



## Full wwPDB EM Validation Report ⓘ

Apr 17, 2024 – 10:24 am BST

PDB ID : 7OTC  
EMDB ID : EMD-13058  
Title : Cryo-EM structure of an Escherichia coli 70S ribosome in complex with elongation factor G and the antibiotic Argyrin B  
Authors : Wieland, M.; Koller, T.O.; Wilson, D.N.  
Deposited on : 2021-06-10  
Resolution : 2.90 Å (reported)  
Based on initial models : 7K00, 4V9P

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

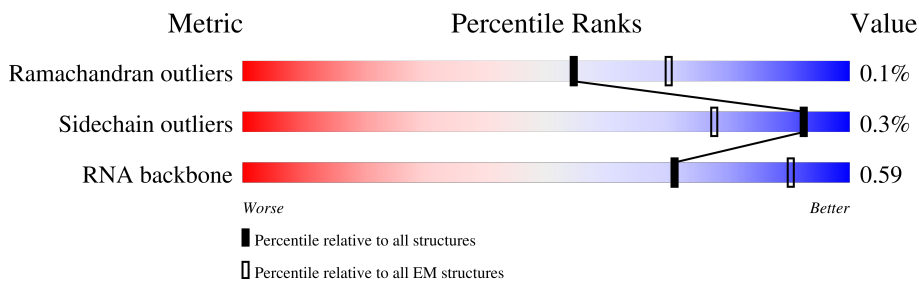
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (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 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a	1533	
2	b	226	
3	c	206	
4	d	205	
5	e	157	
6	f	106	
7	g	156	
8	h	129	

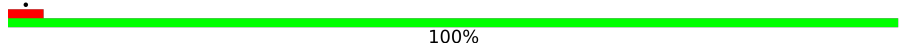
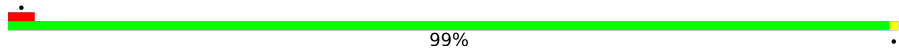
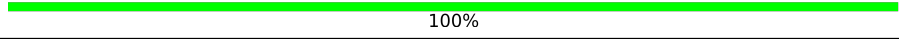
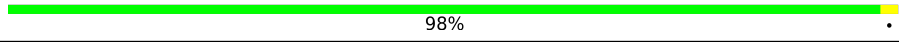
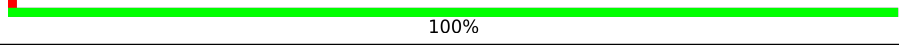
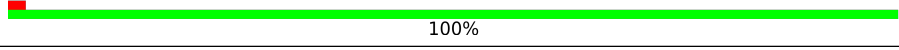
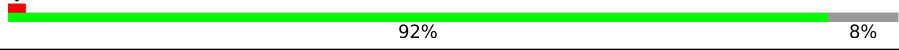
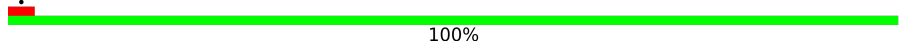
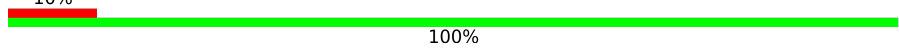
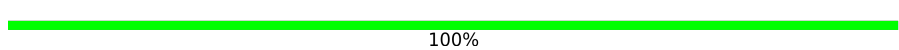
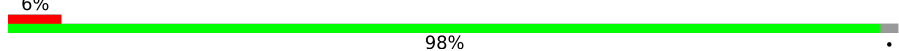
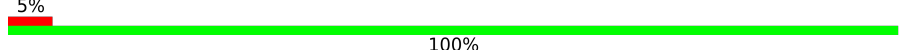
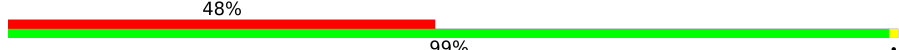
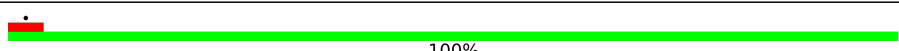
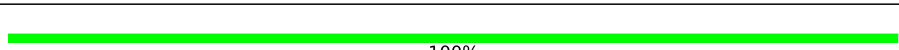

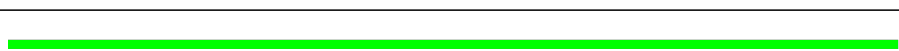
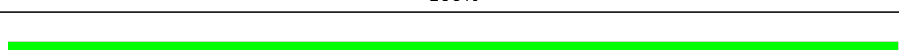
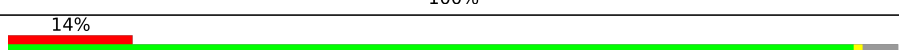
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Mol	Chain	Length	Quality of chain
9	i	127	6% 100%
10	j	99	9% 99%
11	k	117	100%
12	l	123	99%
13	m	115	22% 97%
14	n	101	99%
15	o	88	99%
16	p	82	99%
17	q	80	100%
18	r	67	100%
19	s	92	9% 90% 9%
20	t	86	100%
21	u	70	21% 100%
22	A	2903	84% 15%
23	B	120	88% 12%
24	C	271	100%
25	D	209	100%
26	E	201	100%
27	F	177	15% 99%
28	G	176	100%
29	J	142	100%
30	K	123	100%
31	L	144	100%
32	M	136	99%
33	N	120	100%

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Mol	Chain	Length	Quality of chain
34	O	116	 100%
35	P	114	 99%
36	Q	117	 100%
37	R	103	 98%
38	S	110	 100%
39	T	93	 100%
40	U	102	 92% 8%
41	V	94	 100%
42	W	84	 10% 100%
43	X	77	 100%
44	Y	63	 6% 98%
45	Z	58	 5% 100%
46	5	67	 48% 99%
47	0	56	 100%
48	1	50	 100%
49	2	46	 100%
50	3	64	 100%
51	4	38	 100%
52	w	704	 14% 95%

## 2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 147132 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1533	32907	14683	6036	10655	1533	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	226	1769	1119	317	325	8	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	205	1642	1026	315	297	4	0	0

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	151	GLU	ALA	conflict	UNP A0A140N6Z9

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	156	Total	C	N	O	S	0	0
			1236	773	238	221	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	157	LEU	-	expression tag	UNP A0A140N6W8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	129	Total	C	N	O	S	0	0
			978	616	173	183	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	127	Total	C	N	O	S	0	0
			1021	634	206	178	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	99	Total	C	N	O	S	1	0
			806	504	156	145	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	117	Total	C	N	O	S	0	0
			876	540	174	159	3		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	n	100	804	499	164	138	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	1	MET	-	initiating methionine	UNP A0A140N7K8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	o	88	713	439	144	129	1	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	r	67	555	351	106	97	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	s	84	668	427	127	112	2	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
23	B	120	2570	1144	468	838	120	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	C	271	2090	1292	425	366	7	1	0

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



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

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

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

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

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

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

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

- Molecule 29 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	J	142	1139	720	215	200	4	1	0

- Molecule 30 is a protein called 50S ribosomal protein L14.

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

- Molecule 31 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	L	144	1064	660	211	191	2	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	77	ILE	VAL	conflict	UNP A0A140N711

- Molecule 32 is a protein called 50S ribosomal protein L16.

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

- Molecule 33 is a protein called 50S ribosomal protein L17.

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

- Molecule 34 is a protein called 50S ribosomal protein L18.

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

- Molecule 35 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	P	114	916	574	179	162	1	0	0

- Molecule 36 is a protein called 50S ribosomal protein L20.

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

- Molecule 37 is a protein called 50S ribosomal protein L21.

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

- Molecule 38 is a protein called 50S ribosomal protein L22.

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

- Molecule 39 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 40 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	U	94	Total	C	N	O	0	0
			721	454	136	131		

- Molecule 41 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	V	94	Total	C	N	O	S	0	0
			752	479	137	133	3		

- Molecule 42 is a protein called 50S ribosomal protein L27.

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

- Molecule 43 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	X	77	Total	C	N	O	S	0	0
			624	388	129	105	2		

- Molecule 44 is a protein called 50S ribosomal protein L29.

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

- Molecule 45 is a protein called 50S ribosomal protein L30.

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

- Molecule 46 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	5	67	Total	C	N	O	S	0	0
			529	328	100	95	6		

- Molecule 47 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3	64	Total	C	N	O	S	1	0
			512	329	107	74	2		

- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 52 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	w	675	5196	3277	899	997	23	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
w	1	SER	-	expression tag	UNP A0A140N7C7
w	237	THR	TYR	variant	UNP A0A140N7C7
w	258	ASP	ASN	variant	UNP A0A140N7C7

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	a	61	Total	Mg	0
			61	61	
53	n	1	Total	Mg	0
			1	1	
53	A	219	Total	Mg	0
			219	219	
53	B	4	Total	Mg	0
			4	4	
53	C	2	Total	Mg	0
			2	2	
53	D	1	Total	Mg	0
			1	1	
53	N	1	Total	Mg	0
			1	1	
53	Q	1	Total	Mg	0
			1	1	
53	0	1	Total	Mg	0
			1	1	
53	w	1	Total	Mg	0
			1	1	

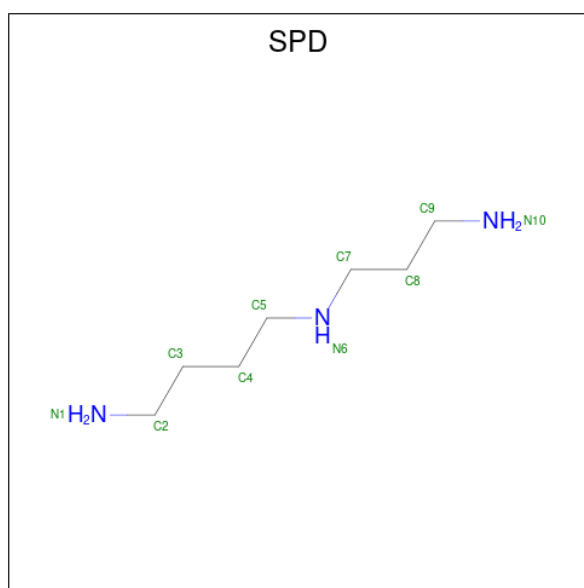
- Molecule 54 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
55	A	1	6	4	2	0
55	A	1	6	4	2	0
55	A	1	6	4	2	0
55	A	1	6	4	2	0
55	A	1	6	4	2	0

- Molecule 56 is SPERMIDINE (three-letter code: SPD) (formula:  $C_7H_{19}N_3$ ).

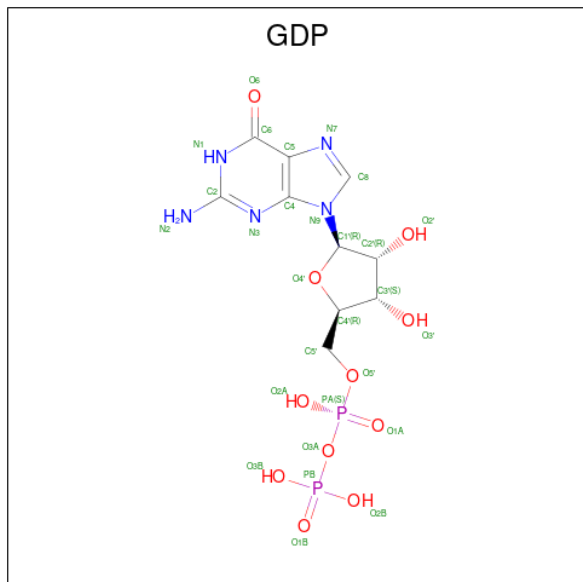


Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
56	A	1	10	7	3	0
56	A	1	10	7	3	0

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

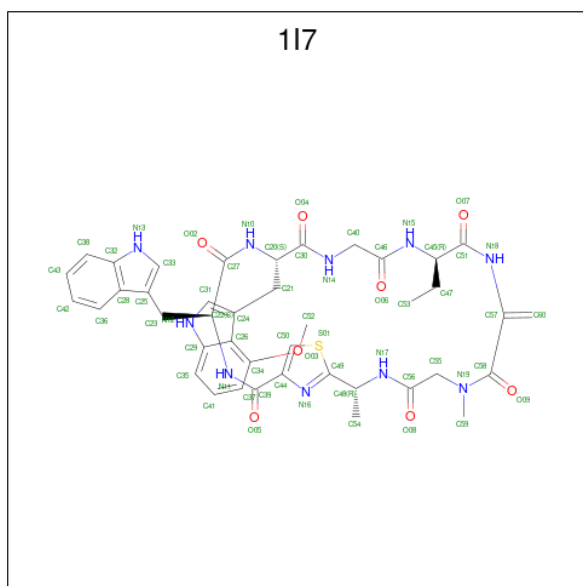
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
57	5	1	1	1	0
57	4	1	1	1	0

- Molecule 58 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	w	1	28	10	5	11	2	0

- Molecule 59 is Argyrin B (three-letter code: 1I7) (formula:  $C_{41}H_{46}N_{10}O_8S$ ) (labeled as "Ligand of Interest" by depositor).



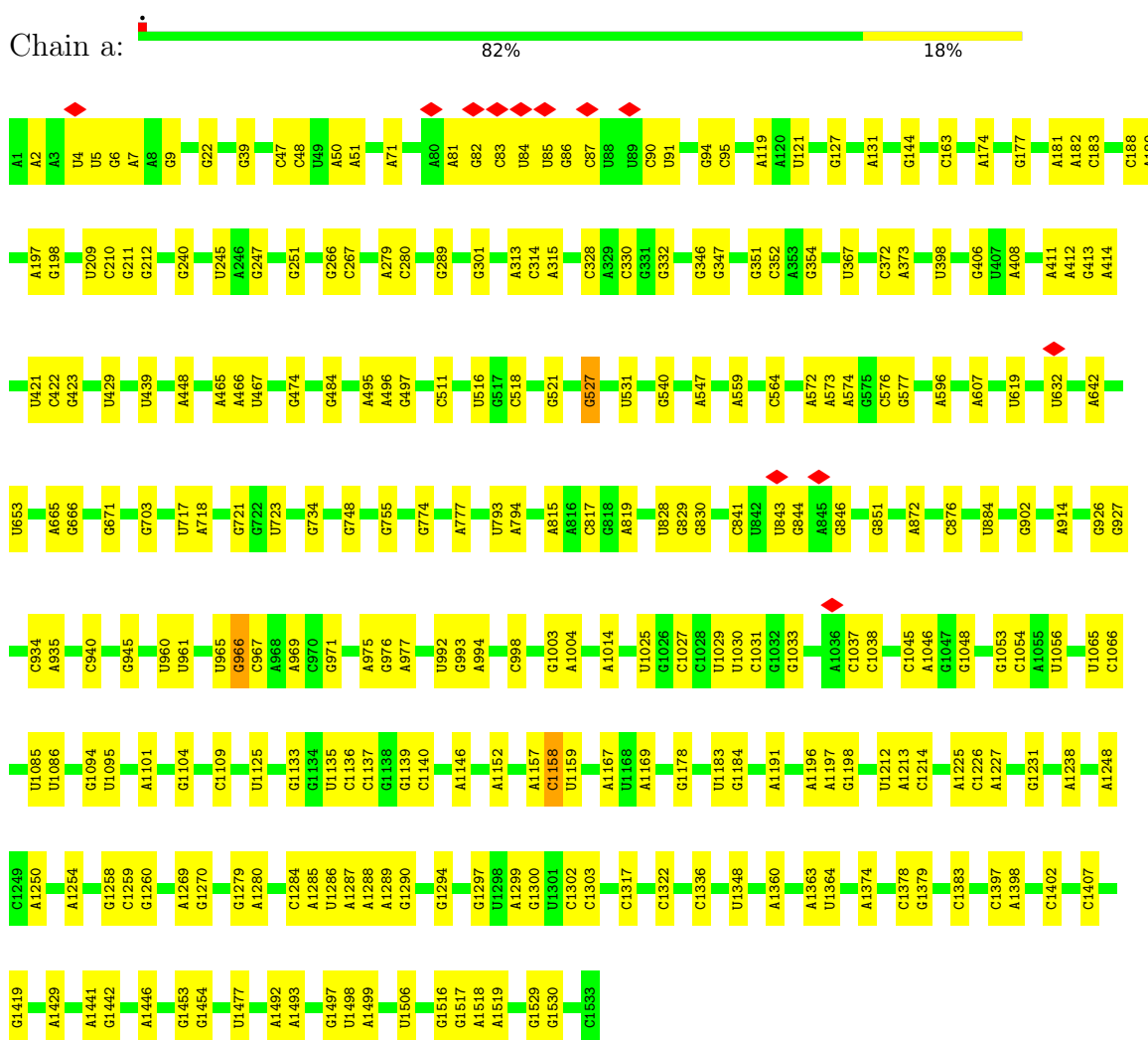
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
59	w	1	60	41	10	8	1	0



### 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: 16S ribosomal RNA



- Molecule 2: 30S ribosomal protein S2





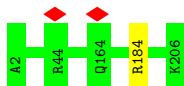
- Molecule 3: 30S ribosomal protein S3

Chain c: 100%

There are no outlier residues recorded for this chain.

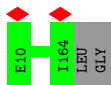
- Molecule 4: 30S ribosomal protein S4

Chain d: 100%



- Molecule 5: 30S ribosomal protein S5

Chain e: 99%



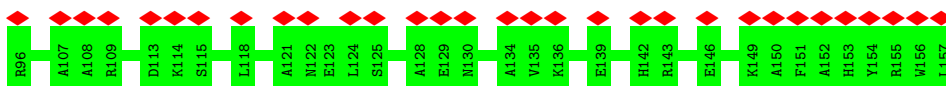
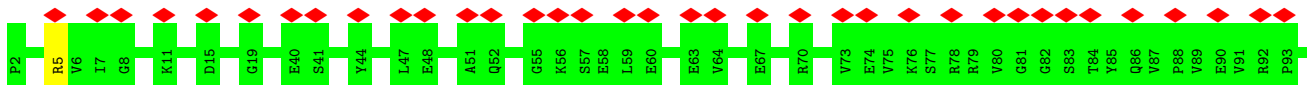
- Molecule 6: 30S ribosomal protein S6

Chain f: 8% 99%



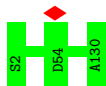
- Molecule 7: 30S ribosomal protein S7

Chain g: 43% 99%

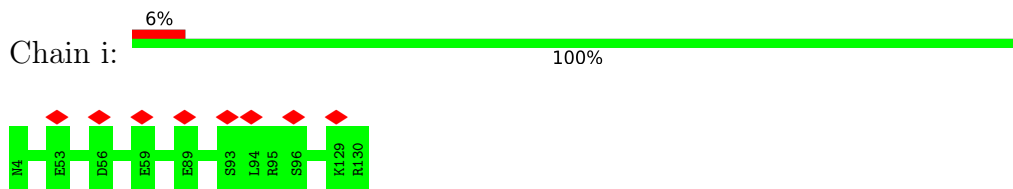


- Molecule 8: 30S ribosomal protein S8

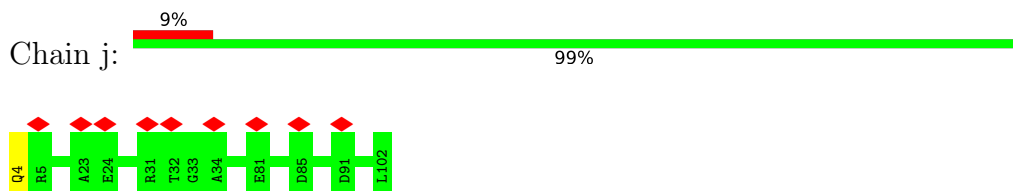
Chain h: 100%



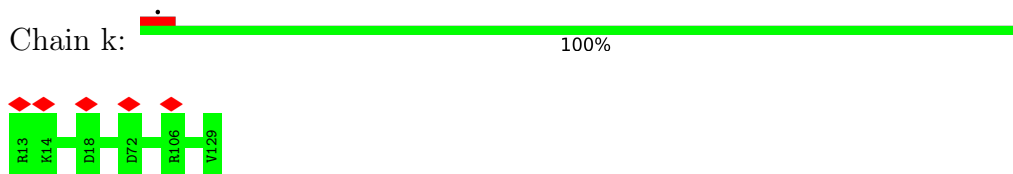
- Molecule 9: 30S ribosomal protein S9



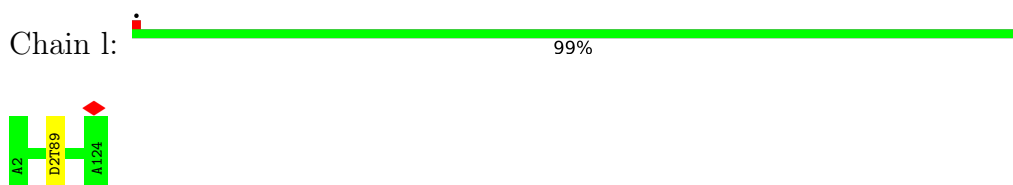
- Molecule 10: 30S ribosomal protein S10



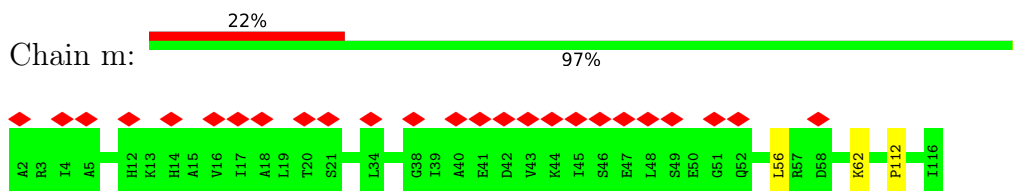
- Molecule 11: 30S ribosomal protein S11



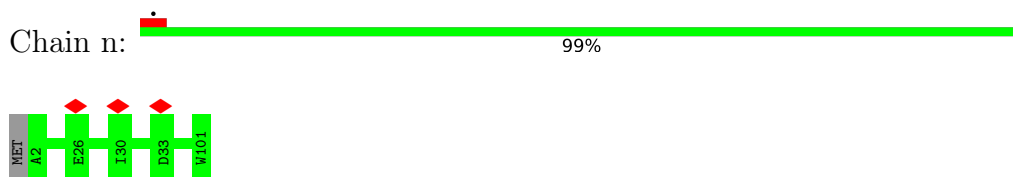
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14



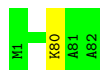
- Molecule 15: 30S ribosomal protein S15





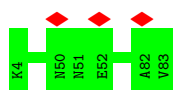
- Molecule 16: 30S ribosomal protein S16

Chain p: 99%



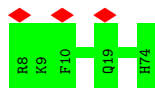
- Molecule 17: 30S ribosomal protein S17

Chain q: 100%



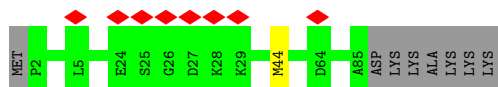
- Molecule 18: 30S ribosomal protein S18

Chain r: 100%



- Molecule 19: 30S ribosomal protein S19

Chain s: 9% 90% 9%



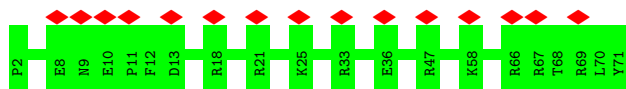
- Molecule 20: 30S ribosomal protein S20

Chain t: 100%

There are no outlier residues recorded for this chain.

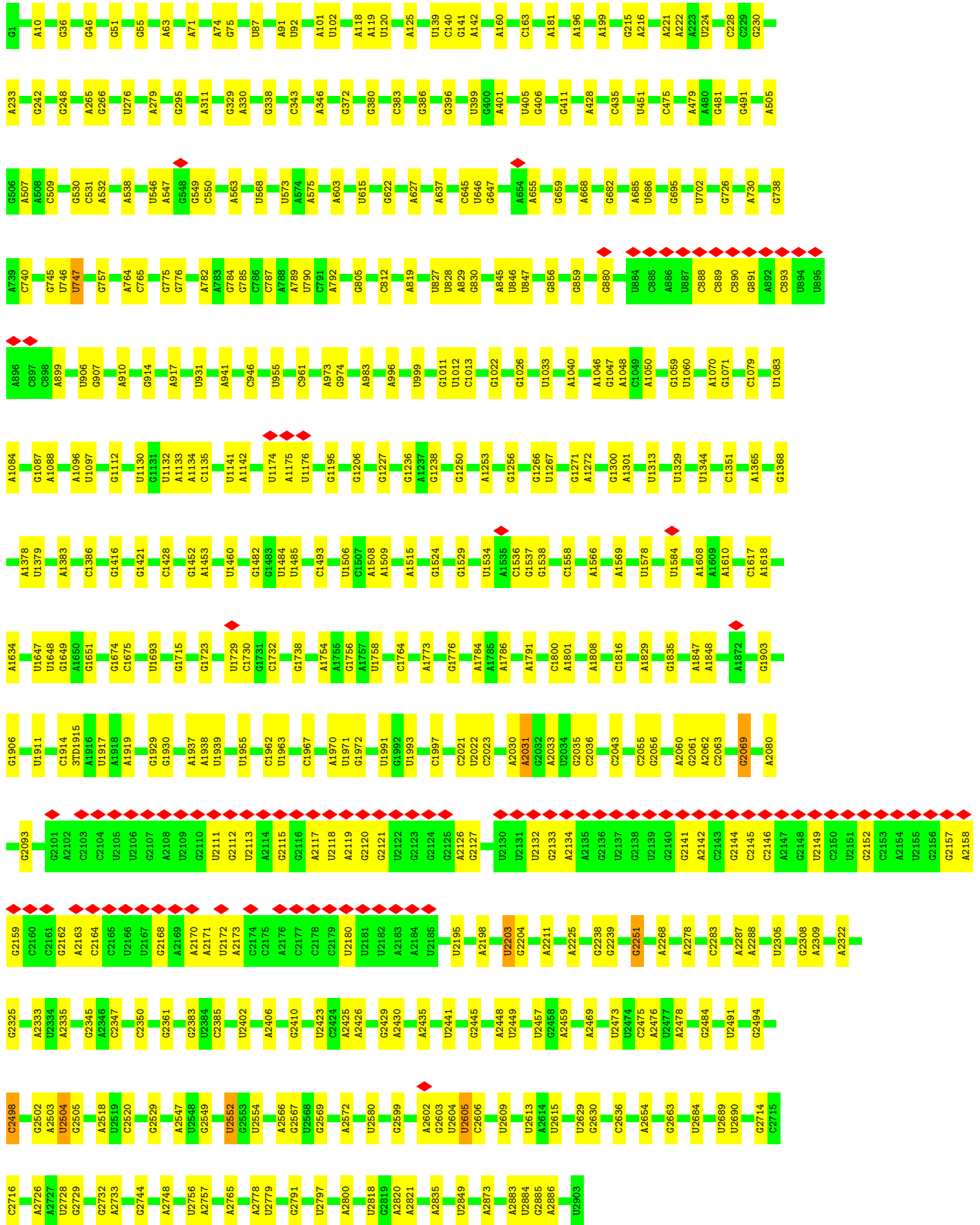
- Molecule 21: 30S ribosomal protein S21

Chain u: 21% 100%




- Molecule 22: 23S ribosomal RNA

Chain A: 84% 15%



- Molecule 23: 5S ribosomal RNA

Chain B:  88% 12%



- Molecule 24: 50S ribosomal protein L2

Chain C:  100%

There are no outlier residues recorded for this chain.

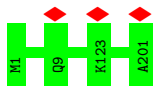
- Molecule 25: 50S ribosomal protein L3

Chain D:  100%



- Molecule 26: 50S ribosomal protein L4

Chain E:  100%



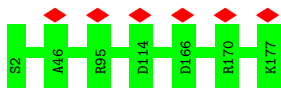
- Molecule 27: 50S ribosomal protein L5

Chain F:  15% 99%



- Molecule 28: 50S ribosomal protein L6

Chain G:  100%



- Molecule 29: 50S ribosomal protein L13

Chain J:  100%

There are no outlier residues recorded for this chain.

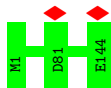
- Molecule 30: 50S ribosomal protein L14

Chain K:  100%

There are no outlier residues recorded for this chain.

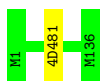
- Molecule 31: 50S ribosomal protein L15

Chain L:  100%



- Molecule 32: 50S ribosomal protein L16

Chain M:  99%



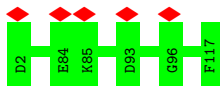
- Molecule 33: 50S ribosomal protein L17

Chain N:  100%

There are no outlier residues recorded for this chain.

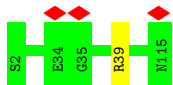
- Molecule 34: 50S ribosomal protein L18

Chain O:  100%



- Molecule 35: 50S ribosomal protein L19

Chain P:  99%



- Molecule 36: 50S ribosomal protein L20

Chain Q:  100%

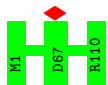
There are no outlier residues recorded for this chain.

- Molecule 37: 50S ribosomal protein L21

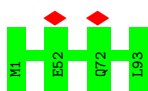
Chain R:  98%



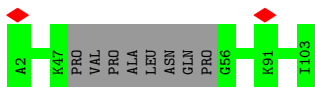
- Molecule 38: 50S ribosomal protein L22



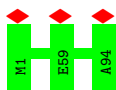
- Molecule 39: 50S ribosomal protein L23



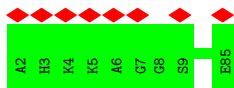
- Molecule 40: 50S ribosomal protein L24



- Molecule 41: 50S ribosomal protein L25



- Molecule 42: 50S ribosomal protein L27



- Molecule 43: 50S ribosomal protein L28

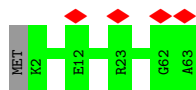


There are no outlier residues recorded for this chain.

- Molecule 44: 50S ribosomal protein L29



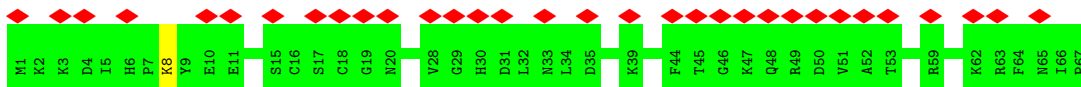




- Molecule 45: 50S ribosomal protein L30



- Molecule 46: 50S ribosomal protein L31



- Molecule 47: 50S ribosomal protein L32



- Molecule 48: 50S ribosomal protein L33



There are no outlier residues recorded for this chain.

- Molecule 49: 50S ribosomal protein L34



There are no outlier residues recorded for this chain.

- Molecule 50: 50S ribosomal protein L35



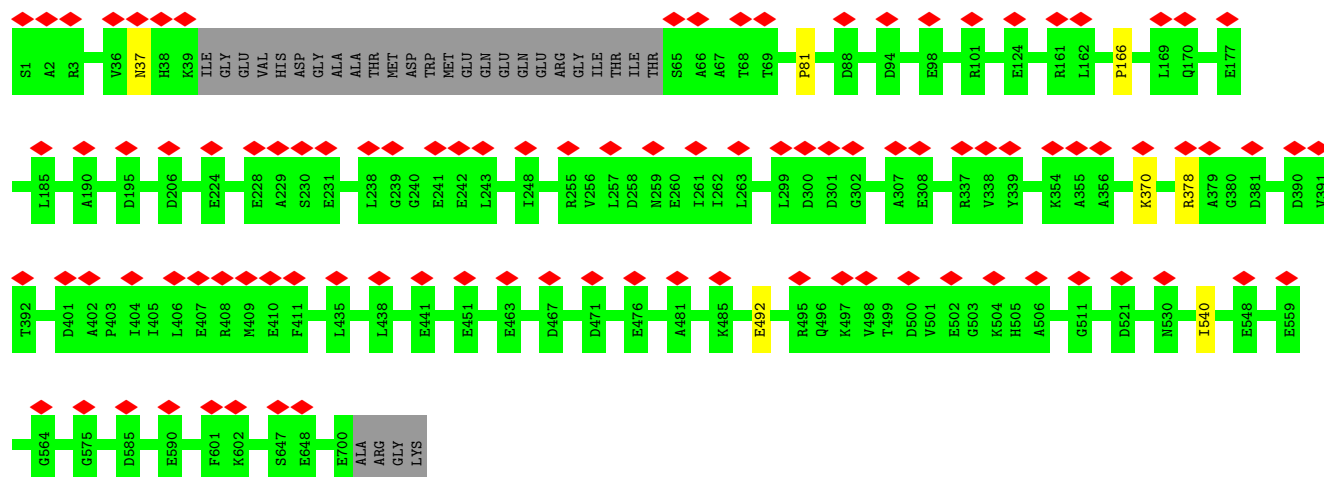
There are no outlier residues recorded for this chain.

- Molecule 51: 50S ribosomal protein L36



There are no outlier residues recorded for this chain.

- Molecule 52: Elongation factor G



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	153360	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	28	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.614	Depositor
Minimum map value	-0.390	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.026	Depositor
Map size ( $\text{\AA}$ )	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.084, 1.084, 1.084	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: G7M, H2U, OMG, D2T, UR3, 3TD, OMU, SPD, 2MA, 6MZ, MG, GDP, PUT, MA6, 2MG, 1I7, OMC, ATP, PSU, ZN, 1MG, 4OC, 4D4, 5MU, 5MC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	a	0.36	0/36594	0.75	4/57083 (0.0%)
2	b	0.29	0/1800	0.65	3/2425 (0.1%)
3	c	0.27	0/1651	0.59	0/2225
4	d	0.28	0/1664	0.61	0/2227
5	e	0.28	0/1157	0.58	0/1557
6	f	0.32	0/881	0.68	0/1189
7	g	0.26	0/1254	0.62	0/1683
8	h	0.29	0/988	0.59	0/1326
9	i	0.31	0/1033	0.68	0/1375
10	j	0.30	0/816	0.72	0/1103
11	k	0.29	0/892	0.66	0/1205
12	l	0.31	0/960	0.64	0/1286
13	m	0.32	0/900	0.81	3/1204 (0.2%)
14	n	0.29	0/816	0.68	0/1088
15	o	0.26	0/721	0.57	0/964
16	p	0.30	0/659	0.64	0/884
17	q	0.31	0/657	0.65	0/881
18	r	0.29	0/564	0.57	0/756
19	s	0.32	0/685	0.66	0/922
20	t	0.27	0/675	0.51	0/895
21	u	0.28	0/597	0.64	0/792
22	A	0.37	0/69239	0.74	7/108014 (0.0%)
23	B	0.32	1/2873 (0.0%)	0.74	0/4478
24	C	0.32	0/2129	0.60	0/2863
25	D	0.30	0/1586	0.56	0/2134
26	E	0.27	0/1571	0.55	0/2113
27	F	0.34	0/1434	0.78	1/1926 (0.1%)
28	G	0.29	0/1343	0.57	0/1816
29	J	0.29	0/1163	0.52	0/1566
30	K	0.30	0/955	0.59	0/1279
31	L	0.29	0/1073	0.63	0/1427

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	M	0.28	0/1081	0.58	0/1443
33	N	0.27	0/973	0.58	0/1301
34	O	0.30	0/902	0.65	0/1209
35	P	0.31	0/928	0.65	1/1242 (0.1%)
36	Q	0.30	0/960	0.56	0/1278
37	R	0.29	0/829	0.59	0/1107
38	S	0.27	0/864	0.56	0/1156
39	T	0.27	0/744	0.60	0/994
40	U	0.29	0/725	0.61	0/961
41	V	0.28	0/765	0.56	0/1025
42	W	0.29	0/642	0.57	0/848
43	X	0.29	0/634	0.65	0/848
44	Y	0.25	0/502	0.64	0/667
45	Z	0.27	0/452	0.57	0/605
46	5	0.27	0/539	0.65	0/721
47	0	0.27	0/450	0.60	0/599
48	1	0.27	0/416	0.55	0/554
49	2	0.27	0/380	0.67	0/498
50	3	0.26	0/521	0.57	0/687
51	4	0.28	0/303	0.58	0/397
52	w	0.30	0/5293	0.63	0/7166
All	All	0.34	1/158233 (0.0%)	0.71	19/235992 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
37	R	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	1	U	OP3-P	-10.64	1.48	1.61

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	129	LEU	CA-CB-CG	8.95	135.88	115.30
2	b	21	ARG	CB-CG-CD	-8.77	88.79	111.60
13	m	112	PRO	CA-N-CD	-7.81	100.56	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	21	ARG	CG-CD-NE	-7.32	96.42	111.80
22	A	790	U	C2-N1-C1'	6.73	125.78	117.70
13	m	112	PRO	N-CD-CG	-6.50	93.45	103.20
22	A	1313	U	N1-C2-O2	6.47	127.33	122.80
22	A	1313	U	C2-N1-C1'	6.46	125.45	117.70
35	P	39	ARG	N-CA-CB	6.25	121.85	110.60
22	A	1313	U	N3-C2-O2	-5.90	118.07	122.20
1	a	330	C	C2-N1-C1'	5.73	125.10	118.80
22	A	2203	U	C2-N1-C1'	5.70	124.55	117.70
1	a	830	G	C4-C5-N7	5.43	112.97	110.80
13	m	56	LEU	CA-CB-CG	5.28	127.44	115.30
1	a	1109	C	C2-N1-C1'	5.26	124.59	118.80
22	A	790	U	N1-C2-O2	5.22	126.45	122.80
22	A	2031	A	P-O5'-C5'	5.13	129.11	120.90
27	F	113	ASP	CB-CG-OD1	5.09	122.88	118.30
1	a	1158	C	C2-N1-C1'	5.03	124.33	118.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
37	R	51	VAL	Peptide

## 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
2	b	224/226 (99%)	210 (94%)	14 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	204/206 (99%)	199 (98%)	5 (2%)	0	100	100
4	d	203/205 (99%)	201 (99%)	2 (1%)	0	100	100
5	e	153/157 (98%)	144 (94%)	9 (6%)	0	100	100
6	f	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
7	g	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
8	h	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
9	i	125/127 (98%)	115 (92%)	10 (8%)	0	100	100
10	j	98/99 (99%)	92 (94%)	6 (6%)	0	100	100
11	k	115/117 (98%)	107 (93%)	8 (7%)	0	100	100
12	l	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
13	m	113/115 (98%)	103 (91%)	10 (9%)	0	100	100
14	n	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
15	o	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
16	p	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
17	q	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
18	r	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
19	s	82/92 (89%)	82 (100%)	0	0	100	100
20	t	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
21	u	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
24	C	270/271 (100%)	260 (96%)	10 (4%)	0	100	100
25	D	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
26	E	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
27	F	175/177 (99%)	166 (95%)	9 (5%)	0	100	100
28	G	174/176 (99%)	168 (97%)	6 (3%)	0	100	100
29	J	141/142 (99%)	140 (99%)	1 (1%)	0	100	100
30	K	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
31	L	143/144 (99%)	140 (98%)	3 (2%)	0	100	100
32	M	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
33	N	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
34	O	114/116 (98%)	113 (99%)	1 (1%)	0	100	100
35	P	112/114 (98%)	107 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	Q	115/117 (98%)	115 (100%)	0	0	100	100
37	R	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	15	45
38	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
39	T	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
40	U	90/102 (88%)	86 (96%)	4 (4%)	0	100	100
41	V	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
42	W	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
43	X	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
44	Y	60/63 (95%)	60 (100%)	0	0	100	100
45	Z	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
46	5	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
47	0	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
48	1	48/50 (96%)	48 (100%)	0	0	100	100
49	2	44/46 (96%)	44 (100%)	0	0	100	100
50	3	63/64 (98%)	58 (92%)	5 (8%)	0	100	100
51	4	36/38 (95%)	36 (100%)	0	0	100	100
52	w	671/704 (95%)	634 (94%)	33 (5%)	4 (1%)	25	58
All	All	6139/6287 (98%)	5914 (96%)	220 (4%)	5 (0%)	54	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
52	w	540	ILE
52	w	166	PRO
52	w	81	PRO
52	w	492	GLU
37	R	52	PRO

### 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	
2	b	188/188 (100%)	185 (98%)	3 (2%)	62	86
3	c	170/170 (100%)	170 (100%)	0	100	100
4	d	172/172 (100%)	171 (99%)	1 (1%)	86	96
5	e	118/119 (99%)	118 (100%)	0	100	100
6	f	92/92 (100%)	91 (99%)	1 (1%)	73	92
7	g	129/129 (100%)	128 (99%)	1 (1%)	81	94
8	h	104/104 (100%)	104 (100%)	0	100	100
9	i	105/105 (100%)	105 (100%)	0	100	100
10	j	88/87 (101%)	87 (99%)	1 (1%)	73	92
11	k	90/90 (100%)	90 (100%)	0	100	100
12	l	102/102 (100%)	102 (100%)	0	100	100
13	m	93/93 (100%)	92 (99%)	1 (1%)	73	92
14	n	83/84 (99%)	83 (100%)	0	100	100
15	o	76/76 (100%)	75 (99%)	1 (1%)	69	90
16	p	65/65 (100%)	64 (98%)	1 (2%)	65	87
17	q	74/74 (100%)	74 (100%)	0	100	100
18	r	58/58 (100%)	58 (100%)	0	100	100
19	s	72/79 (91%)	71 (99%)	1 (1%)	67	89
20	t	65/65 (100%)	65 (100%)	0	100	100
21	u	60/60 (100%)	60 (100%)	0	100	100
24	C	217/216 (100%)	217 (100%)	0	100	100
25	D	164/164 (100%)	164 (100%)	0	100	100
26	E	165/165 (100%)	165 (100%)	0	100	100
27	F	148/148 (100%)	147 (99%)	1 (1%)	84	95
28	G	137/137 (100%)	137 (100%)	0	100	100
29	J	117/116 (101%)	117 (100%)	0	100	100
30	K	104/104 (100%)	104 (100%)	0	100	100
31	L	104/103 (101%)	104 (100%)	0	100	100
32	M	108/108 (100%)	108 (100%)	0	100	100
33	N	100/100 (100%)	100 (100%)	0	100	100
34	O	86/86 (100%)	86 (100%)	0	100	100
35	P	99/99 (100%)	99 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	Q	89/89 (100%)	89 (100%)	0	100	100
37	R	84/84 (100%)	84 (100%)	0	100	100
38	S	93/93 (100%)	93 (100%)	0	100	100
39	T	80/80 (100%)	80 (100%)	0	100	100
40	U	76/83 (92%)	76 (100%)	0	100	100
41	V	78/78 (100%)	78 (100%)	0	100	100
42	W	62/62 (100%)	62 (100%)	0	100	100
43	X	67/67 (100%)	67 (100%)	0	100	100
44	Y	54/55 (98%)	54 (100%)	0	100	100
45	Z	48/48 (100%)	48 (100%)	0	100	100
46	5	60/60 (100%)	59 (98%)	1 (2%)	60	86
47	0	47/47 (100%)	47 (100%)	0	100	100
48	1	45/45 (100%)	45 (100%)	0	100	100
49	2	38/38 (100%)	38 (100%)	0	100	100
50	3	52/51 (102%)	52 (100%)	0	100	100
51	4	34/34 (100%)	34 (100%)	0	100	100
52	w	549/578 (95%)	546 (100%)	3 (0%)	88	96
All	All	5109/5150 (99%)	5093 (100%)	16 (0%)	92	98

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	74	ARG
2	b	120	GLN
2	b	208	ARG
4	d	184	ARG
6	f	79	ARG
7	g	5	ARG
10	j	4	GLN
13	m	62	LYS
15	o	88	ARG
16	p	80	LYS
19	s	44	MET
27	F	161	LYS
46	5	8	LYS
52	w	37	ASN

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Mol	Chain	Res	Type
52	w	370	LYS
52	w	378	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	120	GLN
3	c	6	HIS
4	d	100	ASN
6	f	11	HIS
9	i	32	GLN
10	j	35	GLN
11	k	119	ASN
15	o	80	GLN
24	C	115	GLN
24	C	134	ASN
24	C	153	GLN
24	C	251	GLN
27	F	5	HIS
27	F	135	GLN
40	U	99	ASN
41	V	80	HIS
52	w	220	GLN
52	w	496	GLN
52	w	505	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1529/1533 (99%)	262 (17%)	0
22	A	2897/2903 (99%)	427 (14%)	6 (0%)
23	B	119/120 (99%)	13 (10%)	0
All	All	4545/4556 (99%)	702 (15%)	6 (0%)

All (702) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	2	A
1	a	4	U
1	a	5	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	a	6	G
1	a	7	A
1	a	9	G
1	a	22	G
1	a	39	G
1	a	47	C
1	a	48	C
1	a	50	A
1	a	51	A
1	a	71	A
1	a	81	A
1	a	82	G
1	a	83	C
1	a	84	U
1	a	85	U
1	a	86	G
1	a	87	C
1	a	90	C
1	a	91	U
1	a	94	G
1	a	95	C
1	a	119	A
1	a	121	U
1	a	127	G
1	a	131	A
1	a	144	G
1	a	163	C
1	a	174	A
1	a	177	G
1	a	181	A
1	a	182	A
1	a	183	C
1	a	188	C
1	a	189	A
1	a	197	A
1	a	198	G
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	240	G
1	a	245	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	a	247	G
1	a	251	G
1	a	266	G
1	a	267	C
1	a	279	A
1	a	280	C
1	a	289	G
1	a	301	G
1	a	313	A
1	a	314	C
1	a	315	A
1	a	328	C
1	a	332	G
1	a	346	G
1	a	347	G
1	a	351	G
1	a	352	C
1	a	354	G
1	a	367	U
1	a	372	C
1	a	373	A
1	a	398	U
1	a	406	G
1	a	408	A
1	a	411	A
1	a	412	A
1	a	413	G
1	a	414	A
1	a	421	U
1	a	422	C
1	a	423	G
1	a	429	U
1	a	439	U
1	a	448	A
1	a	465	A
1	a	466	A
1	a	467	U
1	a	474	G
1	a	484	G
1	a	495	A
1	a	496	A
1	a	497	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	a	511	C
1	a	518	C
1	a	521	G
1	a	527	G7M
1	a	531	U
1	a	540	G
1	a	547	A
1	a	559	A
1	a	564	C
1	a	572	A
1	a	573	A
1	a	574	A
1	a	576	C
1	a	577	G
1	a	596	A
1	a	607	A
1	a	619	U
1	a	632	U
1	a	642	A
1	a	653	U
1	a	665	A
1	a	666	G
1	a	671	G
1	a	703	G
1	a	717	U
1	a	718	A
1	a	721	G
1	a	723	U
1	a	734	G
1	a	748	G
1	a	755	G
1	a	774	G
1	a	777	A
1	a	793	U
1	a	794	A
1	a	815	A
1	a	817	C
1	a	819	A
1	a	828	U
1	a	829	G
1	a	841	C
1	a	843	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	a	844	G
1	a	846	G
1	a	851	G
1	a	872	A
1	a	876	C
1	a	884	U
1	a	902	G
1	a	914	A
1	a	926	G
1	a	927	G
1	a	934	C
1	a	935	A
1	a	940	C
1	a	945	G
1	a	960	U
1	a	961	U
1	a	965	U
1	a	966	2MG
1	a	969	A
1	a	971	G
1	a	975	A
1	a	976	G
1	a	977	A
1	a	992	U
1	a	993	G
1	a	994	A
1	a	998	C
1	a	1003	G
1	a	1004	A
1	a	1014	A
1	a	1025	U
1	a	1027	C
1	a	1029	U
1	a	1030	U
1	a	1031	C
1	a	1033	G
1	a	1037	C
1	a	1038	C
1	a	1045	C
1	a	1046	A
1	a	1048	G
1	a	1053	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	a	1054	C
1	a	1056	U
1	a	1065	U
1	a	1066	C
1	a	1085	U
1	a	1086	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1104	G
1	a	1125	U
1	a	1133	G
1	a	1135	U
1	a	1136	C
1	a	1137	C
1	a	1139	G
1	a	1140	C
1	a	1146	A
1	a	1152	A
1	a	1157	A
1	a	1158	C
1	a	1159	U
1	a	1167	A
1	a	1169	A
1	a	1178	G
1	a	1183	U
1	a	1184	G
1	a	1191	A
1	a	1196	A
1	a	1197	A
1	a	1198	G
1	a	1212	U
1	a	1213	A
1	a	1214	C
1	a	1225	A
1	a	1226	C
1	a	1227	A
1	a	1231	G
1	a	1238	A
1	a	1248	A
1	a	1250	A
1	a	1254	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	a	1258	G
1	a	1259	C
1	a	1260	G
1	a	1269	A
1	a	1270	G
1	a	1279	G
1	a	1280	A
1	a	1284	C
1	a	1285	A
1	a	1286	U
1	a	1287	A
1	a	1288	A
1	a	1289	A
1	a	1290	G
1	a	1294	G
1	a	1297	G
1	a	1299	A
1	a	1300	G
1	a	1302	C
1	a	1303	C
1	a	1317	C
1	a	1322	C
1	a	1336	C
1	a	1348	U
1	a	1360	A
1	a	1363	A
1	a	1364	U
1	a	1374	A
1	a	1378	C
1	a	1379	G
1	a	1383	C
1	a	1397	C
1	a	1398	A
1	a	1419	G
1	a	1429	A
1	a	1441	A
1	a	1442	G
1	a	1446	A
1	a	1453	G
1	a	1454	G
1	a	1477	U
1	a	1492	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	a	1493	A
1	a	1497	G
1	a	1499	A
1	a	1506	U
1	a	1517	G
1	a	1529	G
1	a	1530	G
22	A	10	A
22	A	36	G
22	A	46	G
22	A	51	G
22	A	55	G
22	A	63	A
22	A	71	A
22	A	74	A
22	A	75	G
22	A	87	U
22	A	91	A
22	A	92	U
22	A	101	A
22	A	102	U
22	A	118	A
22	A	119	A
22	A	120	U
22	A	125	A
22	A	139	U
22	A	140	C
22	A	141	G
22	A	142	A
22	A	160	A
22	A	163	C
22	A	181	A
22	A	196	A
22	A	199	A
22	A	215	G
22	A	216	A
22	A	221	A
22	A	222	A
22	A	224	U
22	A	228	C
22	A	230	G
22	A	233	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
22	A	242	G
22	A	248	G
22	A	265	A
22	A	266	G
22	A	276	U
22	A	279	A
22	A	295	G
22	A	311	A
22	A	329	G
22	A	330	A
22	A	338	G
22	A	343	C
22	A	346	A
22	A	372	G
22	A	380	G
22	A	383	C
22	A	386	G
22	A	396	G
22	A	399	U
22	A	401	A
22	A	405	U
22	A	406	G
22	A	411	G
22	A	428	A
22	A	435	C
22	A	451	U
22	A	475	C
22	A	479	A
22	A	481	G
22	A	491	G
22	A	505	A
22	A	507	A
22	A	509	C
22	A	530	G
22	A	531	C
22	A	532	A
22	A	538	A
22	A	546	U
22	A	547	A
22	A	549	G
22	A	550	C
22	A	563	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
22	A	568	U
22	A	573	U
22	A	575	A
22	A	603	A
22	A	615	U
22	A	622	G
22	A	627	A
22	A	637	A
22	A	645	C
22	A	646	U
22	A	647	G
22	A	655	A
22	A	659	G
22	A	668	A
22	A	682	G
22	A	685	A
22	A	686	U
22	A	695	G
22	A	702	U
22	A	726	G
22	A	730	A
22	A	738	G
22	A	740	C
22	A	747	5MU
22	A	757	G
22	A	764	A
22	A	765	C
22	A	775	G
22	A	776	G
22	A	782	A
22	A	784	G
22	A	785	G
22	A	787	C
22	A	789	A
22	A	792	A
22	A	805	G
22	A	812	C
22	A	819	A
22	A	827	U
22	A	828	U
22	A	829	A
22	A	830	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
22	A	845	A
22	A	846	U
22	A	847	U
22	A	856	G
22	A	859	G
22	A	880	G
22	A	889	C
22	A	890	C
22	A	891	G
22	A	893	C
22	A	899	A
22	A	906	U
22	A	907	G
22	A	910	A
22	A	914	G
22	A	917	A
22	A	931	U
22	A	941	A
22	A	946	C
22	A	961	C
22	A	973	A
22	A	974	G
22	A	983	A
22	A	996	A
22	A	999	U
22	A	1011	G
22	A	1012	U
22	A	1013	C
22	A	1022	G
22	A	1026	G
22	A	1033	U
22	A	1040	A
22	A	1046	A
22	A	1047	G
22	A	1048	A
22	A	1050	A
22	A	1059	G
22	A	1060	U
22	A	1070	A
22	A	1071	G
22	A	1079	C
22	A	1083	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
22	A	1084	A
22	A	1087	G
22	A	1088	A
22	A	1096	A
22	A	1097	U
22	A	1112	G
22	A	1130	U
22	A	1132	U
22	A	1133	A
22	A	1134	A
22	A	1135	C
22	A	1141	U
22	A	1142	A
22	A	1174	U
22	A	1175	A
22	A	1176	U
22	A	1195	G
22	A	1206	G
22	A	1227	G
22	A	1236	G
22	A	1238	G
22	A	1250	G
22	A	1253	A
22	A	1256	G
22	A	1266	G
22	A	1267	U
22	A	1271	G
22	A	1272	A
22	A	1300	G
22	A	1301	A
22	A	1329	U
22	A	1344	U
22	A	1351	C
22	A	1365	A
22	A	1368	G
22	A	1378	A
22	A	1379	U
22	A	1383	A
22	A	1386	C
22	A	1416	G
22	A	1421	G
22	A	1428	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
22	A	1452	G
22	A	1453	A
22	A	1460	U
22	A	1482	G
22	A	1485	U
22	A	1493	C
22	A	1506	U
22	A	1508	A
22	A	1509	A
22	A	1515	A
22	A	1524	G
22	A	1529	G
22	A	1534	U
22	A	1536	C
22	A	1537	G
22	A	1538	G
22	A	1558	C
22	A	1566	A
22	A	1569	A
22	A	1578	U
22	A	1584	U
22	A	1608	A
22	A	1610	A
22	A	1617	C
22	A	1634	A
22	A	1647	U
22	A	1648	U
22	A	1649	G
22	A	1651	G
22	A	1674	G
22	A	1675	C
22	A	1693	U
22	A	1715	G
22	A	1723	G
22	A	1729	U
22	A	1730	C
22	A	1732	C
22	A	1738	G
22	A	1754	A
22	A	1756	G
22	A	1758	U
22	A	1764	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
22	A	1773	A
22	A	1776	G
22	A	1784	A
22	A	1786	A
22	A	1791	A
22	A	1800	C
22	A	1801	A
22	A	1808	A
22	A	1816	C
22	A	1829	A
22	A	1848	A
22	A	1903	G
22	A	1906	G
22	A	1914	C
22	A	1919	A
22	A	1929	G
22	A	1930	G
22	A	1937	A
22	A	1938	A
22	A	1955	U
22	A	1963	U
22	A	1967	C
22	A	1970	A
22	A	1971	U
22	A	1972	G
22	A	1991	U
22	A	1993	U
22	A	1997	C
22	A	2021	C
22	A	2022	U
22	A	2023	C
22	A	2031	A
22	A	2033	A
22	A	2035	G
22	A	2036	C
22	A	2043	C
22	A	2055	C
22	A	2056	G
22	A	2060	A
22	A	2061	G
22	A	2062	A
22	A	2063	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
22	A	2069	G7M
22	A	2080	A
22	A	2093	G
22	A	2111	U
22	A	2112	G
22	A	2113	U
22	A	2115	G
22	A	2117	A
22	A	2118	U
22	A	2119	A
22	A	2120	G
22	A	2121	G
22	A	2126	A
22	A	2127	G
22	A	2132	U
22	A	2133	G
22	A	2134	A
22	A	2141	G
22	A	2142	A
22	A	2144	G
22	A	2145	C
22	A	2146	C
22	A	2149	U
22	A	2152	G
22	A	2157	G
22	A	2158	A
22	A	2159	G
22	A	2162	G
22	A	2163	A
22	A	2164	C
22	A	2168	G
22	A	2170	A
22	A	2171	A
22	A	2172	U
22	A	2173	A
22	A	2180	U
22	A	2195	U
22	A	2198	A
22	A	2203	U
22	A	2204	G
22	A	2211	A
22	A	2225	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
22	A	2238	G
22	A	2239	G
22	A	2251	OMG
22	A	2268	A
22	A	2278	A
22	A	2283	C
22	A	2287	A
22	A	2288	A
22	A	2305	U
22	A	2308	G
22	A	2309	A
22	A	2322	A
22	A	2325	G
22	A	2333	A
22	A	2335	A
22	A	2345	G
22	A	2347	C
22	A	2350	C
22	A	2361	G
22	A	2383	G
22	A	2385	C
22	A	2402	U
22	A	2406	A
22	A	2410	G
22	A	2423	U
22	A	2425	A
22	A	2426	A
22	A	2429	G
22	A	2430	A
22	A	2435	A
22	A	2441	U
22	A	2448	A
22	A	2459	A
22	A	2469	A
22	A	2473	U
22	A	2475	C
22	A	2476	A
22	A	2478	A
22	A	2484	G
22	A	2491	U
22	A	2494	G
22	A	2498	OMC

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
22	A	2502	G
22	A	2504	PSU
22	A	2505	G
22	A	2518	A
22	A	2520	C
22	A	2529	G
22	A	2547	A
22	A	2549	G
22	A	2552	OMU
22	A	2554	U
22	A	2566	A
22	A	2567	G
22	A	2569	G
22	A	2572	A
22	A	2599	G
22	A	2602	A
22	A	2603	G
22	A	2605	PSU
22	A	2606	C
22	A	2609	U
22	A	2613	U
22	A	2615	U
22	A	2629	U
22	A	2630	G
22	A	2636	C
22	A	2654	A
22	A	2663	G
22	A	2684	U
22	A	2689	U
22	A	2690	U
22	A	2714	G
22	A	2716	C
22	A	2726	A
22	A	2728	U
22	A	2729	G
22	A	2732	G
22	A	2733	A
22	A	2744	G
22	A	2748	A
22	A	2757	A
22	A	2765	A
22	A	2778	A

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Mol	Chain	Res	Type
22	A	2779	U
22	A	2791	G
22	A	2797	U
22	A	2800	A
22	A	2818	U
22	A	2820	A
22	A	2821	A
22	A	2835	A
22	A	2849	U
22	A	2873	A
22	A	2883	A
22	A	2884	U
22	A	2885	G
22	A	2886	A
23	B	13	G
23	B	16	G
23	B	25	U
23	B	35	C
23	B	36	C
23	B	51	G
23	B	53	A
23	B	56	G
23	B	67	G
23	B	89	U
23	B	90	C
23	B	99	A
23	B	109	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	A	784	G
22	A	888	C
22	A	1484	U
22	A	1847	A
22	A	2602	A
22	A	2756	U

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

36 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
22	G7M	A	2069	22	20,26,27	2.41	7 (35%)	17,39,42	1.13	1 (5%)
1	2MG	a	1516	1	18,26,27	2.46	3 (16%)	16,38,41	1.31	3 (18%)
22	PSU	A	2605	22	18,21,22	2.69	6 (33%)	22,30,33	1.84	5 (22%)
1	UR3	a	1498	1	19,22,23	2.89	7 (36%)	26,32,35	1.30	2 (7%)
1	5MC	a	1407	1	18,22,23	3.17	7 (38%)	26,32,35	2.32	7 (26%)
22	PSU	A	2457	22	18,21,22	2.68	6 (33%)	22,30,33	1.87	5 (22%)
22	2MA	A	2503	53,22	17,25,26	2.47	5 (29%)	17,37,40	1.31	2 (11%)
22	2MG	A	2445	22	18,26,27	2.41	3 (16%)	16,38,41	1.36	3 (18%)
12	D2T	l	89	12	7,9,10	1.34	1 (14%)	6,11,13	1.48	0
1	PSU	a	516	1	18,21,22	2.72	7 (38%)	22,30,33	1.83	6 (27%)
22	3TD	A	1915	22	18,22,23	4.09	7 (38%)	22,32,35	1.86	3 (13%)
1	MA6	a	1519	1	18,26,27	1.16	2 (11%)	19,38,41	3.20	2 (10%)
22	PSU	A	746	53,22	18,21,22	2.70	6 (33%)	22,30,33	1.73	5 (22%)
22	PSU	A	1917	22	18,21,22	2.73	6 (33%)	22,30,33	1.89	5 (22%)
1	MA6	a	1518	1	18,26,27	1.16	2 (11%)	19,38,41	3.09	2 (10%)
22	6MZ	A	2030	22	18,25,26	2.48	2 (11%)	16,36,39	2.40	4 (25%)
1	5MC	a	967	1	18,22,23	3.25	7 (38%)	26,32,35	2.33	7 (26%)
22	OMC	A	2498	53,22	19,22,23	2.93	6 (31%)	26,31,34	2.00	5 (19%)
22	OMG	A	2251	53,22	18,26,27	1.16	2 (11%)	19,38,41	0.85	1 (5%)
1	G7M	a	527	1	20,26,27	2.42	7 (35%)	17,39,42	1.10	1 (5%)
22	5MC	A	1962	22	18,22,23	3.15	7 (38%)	26,32,35	2.41	6 (23%)
22	PSU	A	2580	22	18,21,22	2.66	7 (38%)	22,30,33	1.96	6 (27%)
22	H2U	A	2449	22	18,21,22	2.11	4 (22%)	21,30,33	2.11	4 (19%)
22	2MG	A	1835	22	18,26,27	2.42	3 (16%)	16,38,41	1.25	3 (18%)
1	2MG	a	966	1	18,26,27	2.53	3 (16%)	16,38,41	1.30	2 (12%)
22	PSU	A	2604	22	18,21,22	2.68	6 (33%)	22,30,33	1.90	5 (22%)
1	4OC	a	1402	1	20,23,24	3.12	8 (40%)	26,32,35	0.94	1 (3%)
22	PSU	A	2504	22	18,21,22	2.70	6 (33%)	22,30,33	1.87	5 (22%)
22	PSU	A	1911	22	18,21,22	2.76	6 (33%)	22,30,33	1.84	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	5MU	A	747	22	19,22,23	2.29	6 (31%)	28,32,35	2.28	8 (28%)
22	PSU	A	955	22	18,21,22	2.68	6 (33%)	22,30,33	1.92	5 (22%)
22	OMU	A	2552	22	19,22,23	2.04	6 (31%)	26,31,34	1.73	5 (19%)
22	5MU	A	1939	22	19,22,23	2.29	6 (31%)	28,32,35	2.24	8 (28%)
22	1MG	A	745	22	18,26,27	2.78	6 (33%)	19,39,42	1.43	4 (21%)
22	6MZ	A	1618	22	18,25,26	2.51	3 (16%)	16,36,39	2.04	3 (18%)
32	4D4	M	81	32	9,11,12	2.11	2 (22%)	8,13,15	2.09	4 (50%)

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
22	G7M	A	2069	22	-	2/3/25/26	0/3/3/3
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
22	PSU	A	2605	22	-	2/7/25/26	0/2/2/2
1	UR3	a	1498	1	-	0/7/25/26	0/2/2/2
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
22	PSU	A	2457	22	-	0/7/25/26	0/2/2/2
22	2MA	A	2503	53,22	-	2/3/25/26	0/3/3/3
22	2MG	A	2445	22	-	2/5/27/28	0/3/3/3
12	D2T	l	89	12	-	1/7/12/14	-
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
22	3TD	A	1915	22	-	2/7/25/26	0/2/2/2
1	MA6	a	1519	1	-	2/7/29/30	0/3/3/3
22	PSU	A	746	53,22	-	1/7/25/26	0/2/2/2
22	PSU	A	1917	22	-	0/7/25/26	0/2/2/2
1	MA6	a	1518	1	-	0/7/29/30	0/3/3/3
22	6MZ	A	2030	22	-	2/5/27/28	0/3/3/3
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
22	OMC	A	2498	53,22	-	2/9/27/28	0/2/2/2
22	OMG	A	2251	53,22	-	3/5/27/28	0/3/3/3
1	G7M	a	527	1	-	2/3/25/26	0/3/3/3
22	5MC	A	1962	22	-	1/7/25/26	0/2/2/2
22	PSU	A	2580	22	-	0/7/25/26	0/2/2/2
22	H2U	A	2449	22	-	0/7/38/39	0/2/2/2
22	2MG	A	1835	22	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	a	966	1	-	0/5/27/28	0/3/3/3
22	PSU	A	2604	22	-	0/7/25/26	0/2/2/2
1	4OC	a	1402	1	-	1/9/29/30	0/2/2/2
22	PSU	A	2504	22	-	0/7/25/26	0/2/2/2
22	PSU	A	1911	22	-	1/7/25/26	0/2/2/2
22	5MU	A	747	22	-	2/7/25/26	0/2/2/2
22	PSU	A	955	22	-	0/7/25/26	0/2/2/2
22	OMU	A	2552	22	-	2/9/27/28	0/2/2/2
22	5MU	A	1939	22	-	0/7/25/26	0/2/2/2
22	1MG	A	745	22	-	0/3/25/26	0/3/3/3
22	6MZ	A	1618	22	-	3/5/27/28	0/3/3/3
32	4D4	M	81	32	-	5/11/12/14	-

All (184) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1915	3TD	C6-C5	12.20	1.49	1.35
22	A	1618	6MZ	C6-N6	9.58	1.50	1.35
22	A	2030	6MZ	C6-N6	9.34	1.50	1.35
1	a	967	5MC	O2-C2	9.02	1.40	1.23
22	A	2498	OMC	O2-C2	8.92	1.40	1.23
22	A	1962	5MC	O2-C2	8.88	1.40	1.23
22	A	1915	3TD	C2-N1	8.88	1.48	1.37
1	a	1407	5MC	O2-C2	8.83	1.40	1.23
1	a	966	2MG	O6-C6	8.34	1.40	1.23
1	a	1516	2MG	O6-C6	8.29	1.40	1.23
22	A	1835	2MG	O6-C6	8.12	1.39	1.23
22	A	2445	2MG	O6-C6	8.11	1.39	1.23
22	A	1911	PSU	C6-N1	7.60	1.48	1.36
1	a	1498	UR3	C2-N1	7.57	1.49	1.38
22	A	1917	PSU	C6-N1	7.53	1.48	1.36
22	A	2504	PSU	C6-N1	7.45	1.48	1.36
22	A	2604	PSU	C6-N1	7.43	1.48	1.36
22	A	746	PSU	C6-N1	7.40	1.48	1.36
22	A	2449	H2U	C2-N1	7.38	1.46	1.35
1	a	516	PSU	C6-N1	7.37	1.48	1.36
22	A	2605	PSU	C6-N1	7.37	1.48	1.36
22	A	955	PSU	C6-N1	7.30	1.48	1.36
22	A	2457	PSU	C6-N1	7.28	1.48	1.36
22	A	2580	PSU	C6-N1	7.23	1.48	1.36
22	A	2503	2MA	C2-N3	6.93	1.45	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1402	4OC	C4-N3	6.90	1.44	1.32
22	A	745	1MG	C2-N3	6.84	1.47	1.34
22	A	1911	PSU	C2-N1	6.68	1.45	1.36
1	a	967	5MC	C6-N1	6.61	1.49	1.38
1	a	516	PSU	C2-N1	6.54	1.45	1.36
22	A	1917	PSU	C2-N1	6.52	1.45	1.36
22	A	2605	PSU	C2-N1	6.48	1.45	1.36
22	A	955	PSU	C2-N1	6.44	1.45	1.36
22	A	746	PSU	C2-N1	6.42	1.45	1.36
22	A	2504	PSU	C2-N1	6.41	1.45	1.36
1	a	1407	5MC	C6-N1	6.38	1.48	1.38
22	A	2604	PSU	C2-N1	6.36	1.45	1.36
22	A	1962	5MC	C6-N1	6.36	1.48	1.38
22	A	2457	PSU	C2-N1	6.27	1.45	1.36
1	a	1498	UR3	C6-C5	6.23	1.49	1.35
22	A	1939	5MU	C6-N1	6.20	1.48	1.38
1	a	1402	4OC	C6-C5	6.20	1.49	1.35
22	A	2580	PSU	C2-N1	6.12	1.45	1.36
22	A	747	5MU	C6-N1	6.09	1.48	1.38
1	a	1402	4OC	C2-N3	6.03	1.48	1.36
22	A	2498	OMC	C6-C5	6.02	1.49	1.35
22	A	745	1MG	C2-N2	5.75	1.44	1.34
22	A	2503	2MA	C4-N3	5.57	1.50	1.37
1	a	966	2MG	C2-N2	5.43	1.45	1.33
22	A	1915	3TD	C6-N1	5.32	1.45	1.36
1	a	527	G7M	C2-N3	5.27	1.46	1.33
22	A	2069	G7M	C2-N3	5.21	1.45	1.33
1	a	1498	UR3	C2-N3	5.19	1.49	1.39
1	a	1516	2MG	C2-N2	5.18	1.44	1.33
22	A	1835	2MG	C2-N2	5.14	1.44	1.33
22	A	2445	2MG	C2-N2	5.11	1.44	1.33
32	M	81	4D4	CZ-NE	5.07	1.43	1.33
22	A	2069	G7M	C4-N3	4.94	1.49	1.37
1	a	527	G7M	C4-N3	4.85	1.49	1.37
1	a	967	5MC	C6-C5	4.81	1.42	1.34
22	A	2498	OMC	C4-N4	4.80	1.45	1.33
1	a	527	G7M	C2-N2	4.69	1.45	1.34
1	a	1407	5MC	C6-C5	4.67	1.42	1.34
22	A	1939	5MU	C4-C5	4.63	1.52	1.44
22	A	2069	G7M	C2-N2	4.62	1.45	1.34
22	A	747	5MU	C4-C5	4.60	1.52	1.44
22	A	1915	3TD	C2-N3	4.58	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1402	4OC	C4-N4	4.56	1.45	1.35
22	A	745	1MG	C4-N3	4.47	1.48	1.37
1	a	967	5MC	C4-N4	4.46	1.45	1.34
22	A	1962	5MC	C4-N4	4.41	1.45	1.34
1	a	527	G7M	C6-N1	4.41	1.44	1.37
1	a	1407	5MC	C4-N4	4.36	1.45	1.34
22	A	2552	OMU	C6-N1	4.35	1.48	1.38
22	A	1962	5MC	C6-C5	4.33	1.41	1.34
22	A	2552	OMU	C2-N1	4.33	1.45	1.38
22	A	2069	G7M	C6-N1	4.25	1.44	1.37
22	A	747	5MU	C2-N1	4.24	1.45	1.38
22	A	1939	5MU	C2-N1	4.09	1.45	1.38
1	a	1402	4OC	C2-N1	4.07	1.48	1.40
22	A	745	1MG	O6-C6	-4.07	1.14	1.22
22	A	2552	OMU	C5-C4	3.99	1.52	1.43
1	a	1402	4OC	C5-C4	3.92	1.49	1.40
22	A	745	1MG	C5-C4	-3.24	1.34	1.43
22	A	2503	2MA	C2-N1	3.10	1.46	1.36
1	a	1402	4OC	C6-N1	3.08	1.45	1.38
32	M	81	4D4	CZ-NH2	3.08	1.44	1.32
22	A	2457	PSU	C4-C5	3.04	1.52	1.44
22	A	2552	OMU	O4-C4	-3.00	1.18	1.24
1	a	966	2MG	C2-N1	2.98	1.41	1.36
1	a	1407	5MC	C4-N3	-2.98	1.29	1.34
22	A	2580	PSU	C4-C5	2.94	1.52	1.44
22	A	2604	PSU	C4-C5	2.93	1.52	1.44
22	A	2504	PSU	C4-C5	2.93	1.52	1.44
1	a	1516	2MG	C2-N1	2.91	1.41	1.36
22	A	745	1MG	C5-C6	2.89	1.56	1.47
22	A	746	PSU	C4-C5	2.88	1.52	1.44
1	a	1402	4OC	O2-C2	-2.88	1.18	1.23
22	A	1911	PSU	C4-C5	2.87	1.52	1.44
22	A	1962	5MC	C4-N3	-2.87	1.29	1.34
1	a	1518	MA6	C5-C4	-2.86	1.33	1.40
22	A	1917	PSU	C2-N3	2.84	1.42	1.37
22	A	1917	PSU	C4-C5	2.83	1.52	1.44
1	a	516	PSU	C4-C5	2.82	1.52	1.44
22	A	955	PSU	C4-C5	2.82	1.52	1.44
22	A	2030	6MZ	C5-C4	-2.82	1.33	1.40
22	A	1911	PSU	C2-N3	2.81	1.42	1.37
22	A	2251	OMG	C8-N7	-2.80	1.30	1.35
22	A	1835	2MG	C2-N1	2.79	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	2069	G7M	C5-C6	2.78	1.52	1.45
1	a	527	G7M	C5-C6	2.78	1.52	1.45
1	a	1519	MA6	C5-C4	-2.77	1.33	1.40
1	a	1498	UR3	C6-N1	2.76	1.44	1.38
22	A	2498	OMC	C5-C4	2.75	1.49	1.42
22	A	2605	PSU	C4-C5	2.75	1.52	1.44
1	a	1498	UR3	O2-C2	-2.74	1.17	1.22
1	a	967	5MC	C4-N3	-2.74	1.29	1.34
1	a	516	PSU	C2-N3	2.73	1.42	1.37
22	A	2580	PSU	C2-N3	2.72	1.42	1.37
22	A	2503	2MA	C5-C4	-2.72	1.36	1.43
22	A	2457	PSU	O4-C4	-2.71	1.18	1.23
22	A	2445	2MG	C2-N1	2.71	1.41	1.36
22	A	2504	PSU	C2-N3	2.71	1.42	1.37
22	A	955	PSU	O4-C4	-2.68	1.18	1.23
1	a	1498	UR3	O4-C4	-2.68	1.17	1.23
22	A	2605	PSU	O4-C4	-2.67	1.18	1.23
22	A	2457	PSU	C2-N3	2.65	1.42	1.37
22	A	1618	6MZ	C5-C4	-2.64	1.33	1.40
22	A	746	PSU	O4-C4	-2.63	1.18	1.23
22	A	2580	PSU	O4-C4	-2.62	1.18	1.23
1	a	516	PSU	O4-C4	-2.60	1.18	1.23
22	A	747	5MU	O4-C4	-2.60	1.18	1.23
1	a	967	5MC	C2-N3	2.58	1.41	1.36
22	A	1939	5MU	O4-C4	-2.58	1.18	1.23
22	A	746	PSU	C2-N3	2.57	1.41	1.37
22	A	1911	PSU	O4-C4	-2.55	1.18	1.23
22	A	1939	5MU	O2-C2	-2.53	1.18	1.23
22	A	1917	PSU	O4-C4	-2.53	1.18	1.23
22	A	2604	PSU	O4-C4	-2.51	1.18	1.23
1	a	527	G7M	C2-N1	2.50	1.43	1.37
22	A	2504	PSU	O4-C4	-2.50	1.18	1.23
22	A	1915	3TD	O2-C2	-2.49	1.18	1.23
22	A	2605	PSU	C2-N3	2.49	1.41	1.37
22	A	955	PSU	C2-N3	2.48	1.41	1.37
1	a	1498	UR3	C5-C4	2.47	1.50	1.43
22	A	747	5MU	O2-C2	-2.46	1.18	1.23
22	A	2449	H2U	O2-C2	-2.44	1.18	1.23
22	A	2552	OMU	O2-C2	-2.44	1.18	1.23
22	A	2604	PSU	C2-N3	2.42	1.41	1.37
22	A	1962	5MC	C2-N3	2.42	1.41	1.36
22	A	2251	OMG	C5-C6	-2.41	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	2580	PSU	O2-C2	-2.41	1.18	1.23
1	a	1407	5MC	C2-N3	2.37	1.41	1.36
22	A	2498	OMC	C2-N1	-2.35	1.34	1.40
22	A	955	PSU	O2-C2	-2.34	1.18	1.23
22	A	2069	G7M	C2-N1	2.33	1.43	1.37
1	a	516	PSU	O4'-C1'	-2.33	1.40	1.43
22	A	2604	PSU	O2-C2	-2.32	1.18	1.23
1	a	967	5MC	C2-N1	2.30	1.45	1.40
22	A	747	5MU	C2-N3	2.29	1.42	1.38
22	A	1962	5MC	C2-N1	2.29	1.45	1.40
22	A	2605	PSU	O2-C2	-2.27	1.18	1.23
22	A	1915	3TD	C4-N3	2.27	1.45	1.40
22	A	2552	OMU	C2-N3	2.27	1.42	1.38
22	A	2449	H2U	C2-N3	2.26	1.42	1.38
22	A	2457	PSU	O2-C2	-2.24	1.18	1.23
22	A	2449	H2U	O4-C4	-2.24	1.18	1.23
22	A	1939	5MU	C2-N3	2.24	1.42	1.38
22	A	2069	G7M	O6-C6	-2.22	1.18	1.23
22	A	2504	PSU	O2-C2	-2.20	1.18	1.23
22	A	1917	PSU	O2-C2	-2.19	1.18	1.23
22	A	2580	PSU	O4'-C1'	-2.17	1.40	1.43
22	A	746	PSU	O2-C2	-2.16	1.18	1.23
22	A	1911	PSU	O2-C2	-2.13	1.18	1.23
22	A	1618	6MZ	C2-N3	2.12	1.35	1.32
22	A	2503	2MA	C6-N1	2.11	1.42	1.38
22	A	2498	OMC	C2-N3	-2.09	1.32	1.36
12	l	89	D2T	CB1-SB	-2.09	1.75	1.79
1	a	516	PSU	O2-C2	-2.06	1.19	1.23
1	a	527	G7M	O6-C6	-2.05	1.19	1.23
1	a	1519	MA6	C10-N6	2.04	1.50	1.45
1	a	1407	5MC	C2-N1	2.04	1.44	1.40
1	a	1518	MA6	C2-N3	2.02	1.35	1.32
22	A	1915	3TD	O4-C4	-2.01	1.18	1.23

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1519	MA6	N1-C6-N6	-12.29	104.12	117.06
1	a	1518	MA6	N1-C6-N6	-12.01	104.41	117.06
22	A	1962	5MC	C6-N1-C2	-7.99	109.81	120.87
1	a	967	5MC	C6-N1-C2	-7.84	110.02	120.87
1	a	1407	5MC	C6-N1-C2	-7.78	110.09	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	747	5MU	C4-N3-C2	-6.14	119.40	127.35
22	A	2449	H2U	C4-N3-C2	-6.10	120.73	125.79
22	A	1939	5MU	C4-N3-C2	-6.05	119.52	127.35
1	a	1519	MA6	N3-C2-N1	-5.75	119.69	128.68
22	A	1915	3TD	N1-C2-N3	5.70	120.64	116.14
22	A	1939	5MU	C5-C4-N3	5.65	120.13	115.31
22	A	1618	6MZ	N3-C2-N1	-5.63	119.87	128.68
22	A	747	5MU	C5-C4-N3	5.56	120.06	115.31
22	A	2030	6MZ	N3-C2-N1	-5.56	119.99	128.68
1	a	1518	MA6	N3-C2-N1	-5.51	120.06	128.68
22	A	2030	6MZ	C9-N6-C6	-5.46	118.17	122.87
22	A	1962	5MC	C5-C4-N3	5.27	127.36	121.67
1	a	967	5MC	C5-C4-N3	5.24	127.33	121.67
1	a	1407	5MC	C5-C4-N3	5.18	127.26	121.67
22	A	2449	H2U	N3-C2-N1	5.11	122.06	116.65
22	A	2552	OMU	C4-N3-C2	-5.01	119.97	126.58
22	A	2498	OMC	N1-C2-N3	4.97	127.87	118.81
22	A	2498	OMC	C6-C5-C4	-4.84	109.70	117.50
1	a	1498	UR3	C4-N3-C2	-4.84	120.01	124.56
22	A	2580	PSU	N1-C2-N3	4.78	120.55	115.13
22	A	955	PSU	C4-N3-C2	-4.74	119.51	126.34
22	A	2604	PSU	C4-N3-C2	-4.74	119.51	126.34
22	A	2504	PSU	C4-N3-C2	-4.67	119.61	126.34
22	A	2457	PSU	N1-C2-N3	4.63	120.38	115.13
22	A	955	PSU	N1-C2-N3	4.63	120.38	115.13
22	A	1911	PSU	C4-N3-C2	-4.63	119.67	126.34
22	A	2605	PSU	C4-N3-C2	-4.61	119.70	126.34
22	A	1917	PSU	C4-N3-C2	-4.57	119.76	126.34
22	A	2580	PSU	C4-N3-C2	-4.57	119.76	126.34
22	A	2498	OMC	O2-C2-N3	-4.56	114.92	122.33
22	A	2604	PSU	N1-C2-N3	4.54	120.27	115.13
22	A	2457	PSU	C4-N3-C2	-4.50	119.86	126.34
22	A	746	PSU	C4-N3-C2	-4.44	119.94	126.34
22	A	2504	PSU	N1-C2-N3	4.44	120.16	115.13
22	A	1917	PSU	N1-C2-N3	4.42	120.14	115.13
1	a	516	PSU	C4-N3-C2	-4.40	120.00	126.34
22	A	747	5MU	O4-C4-C5	-4.39	119.81	124.90
22	A	2605	PSU	N1-C2-N3	4.32	120.03	115.13
22	A	1915	3TD	C4-N3-C2	-4.31	119.93	124.61
22	A	746	PSU	N1-C2-N3	4.29	119.99	115.13
22	A	1911	PSU	N1-C2-N3	4.24	119.94	115.13
22	A	1939	5MU	O4-C4-C5	-4.21	120.02	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1939	5MU	N3-C2-N1	4.19	120.45	114.89
22	A	745	1MG	C5-C6-N1	4.17	120.16	113.90
22	A	747	5MU	N3-C2-N1	4.14	120.39	114.89
22	A	2552	OMU	N3-C2-N1	4.12	120.36	114.89
1	a	516	PSU	N1-C2-N3	4.11	119.78	115.13
22	A	1618	6MZ	C9-N6-C6	-4.01	119.42	122.87
22	A	1962	5MC	C5-C4-N4	-3.93	115.60	121.48
22	A	1962	5MC	C1'-N1-C2	3.82	126.94	118.42
22	A	2030	6MZ	C2-N1-C6	3.72	119.78	116.59
22	A	2498	OMC	C6-N1-C2	-3.68	114.11	120.49
22	A	747	5MU	C5-C6-N1	-3.61	119.63	123.34
32	M	81	4D4	NE-CZ-NH2	-3.58	114.40	120.70
22	A	2449	H2U	C5-C4-N3	3.58	120.67	116.65
22	A	2503	2MA	C5-C6-N1	3.53	120.12	114.02
1	a	967	5MC	C5-C4-N4	-3.51	116.23	121.48
22	A	1939	5MU	C5-C6-N1	-3.51	119.73	123.34
22	A	2445	2MG	C5-C6-N1	3.48	120.09	113.95
1	a	1407	5MC	C5-C4-N4	-3.45	116.32	121.48
1	a	966	2MG	C5-C6-N1	3.41	119.97	113.95
22	A	2552	OMU	C5-C4-N3	3.40	119.92	114.84
32	M	81	4D4	NH1-CZ-NE	3.30	126.81	119.19
1	a	1516	2MG	C5-C6-N1	3.29	119.76	113.95
22	A	1835	2MG	C5-C6-N1	3.27	119.72	113.95
22	A	1618	6MZ	C2-N1-C6	3.25	119.38	116.59
1	a	1407	5MC	N1-C2-N3	3.14	124.53	118.81
22	A	2030	6MZ	C1'-N9-C4	-3.13	121.13	126.64
22	A	2580	PSU	C6-N1-C2	-3.13	119.48	122.68
1	a	967	5MC	N1-C2-N3	3.05	124.36	118.81
22	A	2449	H2U	O2-C2-N1	-3.04	119.28	123.11
22	A	1962	5MC	O2-C2-N3	-3.02	117.41	122.33
22	A	2457	PSU	C6-N1-C2	-3.02	119.59	122.68
22	A	2580	PSU	O2-C2-N1	-3.02	119.47	122.79
22	A	1962	5MC	N1-C2-N3	3.02	124.30	118.81
22	A	1915	3TD	C6-C5-C4	3.00	120.30	118.22
22	A	1917	PSU	C6-C5-C4	2.97	120.28	118.20
22	A	2552	OMU	O4-C4-C5	-2.89	120.08	125.16
22	A	955	PSU	C6-C5-C4	2.87	120.20	118.20
22	A	2069	G7M	C2-N1-C6	-2.87	119.82	125.10
22	A	2457	PSU	O2-C2-N1	-2.84	119.67	122.79
22	A	747	5MU	C6-C5-C4	2.82	120.39	118.03
1	a	527	G7M	C2-N1-C6	-2.81	119.92	125.10
22	A	2604	PSU	O2-C2-N1	-2.80	119.71	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	967	5MC	C1'-N1-C2	2.78	124.62	118.42
1	a	1407	5MC	C1'-N1-C2	2.76	124.59	118.42
22	A	2498	OMC	C1'-N1-C2	2.75	124.56	118.42
22	A	1917	PSU	C6-N1-C2	-2.74	119.88	122.68
22	A	955	PSU	C6-N1-C2	-2.74	119.89	122.68
1	a	516	PSU	C6-C5-C4	2.73	120.11	118.20
1	a	967	5MC	O2-C2-N3	-2.72	117.90	122.33
22	A	2605	PSU	C6-C5-C4	2.70	120.08	118.20
22	A	746	PSU	C6-N1-C2	-2.69	119.93	122.68
1	a	1407	5MC	O2-C2-N3	-2.67	117.98	122.33
22	A	1917	PSU	O2-C2-N1	-2.67	119.85	122.79
22	A	1911	PSU	C6-C5-C4	2.66	120.06	118.20
22	A	2504	PSU	C6-C5-C4	2.64	120.04	118.20
22	A	2504	PSU	O2-C2-N1	-2.64	119.89	122.79
22	A	2580	PSU	C6-C5-C4	2.62	120.03	118.20
22	A	745	1MG	C8-N7-C5	2.61	107.96	102.99
22	A	2503	2MA	C8-N7-C5	2.59	107.92	102.99
22	A	2604	PSU	C6-N1-C2	-2.56	120.06	122.68
22	A	2605	PSU	C6-N1-C2	-2.55	120.07	122.68
1	a	967	5MC	C1'-N1-C6	2.54	125.36	121.12
1	a	516	PSU	C6-N1-C2	-2.53	120.09	122.68
22	A	2504	PSU	C6-N1-C2	-2.52	120.11	122.68
1	a	1407	5MC	C1'-N1-C6	2.52	125.31	121.12
22	A	2604	PSU	C6-C5-C4	2.52	119.96	118.20
22	A	1939	5MU	C6-C5-C4	2.51	120.13	118.03
1	a	516	PSU	O2-C2-N1	-2.51	120.03	122.79
22	A	747	5MU	O2-C2-N1	-2.50	119.46	122.79
22	A	955	PSU	O2-C2-N1	-2.49	120.05	122.79
1	a	1516	2MG	O6-C6-C5	-2.49	119.51	124.37
22	A	2445	2MG	CM2-N2-C2	-2.49	118.37	123.86
22	A	1911	PSU	C6-N1-C2	-2.44	120.18	122.68
22	A	2251	OMG	O6-C6-C5	2.36	128.99	124.37
22	A	1911	PSU	O2-C2-N1	-2.36	120.20	122.79
22	A	1939	5MU	O2-C2-N1	-2.35	119.66	122.79
1	a	1402	4OC	C6-C5-C4	2.35	119.84	116.96
22	A	747	5MU	C5M-C5-C6	-2.33	119.73	122.85
32	M	81	4D4	O-C-CA	-2.29	118.78	124.78
1	a	516	PSU	O4'-C1'-C2'	2.29	108.37	105.14
22	A	1835	2MG	O6-C6-C5	-2.28	119.92	124.37
22	A	2445	2MG	O6-C6-C5	-2.27	119.93	124.37
22	A	2605	PSU	O2-C2-N1	-2.26	120.31	122.79
22	A	746	PSU	O2-C2-N1	-2.25	120.32	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	746	PSU	C6-C5-C4	2.24	119.76	118.20
1	a	1516	2MG	CM2-N2-C2	-2.23	118.93	123.86
22	A	2580	PSU	O4'-C1'-C2'	2.22	108.28	105.14
1	a	966	2MG	O6-C6-C5	-2.22	120.04	124.37
22	A	2457	PSU	C6-C5-C4	2.22	119.75	118.20
22	A	1939	5MU	C5M-C5-C6	-2.16	119.96	122.85
22	A	1835	2MG	CM2-N2-C2	-2.15	119.11	123.86
22	A	745	1MG	O6-C6-C5	-2.15	120.38	124.19
32	M	81	4D4	CB-CA-C	-2.10	108.42	111.77
1	a	1498	UR3	C6-N1-C2	-2.02	119.98	121.79
22	A	2552	OMU	O2-C2-N1	-2.02	120.11	122.79
22	A	745	1MG	CM1-N1-C6	2.00	120.29	117.55

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	527	G7M	O4'-C4'-C5'-O5'
1	a	527	G7M	C3'-C4'-C5'-O5'
32	M	81	4D4	NE-CD-CG-CB
22	A	747	5MU	C3'-C4'-C5'-O5'
22	A	747	5MU	O4'-C4'-C5'-O5'
22	A	1618	6MZ	O4'-C4'-C5'-O5'
22	A	1618	6MZ	C3'-C4'-C5'-O5'
22	A	2030	6MZ	O4'-C4'-C5'-O5'
22	A	2251	OMG	O4'-C4'-C5'-O5'
22	A	2251	OMG	C3'-C4'-C5'-O5'
22	A	2251	OMG	C1'-C2'-O2'-CM2
22	A	2498	OMC	O4'-C4'-C5'-O5'
22	A	2552	OMU	C3'-C4'-C5'-O5'
22	A	2552	OMU	O4'-C4'-C5'-O5'
22	A	2605	PSU	C3'-C4'-C5'-O5'
22	A	2605	PSU	O4'-C4'-C5'-O5'
22	A	2069	G7M	O4'-C4'-C5'-O5'
22	A	2069	G7M	C3'-C4'-C5'-O5'
22	A	2030	6MZ	C3'-C4'-C5'-O5'
22	A	2498	OMC	C3'-C4'-C5'-O5'
1	a	1519	MA6	O4'-C4'-C5'-O5'
22	A	1915	3TD	O4'-C4'-C5'-O5'
22	A	2445	2MG	C3'-C4'-C5'-O5'
22	A	1835	2MG	O4'-C4'-C5'-O5'
12	l	89	D2T	CG-CB-SB-CB1

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Mol	Chain	Res	Type	Atoms
22	A	1835	2MG	C3'-C4'-C5'-O5'
1	a	1519	MA6	C3'-C4'-C5'-O5'
32	M	81	4D4	CG-CD-NE-CZ
32	M	81	4D4	OB-CB-CG-CD
22	A	1911	PSU	O4'-C1'-C5-C4
1	a	1402	4OC	O4'-C4'-C5'-O5'
32	M	81	4D4	CA-CB-CG-CD
22	A	1915	3TD	C3'-C4'-C5'-O5'
22	A	2445	2MG	O4'-C4'-C5'-O5'
22	A	2503	2MA	O4'-C4'-C5'-O5'
22	A	746	PSU	O4'-C1'-C5-C6
22	A	1962	5MC	C2'-C1'-N1-C6
32	M	81	4D4	O-C-CA-CB
22	A	1618	6MZ	C4'-C5'-O5'-P
22	A	2503	2MA	C4'-C5'-O5'-P

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 307 ligands modelled in this entry, 294 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
55	PUT	A	3008	-	5,5,5	0.17	0	4,4,4	0.17	0
56	SPD	A	3010	-	9,9,9	0.31	0	8,8,8	0.88	0
55	PUT	A	3002	-	5,5,5	0.15	0	4,4,4	0.15	0
55	PUT	A	3005	-	5,5,5	0.12	0	4,4,4	0.16	0
55	PUT	A	3144	-	5,5,5	0.13	0	4,4,4	0.15	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
55	PUT	A	3003	-	5,5,5	0.10	0	4,4,4	0.17	0
55	PUT	A	3007	-	5,5,5	0.11	0	4,4,4	0.16	0
55	PUT	A	3004	-	5,5,5	0.09	0	4,4,4	0.18	0
56	SPD	A	3009	-	9,9,9	0.33	0	8,8,8	0.91	0
58	GDP	w	802	-	24,30,30	2.48	7 (29%)	30,47,47	1.71	9 (30%)
59	1I7	w	803	-	58,65,65	2.63	22 (37%)	69,92,92	1.42	9 (13%)
55	PUT	A	3006	-	5,5,5	0.14	0	4,4,4	0.16	0
54	ATP	A	3001	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)

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
55	PUT	A	3008	-	-	1/3/3/3	-
56	SPD	A	3010	-	-	2/7/7/7	-
55	PUT	A	3002	-	-	0/3/3/3	-
55	PUT	A	3005	-	-	0/3/3/3	-
55	PUT	A	3144	-	-	0/3/3/3	-
55	PUT	A	3003	-	-	0/3/3/3	-
55	PUT	A	3007	-	-	1/3/3/3	-
55	PUT	A	3004	-	-	1/3/3/3	-
56	SPD	A	3009	-	-	0/7/7/7	-
58	GDP	w	802	-	-	1/12/32/32	0/3/3/3
59	1I7	w	803	-	-	12/58/69/69	0/5/6/6
55	PUT	A	3006	-	-	1/3/3/3	-
54	ATP	A	3001	-	-	2/18/38/38	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	w	802	GDP	O6-C6	8.28	1.40	1.23
59	w	803	1I7	C51-N18	7.19	1.49	1.36
59	w	803	1I7	C27-N10	6.72	1.48	1.34
59	w	803	1I7	C46-N15	6.64	1.48	1.34
59	w	803	1I7	C56-N17	6.61	1.48	1.34
59	w	803	1I7	C30-N14	6.50	1.47	1.33
59	w	803	1I7	C57-N18	5.49	1.49	1.40
59	w	803	1I7	C39-N11	5.48	1.46	1.34
58	w	802	GDP	C2-N2	4.76	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	w	802	GDP	O4'-C1'	3.87	1.46	1.41
59	w	803	1I7	C55-N19	2.67	1.50	1.46
59	w	803	1I7	O07-C51	-2.59	1.18	1.23
58	w	802	GDP	C2'-C1'	-2.58	1.49	1.53
59	w	803	1I7	O08-C56	-2.57	1.18	1.23
59	w	803	1I7	O03-C34	2.56	1.41	1.36
59	w	803	1I7	O06-C46	-2.53	1.18	1.23
59	w	803	1I7	C44-N16	2.43	1.45	1.37
59	w	803	1I7	C23-C25	2.41	1.58	1.51
59	w	803	1I7	C50-S01	-2.31	1.67	1.70
59	w	803	1I7	C42-C36	2.26	1.41	1.36
59	w	803	1I7	O05-C39	-2.21	1.18	1.23
59	w	803	1I7	O02-C27	-2.20	1.19	1.23
58	w	802	GDP	PB-O3B	-2.19	1.46	1.54
58	w	802	GDP	PB-O2B	-2.19	1.46	1.54
59	w	803	1I7	O04-C30	-2.18	1.19	1.23
59	w	803	1I7	O09-C58	-2.18	1.18	1.23
59	w	803	1I7	C55-C56	2.11	1.55	1.52
59	w	803	1I7	C43-C38	2.06	1.41	1.36
58	w	802	GDP	C2'-C3'	-2.01	1.47	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	w	803	1I7	C60-C57-N18	-3.89	117.10	126.07
59	w	803	1I7	C44-C50-S01	3.77	116.42	111.79
58	w	802	GDP	C5-C6-N1	3.45	120.04	113.95
58	w	802	GDP	C3'-C2'-C1'	3.45	106.17	100.98
59	w	803	1I7	C52-O03-C34	-3.27	113.18	117.75
59	w	803	1I7	O03-C34-C26	3.05	120.38	115.89
58	w	802	GDP	PA-O3A-PB	-2.92	122.80	132.83
59	w	803	1I7	O03-C34-C37	-2.90	119.44	124.24
58	w	802	GDP	C2-N1-C6	-2.86	119.83	125.10
58	w	802	GDP	O2B-PB-O3A	2.86	114.22	104.64
58	w	802	GDP	O3B-PB-O3A	2.84	114.15	104.64
59	w	803	1I7	C57-C58-N19	2.83	126.77	120.13
59	w	803	1I7	C54-C48-C49	-2.48	108.08	110.95
59	w	803	1I7	O09-C58-C57	-2.46	114.70	119.16
59	w	803	1I7	C20-C30-N14	2.30	121.19	116.54
54	A	3001	ATP	C5-C6-N6	2.30	123.84	120.35
58	w	802	GDP	C2'-C3'-C4'	2.27	107.06	102.64
58	w	802	GDP	O2A-PA-O1A	-2.15	101.60	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	A	3001	ATP	PB-O3B-PG	2.04	139.83	132.83
58	w	802	GDP	O6-C6-C5	-2.00	120.46	124.37

There are no chirality outliers.

All (21) torsion outliers are listed below:

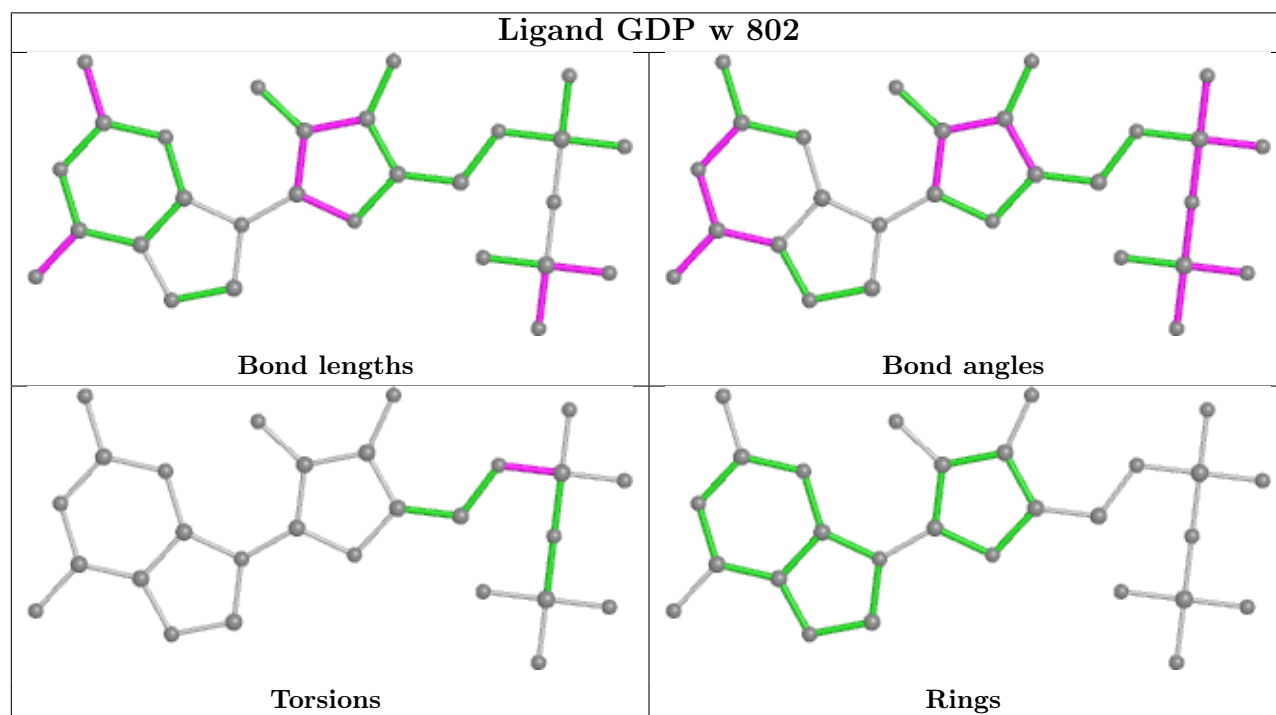
Mol	Chain	Res	Type	Atoms
59	w	803	1I7	C26-C34-O03-C52
59	w	803	1I7	C49-C48-N17-C56
59	w	803	1I7	C56-C55-N19-C58
59	w	803	1I7	C56-C55-N19-C59
59	w	803	1I7	N18-C57-C58-N19
59	w	803	1I7	C58-C57-N18-C51
59	w	803	1I7	C60-C57-N18-C51
59	w	803	1I7	C37-C34-O03-C52
56	A	3010	SPD	N6-C7-C8-C9
55	A	3006	PUT	C1-C2-C3-C4
59	w	803	1I7	N11-C22-C27-O02
55	A	3007	PUT	C1-C2-C3-C4
59	w	803	1I7	N11-C22-C27-N10
59	w	803	1I7	C23-C22-C27-O02
55	A	3004	PUT	N1-C1-C2-C3
55	A	3008	PUT	N1-C1-C2-C3
54	A	3001	ATP	O4'-C4'-C5'-O5'
59	w	803	1I7	C23-C22-C27-N10
56	A	3010	SPD	C2-C3-C4-C5
58	w	802	GDP	C5'-O5'-PA-O1A
54	A	3001	ATP	C3'-C4'-C5'-O5'

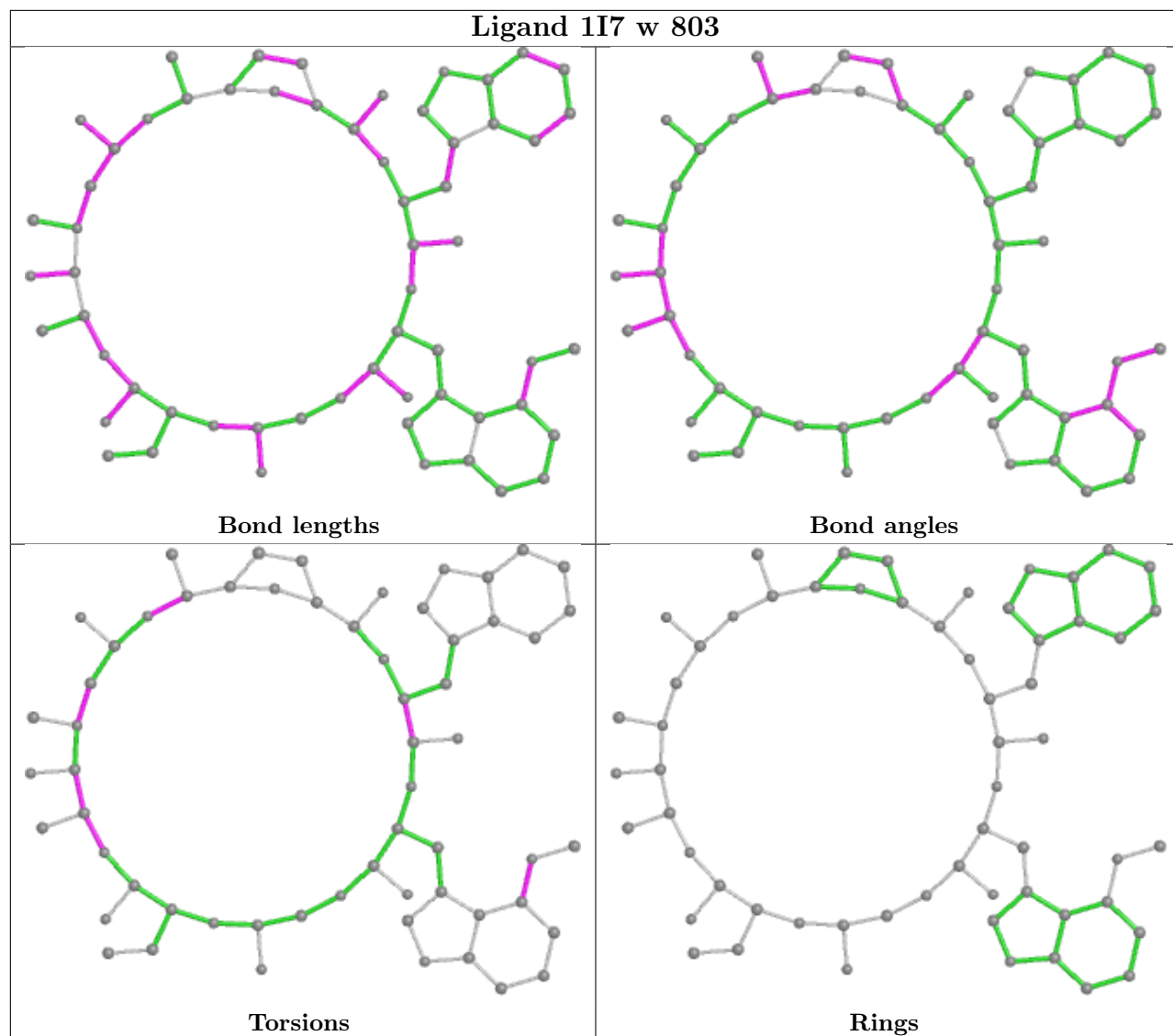
There are no ring outliers.

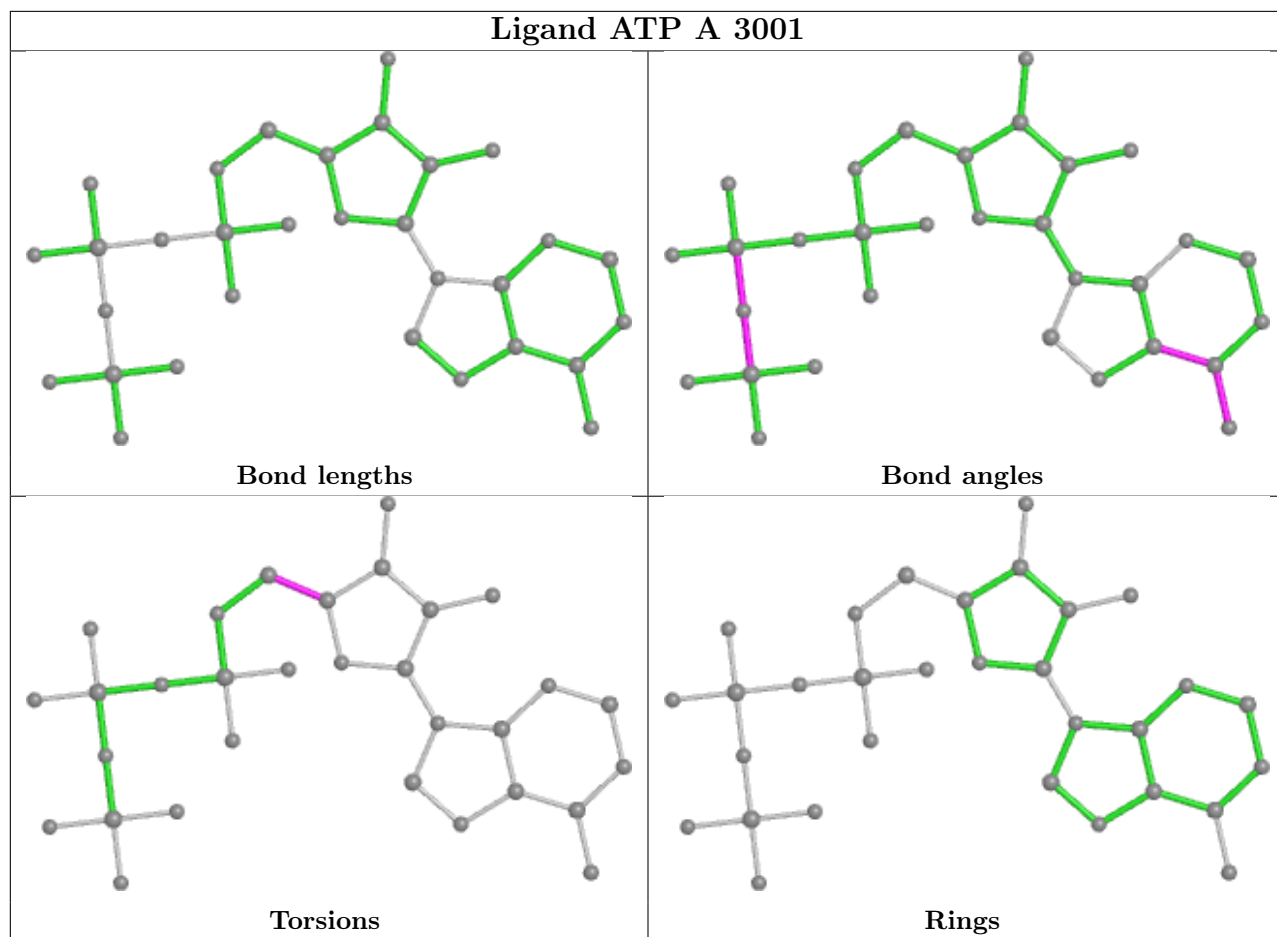
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1618:6MZ	O3'	1619:G	P	4.10

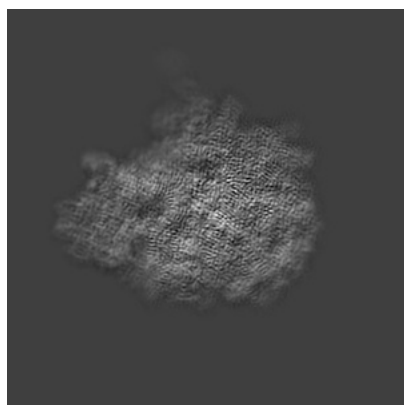
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13058. These allow visual inspection of the internal detail of the map and identification of artifacts.

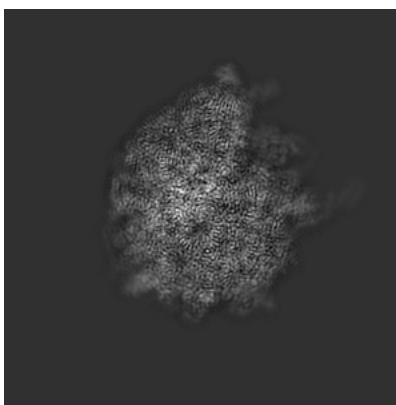
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

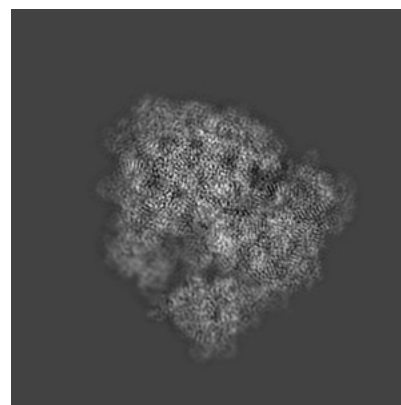
#### 6.1.1 Primary map



X



Y

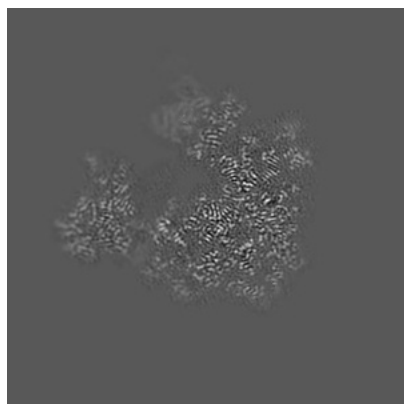


Z

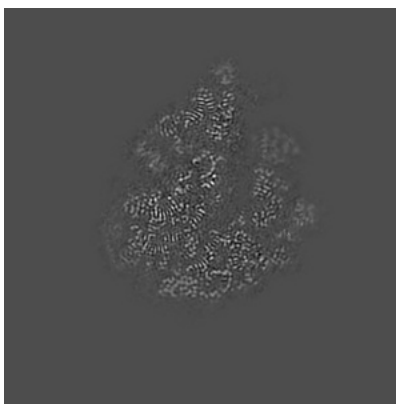
The images above show the map projected in three orthogonal directions.

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

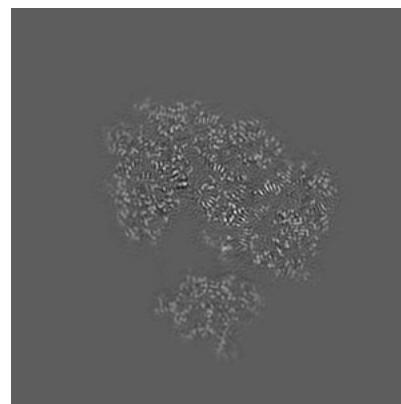
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

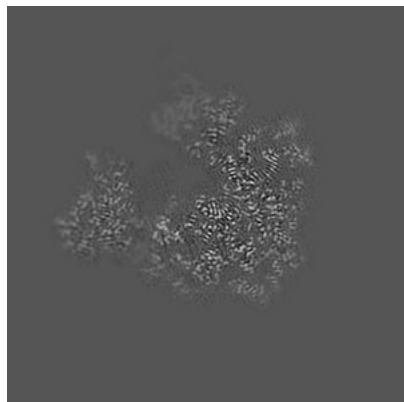


Z Index: 180

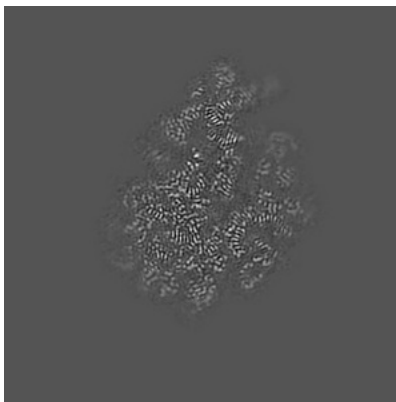
The images above show central slices of the map in three orthogonal directions.

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

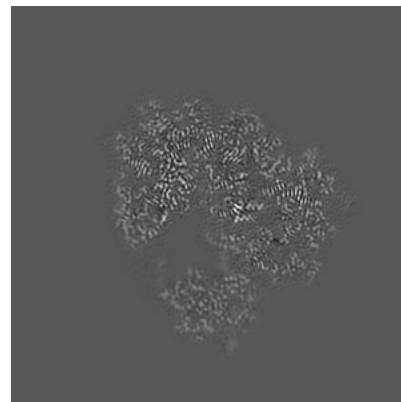
### 6.3.1 Primary map



X Index: 179



Y Index: 187

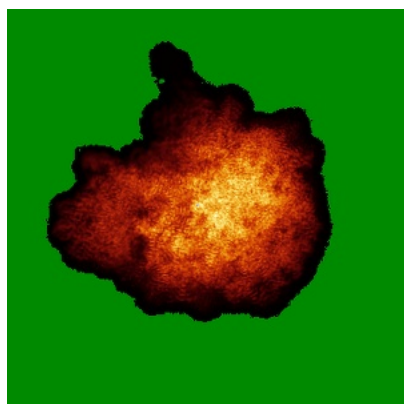


Z Index: 187

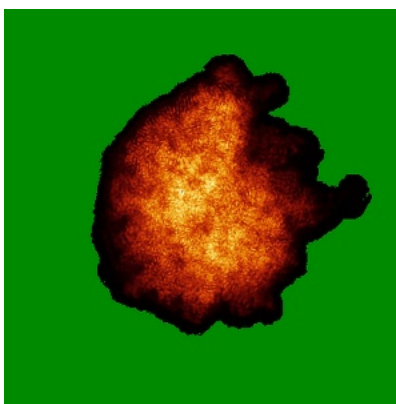
The images above show the largest variance slices of the map in three orthogonal directions.

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

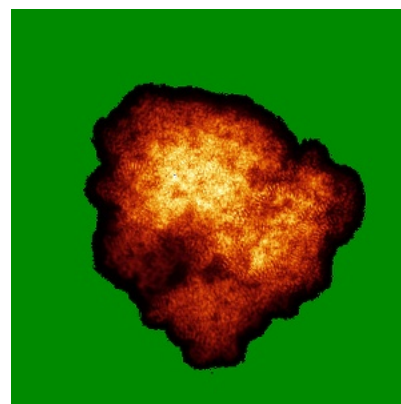
### 6.4.1 Primary map



X



Y



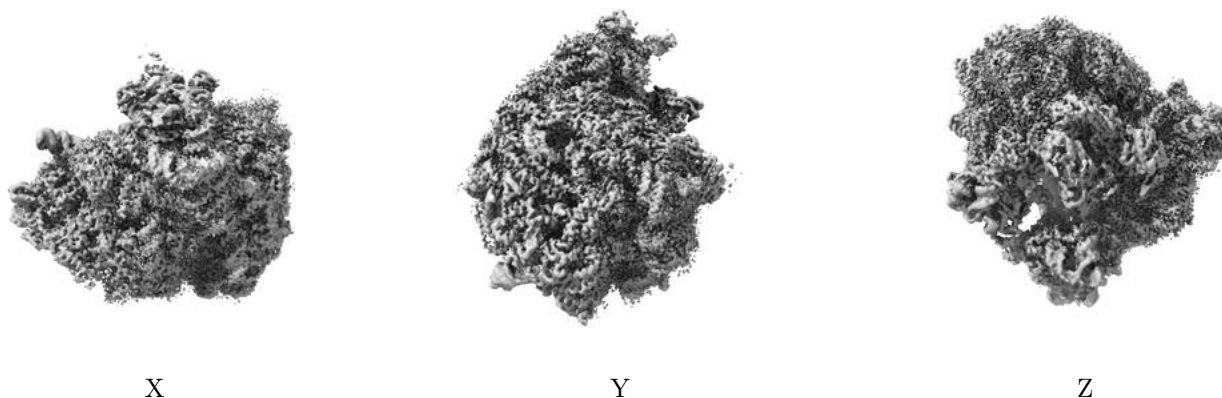
Z

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



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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

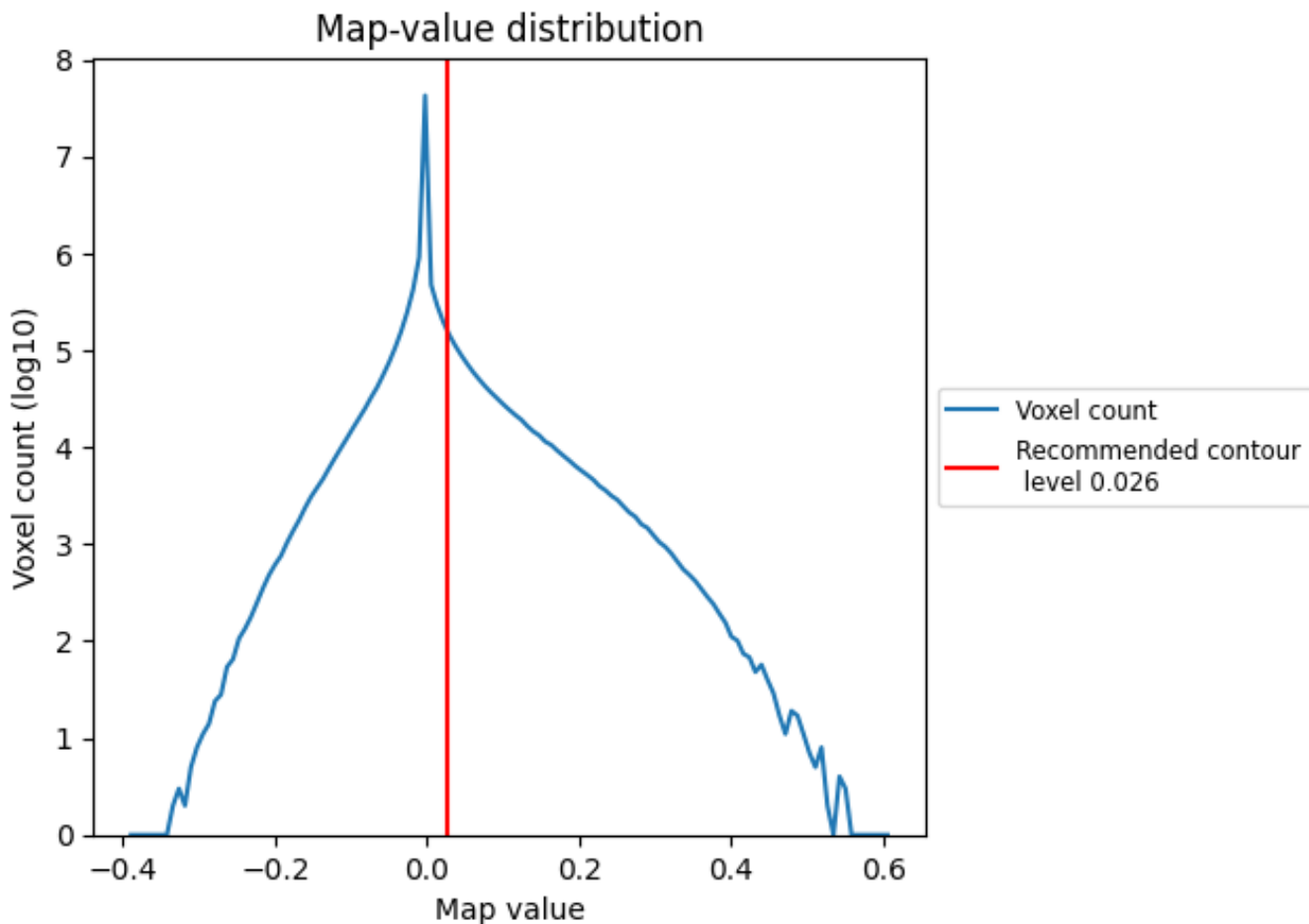
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

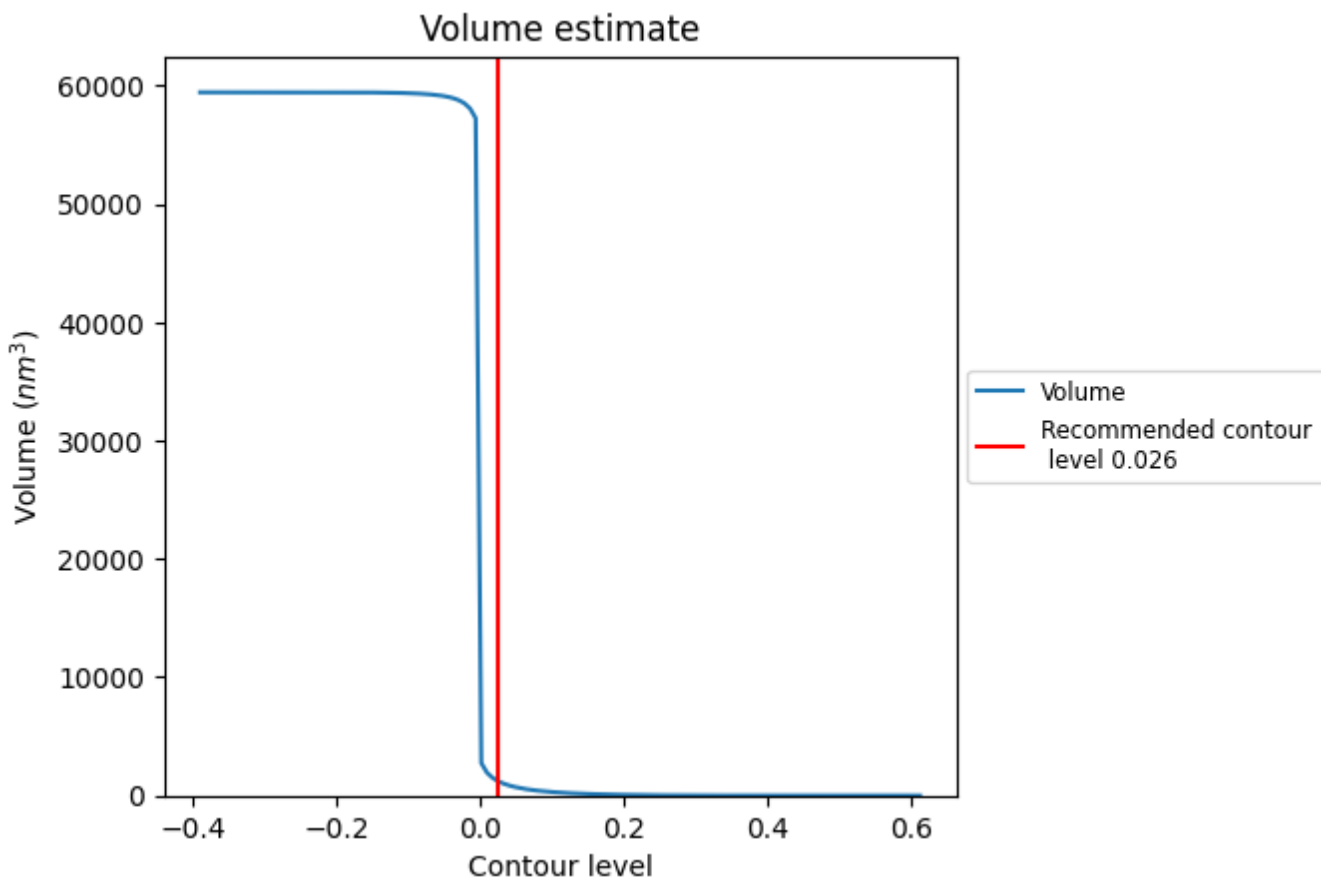
This section contains the results of statistical analysis of the map.

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



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

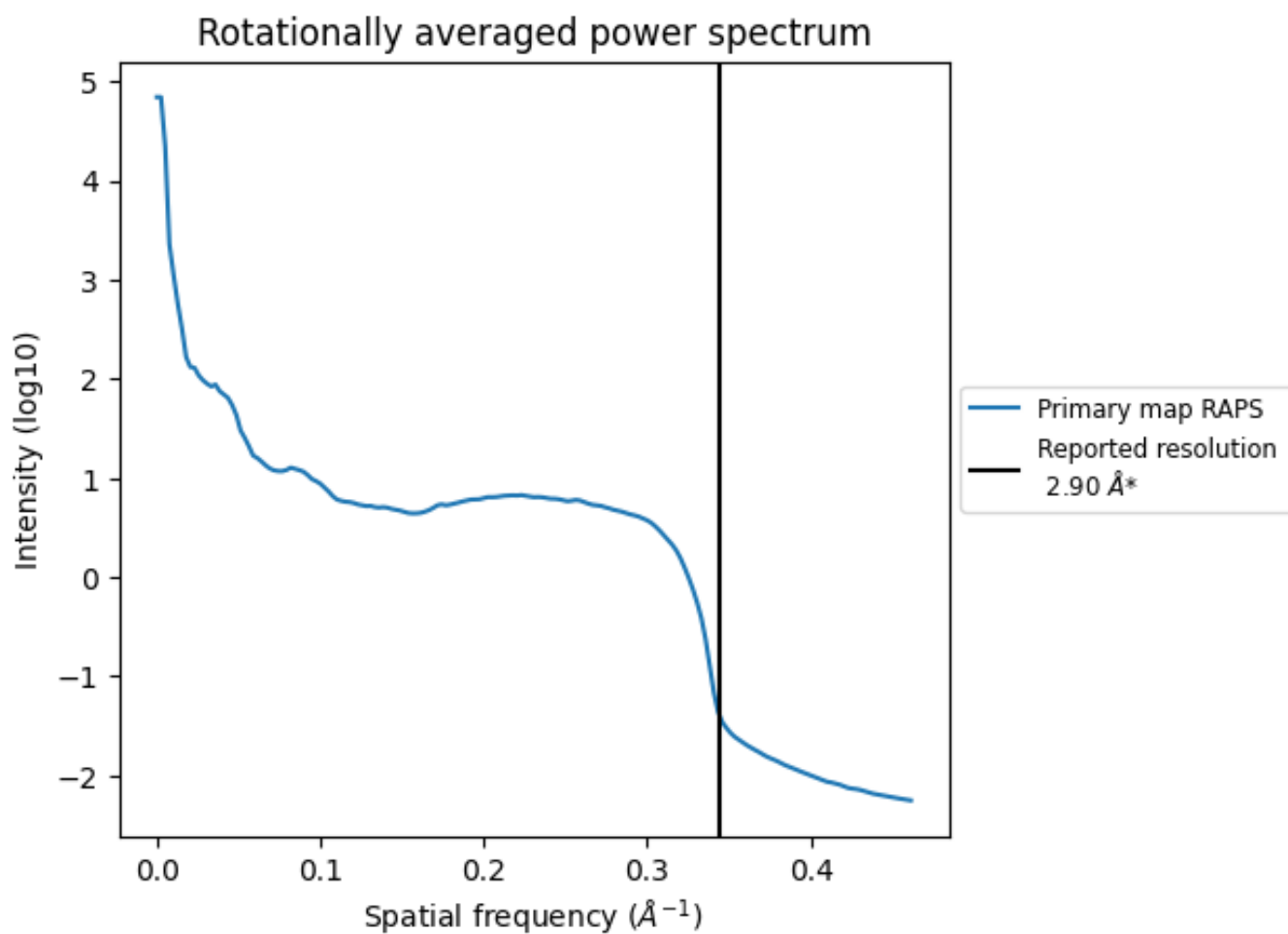
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1206 nm<sup>3</sup>; this corresponds to an approximate mass of 1089 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<sup>-1</sup>

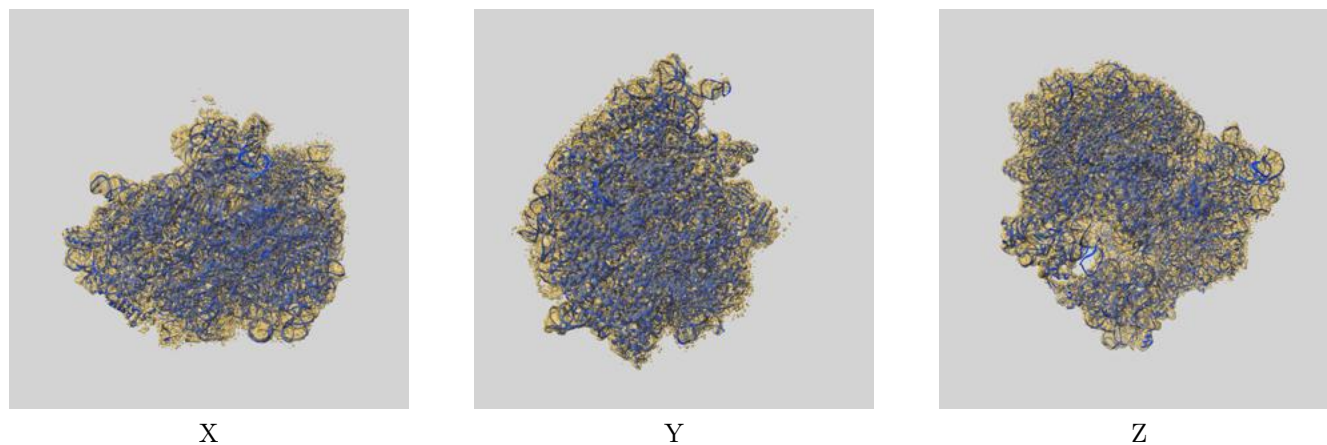
## 8 Fourier-Shell correlation

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

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

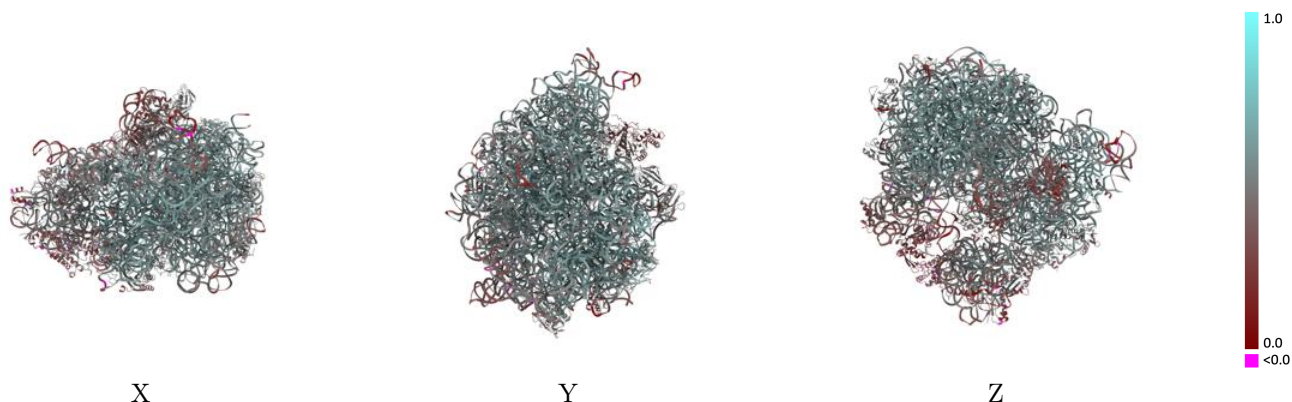
This section contains information regarding the fit between EMDB map EMD-13058 and PDB model 7OTC. Per-residue inclusion information can be found in section 3 on page 17.

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



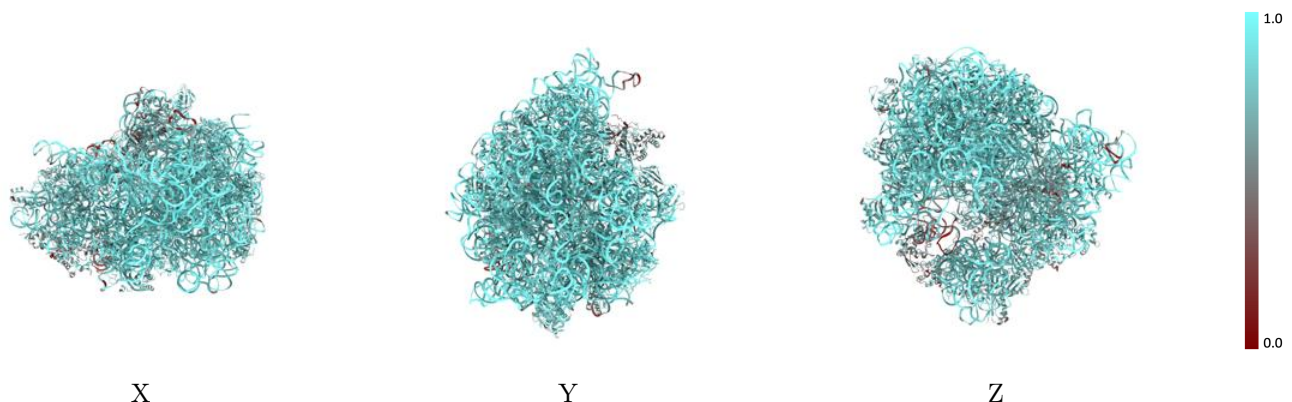
The images above show the 3D surface view of the map at the recommended contour level 0.026 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



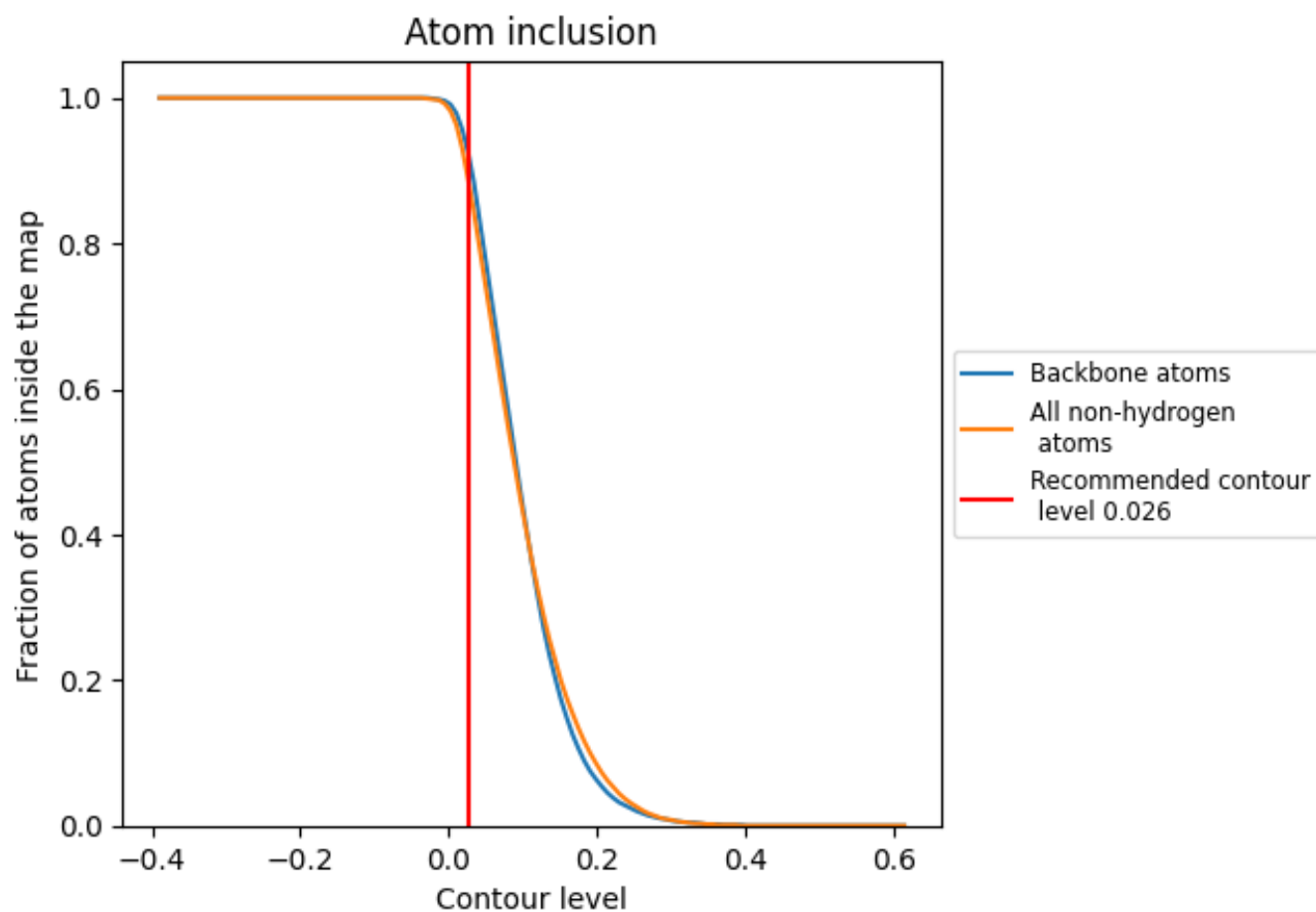
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.026).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 92% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary



































The table lists the average atom inclusion at the recommended contour level (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8880	 0.5040
0	 0.8790	 0.5420
1	 0.8050	 0.4840
2	 0.9350	 0.5890
3	 0.9180	 0.5670
4	 0.8870	 0.5380
5	 0.4260	 0.2120
A	 0.9300	 0.5330
B	 0.9260	 0.4250
C	 0.9450	 0.5780
D	 0.9040	 0.5610
E	 0.8320	 0.5020
F	 0.5880	 0.2800
G	 0.8090	 0.4730
J	 0.9320	 0.5780
K	 0.8940	 0.5630
L	 0.8640	 0.5080
M	 0.8730	 0.5210
N	 0.8940	 0.5420
O	 0.7490	 0.3620
P	 0.8480	 0.5100
Q	 0.9480	 0.5930
R	 0.9170	 0.5610
S	 0.9010	 0.5600
T	 0.7840	 0.4580
U	 0.8170	 0.4600
V	 0.8140	 0.4830
W	 0.7880	 0.5020
X	 0.8650	 0.5310
Y	 0.7300	 0.4010
Z	 0.8490	 0.5380
a	 0.9460	 0.5250
b	 0.6710	 0.3800
c	 0.8140	 0.4470
d	 0.8280	 0.4670



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Chain	Atom inclusion	Q-score
e	 0.8590	 0.4970
f	 0.7420	 0.3890
g	 0.4920	 0.2280
h	 0.8580	 0.5250
i	 0.7850	 0.4000
j	 0.7350	 0.3630
k	 0.8150	 0.4140
l	 0.9090	 0.5340
m	 0.6270	 0.2860
n	 0.8220	 0.4360
o	 0.8810	 0.5020
p	 0.8820	 0.5060
q	 0.8560	 0.4920
r	 0.8200	 0.4580
s	 0.7670	 0.3880
t	 0.8930	 0.5310
u	 0.6010	 0.3710
w	 0.6170	 0.3470