Full wwPDB EM Validation Report (i)

Nov 9, 2022 – 07:51 AM EST

PDB ID	:	6ORE
EMDB ID	:	EMD-20173
Title	:	Release complex 70S
Authors	:	Fu, Z.
Deposited on	:	2019-04-30
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

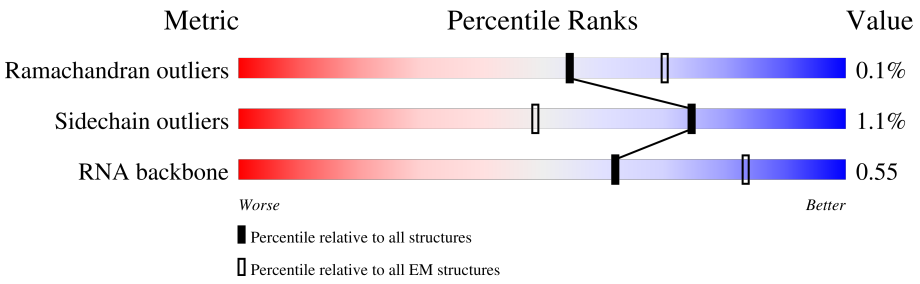
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	1	2903	82% 18%
2	2	1534	83% 17%
3	3	120	88% 12%
4	4	9	11% 78% 22%
5	5	76	8% 75% 21%
6	A	3	100% 100%
7	B	271	99%
8	C	209	97%

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Mol	Chain	Length	Quality of chain
9	D	201	99%
10	E	177	6%, 99%
11	F	175	98%
12	G	149	87%, 99%
13	J	142	100%
14	K	123	99%
15	L	144	99%
16	M	136	100%
17	N	119	100%
18	O	116	98%
19	P	114	99%
20	Q	117	99%
21	R	103	96%
22	S	110	100%
23	T	94	100%
24	U	103	99%
25	V	94	99%
26	W	76	99%
27	X	77	99%
28	Y	62	100%
29	Z	58	98%
30	a	66	39%, 97%
31	b	56	98%
32	c	52	98%
33	d	46	100%

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Mol	Chain	Length	Quality of chain
34	e	64	100%
35	f	38	100%
36	g	225	66% 100%
37	h	208	6% 99%
38	i	205	6% 100%
39	j	156	97%
40	k	104	5% 100%
41	l	151	13% 99%
42	m	129	100%
43	n	127	98%
44	o	99	27% 99%
45	p	117	5% 98%
46	q	123	5% 99%
47	r	116	7% 100%
48	s	100	100%
49	t	88	8% 98%
50	u	82	5% 99%
51	v	80	5% 100%
52	w	66	20% 100%
53	x	83	98%
54	y	86	6% 99%
55	z	70	40% 100%

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 144774 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	2903	62336	27816	11470	20147	2903	0	0

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	1534	32929	14693	6041	10661	1534	0	0

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	3	120	2569	1144	468	837	120	0	0

- Molecule 4 is a RNA chain called RNA (5'-R(P*UP*UP*CP*UP*UP*CP*UP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	4	9	184	83	26	66	9	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
5	5	76	1627	727	296	527	76	1	0	0

- Molecule 6 is a protein called FME-PHE-PHE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	3	32	24	3	4	1	0	0

- Molecule 7 is a protein called 50S ribosomal protein L2.

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

- Molecule 8 is a protein called 50S ribosomal protein L3.

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

- Molecule 9 is a protein called 50S ribosomal protein L4.

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

- Molecule 10 is a protein called 50S ribosomal protein L5.

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

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	F	175	1313	826	241	244	2	0	0

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	G	149	1111	699	197	214	1	0	0

- Molecule 13 is a protein called 50S ribosomal protein L13.

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

- Molecule 14 is a protein called 50S ribosomal protein L14.

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

- Molecule 15 is a protein called 50S ribosomal protein L15.

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

- Molecule 16 is a protein called 50S ribosomal protein L16.

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

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	N	119	951	588	195	163	5	0	0

- Molecule 18 is a protein called 50S ribosomal protein L18.

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

- Molecule 19 is a protein called 50S ribosomal protein L19.

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

- Molecule 20 is a protein called 50S ribosomal protein L20.

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

- Molecule 21 is a protein called 50S ribosomal protein L21.

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

- Molecule 22 is a protein called 50S ribosomal protein L22.

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

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	T	94	746	470	140	134	2	0	0

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	U	103	788	498	148	142	0	0

- Molecule 25 is a protein called 50S ribosomal protein L25.

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

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	W	76	582	360	117	104	1	0	0

- Molecule 27 is a protein called 50S ribosomal protein L28.

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

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

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

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Z	58	448	281	87	78	2	0	0

- Molecule 30 is a protein called 50S ribosomal protein L31.

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

- Molecule 31 is a protein called 50S ribosomal protein L32.

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

- Molecule 32 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	c	52	426	275	78	73	0	0

- Molecule 33 is a protein called 50S ribosomal protein L34.

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

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L36.

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

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	g	225	1760	1113	316	323	8	0	0

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	h	208	1636	1036	307	290	3	0	0

- Molecule 38 is a protein called 30S ribosomal protein S4.

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

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	j	156	1152	717	217	212	6	0	0

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	k	104	848	536	153	152	7	0	0

- Molecule 41 is a protein called 30S ribosomal protein S7.

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

- Molecule 42 is a protein called 30S ribosomal protein S8.

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

- Molecule 43 is a protein called 30S ribosomal protein S9.

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

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	o	99	790	495	151	143	1	0	0

- Molecule 45 is a protein called 30S ribosomal protein S11.

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

- Molecule 46 is a protein called 30S ribosomal protein S12.

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

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	r	116	900	558	181	158	3	0	0

- Molecule 48 is a protein called 30S ribosomal protein S14.

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

- Molecule 49 is a protein called 30S ribosomal protein S15.

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

- Molecule 50 is a protein called 30S ribosomal protein S16.

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

- Molecule 51 is a protein called 30S ribosomal protein S17.

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

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	w	66	544	344	102	97	1	0	0

- Molecule 53 is a protein called 30S ribosomal protein S19.

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

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	y	86	669	414	138	114	3	0	0

- Molecule 55 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	z	70	589	366	125	97	1	0	0

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
56	1	290	290	290	0
56	2	126	126	126	0
56	3	8	8	8	0
56	5	4	4	4	0
56	B	1	1	1	0
56	C	1	1	1	0
56	Q	1	1	1	0
56	b	2	2	2	0
56	f	1	1	1	0
56	i	1	1	1	0
56	r	1	1	1	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

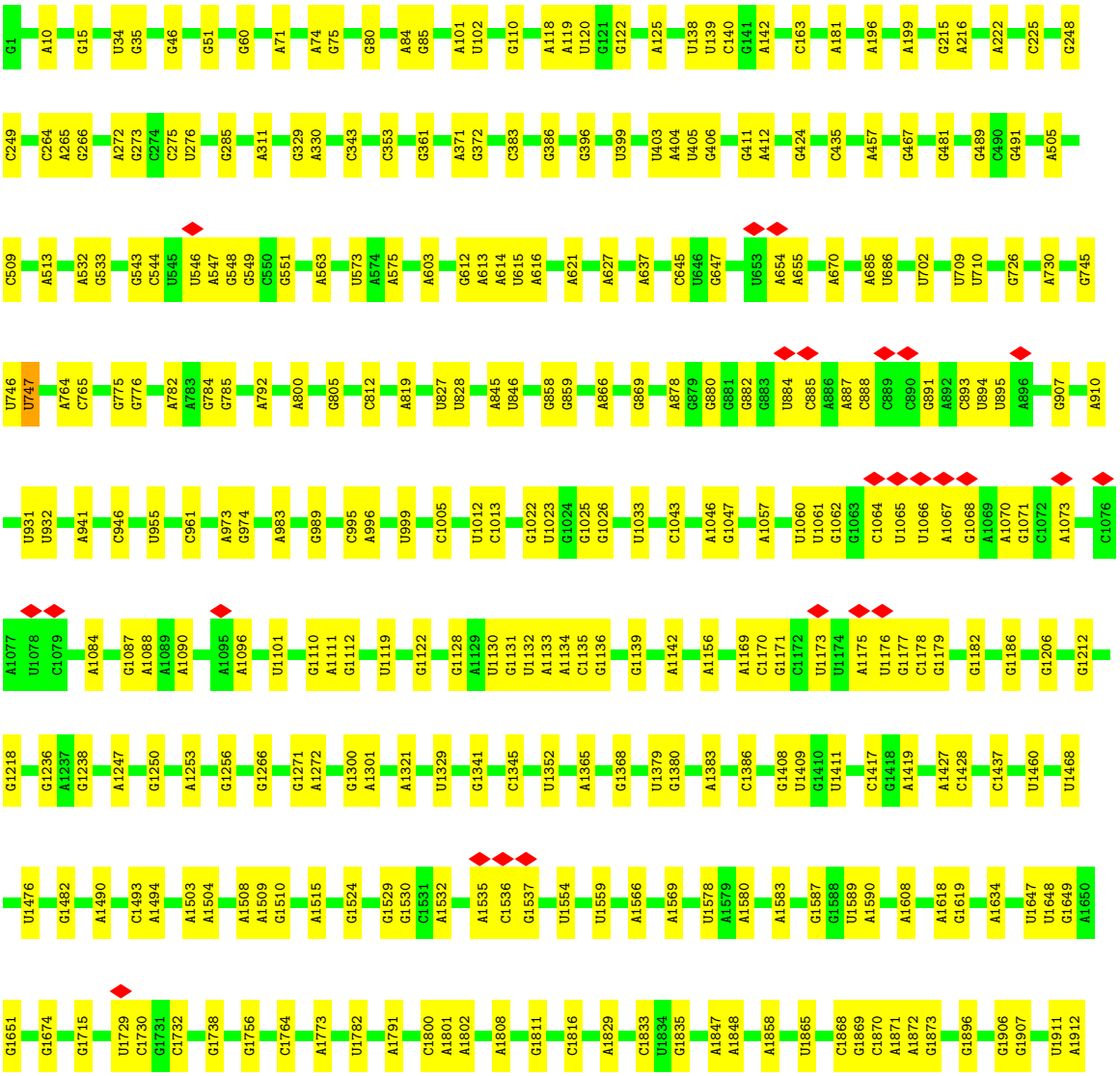
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
57	a	1	1	1	0
57	f	1	1	1	0

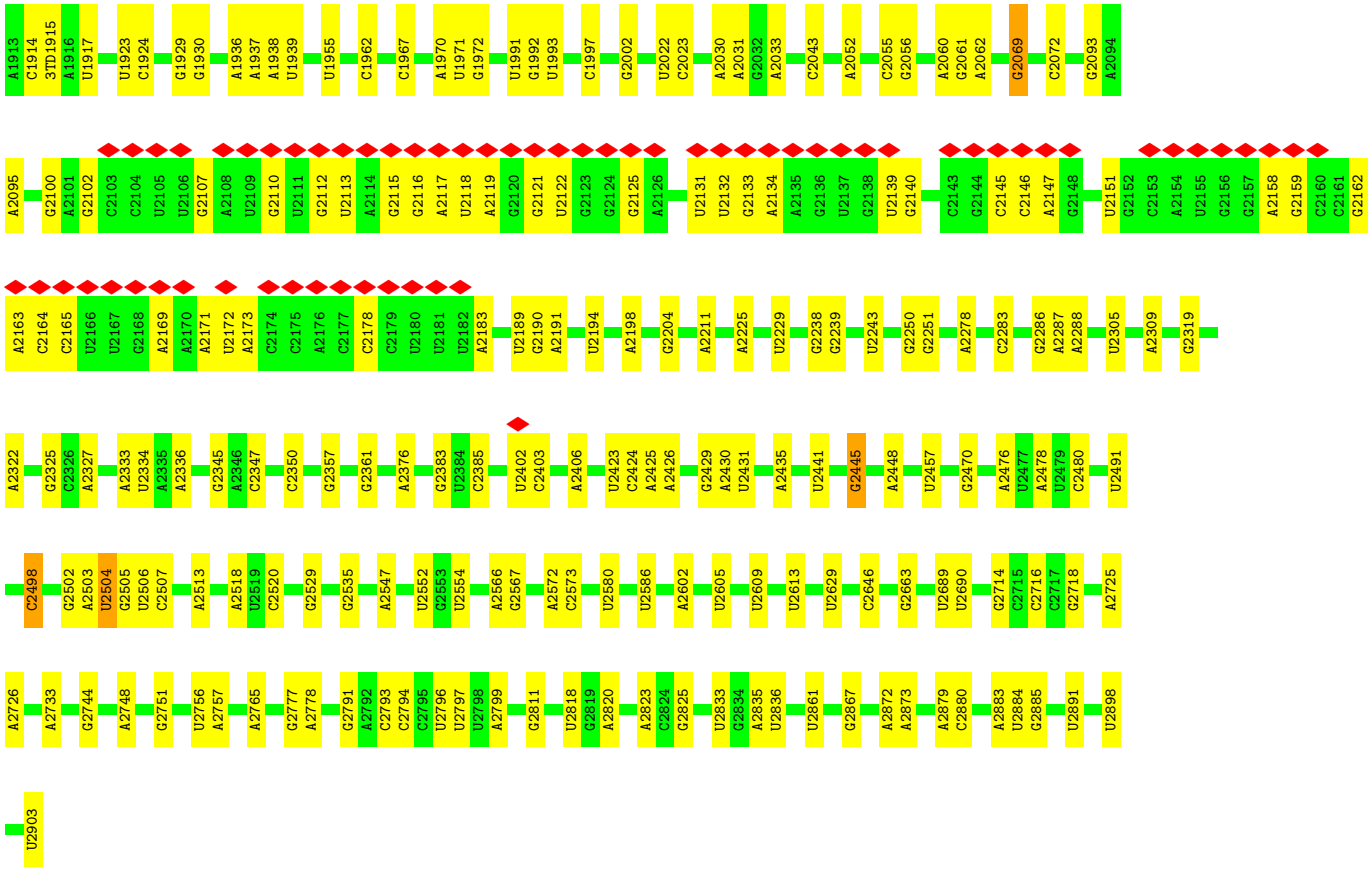
3 Residue-property plots (i)

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

- Molecule 1: 23S ribosomal RNA

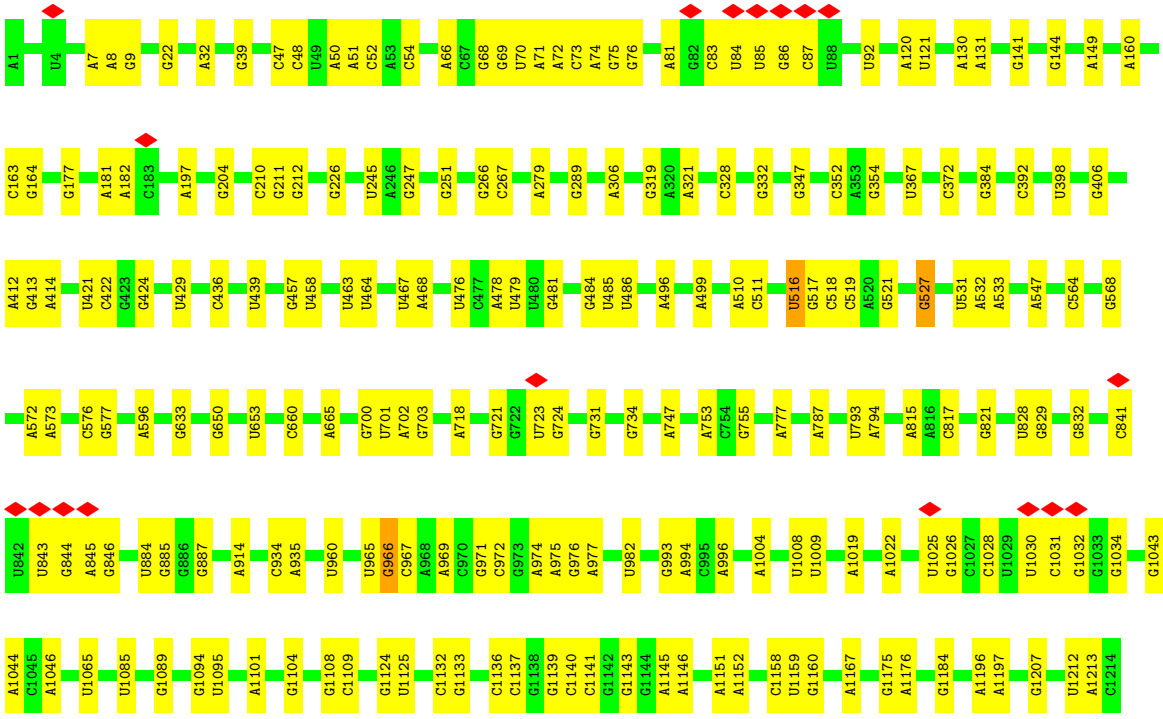
Chain 1:

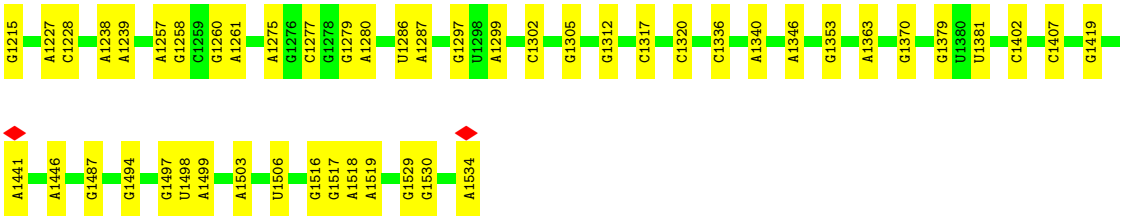




- Molecule 2: 16S ribosomal RNA

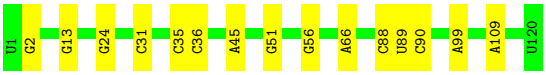
Chain 2:





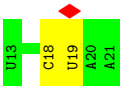
• Molecule 3: 5S ribosomal RNA

Chain 3:



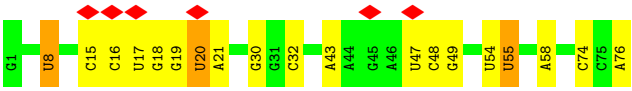
• Molecule 4: RNA (5'-R(P*UP*UP*CP*UP*UP*CP*UP*AP*A)-3')

Chain 4:



• Molecule 5: P-tRNA

Chain 5:

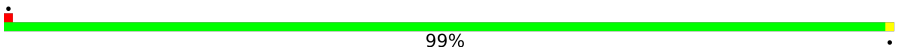


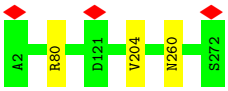
• Molecule 6: FME-PHE-PHE

Chain A:

• Molecule 7: 50S ribosomal protein L2

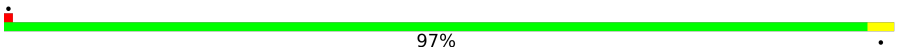
Chain B:

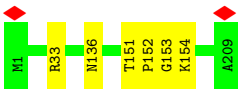




• Molecule 8: 50S ribosomal protein L3

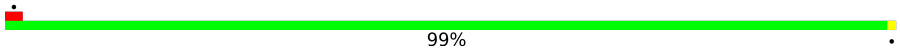
Chain C:

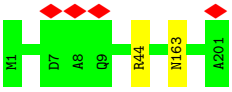




• Molecule 9: 50S ribosomal protein L4

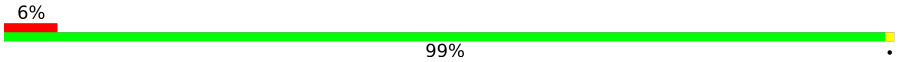
Chain D:

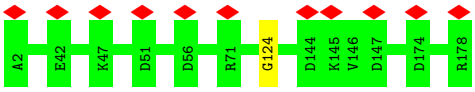




• Molecule 10: 50S ribosomal protein L5

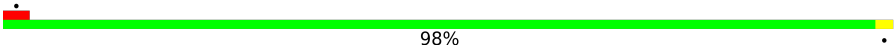
Chain E:

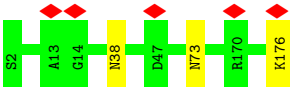




• Molecule 11: 50S ribosomal protein L6

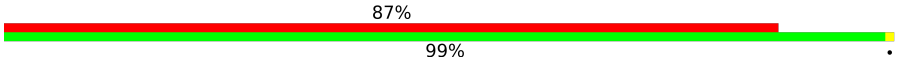
Chain F:

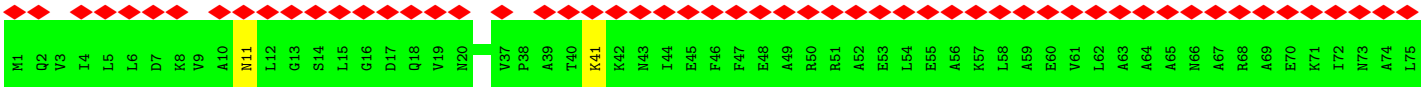


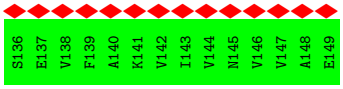


• Molecule 12: 50S ribosomal protein L9

Chain G:

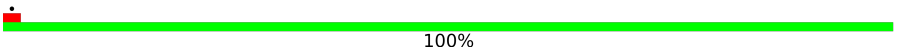




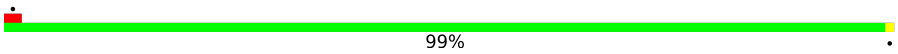


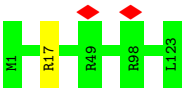
• Molecule 13: 50S ribosomal protein L13

Chain J:

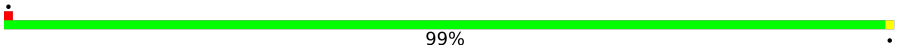


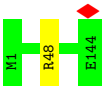
• Molecule 14: 50S ribosomal protein L14

Chain K: 

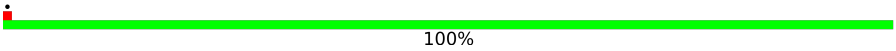


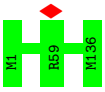
• Molecule 15: 50S ribosomal protein L15

Chain L: 

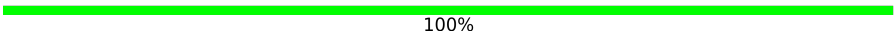


• Molecule 16: 50S ribosomal protein L16

Chain M: 

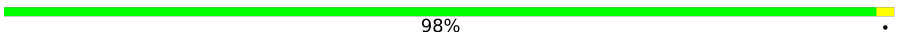


• Molecule 17: 50S ribosomal protein L17

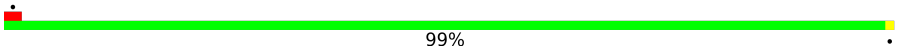
Chain N: 

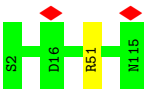
There are no outlier residues recorded for this chain.

• Molecule 18: 50S ribosomal protein L18

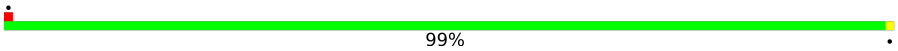
Chain O: 

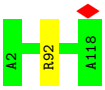
• Molecule 19: 50S ribosomal protein L19

Chain P: 

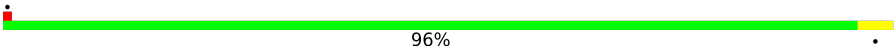


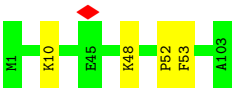
• Molecule 20: 50S ribosomal protein L20

Chain Q: 

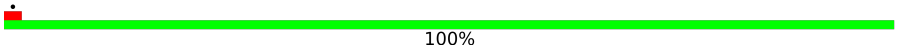


• Molecule 21: 50S ribosomal protein L21

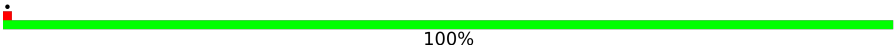
Chain R: 



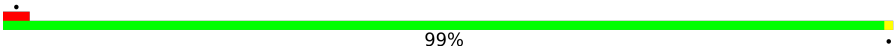
• Molecule 22: 50S ribosomal protein L22

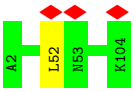
Chain S: 

• Molecule 23: 50S ribosomal protein L23

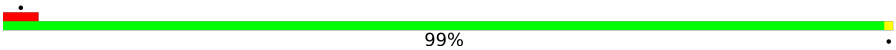
Chain T: 

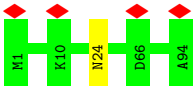
• Molecule 24: 50S ribosomal protein L24

Chain U: 

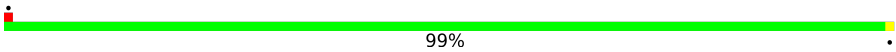


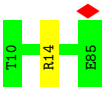
• Molecule 25: 50S ribosomal protein L25

Chain V: 

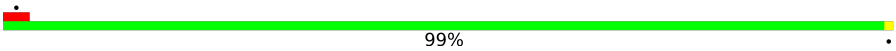


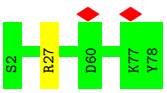
• Molecule 26: 50S ribosomal protein L27

Chain W: 



• Molecule 27: 50S ribosomal protein L28

Chain X: 

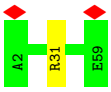


• Molecule 28: 50S ribosomal protein L29

Chain Y: 100%

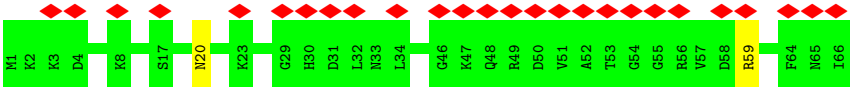
• Molecule 29: 50S ribosomal protein L30

Chain Z: 98%



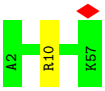
• Molecule 30: 50S ribosomal protein L31

Chain a: 39% 97%



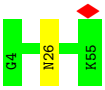
• Molecule 31: 50S ribosomal protein L32

Chain b: 98%



• Molecule 32: 50S ribosomal protein L33

Chain c: 98%

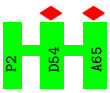


• Molecule 33: 50S ribosomal protein L34

Chain d: 100%

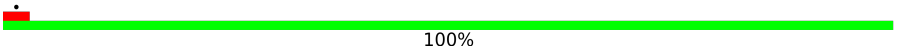
• Molecule 34: 50S ribosomal protein L35

Chain e: 100%



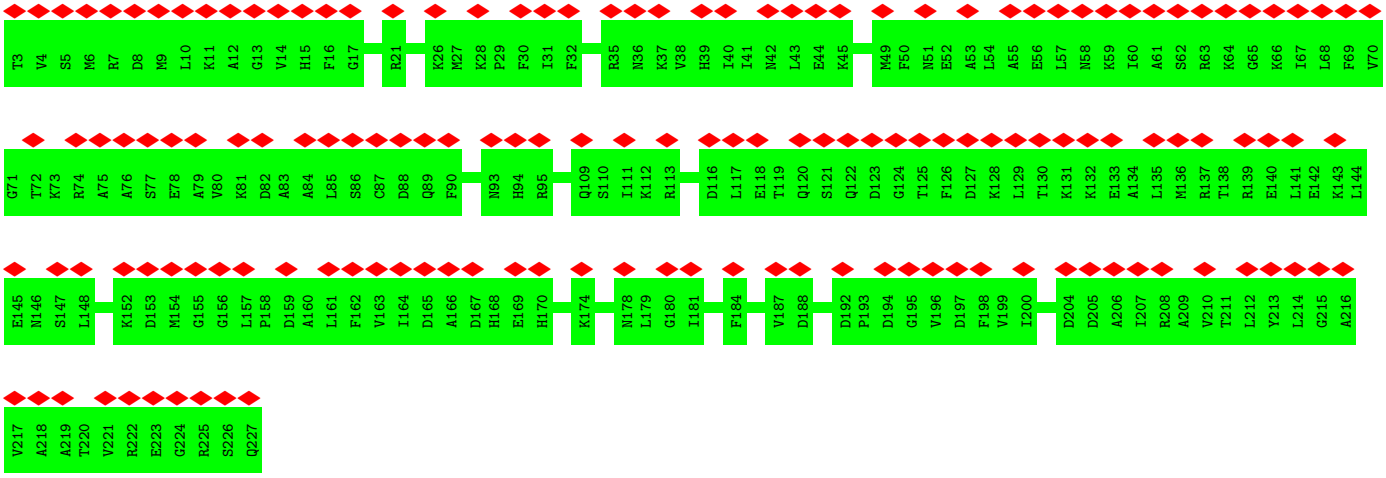
• Molecule 35: 50S ribosomal protein L36

Chain f:



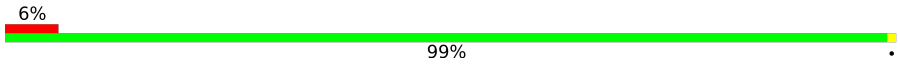
• Molecule 36: 30S ribosomal protein S2

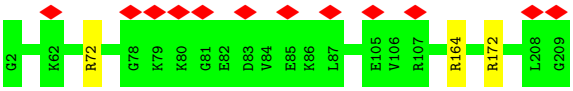
Chain g:



• Molecule 37: 30S ribosomal protein S3

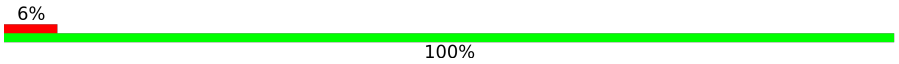
Chain h:

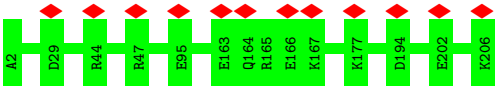




• Molecule 38: 30S ribosomal protein S4

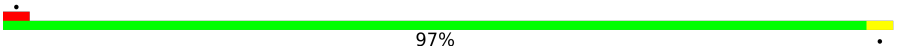
Chain i:

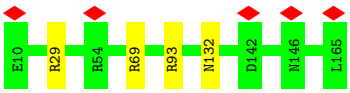




• Molecule 39: 30S ribosomal protein S5

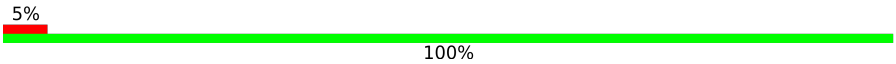
Chain j:

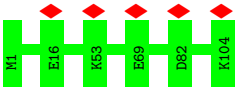




• Molecule 40: 30S ribosomal protein S6

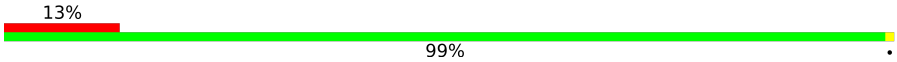
Chain k:

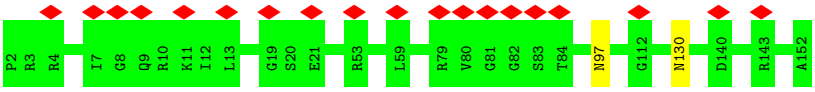




• Molecule 41: 30S ribosomal protein S7

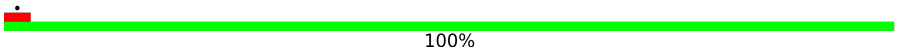
Chain l:

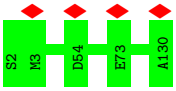




• Molecule 42: 30S ribosomal protein S8

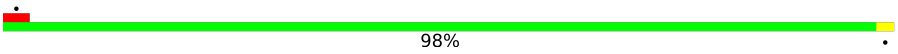
Chain m:

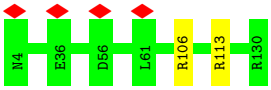




• Molecule 43: 30S ribosomal protein S9

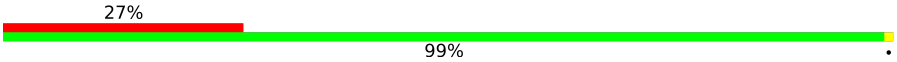
Chain n:

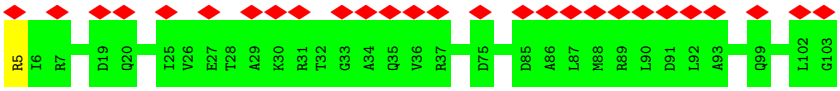




• Molecule 44: 30S ribosomal protein S10

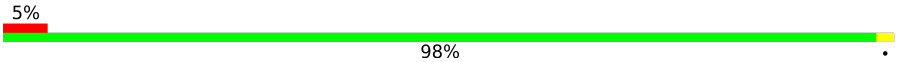
Chain o:

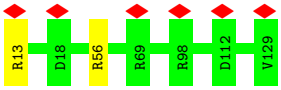




• Molecule 45: 30S ribosomal protein S11

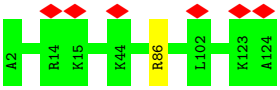
Chain p:





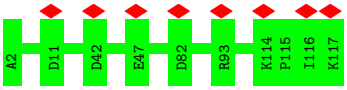
• Molecule 46: 30S ribosomal protein S12

Chain q: 5% 99%



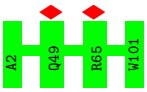
• Molecule 47: 30S ribosomal protein S13

Chain r: 7% 100%



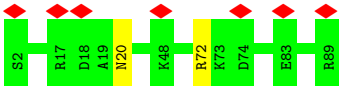
• Molecule 48: 30S ribosomal protein S14

Chain s: 100%



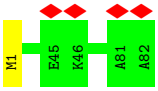
• Molecule 49: 30S ribosomal protein S15

Chain t: 8% 98%



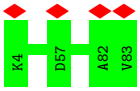
• Molecule 50: 30S ribosomal protein S16

Chain u: 5% 99%



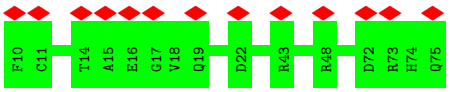
• Molecule 51: 30S ribosomal protein S17

Chain v: 5% 100%



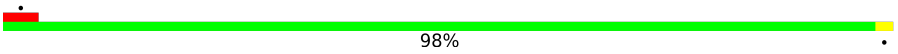
• Molecule 52: 30S ribosomal protein S18

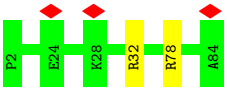
Chain w: 20% 100%



• Molecule 53: 30S ribosomal protein S19

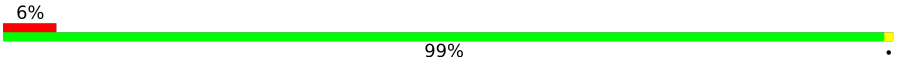
Chain x:

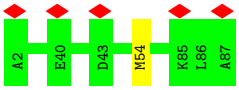




• Molecule 54: 30S ribosomal protein S20

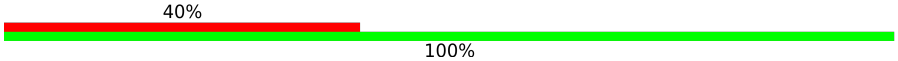
Chain y:

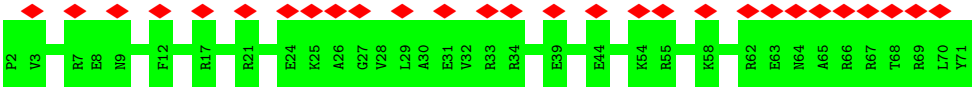




• Molecule 55: 30S ribosomal protein S21

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	135250	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	41.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.081	Depositor
Minimum map value	-0.028	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	475.008, 475.008, 475.008	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.237, 1.237, 1.237	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 4OC, G7M, OMU, FME, 1MG, 2MG, H2U, OMG, UR3, 6MZ, 0TD, PSU, MA6, 3TD, 5MC, 5MU, ZN, MG, 2MA, 4SU, OMC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	1	0.92	0/69286	0.92	0/108087
2	2	0.73	0/36590	0.90	0/57074
3	3	0.78	0/2872	0.93	0/4478
4	4	0.53	0/203	0.95	0/312
5	5	0.58	0/1704	0.92	0/2654
6	A	0.48	0/23	0.30	0/29
7	B	0.49	0/2121	0.58	0/2852
8	C	0.48	0/1586	0.60	0/2134
9	D	0.45	0/1571	0.53	0/2113
10	E	0.38	0/1434	0.54	0/1926
11	F	0.37	0/1333	0.52	0/1805
12	G	0.29	0/1122	0.55	0/1515
13	J	0.47	0/1152	0.51	0/1551
14	K	0.46	0/955	0.57	0/1279
15	L	0.44	0/1062	0.61	0/1413
16	M	0.46	0/1093	0.55	0/1460
17	N	0.45	0/964	0.58	0/1289
18	O	0.41	0/902	0.53	0/1209
19	P	0.47	0/929	0.52	0/1242
20	Q	0.52	0/960	0.51	0/1278
21	R	0.48	0/829	0.59	0/1107
22	S	0.44	0/864	0.53	0/1156
23	T	0.41	0/752	0.53	0/1005
24	U	0.43	0/796	0.54	0/1062
25	V	0.40	0/766	0.52	0/1025
26	W	0.47	0/589	0.54	0/779
27	X	0.43	0/635	0.51	0/848
28	Y	0.35	0/502	0.49	0/667
29	Z	0.39	0/452	0.55	0/605
30	a	0.35	0/531	0.47	0/709
31	b	0.44	0/450	0.57	0/599

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	c	0.42	0/433	0.53	0/576
33	d	0.46	0/380	0.57	0/498
34	e	0.47	0/513	0.58	0/676
35	f	0.45	0/303	0.51	0/397
36	g	0.30	0/1791	0.52	0/2413
37	h	0.37	0/1663	0.52	0/2241
38	i	0.35	0/1665	0.48	0/2227
39	j	0.42	0/1165	0.59	0/1568
40	k	0.39	0/867	0.56	0/1171
41	l	0.33	0/1195	0.51	0/1602
42	m	0.39	0/989	0.53	0/1326
43	n	0.36	0/1034	0.56	0/1375
44	o	0.38	0/800	0.57	0/1082
45	p	0.38	0/893	0.51	0/1205
46	q	0.40	0/960	0.59	0/1286
47	r	0.35	0/909	0.55	0/1215
48	s	0.36	0/817	0.49	0/1088
49	t	0.34	0/722	0.49	0/964
50	u	0.38	0/659	0.56	0/884
51	v	0.37	0/657	0.56	0/881
52	w	0.37	0/553	0.48	0/743
53	x	0.34	0/680	0.51	0/915
54	y	0.32	0/675	0.44	0/895
55	z	0.32	0/597	0.46	0/792
All	All	0.75	0/155948	0.83	0/233282

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
6	A	1/3 (33%)	1 (100%)	0	0	100	100
7	B	269/271 (99%)	257 (96%)	12 (4%)	0	100	100
8	C	207/209 (99%)	201 (97%)	3 (1%)	3 (1%)	11	36
9	D	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
10	E	175/177 (99%)	164 (94%)	10 (6%)	1 (1%)	25	58
11	F	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
12	G	147/149 (99%)	141 (96%)	6 (4%)	0	100	100
13	J	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
14	K	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
15	L	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
16	M	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
17	N	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
18	O	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
19	P	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
20	Q	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
21	R	101/103 (98%)	93 (92%)	6 (6%)	2 (2%)	7	27
22	S	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
23	T	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
24	U	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
25	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
26	W	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
27	X	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
28	Y	60/62 (97%)	60 (100%)	0	0	100	100
29	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
30	a	64/66 (97%)	59 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	b	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
32	c	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
33	d	44/46 (96%)	44 (100%)	0	0	100	100
34	e	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
35	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
36	g	223/225 (99%)	208 (93%)	15 (7%)	0	100	100
37	h	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
38	i	203/205 (99%)	200 (98%)	3 (2%)	0	100	100
39	j	154/156 (99%)	145 (94%)	9 (6%)	0	100	100
40	k	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
41	l	149/151 (99%)	146 (98%)	3 (2%)	0	100	100
42	m	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
43	n	125/127 (98%)	119 (95%)	6 (5%)	0	100	100
44	o	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
45	p	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
46	q	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
47	r	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
48	s	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
49	t	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
50	u	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
51	v	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
52	w	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
53	x	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
54	y	84/86 (98%)	84 (100%)	0	0	100	100
55	z	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
All	All	5609/5710 (98%)	5415 (96%)	188 (3%)	6 (0%)	54	82

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	C	152	PRO
8	C	153	GLY
8	C	154	LYS

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Mol	Chain	Res	Type
21	R	52	PRO
21	R	53	PHE
10	E	124	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	A	2/2 (100%)	0	2 (100%)	0 0
7	B	216/216 (100%)	213 (99%)	3 (1%)	67 89
8	C	164/164 (100%)	161 (98%)	3 (2%)	59 85
9	D	165/165 (100%)	163 (99%)	2 (1%)	71 91
10	E	148/148 (100%)	148 (100%)	0	100 100
11	F	136/136 (100%)	133 (98%)	3 (2%)	52 81
12	G	114/114 (100%)	112 (98%)	2 (2%)	59 85
13	J	116/116 (100%)	116 (100%)	0	100 100
14	K	104/104 (100%)	103 (99%)	1 (1%)	76 92
15	L	103/103 (100%)	102 (99%)	1 (1%)	76 92
16	M	109/109 (100%)	109 (100%)	0	100 100
17	N	99/99 (100%)	99 (100%)	0	100 100
18	O	86/86 (100%)	84 (98%)	2 (2%)	50 80
19	P	99/99 (100%)	98 (99%)	1 (1%)	76 92
20	Q	89/89 (100%)	88 (99%)	1 (1%)	73 92
21	R	84/84 (100%)	82 (98%)	2 (2%)	49 79
22	S	93/93 (100%)	93 (100%)	0	100 100
23	T	81/81 (100%)	81 (100%)	0	100 100
24	U	84/84 (100%)	83 (99%)	1 (1%)	71 91
25	V	78/78 (100%)	77 (99%)	1 (1%)	69 90
26	W	58/58 (100%)	57 (98%)	1 (2%)	60 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	X	67/67 (100%)	66 (98%)	1 (2%)	65	87
28	Y	54/54 (100%)	54 (100%)	0	100	100
29	Z	48/48 (100%)	47 (98%)	1 (2%)	53	81
30	a	59/59 (100%)	57 (97%)	2 (3%)	37	71
31	b	47/47 (100%)	46 (98%)	1 (2%)	53	81
32	c	47/47 (100%)	46 (98%)	1 (2%)	53	81
33	d	38/38 (100%)	38 (100%)	0	100	100
34	e	51/51 (100%)	51 (100%)	0	100	100
35	f	34/34 (100%)	34 (100%)	0	100	100
36	g	187/187 (100%)	187 (100%)	0	100	100
37	h	171/171 (100%)	168 (98%)	3 (2%)	59	85
38	i	172/172 (100%)	172 (100%)	0	100	100
39	j	119/119 (100%)	115 (97%)	4 (3%)	37	71
40	k	91/91 (100%)	91 (100%)	0	100	100
41	l	124/124 (100%)	122 (98%)	2 (2%)	62	86
42	m	104/104 (100%)	104 (100%)	0	100	100
43	n	105/105 (100%)	103 (98%)	2 (2%)	57	84
44	o	86/86 (100%)	85 (99%)	1 (1%)	71	91
45	p	90/90 (100%)	88 (98%)	2 (2%)	52	81
46	q	102/102 (100%)	101 (99%)	1 (1%)	76	92
47	r	94/94 (100%)	94 (100%)	0	100	100
48	s	83/83 (100%)	83 (100%)	0	100	100
49	t	76/76 (100%)	74 (97%)	2 (3%)	46	77
50	u	65/65 (100%)	64 (98%)	1 (2%)	65	87
51	v	74/74 (100%)	74 (100%)	0	100	100
52	w	57/57 (100%)	57 (100%)	0	100	100
53	x	72/72 (100%)	70 (97%)	2 (3%)	43	76
54	y	65/65 (100%)	64 (98%)	1 (2%)	65	87
55	z	60/60 (100%)	60 (100%)	0	100	100
All	All	4670/4670 (100%)	4617 (99%)	53 (1%)	74	92

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	A	78	PHE
6	A	77	PHE
7	B	80	ARG
7	B	204	VAL
7	B	260	ASN
8	C	33	ARG
8	C	136	ASN
8	C	151	THR
9	D	44	ARG
9	D	163	ASN
11	F	38	ASN
11	F	73	ASN
11	F	176	LYS
12	G	11	ASN
12	G	41	LYS
14	K	17	ARG
15	L	48	ARG
18	O	25	ARG
18	O	94	ARG
19	P	51	ARG
20	Q	92	ARG
21	R	10	LYS
21	R	48	LYS
24	U	52	LEU
25	V	24	ASN
26	W	14	ARG
27	X	27	ARG
29	Z	31	ARG
30	a	20	ASN
30	a	59	ARG
31	b	10	ARG
32	c	26	ASN
37	h	72	ARG
37	h	164	ARG
37	h	172	ARG
39	j	29	ARG
39	j	69	ARG
39	j	93	ARG
39	j	132	ASN
41	l	97	ASN
41	l	130	ASN
43	n	106	ARG
43	n	113	ARG

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Mol	Chain	Res	Type
44	o	5	ARG
45	p	13	ARG
45	p	56	ARG
46	q	86	ARG
49	t	20	ASN
49	t	72	ARG
50	u	1	MET
53	x	32	ARG
53	x	78	ARG
54	y	54	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
7	B	53	HIS
7	B	86	ASN
7	B	260	ASN
8	C	32	ASN
8	C	49	GLN
8	C	136	ASN
8	C	150	GLN
9	D	163	ASN
11	F	38	ASN
11	F	88	GLN
12	G	11	ASN
18	O	29	HIS
18	O	38	GLN
20	Q	44	GLN
22	S	61	ASN
25	V	24	ASN
29	Z	20	HIS
30	a	20	ASN
32	c	26	ASN
36	g	39	HIS
36	g	177	ASN
38	i	59	GLN
38	i	116	GLN
39	j	132	ASN
40	k	63	ASN
41	l	97	ASN
41	l	130	ASN
43	n	32	GLN

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Mol	Chain	Res	Type
45	p	119	ASN
46	q	5	ASN
49	t	20	ASN
53	x	52	HIS
53	x	57	HIS
54	y	3	ASN
54	y	52	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2898/2903 (99%)	495 (17%)	9 (0%)
2	2	1529/1534 (99%)	255 (16%)	3 (0%)
3	3	119/120 (99%)	15 (12%)	0
4	4	8/9 (88%)	2 (25%)	0
5	5	74/76 (97%)	17 (22%)	1 (1%)
All	All	4628/4642 (99%)	784 (16%)	13 (0%)

All (784) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	15	G
1	1	34	U
1	1	35	G
1	1	46	G
1	1	51	G
1	1	60	G
1	1	71	A
1	1	74	A
1	1	75	G
1	1	80	G
1	1	84	A
1	1	85	G
1	1	101	A
1	1	102	U
1	1	110	G
1	1	118	A
1	1	119	A
1	1	120	U
1	1	122	G

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Mol	Chain	Res	Type
1	1	125	A
1	1	138	U
1	1	139	U
1	1	140	C
1	1	142	A
1	1	163	C
1	1	181	A
1	1	196	A
1	1	199	A
1	1	215	G
1	1	216	A
1	1	222	A
1	1	225	C
1	1	248	G
1	1	249	C
1	1	264	C
1	1	265	A
1	1	266	G
1	1	272	A
1	1	273	G
1	1	275	C
1	1	276	U
1	1	285	G
1	1	311	A
1	1	329	G
1	1	330	A
1	1	343	C
1	1	353	C
1	1	361	G
1	1	371	A
1	1	372	G
1	1	383	C
1	1	386	G
1	1	396	G
1	1	399	U
1	1	403	U
1	1	405	U
1	1	406	G
1	1	411	G
1	1	412	A
1	1	424	G
1	1	435	C

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Mol	Chain	Res	Type
1	1	457	A
1	1	467	G
1	1	481	G
1	1	489	G
1	1	491	G
1	1	505	A
1	1	509	C
1	1	513	A
1	1	532	A
1	1	533	G
1	1	543	G
1	1	544	C
1	1	546	U
1	1	547	A
1	1	548	G
1	1	549	G
1	1	551	G
1	1	563	A
1	1	573	U
1	1	575	A
1	1	603	A
1	1	612	G
1	1	613	A
1	1	614	A
1	1	615	U
1	1	616	A
1	1	621	A
1	1	627	A
1	1	637	A
1	1	645	C
1	1	647	G
1	1	654	A
1	1	655	A
1	1	670	A
1	1	685	A
1	1	686	U
1	1	702	U
1	1	709	U
1	1	710	U
1	1	726	G
1	1	730	A
1	1	747	5MU

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Mol	Chain	Res	Type
1	1	764	A
1	1	765	C
1	1	775	G
1	1	776	G
1	1	782	A
1	1	784	G
1	1	785	G
1	1	792	A
1	1	800	A
1	1	805	G
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	845	A
1	1	846	U
1	1	858	G
1	1	859	G
1	1	866	A
1	1	869	G
1	1	878	A
1	1	880	G
1	1	882	G
1	1	884	U
1	1	885	C
1	1	887	A
1	1	888	C
1	1	891	G
1	1	893	C
1	1	895	U
1	1	907	G
1	1	910	A
1	1	931	U
1	1	932	U
1	1	941	A
1	1	946	C
1	1	961	C
1	1	973	A
1	1	974	G
1	1	983	A
1	1	989	G
1	1	995	C

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Mol	Chain	Res	Type
1	1	996	A
1	1	999	U
1	1	1005	C
1	1	1012	U
1	1	1013	C
1	1	1022	G
1	1	1023	U
1	1	1025	G
1	1	1026	G
1	1	1033	U
1	1	1043	C
1	1	1046	A
1	1	1047	G
1	1	1057	A
1	1	1060	U
1	1	1061	U
1	1	1062	G
1	1	1064	C
1	1	1065	U
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1070	A
1	1	1071	G
1	1	1073	A
1	1	1084	A
1	1	1087	G
1	1	1088	A
1	1	1090	A
1	1	1096	A
1	1	1101	U
1	1	1110	G
1	1	1111	A
1	1	1112	G
1	1	1119	U
1	1	1122	G
1	1	1128	G
1	1	1130	U
1	1	1131	G
1	1	1132	U
1	1	1133	A
1	1	1134	A

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Mol	Chain	Res	Type
1	1	1135	C
1	1	1136	G
1	1	1139	G
1	1	1142	A
1	1	1156	A
1	1	1169	A
1	1	1170	C
1	1	1171	G
1	1	1173	U
1	1	1175	A
1	1	1176	U
1	1	1177	G
1	1	1178	C
1	1	1179	G
1	1	1182	G
1	1	1186	G
1	1	1206	G
1	1	1212	G
1	1	1218	G
1	1	1236	G
1	1	1238	G
1	1	1247	A
1	1	1250	G
1	1	1253	A
1	1	1256	G
1	1	1266	G
1	1	1271	G
1	1	1272	A
1	1	1300	G
1	1	1301	A
1	1	1321	A
1	1	1329	U
1	1	1341	G
1	1	1345	C
1	1	1352	U
1	1	1365	A
1	1	1368	G
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1386	C
1	1	1408	G

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Mol	Chain	Res	Type
1	1	1409	U
1	1	1411	U
1	1	1417	C
1	1	1419	A
1	1	1427	A
1	1	1428	C
1	1	1437	C
1	1	1460	U
1	1	1468	U
1	1	1476	U
1	1	1482	G
1	1	1490	A
1	1	1493	C
1	1	1494	A
1	1	1503	A
1	1	1504	A
1	1	1508	A
1	1	1509	A
1	1	1510	G
1	1	1515	A
1	1	1524	G
1	1	1529	G
1	1	1530	G
1	1	1532	A
1	1	1535	A
1	1	1536	C
1	1	1537	G
1	1	1554	U
1	1	1559	U
1	1	1566	A
1	1	1569	A
1	1	1578	U
1	1	1580	A
1	1	1583	A
1	1	1587	G
1	1	1589	U
1	1	1590	A
1	1	1608	A
1	1	1619	G
1	1	1634	A
1	1	1647	U
1	1	1648	U

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Mol	Chain	Res	Type
1	1	1649	G
1	1	1651	G
1	1	1674	G
1	1	1715	G
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1738	G
1	1	1756	G
1	1	1764	C
1	1	1773	A
1	1	1782	U
1	1	1791	A
1	1	1800	C
1	1	1801	A
1	1	1802	A
1	1	1808	A
1	1	1811	G
1	1	1816	C
1	1	1829	A
1	1	1833	C
1	1	1847	A
1	1	1848	A
1	1	1858	A
1	1	1865	U
1	1	1868	C
1	1	1869	G
1	1	1870	C
1	1	1871	A
1	1	1872	A
1	1	1873	G
1	1	1896	G
1	1	1906	G
1	1	1907	G
1	1	1912	A
1	1	1914	C
1	1	1923	U
1	1	1924	C
1	1	1929	G
1	1	1930	G
1	1	1936	A
1	1	1937	A

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Mol	Chain	Res	Type
1	1	1938	A
1	1	1955	U
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1991	U
1	1	1992	G
1	1	1993	U
1	1	1997	C
1	1	2002	G
1	1	2022	U
1	1	2023	C
1	1	2031	A
1	1	2033	A
1	1	2043	C
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2069	G7M
1	1	2072	C
1	1	2093	G
1	1	2095	A
1	1	2100	G
1	1	2102	G
1	1	2107	G
1	1	2110	G
1	1	2112	G
1	1	2113	U
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2119	A
1	1	2121	G
1	1	2122	U
1	1	2125	G
1	1	2131	U
1	1	2132	U

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Mol	Chain	Res	Type
1	1	2133	G
1	1	2134	A
1	1	2139	U
1	1	2140	G
1	1	2145	C
1	1	2146	C
1	1	2147	A
1	1	2151	U
1	1	2158	A
1	1	2159	G
1	1	2162	G
1	1	2163	A
1	1	2164	C
1	1	2165	C
1	1	2169	A
1	1	2171	A
1	1	2172	U
1	1	2173	A
1	1	2178	C
1	1	2183	A
1	1	2189	U
1	1	2190	G
1	1	2191	A
1	1	2194	U
1	1	2198	A
1	1	2204	G
1	1	2211	A
1	1	2225	A
1	1	2229	U
1	1	2238	G
1	1	2239	G
1	1	2243	U
1	1	2250	G
1	1	2278	A
1	1	2283	C
1	1	2286	G
1	1	2287	A
1	1	2288	A
1	1	2305	U
1	1	2309	A
1	1	2319	G
1	1	2322	A

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Mol	Chain	Res	Type
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2334	U
1	1	2336	A
1	1	2345	G
1	1	2347	C
1	1	2350	C
1	1	2357	G
1	1	2361	G
1	1	2376	A
1	1	2383	G
1	1	2385	C
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2423	U
1	1	2424	C
1	1	2425	A
1	1	2426	A
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2435	A
1	1	2441	U
1	1	2445	2MG
1	1	2448	A
1	1	2470	G
1	1	2476	A
1	1	2478	A
1	1	2480	C
1	1	2491	U
1	1	2498	OMC
1	1	2502	G
1	1	2504	PSU
1	1	2505	G
1	1	2506	U
1	1	2507	C
1	1	2513	A
1	1	2518	A
1	1	2520	C
1	1	2529	G

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Mol	Chain	Res	Type
1	1	2535	G
1	1	2547	A
1	1	2554	U
1	1	2566	A
1	1	2567	G
1	1	2572	A
1	1	2573	C
1	1	2586	U
1	1	2602	A
1	1	2609	U
1	1	2613	U
1	1	2629	U
1	1	2646	C
1	1	2663	G
1	1	2689	U
1	1	2690	U
1	1	2714	G
1	1	2716	C
1	1	2718	G
1	1	2725	A
1	1	2726	A
1	1	2733	A
1	1	2744	G
1	1	2748	A
1	1	2751	G
1	1	2757	A
1	1	2765	A
1	1	2777	G
1	1	2778	A
1	1	2791	G
1	1	2793	C
1	1	2794	C
1	1	2796	U
1	1	2797	U
1	1	2799	A
1	1	2811	G
1	1	2818	U
1	1	2820	A
1	1	2823	A
1	1	2825	G
1	1	2833	U
1	1	2835	A

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Mol	Chain	Res	Type
1	1	2836	U
1	1	2861	U
1	1	2867	G
1	1	2872	A
1	1	2873	A
1	1	2879	A
1	1	2880	C
1	1	2883	A
1	1	2884	U
1	1	2885	G
1	1	2891	U
1	1	2898	U
1	1	2903	U
2	2	7	A
2	2	8	A
2	2	9	G
2	2	22	G
2	2	32	A
2	2	39	G
2	2	47	C
2	2	48	C
2	2	50	A
2	2	51	A
2	2	52	C
2	2	54	C
2	2	66	A
2	2	68	G
2	2	69	G
2	2	70	U
2	2	71	A
2	2	72	A
2	2	73	C
2	2	74	A
2	2	75	G
2	2	76	G
2	2	81	A
2	2	83	C
2	2	84	U
2	2	85	U
2	2	86	G
2	2	87	C
2	2	92	U

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Mol	Chain	Res	Type
2	2	120	A
2	2	121	U
2	2	130	A
2	2	131	A
2	2	141	G
2	2	144	G
2	2	149	A
2	2	160	A
2	2	163	C
2	2	164	G
2	2	177	G
2	2	181	A
2	2	182	A
2	2	197	A
2	2	204	G
2	2	210	C
2	2	211	G
2	2	212	G
2	2	226	G
2	2	245	U
2	2	247	G
2	2	251	G
2	2	266	G
2	2	267	C
2	2	279	A
2	2	289	G
2	2	306	A
2	2	319	G
2	2	321	A
2	2	328	C
2	2	332	G
2	2	347	G
2	2	352	C
2	2	354	G
2	2	367	U
2	2	372	C
2	2	384	G
2	2	392	C
2	2	398	U
2	2	406	G
2	2	412	A
2	2	413	G

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Mol	Chain	Res	Type
2	2	414	A
2	2	421	U
2	2	422	C
2	2	424	G
2	2	429	U
2	2	436	C
2	2	439	U
2	2	457	G
2	2	458	U
2	2	463	U
2	2	464	U
2	2	467	U
2	2	468	A
2	2	476	U
2	2	478	A
2	2	479	U
2	2	481	G
2	2	484	G
2	2	485	U
2	2	486	U
2	2	496	A
2	2	499	A
2	2	510	A
2	2	511	C
2	2	517	G
2	2	518	C
2	2	519	C
2	2	521	G
2	2	527	G7M
2	2	531	U
2	2	532	A
2	2	533	A
2	2	547	A
2	2	564	C
2	2	568	G
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	596	A
2	2	633	G
2	2	650	G

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Mol	Chain	Res	Type
2	2	653	U
2	2	660	C
2	2	665	A
2	2	700	G
2	2	701	U
2	2	702	A
2	2	703	G
2	2	718	A
2	2	721	G
2	2	723	U
2	2	724	G
2	2	731	G
2	2	734	G
2	2	747	A
2	2	753	A
2	2	755	G
2	2	777	A
2	2	787	A
2	2	793	U
2	2	794	A
2	2	815	A
2	2	817	C
2	2	821	G
2	2	828	U
2	2	829	G
2	2	832	G
2	2	841	C
2	2	843	U
2	2	844	G
2	2	845	A
2	2	846	G
2	2	884	U
2	2	885	G
2	2	887	G
2	2	914	A
2	2	934	C
2	2	935	A
2	2	960	U
2	2	965	U
2	2	966	2MG
2	2	969	A
2	2	971	G

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Mol	Chain	Res	Type
2	2	972	C
2	2	974	A
2	2	975	A
2	2	976	G
2	2	977	A
2	2	982	U
2	2	993	G
2	2	994	A
2	2	996	A
2	2	1004	A
2	2	1008	U
2	2	1009	U
2	2	1019	A
2	2	1022	A
2	2	1025	U
2	2	1026	G
2	2	1028	C
2	2	1030	U
2	2	1031	C
2	2	1032	G
2	2	1034	G
2	2	1043	G
2	2	1044	A
2	2	1046	A
2	2	1065	U
2	2	1085	U
2	2	1089	G
2	2	1094	G
2	2	1095	U
2	2	1101	A
2	2	1104	G
2	2	1108	G
2	2	1124	G
2	2	1125	U
2	2	1132	C
2	2	1133	G
2	2	1136	C
2	2	1137	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1143	G

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Mol	Chain	Res	Type
2	2	1145	A
2	2	1146	A
2	2	1151	A
2	2	1152	A
2	2	1158	C
2	2	1159	U
2	2	1160	G
2	2	1167	A
2	2	1175	G
2	2	1176	A
2	2	1184	G
2	2	1196	A
2	2	1197	A
2	2	1212	U
2	2	1213	A
2	2	1215	G
2	2	1227	A
2	2	1228	C
2	2	1238	A
2	2	1239	A
2	2	1257	A
2	2	1258	G
2	2	1260	G
2	2	1261	A
2	2	1275	A
2	2	1277	C
2	2	1279	G
2	2	1280	A
2	2	1286	U
2	2	1287	A
2	2	1297	G
2	2	1299	A
2	2	1302	C
2	2	1305	G
2	2	1312	G
2	2	1317	C
2	2	1320	C
2	2	1336	C
2	2	1340	A
2	2	1346	A
2	2	1353	G
2	2	1363	A

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Mol	Chain	Res	Type
2	2	1370	G
2	2	1379	G
2	2	1381	U
2	2	1419	G
2	2	1441	A
2	2	1446	A
2	2	1487	G
2	2	1494	G
2	2	1497	G
2	2	1499	A
2	2	1503	A
2	2	1506	U
2	2	1517	G
2	2	1529	G
2	2	1530	G
2	2	1534	A
3	3	2	G
3	3	13	G
3	3	24	G
3	3	31	C
3	3	35	C
3	3	36	C
3	3	45	A
3	3	51	G
3	3	56	G
3	3	66	A
3	3	88	C
3	3	89	U
3	3	90	C
3	3	99	A
3	3	109	A
4	4	18	C
4	4	19	U
5	5	8	4SU
5	5	15	C
5	5	16	C
5	5	17	U
5	5	18	G
5	5	19	G
5	5	20	H2U
5	5	21	A
5	5	30	G

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Mol	Chain	Res	Type
5	5	43	A
5	5	47	U
5	5	48	C
5	5	49	G
5	5	55	PSU
5	5	58	A
5	5	74	C
5	5	76	A

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	404	A
1	1	613	A
1	1	784	G
1	1	894	U
1	1	1379	U
1	1	2146	C
1	1	2189	U
1	1	2425	A
1	1	2756	U
2	2	516	PSU
2	2	1109	C
2	2	1145	A
5	5	17	U

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

40 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	$\#\|Z\| > 2$
1	PSU	1	2504	56,1	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
1	PSU	1	746	56,1	18,21,22	1.04	2 (11%)	22,30,33	1.76	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
46	0TD	q	89	46	7,9,10	1.46	0	6,11,13	1.06	0
6	FME	A	79	6	8,9,10	0.66	0	7,9,11	1.36	1 (14%)
2	5MC	2	1407	2	18,22,23	3.61	7 (38%)	26,32,35	1.00	1 (3%)
1	2MG	1	2445	1	18,26,27	2.49	7 (38%)	16,38,41	1.54	4 (25%)
1	6MZ	1	2030	1	18,25,26	2.14	4 (22%)	16,36,39	2.29	3 (18%)
2	2MG	2	1207	2	18,26,27	2.52	7 (38%)	16,38,41	1.40	4 (25%)
2	G7M	2	527	2	20,26,27	3.92	10 (50%)	17,39,42	1.09	2 (11%)
1	PSU	1	2580	1	18,21,22	1.07	2 (11%)	22,30,33	1.82	5 (22%)
1	5MU	1	747	1	19,22,23	4.56	7 (36%)	28,32,35	3.78	10 (35%)
1	PSU	1	1917	1	18,21,22	1.07	1 (5%)	22,30,33	1.70	4 (18%)
2	PSU	2	516	56,2	18,21,22	1.34	2 (11%)	22,30,33	1.96	5 (22%)
2	MA6	2	1518	2	19,26,27	1.05	1 (5%)	18,38,41	2.85	2 (11%)
1	5MU	1	1939	56,1	19,22,23	4.56	7 (36%)	28,32,35	3.84	10 (35%)
2	5MC	2	967	2	18,22,23	3.58	7 (38%)	26,32,35	1.08	2 (7%)
5	PSU	5	55	5	18,21,22	1.07	1 (5%)	22,30,33	1.72	4 (18%)
1	1MG	1	745	1	18,26,27	2.54	4 (22%)	19,39,42	1.39	3 (15%)
5	4SU	5	8	5	18,21,22	3.60	8 (44%)	26,30,33	2.26	7 (26%)
1	OMU	1	2552	1	19,22,23	2.75	8 (42%)	26,31,34	1.83	5 (19%)
1	OMC	1	2498	56,1	19,22,23	2.70	7 (36%)	26,31,34	1.03	1 (3%)
1	PSU	1	2457	1	18,21,22	1.08	3 (16%)	22,30,33	2.03	5 (22%)
1	6MZ	1	1618	1	18,25,26	2.13	3 (16%)	16,36,39	2.02	3 (18%)
1	3TD	1	1915	56,1	18,22,23	4.29	5 (27%)	22,32,35	1.62	3 (13%)
2	UR3	2	1498	2	19,22,23	2.54	6 (31%)	26,32,35	1.23	1 (3%)
5	4OC	5	32	5	20,23,24	2.94	8 (40%)	26,32,35	0.92	0
2	2MG	2	1516	2	18,26,27	2.54	7 (38%)	16,38,41	1.50	4 (25%)
2	4OC	2	1402	2	20,23,24	2.91	8 (40%)	26,32,35	0.94	2 (7%)
1	OMG	1	2251	1,5	18,26,27	2.39	8 (44%)	19,38,41	1.55	4 (21%)
1	2MA	1	2503	56,1	17,25,26	2.30	4 (23%)	17,37,40	1.28	2 (11%)
1	PSU	1	955	56,1	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
1	G7M	1	2069	1	20,26,27	2.25	7 (35%)	17,39,42	1.25	1 (5%)
5	5MU	5	54	5	19,22,23	4.71	7 (36%)	28,32,35	3.61	9 (32%)
5	H2U	5	20	5	18,21,22	3.13	5 (27%)	21,30,33	1.94	4 (19%)
2	MA6	2	1519	2	19,26,27	1.02	1 (5%)	18,38,41	2.79	2 (11%)
1	2MG	1	1835	1	18,26,27	2.47	7 (38%)	16,38,41	1.57	4 (25%)
1	PSU	1	1911	1	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	1	2605	1	18,21,22	1.02	1 (5%)	22,30,33	1.79	4 (18%)
1	5MC	1	1962	1	18,22,23	3.53	7 (38%)	26,32,35	1.10	2 (7%)
2	2MG	2	966	2	18,26,27	2.56	7 (38%)	16,38,41	1.46	3 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1	2504	56,1	-	2/7/25/26	0/2/2/2
1	PSU	1	746	56,1	-	1/7/25/26	0/2/2/2
46	0TD	q	89	46	-	2/7/12/14	-
6	FME	A	79	6	-	2/7/9/11	-
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
1	2MG	1	2445	1	-	2/5/27/28	0/3/3/3
1	6MZ	1	2030	1	-	2/5/27/28	0/3/3/3
2	2MG	2	1207	2	-	0/5/27/28	0/3/3/3
2	G7M	2	527	2	-	3/3/25/26	0/3/3/3
1	PSU	1	2580	1	-	0/7/25/26	0/2/2/2
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
2	PSU	2	516	56,2	-	2/7/25/26	0/2/2/2
2	MA6	2	1518	2	-	0/7/29/30	0/3/3/3
1	5MU	1	1939	56,1	-	0/7/25/26	0/2/2/2
2	5MC	2	967	2	-	0/7/25/26	0/2/2/2
5	PSU	5	55	5	-	2/7/25/26	0/2/2/2
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
5	4SU	5	8	5	-	3/7/25/26	0/2/2/2
1	OMU	1	2552	1	-	0/9/27/28	0/2/2/2
1	OMC	1	2498	56,1	-	1/9/27/28	0/2/2/2
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
1	6MZ	1	1618	1	-	2/5/27/28	0/3/3/3
1	3TD	1	1915	56,1	-	2/7/25/26	0/2/2/2
2	UR3	2	1498	2	-	0/7/25/26	0/2/2/2
5	4OC	5	32	5	-	0/9/29/30	0/2/2/2
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
2	4OC	2	1402	2	-	2/9/29/30	0/2/2/2
1	OMG	1	2251	1,5	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MA	1	2503	56,1	-	2/3/25/26	0/3/3/3
1	PSU	1	955	56,1	-	0/7/25/26	0/2/2/2
1	G7M	1	2069	1	-	1/3/25/26	0/3/3/3
5	5MU	5	54	5	-	0/7/25/26	0/2/2/2
5	H2U	5	20	5	-	4/7/38/39	0/2/2/2
2	MA6	2	1519	2	-	3/7/29/30	0/3/3/3
1	2MG	1	1835	1	-	2/5/27/28	0/3/3/3
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	1	1962	1	-	0/7/25/26	0/2/2/2
2	2MG	2	966	2	-	2/5/27/28	0/3/3/3

All (189) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1915	3TD	C6-C5	13.00	1.50	1.35
5	5	54	5MU	C2-N1	10.62	1.55	1.38
5	5	54	5MU	C6-N1	10.14	1.55	1.38
1	1	747	5MU	C2-N1	10.01	1.54	1.38
5	5	20	H2U	C2-N1	9.82	1.49	1.35
1	1	1939	5MU	C6-N1	9.78	1.54	1.38
2	2	527	G7M	C8-N7	9.78	1.51	1.33
1	1	747	5MU	C6-N1	9.76	1.54	1.38
1	1	1939	5MU	C2-N1	9.71	1.54	1.38
5	5	54	5MU	C4-C5	9.67	1.60	1.44
2	2	527	G7M	C8-N9	9.54	1.50	1.33
1	1	1915	3TD	C2-N1	9.44	1.49	1.37
1	1	1939	5MU	C4-C5	9.21	1.60	1.44
2	2	1407	5MC	C6-C5	9.08	1.49	1.34
2	2	967	5MC	C6-C5	8.90	1.49	1.34
1	1	1962	5MC	C6-C5	8.89	1.49	1.34
1	1	747	5MU	C4-C5	8.88	1.59	1.44
1	1	747	5MU	C4-N3	-8.52	1.23	1.38
1	1	1939	5MU	C4-N3	-8.40	1.23	1.38
5	5	54	5MU	C4-N3	-8.01	1.24	1.38
5	5	8	4SU	C2-N1	7.98	1.51	1.38
5	5	8	4SU	C4-N3	7.59	1.45	1.37
1	1	1618	6MZ	C6-N6	7.39	1.47	1.35
1	1	2030	6MZ	C6-N6	7.17	1.46	1.35
1	1	745	1MG	C2-N2	6.96	1.46	1.34
1	1	2503	2MA	C2-N3	6.81	1.45	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1962	5MC	C4-N3	6.77	1.45	1.34
2	2	967	5MC	C4-N3	6.73	1.45	1.34
5	5	32	4OC	C4-N3	6.64	1.44	1.32
2	2	1402	4OC	C4-N3	6.56	1.44	1.32
5	5	20	H2U	C2-N3	6.52	1.49	1.38
2	2	1407	5MC	C4-N3	6.47	1.45	1.34
2	2	966	2MG	C2-N2	6.23	1.47	1.33
1	1	2552	OMU	C2-N3	6.22	1.49	1.38
2	2	967	5MC	C2-N3	6.06	1.48	1.36
2	2	1207	2MG	C2-N2	6.05	1.46	1.33
2	2	1516	2MG	C2-N2	6.02	1.46	1.33
2	2	1498	UR3	C2-N1	6.00	1.47	1.38
2	2	1407	5MC	C2-N3	5.99	1.48	1.36
2	2	1498	UR3	C6-C5	5.97	1.48	1.35
1	1	2498	OMC	C6-C5	5.88	1.48	1.35
1	1	1915	3TD	C6-N1	5.88	1.46	1.36
5	5	8	4SU	C6-C5	5.87	1.48	1.35
2	2	1402	4OC	C6-C5	5.85	1.48	1.35
1	1	1835	2MG	C2-N2	5.81	1.46	1.33
5	5	32	4OC	C6-C5	5.77	1.48	1.35
1	1	1962	5MC	C2-N3	5.76	1.48	1.36
5	5	32	4OC	C2-N3	5.76	1.48	1.36
1	1	2445	2MG	C2-N2	5.73	1.46	1.33
2	2	527	G7M	C2-N3	5.73	1.47	1.33
1	1	2552	OMU	C2-N1	5.68	1.47	1.38
5	5	54	5MU	C6-C5	5.63	1.43	1.34
2	2	1402	4OC	C2-N3	5.60	1.47	1.36
5	5	8	4SU	C2-N3	5.56	1.47	1.38
1	1	2498	OMC	C2-N3	5.56	1.47	1.36
1	1	747	5MU	C6-C5	5.39	1.43	1.34
1	1	2552	OMU	C6-C5	5.38	1.47	1.35
1	1	1939	5MU	C6-C5	5.35	1.43	1.34
1	1	745	1MG	C2-N3	5.20	1.43	1.34
2	2	966	2MG	C4-N3	5.11	1.49	1.37
5	5	8	4SU	C4-S4	-5.11	1.58	1.68
1	1	2251	OMG	C2-N3	5.02	1.45	1.33
1	1	2069	G7M	C2-N3	5.02	1.45	1.33
1	1	2498	OMC	C4-N3	4.93	1.44	1.34
2	2	1207	2MG	C4-N3	4.82	1.49	1.37
5	5	20	H2U	C4-N3	4.78	1.45	1.37
2	2	967	5MC	C4-N4	4.78	1.46	1.34
1	1	1915	3TD	C2-N3	4.76	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2069	G7M	C4-N3	4.74	1.48	1.37
1	1	1962	5MC	C4-N4	4.74	1.46	1.34
2	2	1407	5MC	C4-N4	4.72	1.46	1.34
2	2	1516	2MG	C4-N3	4.72	1.48	1.37
1	1	2445	2MG	C4-N3	4.71	1.48	1.37
1	1	1835	2MG	C4-N3	4.70	1.48	1.37
1	1	745	1MG	C4-N3	4.63	1.48	1.37
2	2	527	G7M	C2-N2	4.63	1.45	1.34
2	2	1498	UR3	C2-N3	4.58	1.47	1.39
1	1	2503	2MA	C4-N3	4.57	1.48	1.37
2	2	1407	5MC	C6-N1	4.49	1.45	1.38
1	1	2251	OMG	C4-N3	4.44	1.48	1.37
1	1	2251	OMG	C2-N2	4.42	1.44	1.34
2	2	1516	2MG	C2-N1	4.29	1.43	1.36
2	2	967	5MC	C6-N1	4.22	1.45	1.38
2	2	1207	2MG	C2-N1	4.17	1.43	1.36
2	2	527	G7M	C6-N1	4.14	1.44	1.37
1	1	2069	G7M	C2-N2	4.10	1.44	1.34
2	2	966	2MG	C2-N1	4.08	1.43	1.36
2	2	1407	5MC	C2-N1	4.04	1.48	1.40
5	5	32	4OC	C4-N4	4.03	1.44	1.35
1	1	1835	2MG	C2-N1	3.94	1.43	1.36
1	1	1962	5MC	C6-N1	3.94	1.44	1.38
2	2	967	5MC	C2-N1	3.92	1.48	1.40
2	2	1402	4OC	C4-N4	3.92	1.43	1.35
2	2	527	G7M	C4-N3	3.88	1.46	1.37
1	1	2445	2MG	C2-N1	3.88	1.42	1.36
5	5	32	4OC	C2-N1	3.76	1.48	1.40
1	1	1962	5MC	C2-N1	3.64	1.47	1.40
1	1	2498	OMC	C4-N4	3.59	1.42	1.33
5	5	32	4OC	C5-C4	3.56	1.48	1.40
2	2	1402	4OC	C2-N1	3.52	1.47	1.40
2	2	1402	4OC	C5-C4	3.52	1.48	1.40
1	1	2552	OMU	C4-N3	3.50	1.44	1.38
1	1	2030	6MZ	C5-C4	-3.48	1.31	1.40
1	1	1962	5MC	O2-C2	-3.47	1.17	1.23
2	2	516	PSU	C6-C5	3.45	1.39	1.35
2	2	1407	5MC	O2-C2	-3.44	1.17	1.23
1	1	2445	2MG	O6-C6	-3.42	1.16	1.23
1	1	2498	OMC	C2-N1	3.40	1.47	1.40
2	2	527	G7M	C2-N1	3.38	1.46	1.37
5	5	55	PSU	C6-C5	3.33	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2445	2MG	C5-C4	-3.31	1.34	1.43
1	1	1835	2MG	C5-C4	-3.27	1.34	1.43
2	2	967	5MC	O2-C2	-3.26	1.17	1.23
1	1	1917	PSU	C6-C5	3.24	1.39	1.35
1	1	1835	2MG	O6-C6	-3.24	1.16	1.23
2	2	1516	2MG	C5-C4	-3.22	1.34	1.43
1	1	2498	OMC	O2-C2	-3.18	1.17	1.23
2	2	966	2MG	O6-C6	-3.17	1.16	1.23
2	2	1207	2MG	O6-C6	-3.16	1.16	1.23
1	1	745	1MG	C5-C4	-3.14	1.35	1.43
1	1	2251	OMG	C5-C4	-3.13	1.35	1.43
1	1	2552	OMU	O4-C4	-3.13	1.18	1.24
2	2	1516	2MG	O6-C6	-3.11	1.17	1.23
1	1	1618	6MZ	C5-C4	-3.11	1.32	1.40
2	2	1402	4OC	O2-C2	-3.10	1.18	1.23
2	2	1516	2MG	C6-N1	3.09	1.42	1.37
1	1	2498	OMC	C6-N1	3.08	1.45	1.38
1	1	1939	5MU	O4-C4	-3.07	1.17	1.23
2	2	1207	2MG	C5-C4	-3.07	1.35	1.43
1	1	2069	G7M	C5-C6	3.06	1.53	1.45
1	1	1911	PSU	C6-C5	3.04	1.38	1.35
1	1	2504	PSU	C6-C5	3.00	1.38	1.35
1	1	2069	G7M	C6-N1	3.00	1.42	1.37
1	1	747	5MU	O4-C4	-2.99	1.17	1.23
5	5	8	4SU	C5-C4	2.99	1.46	1.42
2	2	966	2MG	C6-N1	2.98	1.42	1.37
1	1	1939	5MU	O2-C2	-2.98	1.17	1.23
1	1	2503	2MA	C5-C4	-2.97	1.35	1.43
2	2	1207	2MG	C6-N1	2.96	1.42	1.37
1	1	1835	2MG	C6-N1	2.94	1.42	1.37
1	1	2552	OMU	O2-C2	-2.92	1.17	1.23
5	5	32	4OC	O2-C2	-2.90	1.18	1.23
1	1	2251	OMG	C6-N1	2.88	1.42	1.37
2	2	966	2MG	C5-C4	-2.87	1.35	1.43
5	5	32	4OC	C6-N1	2.85	1.44	1.38
2	2	1519	MA6	C5-C4	-2.83	1.33	1.40
1	1	747	5MU	O2-C2	-2.83	1.17	1.23
2	2	1402	4OC	C6-N1	2.80	1.44	1.38
2	2	527	G7M	C5-C6	2.80	1.52	1.45
2	2	1518	MA6	C5-C4	-2.79	1.33	1.40
1	1	955	PSU	C6-C5	2.77	1.38	1.35
1	1	1915	3TD	C4-N3	2.76	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	54	5MU	O4-C4	-2.75	1.18	1.23
1	1	2445	2MG	C6-N1	2.68	1.41	1.37
1	1	2605	PSU	C6-C5	2.64	1.38	1.35
2	2	1498	UR3	C6-N1	2.63	1.44	1.38
1	1	2251	OMG	O6-C6	-2.59	1.18	1.23
2	2	1516	2MG	C5-C6	2.53	1.52	1.47
1	1	2069	G7M	O6-C6	-2.53	1.18	1.23
2	2	1207	2MG	C5-C6	2.52	1.52	1.47
1	1	746	PSU	C6-C5	2.52	1.38	1.35
1	1	2457	PSU	C6-C5	2.51	1.38	1.35
1	1	2445	2MG	C5-C6	2.51	1.52	1.47
1	1	1618	6MZ	C2-N3	2.50	1.36	1.32
5	5	8	4SU	O2-C2	-2.49	1.18	1.23
2	2	1498	UR3	O4-C4	-2.49	1.18	1.23
1	1	2580	PSU	C6-C5	2.47	1.38	1.35
2	2	966	2MG	C5-C6	2.46	1.52	1.47
2	2	1498	UR3	O2-C2	-2.45	1.18	1.22
5	5	54	5MU	O2-C2	-2.43	1.18	1.23
1	1	2251	OMG	C5-C6	2.43	1.52	1.47
1	1	1835	2MG	C5-C6	2.40	1.52	1.47
2	2	527	G7M	O6-C6	-2.39	1.18	1.23
1	1	2552	OMU	C6-N1	2.36	1.43	1.38
2	2	516	PSU	C4-N3	-2.34	1.34	1.38
1	1	2030	6MZ	C2-N3	2.33	1.35	1.32
1	1	2030	6MZ	C6-N1	-2.32	1.30	1.34
5	5	20	H2U	O2-C2	-2.32	1.18	1.23
5	5	20	H2U	O4-C4	-2.28	1.18	1.23
1	1	2251	OMG	C2-N1	2.27	1.43	1.37
1	1	2503	2MA	C2-N1	2.27	1.43	1.36
1	1	2580	PSU	O4'-C1'	-2.24	1.40	1.43
2	2	527	G7M	C5-C4	2.23	1.43	1.39
1	1	2069	G7M	C2-N1	2.18	1.43	1.37
1	1	746	PSU	C4-C5	-2.16	1.38	1.44
1	1	2457	PSU	C4-C5	-2.07	1.38	1.44
1	1	2552	OMU	C5-C4	2.05	1.48	1.43
5	5	8	4SU	C6-N1	2.02	1.42	1.38
1	1	2457	PSU	O4'-C1'	-2.01	1.41	1.43

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1939	5MU	C5-C4-N3	12.76	126.20	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	747	5MU	C5-C4-N3	12.51	125.99	115.31
5	5	54	5MU	C5-C4-N3	12.17	125.70	115.31
1	1	1939	5MU	C5-C6-N1	-11.19	111.83	123.34
1	1	747	5MU	C5-C6-N1	-11.11	111.91	123.34
2	2	1518	MA6	N1-C6-N6	-10.14	106.38	117.06
5	5	54	5MU	C5-C6-N1	-10.09	112.96	123.34
2	2	1519	MA6	N1-C6-N6	-9.87	106.67	117.06
5	5	8	4SU	C4-N3-C2	-6.96	120.58	127.34
5	5	20	H2U	C4-N3-C2	-6.73	120.21	125.79
2	2	1518	MA6	N3-C2-N1	-6.06	119.21	128.68
2	2	1519	MA6	N3-C2-N1	-5.95	119.37	128.68
1	1	2552	OMU	C4-N3-C2	-5.69	119.08	126.58
1	1	2030	6MZ	C9-N6-C6	-5.66	117.99	122.87
1	1	2030	6MZ	N3-C2-N1	-5.64	119.86	128.68
1	1	747	5MU	O4-C4-C5	-5.52	118.50	124.90
1	1	1618	6MZ	N3-C2-N1	-5.50	120.08	128.68
1	1	1939	5MU	C4-N3-C2	-5.48	120.25	127.35
1	1	1939	5MU	O4-C4-C5	-5.43	118.61	124.90
5	5	54	5MU	O4-C4-C5	-5.39	118.66	124.90
2	2	516	PSU	N1-C2-N3	5.31	121.15	115.13
5	5	8	4SU	C5-C4-N3	5.26	119.57	114.69
1	1	2457	PSU	N1-C2-N3	5.23	121.06	115.13
1	1	747	5MU	C4-N3-C2	-5.23	120.59	127.35
1	1	2457	PSU	C4-N3-C2	-5.11	118.98	126.34
1	1	1915	3TD	N1-C2-N3	4.94	120.04	116.14
1	1	746	PSU	C4-N3-C2	-4.86	119.34	126.34
1	1	2605	PSU	C4-N3-C2	-4.86	119.34	126.34
1	1	1911	PSU	C4-N3-C2	-4.77	119.46	126.34
1	1	2580	PSU	N1-C2-N3	4.75	120.51	115.13
1	1	1618	6MZ	C9-N6-C6	-4.73	118.80	122.87
5	5	54	5MU	C4-N3-C2	-4.69	121.28	127.35
1	1	2580	PSU	C4-N3-C2	-4.66	119.62	126.34
2	2	1498	UR3	C4-N3-C2	-4.63	120.20	124.56
1	1	955	PSU	C4-N3-C2	-4.63	119.67	126.34
1	1	955	PSU	N1-C2-N3	4.60	120.34	115.13
1	1	1939	5MU	N3-C2-N1	4.60	120.99	114.89
1	1	2504	PSU	N1-C2-N3	4.57	120.31	115.13
1	1	2605	PSU	N1-C2-N3	4.52	120.26	115.13
1	1	1917	PSU	C4-N3-C2	-4.52	119.83	126.34
1	1	1911	PSU	N1-C2-N3	4.50	120.22	115.13
1	1	747	5MU	N3-C2-N1	4.49	120.85	114.89
1	1	1917	PSU	N1-C2-N3	4.48	120.21	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	5	55	PSU	N1-C2-N3	4.45	120.17	115.13
5	5	55	PSU	C4-N3-C2	-4.39	120.02	126.34
1	1	746	PSU	N1-C2-N3	4.35	120.06	115.13
1	1	2504	PSU	C4-N3-C2	-4.25	120.22	126.34
5	5	54	5MU	N3-C2-N1	4.16	120.41	114.89
1	1	2552	OMU	N3-C2-N1	4.12	120.36	114.89
5	5	8	4SU	C1'-N1-C2	4.07	124.94	117.57
2	2	516	PSU	O3'-C3'-C4'	4.06	122.80	111.05
1	1	1915	3TD	C4-N3-C2	-4.04	120.23	124.61
1	1	745	1MG	C5-C6-N1	3.97	119.88	113.90
1	1	2030	6MZ	C1'-N9-C4	-3.89	119.80	126.64
2	2	966	2MG	C5-C6-N1	3.82	120.69	113.95
1	1	1835	2MG	C5-C6-N1	3.72	120.52	113.95
2	2	967	5MC	C5-C6-N1	-3.71	119.52	123.34
1	1	2445	2MG	C5-C6-N1	3.70	120.49	113.95
5	5	54	5MU	C5M-C5-C6	-3.67	117.95	122.85
1	1	2503	2MA	C5-C6-N1	3.66	120.34	114.02
1	1	2251	OMG	C5-C6-N1	3.64	120.37	113.95
5	5	54	5MU	C5M-C5-C4	3.62	122.75	118.77
1	1	2552	OMU	C5-C4-N3	3.56	120.17	114.84
5	5	8	4SU	N3-C2-N1	3.55	119.61	114.89
1	1	1962	5MC	C5-C6-N1	-3.55	119.69	123.34
2	2	516	PSU	C4-N3-C2	-3.48	121.33	126.34
2	2	1207	2MG	C5-C6-N1	3.47	120.08	113.95
1	1	747	5MU	C5M-C5-C6	-3.47	118.22	122.85
2	2	1516	2MG	C5-C6-N1	3.40	119.95	113.95
1	1	1939	5MU	C5M-C5-C6	-3.37	118.34	122.85
1	1	2069	G7M	C2-N1-C6	-3.35	118.93	125.10
1	1	1835	2MG	CM2-N2-C2	-3.28	116.62	123.86
5	5	20	H2U	N3-C2-N1	3.28	120.12	116.65
1	1	2251	OMG	C2-N1-C6	-3.26	119.10	125.10
5	5	8	4SU	C5-C4-S4	-3.18	120.37	124.47
1	1	2445	2MG	CM2-N2-C2	-3.10	117.01	123.86
2	2	516	PSU	O2-C2-N1	-3.04	119.45	122.79
1	1	2552	OMU	O4-C4-C5	-3.02	119.84	125.16
1	1	2504	PSU	C6-N1-C2	-2.97	119.65	122.68
1	1	2552	OMU	O2-C2-N1	-2.97	118.84	122.79
2	2	1516	2MG	CM2-N2-C2	-2.94	117.37	123.86
1	1	1939	5MU	O2-C2-N1	-2.93	118.89	122.79
1	1	2457	PSU	O2-C2-N1	-2.92	119.58	122.79
1	1	1939	5MU	C5M-C5-C4	2.86	121.92	118.77
1	1	746	PSU	O2-C2-N1	-2.84	119.66	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	5	55	PSU	O2-C2-N1	-2.81	119.69	122.79
1	1	2504	PSU	O2-C2-N1	-2.79	119.72	122.79
2	2	527	G7M	C2-N1-C6	-2.76	120.01	125.10
2	2	966	2MG	O6-C6-C5	-2.76	118.98	124.37
1	1	747	5MU	C5M-C5-C4	2.74	121.78	118.77
5	5	20	H2U	C5-C6-N1	2.72	120.59	111.61
1	1	745	1MG	C8-N7-C5	2.71	108.16	102.99
1	1	2498	OMC	O2-C2-N3	-2.69	117.95	122.33
1	1	2251	OMG	C8-N7-C5	2.69	108.11	102.99
1	1	2503	2MA	C8-N7-C5	2.67	108.07	102.99
2	2	1407	5MC	C5-C6-N1	-2.65	120.61	123.34
1	1	2580	PSU	O2-C2-N1	-2.64	119.88	122.79
1	1	2445	2MG	C8-N7-C5	2.64	108.01	102.99
5	5	20	H2U	C5-C4-N3	2.62	119.59	116.65
1	1	1911	PSU	O2-C2-N1	-2.58	119.95	122.79
1	1	1939	5MU	O4-C4-N3	-2.57	115.18	120.12
1	1	2580	PSU	C6-N1-C2	-2.53	120.09	122.68
1	1	1835	2MG	O6-C6-C5	-2.52	119.44	124.37
2	2	1516	2MG	C8-N7-C5	2.51	107.77	102.99
1	1	955	PSU	O2-C2-N1	-2.50	120.04	122.79
2	2	516	PSU	O4'-C4'-C3'	-2.50	100.17	105.11
2	2	1207	2MG	C8-N7-C5	2.49	107.73	102.99
1	1	1618	6MZ	C1'-N9-C4	-2.48	122.28	126.64
1	1	1835	2MG	C8-N7-C5	2.48	107.72	102.99
1	1	2457	PSU	C6-C5-C4	2.46	119.92	118.20
1	1	747	5MU	O2-C2-N1	-2.46	119.52	122.79
1	1	2457	PSU	C6-N1-C2	-2.44	120.19	122.68
5	5	55	PSU	C6-N1-C2	-2.43	120.20	122.68
2	2	527	G7M	O6-C6-N1	-2.40	117.81	120.65
1	1	747	5MU	O4-C4-N3	-2.40	115.52	120.12
2	2	1207	2MG	O6-C6-C5	-2.38	119.72	124.37
1	1	2605	PSU	O2-C2-N1	-2.38	120.17	122.79
2	2	966	2MG	C8-N7-C5	2.37	107.50	102.99
1	1	747	5MU	C6-C5-C4	2.35	120.00	118.03
2	2	1207	2MG	CM2-N2-C2	-2.35	118.67	123.86
1	1	2251	OMG	O6-C6-C5	-2.34	119.81	124.37
5	5	54	5MU	O4-C4-N3	-2.34	115.64	120.12
1	1	955	PSU	C6-N1-C2	-2.32	120.31	122.68
5	5	8	4SU	O2-C2-N3	-2.32	117.18	121.50
2	2	1516	2MG	O6-C6-C5	-2.27	119.94	124.37
1	1	1911	PSU	C6-N1-C2	-2.24	120.39	122.68
1	1	745	1MG	O6-C6-C5	-2.23	120.25	124.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2445	2MG	O6-C6-C5	-2.22	120.03	124.37
1	1	1917	PSU	O2-C2-N1	-2.22	120.35	122.79
1	1	1917	PSU	C6-N1-C2	-2.19	120.44	122.68
2	2	1402	4OC	C6-C5-C4	2.14	119.58	116.96
5	5	54	5MU	O2-C2-N1	-2.06	120.05	122.79
2	2	1402	4OC	CM4-N4-C4	-2.05	118.44	122.45
1	1	1962	5MC	CM5-C5-C6	-2.05	120.11	122.85
1	1	2605	PSU	C6-N1-C2	-2.05	120.59	122.68
6	A	79	FME	O1-CN-N	-2.04	119.89	125.27
1	1	1939	5MU	C6-C5-C4	2.04	119.74	118.03
2	2	967	5MC	CM5-C5-C6	-2.04	120.12	122.85
1	1	2580	PSU	O4'-C1'-C2'	2.04	108.02	105.14
5	5	8	4SU	C1'-N1-C6	-2.03	116.42	120.84
1	1	1915	3TD	O4-C4-N3	-2.01	116.63	120.30

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	1618	6MZ	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C3'-C4'-C5'-O5'
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C6
1	1	2445	2MG	C3'-C4'-C5'-O5'
1	1	2504	PSU	O4'-C4'-C5'-O5'
2	2	516	PSU	O4'-C1'-C5-C4
2	2	516	PSU	O4'-C1'-C5-C6
2	2	527	G7M	C3'-C4'-C5'-O5'
2	2	1519	MA6	O4'-C4'-C5'-O5'
5	5	20	H2U	O4'-C1'-N1-C6
6	A	79	FME	O1-CN-N-CA
1	1	2030	6MZ	O4'-C4'-C5'-O5'
1	1	2030	6MZ	C3'-C4'-C5'-O5'
1	1	2504	PSU	C3'-C4'-C5'-O5'
2	2	1402	4OC	O4'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
2	2	527	G7M	O4'-C4'-C5'-O5'
2	2	1402	4OC	C3'-C4'-C5'-O5'
6	A	79	FME	CA-CB-CG-SD
1	1	2445	2MG	O4'-C4'-C5'-O5'
5	5	20	H2U	C3'-C4'-C5'-O5'
1	1	1835	2MG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	5	20	H2U	O4'-C4'-C5'-O5'
2	2	1519	MA6	C5-C6-N6-C10
1	1	2503	2MA	O4'-C4'-C5'-O5'
1	1	1835	2MG	C3'-C4'-C5'-O5'
2	2	966	2MG	C3'-C4'-C5'-O5'
46	q	89	0TD	CG-CB-SB-CSB
2	2	527	G7M	C4'-C5'-O5'-P
2	2	966	2MG	O4'-C4'-C5'-O5'
46	q	89	0TD	SB-CB-CG-OD1
5	5	20	H2U	O4'-C1'-N1-C2
5	5	8	4SU	O4'-C1'-N1-C6
5	5	55	PSU	C3'-C4'-C5'-O5'
5	5	55	PSU	C4'-C5'-O5'-P
1	1	2069	G7M	O4'-C4'-C5'-O5'
1	1	2503	2MA	C3'-C4'-C5'-O5'
5	5	8	4SU	O4'-C1'-N1-C2
1	1	2498	OMC	O4'-C4'-C5'-O5'
1	1	746	PSU	O4'-C1'-C5-C6
5	5	8	4SU	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 438 ligands modelled in this entry, 438 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

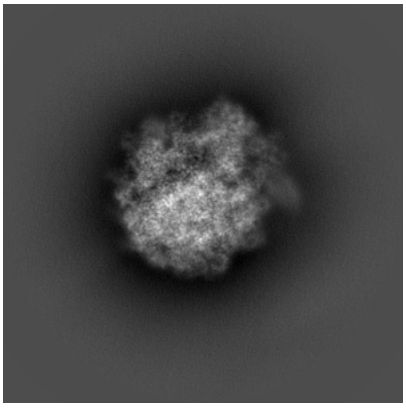
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20173. These allow visual inspection of the internal detail of the map and identification of artifacts.

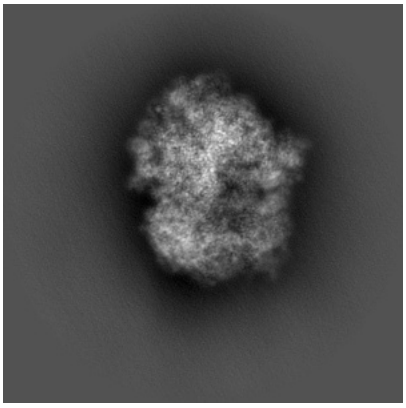
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

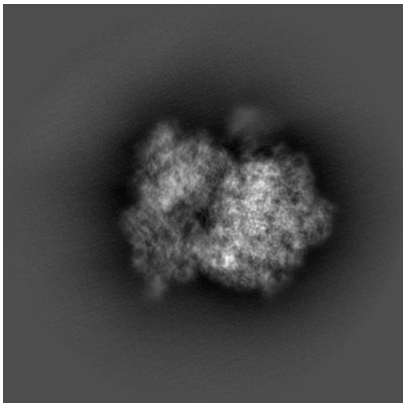
6.1.1 Primary map



X



Y

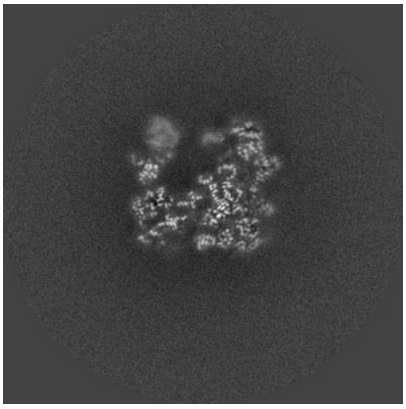


Z

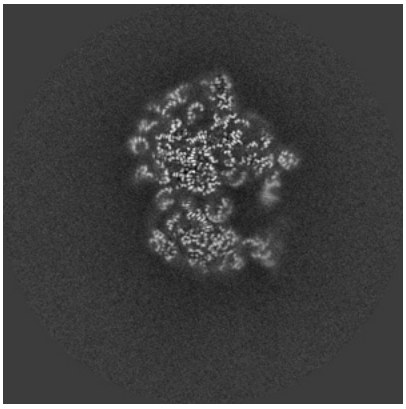
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

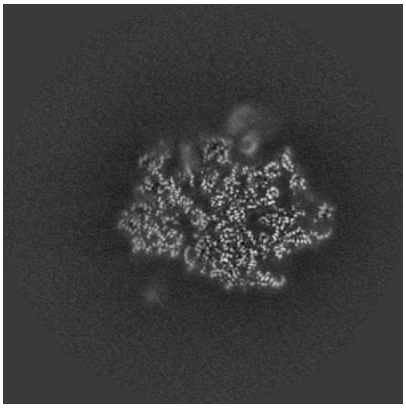
6.2.1 Primary map



X Index: 192



Y Index: 192

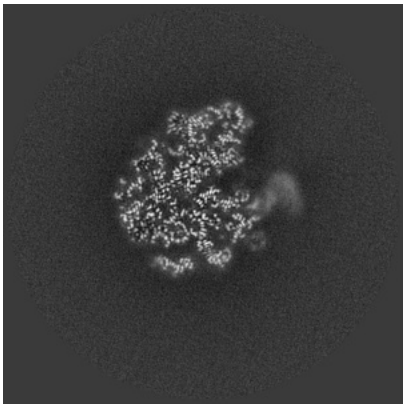


Z Index: 192

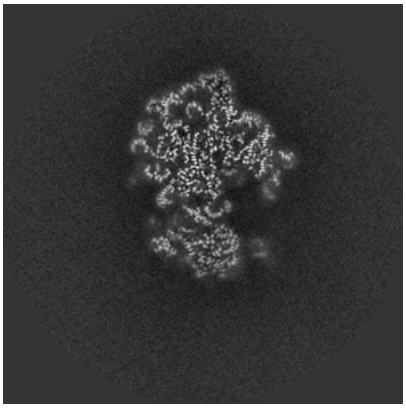
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

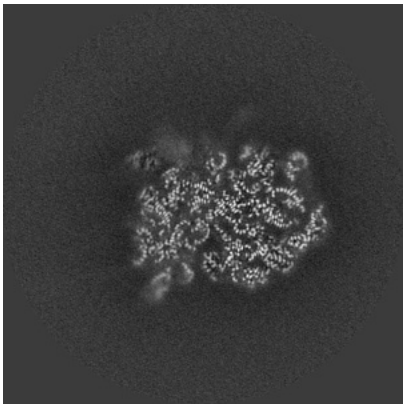
6.3.1 Primary map



X Index: 236



Y Index: 188

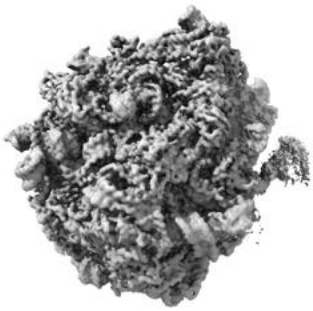


Z Index: 179

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

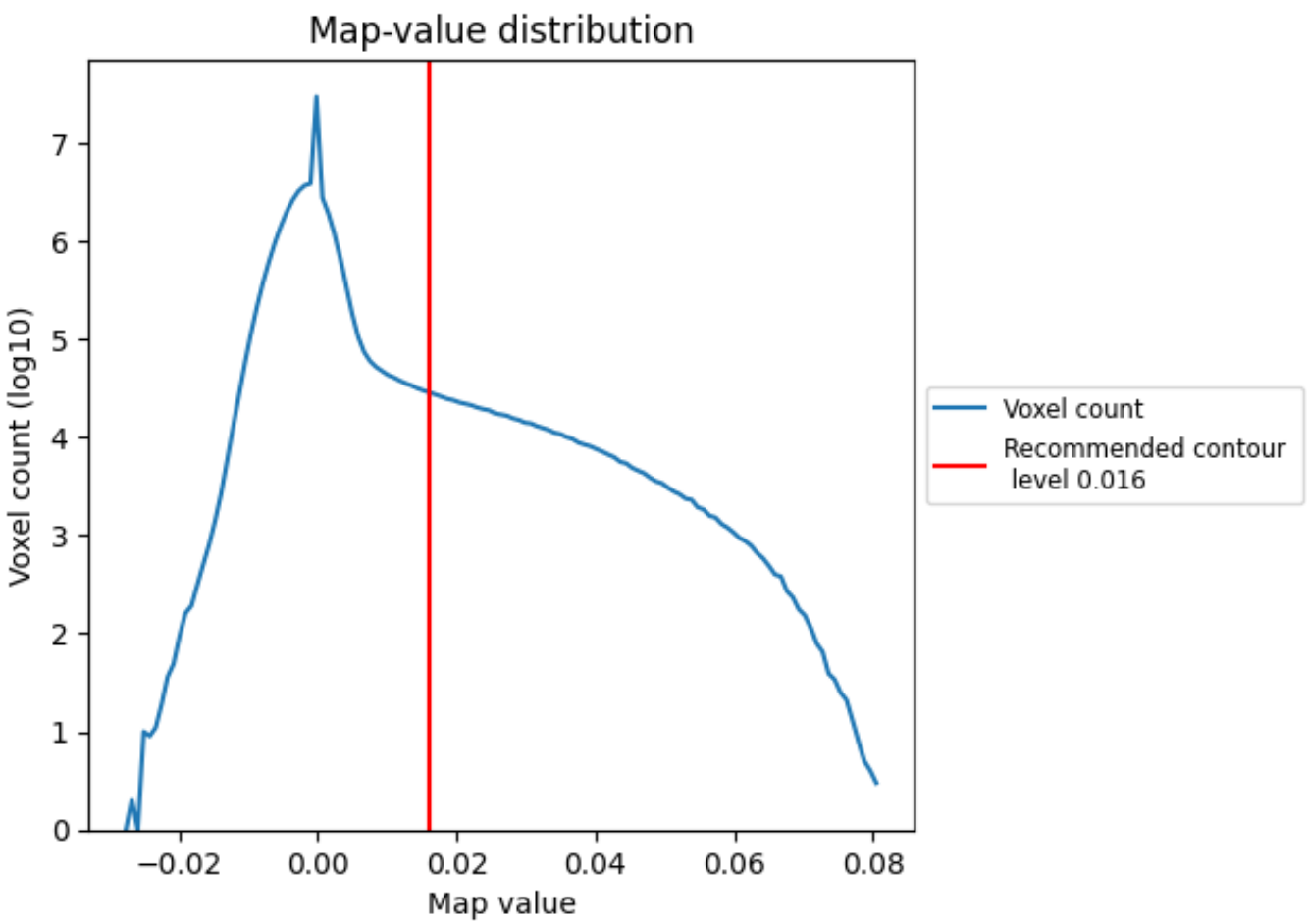
6.5 Mask visualisation (i)

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

7 Map analysis (i)

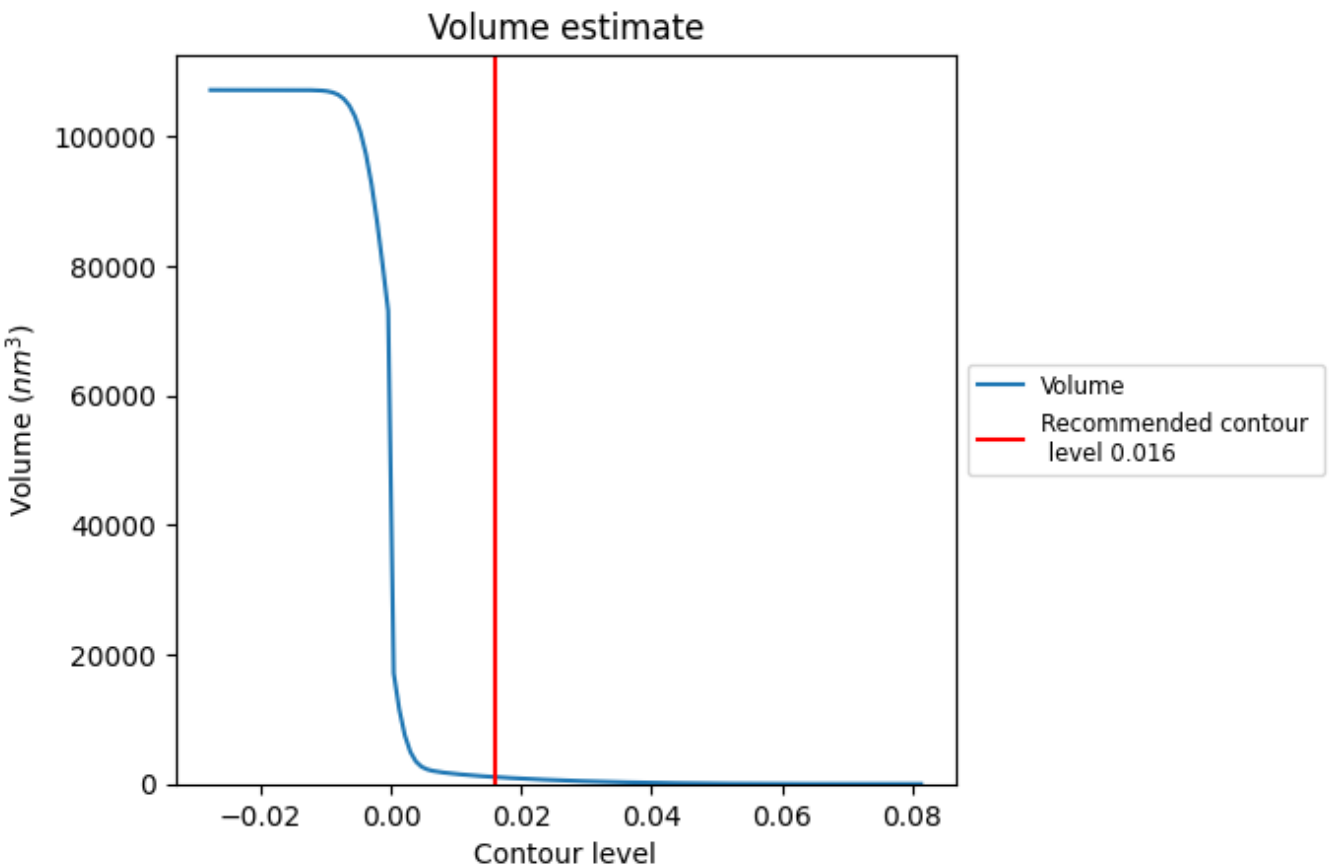
This section contains the results of statistical analysis of the map.

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.

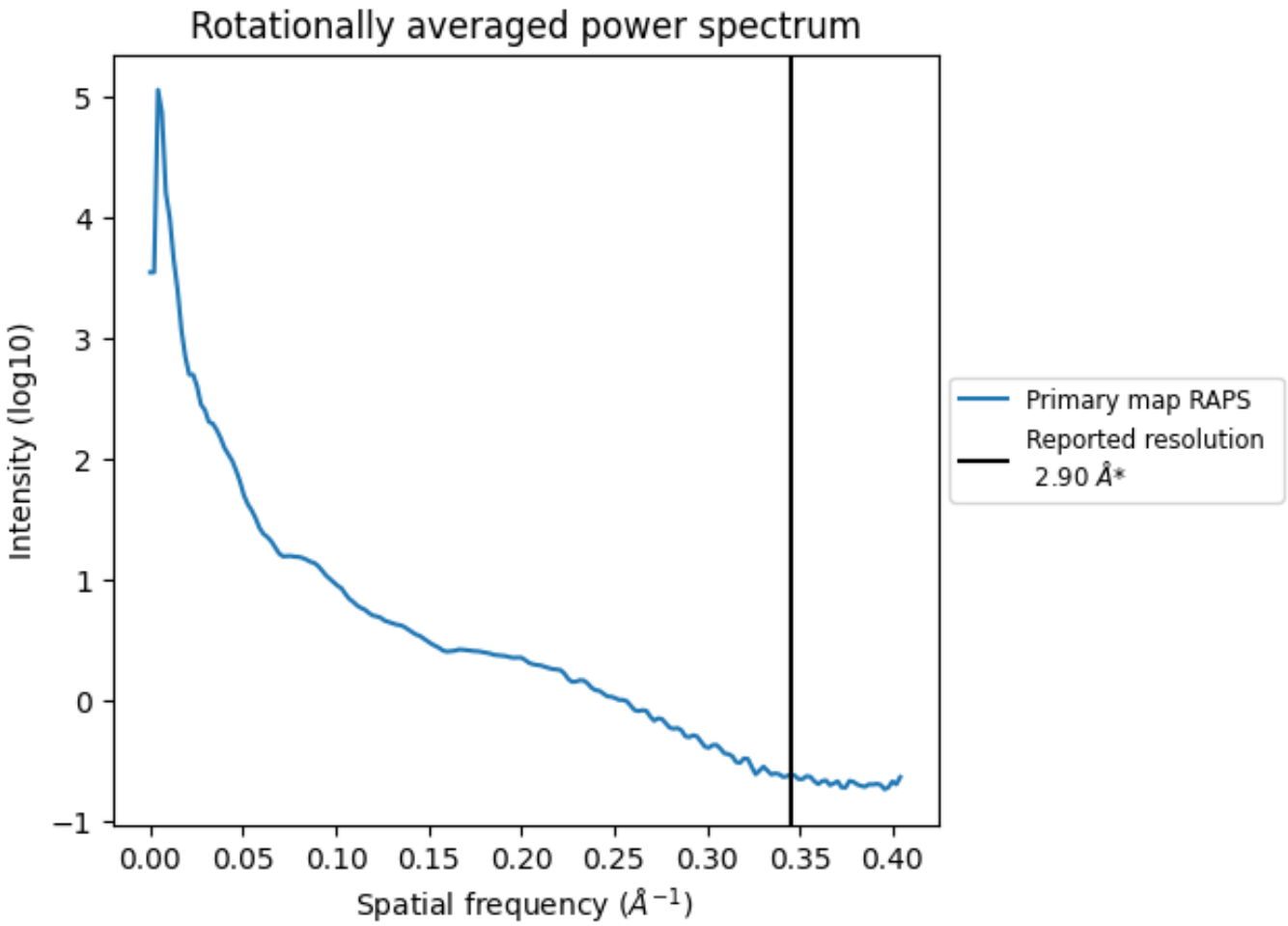
7.2 Volume estimate (i)



The volume at the recommended contour level is 1068 nm^3; this corresponds to an approximate mass of 965 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 (i)



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

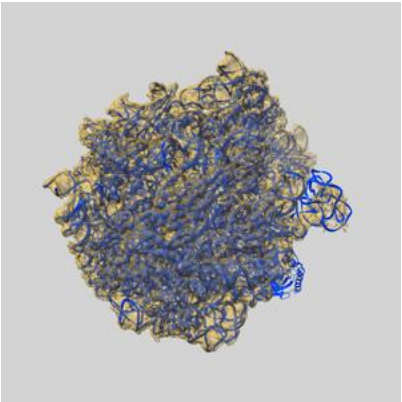
8 Fourier-Shell correlation (i)

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

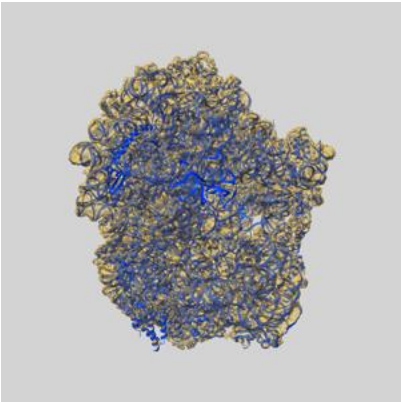
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20173 and PDB model 6ORE. Per-residue inclusion information can be found in section 3 on page 14.

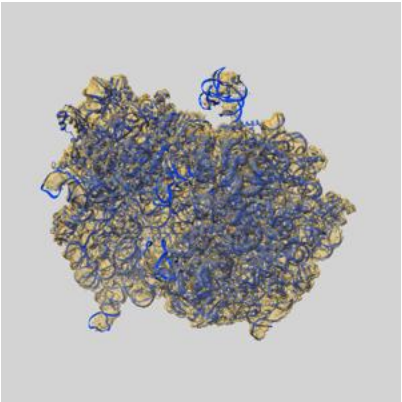
9.1 Map-model overlay (i)



X



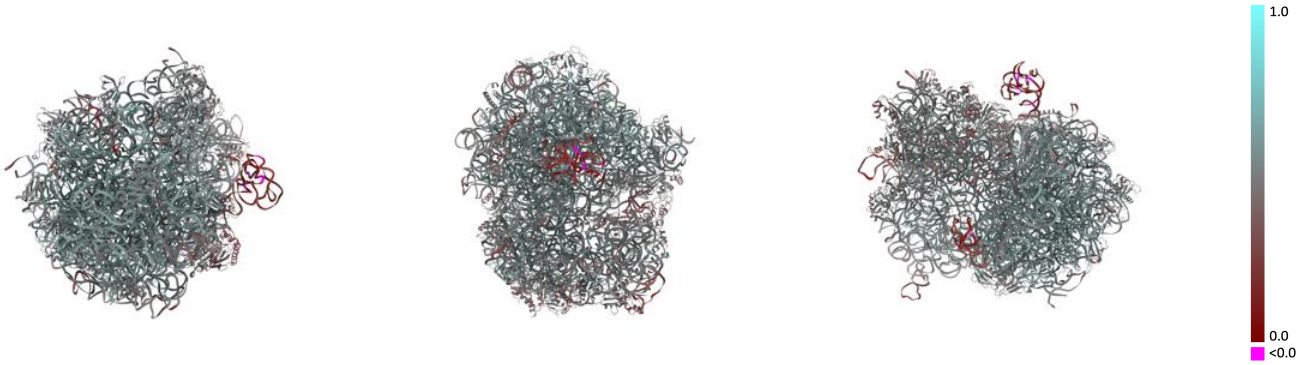
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016 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.

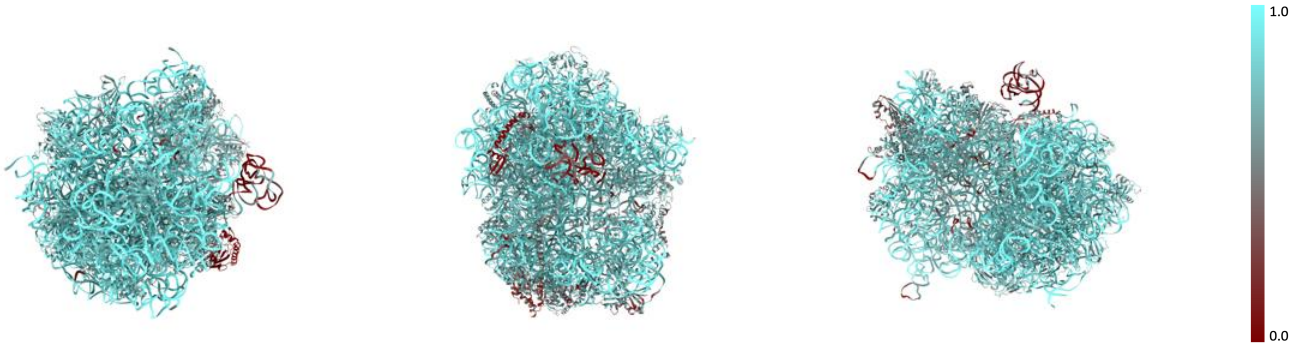
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

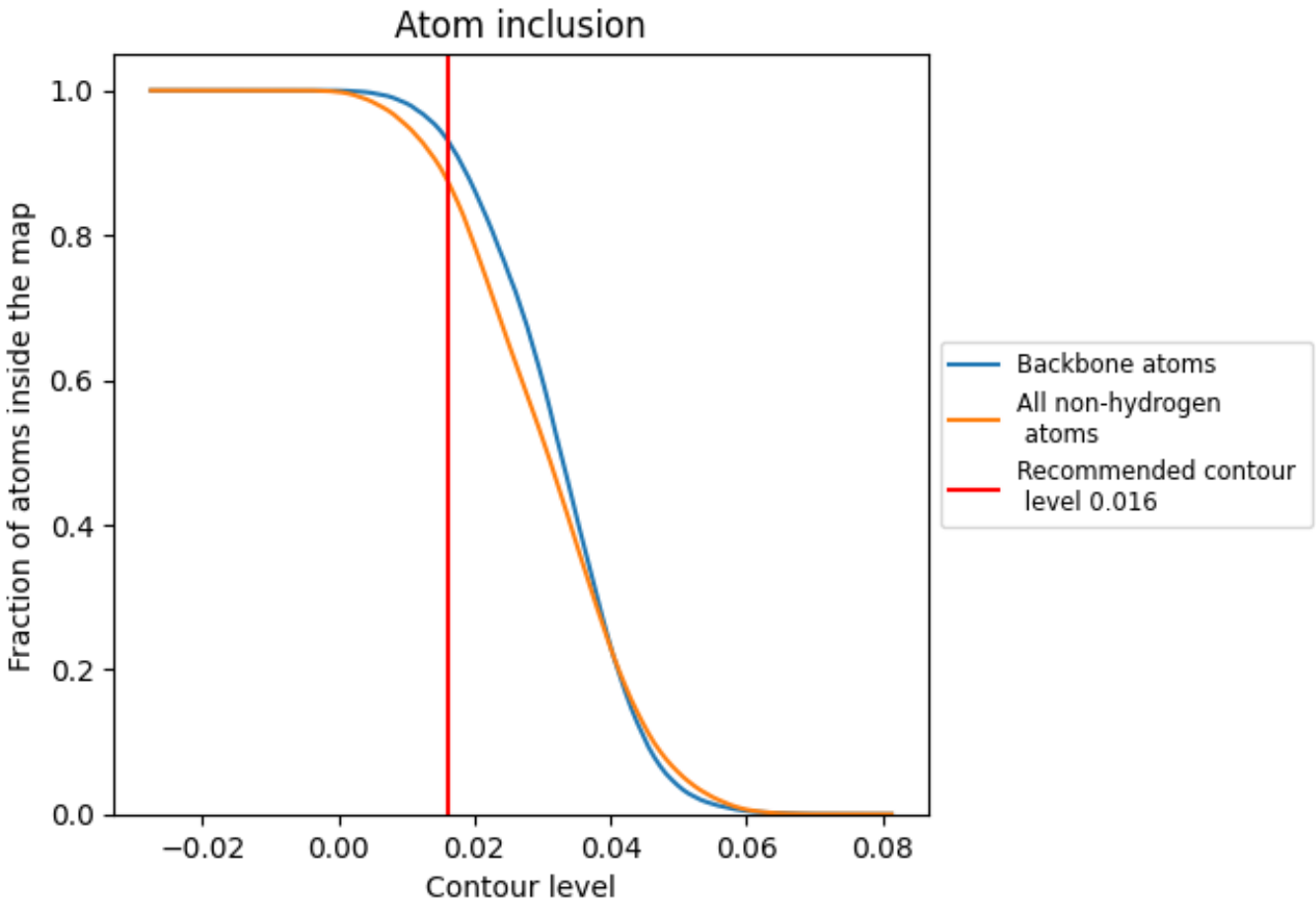
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8757	0.5160
1	0.9462	0.5310
2	0.9455	0.5070
3	0.9759	0.5190
4	0.7120	0.4110
5	0.7977	0.4820
A	0.2500	0.4220
B	0.8240	0.5620
C	0.8363	0.5540
D	0.7862	0.5280
E	0.7021	0.4570
F	0.7537	0.4840
G	0.1068	0.3720
J	0.8382	0.5550
K	0.7568	0.5390
L	0.8291	0.5390
M	0.8186	0.5380
N	0.8631	0.5610
O	0.8146	0.5040
P	0.8086	0.5500
Q	0.8647	0.5530
R	0.8319	0.5420
S	0.7739	0.5480
T	0.7726	0.5250
U	0.7848	0.5230
V	0.7940	0.5180
W	0.8322	0.5570
X	0.8053	0.5480
Y	0.7546	0.4860
Z	0.8257	0.5410
a	0.4629	0.4090
b	0.8140	0.5490
c	0.7584	0.5220
d	0.8563	0.5710
e	0.8473	0.5750

Continued on next page...

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Chain	Atom inclusion	Q-score
f	0.8129	0.5490
g	0.3320	0.4320
h	0.6830	0.4840
i	0.6996	0.4820
j	0.7381	0.5100
k	0.6723	0.4500
l	0.6329	0.4430
m	0.7438	0.5120
n	0.7211	0.4680
o	0.5621	0.4410
p	0.6928	0.4870
q	0.7216	0.5160
r	0.6812	0.4600
s	0.7287	0.4860
t	0.7203	0.4750
u	0.7624	0.5040
v	0.6915	0.4850
w	0.6367	0.4910
x	0.6909	0.4780
y	0.7508	0.4890
z	0.4794	0.4210