31	123.42	115.13
22	23S1	1911	PSU	N1-C2-N3	7.17	123.26	115.13
53	ATR1	36	PSU	N1-C2-N3	7.09	123.17	115.13
1	16S1	1519	MA6	N1-C6-N6	-7.08	109.61	117.06
22	23S1	1917	PSU	N1-C2-N3	7.08	123.15	115.13
53	ATR1	29	PSU	N1-C2-N3	7.07	123.14	115.13
22	23S1	2504	PSU	N1-C2-N3	7.03	123.10	115.13
53	ATR1	51	PSU	N1-C2-N3	7.01	123.08	115.13
56	ETR1	54	PSU	N1-C2-N3	7.00	123.06	115.13
54	PTR1	39	PSU	N1-C2-N3	7.00	123.06	115.13
53	ATR1	34	MIA	C11-S10-C2	6.99	107.49	102.27
56	ETR1	37	PSU	N1-C2-N3	6.91	122.96	115.13
56	ETR1	38	PSU	N1-C2-N3	6.81	122.84	115.13
22	23S1	746	PSU	N1-C2-N3	6.75	122.77	115.13
54	PTR1	55	PSU	N1-C2-N3	6.71	122.73	115.13
53	ATR1	50	5MU	N3-C2-N1	6.68	123.76	114.89
53	ATR1	50	5MU	O4-C4-C5	-6.55	117.31	124.90
22	23S1	2457	PSU	C4-N3-C2	-6.34	117.20	126.34
22	23S1	2605	PSU	C4-N3-C2	-6.34	117.21	126.34
54	PTR1	37	T6A	N6-C10-N11	6.33	122.61	113.76
22	23S1	955	PSU	C4-N3-C2	-6.29	117.27	126.34
56	ETR1	53	5MU	N3-C2-N1	6.26	123.20	114.89
22	23S1	2604	PSU	C4-N3-C2	-6.18	117.44	126.34
53	ATR1	51	PSU	C4-N3-C2	-6.14	117.49	126.34
1	16S1	1518	MA6	N1-C6-N6	-6.13	110.61	117.06
1	16S1	516	PSU	N1-C2-N3	6.12	122.06	115.13
54	PTR1	39	PSU	C4-N3-C2	-6.10	117.56	126.34
22	23S1	1917	PSU	C4-N3-C2	-6.07	117.59	126.34
53	ATR1	29	PSU	C4-N3-C2	-6.07	117.60	126.34
22	23S1	2580	PSU	C4-N3-C2	-6.03	117.66	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1911	PSU	C4-N3-C2	-6.02	117.67	126.34
56	ETR1	8	4SU	C5-C4-N3	5.99	120.24	114.69
56	ETR1	37	PSU	C4-N3-C2	-5.96	117.75	126.34
53	ATR1	36	PSU	C4-N3-C2	-5.94	117.78	126.34
56	ETR1	53	5MU	O4-C4-C5	-5.92	118.04	124.90
22	23S1	2504	PSU	C4-N3-C2	-5.89	117.85	126.34
22	23S1	746	PSU	C4-N3-C2	-5.88	117.87	126.34
56	ETR1	54	PSU	C4-N3-C2	-5.85	117.91	126.34
56	ETR1	38	PSU	C4-N3-C2	-5.84	117.93	126.34
1	16S1	1519	MA6	N3-C2-N1	-5.83	119.57	128.68
22	23S1	747	5MU	C4-N3-C2	-5.79	119.86	127.35
22	23S1	2552	OMU	C4-N3-C2	-5.74	119.00	126.58
54	PTR1	55	PSU	C4-N3-C2	-5.74	118.08	126.34
1	16S1	1518	MA6	N3-C2-N1	-5.73	119.72	128.68
1	16S1	516	PSU	C4-N3-C2	-5.71	118.11	126.34
22	23S1	747	5MU	O4-C4-C5	-5.63	118.37	124.90
54	PTR1	37	T6A	N3-C2-N1	-5.62	119.90	128.68
22	23S1	1915	3TD	N1-C2-N3	5.57	120.54	116.14
54	PTR1	54	5MU	O4-C4-C5	-5.55	118.47	124.90
53	ATR1	34	MIA	C12-C13-C14	-5.48	116.47	127.14
53	ATR1	8	4SU	C5-C4-N3	5.44	119.73	114.69
22	23S1	1939	5MU	O4-C4-C5	-5.42	118.61	124.90
22	23S1	2030	6MZ	N3-C2-N1	-5.26	120.45	128.68
22	23S1	1618	6MZ	N3-C2-N1	-5.24	120.49	128.68
56	ETR1	31	OMU	C4-N3-C2	-5.21	119.71	126.58
53	ATR1	34	MIA	C16-C14-C13	-5.14	107.79	122.65
22	23S1	1939	5MU	C4-N3-C2	-5.08	120.77	127.35
22	23S1	2580	PSU	C6-N1-C2	-5.07	117.50	122.68
22	23S1	2457	PSU	C6-N1-C2	-5.06	117.51	122.68
22	23S1	955	PSU	C6-N1-C2	-5.04	117.53	122.68
54	PTR1	54	5MU	C4-N3-C2	-5.02	120.86	127.35
1	16S1	1498	UR3	C4-N3-C2	-4.97	119.89	124.56
22	23S1	1939	5MU	N3-C2-N1	4.96	121.47	114.89
22	23S1	1911	PSU	C6-N1-C2	-4.95	117.63	122.68
54	PTR1	37	T6A	C2-N1-C6	4.91	120.80	116.59
22	23S1	747	5MU	N3-C2-N1	4.91	121.40	114.89
22	23S1	2604	PSU	C6-N1-C2	-4.88	117.69	122.68
22	23S1	1917	PSU	C6-N1-C2	-4.78	117.79	122.68
22	23S1	2504	PSU	C6-N1-C2	-4.78	117.80	122.68
53	ATR1	29	PSU	C6-N1-C2	-4.76	117.82	122.68
53	ATR1	51	PSU	C6-N1-C2	-4.76	117.82	122.68
56	ETR1	54	PSU	C6-N1-C2	-4.73	117.85	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	ATR1	36	PSU	C6-N1-C2	-4.71	117.86	122.68
53	ATR1	29	PSU	C6-C5-C4	4.70	121.49	118.20
56	ETR1	37	PSU	C6-N1-C2	-4.70	117.88	122.68
22	23S1	2457	PSU	C6-C5-C4	4.70	121.48	118.20
54	PTR1	39	PSU	C6-N1-C2	-4.69	117.89	122.68
22	23S1	2604	PSU	C6-C5-C4	4.68	121.47	118.20
22	23S1	746	PSU	C6-N1-C2	-4.68	117.90	122.68
54	PTR1	55	PSU	C6-N1-C2	-4.62	117.96	122.68
22	23S1	2605	PSU	C6-N1-C2	-4.61	117.97	122.68
56	ETR1	38	PSU	C6-N1-C2	-4.59	117.99	122.68
22	23S1	955	PSU	C6-C5-C4	4.55	121.38	118.20
22	23S1	2605	PSU	C6-C5-C4	4.54	121.37	118.20
22	23S1	2604	PSU	O2-C2-N1	-4.52	117.82	122.79
56	ETR1	37	PSU	C6-C5-C4	4.51	121.35	118.20
53	ATR1	36	PSU	C6-C5-C4	4.50	121.35	118.20
53	ATR1	51	PSU	C6-C5-C4	4.46	121.32	118.20
54	PTR1	54	5MU	N3-C2-N1	4.45	120.80	114.89
56	ETR1	17	OMG	N2-C2-N3	4.42	128.34	119.74
22	23S1	747	5MU	C5M-C5-C6	-4.41	116.96	122.85
22	23S1	2457	PSU	O2-C2-N1	-4.33	118.02	122.79
22	23S1	1917	PSU	C6-C5-C4	4.32	121.22	118.20
22	23S1	2580	PSU	O2-C2-N1	-4.31	118.04	122.79
1	16S1	516	PSU	C6-N1-C2	-4.31	118.28	122.68
54	PTR1	55	PSU	C6-C5-C4	4.29	121.20	118.20
56	ETR1	54	PSU	C6-C5-C4	4.28	121.19	118.20
22	23S1	1917	PSU	O2-C2-N1	-4.28	118.08	122.79
22	23S1	1911	PSU	C6-C5-C4	4.23	121.16	118.20
53	ATR1	51	PSU	O2-C2-N1	-4.23	118.14	122.79
53	ATR1	36	PSU	O2-C2-N1	-4.19	118.17	122.79
22	23S1	1915	3TD	C4-N3-C2	-4.16	120.09	124.61
22	23S1	2580	PSU	C6-C5-C4	4.14	121.09	118.20
54	PTR1	39	PSU	O2-C2-N1	-4.13	118.24	122.79
53	ATR1	29	PSU	O2-C2-N1	-4.13	118.24	122.79
22	23S1	747	5MU	C5M-C5-C4	4.11	123.29	118.77
22	23S1	745	1MG	C5-C6-N1	4.09	120.05	113.90
12	S121	89	D2T	CB-CA-N	4.07	117.78	109.10
54	PTR1	54	5MU	C5M-C5-C4	4.06	123.24	118.77
22	23S1	2030	6MZ	C2-N1-C6	4.06	120.07	116.59
22	23S1	2552	OMU	N3-C2-N1	4.05	120.27	114.89
22	23S1	2504	PSU	C6-C5-C4	4.04	121.02	118.20
22	23S1	746	PSU	O2-C2-N1	-4.02	118.36	122.79
1	16S1	516	PSU	O2-C2-N1	-3.99	118.40	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	747	5MU	O2-C2-N1	-3.98	117.49	122.79
22	23S1	1939	5MU	C5M-C5-C4	3.97	123.13	118.77
56	ETR1	53	5MU	C5M-C5-C6	-3.94	117.58	122.85
56	ETR1	37	PSU	O2-C2-N1	-3.91	118.48	122.79
56	ETR1	54	PSU	O2-C2-N1	-3.91	118.49	122.79
12	S121	89	D2T	CB1-SB-CB	3.91	109.51	102.44
56	ETR1	38	PSU	C6-C5-C4	3.89	120.92	118.20
22	23S1	955	PSU	O2-C2-N1	-3.87	118.53	122.79
54	PTR1	55	PSU	O2-C2-N1	-3.87	118.53	122.79
22	23S1	2504	PSU	O2-C2-N1	-3.86	118.54	122.79
22	23S1	1835	2MG	C5-C6-N1	3.84	120.73	113.95
56	ETR1	17	OMG	N1-C2-N3	-3.81	116.19	123.32
53	ATR1	50	5MU	C5M-C5-C6	-3.81	117.76	122.85
22	23S1	2445	2MG	C5-C6-N1	3.79	120.64	113.95
22	23S1	1911	PSU	O2-C2-N1	-3.78	118.62	122.79
56	ETR1	31	OMU	N3-C2-N1	3.74	119.86	114.89
22	23S1	2552	OMU	C5-C4-N3	3.74	120.43	114.84
53	ATR1	50	5MU	C1'-N1-C2	3.73	124.32	117.57
22	23S1	1618	6MZ	C2-N1-C6	3.73	119.78	116.59
53	ATR1	50	5MU	O2-C2-N1	-3.69	117.88	122.79
22	23S1	2605	PSU	O2-C2-N1	-3.69	118.73	122.79
1	16S1	1207	2MG	C5-C6-N1	3.67	120.43	113.95
22	23S1	2503	2MA	C5-C6-N1	3.64	120.30	114.02
22	23S1	2251	OMG	C5-C6-N1	3.60	120.31	113.95
53	ATR1	8	4SU	N3-C2-N1	3.58	119.64	114.89
53	ATR1	8	4SU	C5-C4-S4	-3.57	119.87	124.47
1	16S1	966	2MG	C5-C6-N1	3.56	120.23	113.95
56	ETR1	38	PSU	O2-C2-N1	-3.55	118.89	122.79
22	23S1	2030	6MZ	C1'-N9-C4	-3.53	120.43	126.64
56	ETR1	8	4SU	N3-C2-N1	3.53	119.58	114.89
22	23S1	1939	5MU	C5M-C5-C6	-3.52	118.14	122.85
53	ATR1	34	MIA	N3-C2-N1	-3.52	120.51	126.98
22	23S1	746	PSU	C6-C5-C4	3.52	120.66	118.20
1	16S1	1516	2MG	C5-C6-N1	3.50	120.13	113.95
22	23S1	2030	6MZ	C9-N6-C6	-3.48	119.88	122.87
56	ETR1	8	4SU	C5-C4-S4	-3.47	119.99	124.47
22	23S1	1618	6MZ	C1'-N9-C4	-3.44	120.60	126.64
54	PTR1	34	U8U	C5-C4-N3	3.44	119.80	114.97
54	PTR1	34	U8U	O4-C4-C5	-3.40	119.91	124.96
56	ETR1	36	2MA	C5-C6-N1	3.37	119.84	114.02
56	ETR1	31	OMU	C5-C4-N3	3.37	119.88	114.84
54	PTR1	54	5MU	C5M-C5-C6	-3.32	118.41	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	967	5MC	C5-C6-N1	-3.30	119.94	123.34
54	PTR1	39	PSU	C6-C5-C4	3.27	120.49	118.20
22	23S1	1618	6MZ	C9-N6-C6	-3.27	120.06	122.87
56	ETR1	53	5MU	C1'-N1-C2	3.22	123.40	117.57
53	ATR1	34	MIA	S10-C2-N1	3.14	126.88	116.01
56	ETR1	53	5MU	O2-C2-N1	-3.14	118.61	122.79
22	23S1	1939	5MU	O2-C2-N1	-3.12	118.64	122.79
53	ATR1	34	MIA	C2-N3-C4	3.07	119.56	115.32
1	16S1	516	PSU	C6-C5-C4	3.05	120.33	118.20
22	23S1	2251	OMG	C2-N1-C6	-3.03	119.52	125.10
22	23S1	2069	G7M	C2-N1-C6	-3.02	119.53	125.10
12	S121	89	D2T	OD2-CG-CB	3.02	119.68	113.15
53	ATR1	34	MIA	C16-C14-C15	-3.01	107.95	114.60
54	PTR1	37	T6A	O10-C10-N6	-3.01	118.53	123.62
1	16S1	527	G7M	C2-N1-C6	-2.95	119.67	125.10
22	23S1	2552	OMU	O4-C4-C5	-2.91	120.03	125.16
54	PTR1	46	G7M	C2-N1-C6	-2.91	119.73	125.10
56	ETR1	31	OMU	O4-C4-C5	-2.91	120.04	125.16
1	16S1	1407	5MC	C5-C6-N1	-2.90	120.36	123.34
22	23S1	1962	5MC	C5-C6-N1	-2.82	120.43	123.34
22	23S1	2503	2MA	C8-N7-C5	2.73	108.20	102.99
56	ETR1	17	OMG	C5-C6-N1	2.71	118.74	113.95
1	16S1	1516	2MG	C8-N7-C5	2.66	108.06	102.99
22	23S1	2251	OMG	C8-N7-C5	2.66	108.06	102.99
53	ATR1	34	MIA	C15-C14-C13	-2.65	114.98	122.65
22	23S1	2445	2MG	CM2-N2-C2	-2.63	118.05	123.86
56	ETR1	17	OMG	C8-N7-C5	2.61	107.97	102.99
22	23S1	1835	2MG	C8-N7-C5	2.60	107.94	102.99
1	16S1	966	2MG	C8-N7-C5	2.60	107.93	102.99
1	16S1	1207	2MG	C8-N7-C5	2.59	107.92	102.99
54	PTR1	54	5MU	O4-C4-N3	-2.56	115.21	120.12
22	23S1	1962	5MC	CM5-C5-C6	-2.52	119.48	122.85
1	16S1	966	2MG	O6-C6-C5	-2.49	119.50	124.37
22	23S1	2445	2MG	O6-C6-C5	-2.48	119.54	124.37
22	23S1	745	1MG	C8-N7-C5	2.47	107.69	102.99
22	23S1	2445	2MG	C8-N7-C5	2.46	107.68	102.99
22	23S1	1939	5MU	O4-C4-N3	-2.46	115.40	120.12
22	23S1	745	1MG	O6-C6-C5	-2.46	119.84	124.19
56	ETR1	36	2MA	C8-N7-C5	2.45	107.65	102.99
54	PTR1	20	H2U	C4-N3-C2	-2.44	123.77	125.79
22	23S1	1835	2MG	O6-C6-C5	-2.41	119.66	124.37
54	PTR1	54	5MU	O2-C2-N1	-2.40	119.59	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	ETR1	53	5MU	C1'-N1-C6	2.40	125.11	121.12
22	23S1	2552	OMU	C2'-C1'-N1	-2.39	109.59	114.22
22	23S1	747	5MU	O4-C4-N3	-2.38	115.55	120.12
22	23S1	1915	3TD	C6-C5-C4	2.38	119.87	118.22
1	16S1	527	G7M	N2-C2-N1	2.38	121.78	116.71
1	16S1	1516	2MG	O6-C6-C5	-2.37	119.73	124.37
22	23S1	2449	H2U	O2-C2-N1	2.35	126.06	123.11
56	ETR1	17	OMG	O6-C6-N1	-2.34	117.89	120.65
22	23S1	2449	H2U	O2-C2-N3	-2.33	117.16	121.50
1	16S1	1207	2MG	O6-C6-C5	-2.31	119.86	124.37
22	23S1	2251	OMG	O6-C6-C5	-2.30	119.89	124.37
1	16S1	1516	2MG	CM2-N2-C2	-2.27	118.84	123.86
22	23S1	2580	PSU	O4'-C1'-C2'	2.27	108.35	105.14
1	16S1	1402	4OC	C6-C5-C4	2.26	119.72	116.96
22	23S1	2503	2MA	CM2-C2-N1	2.25	121.24	116.23
54	PTR1	20	H2U	O2-C2-N3	-2.23	117.34	121.50
22	23S1	1835	2MG	CM2-N2-C2	-2.22	118.95	123.86
53	ATR1	50	5MU	C1'-N1-C6	2.21	124.81	121.12
1	16S1	1498	UR3	C6-N1-C2	-2.20	119.82	121.79
22	23S1	1939	5MU	C6-N1-C2	-2.19	119.08	121.30
22	23S1	955	PSU	O2-C2-N3	-2.17	117.72	121.82
22	23S1	2503	2MA	N1-C2-N3	-2.16	119.47	123.06
53	ATR1	8	4SU	O2-C2-N1	-2.14	119.95	122.79
22	23S1	2552	OMU	O2-C2-N1	-2.13	119.96	122.79
54	PTR1	34	U8U	C1'-N1-C6	-2.12	117.60	121.12
22	23S1	2605	PSU	O2-C2-N3	-2.10	117.85	121.82
53	ATR1	29	PSU	O4'-C1'-C2'	2.07	108.06	105.14
54	PTR1	37	T6A	O10-C10-N11	-2.06	118.86	122.62
22	23S1	747	5MU	C6-C5-C4	2.06	119.75	118.03
54	PTR1	34	U8U	C5-C6-N1	-2.02	120.20	122.91

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16S1	527	G7M	O4'-C4'-C5'-O5'
1	16S1	527	G7M	C3'-C4'-C5'-O5'
1	16S1	966	2MG	O4'-C4'-C5'-O5'
1	16S1	966	2MG	C3'-C4'-C5'-O5'
12	S121	89	D2T	CG-CB-SB-CB1
12	S121	89	D2T	SB-CB-CG-OD2
25	L031	150	MEQ	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
25	L031	150	MEQ	C-CA-CB-CG
53	ATR1	34	MIA	C12-C13-C14-C16
56	ETR1	38	PSU	C3'-C4'-C5'-O5'
56	ETR1	38	PSU	O4'-C4'-C5'-O5'
22	23S1	1915	3TD	O4'-C4'-C5'-O5'
54	PTR1	20	H2U	O4'-C4'-C5'-O5'
54	PTR1	20	H2U	C3'-C4'-C5'-O5'
54	PTR1	20	H2U	O4'-C1'-N1-C6
54	PTR1	20	H2U	C2'-C1'-N1-C2
54	PTR1	20	H2U	C2'-C1'-N1-C6
54	PTR1	37	T6A	O4'-C4'-C5'-O5'
54	PTR1	39	PSU	C3'-C4'-C5'-O5'
54	PTR1	39	PSU	O4'-C4'-C5'-O5'
1	16S1	1519	MA6	O4'-C4'-C5'-O5'
1	16S1	1519	MA6	C3'-C4'-C5'-O5'
22	23S1	1915	3TD	C3'-C4'-C5'-O5'
22	23S1	2030	6MZ	O4'-C4'-C5'-O5'
22	23S1	2030	6MZ	C3'-C4'-C5'-O5'
22	23S1	2445	2MG	C3'-C4'-C5'-O5'
22	23S1	2504	PSU	O4'-C4'-C5'-O5'
54	PTR1	37	T6A	C3'-C4'-C5'-O5'
22	23S1	1939	5MU	O4'-C4'-C5'-O5'
22	23S1	2504	PSU	C3'-C4'-C5'-O5'
22	23S1	1939	5MU	C3'-C4'-C5'-O5'
54	PTR1	37	T6A	N11-C12-C13-ODA
54	PTR1	37	T6A	N11-C12-C13-ODB
1	16S1	1402	4OC	O4'-C4'-C5'-O5'
22	23S1	2445	2MG	O4'-C4'-C5'-O5'
33	L161	81	4D4	OB-CB-CG-CD
56	ETR1	17	OMG	O4'-C4'-C5'-O5'
53	ATR1	34	MIA	C12-C13-C14-C15
22	23S1	2580	PSU	O4'-C4'-C5'-O5'
56	ETR1	17	OMG	C3'-C4'-C5'-O5'
54	PTR1	46	G7M	C4'-C5'-O5'-P
33	L161	81	4D4	CA-CB-CG-CD
22	23S1	2503	2MA	O4'-C4'-C5'-O5'
54	PTR1	20	H2U	C4'-C5'-O5'-P
22	23S1	2069	G7M	O4'-C4'-C5'-O5'
54	PTR1	20	H2U	O4'-C1'-N1-C2
22	23S1	2503	2MA	C4'-C5'-O5'-P
1	16S1	1498	UR3	O4'-C4'-C5'-O5'
1	16S1	1402	4OC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	16S1	1518	MA6	O4'-C4'-C5'-O5'
56	ETR1	31	OMU	O4'-C4'-C5'-O5'
22	23S1	2457	PSU	O4'-C4'-C5'-O5'
22	23S1	2069	G7M	C4'-C5'-O5'-P
22	23S1	746	PSU	O4'-C1'-C5-C6
56	ETR1	31	OMU	C2'-C1'-N1-C2
22	23S1	2069	G7M	C3'-C4'-C5'-O5'
22	23S1	1962	5MC	O4'-C1'-N1-C6
22	23S1	1962	5MC	C2'-C1'-N1-C6

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 410 ligands modelled in this entry, 407 are monoatomic - leaving 3 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	$\# Z  > 2$
63	GLN	ETR1	101	56	7,8,9	0.45	0	4,9,11	0.04	0
61	OCW	23S1	3001	58	34,38,38	0.50	0	41,61,61	0.95	2 (4%)
62	CYS	ATR1	101	53	4,5,6	0.55	0	1,5,7	0.12	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
63	GLN	ETR1	101	56	-	3/6/7/9	-
61	OCW	23S1	3001	58	-	2/13/62/62	0/4/4/4
62	CYS	ATR1	101	53	-	0/1/4/6	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	23S1	3001	OCW	O04-C20-C14	3.45	112.99	110.06
61	23S1	3001	OCW	C12-C14-C20	2.85	114.87	110.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

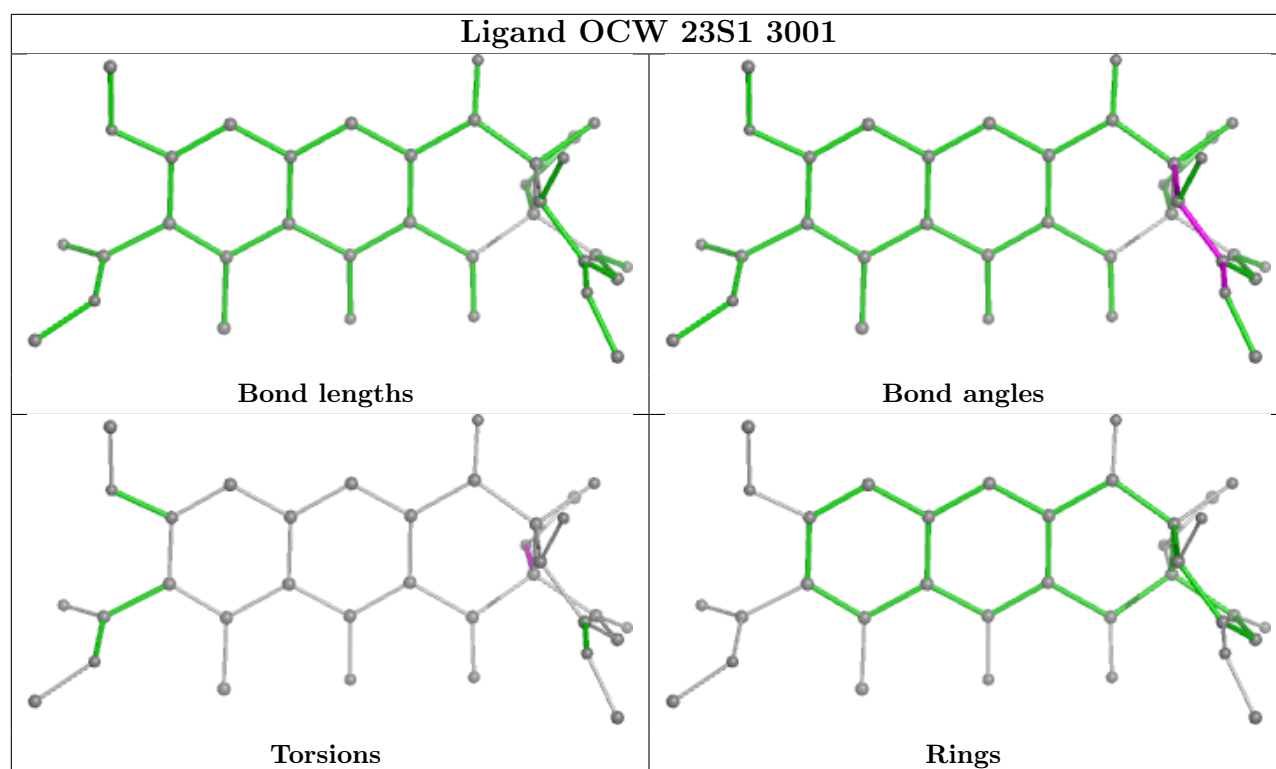
Mol	Chain	Res	Type	Atoms
61	23S1	3001	OCW	C12-C13-O01-C27
63	ETR1	101	GLN	CA-CB-CG-CD
63	ETR1	101	GLN	OE1-CD-CG-CB
63	ETR1	101	GLN	NE2-CD-CG-CB
61	23S1	3001	OCW	C16-C13-O01-C27

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.





## 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.

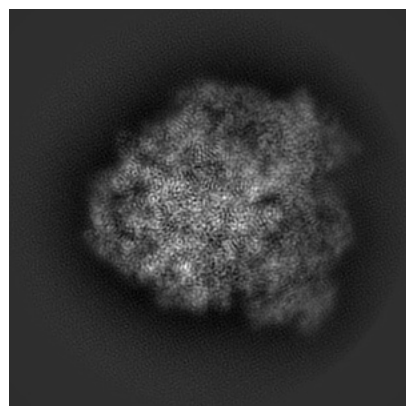
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14956. These allow visual inspection of the internal detail of the map and identification of artifacts.

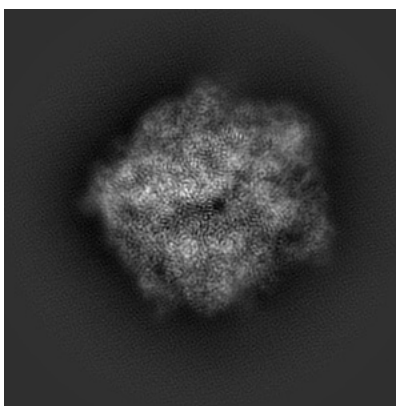
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

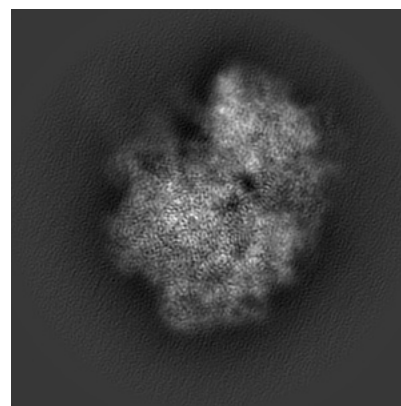
#### 6.1.1 Primary map



X

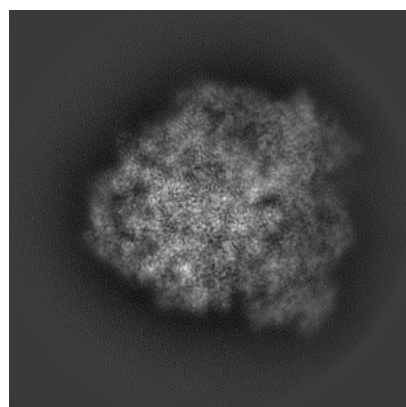


Y

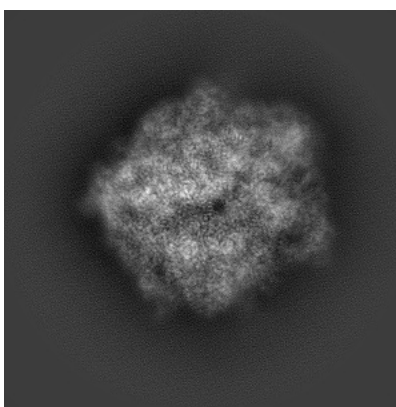


Z

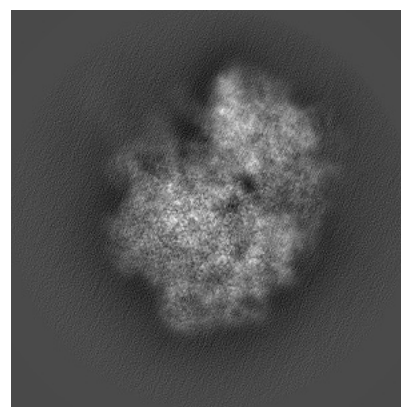
#### 6.1.2 Raw map



X



Y

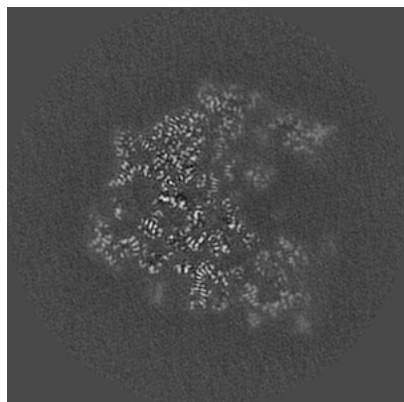


Z

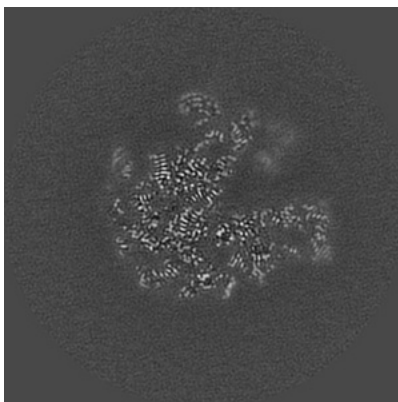
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

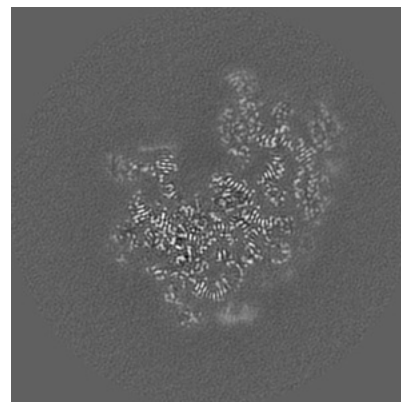
### 6.2.1 Primary map



X Index: 204

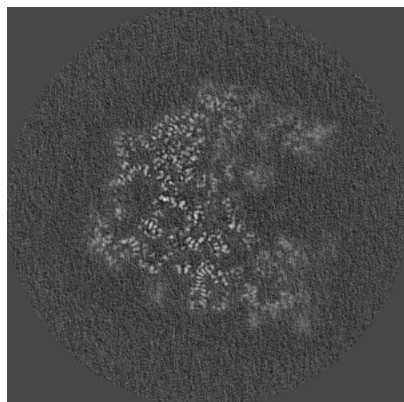


Y Index: 204

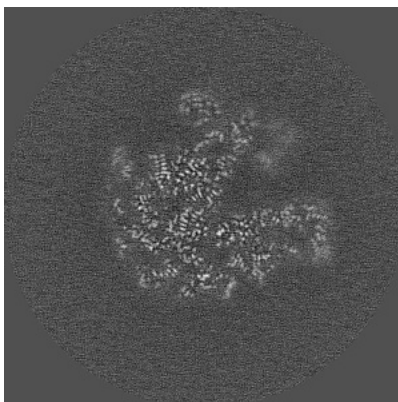


Z Index: 204

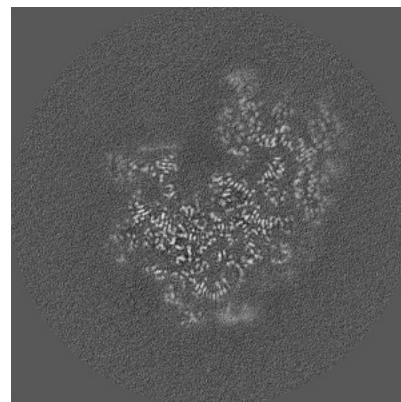
### 6.2.2 Raw map



X Index: 204



Y Index: 204

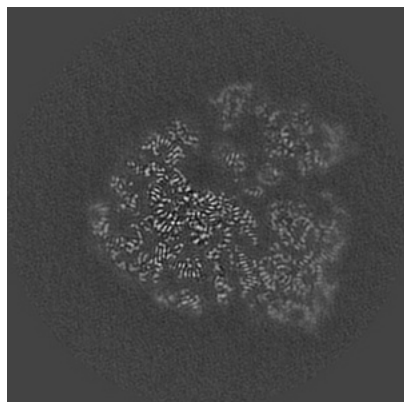


Z Index: 204

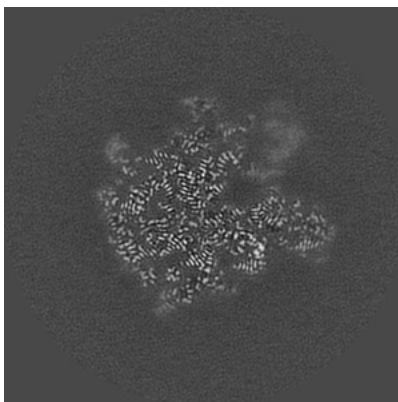
The images above show central slices of the map in three orthogonal directions.

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

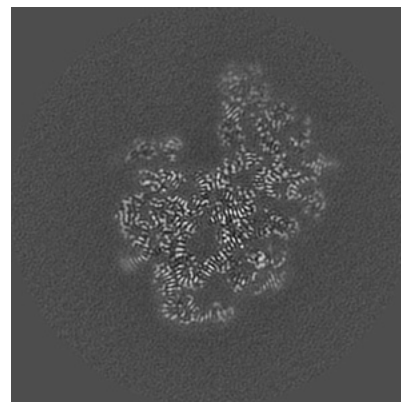
### 6.3.1 Primary map



X Index: 218

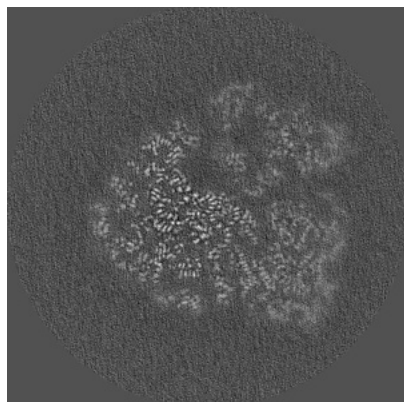


Y Index: 194

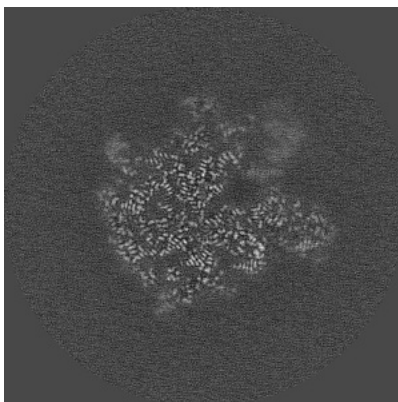


Z Index: 188

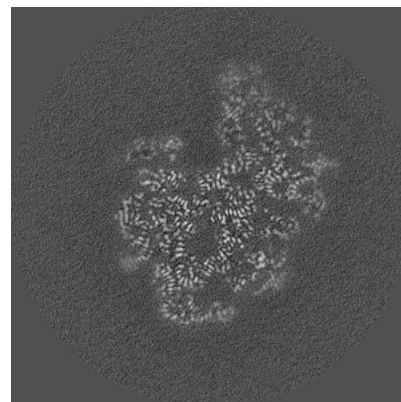
### 6.3.2 Raw map



X Index: 218



Y Index: 194



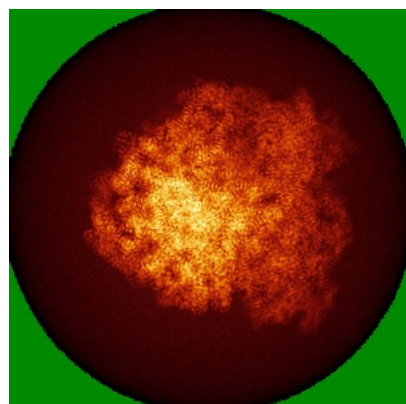
Z Index: 188

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

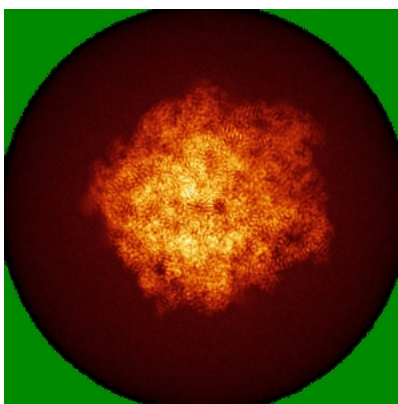


## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

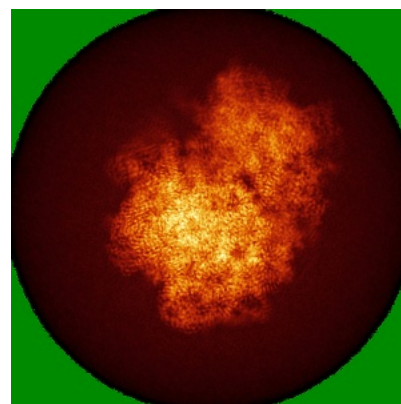
### 6.4.1 Primary map



X

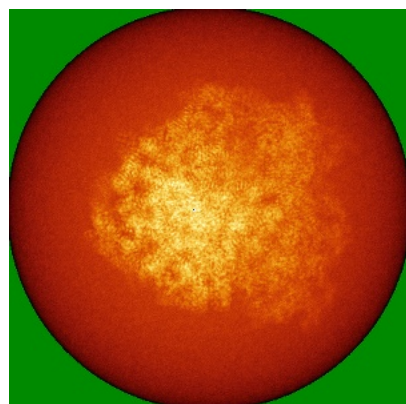


Y

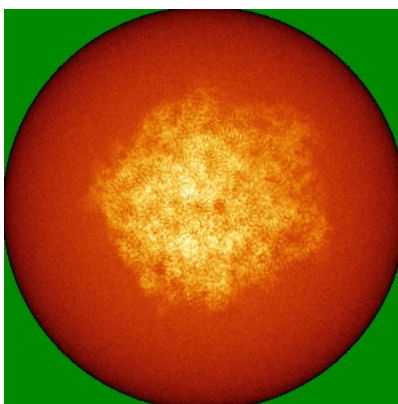


Z

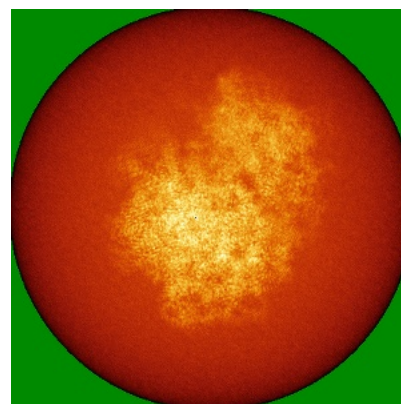
### 6.4.2 Raw map



X



Y

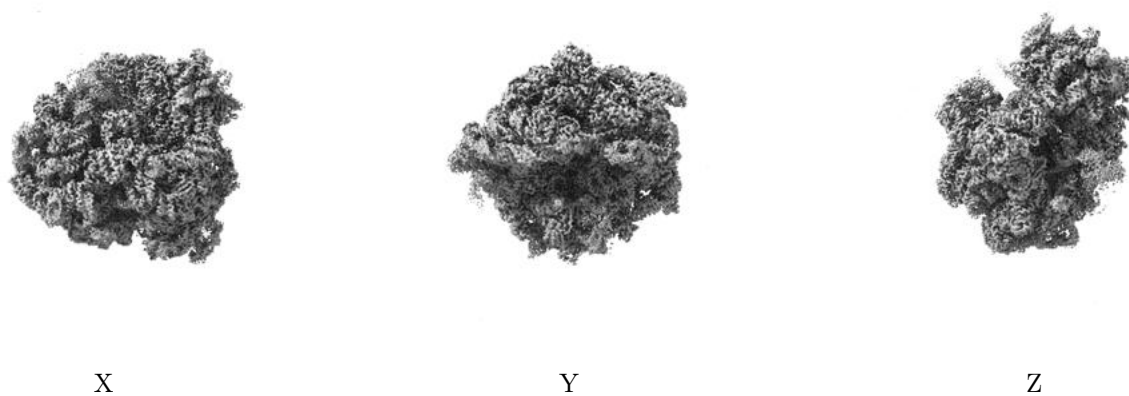


Z

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

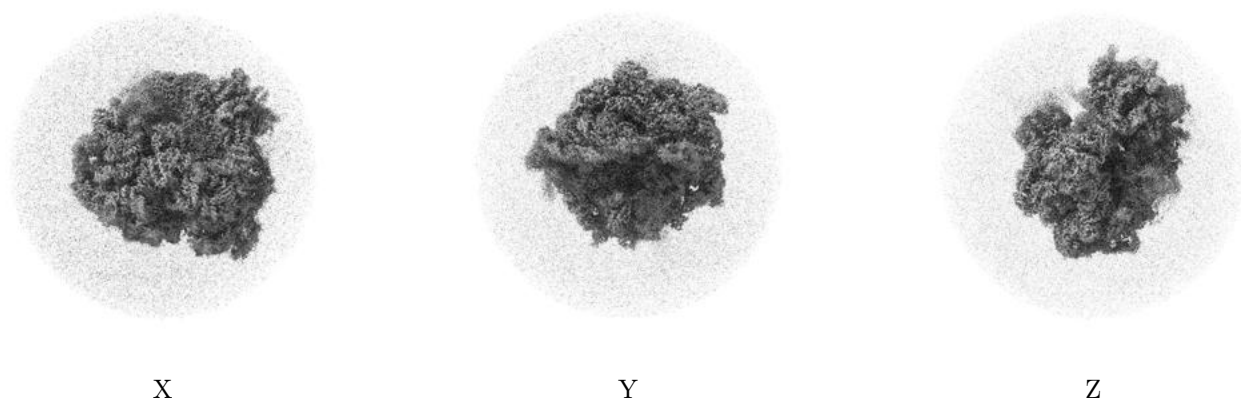
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

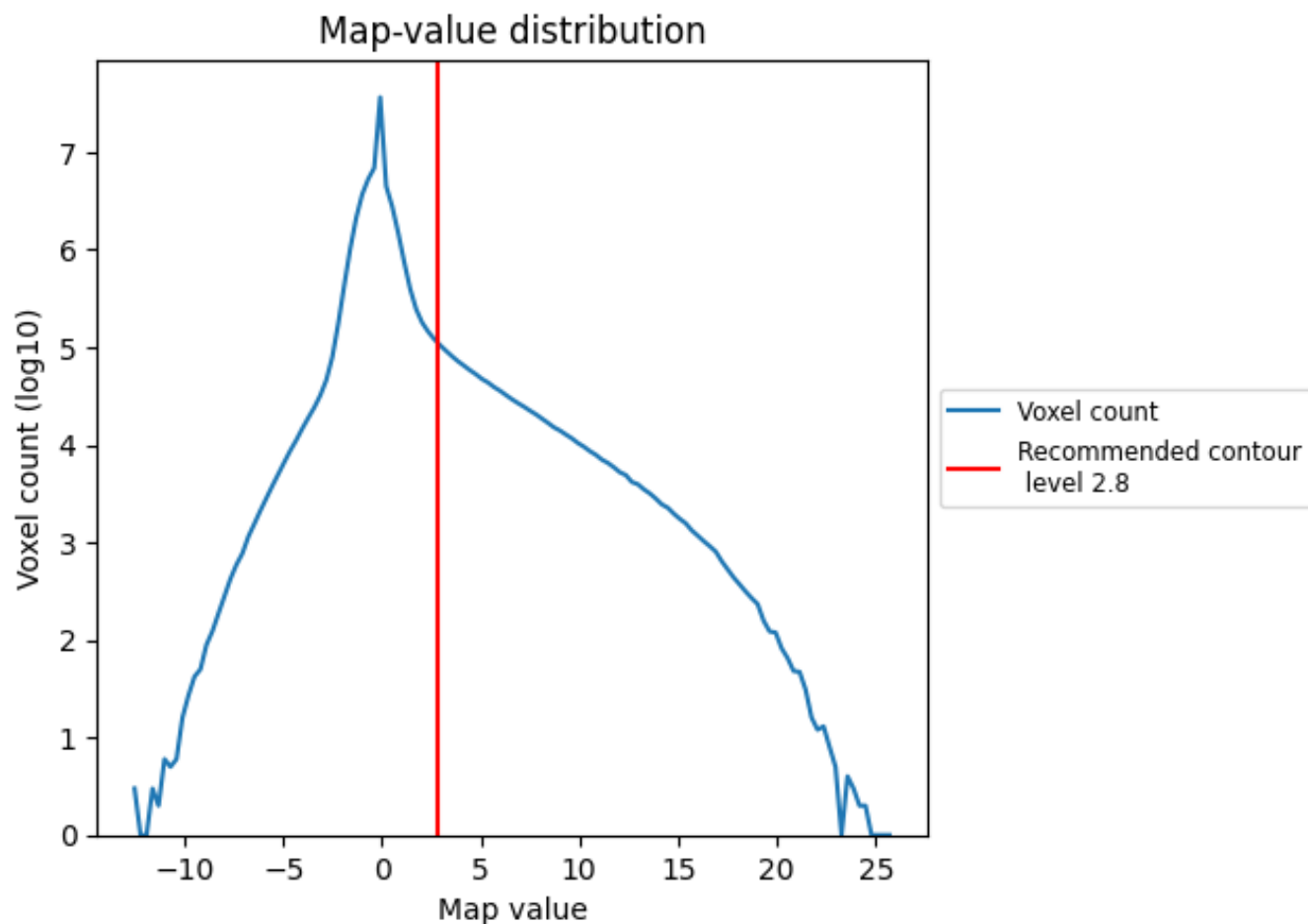
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

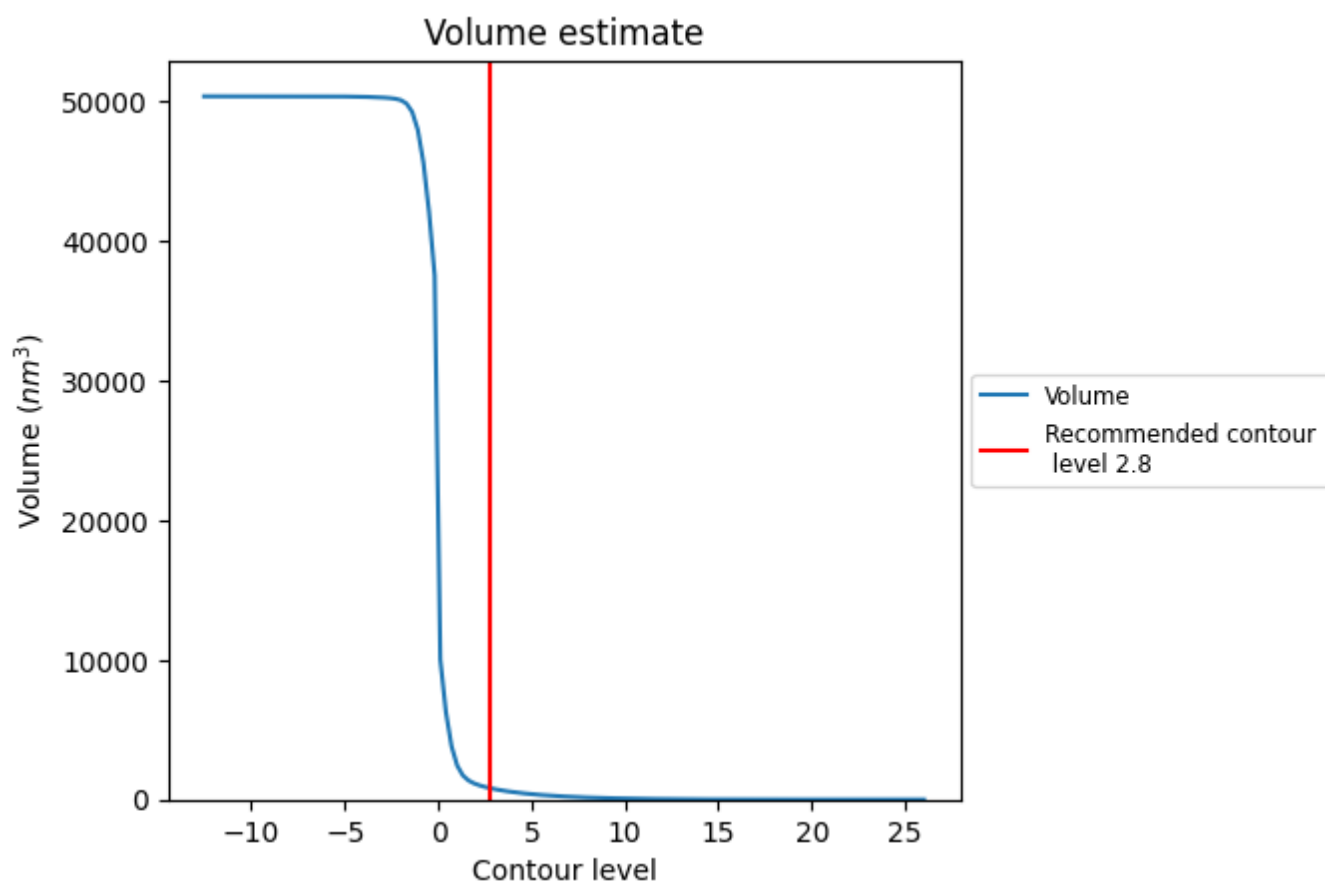
This section contains the results of statistical analysis of the map.

### 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](#)

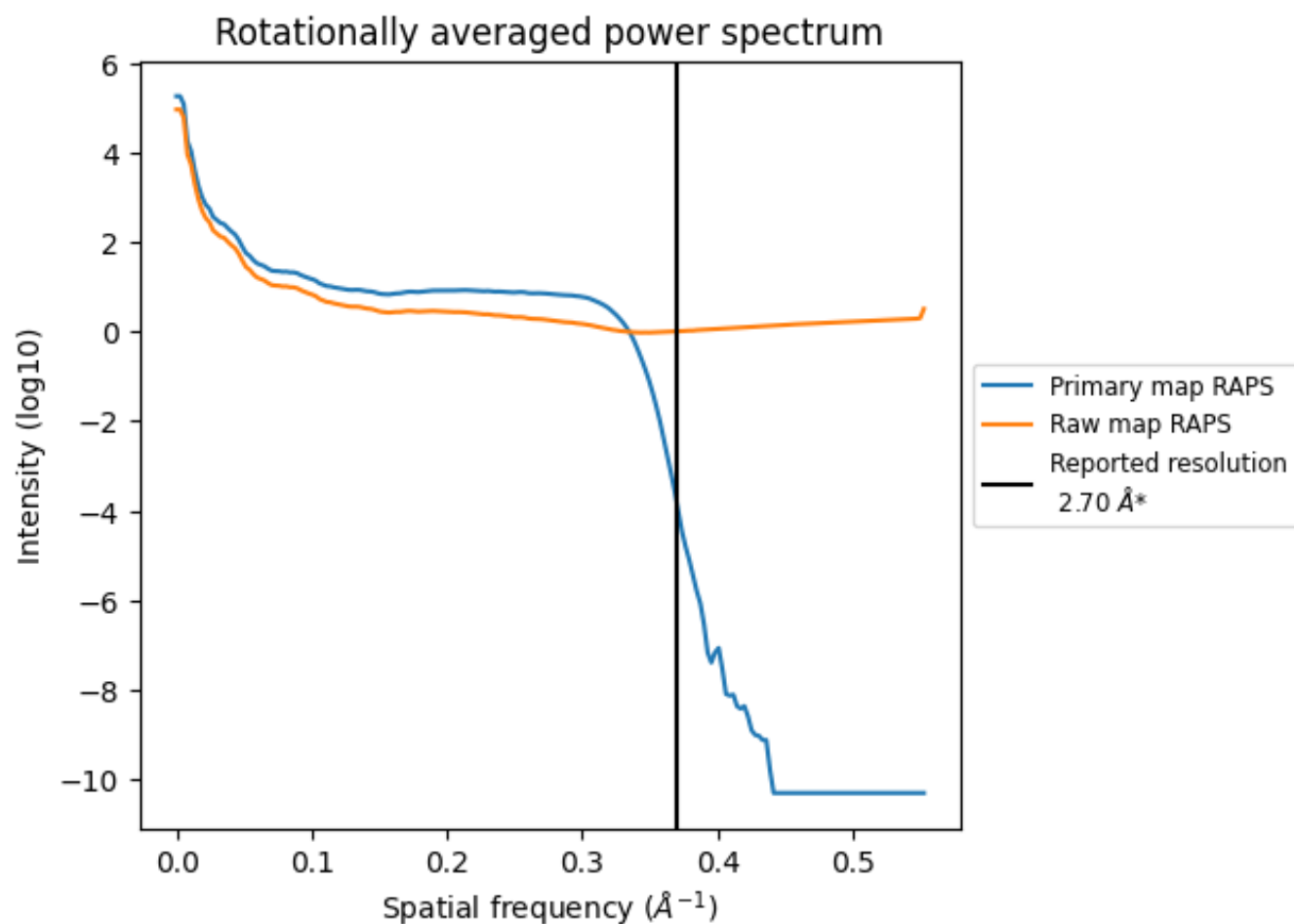


The volume at the recommended contour level is 810 nm<sup>3</sup>; this corresponds to an approximate mass of 732 kDa.

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 ⓘ

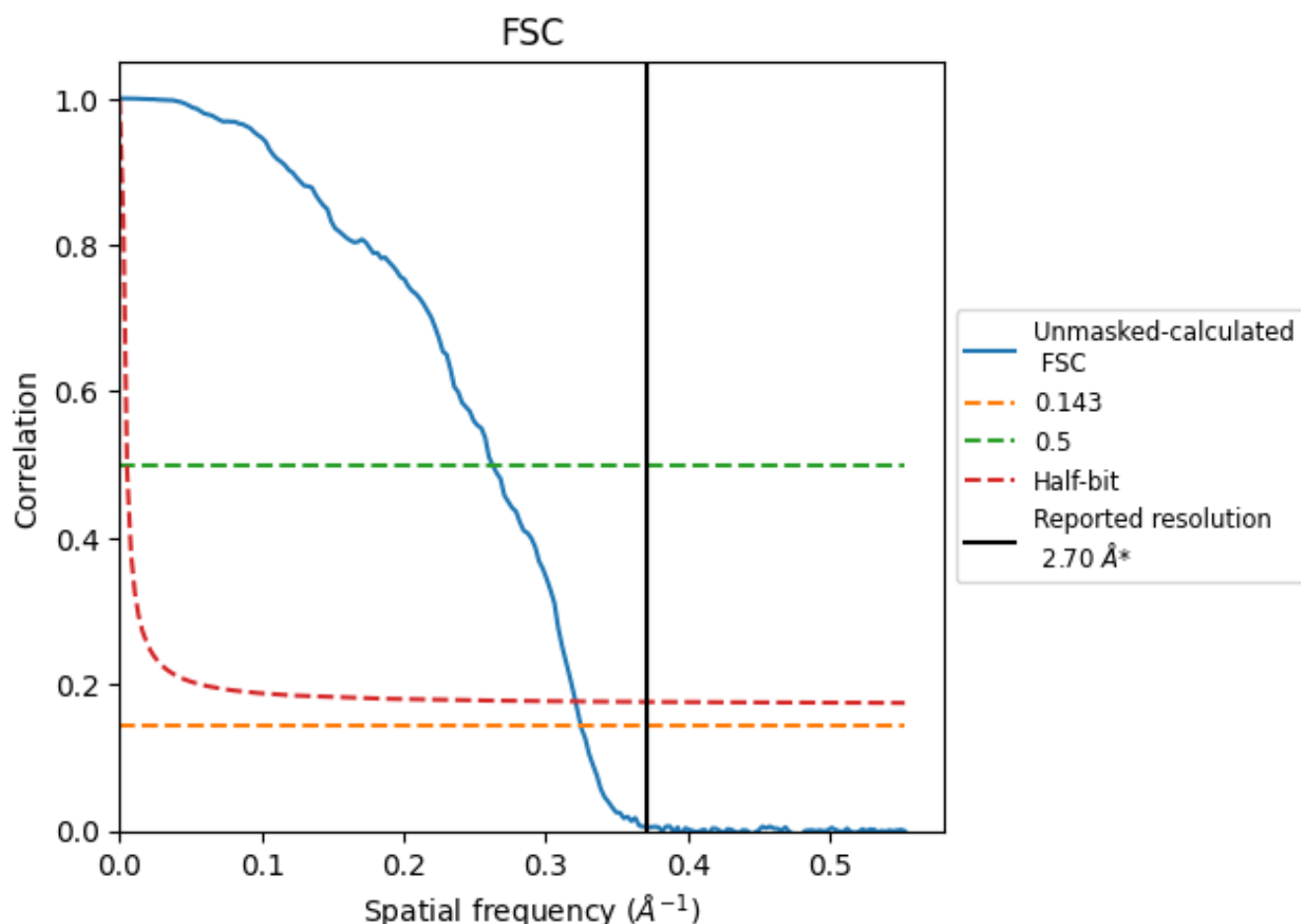


\*Reported resolution corresponds to spatial frequency of 0.370 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

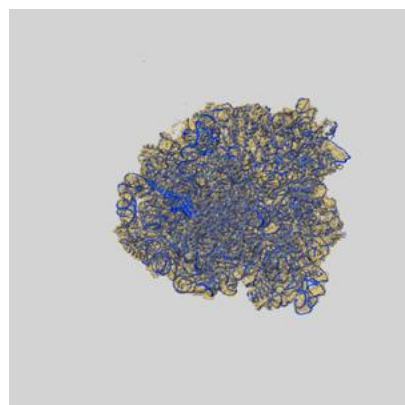
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.08	3.81	3.12

\*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 3.08 differs from the reported value 2.7 by more than 10 %

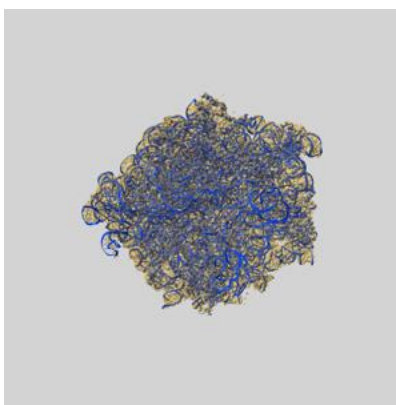
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14956 and PDB model 7ZTA. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

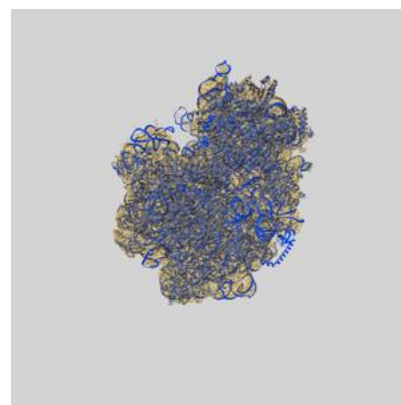
### 9.1 Map-model overlay [i](#)



X



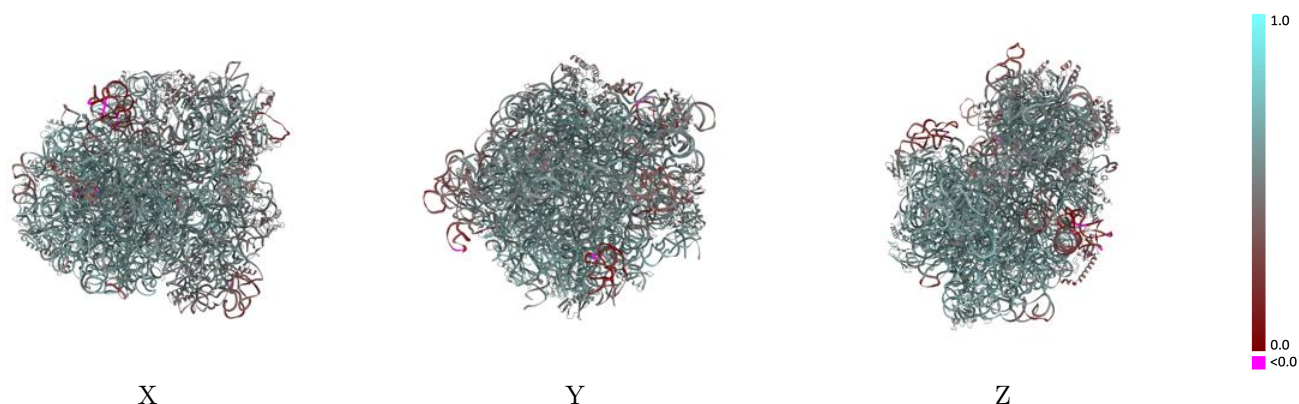
Y



Z

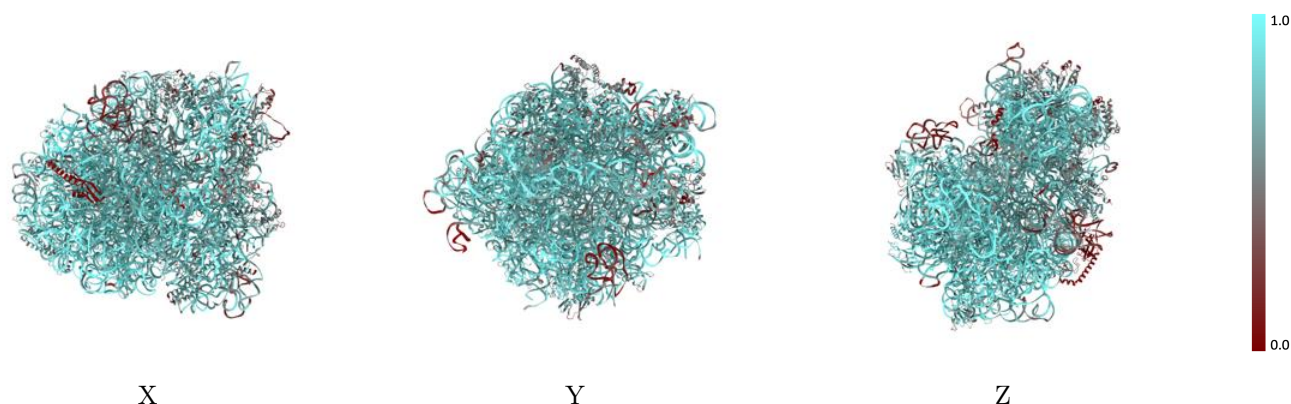
The images above show the 3D surface view of the map at the recommended contour level 2.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



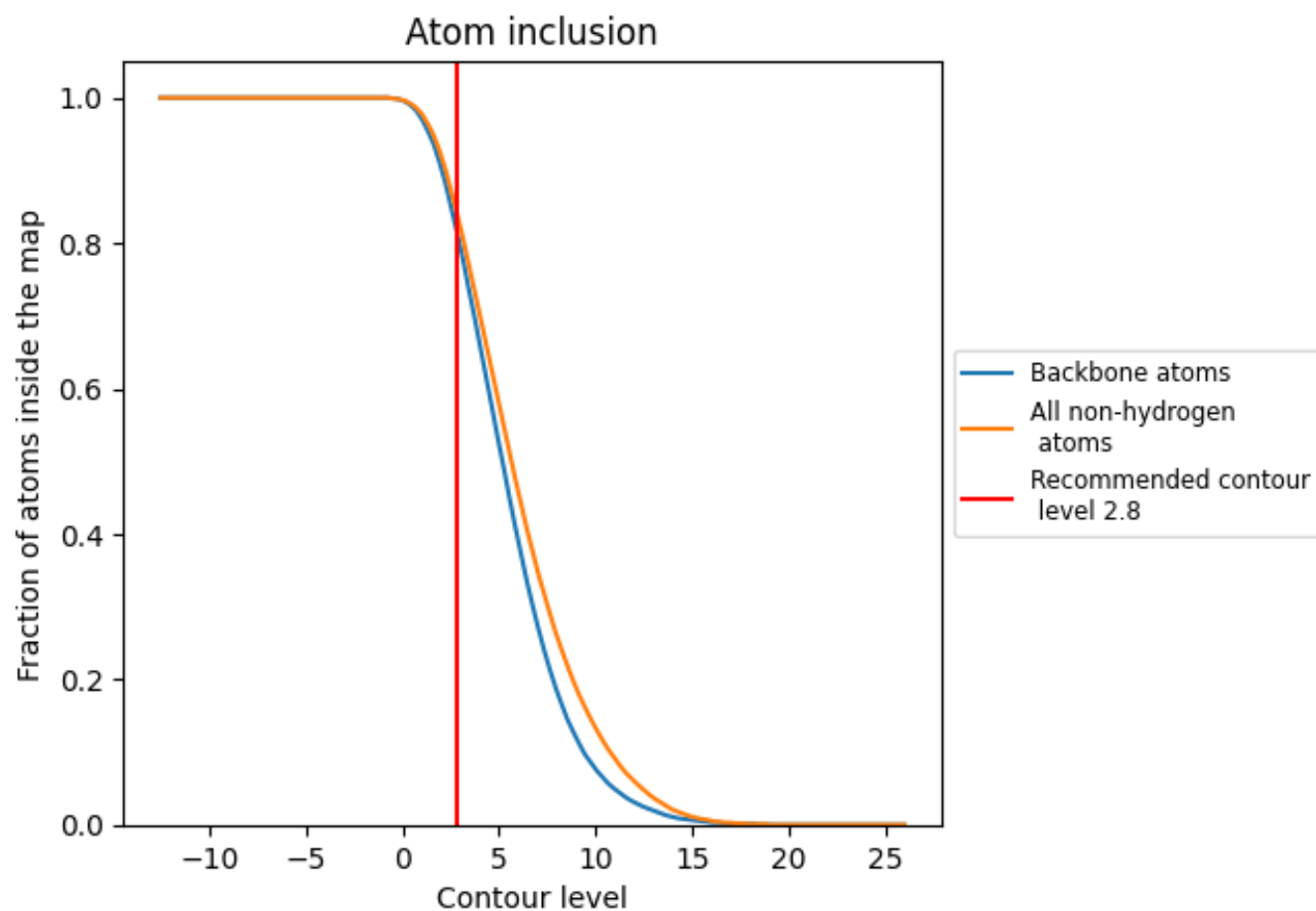
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.8).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 84% 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 (2.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8440	 0.5650
05S1	 0.9330	 0.5890
16S1	 0.8840	 0.5520
23S1	 0.9190	 0.5900
ATR1	 0.8070	 0.5630
ETR1	 0.5300	 0.4180
L021	 0.8790	 0.6120
L031	 0.8720	 0.6030
L041	 0.7740	 0.5670
L051	 0.6610	 0.5060
L061	 0.6530	 0.5120
L091	 0.1460	 0.3570
L131	 0.8730	 0.6050
L141	 0.8030	 0.5880
L151	 0.8490	 0.5980
L161	 0.8410	 0.5980
L171	 0.9030	 0.6100
L181	 0.7770	 0.5580
L191	 0.8110	 0.5840
L201	 0.9070	 0.6140
L211	 0.8220	 0.5860
L221	 0.8400	 0.5900
L231	 0.7750	 0.5660
L241	 0.7550	 0.5460
L251	 0.7720	 0.5660
L271	 0.8400	 0.5980
L281	 0.8700	 0.5990
L291	 0.7160	 0.5530
L301	 0.8350	 0.5840
L311	 0.4100	 0.4020
L321	 0.8550	 0.5930
L331	 0.7730	 0.5700
L341	 0.8930	 0.6230
L351	 0.9140	 0.6270
L361	 0.8640	 0.6010



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Chain	Atom inclusion	Q-score
MRN1	 0.7990	 0.5830
PQK1	 0.8570	 0.6000
PTR1	 0.8310	 0.5770
S021	 0.5400	 0.4690
S031	 0.6730	 0.5230
S041	 0.5500	 0.4780
S051	 0.7480	 0.5540
S061	 0.6750	 0.5050
S071	 0.5680	 0.4720
S081	 0.7290	 0.5490
S091	 0.6950	 0.5090
S101	 0.5580	 0.4690
S111	 0.7220	 0.5560
S121	 0.6960	 0.5540
S131	 0.6400	 0.4890
S141	 0.7030	 0.5150
S151	 0.7350	 0.5390
S161	 0.6250	 0.4860
S171	 0.6350	 0.5070
S181	 0.7400	 0.5540
S191	 0.6460	 0.5040
S201	 0.6460	 0.4820
S211	 0.5290	 0.4670