



Full wwPDB EM Validation Report ⓘ

Apr 17, 2024 – 01:53 am BST

PDB ID : 7AC7
EMDB ID : EMD-11713
Title : Structure of accomodated trans-translation complex on E. Coli stalled ribosome.
Authors : Guyomar, C.; D'Urso, G.; Chat, S.; Giudice, E.; Gillet, R.
Deposited on : 2020-09-10
Resolution : 3.08 Å(reported)
Based on initial model : 4YBB

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 ⓘ symbol.

The types of validation reports are described at

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

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

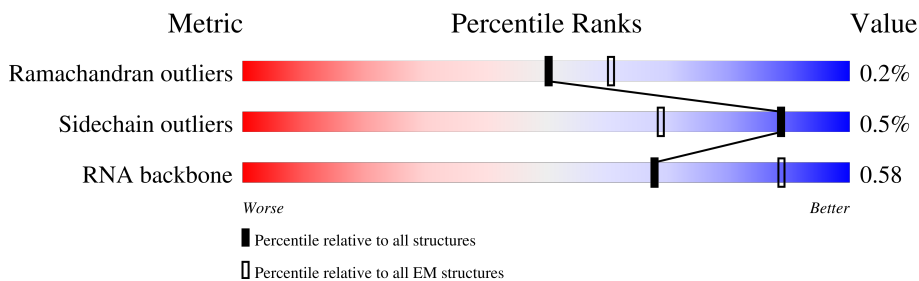
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 3.08 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 $\leq 5\%$. 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	1	2903	
2	2	1540	
3	3	120	
4	4	363	
5	5	147	
6	7	76	
7	8	15	
8	A	84	
















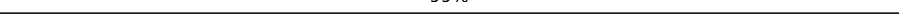
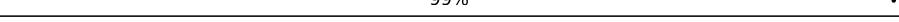
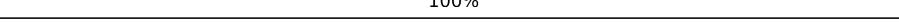
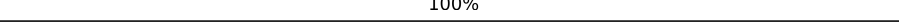
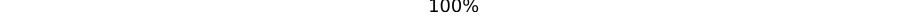
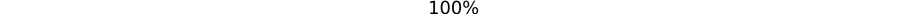
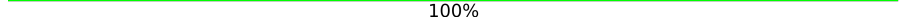
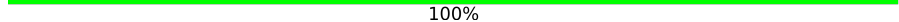


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Mol	Chain	Length	Quality of chain
9	B	271	100%
10	C	209	100%
11	D	201	100%
12	E	177	100%
13	F	175	97%
14	G	149	99%
15	H	130	92% 8%
16	J	141	100%
17	K	123	100%
18	L	144	100%
19	M	136	99%
20	N	119	100%
21	O	115	100%
22	P	114	100%
23	Q	117	100%
24	R	103	100%
25	S	109	100%
26	T	94	100%
27	U	103	100%
28	V	94	100%
29	W	2	50% 50%
30	X	77	100%
31	Y	58	100%
32	Z	56	100%
33	a	66	6% 100%

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Mol	Chain	Length	Quality of chain
34	b	54	 100%
35	c	52	 100%
36	d	46	 100%
37	e	64	 95% 5%
38	f	37	 100%
39	g	225	 100%
40	h	208	 100%
41	i	205	 100%
42	j	156	 100%
43	k	104	 100%
44	l	151	 100%
45	m	129	 100%
46	n	126	 98%
47	o	99	 100%
48	p	117	 99%
49	q	123	 99%
50	r	115	 100%
51	s	100	 100%
52	t	87	 100%
53	u	81	 100%
54	v	80	 100%
55	w	65	 100%
56	x	82	 100%
57	y	85	 100%
58	z	70	 10% 100%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 154883 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	1540	33049	14747	6057	10705	1540	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 transfer-messenger RNA (tmRNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	4	363	7759	3466	1410	2520	363	0	0

- Molecule 5 is a protein called SsrA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	147	1191	753	223	211	4	0	0

- Molecule 6 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
6	7	76	1635	735	291	532	75	2	0	0

- Molecule 7 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	15	Total	C	N	O	P	0	0
			324	145	60	105	14		

- Molecule 8 is a protein called 50S ribosomal protein L27.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 15 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	130	Total	C	N	O	S	0	0
			980	620	174	182	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	141	Total	C	N	O	S	0	0
			1121	709	211	198	3		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
21	O	115	Total	C	N	O	0	0
			884	548	177	159		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	109	Total	C	N	O	S	0	0
			849	527	165	155	2		

- Molecule 26 is a protein called 50S ribosomal protein L23.

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

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

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

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

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

- Molecule 29 is a protein called Nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	W	2	Total	C	N	O	0	0
			16	12	2	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	58	Total	C	N	O	S	0	0
			477	294	93	89	1		

- Molecule 32 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	56	Total	C	N	O	S	0	0
			434	272	84	76	2		

- Molecule 33 is a protein called 50S ribosomal protein L31.

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

- Molecule 34 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	54	Total	C	N	O	S	0	0
			429	260	91	77	1		

- Molecule 35 is a protein called 50S ribosomal protein L33.

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

- Molecule 36 is a protein called 50S ribosomal protein L34.

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

- Molecule 37 is a protein called 50S ribosomal protein L35.

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

- Molecule 38 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	37	Total	C	N	O	S	0	0
			297	183	64	46	4		

- Molecule 39 is a protein called 30S ribosomal protein S2.

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

- Molecule 40 is a protein called 30S ribosomal protein S3.

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

- Molecule 41 is a protein called 30S ribosomal protein S4.

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

- Molecule 42 is a protein called 30S ribosomal protein S5.

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

- Molecule 43 is a protein called 30S ribosomal protein S6.

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

- Molecule 44 is a protein called 30S ribosomal protein S7.

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

- Molecule 45 is a protein called 30S ribosomal protein S8.

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

- Molecule 46 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	n	126	1010	628	202	177	3	0	0

- Molecule 47 is a protein called 30S ribosomal protein S10.

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

- Molecule 48 is a protein called 30S ribosomal protein S11.

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

- Molecule 49 is a protein called 30S ribosomal protein S12.

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

- Molecule 50 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	r	115	891	552	179	157	3	0	0

- Molecule 51 is a protein called 30S ribosomal protein S14.

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

- Molecule 52 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	t	87	708	436	143	128	1	0	0

- Molecule 53 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	u	81	643	403	127	112	1	0	0

- Molecule 54 is a protein called 30S ribosomal protein S17.

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

- Molecule 55 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	w	65	535	339	100	95	1	0	0

- Molecule 56 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	x	82	658	421	125	110	2	0	0

- Molecule 57 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	y	85	664	411	137	113	3	0	0

- Molecule 58 is a protein called 30S ribosomal protein S21.

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

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	1	303	Total 303	Mg 303	0
59	2	118	Total 118	Mg 118	0
59	3	9	Total 9	Mg 9	0
59	7	1	Total 1	Mg 1	0
59	B	2	Total 2	Mg 2	0
59	C	1	Total 1	Mg 1	0
59	D	1	Total 1	Mg 1	0
59	L	1	Total 1	Mg 1	0
59	Q	2	Total 2	Mg 2	0
59	Z	1	Total 1	Mg 1	0
59	b	2	Total 2	Mg 2	0

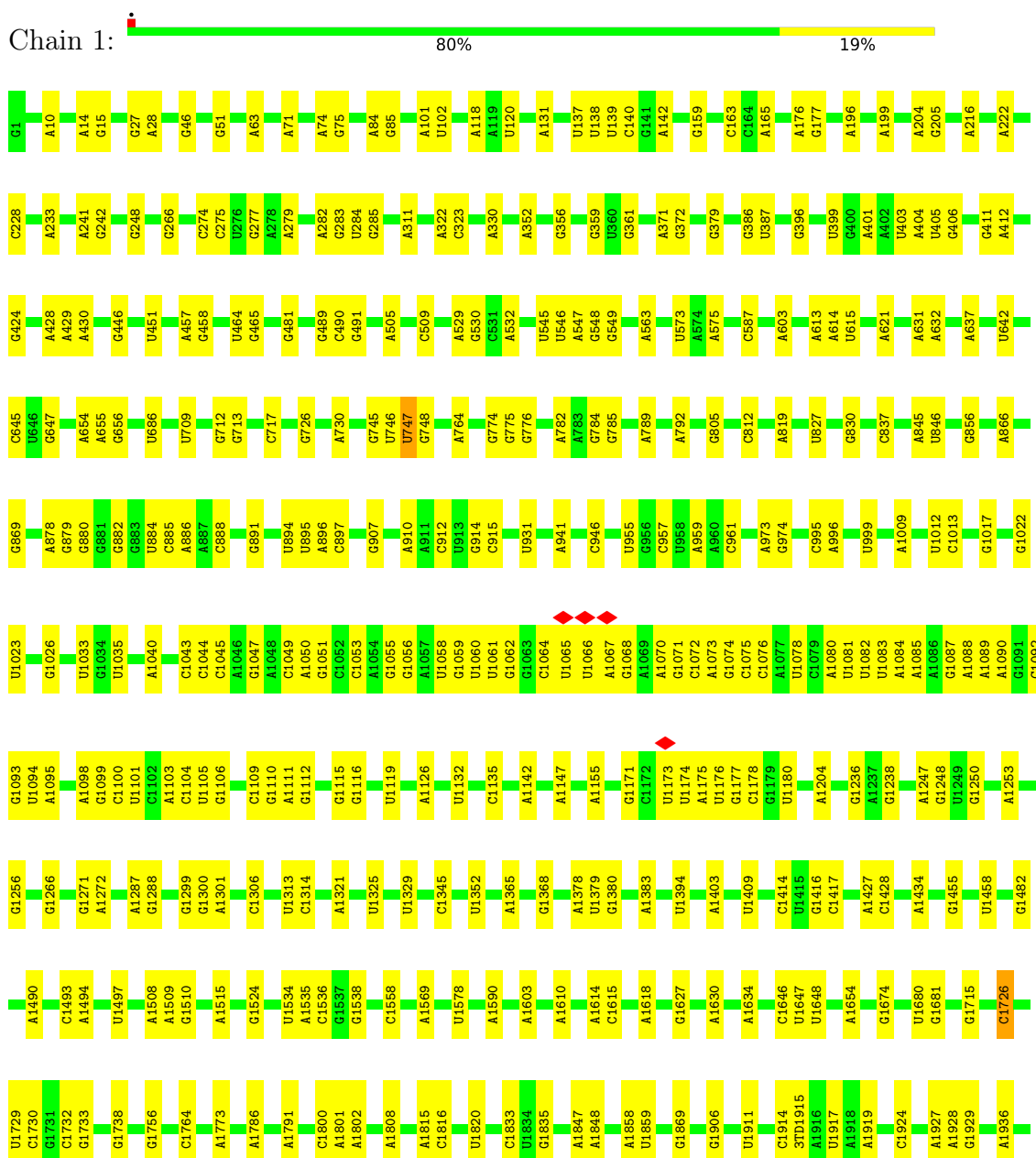
- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

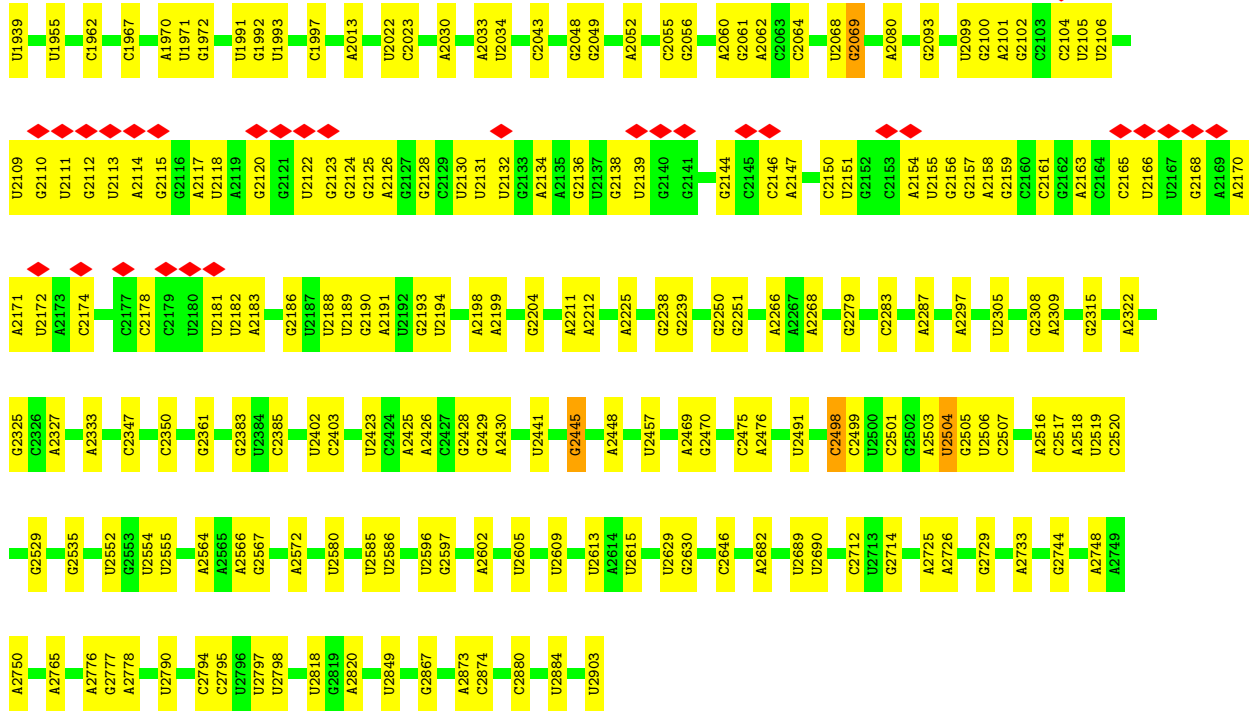
Mol	Chain	Residues	Atoms		AltConf
60	a	1	Total 1	Zn 1	0
60	f	1	Total 1	Zn 1	0

3 Residue-property plots i

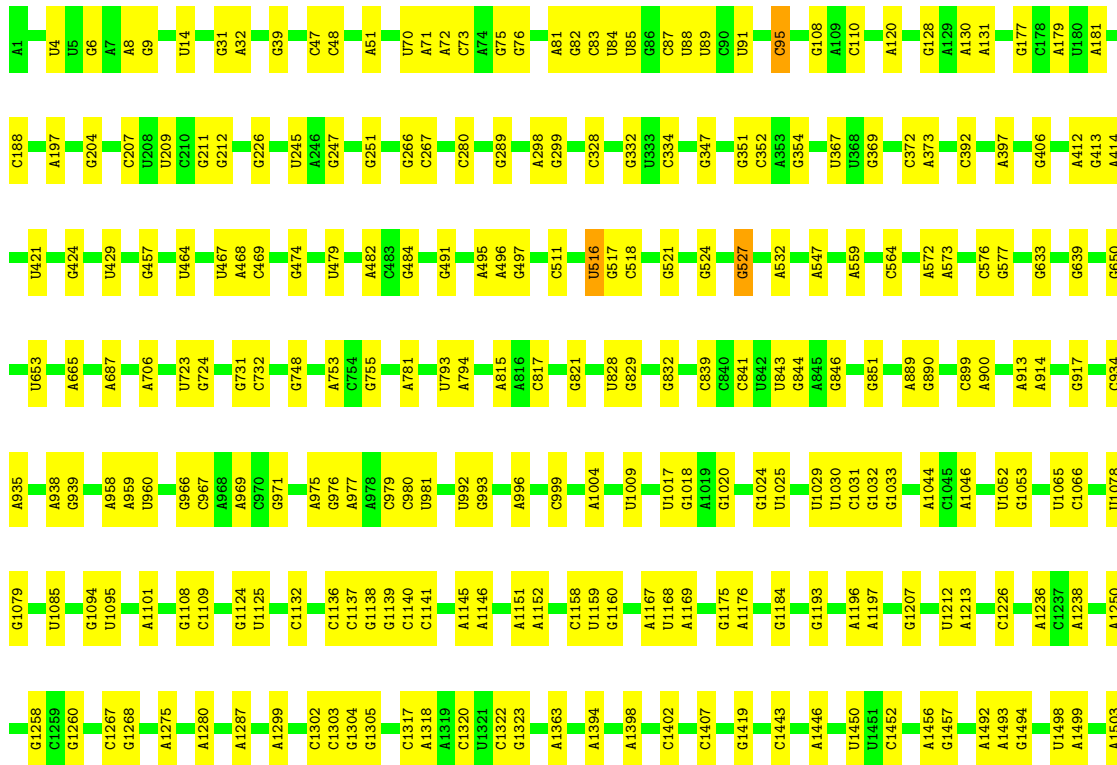
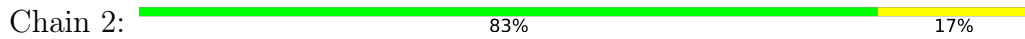
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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





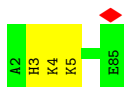
• Molecule 2: 16S ribosomal RNA



- Molecule 7: mRNA



- Molecule 8: 50S ribosomal protein L27



- Molecule 9: 50S ribosomal protein L2

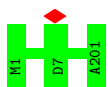


- Molecule 10: 50S ribosomal protein L3



There are no outlier residues recorded for this chain.

- Molecule 11: 50S ribosomal protein L4

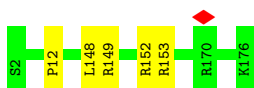


- Molecule 12: 50S ribosomal protein L5

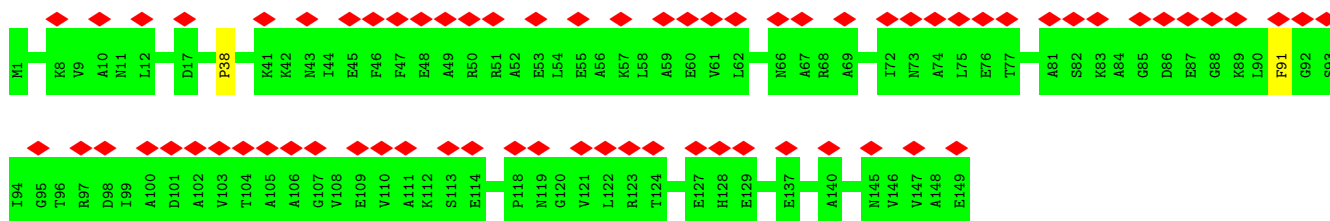


There are no outlier residues recorded for this chain.

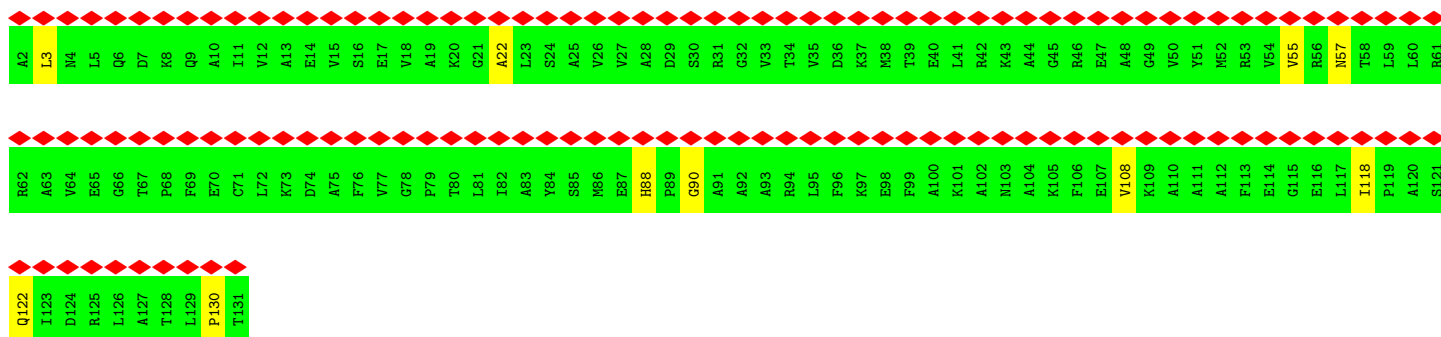
- Molecule 13: 50S ribosomal protein L6



- Molecule 14: 50S ribosomal protein L9



- Molecule 15: 50S ribosomal protein L10



- Molecule 16: 50S ribosomal protein L13



There are no outlier residues recorded for this chain.

- Molecule 17: 50S ribosomal protein L14



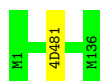
There are no outlier residues recorded for this chain.

- Molecule 18: 50S ribosomal protein L15



There are no outlier residues recorded for this chain.

- Molecule 19: 50S ribosomal protein L16



- Molecule 20: 50S ribosomal protein L17

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 21: 50S ribosomal protein L18

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 22: 50S ribosomal protein L19

Chain P:  100%



- Molecule 23: 50S ribosomal protein L20

Chain Q:  100%

There are no outlier residues recorded for this chain.

- Molecule 24: 50S ribosomal protein L21

Chain R:  100%

There are no outlier residues recorded for this chain.

- Molecule 25: 50S ribosomal protein L22

Chain S:  100%

There are no outlier residues recorded for this chain.

- Molecule 26: 50S ribosomal protein L23

Chain T:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: 50S ribosomal protein L24

Chain U:  100%



- Molecule 28: 50S ribosomal protein L25

Chain V:  100%

There are no outlier residues recorded for this chain.

- Molecule 29: Nascent peptide



- Molecule 30: 50S ribosomal protein L28



There are no outlier residues recorded for this chain.

- Molecule 31: 50S ribosomal protein L29



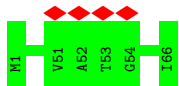
There are no outlier residues recorded for this chain.

- Molecule 32: 50S ribosomal protein L30



There are no outlier residues recorded for this chain.

- Molecule 33: 50S ribosomal protein L31



- Molecule 34: 50S ribosomal protein L32



There are no outlier residues recorded for this chain.

- Molecule 35: 50S ribosomal protein L33



There are no outlier residues recorded for this chain.

- Molecule 36: 50S ribosomal protein L34



- Molecule 37: 50S ribosomal protein L35

Chain e:  95% 5%



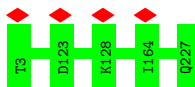
- Molecule 38: 50S ribosomal protein L36

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 39: 30S ribosomal protein S2

Chain g:  100%



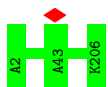
- Molecule 40: 30S ribosomal protein S3

Chain h:  100%



- Molecule 41: 30S ribosomal protein S4

Chain i:  100%



- Molecule 42: 30S ribosomal protein S5

Chain j:  100%

There are no outlier residues recorded for this chain.

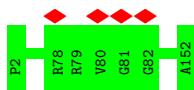
- Molecule 43: 30S ribosomal protein S6

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 44: 30S ribosomal protein S7

Chain l:  100%



- Molecule 45: 30S ribosomal protein S8

Chain m: 100%

There are no outlier residues recorded for this chain.

- Molecule 46: 30S ribosomal protein S9

Chain n: 98%



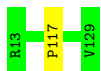
- Molecule 47: 30S ribosomal protein S10

Chain o: 100%

There are no outlier residues recorded for this chain.

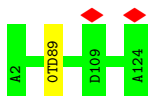
- Molecule 48: 30S ribosomal protein S11

Chain p: 99%



- Molecule 49: 30S ribosomal protein S12

Chain q: 99%



- Molecule 50: 30S ribosomal protein S13

Chain r: 100%

There are no outlier residues recorded for this chain.

- Molecule 51: 30S ribosomal protein S14

Chain s: 100%

There are no outlier residues recorded for this chain.

- Molecule 52: 30S ribosomal protein S15

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 53: 30S ribosomal protein S16

Chain u:  100%

There are no outlier residues recorded for this chain.

- Molecule 54: 30S ribosomal protein S17

Chain v:  100%

There are no outlier residues recorded for this chain.

- Molecule 55: 30S ribosomal protein S18

Chain w:  100%

There are no outlier residues recorded for this chain.

- Molecule 56: 30S ribosomal protein S19

Chain x:  100%

There are no outlier residues recorded for this chain.

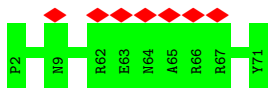
- Molecule 57: 30S ribosomal protein S20

Chain y:  100%

There are no outlier residues recorded for this chain.

- Molecule 58: 30S ribosomal protein S21

Chain z:  10%  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36069	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	29	Depositor
Minimum defocus (nm)	-700	Depositor
Maximum defocus (nm)	-2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	27.267	Depositor
Minimum map value	-12.720	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.5	Depositor
Map size (\AA)	499.20026, 499.20026, 499.20026	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0400006, 1.0400006, 1.0400006	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: 4D4, UR3, G7M, 5MC, 4SU, MG, 3AU, 5MU, 3TD, ZN, OMU, H2U, 2MA, PSU, OMG, MIA, 6MZ, 4OC, 2MG, 1MG, OMC, 0TD, MA6

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	0.17	0/69286	0.74	5/108087 (0.0%)
2	2	0.17	0/36722	0.75	3/57278 (0.0%)
3	3	0.16	0/2872	0.75	0/4478
4	4	0.21	1/8615 (0.0%)	0.78	4/13430 (0.0%)
5	5	0.33	0/1213	0.64	1/1630 (0.1%)
6	7	0.18	0/1580	0.74	0/2459
7	8	0.20	0/363	0.76	0/566
8	A	0.26	0/642	0.45	0/848
9	B	0.27	1/2122 (0.0%)	0.44	0/2852
10	C	0.24	0/1586	0.45	0/2134
11	D	0.23	0/1571	0.40	0/2113
12	E	0.24	0/1435	0.43	0/1926
13	F	0.32	1/1333 (0.1%)	0.47	0/1805
14	G	0.34	1/1122 (0.1%)	0.52	2/1515 (0.1%)
15	H	0.25	0/993	0.45	0/1340
16	J	0.23	0/1144	0.41	0/1541
17	K	0.23	0/955	0.45	0/1279
18	L	0.24	0/1062	0.44	0/1413
19	M	0.25	0/1081	0.42	0/1443
20	N	0.23	0/964	0.41	0/1289
21	O	0.23	0/894	0.40	0/1198
22	P	0.23	0/929	0.44	0/1242
23	Q	0.23	0/960	0.34	0/1278
24	R	0.24	0/829	0.45	0/1107
25	S	0.23	0/856	0.44	0/1146
26	T	0.23	0/752	0.43	0/1005
27	U	0.24	0/796	0.42	0/1062
28	V	0.23	0/766	0.41	0/1025
29	W	1.13	0/16	1.22	0/20
30	X	0.23	0/635	0.47	0/848
31	Y	0.22	0/478	0.36	0/637

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Z	0.22	0/438	0.42	0/587
33	a	0.23	0/531	0.44	0/709
34	b	0.22	0/435	0.43	0/581
35	c	0.23	0/433	0.48	0/576
36	d	0.23	0/380	0.41	0/498
37	e	0.28	0/513	0.54	0/676
38	f	0.23	0/298	0.45	0/392
39	g	0.24	0/1791	0.39	0/2413
40	h	0.23	0/1663	0.41	0/2241
41	i	0.23	0/1665	0.42	0/2227
42	j	0.24	0/1165	0.43	0/1568
43	k	0.27	0/867	0.45	0/1171
44	l	0.23	0/1195	0.39	0/1602
45	m	0.24	0/989	0.46	0/1326
46	n	0.26	0/1022	0.47	0/1361
47	o	0.24	0/800	0.46	0/1082
48	p	0.36	1/893 (0.1%)	0.48	1/1205 (0.1%)
49	q	0.23	0/960	0.45	0/1286
50	r	0.23	0/900	0.43	0/1204
51	s	0.23	0/817	0.37	0/1088
52	t	0.22	0/716	0.36	0/956
53	u	0.23	0/653	0.43	0/877
54	v	0.22	0/658	0.45	0/881
55	w	0.23	0/544	0.39	0/731
56	x	0.23	0/675	0.44	0/908
57	y	0.24	0/670	0.35	0/888
58	z	0.23	0/597	0.41	0/792
All	All	0.20	5/166840 (0.0%)	0.68	16/249820 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	p	117	PRO	N-CD	-8.10	1.36	1.47
14	G	38	PRO	N-CD	-8.02	1.36	1.47
13	F	12	PRO	N-CD	-6.70	1.38	1.47
4	4	363	A	C3'-O3'	6.41	1.51	1.42
9	B	247	PRO	N-CD	-5.83	1.39	1.47

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1313	U	C2-N1-C1'	5.87	124.75	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	112	VAL	N-CA-CB	-5.82	98.71	111.50
1	1	837	C	N3-C2-O2	-5.63	117.96	121.90
4	4	142	U	N3-C4-O4	-5.62	115.47	119.40
2	2	979	C	C2-N1-C1'	5.56	124.92	118.80
2	2	979	C	N1-C2-O2	5.38	122.12	118.90
48	p	117	PRO	CA-N-CD	5.36	119.21	111.70
14	G	38	PRO	CA-N-CD	5.31	119.14	111.70
14	G	91	PHE	N-CA-CB	-5.30	101.07	110.60
4	4	353	C	C2-N1-C1'	5.25	124.58	118.80
1	1	1726	C	N1-C2-O2	5.22	122.03	118.90
1	1	837	C	N1-C2-O2	5.07	121.94	118.90
4	4	363	A	C2'-C3'-O3'	5.06	121.80	113.70
4	4	156	G	C4-N9-C1'	5.04	133.05	126.50
1	1	1313	U	N3-C2-O2	-5.03	118.68	122.20
2	2	95	C	N1-C2-O2	5.02	121.91	118.90

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	
5	5	145/147 (99%)	114 (79%)	29 (20%)	2 (1%)	11	38
8	A	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
9	B	269/271 (99%)	266 (99%)	3 (1%)	0	100	100
10	C	207/209 (99%)	204 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	D	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
12	E	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
13	F	173/175 (99%)	165 (95%)	8 (5%)	0	100	100
14	G	147/149 (99%)	137 (93%)	10 (7%)	0	100	100
15	H	128/130 (98%)	98 (77%)	23 (18%)	7 (6%)	2	10
16	J	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
17	K	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
18	L	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
19	M	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
20	N	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
21	O	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
22	P	112/114 (98%)	112 (100%)	0	0	100	100
23	Q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
24	R	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
25	S	107/109 (98%)	103 (96%)	4 (4%)	0	100	100
26	T	92/94 (98%)	92 (100%)	0	0	100	100
27	U	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
28	V	92/94 (98%)	92 (100%)	0	0	100	100
30	X	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
31	Y	56/58 (97%)	56 (100%)	0	0	100	100
32	Z	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
33	a	64/66 (97%)	61 (95%)	3 (5%)	0	100	100
34	b	52/54 (96%)	52 (100%)	0	0	100	100
35	c	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
36	d	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
37	e	62/64 (97%)	57 (92%)	2 (3%)	3 (5%)	2	12
38	f	35/37 (95%)	35 (100%)	0	0	100	100
39	g	223/225 (99%)	219 (98%)	4 (2%)	0	100	100
40	h	206/208 (99%)	202 (98%)	4 (2%)	0	100	100
41	i	203/205 (99%)	198 (98%)	5 (2%)	0	100	100
42	j	154/156 (99%)	147 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	k	102/104 (98%)	102 (100%)	0	0	100	100
44	l	149/151 (99%)	147 (99%)	2 (1%)	0	100	100
45	m	127/129 (98%)	127 (100%)	0	0	100	100
46	n	124/126 (98%)	120 (97%)	4 (3%)	0	100	100
47	o	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
48	p	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
49	q	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
50	r	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
51	s	98/100 (98%)	98 (100%)	0	0	100	100
52	t	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
53	u	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
54	v	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
55	w	63/65 (97%)	63 (100%)	0	0	100	100
56	x	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
57	y	83/85 (98%)	82 (99%)	1 (1%)	0	100	100
58	z	68/70 (97%)	68 (100%)	0	0	100	100
All	All	5869/5973 (98%)	5678 (97%)	179 (3%)	12 (0%)	50	77

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
37	e	32	ILE
15	H	55	VAL
15	H	88	HIS
15	H	118	ILE
37	e	33	LEU
15	H	22	ALA
15	H	90	GLY
15	H	130	PRO
37	e	34	THR
5	5	111	VAL
5	5	68	ALA
15	H	108	VAL

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	
5	5	123/123 (100%)	112 (91%)	11 (9%)	9	33
8	A	62/62 (100%)	59 (95%)	3 (5%)	25	57
9	B	216/216 (100%)	216 (100%)	0	100	100
10	C	164/164 (100%)	164 (100%)	0	100	100
11	D	165/165 (100%)	165 (100%)	0	100	100
12	E	148/148 (100%)	148 (100%)	0	100	100
13	F	136/136 (100%)	132 (97%)	4 (3%)	42	70
14	G	114/114 (100%)	114 (100%)	0	100	100
15	H	99/99 (100%)	96 (97%)	3 (3%)	41	70
16	J	115/115 (100%)	115 (100%)	0	100	100
17	K	104/104 (100%)	104 (100%)	0	100	100
18	L	103/103 (100%)	103 (100%)	0	100	100
19	M	108/108 (100%)	108 (100%)	0	100	100
20	N	99/99 (100%)	99 (100%)	0	100	100
21	O	85/85 (100%)	85 (100%)	0	100	100
22	P	99/99 (100%)	99 (100%)	0	100	100
23	Q	89/89 (100%)	89 (100%)	0	100	100
24	R	84/84 (100%)	84 (100%)	0	100	100
25	S	92/92 (100%)	92 (100%)	0	100	100
26	T	81/81 (100%)	81 (100%)	0	100	100
27	U	84/84 (100%)	84 (100%)	0	100	100
28	V	78/78 (100%)	78 (100%)	0	100	100
29	W	1/1 (100%)	0	1 (100%)	0	0
30	X	67/67 (100%)	67 (100%)	0	100	100
31	Y	53/53 (100%)	53 (100%)	0	100	100
32	Z	47/47 (100%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	a	59/59 (100%)	59 (100%)	0	100	100
34	b	46/46 (100%)	46 (100%)	0	100	100
35	c	47/47 (100%)	47 (100%)	0	100	100
36	d	38/38 (100%)	38 (100%)	0	100	100
37	e	51/51 (100%)	51 (100%)	0	100	100
38	f	34/34 (100%)	34 (100%)	0	100	100
39	g	187/187 (100%)	187 (100%)	0	100	100
40	h	171/171 (100%)	170 (99%)	1 (1%)	86	93
41	i	172/172 (100%)	172 (100%)	0	100	100
42	j	119/119 (100%)	119 (100%)	0	100	100
43	k	91/91 (100%)	91 (100%)	0	100	100
44	l	124/124 (100%)	124 (100%)	0	100	100
45	m	104/104 (100%)	104 (100%)	0	100	100
46	n	104/104 (100%)	102 (98%)	2 (2%)	57	79
47	o	86/86 (100%)	86 (100%)	0	100	100
48	p	90/90 (100%)	90 (100%)	0	100	100
49	q	102/102 (100%)	102 (100%)	0	100	100
50	r	93/93 (100%)	93 (100%)	0	100	100
51	s	83/83 (100%)	83 (100%)	0	100	100
52	t	75/75 (100%)	75 (100%)	0	100	100
53	u	65/65 (100%)	65 (100%)	0	100	100
54	v	74/74 (100%)	74 (100%)	0	100	100
55	w	56/56 (100%)	56 (100%)	0	100	100
56	x	72/72 (100%)	72 (100%)	0	100	100
57	y	65/65 (100%)	65 (100%)	0	100	100
58	z	60/60 (100%)	60 (100%)	0	100	100
All	All	4884/4884 (100%)	4859 (100%)	25 (0%)	89	94

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	5	34	LEU
5	5	36	LEU

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Mol	Chain	Res	Type
5	5	37	GLN
5	5	110	THR
5	5	134	LYS
5	5	135	GLN
5	5	136	HIS
5	5	137	ASP
5	5	138	LYS
5	5	139	ARG
5	5	143	LYS
8	A	3	HIS
8	A	4	LYS
8	A	5	LYS
13	F	148	LEU
13	F	149	ARG
13	F	152	ARG
13	F	153	ARG
15	H	3	LEU
15	H	57	ASN
15	H	122	GLN
29	W	1	PHE
40	h	29	PHE
46	n	43	THR
46	n	107	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
5	5	37	GLN
21	O	38	GLN
27	U	74	ASN
31	Y	20	ASN
34	b	42	HIS
42	j	97	GLN
42	j	146	ASN
43	k	58	HIS
50	r	100	GLN
56	x	14	HIS
57	y	55	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2898/2903 (99%)	535 (18%)	25 (0%)
2	2	1535/1540 (99%)	244 (15%)	13 (0%)
3	3	119/120 (99%)	13 (10%)	0
4	4	362/363 (99%)	164 (45%)	14 (3%)
6	7	73/76 (96%)	12 (16%)	2 (2%)
7	8	14/15 (93%)	4 (28%)	2 (14%)
All	All	5001/5017 (99%)	972 (19%)	56 (1%)

All (972) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	14	A
1	1	15	G
1	1	27	G
1	1	28	A
1	1	46	G
1	1	51	G
1	1	63	A
1	1	71	A
1	1	74	A
1	1	75	G
1	1	84	A
1	1	85	G
1	1	101	A
1	1	102	U
1	1	118	A
1	1	120	U
1	1	131	A
1	1	137	U
1	1	138	U
1	1	139	U
1	1	140	C
1	1	142	A
1	1	159	G
1	1	163	C
1	1	165	A
1	1	177	G
1	1	196	A
1	1	199	A
1	1	204	A
1	1	205	G
1	1	216	A

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Mol	Chain	Res	Type
1	1	222	A
1	1	228	C
1	1	233	A
1	1	241	A
1	1	242	G
1	1	248	G
1	1	266	G
1	1	274	C
1	1	275	C
1	1	277	G
1	1	279	A
1	1	282	A
1	1	283	G
1	1	284	U
1	1	285	G
1	1	311	A
1	1	322	A
1	1	323	C
1	1	330	A
1	1	352	A
1	1	356	G
1	1	359	G
1	1	361	G
1	1	371	A
1	1	372	G
1	1	379	G
1	1	386	G
1	1	387	U
1	1	396	G
1	1	399	U
1	1	401	A
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	429	A
1	1	430	A
1	1	446	G
1	1	451	U
1	1	457	A

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Mol	Chain	Res	Type
1	1	458	G
1	1	464	U
1	1	465	G
1	1	481	G
1	1	489	G
1	1	490	C
1	1	491	G
1	1	505	A
1	1	509	C
1	1	529	A
1	1	530	G
1	1	532	A
1	1	545	U
1	1	546	U
1	1	547	A
1	1	548	G
1	1	549	G
1	1	563	A
1	1	573	U
1	1	575	A
1	1	587	C
1	1	603	A
1	1	613	A
1	1	614	A
1	1	615	U
1	1	621	A
1	1	632	A
1	1	637	A
1	1	642	U
1	1	645	C
1	1	647	G
1	1	654	A
1	1	655	A
1	1	656	G
1	1	686	U
1	1	709	U
1	1	712	G
1	1	713	G
1	1	717	C
1	1	726	G
1	1	730	A
1	1	747	5MU

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Mol	Chain	Res	Type
1	1	748	G
1	1	764	A
1	1	775	G
1	1	776	G
1	1	782	A
1	1	784	G
1	1	785	G
1	1	789	A
1	1	792	A
1	1	805	G
1	1	812	C
1	1	819	A
1	1	827	U
1	1	830	G
1	1	845	A
1	1	846	U
1	1	856	G
1	1	866	A
1	1	869	G
1	1	878	A
1	1	879	G
1	1	880	G
1	1	882	G
1	1	884	U
1	1	885	C
1	1	886	A
1	1	888	C
1	1	891	G
1	1	894	U
1	1	895	U
1	1	896	A
1	1	897	C
1	1	907	G
1	1	910	A
1	1	912	C
1	1	914	G
1	1	915	C
1	1	931	U
1	1	941	A
1	1	946	C
1	1	957	C
1	1	959	A

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Mol	Chain	Res	Type
1	1	961	C
1	1	973	A
1	1	974	G
1	1	995	C
1	1	996	A
1	1	999	U
1	1	1009	A
1	1	1012	U
1	1	1013	C
1	1	1017	G
1	1	1022	G
1	1	1023	U
1	1	1026	G
1	1	1033	U
1	1	1035	U
1	1	1040	A
1	1	1043	C
1	1	1044	C
1	1	1045	C
1	1	1047	G
1	1	1049	C
1	1	1050	A
1	1	1051	G
1	1	1053	C
1	1	1055	G
1	1	1056	G
1	1	1058	U
1	1	1059	G
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	1072	C
1	1	1073	A
1	1	1074	G
1	1	1075	C

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Mol	Chain	Res	Type
1	1	1076	C
1	1	1078	U
1	1	1080	A
1	1	1081	U
1	1	1082	U
1	1	1083	U
1	1	1084	A
1	1	1085	A
1	1	1087	G
1	1	1088	A
1	1	1089	A
1	1	1090	A
1	1	1092	C
1	1	1093	G
1	1	1094	U
1	1	1095	A
1	1	1098	A
1	1	1099	G
1	1	1100	C
1	1	1101	U
1	1	1103	A
1	1	1104	C
1	1	1105	U
1	1	1106	G
1	1	1110	G
1	1	1111	A
1	1	1112	G
1	1	1115	G
1	1	1116	G
1	1	1119	U
1	1	1126	A
1	1	1132	U
1	1	1135	C
1	1	1142	A
1	1	1147	A
1	1	1155	A
1	1	1171	G
1	1	1173	U
1	1	1174	U
1	1	1175	A
1	1	1176	U
1	1	1177	G

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Mol	Chain	Res	Type
1	1	1178	C
1	1	1180	U
1	1	1204	A
1	1	1236	G
1	1	1238	G
1	1	1247	A
1	1	1248	G
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	1288	G
1	1	1299	G
1	1	1300	G
1	1	1301	A
1	1	1306	C
1	1	1314	C
1	1	1321	A
1	1	1325	U
1	1	1329	U
1	1	1345	C
1	1	1352	U
1	1	1365	A
1	1	1368	G
1	1	1378	A
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1394	U
1	1	1403	A
1	1	1409	U
1	1	1414	C
1	1	1416	G
1	1	1417	C
1	1	1427	A
1	1	1428	C
1	1	1434	A
1	1	1455	G
1	1	1458	U
1	1	1482	G

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Mol	Chain	Res	Type
1	1	1490	A
1	1	1493	C
1	1	1494	A
1	1	1497	U
1	1	1508	A
1	1	1509	A
1	1	1510	G
1	1	1515	A
1	1	1524	G
1	1	1534	U
1	1	1535	A
1	1	1536	C
1	1	1538	G
1	1	1558	C
1	1	1569	A
1	1	1578	U
1	1	1590	A
1	1	1603	A
1	1	1610	A
1	1	1615	C
1	1	1627	G
1	1	1630	A
1	1	1634	A
1	1	1646	C
1	1	1647	U
1	1	1648	U
1	1	1654	A
1	1	1674	G
1	1	1681	G
1	1	1715	G
1	1	1726	C
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1733	G
1	1	1738	G
1	1	1756	G
1	1	1764	C
1	1	1773	A
1	1	1786	A
1	1	1791	A
1	1	1800	C

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Mol	Chain	Res	Type
1	1	1801	A
1	1	1802	A
1	1	1808	A
1	1	1815	A
1	1	1816	C
1	1	1820	U
1	1	1833	C
1	1	1847	A
1	1	1848	A
1	1	1858	A
1	1	1859	U
1	1	1869	G
1	1	1906	G
1	1	1914	C
1	1	1919	A
1	1	1924	C
1	1	1927	A
1	1	1928	A
1	1	1929	G
1	1	1936	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	2013	A
1	1	2022	U
1	1	2023	C
1	1	2033	A
1	1	2034	U
1	1	2043	C
1	1	2049	G
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2060	A
1	1	2061	G
1	1	2062	A

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Mol	Chain	Res	Type
1	1	2064	C
1	1	2068	U
1	1	2069	G7M
1	1	2080	A
1	1	2093	G
1	1	2099	U
1	1	2100	G
1	1	2101	A
1	1	2102	G
1	1	2104	C
1	1	2105	U
1	1	2106	U
1	1	2109	U
1	1	2110	G
1	1	2111	U
1	1	2112	G
1	1	2113	U
1	1	2114	A
1	1	2115	G
1	1	2117	A
1	1	2118	U
1	1	2120	G
1	1	2122	U
1	1	2123	G
1	1	2124	G
1	1	2125	G
1	1	2126	A
1	1	2128	G
1	1	2130	U
1	1	2131	U
1	1	2132	U
1	1	2134	A
1	1	2136	G
1	1	2138	G
1	1	2139	U
1	1	2144	G
1	1	2146	C
1	1	2147	A
1	1	2151	U
1	1	2154	A
1	1	2155	U
1	1	2156	G

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Mol	Chain	Res	Type
1	1	2157	G
1	1	2158	A
1	1	2159	G
1	1	2161	C
1	1	2163	A
1	1	2165	C
1	1	2166	U
1	1	2168	G
1	1	2170	A
1	1	2171	A
1	1	2172	U
1	1	2174	C
1	1	2178	C
1	1	2181	U
1	1	2182	U
1	1	2183	A
1	1	2186	G
1	1	2188	U
1	1	2189	U
1	1	2190	G
1	1	2191	A
1	1	2193	G
1	1	2194	U
1	1	2198	A
1	1	2199	A
1	1	2204	G
1	1	2211	A
1	1	2212	A
1	1	2225	A
1	1	2238	G
1	1	2239	G
1	1	2250	G
1	1	2266	A
1	1	2268	A
1	1	2279	G
1	1	2283	C
1	1	2287	A
1	1	2297	A
1	1	2305	U
1	1	2308	G
1	1	2309	A
1	1	2315	G

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Mol	Chain	Res	Type
1	1	2322	A
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2347	C
1	1	2350	C
1	1	2361	G
1	1	2383	G
1	1	2385	C
1	1	2402	U
1	1	2403	C
1	1	2423	U
1	1	2425	A
1	1	2426	A
1	1	2428	G
1	1	2429	G
1	1	2430	A
1	1	2441	U
1	1	2445	2MG
1	1	2448	A
1	1	2469	A
1	1	2470	G
1	1	2475	C
1	1	2476	A
1	1	2491	U
1	1	2498	OMC
1	1	2499	C
1	1	2501	C
1	1	2504	PSU
1	1	2506	U
1	1	2507	C
1	1	2517	C
1	1	2518	A
1	1	2519	U
1	1	2520	C
1	1	2529	G
1	1	2535	G
1	1	2554	U
1	1	2555	U
1	1	2564	A
1	1	2566	A
1	1	2567	G

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Mol	Chain	Res	Type
1	1	2572	A
1	1	2585	U
1	1	2586	U
1	1	2597	G
1	1	2602	A
1	1	2609	U
1	1	2613	U
1	1	2615	U
1	1	2629	U
1	1	2630	G
1	1	2646	C
1	1	2682	A
1	1	2689	U
1	1	2690	U
1	1	2712	C
1	1	2714	G
1	1	2725	A
1	1	2726	A
1	1	2729	G
1	1	2733	A
1	1	2744	G
1	1	2748	A
1	1	2750	A
1	1	2765	A
1	1	2776	A
1	1	2777	G
1	1	2778	A
1	1	2790	U
1	1	2794	C
1	1	2795	C
1	1	2797	U
1	1	2798	U
1	1	2818	U
1	1	2820	A
1	1	2849	U
1	1	2867	G
1	1	2873	A
1	1	2874	C
1	1	2880	C
1	1	2884	U
1	1	2903	U
2	2	4	U

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Mol	Chain	Res	Type
2	2	6	G
2	2	8	A
2	2	9	G
2	2	14	U
2	2	31	G
2	2	32	A
2	2	39	G
2	2	47	C
2	2	48	C
2	2	51	A
2	2	70	U
2	2	71	A
2	2	72	A
2	2	73	C
2	2	75	G
2	2	76	G
2	2	81	A
2	2	82	G
2	2	83	C
2	2	84	U
2	2	85	U
2	2	87	C
2	2	88	U
2	2	89	U
2	2	91	U
2	2	95	C
2	2	108	G
2	2	110	C
2	2	120	A
2	2	128	G
2	2	130	A
2	2	131	A
2	2	177	G
2	2	179	A
2	2	181	A
2	2	188	C
2	2	197	A
2	2	204	G
2	2	207	C
2	2	209	U
2	2	211	G
2	2	212	G

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Mol	Chain	Res	Type
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	280	C
2	2	289	G
2	2	299	G
2	2	328	C
2	2	332	G
2	2	334	C
2	2	347	G
2	2	351	G
2	2	352	C
2	2	354	G
2	2	367	U
2	2	369	G
2	2	372	C
2	2	373	A
2	2	392	C
2	2	397	A
2	2	406	G
2	2	412	A
2	2	413	G
2	2	414	A
2	2	421	U
2	2	424	G
2	2	429	U
2	2	457	G
2	2	464	U
2	2	467	U
2	2	468	A
2	2	469	C
2	2	474	G
2	2	479	U
2	2	482	A
2	2	484	G
2	2	491	G
2	2	495	A
2	2	496	A
2	2	497	G

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Mol	Chain	Res	Type
2	2	511	C
2	2	517	G
2	2	518	C
2	2	521	G
2	2	524	G
2	2	527	G7M
2	2	532	A
2	2	547	A
2	2	559	A
2	2	564	C
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	633	G
2	2	639	G
2	2	650	G
2	2	653	U
2	2	665	A
2	2	687	A
2	2	706	A
2	2	723	U
2	2	724	G
2	2	731	G
2	2	732	C
2	2	748	G
2	2	753	A
2	2	755	G
2	2	781	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	839	C
2	2	841	C
2	2	843	U
2	2	844	G
2	2	846	G

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Mol	Chain	Res	Type
2	2	851	G
2	2	889	A
2	2	890	G
2	2	900	A
2	2	913	A
2	2	914	A
2	2	917	G
2	2	934	C
2	2	935	A
2	2	939	G
2	2	959	A
2	2	960	U
2	2	969	A
2	2	971	G
2	2	975	A
2	2	976	G
2	2	977	A
2	2	981	U
2	2	992	U
2	2	993	G
2	2	996	A
2	2	999	C
2	2	1004	A
2	2	1009	U
2	2	1017	U
2	2	1018	G
2	2	1020	G
2	2	1024	G
2	2	1025	U
2	2	1029	U
2	2	1030	U
2	2	1031	C
2	2	1032	G
2	2	1033	G
2	2	1044	A
2	2	1046	A
2	2	1052	U
2	2	1053	G
2	2	1065	U
2	2	1066	C
2	2	1078	U
2	2	1079	G

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Mol	Chain	Res	Type
2	2	1085	U
2	2	1094	G
2	2	1095	U
2	2	1101	A
2	2	1108	G
2	2	1124	G
2	2	1125	U
2	2	1132	C
2	2	1136	C
2	2	1137	C
2	2	1138	G
2	2	1139	G
2	2	1140	C
2	2	1141	C
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	1168	U
2	2	1169	A
2	2	1175	G
2	2	1176	A
2	2	1184	G
2	2	1193	G
2	2	1196	A
2	2	1197	A
2	2	1212	U
2	2	1213	A
2	2	1226	C
2	2	1236	A
2	2	1238	A
2	2	1250	A
2	2	1258	G
2	2	1260	G
2	2	1267	C
2	2	1268	G
2	2	1275	A
2	2	1280	A
2	2	1287	A

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Mol	Chain	Res	Type
2	2	1299	A
2	2	1302	C
2	2	1304	G
2	2	1305	G
2	2	1317	C
2	2	1318	A
2	2	1320	C
2	2	1322	C
2	2	1323	G
2	2	1363	A
2	2	1394	A
2	2	1398	A
2	2	1419	G
2	2	1443	C
2	2	1446	A
2	2	1450	U
2	2	1452	C
2	2	1456	A
2	2	1457	G
2	2	1492	A
2	2	1493	A
2	2	1494	G
2	2	1499	A
2	2	1503	A
2	2	1506	U
2	2	1507	A
2	2	1517	G
2	2	1529	G
2	2	1530	G
2	2	1532	U
2	2	1533	C
2	2	1534	A
2	2	1535	C
3	3	9	G
3	3	13	G
3	3	35	C
3	3	36	C
3	3	37	C
3	3	41	G
3	3	44	G
3	3	53	A
3	3	67	G

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Mol	Chain	Res	Type
3	3	85	G
3	3	89	U
3	3	99	A
3	3	109	A
4	4	4	G
4	4	7	G
4	4	8	A
4	4	11	C
4	4	14	G
4	4	15	A
4	4	18	C
4	4	20	A
4	4	21	C
4	4	28	U
4	4	29	G
4	4	30	C
4	4	31	G
4	4	32	A
4	4	33	A
4	4	34	A
4	4	36	C
4	4	39	A
4	4	41	G
4	4	44	C
4	4	50	G
4	4	53	G
4	4	54	G
4	4	55	G
4	4	56	C
4	4	61	G
4	4	63	C
4	4	64	C
4	4	67	G
4	4	68	U
4	4	69	A
4	4	70	A
4	4	71	A
4	4	74	G
4	4	75	C
4	4	77	G
4	4	78	C
4	4	79	A

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Mol	Chain	Res	Type
4	4	80	A
4	4	81	A
4	4	82	A
4	4	83	A
4	4	84	A
4	4	85	U
4	4	86	A
4	4	87	G
4	4	88	U
4	4	89	C
4	4	90	G
4	4	93	A
4	4	96	G
4	4	97	A
4	4	98	C
4	4	99	G
4	4	100	A
4	4	101	A
4	4	102	A
4	4	103	A
4	4	104	C
4	4	105	U
4	4	106	A
4	4	107	C
4	4	122	A
4	4	123	U
4	4	125	A
4	4	128	U
4	4	130	C
4	4	131	U
4	4	134	G
4	4	138	C
4	4	139	C
4	4	140	U
4	4	142	U
4	4	144	U
4	4	149	A
4	4	154	C
4	4	155	C
4	4	157	C
4	4	159	C
4	4	160	U

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Mol	Chain	Res	Type
4	4	164	G
4	4	165	A
4	4	166	C
4	4	167	G
4	4	170	G
4	4	173	C
4	4	175	A
4	4	180	G
4	4	181	G
4	4	182	U
4	4	184	A
4	4	186	A
4	4	187	C
4	4	188	C
4	4	189	C
4	4	190	A
4	4	191	A
4	4	195	A
4	4	197	A
4	4	200	G
4	4	202	G
4	4	204	G
4	4	206	A
4	4	209	C
4	4	213	G
4	4	214	C
4	4	223	G
4	4	224	A
4	4	225	A
4	4	227	C
4	4	228	G
4	4	229	U
4	4	230	U
4	4	231	A
4	4	233	A
4	4	234	A
4	4	237	U
4	4	240	U
4	4	245	C
4	4	246	U
4	4	252	G
4	4	257	U

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Mol	Chain	Res	Type
4	4	261	G
4	4	262	U
4	4	263	G
4	4	264	U
4	4	267	G
4	4	274	G
4	4	278	G
4	4	281	A
4	4	285	A
4	4	290	A
4	4	291	A
4	4	293	G
4	4	299	C
4	4	300	U
4	4	301	A
4	4	302	A
4	4	303	G
4	4	304	C
4	4	308	U
4	4	310	G
4	4	311	U
4	4	313	C
4	4	314	C
4	4	315	G
4	4	316	A
4	4	317	G
4	4	318	G
4	4	321	G
4	4	322	U
4	4	323	A
4	4	327	A
4	4	328	U
4	4	333	G
4	4	336	G
4	4	344	A
4	4	346	C
4	4	347	PSU
4	4	348	C
4	4	356	C
4	4	360	A
4	4	361	C
4	4	362	C

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Mol	Chain	Res	Type
6	7	17	C
6	7	18	G
6	7	19	G
6	7	20	H2U
6	7	22	G
6	7	43	C
6	7	45	U
6	7	46	G7M
6	7	48	C
6	7	61	C
6	7	75	C
6	7	76	A
7	8	6	G
7	8	8	G
7	8	9	A
7	8	10	G

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	176	A
1	1	404	A
1	1	428	A
1	1	464	U
1	1	631	A
1	1	774	G
1	1	784	G
1	1	894	U
1	1	1070	A
1	1	1088	A
1	1	1109	C
1	1	1287	A
1	1	1379	U
1	1	1614	A
1	1	1680	U
1	1	1927	A
1	1	2048	G
1	1	2100	G
1	1	2150	C
1	1	2193	G
1	1	2425	A
1	1	2505	G

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Mol	Chain	Res	Type
1	1	2506	U
1	1	2516	A
1	1	2596	U
2	2	298	A
2	2	516	PSU
2	2	899	C
2	2	938	A
2	2	958	A
2	2	980	C
2	2	1078	U
2	2	1109	C
2	2	1145	A
2	2	1267	C
2	2	1303	C
2	2	1492	A
2	2	1533	C
4	4	14	G
4	4	19	G
4	4	43	G
4	4	78	C
4	4	79	A
4	4	80	A
4	4	92	A
4	4	96	G
4	4	101	A
4	4	224	A
4	4	310	G
4	4	314	C
4	4	316	A
4	4	343	C
6	7	19	G
6	7	20	H2U
7	8	7	U
7	8	9	A

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

48 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
6	G7M	7	46	6	20,26,27	4.14	10 (50%)	17,39,42	0.98	1 (5%)
2	4OC	2	1402	2	20,23,24	3.28	9 (45%)	26,32,35	0.91	1 (3%)
19	4D4	M	81	19	9,11,12	2.05	2 (22%)	8,13,15	1.84	3 (37%)
1	2MG	1	1835	1	18,26,27	2.77	6 (33%)	16,38,41	1.36	3 (18%)
1	PSU	1	1917	1	18,21,22	1.11	1 (5%)	22,30,33	1.77	4 (18%)
2	5MC	2	967	2	18,22,23	3.60	7 (38%)	26,32,35	0.98	1 (3%)
1	PSU	1	746	1,59	18,21,22	1.10	1 (5%)	22,30,33	1.79	5 (22%)
1	PSU	1	2457	1	18,21,22	1.04	1 (5%)	22,30,33	1.71	3 (13%)
6	H2U	7	20	6	18,21,22	1.10	2 (11%)	21,30,33	2.54	2 (9%)
6	MIA	7	37	6	24,31,32	2.61	4 (16%)	26,44,47	3.13	8 (30%)
2	UR3	2	1498	2	19,22,23	2.99	6 (31%)	26,32,35	1.31	1 (3%)
1	PSU	1	1911	1	18,21,22	1.10	1 (5%)	22,30,33	1.76	4 (18%)
1	PSU	1	2504	1	18,21,22	1.08	1 (5%)	22,30,33	1.76	4 (18%)
1	5MU	1	747	1	19,22,23	4.90	7 (36%)	28,32,35	3.62	8 (28%)
4	5MU	4	341	4	19,22,23	4.89	7 (36%)	28,32,35	3.56	9 (32%)
4	PSU	4	342	4	18,21,22	1.11	1 (5%)	22,30,33	1.74	4 (18%)
2	5MC	2	1407	2	18,22,23	3.62	7 (38%)	26,32,35	1.00	2 (7%)
1	5MC	1	1962	1	18,22,23	3.61	7 (38%)	26,32,35	1.04	2 (7%)
6	PSU	7	39	6	18,21,22	1.08	1 (5%)	22,30,33	1.70	4 (18%)
1	PSU	1	2580	1	18,21,22	1.07	1 (5%)	22,30,33	1.65	4 (18%)
6	3AU	7	47	6	24,28,29	3.03	9 (37%)	33,40,43	1.30	3 (9%)
6	PSU	7	55	6	18,21,22	1.10	1 (5%)	22,30,33	1.73	4 (18%)
2	2MG	2	1516	2	18,26,27	2.79	6 (33%)	16,38,41	1.35	3 (18%)
1	2MA	1	2503	1,59	17,25,26	2.47	5 (29%)	17,37,40	1.30	2 (11%)
1	3TD	1	1915	1	18,22,23	4.33	7 (38%)	22,32,35	1.60	3 (13%)
1	PSU	1	955	1	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
1	5MU	1	1939	1	19,22,23	4.87	7 (36%)	28,32,35	3.63	9 (32%)
1	2MG	1	2445	1	18,26,27	2.76	6 (33%)	16,38,41	1.37	4 (25%)
6	4SU	7	8	6	18,21,22	3.74	8 (44%)	26,30,33	2.20	4 (15%)
1	PSU	1	2605	1	18,21,22	1.10	1 (5%)	22,30,33	1.76	4 (18%)
2	2MG	2	966	2	18,26,27	2.80	6 (33%)	16,38,41	1.44	3 (18%)
1	1MG	1	745	1	18,26,27	2.69	6 (33%)	19,39,42	1.44	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2MG	2	1207	2	18,26,27	2.79	6 (33%)	16,38,41	1.32	3 (18%)
6	H2U	7	16	6	18,21,22	1.22	3 (16%)	21,30,33	1.79	3 (14%)
6	PSU	7	32	6	18,21,22	1.07	1 (5%)	22,30,33	1.74	4 (18%)
6	5MU	7	54	6	19,22,23	4.88	7 (36%)	28,32,35	3.56	9 (32%)
2	MA6	2	1519	2	18,26,27	1.08	2 (11%)	19,38,41	4.39	3 (15%)
1	OMU	1	2552	1	19,22,23	3.21	7 (36%)	26,31,34	1.67	5 (19%)
1	G7M	1	2069	1	20,26,27	2.33	7 (35%)	17,39,42	1.07	1 (5%)
1	OMC	1	2498	1,59	19,22,23	3.05	8 (42%)	26,31,34	0.77	0
49	0TD	q	89	49	7,9,10	1.43	0	6,11,13	1.98	2 (33%)
1	6MZ	1	2030	1	18,25,26	2.05	3 (16%)	16,36,39	2.28	3 (18%)
2	G7M	2	527	2	20,26,27	2.34	7 (35%)	17,39,42	1.06	1 (5%)
1	OMG	1	2251	6,1	18,26,27	2.65	8 (44%)	19,38,41	1.51	4 (21%)
4	PSU	4	347	4	18,21,22	1.12	1 (5%)	22,30,33	1.75	4 (18%)
2	PSU	2	516	2	18,21,22	1.07	1 (5%)	22,30,33	1.69	5 (22%)
2	MA6	2	1518	2	18,26,27	1.05	2 (11%)	19,38,41	4.41	3 (15%)
1	6MZ	1	1618	1	18,25,26	2.10	3 (16%)	16,36,39	2.06	4 (25%)

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. ^{1,2} means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	G7M	7	46	6	-	3/3/25/26	0/3/3/3
2	4OC	2	1402	2	-	2/9/29/30	0/2/2/2
19	4D4	M	81	19	-	5/11/12/14	-
1	2MG	1	1835	1	-	2/5/27/28	0/3/3/3
1	PSU	1	1917	1	-	2/7/25/26	0/2/2/2
2	5MC	2	967	2	-	0/7/25/26	0/2/2/2
1	PSU	1	746	1,59	-	0/7/25/26	0/2/2/2
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
6	H2U	7	20	6	-	6/7/38/39	0/2/2/2
6	MIA	7	37	6	-	5/11/33/34	0/3/3/3
2	UR3	2	1498	2	-	2/7/25/26	0/2/2/2
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2504	1	-	2/7/25/26	0/2/2/2
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	5MU	4	341	4	-	0/7/25/26	0/2/2/2
4	PSU	4	342	4	-	1/7/25/26	0/2/2/2
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
1	5MC	1	1962	1	-	0/7/25/26	0/2/2/2
6	PSU	7	39	6	-	0/7/25/26	0/2/2/2
1	PSU	1	2580	1	-	3/7/25/26	0/2/2/2
6	3AU	7	47	6	-	2/16/34/35	0/2/2/2
6	PSU	7	55	6	-	0/7/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
1	2MA	1	2503	1,59	-	2/3/25/26	0/3/3/3
1	3TD	1	1915	1	-	2/7/25/26	0/2/2/2
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
1	5MU	1	1939	1	-	0/7/25/26	0/2/2/2
1	2MG	1	2445	1	-	2/5/27/28	0/3/3/3
6	4SU	7	8	6	-	0/7/25/26	0/2/2/2
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
2	2MG	2	966	2	-	0/5/27/28	0/3/3/3
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
2	2MG	2	1207	2	-	0/5/27/28	0/3/3/3
6	H2U	7	16	6	-	1/7/38/39	0/2/2/2
6	PSU	7	32	6	-	0/7/25/26	0/2/2/2
6	5MU	7	54	6	-	2/7/25/26	0/2/2/2
2	MA6	2	1519	2	-	2/7/29/30	0/3/3/3
1	OMU	1	2552	1	-	1/9/27/28	0/2/2/2
1	G7M	1	2069	1	-	2/3/25/26	0/3/3/3
1	OMC	1	2498	1,59	-	2/9/27/28	0/2/2/2
49	0TD	q	89	49	-	4/7/12/14	-
1	6MZ	1	2030	1	-	2/5/27/28	0/3/3/3
2	G7M	2	527	2	-	3/3/25/26	0/3/3/3
1	OMG	1	2251	6,1	-	0/5/27/28	0/3/3/3
4	PSU	4	347	4	-	2/7/25/26	0/2/2/2
2	PSU	2	516	2	-	2/7/25/26	0/2/2/2
2	MA6	2	1518	2	-	0/7/29/30	0/3/3/3
1	6MZ	1	1618	1	-	3/5/27/28	0/3/3/3

All (211) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1915	3TD	C6-C5	12.55	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	747	5MU	C2-N1	11.45	1.56	1.38
6	7	54	5MU	C2-N1	11.29	1.56	1.38
4	4	341	5MU	C2-N1	11.23	1.56	1.38
1	1	1939	5MU	C2-N1	11.12	1.56	1.38
6	7	54	5MU	C6-N1	10.73	1.56	1.38
4	4	341	5MU	C6-N1	10.63	1.56	1.38
1	1	1939	5MU	C6-N1	10.59	1.56	1.38
1	1	747	5MU	C6-N1	10.52	1.56	1.38
1	1	1939	5MU	C4-C5	10.26	1.61	1.44
4	4	341	5MU	C4-C5	10.20	1.61	1.44
1	1	747	5MU	C4-C5	10.15	1.61	1.44
6	7	46	G7M	C8-N9	10.12	1.51	1.33
6	7	46	G7M	C8-N7	10.11	1.51	1.33
6	7	54	5MU	C4-C5	10.09	1.61	1.44
1	1	1915	3TD	C2-N1	9.37	1.49	1.37
2	2	1407	5MC	C6-C5	9.23	1.49	1.34
1	1	1962	5MC	C6-C5	9.16	1.49	1.34
2	2	967	5MC	C6-C5	9.15	1.49	1.34
6	7	47	3AU	C2-N1	8.48	1.50	1.38
6	7	8	4SU	C4-N3	7.90	1.46	1.37
1	1	747	5MU	C4-N3	-7.78	1.24	1.38
1	1	1618	6MZ	C6-N6	7.75	1.47	1.35
1	1	1939	5MU	C4-N3	-7.74	1.24	1.38
4	4	341	5MU	C4-N3	-7.72	1.24	1.38
6	7	54	5MU	C4-N3	-7.69	1.24	1.38
1	1	2503	2MA	C2-N3	7.64	1.47	1.31
1	1	2030	6MZ	C6-N6	7.58	1.47	1.35
2	2	1498	UR3	C2-N1	7.57	1.49	1.38
1	1	2552	OMU	C2-N3	7.50	1.51	1.38
6	7	37	MIA	C2-S10	7.48	1.82	1.75
1	1	2552	OMU	C2-N1	7.46	1.50	1.38
6	7	37	MIA	C13-C14	7.30	1.53	1.32
6	7	8	4SU	C2-N1	7.08	1.49	1.38
2	2	966	2MG	C2-N2	6.88	1.48	1.33
6	7	8	4SU	C2-N3	6.86	1.50	1.38
2	2	1207	2MG	C2-N2	6.86	1.48	1.33
2	2	1516	2MG	C2-N2	6.85	1.48	1.33
1	1	1835	2MG	C2-N2	6.83	1.48	1.33
2	2	1498	UR3	C6-C5	6.77	1.50	1.35
1	1	2445	2MG	C2-N2	6.76	1.48	1.33
6	7	47	3AU	C6-C5	6.66	1.50	1.35
1	1	745	1MG	C2-N3	6.66	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1962	5MC	C4-N3	6.63	1.45	1.34
2	2	967	5MC	C4-N3	6.62	1.45	1.34
2	2	1407	5MC	C4-N3	6.59	1.45	1.34
2	2	1402	4OC	C4-N3	6.58	1.44	1.32
1	1	2498	OMC	C2-N3	6.46	1.49	1.36
1	1	745	1MG	C2-N2	6.26	1.45	1.34
1	1	1962	5MC	C2-N3	6.25	1.49	1.36
2	2	1407	5MC	C2-N3	6.24	1.49	1.36
2	2	967	5MC	C2-N3	6.22	1.49	1.36
2	2	1498	UR3	C2-N3	6.16	1.50	1.39
2	2	1402	4OC	C2-N3	6.11	1.48	1.36
6	7	37	MIA	C6-N6	6.08	1.45	1.34
1	1	2498	OMC	C6-C5	6.05	1.49	1.35
4	4	341	5MU	C6-C5	6.04	1.44	1.34
6	7	47	3AU	C2-N3	6.04	1.49	1.38
1	1	2552	OMU	C6-C5	6.00	1.49	1.35
1	1	1939	5MU	C6-C5	6.00	1.44	1.34
1	1	747	5MU	C6-C5	6.00	1.44	1.34
6	7	46	G7M	C2-N3	6.00	1.47	1.33
6	7	54	5MU	C6-C5	5.89	1.44	1.34
2	2	1402	4OC	C6-C5	5.86	1.48	1.35
1	1	1915	3TD	C6-N1	5.84	1.45	1.36
6	7	8	4SU	C6-C5	5.77	1.48	1.35
2	2	1402	4OC	C4-N4	5.65	1.47	1.35
1	1	2251	OMG	C2-N3	5.58	1.46	1.33
2	2	966	2MG	C2-N1	5.53	1.45	1.36
2	2	1207	2MG	C2-N1	5.52	1.45	1.36
2	2	1516	2MG	C2-N1	5.52	1.45	1.36
1	1	2445	2MG	C2-N1	5.49	1.45	1.36
1	1	1835	2MG	C2-N1	5.47	1.45	1.36
1	1	1835	2MG	C4-N3	5.35	1.50	1.37
2	2	1207	2MG	C4-N3	5.30	1.50	1.37
19	M	81	4D4	CZ-NE	5.27	1.43	1.33
2	2	966	2MG	C4-N3	5.27	1.50	1.37
2	2	1516	2MG	C4-N3	5.21	1.50	1.37
1	1	1915	3TD	C2-N3	5.20	1.50	1.38
1	1	2498	OMC	C4-N3	5.16	1.44	1.34
1	1	2445	2MG	C4-N3	5.15	1.49	1.37
2	2	527	G7M	C2-N2	5.09	1.46	1.34
1	1	2069	G7M	C2-N2	5.07	1.46	1.34
1	1	2251	OMG	C4-N3	5.07	1.49	1.37
1	1	745	1MG	C4-N3	5.05	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2498	OMC	C4-N4	4.96	1.45	1.33
6	7	8	4SU	C5-C4	4.94	1.48	1.42
1	1	2251	OMG	C2-N2	4.84	1.45	1.34
6	7	46	G7M	C2-N2	4.83	1.45	1.34
6	7	46	G7M	C6-N1	4.82	1.45	1.37
1	1	2503	2MA	C4-N3	4.77	1.48	1.37
1	1	2498	OMC	C2-N1	4.62	1.50	1.40
2	2	1407	5MC	C6-N1	4.61	1.45	1.38
2	2	527	G7M	C4-N3	4.61	1.48	1.37
1	1	1962	5MC	C6-N1	4.59	1.45	1.38
2	2	967	5MC	C6-N1	4.57	1.45	1.38
1	1	2069	G7M	C4-N3	4.55	1.48	1.37
1	1	1962	5MC	C4-N4	4.45	1.45	1.34
2	2	967	5MC	C4-N4	4.44	1.45	1.34
2	2	1407	5MC	C4-N4	4.43	1.45	1.34
2	2	527	G7M	C2-N3	4.43	1.43	1.33
6	7	8	4SU	C4-S4	-4.40	1.60	1.68
2	2	1402	4OC	C2-N1	4.40	1.49	1.40
1	1	2552	OMU	C4-N3	4.38	1.46	1.38
1	1	2069	G7M	C2-N3	4.35	1.43	1.33
6	7	46	G7M	C4-N3	4.33	1.47	1.37
6	7	47	3AU	C4-N3	4.26	1.47	1.40
2	2	967	5MC	C2-N1	4.26	1.49	1.40
2	2	1407	5MC	C2-N1	4.24	1.49	1.40
1	1	1962	5MC	C2-N1	4.20	1.49	1.40
2	2	1402	4OC	C5-C4	4.07	1.49	1.40
2	2	966	2MG	C6-N1	3.92	1.43	1.37
2	2	1516	2MG	C6-N1	3.90	1.43	1.37
2	2	1207	2MG	C6-N1	3.87	1.43	1.37
1	1	2251	OMG	C6-N1	3.85	1.43	1.37
1	1	2445	2MG	C6-N1	3.82	1.43	1.37
6	7	46	G7M	C2-N1	3.81	1.47	1.37
1	1	1915	3TD	O2-C2	-3.78	1.16	1.23
1	1	1835	2MG	C6-N1	3.75	1.43	1.37
4	4	347	PSU	C6-C5	3.68	1.39	1.35
2	2	516	PSU	C6-C5	3.66	1.39	1.35
4	4	342	PSU	C6-C5	3.65	1.39	1.35
1	1	1911	PSU	C6-C5	3.62	1.39	1.35
1	1	1917	PSU	C6-C5	3.62	1.39	1.35
1	1	2580	PSU	C6-C5	3.61	1.39	1.35
1	1	2605	PSU	C6-C5	3.61	1.39	1.35
6	7	55	PSU	C6-C5	3.60	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2504	PSU	C6-C5	3.60	1.39	1.35
6	7	39	PSU	C6-C5	3.60	1.39	1.35
2	2	1402	4OC	CM4-N4	3.59	1.52	1.45
1	1	746	PSU	C6-C5	3.58	1.39	1.35
2	2	1402	4OC	O2-C2	-3.53	1.17	1.23
6	7	32	PSU	C6-C5	3.52	1.39	1.35
1	1	955	PSU	C6-C5	3.46	1.39	1.35
6	7	47	3AU	C6-N1	3.43	1.46	1.38
1	1	2457	PSU	C6-C5	3.41	1.39	1.35
2	2	1516	2MG	C5-C6	3.36	1.54	1.47
2	2	966	2MG	C5-C6	3.36	1.54	1.47
1	1	1835	2MG	C5-C6	3.36	1.54	1.47
2	2	1207	2MG	C5-C6	3.35	1.54	1.47
1	1	2445	2MG	C5-C6	3.33	1.54	1.47
1	1	2498	OMC	C6-N1	3.25	1.45	1.38
1	1	2552	OMU	C6-N1	3.24	1.45	1.38
1	1	2251	OMG	C5-C6	3.21	1.53	1.47
2	2	1498	UR3	C6-N1	3.20	1.45	1.38
1	1	2069	G7M	C6-N1	3.20	1.42	1.37
6	7	16	H2U	C2-N3	-3.12	1.32	1.38
1	1	2069	G7M	C2-N1	3.11	1.45	1.37
2	2	527	G7M	C2-N1	3.10	1.45	1.37
2	2	527	G7M	C6-N1	3.09	1.42	1.37
6	7	20	H2U	C2-N3	-2.98	1.32	1.38
2	2	527	G7M	O6-C6	-2.98	1.17	1.23
1	1	2069	G7M	O6-C6	-2.98	1.17	1.23
6	7	8	4SU	C6-N1	2.95	1.45	1.38
6	7	46	G7M	C5-C6	2.89	1.52	1.45
1	1	2552	OMU	C5-C4	2.86	1.50	1.43
6	7	47	3AU	C5-C4	2.84	1.51	1.43
2	2	1519	MA6	C5-C4	-2.84	1.33	1.40
2	2	1518	MA6	C5-C4	-2.79	1.33	1.40
1	1	2251	OMG	C2-N1	2.78	1.44	1.37
6	7	47	3AU	C11-C10	2.73	1.58	1.52
6	7	16	H2U	C4-N3	-2.72	1.33	1.37
6	7	20	H2U	C4-N3	-2.68	1.33	1.37
1	1	2503	2MA	C2-N1	2.64	1.44	1.36
6	7	37	MIA	C5-C4	-2.62	1.34	1.40
2	2	527	G7M	C5-C6	2.62	1.52	1.45
6	7	47	3AU	O4-C4	-2.59	1.18	1.23
1	1	2498	OMC	O2-C2	-2.59	1.18	1.23
1	1	2069	G7M	C5-C6	2.59	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1962	5MC	O2-C2	-2.58	1.18	1.23
6	7	54	5MU	O4-C4	-2.57	1.18	1.23
6	7	46	G7M	C5-C4	2.55	1.44	1.39
2	2	967	5MC	O2-C2	-2.55	1.19	1.23
1	1	1939	5MU	O4-C4	-2.55	1.18	1.23
1	1	747	5MU	O4-C4	-2.54	1.18	1.23
1	1	2498	OMC	C5-C4	2.54	1.48	1.42
1	1	745	1MG	C5-C4	-2.53	1.36	1.43
2	2	1407	5MC	O2-C2	-2.53	1.19	1.23
4	4	341	5MU	O4-C4	-2.52	1.18	1.23
1	1	2251	OMG	C5-C4	-2.51	1.36	1.43
1	1	1618	6MZ	C2-N3	2.50	1.36	1.32
1	1	2503	2MA	C6-N1	2.45	1.43	1.38
6	7	47	3AU	O2-C2	-2.44	1.18	1.22
1	1	2552	OMU	O4-C4	-2.42	1.19	1.24
1	1	2030	6MZ	C2-N3	2.41	1.36	1.32
2	2	1498	UR3	C5-C4	2.41	1.50	1.43
19	M	81	4D4	CZ-NH1	2.41	1.44	1.34
2	2	1519	MA6	C2-N3	2.41	1.36	1.32
1	1	1939	5MU	O2-C2	-2.32	1.18	1.23
4	4	341	5MU	O2-C2	-2.32	1.18	1.23
6	7	54	5MU	O2-C2	-2.31	1.18	1.23
2	2	966	2MG	C5-C4	-2.29	1.37	1.43
2	2	1498	UR3	C4-N3	2.29	1.45	1.40
2	2	1402	4OC	C6-N1	2.29	1.43	1.38
6	7	16	H2U	C2-N1	-2.28	1.32	1.35
1	1	2445	2MG	C5-C4	-2.27	1.37	1.43
1	1	747	5MU	O2-C2	-2.27	1.18	1.23
2	2	1518	MA6	C2-N3	2.27	1.35	1.32
2	2	1207	2MG	C5-C4	-2.26	1.37	1.43
2	2	1516	2MG	C5-C4	-2.26	1.37	1.43
1	1	1915	3TD	C4-N3	2.24	1.45	1.40
1	1	745	1MG	C6-N1	2.23	1.43	1.39
6	7	8	4SU	O2-C2	-2.18	1.19	1.23
1	1	1915	3TD	O4-C4	-2.15	1.18	1.23
1	1	1835	2MG	C5-C4	-2.15	1.37	1.43
1	1	2251	OMG	O6-C6	-2.15	1.18	1.23
6	7	46	G7M	O6-C6	-2.14	1.18	1.23
1	1	745	1MG	C5-C6	2.14	1.53	1.47
1	1	2503	2MA	C5-C4	-2.06	1.37	1.43
1	1	2030	6MZ	C5-C4	-2.01	1.35	1.40
1	1	1618	6MZ	C5-C4	-2.01	1.35	1.40

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1518	MA6	C1'-N9-C4	14.05	151.33	126.64
2	2	1519	MA6	C1'-N9-C4	13.76	150.82	126.64
1	1	1939	5MU	C5-C4-N3	12.03	125.58	115.31
1	1	747	5MU	C5-C4-N3	11.95	125.52	115.31
6	7	54	5MU	C5-C4-N3	11.93	125.50	115.31
4	4	341	5MU	C5-C4-N3	11.82	125.40	115.31
2	2	1519	MA6	N1-C6-N6	-11.72	104.72	117.06
2	2	1518	MA6	N1-C6-N6	-11.67	104.78	117.06
6	7	20	H2U	C4-N3-C2	-10.62	116.98	125.79
1	1	1939	5MU	C5-C6-N1	-10.23	112.81	123.34
1	1	747	5MU	C5-C6-N1	-10.08	112.96	123.34
4	4	341	5MU	C5-C6-N1	-9.70	113.36	123.34
6	7	54	5MU	C5-C6-N1	-9.55	113.52	123.34
6	7	37	MIA	C11-S10-C2	9.02	109.00	102.27
6	7	37	MIA	C12-C13-C14	-8.63	110.34	127.14
6	7	8	4SU	C4-N3-C2	-7.73	119.83	127.34
6	7	16	H2U	C4-N3-C2	-5.61	121.14	125.79
2	2	1519	MA6	N3-C2-N1	-5.60	119.93	128.68
1	1	2030	6MZ	N3-C2-N1	-5.55	120.01	128.68
1	1	1618	6MZ	N3-C2-N1	-5.53	120.04	128.68
6	7	8	4SU	C5-C4-N3	5.44	119.74	114.69
2	2	1518	MA6	N3-C2-N1	-5.32	120.36	128.68
1	1	2030	6MZ	C9-N6-C6	-5.17	118.42	122.87
1	1	2552	OMU	C4-N3-C2	-5.16	119.77	126.58
6	7	54	5MU	O4-C4-C5	-5.09	119.00	124.90
1	1	1915	3TD	N1-C2-N3	4.93	120.03	116.14
2	2	1498	UR3	C4-N3-C2	-4.89	119.96	124.56
1	1	1939	5MU	C4-N3-C2	-4.84	121.09	127.35
1	1	1939	5MU	O4-C4-C5	-4.82	119.31	124.90
1	1	747	5MU	O4-C4-C5	-4.82	119.32	124.90
4	4	341	5MU	O4-C4-C5	-4.76	119.39	124.90
1	1	747	5MU	C4-N3-C2	-4.71	121.25	127.35
6	7	37	MIA	C15-C14-C13	-4.70	109.06	122.65
6	7	54	5MU	C4-N3-C2	-4.67	121.30	127.35
4	4	341	5MU	C4-N3-C2	-4.66	121.32	127.35
1	1	746	PSU	C4-N3-C2	-4.57	119.75	126.34
1	1	2605	PSU	C4-N3-C2	-4.53	119.82	126.34
1	1	2504	PSU	C4-N3-C2	-4.52	119.82	126.34
1	1	1911	PSU	C4-N3-C2	-4.52	119.83	126.34
4	4	341	5MU	N3-C2-N1	4.51	120.87	114.89
4	4	342	PSU	C4-N3-C2	-4.50	119.85	126.34
1	1	1917	PSU	C4-N3-C2	-4.49	119.87	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	7	55	PSU	C4-N3-C2	-4.48	119.88	126.34
1	1	955	PSU	C4-N3-C2	-4.48	119.88	126.34
4	4	347	PSU	N1-C2-N3	4.48	120.20	115.13
6	7	32	PSU	C4-N3-C2	-4.47	119.90	126.34
6	7	54	5MU	N3-C2-N1	4.47	120.82	114.89
1	1	2457	PSU	C4-N3-C2	-4.46	119.91	126.34
1	1	746	PSU	N1-C2-N3	4.45	120.17	115.13
4	4	347	PSU	C4-N3-C2	-4.45	119.93	126.34
1	1	1917	PSU	N1-C2-N3	4.44	120.16	115.13
1	1	2504	PSU	N1-C2-N3	4.43	120.15	115.13
1	1	1939	5MU	N3-C2-N1	4.41	120.74	114.89
1	1	1911	PSU	N1-C2-N3	4.41	120.12	115.13
6	7	32	PSU	N1-C2-N3	4.41	120.12	115.13
1	1	2605	PSU	N1-C2-N3	4.39	120.11	115.13
6	7	55	PSU	N1-C2-N3	4.38	120.09	115.13
6	7	39	PSU	C4-N3-C2	-4.37	120.04	126.34
1	1	955	PSU	N1-C2-N3	4.37	120.09	115.13
6	7	39	PSU	N1-C2-N3	4.35	120.06	115.13
4	4	342	PSU	N1-C2-N3	4.34	120.05	115.13
1	1	747	5MU	N3-C2-N1	4.32	120.63	114.89
6	7	37	MIA	C16-C14-C13	-4.32	110.16	122.65
1	1	2457	PSU	N1-C2-N3	4.29	119.99	115.13
1	1	2580	PSU	N1-C2-N3	4.25	119.95	115.13
2	2	516	PSU	C4-N3-C2	-4.22	120.27	126.34
1	1	747	5MU	C5M-C5-C6	-4.20	117.24	122.85
2	2	516	PSU	N1-C2-N3	4.18	119.86	115.13
1	1	2580	PSU	C4-N3-C2	-4.18	120.32	126.34
1	1	745	1MG	C5-C6-N1	4.06	120.01	113.90
1	1	2030	6MZ	C2-N1-C6	4.06	120.07	116.59
6	7	16	H2U	O4'-C1'-N1	4.05	114.82	109.30
4	4	341	5MU	C5M-C5-C6	-4.04	117.45	122.85
1	1	1939	5MU	C5M-C5-C6	-3.99	117.52	122.85
4	4	341	5MU	C5M-C5-C4	3.99	123.16	118.77
6	7	54	5MU	C5M-C5-C6	-3.96	117.56	122.85
1	1	747	5MU	C5M-C5-C4	3.95	123.12	118.77
1	1	1618	6MZ	C2-N1-C6	3.95	119.98	116.59
6	7	54	5MU	C5M-C5-C4	3.93	123.09	118.77
1	1	1915	3TD	C4-N3-C2	-3.87	120.41	124.61
1	1	1939	5MU	C5M-C5-C4	3.77	122.91	118.77
1	1	2552	OMU	N3-C2-N1	3.75	119.87	114.89
6	7	8	4SU	N3-C2-N1	3.75	119.87	114.89
6	7	47	3AU	C4-N3-C2	-3.70	119.99	124.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	7	37	MIA	N3-C2-N1	-3.68	120.22	126.98
6	7	37	MIA	S10-C2-N1	3.63	128.57	116.01
1	1	1618	6MZ	C9-N6-C6	-3.59	119.78	122.87
49	q	89	0TD	OD2-CG-CB	3.55	120.81	113.15
1	1	2503	2MA	C5-C6-N1	3.48	120.02	114.02
1	1	1835	2MG	C5-C6-N1	3.46	120.06	113.95
6	7	37	MIA	C2-N3-C4	3.44	120.07	115.32
19	M	81	4D4	NE-CZ-NH2	3.43	126.73	120.70
1	1	2251	OMG	C5-C6-N1	3.43	120.00	113.95
2	2	966	2MG	C5-C6-N1	3.40	119.96	113.95
1	1	1962	5MC	C5-C6-N1	-3.39	119.85	123.34
6	7	8	4SU	C5-C4-S4	-3.37	120.13	124.47
1	1	2445	2MG	C5-C6-N1	3.36	119.88	113.95
2	2	1516	2MG	C5-C6-N1	3.35	119.88	113.95
2	2	1207	2MG	C5-C6-N1	3.31	119.80	113.95
6	7	47	3AU	C5-C4-N3	3.30	119.85	115.50
1	1	2552	OMU	C5-C4-N3	3.27	119.73	114.84
2	2	1407	5MC	C5-C6-N1	-3.16	120.08	123.34
2	2	967	5MC	C5-C6-N1	-2.96	120.30	123.34
1	1	2251	OMG	C8-N7-C5	2.91	108.54	102.99
2	2	527	G7M	C2-N1-C6	-2.88	119.79	125.10
1	1	2251	OMG	C2-N1-C6	-2.88	119.79	125.10
1	1	2069	G7M	C2-N1-C6	-2.87	119.81	125.10
1	1	2552	OMU	O4-C4-C5	-2.83	120.19	125.16
1	1	745	1MG	C8-N7-C5	2.77	108.27	102.99
6	7	46	G7M	C2-N1-C6	-2.73	120.07	125.10
1	1	1917	PSU	O2-C2-N1	-2.73	119.79	122.79
1	1	2503	2MA	C8-N7-C5	2.67	108.07	102.99
4	4	342	PSU	O2-C2-N1	-2.65	119.88	122.79
4	4	347	PSU	O2-C2-N1	-2.64	119.89	122.79
1	1	955	PSU	O2-C2-N1	-2.62	119.91	122.79
1	1	1939	5MU	O4-C4-N3	-2.61	115.11	120.12
1	1	1911	PSU	O2-C2-N1	-2.61	119.92	122.79
2	2	966	2MG	C8-N7-C5	2.61	107.95	102.99
1	1	2605	PSU	O2-C2-N1	-2.60	119.92	122.79
1	1	1835	2MG	C8-N7-C5	2.60	107.95	102.99
2	2	1516	2MG	C8-N7-C5	2.59	107.92	102.99
1	1	747	5MU	O4-C4-N3	-2.58	115.17	120.12
2	2	1207	2MG	C8-N7-C5	2.58	107.91	102.99
6	7	32	PSU	O2-C2-N1	-2.58	119.95	122.79
1	1	746	PSU	O2-C2-N1	-2.56	119.97	122.79
1	1	2457	PSU	O2-C2-N1	-2.56	119.97	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	341	5MU	O4-C4-N3	-2.56	115.21	120.12
6	7	55	PSU	O2-C2-N1	-2.56	119.97	122.79
6	7	39	PSU	O2-C2-N1	-2.56	119.97	122.79
1	1	2445	2MG	C8-N7-C5	2.55	107.85	102.99
1	1	2504	PSU	O2-C2-N1	-2.54	119.99	122.79
1	1	2580	PSU	O2-C2-N1	-2.50	120.04	122.79
1	1	1939	5MU	O2-C2-N1	-2.48	119.49	122.79
6	7	37	MIA	C16-C14-C15	-2.47	109.16	114.60
4	4	341	5MU	O2-C2-N1	-2.41	119.58	122.79
6	7	54	5MU	O4-C4-N3	-2.41	115.50	120.12
6	7	54	5MU	O2-C2-N1	-2.39	119.61	122.79
1	1	745	1MG	O6-C6-C5	-2.38	119.97	124.19
2	2	1402	4OC	C6-C5-C4	2.35	119.84	116.96
1	1	2580	PSU	C6-N1-C2	-2.35	120.28	122.68
4	4	347	PSU	C6-N1-C2	-2.31	120.32	122.68
19	M	81	4D4	CB-CA-C	-2.30	108.10	111.77
2	2	516	PSU	C6-N1-C2	-2.29	120.34	122.68
1	1	1835	2MG	O6-C6-C5	-2.25	119.98	124.37
2	2	966	2MG	O6-C6-C5	-2.24	119.99	124.37
1	1	746	PSU	C6-C5-C4	2.24	119.77	118.20
49	q	89	0TD	OD1-CG-CB	-2.24	117.76	122.44
1	1	2445	2MG	O6-C6-C5	-2.23	120.01	124.37
6	7	39	PSU	C6-N1-C2	-2.22	120.41	122.68
1	1	1917	PSU	C6-N1-C2	-2.22	120.42	122.68
6	7	16	H2U	O2-C2-N1	-2.21	120.33	123.11
1	1	955	PSU	C6-N1-C2	-2.21	120.42	122.68
2	2	1516	2MG	O6-C6-C5	-2.20	120.07	124.37
1	1	2251	OMG	O6-C6-C5	-2.20	120.08	124.37
19	M	81	4D4	O-C-CA	-2.20	119.02	124.78
1	1	2445	2MG	CM2-N2-C2	-2.19	119.03	123.86
1	1	2605	PSU	C6-N1-C2	-2.19	120.45	122.68
1	1	1962	5MC	CM5-C5-C6	-2.19	119.93	122.85
1	1	2504	PSU	C6-N1-C2	-2.18	120.46	122.68
2	2	1207	2MG	O6-C6-C5	-2.17	120.13	124.37
6	7	32	PSU	C6-N1-C2	-2.16	120.47	122.68
6	7	20	H2U	C3'-C2'-C1'	2.14	105.50	101.43
2	2	516	PSU	O4'-C1'-C2'	2.13	108.15	105.14
1	1	1911	PSU	C6-N1-C2	-2.13	120.50	122.68
6	7	55	PSU	C6-N1-C2	-2.10	120.53	122.68
2	2	516	PSU	O2-C2-N1	-2.10	120.48	122.79
4	4	342	PSU	C6-N1-C2	-2.09	120.55	122.68
1	1	746	PSU	C6-N1-C2	-2.09	120.55	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1915	3TD	O4'-C1'-C2'	2.06	108.05	105.14
1	1	2552	OMU	O2-C2-N1	-2.06	120.05	122.79
2	2	1407	5MC	CM5-C5-C6	-2.04	120.12	122.85
1	1	1618	6MZ	C3'-C2'-C1'	2.04	104.05	100.98
6	7	47	3AU	C6-N1-C2	-2.01	119.99	121.79

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	M	81	4D4	C-CA-CB-OB
19	M	81	4D4	C-CA-CB-CG
19	M	81	4D4	N-CA-CB-OB
19	M	81	4D4	N-CA-CB-CG
49	q	89	0TD	SB-CB-CG-OD2
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	2030	6MZ	O4'-C4'-C5'-O5'
1	1	2445	2MG	C3'-C4'-C5'-O5'
1	1	2504	PSU	O4'-C4'-C5'-O5'
1	1	2552	OMU	C1'-C2'-O2'-CM2
1	1	2580	PSU	O4'-C1'-C5-C4
1	1	2580	PSU	C2'-C1'-C5-C6
1	1	2580	PSU	O4'-C1'-C5-C6
2	2	516	PSU	O4'-C1'-C5-C4
2	2	516	PSU	O4'-C1'-C5-C6
2	2	1402	4OC	O4'-C4'-C5'-O5'
2	2	1519	MA6	O4'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
4	4	347	PSU	C3'-C4'-C5'-O5'
4	4	347	PSU	O4'-C4'-C5'-O5'
6	7	20	H2U	O4'-C4'-C5'-O5'
6	7	20	H2U	O4'-C1'-N1-C6
6	7	37	MIA	O4'-C4'-C5'-O5'
6	7	37	MIA	C3'-C4'-C5'-O5'
6	7	37	MIA	C5-C6-N6-C12
6	7	37	MIA	C12-C13-C14-C16
6	7	47	3AU	C10-C11-C12-C13
6	7	47	3AU	C10-C11-C12-N40
1	1	2503	2MA	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	1	2503	2MA	C3'-C4'-C5'-O5'
1	1	2504	PSU	C3'-C4'-C5'-O5'
2	2	527	G7M	C3'-C4'-C5'-O5'
2	2	1402	4OC	C3'-C4'-C5'-O5'
6	7	20	H2U	C3'-C4'-C5'-O5'
6	7	46	G7M	C3'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
6	7	20	H2U	C2'-C1'-N1-C6
6	7	20	H2U	C2'-C1'-N1-C2
6	7	37	MIA	N1-C6-N6-C12
1	1	1835	2MG	O4'-C4'-C5'-O5'
1	1	1917	PSU	C3'-C4'-C5'-O5'
2	2	527	G7M	O4'-C4'-C5'-O5'
6	7	46	G7M	O4'-C4'-C5'-O5'
1	1	1835	2MG	C3'-C4'-C5'-O5'
2	2	1498	UR3	O4'-C4'-C5'-O5'
1	1	2498	OMC	O4'-C4'-C5'-O5'
6	7	54	5MU	O4'-C4'-C5'-O5'
2	2	527	G7M	C4'-C5'-O5'-P
1	1	1917	PSU	O4'-C4'-C5'-O5'
49	q	89	0TD	SB-CB-CG-OD1
6	7	54	5MU	C3'-C4'-C5'-O5'
1	1	2069	G7M	C4'-C5'-O5'-P
6	7	46	G7M	C4'-C5'-O5'-P
2	2	1498	UR3	C3'-C4'-C5'-O5'
6	7	20	H2U	O4'-C1'-N1-C2
19	M	81	4D4	CA-CB-CG-CD
1	1	2069	G7M	O4'-C4'-C5'-O5'
4	4	342	PSU	C3'-C4'-C5'-O5'
1	1	2030	6MZ	C3'-C4'-C5'-O5'
49	q	89	0TD	CA-CB-SB-CSB
1	1	1618	6MZ	C4'-C5'-O5'-P
1	1	2498	OMC	C3'-C4'-C5'-O5'
6	7	16	H2U	C3'-C4'-C5'-O5'
49	q	89	0TD	CG-CB-SB-CSB

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

Of 443 ligands modelled in this entry, 443 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

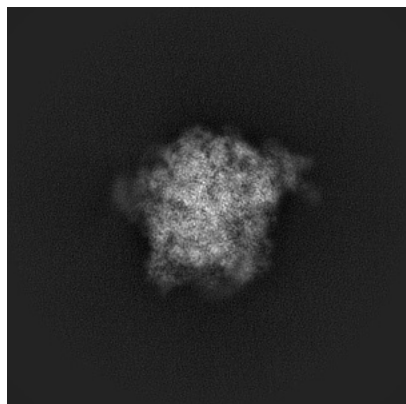
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11713. These allow visual inspection of the internal detail of the map and identification of artifacts.

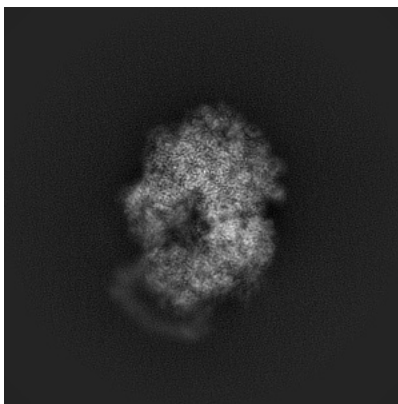
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

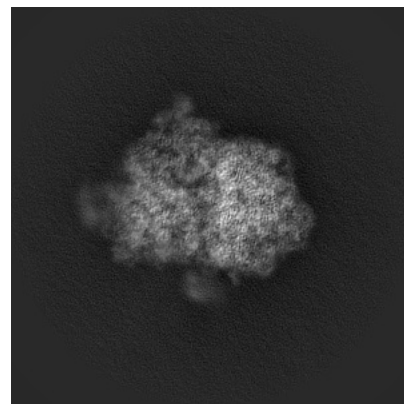
6.1.1 Primary map



X

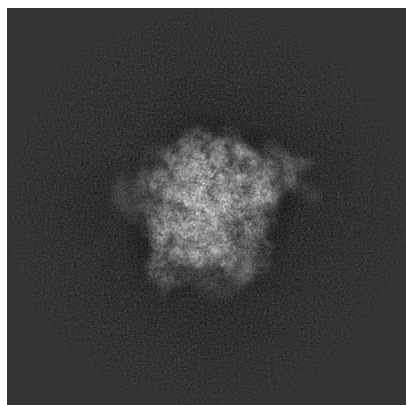


Y

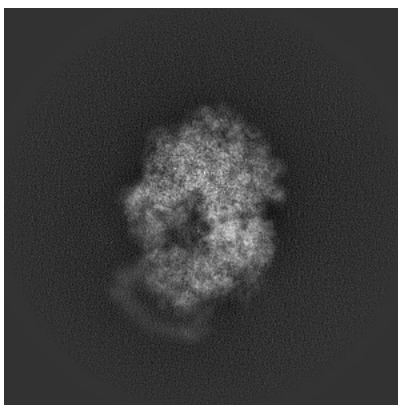


Z

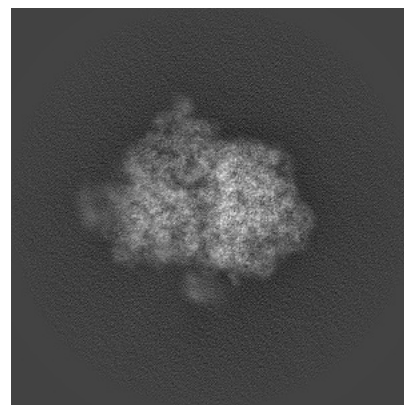
6.1.2 Raw map



X



Y

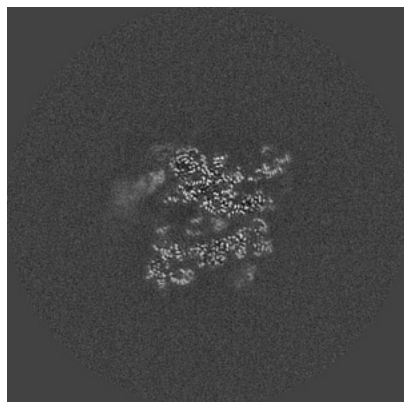


Z

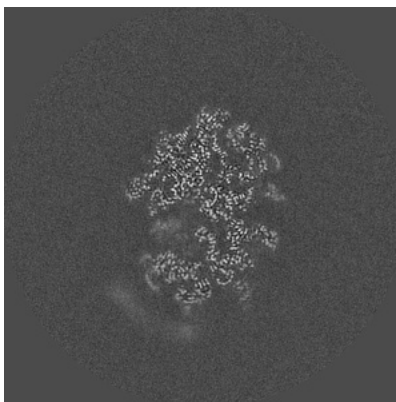
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

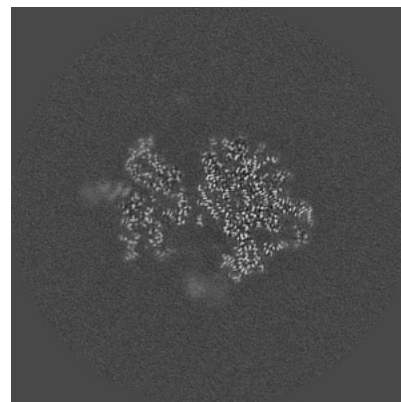
6.2.1 Primary map



X Index: 240

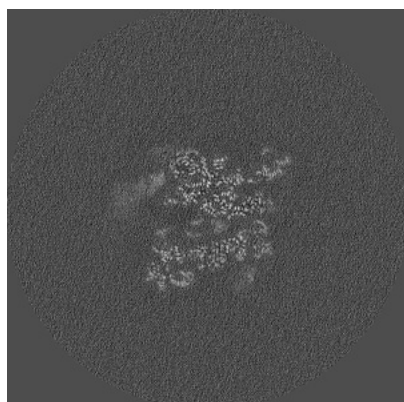


Y Index: 240

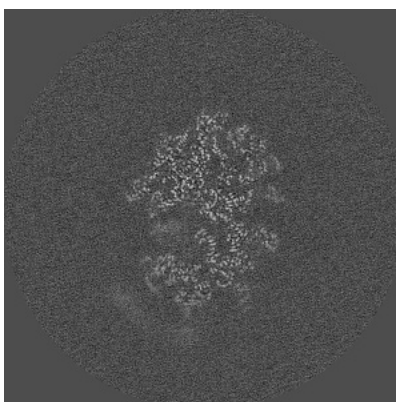


Z Index: 240

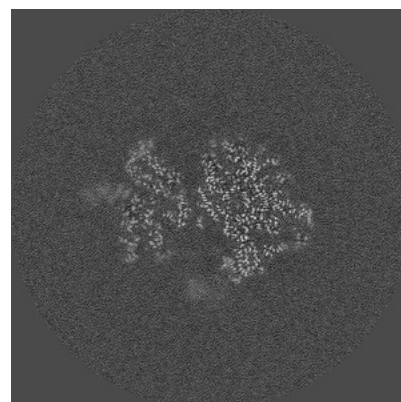
6.2.2 Raw map



X Index: 240



Y Index: 240

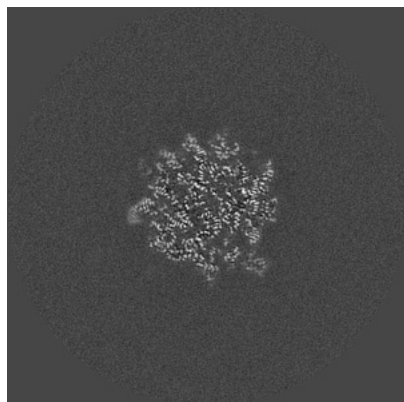


Z Index: 240

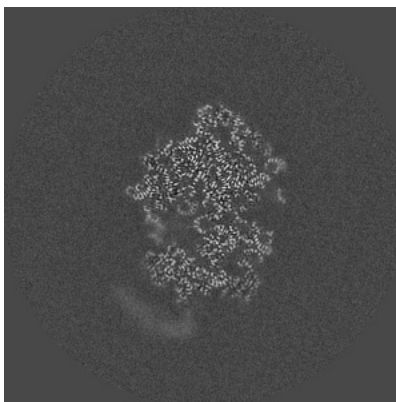
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

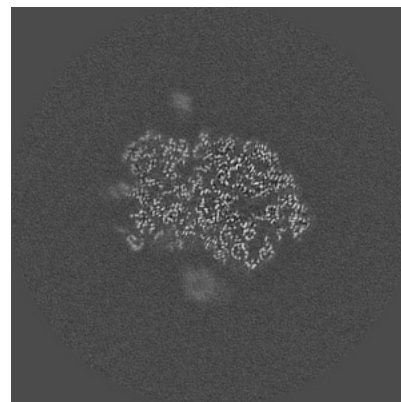
6.3.1 Primary map



X Index: 269

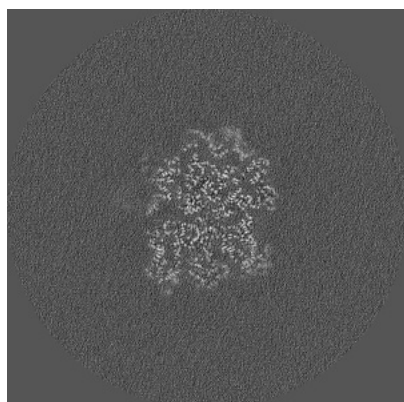


Y Index: 231

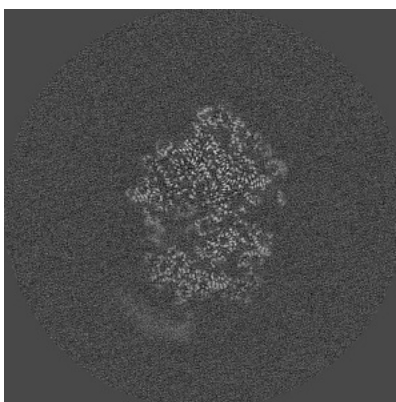


Z Index: 252

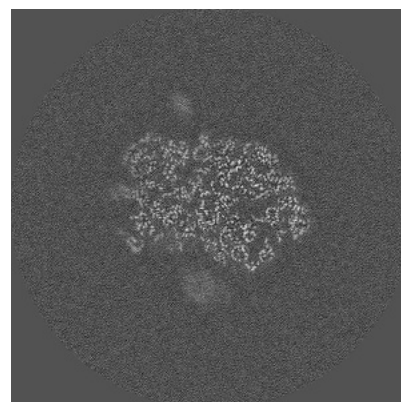
6.3.2 Raw map



X Index: 258



Y Index: 230

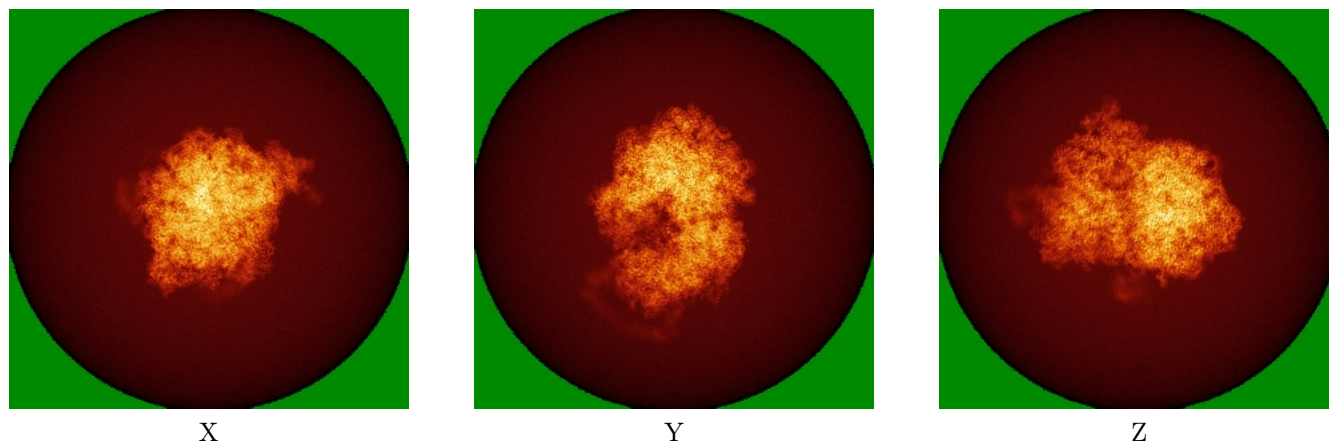


Z Index: 252

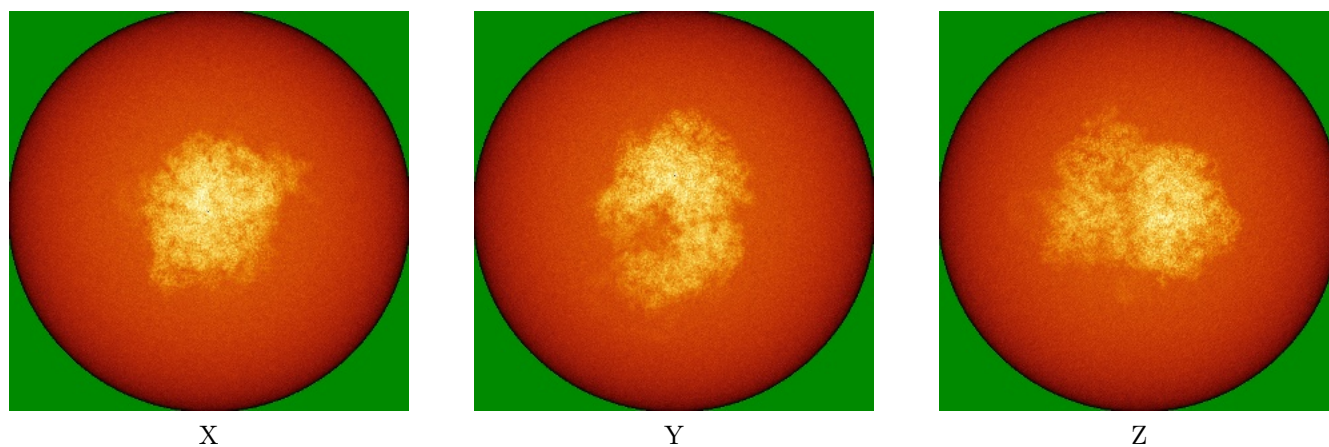
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



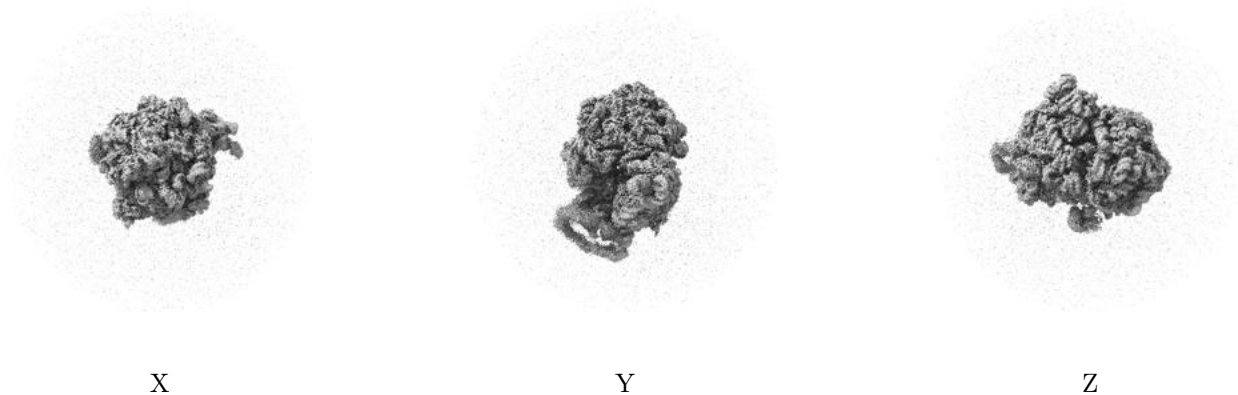
6.4.2 Raw map



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.

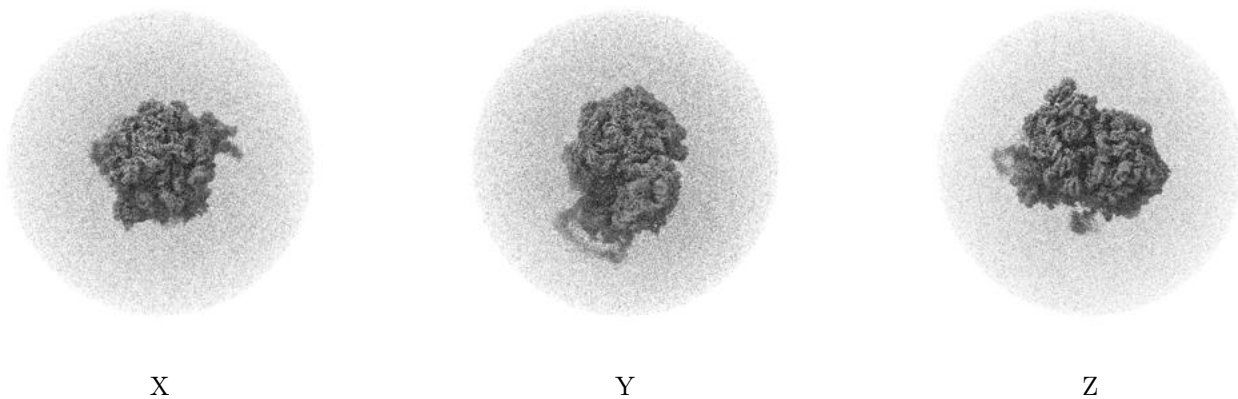
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

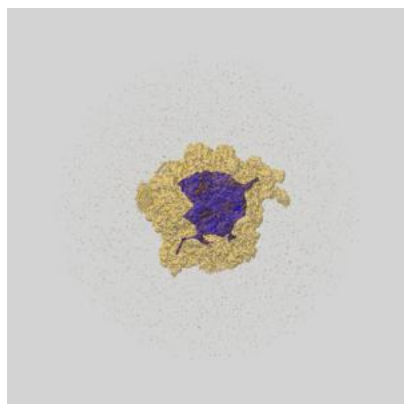
6.6 Mask visualisation [i](#)

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

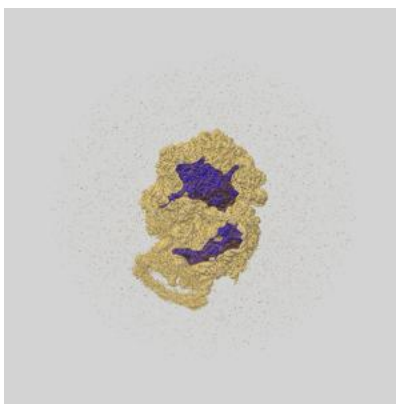
A mask typically either:

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

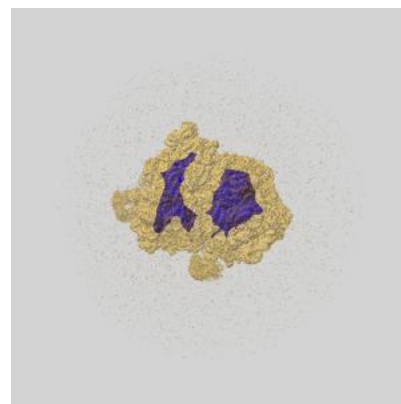
6.6.1 emd_11713_msk_1.map [i](#)



X



Y

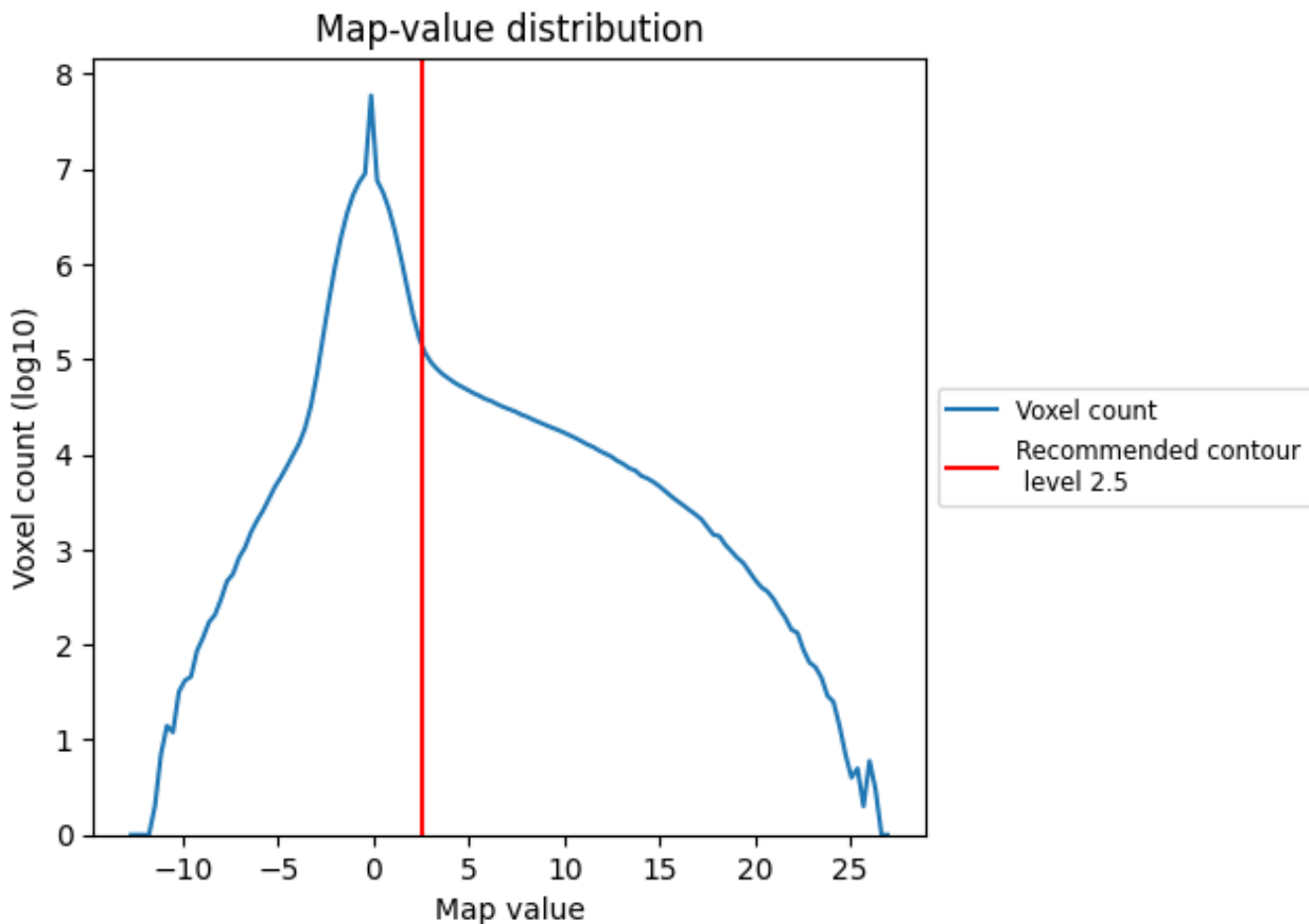


Z

7 Map analysis [i](#)

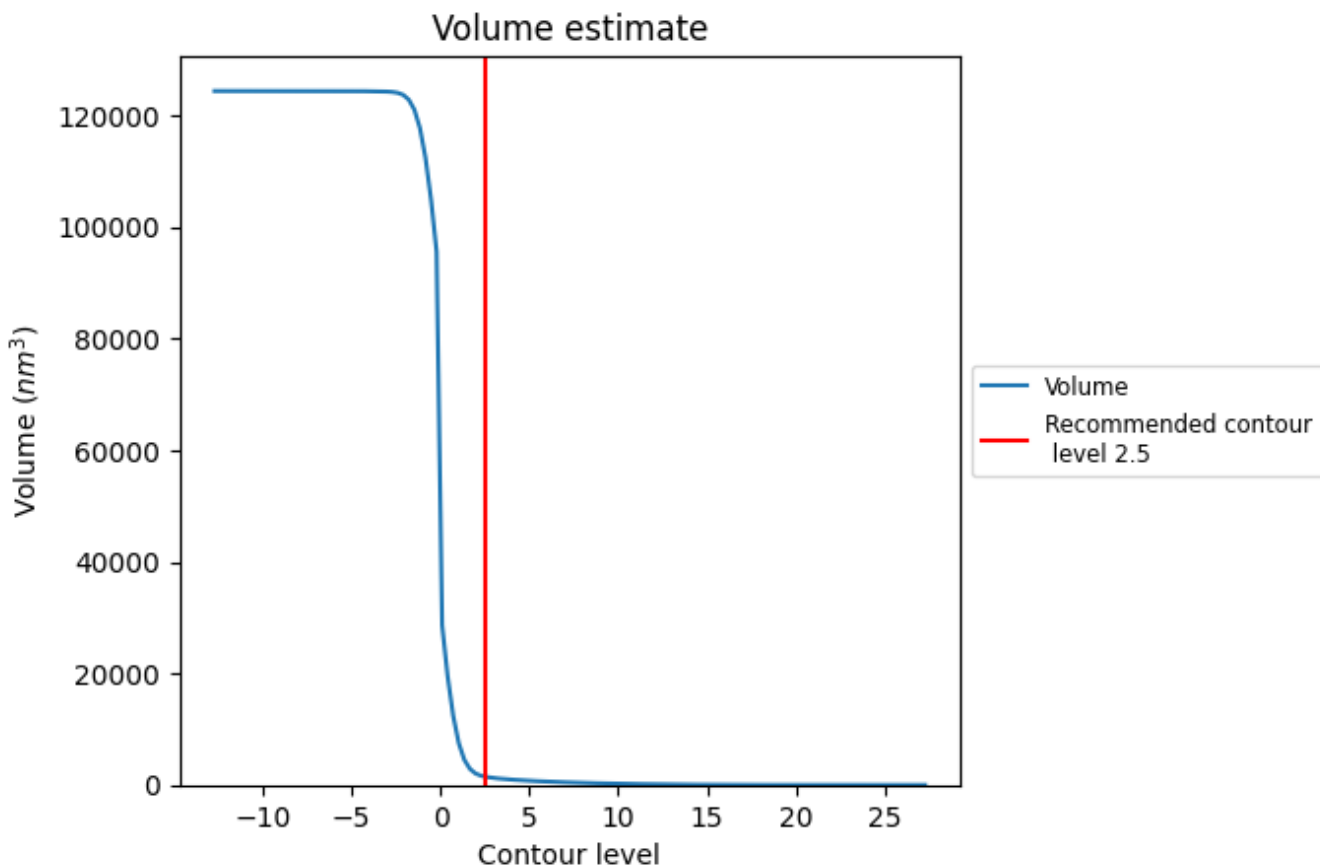
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

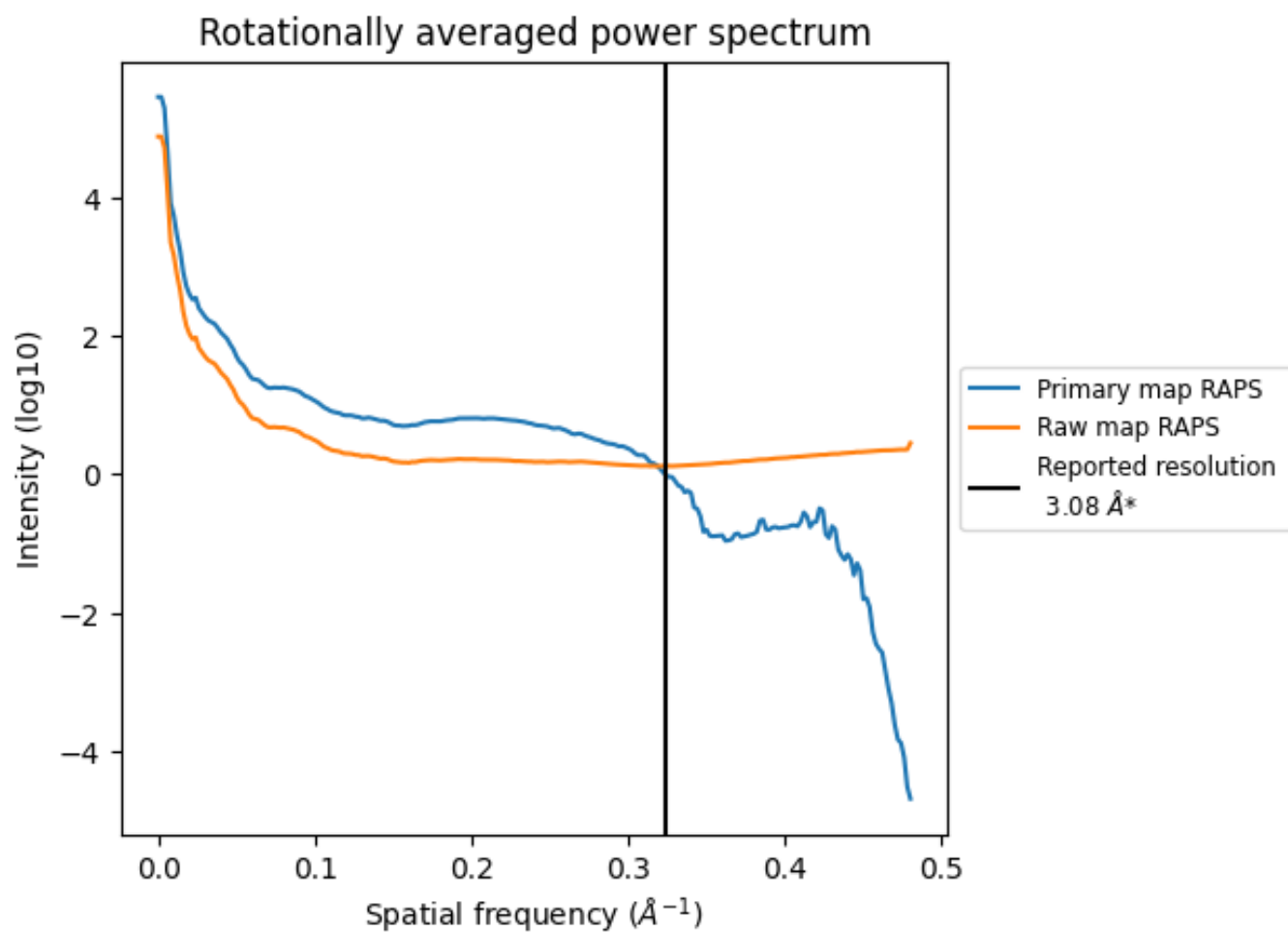
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1491 nm³; this corresponds to an approximate mass of 1347 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

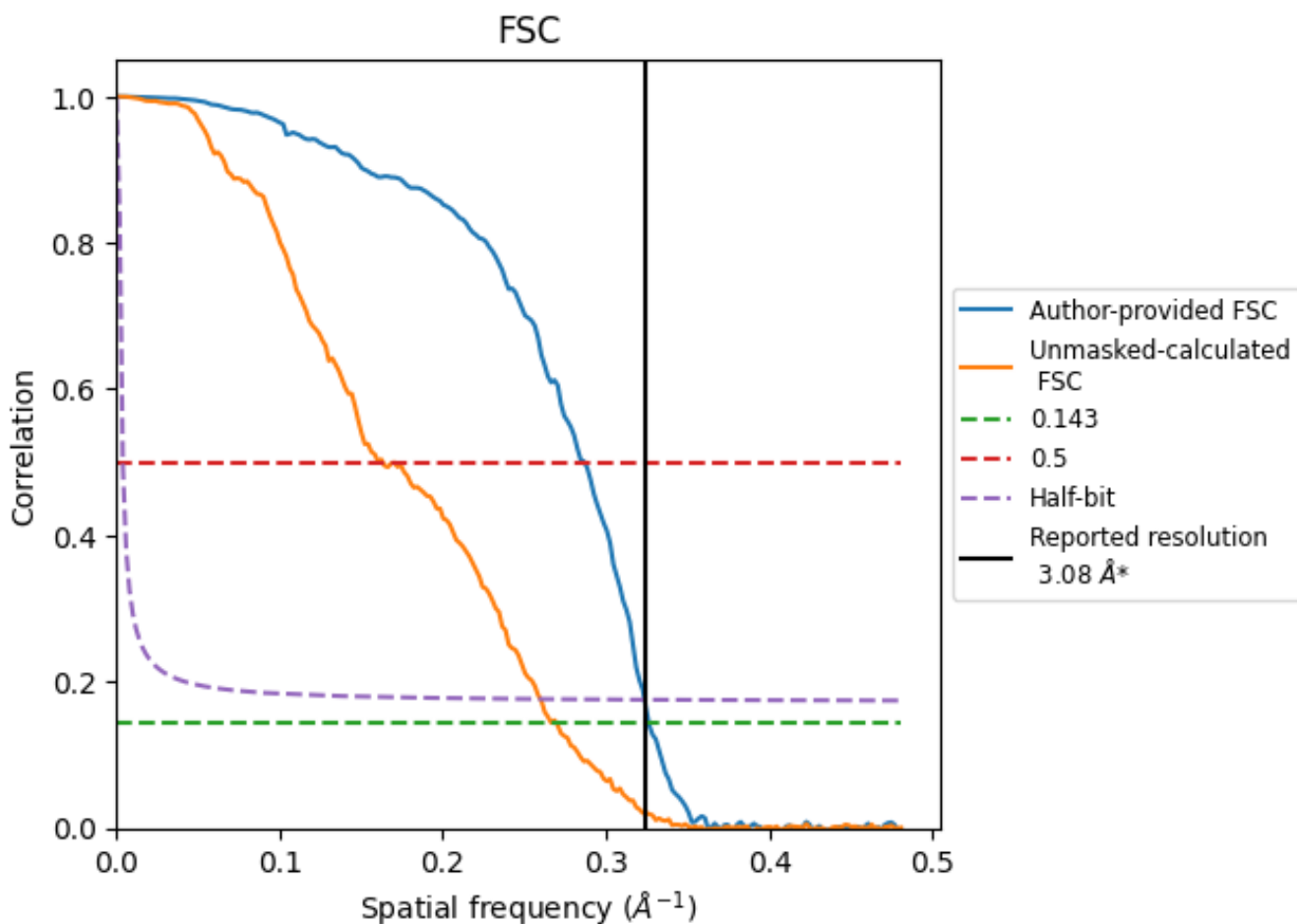


*Reported resolution corresponds to spatial frequency of 0.325 Å⁻¹

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 0.325 Å⁻¹

8.2 Resolution estimates [i](#)

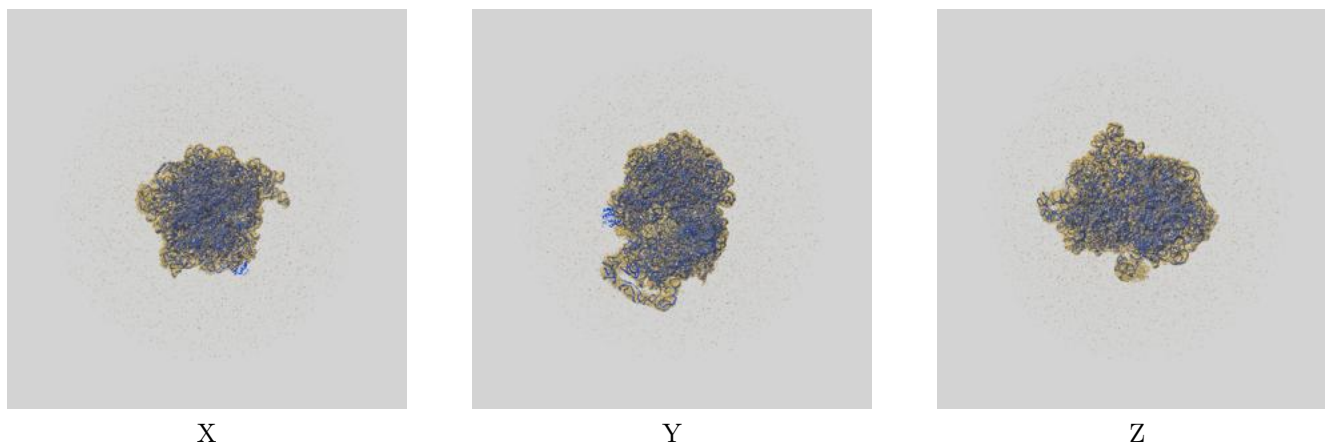
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	3.06	3.49	3.09
Unmasked-calculated*	3.71	6.13	3.85

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

9 Map-model fit [i](#)

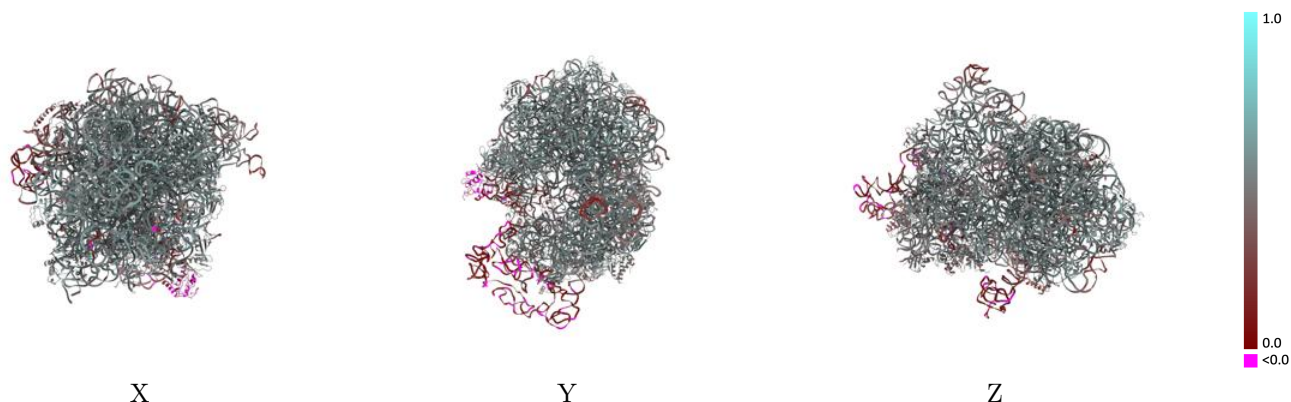
This section contains information regarding the fit between EMDB map EMD-11713 and PDB model 7AC7. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



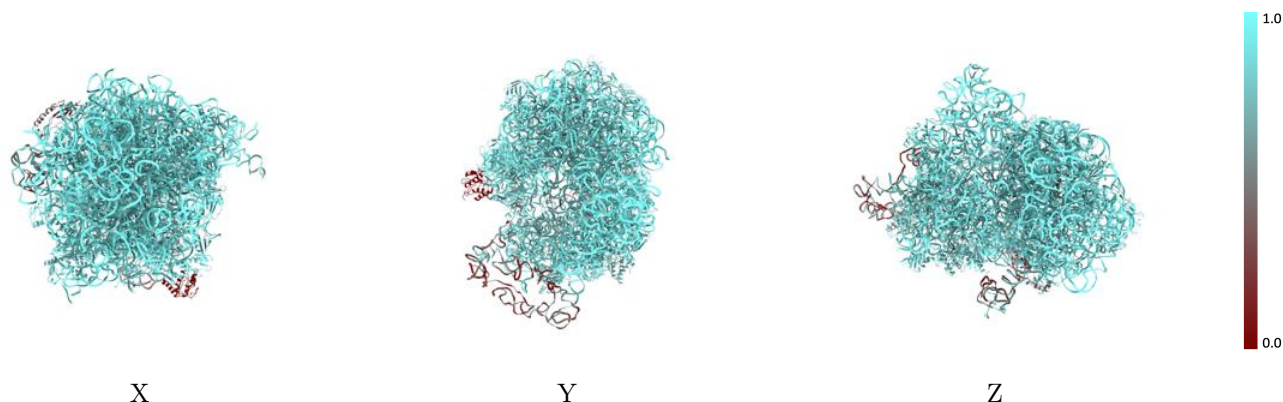
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



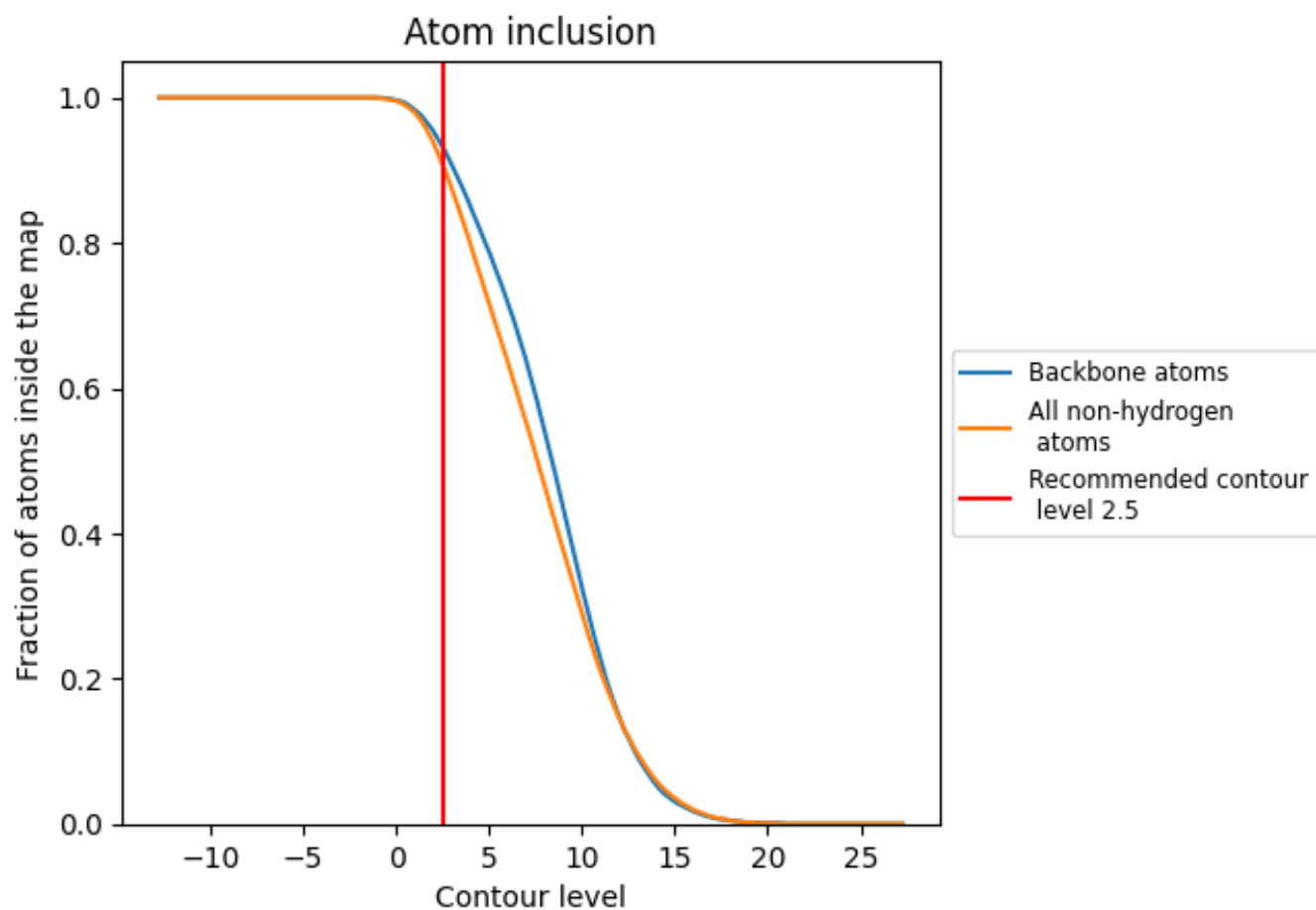
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 91% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9090	 0.4780
1	 0.9590	 0.5010
2	 0.9710	 0.4960
3	 0.9790	 0.5140
4	 0.5090	 0.1570
5	 0.7440	 0.3550
7	 0.9390	 0.5020
8	 0.6850	 0.2610
A	 0.9130	 0.5380
B	 0.9250	 0.5440
C	 0.9140	 0.5270
D	 0.9050	 0.5150
E	 0.8920	 0.4880
F	 0.8810	 0.4740
G	 0.4570	 0.3420
H	 0.0090	 0.0260
J	 0.9070	 0.5240
K	 0.9110	 0.5380
L	 0.9110	 0.5180
M	 0.9150	 0.5370
N	 0.9240	 0.5370
O	 0.9160	 0.5040
P	 0.9140	 0.5300
Q	 0.9190	 0.5300
R	 0.9160	 0.5250
S	 0.8860	 0.5090
T	 0.8860	 0.5110
U	 0.9100	 0.5100
V	 0.9160	 0.5240
W	 0.6880	 0.4110
X	 0.9130	 0.5340
Y	 0.9140	 0.4810
Z	 0.9240	 0.5240
a	 0.8460	 0.4550
b	 0.9200	 0.5280



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Chain	Atom inclusion	Q-score
c	 0.8920	 0.5180
d	 0.9240	 0.5260
e	 0.9040	 0.5340
f	 0.9620	 0.5560
g	 0.7650	 0.4510
h	 0.8900	 0.4950
i	 0.8870	 0.4930
j	 0.9070	 0.5140
k	 0.8790	 0.4710
l	 0.7970	 0.4310
m	 0.9210	 0.5290
n	 0.9080	 0.4780
o	 0.8630	 0.4600
p	 0.8990	 0.4910
q	 0.8890	 0.5090
r	 0.8910	 0.4660
s	 0.9070	 0.4980
t	 0.9080	 0.5030
u	 0.9070	 0.5020
v	 0.8830	 0.4990
w	 0.8790	 0.4890
x	 0.8970	 0.4770
y	 0.8870	 0.4890
z	 0.6830	 0.4030