



Full wwPDB EM Validation Report ⓘ

Jun 20, 2026 – 08:40 pm BST

PDB ID : 8R8M / pdb_00008r8m
EMDB ID : EMD-19004
Title : 70S Escherichia coli ribosome with Paenilamicin B2 bound with hybrid A/P- and hybrid P/E-tRNA.
Authors : Koller, T.O.; Wilson, D.N.
Deposited on : 2023-11-29
Resolution : 2.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

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

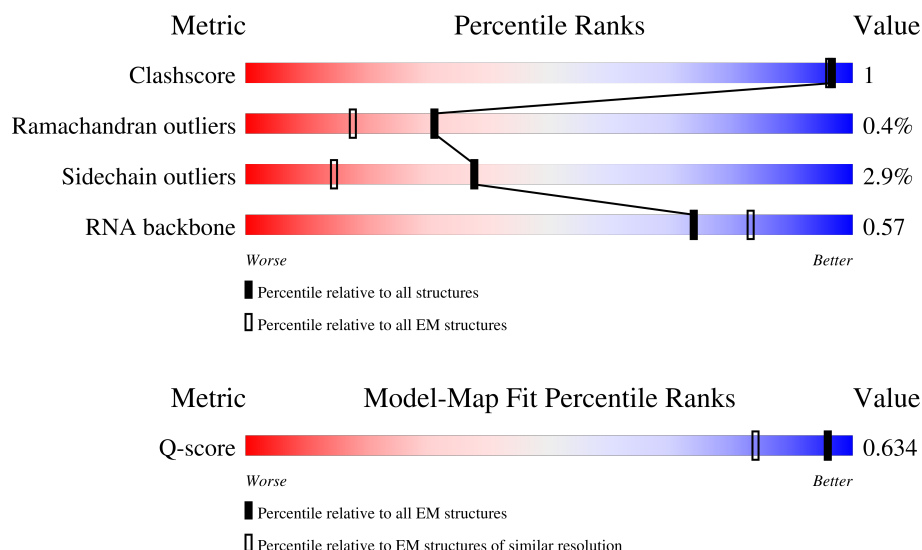
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 Å.

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



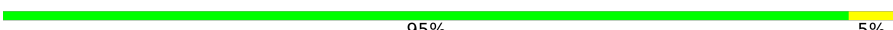
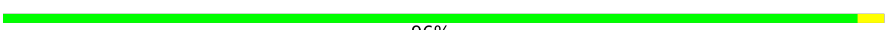
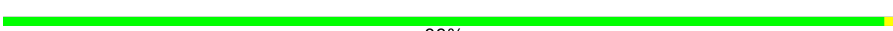
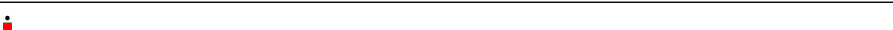
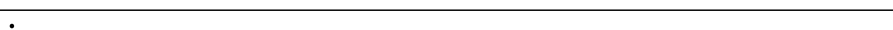
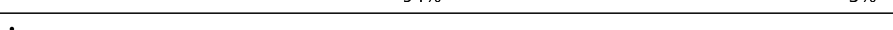
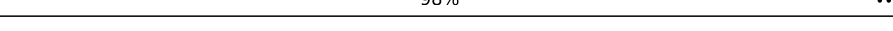
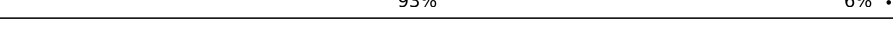
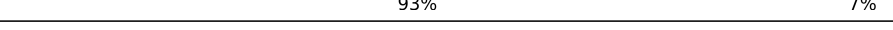
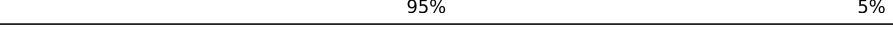
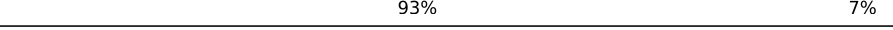
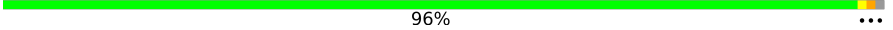
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	0	55	
2	1	46	
3	2	65	

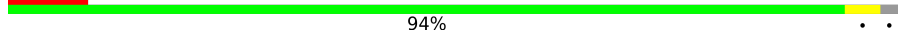
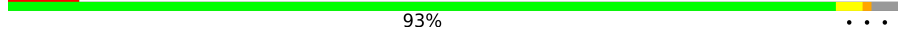
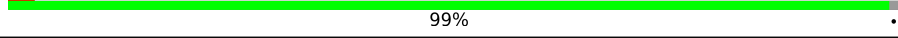
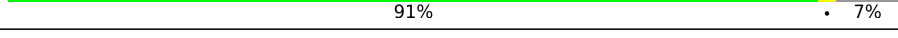
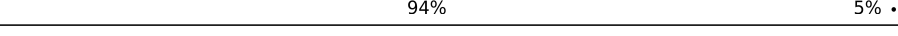
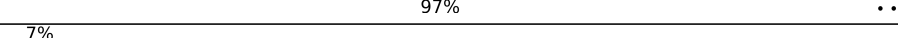
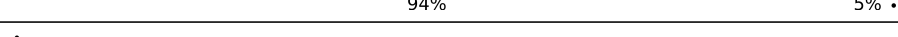
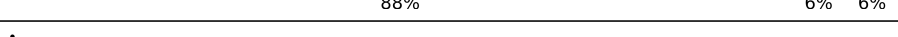
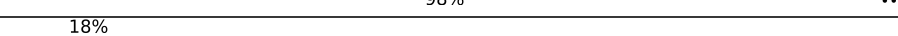
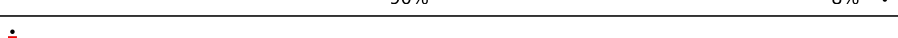
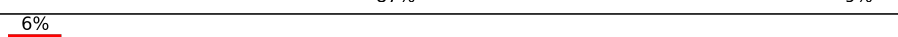
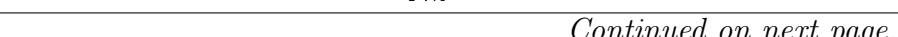
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Mol	Chain	Length	Quality of chain
4	3	38	 89% 11%
5	b	120	 89% 8% ..
6	c	273	 95% 5% .
7	d	209	 96% .
8	e	201	 99% .
9	f	179	 7% 94% ..
10	g	177	 7% 92% 6% ..
11	h	149	 25% . 72%
12	i	142	 92% 8%
13	j	123	 93% 7% .
14	k	144	 97% .
15	l	136	 93% 7%
16	m	127	 90% . 7%
17	n	117	 94% 5% .
18	o	115	 98% ..
19	p	118	 93% 6% .
20	q	103	 93% 7%
21	r	110	 95% 5%
22	s	100	 93% 7%
23	t	104	 90% 8% .
24	u	94	 91% 9%
25	v	85	 87% 5% 8%
26	w	78	 96% ...
27	x	63	 89% 6% ..
28	y	59	 95% ..

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Mol	Chain	Length	Quality of chain
29	z	57	
30	X	10	
31	4	70	
32	a	2903	
33	A	1534	
34	C	233	
35	I	130	
36	J	103	
37	M	118	
38	N	101	
39	S	92	
40	G	179	
41	B	241	
42	D	206	
43	E	167	
44	F	135	
45	H	130	
46	O	89	
47	P	82	
48	Q	84	
49	R	75	
50	T	87	
51	U	71	
52	K	129	
53	L	124	

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Mol	Chain	Length	Quality of chain
54	Z	85	62%19%15%
55	Y	76	28%71%24%
56	5	8	12%75%25%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 141380 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 protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 6 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 8 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 11 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 12 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 13 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 14 is a protein called 50S ribosomal protein L15.

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

- Molecule 15 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	variant	UNP P0ADY7

- Molecule 16 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 17 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 18 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 19 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 20 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 21 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 22 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 23 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	t	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 24 is a protein called 50S ribosomal protein L25.

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

- Molecule 25 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	v	78	Total	C	N	O	S	0	0
			592	365	119	107	1		

- Molecule 26 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 27 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 28 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 29 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 30 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	10	Total	C	N	O	P	0	0
			212	95	35	72	10		

- Molecule 31 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	48	Total	C	N	O	S	0	0
			373	232	66	69	6		

- Molecule 32 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	2738	Total	C	N	O	P	0	0
			58815	26243	10844	18990	2738		

- Molecule 33 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	A	1519	Total	C	N	O	P	0	0
			32608	14548	5986	10555	1519		

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

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

- Molecule 35 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 36 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 37 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 38 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 39 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 41 is a protein called 30S ribosomal protein S2.

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

- Molecule 42 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 43 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 44 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 45 is a protein called Small ribosomal subunit protein uS8.

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

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

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

- Molecule 47 is a protein called 30S ribosomal protein S16.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 50 is a protein called 30S ribosomal protein S20.

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

- Molecule 51 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 52 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	variant	UNP P0A7R9

- Molecule 53 is a protein called Small ribosomal subunit protein uS12.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
54	Z	72	Total	C	N	O	P	S	0	0
			1547	693	281	500	72	1		

- Molecule 55 is a RNA chain called Isoleucine-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	Y	73	Total	C	N	O	P		0	0
			1564	700	283	509	72			

- Molecule 56 is a protein called Paenilamicin B2.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	5	8	Total	C	N	O	0	0
			71	42	16	13		

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

Mol	Chain	Residues	Atoms		AltConf
57	3	1	Total	Zn	0
			1	1	
57	4	1	Total	Zn	0
			1	1	

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	b	5	Total	Mg	0
			5	5	
58	c	1	Total	Mg	0
			1	1	
58	d	1	Total	Mg	0
			1	1	
58	p	1	Total	Mg	0
			1	1	
58	z	1	Total	Mg	0
			1	1	
58	a	207	Total	Mg	0
			207	207	
58	A	91	Total	Mg	0
			91	91	

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
59	d	1	Total 1	K 1	0
59	5	1	Total 1	K 1	0

- Molecule 60 is water.

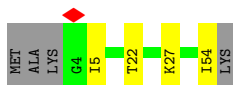
Mol	Chain	Residues	Atoms		AltConf
60	X	3	Total 3	O 3	0
60	a	1	Total 1	O 1	0
60	A	19	Total 19	O 19	0
60	C	1	Total 1	O 1	0
60	Z	2	Total 2	O 2	0
60	5	10	Total 10	O 10	0

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: Large ribosomal subunit protein bL33

Chain 0: 



- Molecule 2: Large ribosomal subunit protein bL34

Chain 1: 



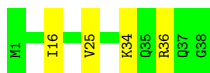
- Molecule 3: Large ribosomal subunit protein bL35

Chain 2: 



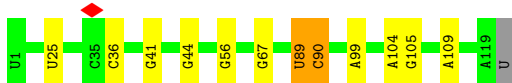
- Molecule 4: Large ribosomal subunit protein bL36A

Chain 3: 



- Molecule 5: 5S ribosomal RNA

Chain b: 

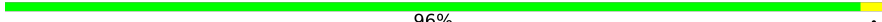


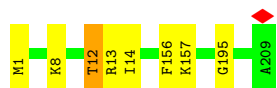
- Molecule 6: Large ribosomal subunit protein uL2

Chain c:  95% 5% .

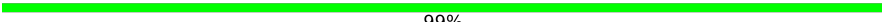


- Molecule 7: Large ribosomal subunit protein uL3

Chain d:  96% .



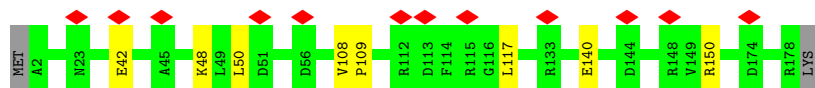
- Molecule 8: Large ribosomal subunit protein uL4

Chain e:  99% .



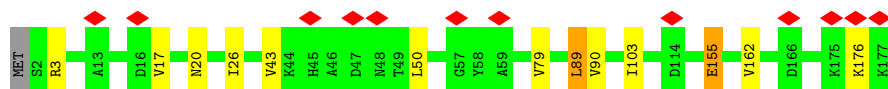
- Molecule 9: Large ribosomal subunit protein uL5

Chain f:  7% 94% . .



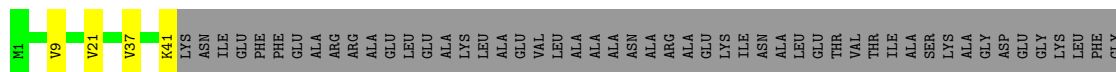
- Molecule 10: Large ribosomal subunit protein uL6

Chain g:  7% 92% 6% ..



- Molecule 11: Large ribosomal subunit protein bL9

Chain h:  25% 72%



- Molecule 12: Large ribosomal subunit protein uL13

Chain i:  92% 8%



- Molecule 13: Large ribosomal subunit protein uL14

Chain j: 93% 7% .



- Molecule 14: 50S ribosomal protein L15

Chain k: 97% .



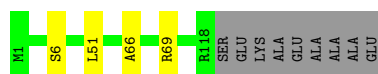
- Molecule 15: Large ribosomal subunit protein uL16

Chain l: 93% 7%



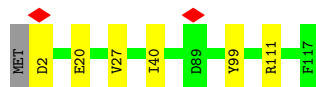
- Molecule 16: Large ribosomal subunit protein bL17

Chain m: 90% 7%



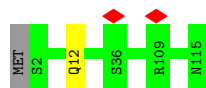
- Molecule 17: Large ribosomal subunit protein uL18

Chain n: 94% 5% .



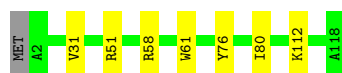
- Molecule 18: Large ribosomal subunit protein bL19

Chain o: 98% ..



- Molecule 19: Large ribosomal subunit protein bL20

Chain p: 93% 6% .



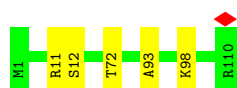
- Molecule 20: Large ribosomal subunit protein bL21

Chain q: 93% 7%



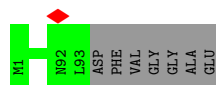
- Molecule 21: Large ribosomal subunit protein uL22

Chain r: 95% 5%



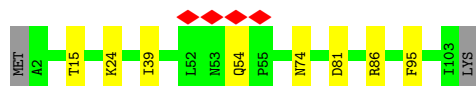
- Molecule 22: Large ribosomal subunit protein uL23

Chain s: 93% 7%



- Molecule 23: Large ribosomal subunit protein uL24

Chain t: 90% 8% .



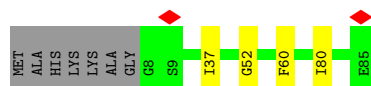
- Molecule 24: 50S ribosomal protein L25

Chain u: 91% 9%

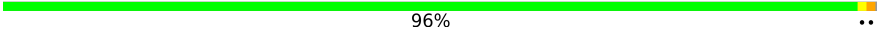


- Molecule 25: Large ribosomal subunit protein bL27

Chain v: 87% 5% 8%



- Molecule 26: Large ribosomal subunit protein bL28

Chain w:  96% ...

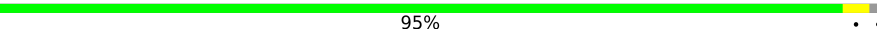


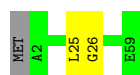
- Molecule 27: Large ribosomal subunit protein uL29

Chain x:  89% 6% ..



- Molecule 28: Large ribosomal subunit protein uL30

Chain y:  95% ..



- Molecule 29: Large ribosomal subunit protein bL32

Chain z:  91% 7% .



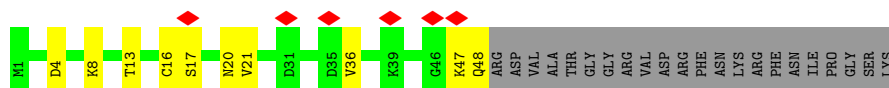
- Molecule 30: mRNA

Chain X:  90% 10%



- Molecule 31: Large ribosomal subunit protein bL31A

Chain 4:  9% 54% 14% 31%

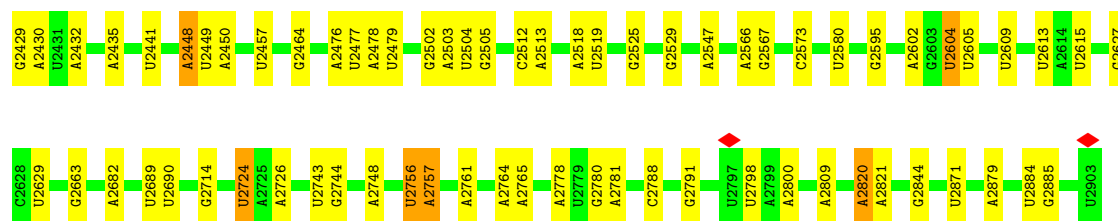


- Molecule 32: 23S ribosomal RNA

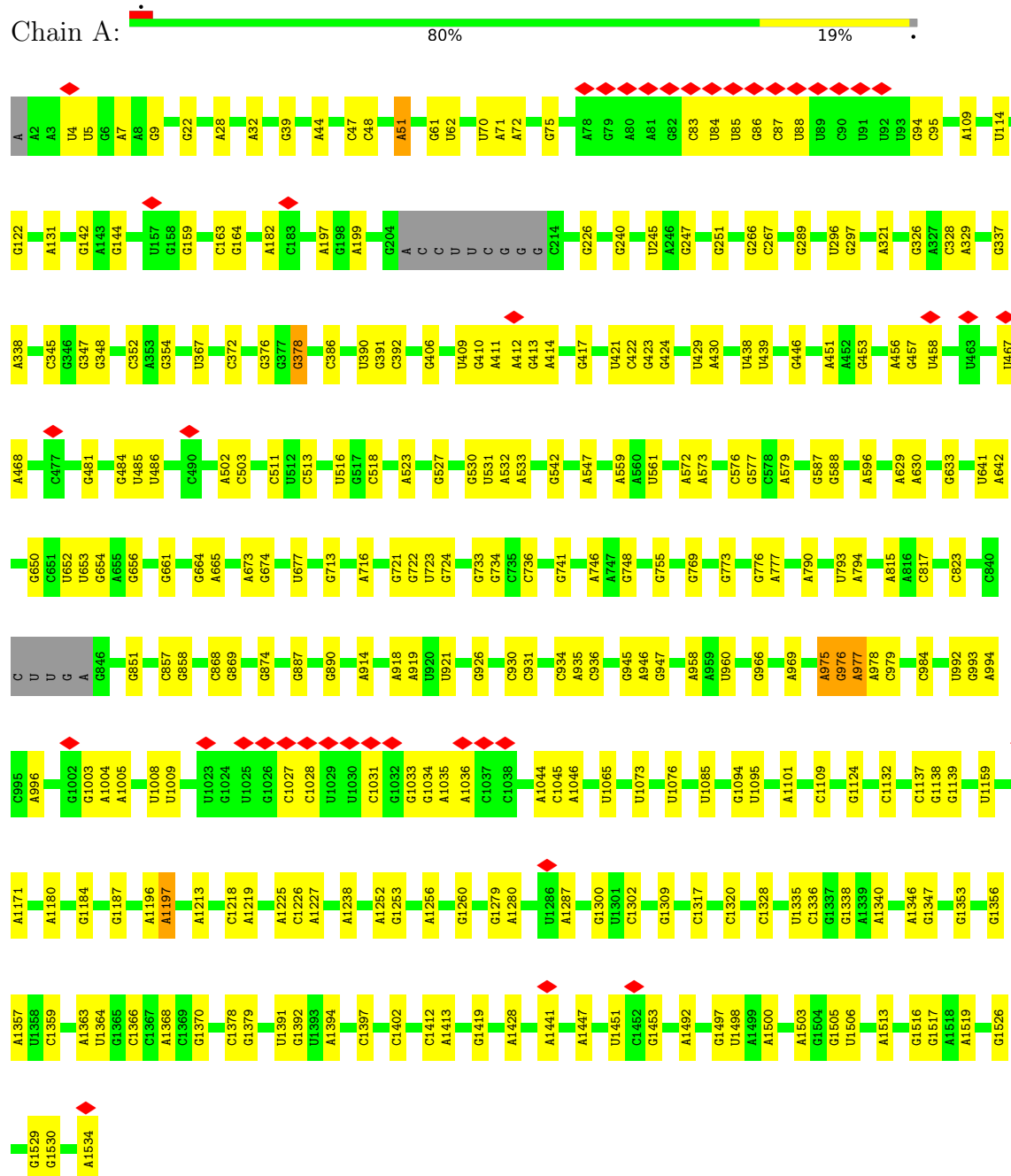
Chain a:  77% 16% • 6%



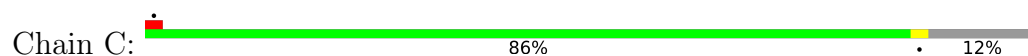


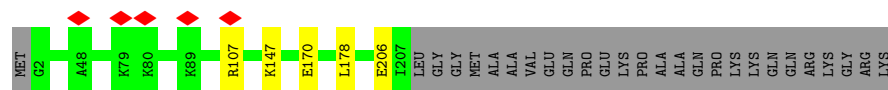


• Molecule 33: 16S ribosomal RNA

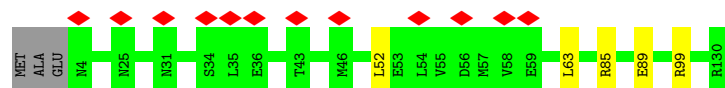
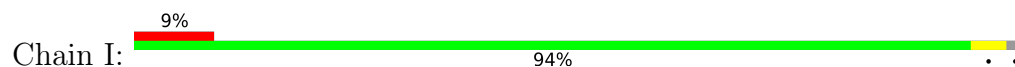


• Molecule 34: Small ribosomal subunit protein uS3

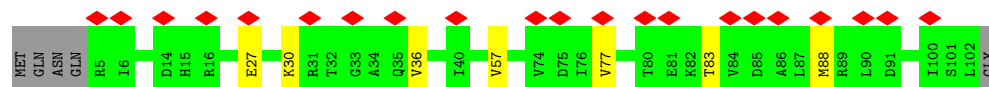
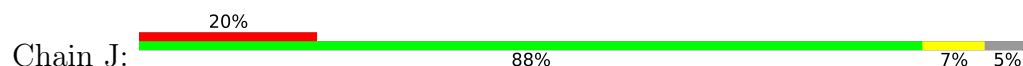




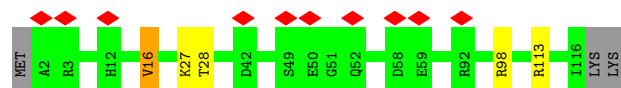
- Molecule 35: Small ribosomal subunit protein uS9



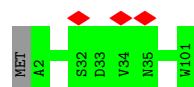
- Molecule 36: Small ribosomal subunit protein uS10



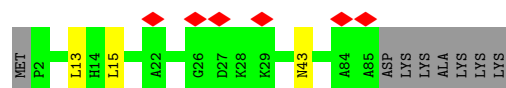
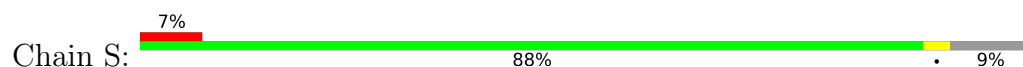
- Molecule 37: Small ribosomal subunit protein uS13



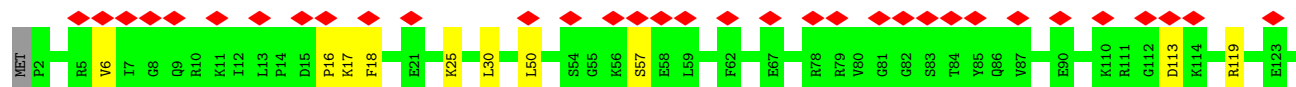
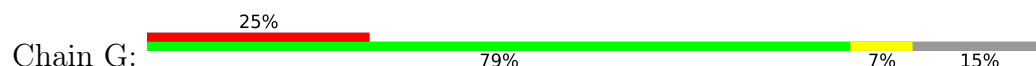
- Molecule 38: Small ribosomal subunit protein uS14

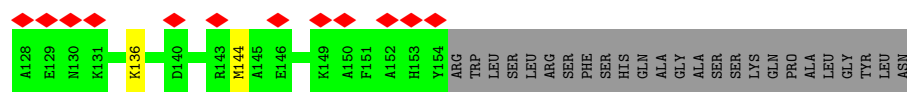


- Molecule 39: Small ribosomal subunit protein uS19

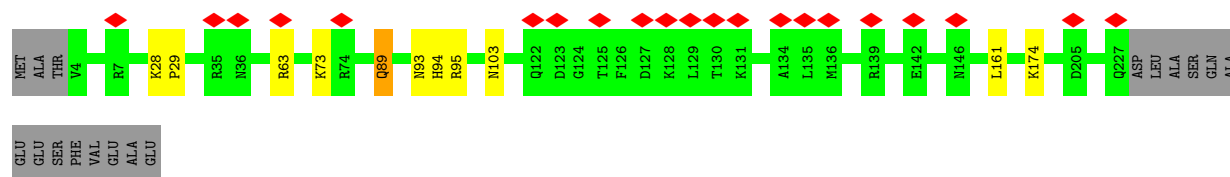
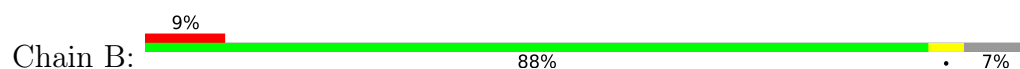


- Molecule 40: 30S ribosomal protein S7

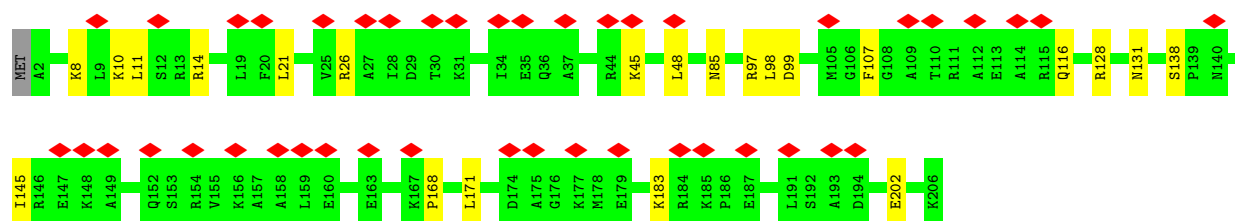
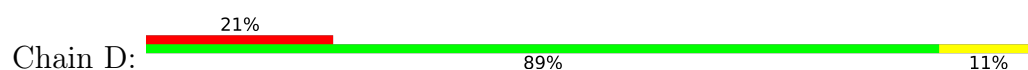




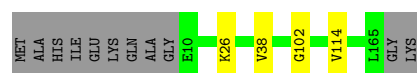
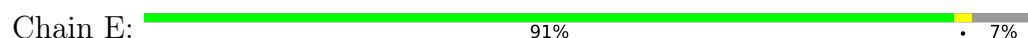
- Molecule 41: 30S ribosomal protein S2



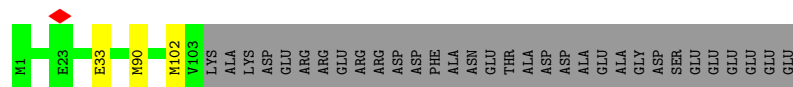
- Molecule 42: Small ribosomal subunit protein uS4



- Molecule 43: Small ribosomal subunit protein uS5



- Molecule 44: 30S ribosomal protein S6, fully modified isoform



- Molecule 45: Small ribosomal subunit protein uS8

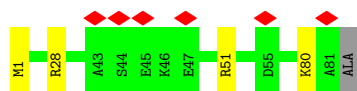
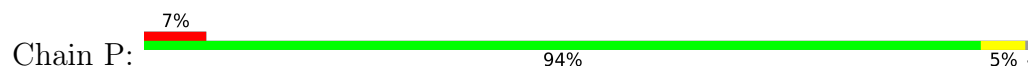


- Molecule 46: Small ribosomal subunit protein uS15

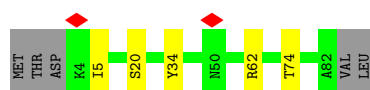
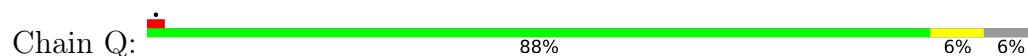




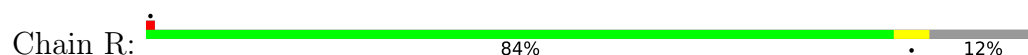
- Molecule 47: 30S ribosomal protein S16



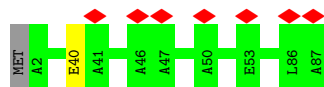
- Molecule 48: Small ribosomal subunit protein uS17



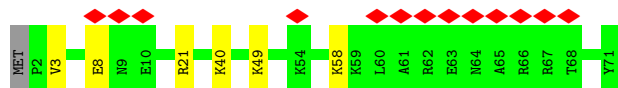
- Molecule 49: Small ribosomal subunit protein bS18



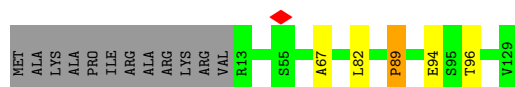
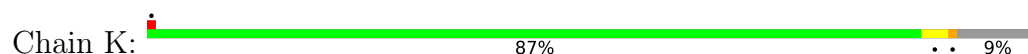
- Molecule 50: 30S ribosomal protein S20



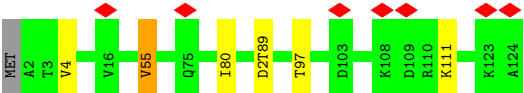
- Molecule 51: Small ribosomal subunit protein bS21



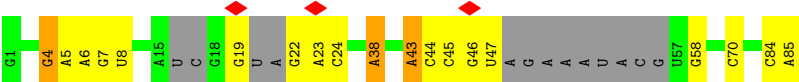
- Molecule 52: Small ribosomal subunit protein uS11



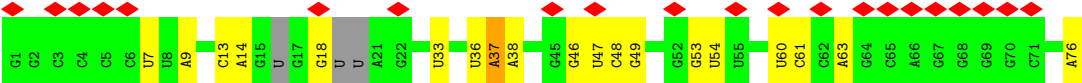
- Molecule 53: Small ribosomal subunit protein uS12



• Molecule 54: Leucine-tRNA



• Molecule 55: Isoleucine-tRNA



• Molecule 56: Paenilamicin B2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13681	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.122	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0055	Depositor
Map size (Å)	480.0, 480.0, 480.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8, 0.8, 0.8	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ORD, MG, OMG, H2U, K, YF5, PSU, 4OC, 5MC, MEQ, 5MU, G7M, D2T, OMU, 2MA, OMC, DAL, 2MG, IAS, ZN, MS6, MKX, 4D4, YFZ, SPD, 6MZ, 1MG, MIA, UR3, 3TD, YFQ

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	0	0.56	0/424	0.87	0/565
2	1	0.67	0/380	0.88	0/498
3	2	0.67	0/513	0.95	0/676
4	3	0.61	0/303	0.81	0/397
5	b	0.52	0/2850	0.88	1/4444 (0.0%)
6	c	0.63	0/2121	0.88	0/2852
7	d	0.60	0/1576	0.84	0/2119
8	e	0.59	0/1571	0.90	0/2113
9	f	0.54	0/1434	0.93	0/1926
10	g	0.54	0/1343	0.92	1/1816 (0.1%)
11	h	0.56	0/306	0.95	0/413
12	i	0.57	0/1152	0.85	0/1551
13	j	0.56	0/955	0.88	0/1279
14	k	0.61	0/1062	0.86	0/1413
15	l	0.55	0/1073	0.84	0/1433
16	m	0.62	0/958	0.93	0/1281
17	n	0.54	0/902	0.89	0/1209
18	o	0.59	0/929	0.83	0/1242
19	p	0.64	0/960	0.91	0/1278
20	q	0.57	0/829	0.82	0/1107
21	r	0.61	0/864	0.87	0/1156
22	s	0.55	0/744	0.82	0/994
23	t	0.56	0/787	0.85	0/1051
24	u	0.54	0/766	0.85	0/1025
25	v	0.61	0/599	0.80	0/792
26	w	0.62	0/635	0.90	0/848
27	x	0.49	0/502	0.97	0/667
28	y	0.57	0/453	0.85	0/605
29	z	0.65	0/450	0.89	0/599
30	X	0.52	0/236	0.79	0/365
31	4	0.57	0/380	0.89	0/508

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	a	0.51	0/65299	0.93	91/101863 (0.1%)
33	A	0.52	0/36287	0.87	19/56602 (0.0%)
34	C	0.53	0/1651	0.87	0/2225
35	I	0.56	0/1034	0.93	0/1375
36	J	0.57	0/796	0.88	0/1077
37	M	0.57	0/900	0.95	1/1204 (0.1%)
38	N	0.54	0/817	0.93	0/1088
39	S	0.55	0/685	0.86	0/922
40	G	0.56	0/1219	0.95	0/1635
41	B	0.55	0/1784	0.94	0/2403
42	D	0.55	0/1665	0.99	0/2227
43	E	0.53	0/1165	0.90	0/1568
44	F	0.53	0/858	0.87	0/1160
45	H	0.53	0/989	0.86	0/1326
46	O	0.52	0/722	0.94	0/964
47	P	0.53	0/653	0.89	0/877
48	Q	0.52	0/650	0.78	0/871
49	R	0.53	0/553	0.93	0/742
50	T	0.54	0/676	1.05	0/895
51	U	0.53	0/597	0.96	0/792
52	K	0.56	0/884	0.85	1/1191 (0.1%)
53	L	0.55	0/960	0.81	0/1286
54	Z	0.56	0/1693	0.89	2/2628 (0.1%)
55	Y	0.60	0/1711	0.82	0/2659
56	5	0.53	0/3	1.01	0/2
All	All	0.53	0/152308	0.90	116/227804 (0.1%)

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
32	a	0	5
52	K	0	1
56	5	0	1
All	All	0	7

There are no bond length outliers.

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	204	A	O3'-P-O5'	-7.96	92.06	104.00
32	a	1565	C	O3'-P-O5'	-7.88	92.18	104.00
32	a	542	C	O3'-P-O5'	-7.71	92.44	104.00
32	a	543	G	O3'-P-O5'	-7.54	92.69	104.00
32	a	1246	A	O3'-P-O5'	-7.51	92.73	104.00
32	a	1025	G	O3'-P-O5'	7.37	115.05	104.00
32	a	1648	U	O3'-P-O5'	-7.20	93.19	104.00
32	a	781	A	O3'-P-O5'	-7.18	93.23	104.00
32	a	2050	C	O3'-P-O5'	-7.13	93.31	104.00
32	a	310	A	O3'-P-O5'	-7.07	93.40	104.00
32	a	1293	C	O3'-P-O5'	-6.94	93.58	104.00
32	a	528	A	O3'-P-O5'	-6.91	93.63	104.00
33	A	561	U	O3'-P-O5'	-6.86	93.72	104.00
32	a	1969	A	O3'-P-O5'	-6.85	93.72	104.00
32	a	2222	C	O3'-P-O5'	-6.84	93.74	104.00
33	A	746	A	O3'-P-O5'	-6.73	93.91	104.00
32	a	1643	G	O3'-P-O5'	-6.72	93.92	104.00
32	a	2382	G	O3'-P-O5'	-6.51	94.24	104.00
52	K	89	PRO	N-CA-CB	-6.51	96.42	103.25
32	a	1025	G	C2'-C3'-O3'	6.50	119.25	109.50
32	a	2761	A	O3'-P-O5'	-6.49	94.26	104.00
32	a	2094	A	O3'-P-O5'	-6.33	94.50	104.00
32	a	503	A	O3'-P-O5'	-6.26	94.60	104.00
32	a	1971	U	C4'-C3'-O3'	-6.24	103.63	113.00
10	g	155	GLU	CB-CA-C	6.24	118.15	108.61
54	Z	4	G	O3'-P-O5'	-6.24	94.65	104.00
32	a	1328	A	O3'-P-O5'	-6.23	94.66	104.00
33	A	921	U	O3'-P-O5'	-6.20	94.69	104.00
32	a	1373	A	O3'-P-O5'	-6.20	94.70	104.00
32	a	2820	A	C2'-C3'-O3'	6.17	118.75	109.50
32	a	9	G	O3'-P-O5'	-6.12	94.82	104.00
32	a	1757	A	C4'-C3'-O3'	-6.08	103.88	113.00
33	A	1279	G	O3'-P-O5'	-6.05	94.92	104.00
32	a	667	U	O3'-P-O5'	-6.02	94.98	104.00
32	a	2479	U	O3'-P-O5'	-5.94	95.10	104.00
32	a	2203	U	O3'-P-O5'	-5.89	95.16	104.00
32	a	456	C	O3'-P-O5'	-5.89	95.16	104.00
32	a	1133	A	O3'-P-O5'	-5.86	95.21	104.00
32	a	2879	A	O3'-P-O5'	-5.86	95.22	104.00
33	A	1197	A	O3'-P-O5'	-5.85	95.22	104.00
5	b	90	C	O3'-P-O5'	-5.85	95.22	104.00
32	a	1187	G	C4'-C3'-O3'	-5.84	104.24	113.00
32	a	701	G	O3'-P-O5'	-5.80	95.30	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	A	930	C	O3'-P-O5'	-5.79	95.32	104.00
32	a	1650	A	O3'-P-O5'	-5.78	95.34	104.00
32	a	62	U	O3'-P-O5'	-5.77	95.35	104.00
32	a	134	G	O3'-P-O5'	-5.76	95.35	104.00
33	A	1359	C	O3'-P-O5'	-5.74	95.40	104.00
32	a	1408	G	O3'-P-O5'	-5.73	95.41	104.00
32	a	1922	G	O3'-P-O5'	-5.69	95.47	104.00
32	a	1468	U	O3'-P-O5'	-5.68	95.48	104.00
32	a	2724	U	C4'-C3'-O3'	-5.66	104.51	113.00
32	a	995	C	O3'-P-O5'	-5.62	95.57	104.00
32	a	388	G	O3'-P-O5'	-5.59	95.61	104.00
32	a	1131	G	O3'-P-O5'	-5.56	95.65	104.00
32	a	385	C	O3'-P-O5'	-5.56	95.66	104.00
32	a	1452	G	O3'-P-O5'	-5.54	95.70	104.00
32	a	1606	C	C2'-C3'-O3'	-5.54	105.40	113.70
32	a	1359	A	O3'-P-O5'	-5.53	95.71	104.00
33	A	1347	G	O3'-P-O5'	-5.53	95.71	104.00
32	a	2278	A	O3'-P-O5'	-5.52	95.72	104.00
33	A	976	G	O3'-P-O5'	-5.51	95.73	104.00
32	a	2238	G	O3'-P-O5'	-5.51	95.73	104.00
33	A	790	A	O3'-P-O5'	-5.51	95.73	104.00
32	a	621	A	O3'-P-O5'	-5.51	95.74	104.00
32	a	855	G	O3'-P-O5'	-5.49	95.76	104.00
32	a	2048	G	O3'-P-O5'	-5.47	95.79	104.00
32	a	1606	C	O3'-P-O5'	-5.47	95.79	104.00
32	a	2871	U	O3'-P-O5'	-5.46	95.80	104.00
32	a	2519	U	O3'-P-O5'	-5.46	95.81	104.00
32	a	2279	G	O3'-P-O5'	-5.44	95.84	104.00
33	A	652	U	O3'-P-O5'	-5.42	95.87	104.00
32	a	1378	A	O3'-P-O5'	-5.40	95.89	104.00
33	A	1394	A	O3'-P-O5'	-5.40	95.90	104.00
32	a	1025	G	C4'-C3'-O3'	-5.39	101.31	109.40
32	a	1923	U	O3'-P-O5'	-5.39	95.91	104.00
32	a	1254	A	C4'-C3'-O3'	-5.39	104.91	113.00
32	a	1436	G	O3'-P-O5'	-5.38	95.93	104.00
32	a	726	G	O3'-P-O5'	-5.38	95.94	104.00
32	a	731	C	O3'-P-O5'	-5.37	95.94	104.00
37	M	16	VAL	N-CA-CB	5.36	116.82	110.55
32	a	2820	A	C4'-C3'-O3'	-5.35	101.38	109.40
32	a	784	G	C2'-C3'-O3'	-5.33	105.70	113.70
32	a	1416	G	O3'-P-O5'	-5.33	96.01	104.00
32	a	404	A	C2'-C3'-O3'	5.30	117.45	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	2764	A	O3'-P-O5'	-5.30	96.06	104.00
33	A	523	A	O3'-P-O5'	-5.29	96.07	104.00
32	a	1135	C	C4'-C3'-O3'	-5.27	105.09	113.00
33	A	297	G	O3'-P-O5'	-5.27	96.09	104.00
32	a	2049	G	O3'-P-O5'	-5.25	96.13	104.00
32	a	376	G	O3'-P-O5'	-5.24	96.14	104.00
32	a	1857	G	O3'-P-O5'	-5.24	96.15	104.00
32	a	2477	U	O3'-P-O5'	-5.22	96.17	104.00
32	a	1377	G	O3'-P-O5'	-5.22	96.18	104.00
32	a	1818	U	O3'-P-O5'	-5.21	96.18	104.00
32	a	73	A	O3'-P-O5'	-5.20	96.21	104.00
32	a	684	G	O3'-P-O5'	-5.18	96.23	104.00
32	a	747	5MU	O3'-P-O5'	-5.18	96.23	104.00
32	a	1974	C	O3'-P-O5'	-5.16	96.26	104.00
33	A	716	A	O3'-P-O5'	-5.14	96.29	104.00
33	A	773	G	O3'-P-O5'	-5.13	96.30	104.00
33	A	1428	A	O3'-P-O5'	-5.12	96.32	104.00
32	a	1467	U	O3'-P-O5'	-5.12	96.32	104.00
32	a	1151	A	O3'-P-O5'	-5.11	96.34	104.00
32	a	2756	U	C4'-C3'-O3'	5.09	117.03	109.40
32	a	1781	U	O3'-P-O5'	-5.05	96.42	104.00
32	a	1016	G	O3'-P-O5'	-5.05	96.43	104.00
32	a	189	G	O3'-P-O5'	-5.04	96.44	104.00
32	a	2001	C	O3'-P-O5'	-5.03	96.45	104.00
33	A	931	C	O3'-P-O5'	-5.03	96.46	104.00
32	a	1409	U	O3'-P-O5'	-5.02	96.47	104.00
32	a	254	G	O3'-P-O5'	-5.01	96.48	104.00
32	a	1810	A	O3'-P-O5'	-5.01	96.49	104.00
32	a	2844	G	O3'-P-O5'	-5.01	96.49	104.00
33	A	378	G	O3'-P-O5'	-5.01	96.49	104.00
54	Z	43	A	O3'-P-O5'	-5.00	96.50	104.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
56	5	4	ORD	Peptide
52	K	82	LEU	Peptide
32	a	249	C	Sidechain
32	a	2595	G	Sidechain
32	a	463	G	Sidechain
32	a	512	G	Sidechain

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Mol	Chain	Res	Type	Group
32	a	980	A	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	417	0	451	1	0
2	1	377	0	418	3	0
3	2	504	0	572	2	0
4	3	302	0	340	2	0
5	b	2549	0	1291	3	0
6	c	2082	0	2154	5	0
7	d	1566	0	1617	4	0
8	e	1552	0	1619	1	0
9	f	1410	0	1444	1	0
10	g	1323	0	1371	4	0
11	h	303	0	327	0	0
12	i	1129	0	1162	7	0
13	j	946	0	1023	4	0
14	k	1053	0	1129	2	0
15	l	1075	0	1145	5	0
16	m	945	0	989	1	0
17	n	892	0	923	2	0
18	o	917	0	962	1	0
19	p	947	0	1019	4	0
20	q	816	0	839	3	0
21	r	857	0	922	2	0
22	s	738	0	807	0	0
23	t	779	0	831	1	0
24	u	753	0	780	3	0
25	v	592	0	607	2	0
26	w	625	0	652	1	0
27	x	501	0	531	1	0
28	y	449	0	488	2	0
29	z	444	0	458	3	0
30	X	212	0	106	0	0
31	4	373	0	370	2	0
32	a	58815	0	29607	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	A	32608	0	16424	37	0
34	C	1624	0	1696	0	0
35	I	1022	0	1070	2	0
36	J	786	0	828	0	0
37	M	891	0	952	2	0
38	N	805	0	844	0	0
39	S	668	0	693	0	0
40	G	1203	0	1254	1	0
41	B	1753	0	1780	5	0
42	D	1643	0	1707	6	0
43	E	1152	0	1196	3	0
44	F	839	0	833	2	0
45	H	979	0	1031	1	0
46	O	714	0	734	1	0
47	P	643	0	661	1	0
48	Q	641	0	682	2	0
49	R	544	0	565	3	0
50	T	670	0	719	0	0
51	U	589	0	629	1	0
52	K	877	0	884	1	0
53	L	957	0	1017	3	0
54	Z	1547	0	794	1	0
55	Y	1564	0	783	3	0
56	5	71	0	35	1	0
57	3	1	0	0	0	0
57	4	1	0	0	0	0
58	A	91	0	0	0	0
58	a	207	0	0	0	0
58	b	5	0	0	0	0
58	c	1	0	0	0	0
58	d	1	0	0	0	0
58	p	1	0	0	0	0
58	z	1	0	0	0	0
59	5	1	0	0	0	0
59	d	1	0	0	0	0
60	5	10	0	0	0	0
60	A	19	0	0	0	0
60	C	1	0	0	0	0
60	X	3	0	0	0	0
60	Z	2	0	0	0	0
60	a	1	0	0	0	0
All	All	141380	0	94765	192	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (192) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:568:U:H1'	32:a:2030:6MZ:H9C1	1.69	0.72
41:B:89:GLN:HE21	41:B:89:GLN:HA	1.54	0.72
32:a:12:U:H2'	32:a:12:U:O2	1.98	0.64
15:l:66:ARG:NH1	15:l:104:GLU:OE2	2.29	0.64
16:m:66:ALA:O	16:m:69:ARG:O	2.16	0.64
33:A:823:C:HO2'	45:H:2:SER:N	2.00	0.59
4:3:16:ILE:HD13	4:3:25:VAL:HG22	1.85	0.59
32:a:1913:A:N1	55:Y:37:MKX:O2'	2.35	0.58
12:i:58:ASN:HD21	12:i:128:ASN:HD22	1.52	0.57
35:I:52:LEU:HD11	35:I:63:LEU:HD11	1.88	0.54
42:D:85:ASN:HD22	43:E:102:GLY:HA3	1.73	0.54
3:2:54:ASP:HB3	14:k:57:LEU:HD22	1.90	0.54
14:k:21:ARG:HA	32:a:811:U:H2'	1.90	0.54
48:Q:34:TYR:HB3	53:L:4:VAL:HG23	1.88	0.53
32:a:717:C:C4	32:a:718:A:H1'	2.44	0.53
32:a:1182:G:H2'	32:a:1183:U:O4'	2.09	0.53
33:A:664:G:H22	33:A:741:G:H1	1.56	0.52
33:A:769:G:H4'	33:A:1513:A:H4'	1.90	0.52
44:F:90:MET:HE1	49:R:23:TYR:CE1	2.45	0.52
29:z:9:THR:CG2	32:a:2020:A:H5'	2.40	0.51
31:4:16:CYS:SG	31:4:17:SER:N	2.84	0.51
27:x:6:LEU:HB3	27:x:56:LEU:HD13	1.92	0.50
33:A:977:A:O2'	33:A:979:C:OP2	2.21	0.50
53:L:55:VAL:HG11	53:L:80:ILE:HD11	1.93	0.50
12:i:125:TYR:OH	12:i:132:HIS:NE2	2.44	0.50
33:A:1076:U:OP1	41:B:174:LYS:NZ	2.41	0.50
7:d:14:ILE:HA	18:o:12:GLN:HE22	1.75	0.50
33:A:1402:4OC:O2	33:A:1500:A:N1	2.44	0.50
32:a:84:A:N1	32:a:98:G:O2'	2.44	0.49
6:c:79:GLU:OE2	6:c:101:ARG:NE	2.44	0.49
10:g:17:VAL:HG11	10:g:50:LEU:HD21	1.95	0.49
32:a:160:A:N3	32:a:2208:C:O2'	2.40	0.49
32:a:395:U:O2'	32:a:396:G:N7	2.40	0.49
32:a:2038:G:H2'	32:a:2039:U:O4'	2.13	0.49
53:L:80:ILE:HD13	53:L:97:THR:HG22	1.94	0.49
33:A:1218:C:H2'	33:A:1219:A:C8	2.47	0.48
33:A:1526:G:N7	51:U:40:LYS:NZ	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:D:97:ARG:O	42:D:99:ASP:N	2.46	0.48
33:A:378:G:C2	33:A:386:C:O2	2.66	0.48
15:l:96:ILE:HG21	15:l:126:ILE:HD12	1.95	0.48
23:t:86:ARG:HG3	23:t:95:PHE:CD1	2.48	0.48
32:a:2273:A:H2'	32:a:2274:A:C8	2.49	0.48
12:i:9:GLU:HG2	12:i:10:THR:HG23	1.96	0.47
32:a:788:A:OP1	32:a:790:U:H5	1.97	0.47
17:n:99:TYR:OH	17:n:111:ARG:NH2	2.47	0.47
33:A:1252:A:H2'	33:A:1253:G:O4'	2.13	0.47
32:a:644:A:H2'	32:a:645:C:O4'	2.14	0.47
33:A:736:C:OP1	49:R:61:ARG:NH1	2.47	0.47
15:l:20:LEU:HD13	24:u:81:PRO:HG3	1.97	0.47
32:a:1434:A:H2'	32:a:1435:G:C8	2.50	0.47
33:A:51:A:N7	33:A:114:U:O2'	2.47	0.47
13:j:67:LYS:NZ	32:a:1664:A:N3	2.63	0.47
19:p:76:TYR:CZ	19:p:80:ILE:HG13	2.50	0.47
28:y:25:LEU:HD11	32:a:930:G:H1'	1.97	0.47
40:G:113:ASP:HB2	40:G:119:ARG:HG2	1.97	0.46
25:v:37:ILE:HG21	25:v:80:ILE:HG21	1.97	0.46
32:a:1020:A:C2	32:a:1141:U:C2	3.02	0.46
33:A:673:A:H2'	33:A:674:G:C8	2.50	0.46
33:A:677:U:H3	33:A:713:G:H22	1.63	0.46
32:a:1939:5MU:OP1	32:a:2604:PSU:O2'	2.30	0.46
55:Y:38:A:N3	56:5:5:YFZ:OH	2.48	0.46
32:a:614:A:H3'	32:a:615:U:C5'	2.46	0.46
7:d:156:PHE:CE1	12:i:81:ILE:HD13	2.51	0.46
13:j:1:MET:HE3	13:j:32:TYR:CZ	2.50	0.46
32:a:493:G:H2'	32:a:494:G:O4'	2.17	0.45
5:b:104:A:H2'	5:b:105:G:O4'	2.17	0.45
32:a:58:G:O2'	32:a:73:A:N1	2.49	0.45
10:g:89:LEU:N	10:g:89:LEU:HD23	2.31	0.45
24:u:47:VAL:HA	24:u:50:MET:HE3	1.98	0.45
20:q:14:VAL:HG11	20:q:20:VAL:HG21	1.98	0.45
32:a:645:C:H2'	32:a:647:G:C8	2.52	0.45
33:A:28:A:O2'	33:A:296:U:OP1	2.23	0.45
17:n:27:VAL:HG21	17:n:40:ILE:HD12	1.98	0.45
2:l:12:ARG:NH1	32:a:465:G:OP1	2.49	0.45
10:g:89:LEU:HD22	10:g:162:VAL:HG22	1.98	0.45
6:c:242:LYS:O	32:a:1902:C:H4'	2.17	0.45
20:q:5:PHE:HB3	20:q:59:ILE:HD12	1.98	0.45
32:a:2328:A:H2'	32:a:2329:U:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:D:107:PHE:HB3	42:D:145:ILE:HD11	1.99	0.45
32:a:570:G:H2'	32:a:2030:6MZ:N7	2.32	0.44
15:l:36:VAL:HG21	15:l:129:THR:HG23	1.99	0.44
33:A:411:A:P	42:D:26:ARG:HH12	2.40	0.44
33:A:975:A:N1	33:A:1366:C:O2'	2.43	0.44
32:a:36:G:N3	32:a:450:G:O2'	2.51	0.44
8:e:162:ARG:NH1	32:a:340:A:O2'	2.50	0.44
32:a:460:A:H2'	32:a:461:C:O4'	2.17	0.44
33:A:1180:A:P	35:I:99:ARG:HH12	2.40	0.44
19:p:51:ARG:NH2	32:a:993:G:OP2	2.48	0.44
33:A:502:A:H2'	33:A:503:C:O4'	2.18	0.44
21:r:93:ALA:HB2	32:a:1614:A:C2	2.53	0.44
26:w:16:ASN:ND2	32:a:381:G:OP1	2.36	0.44
42:D:85:ASN:HD22	43:E:102:GLY:CA	2.31	0.44
19:p:31:VAL:HG13	32:a:580:U:O3'	2.18	0.43
33:A:390:U:O2'	47:P:28:ARG:NH2	2.50	0.43
33:A:1356:G:H2'	33:A:1357:A:C8	2.53	0.43
1:0:22:THR:HG21	32:a:2419:U:H4'	2.00	0.43
5:b:89:U:O2	5:b:89:U:O4'	2.35	0.43
13:j:58:LEU:HD23	13:j:58:LEU:N	2.34	0.43
25:v:52:GLY:HA3	25:v:60:PHE:CZ	2.52	0.43
32:a:945:A:C4	32:a:2448:A:C2	3.06	0.43
32:a:1720:U:H2'	32:a:1721:G:O4'	2.19	0.43
32:a:2063:C:O2	32:a:2450:A:N1	2.51	0.43
33:A:109:A:H2'	33:A:326:G:N2	2.33	0.43
33:A:945:G:C2	33:A:946:A:C8	3.06	0.43
13:j:43:ILE:HD12	13:j:56:ASP:HB2	2.01	0.43
20:q:74:ILE:N	20:q:74:ILE:HD12	2.34	0.43
29:z:43:ILE:HG22	29:z:49:TYR:HB2	2.00	0.43
32:a:340:A:H2'	32:a:341:C:O4'	2.18	0.43
32:a:1778:U:H2'	32:a:1784:A:N6	2.34	0.43
32:a:2395:C:H2'	32:a:2396:G:O4'	2.19	0.43
48:Q:5:ILE:HD11	48:Q:62:ARG:HD3	1.99	0.43
12:i:125:TYR:HH	12:i:132:HIS:HE2	1.62	0.43
32:a:476:G:H4'	32:a:502:A:N1	2.33	0.43
32:a:2432:A:H1'	54:Z:84:C:O4'	2.18	0.43
33:A:1391:U:H2'	33:A:1392:G:C8	2.54	0.43
32:a:627:A:N1	32:a:636:G:O2'	2.50	0.43
21:r:11:ARG:NH2	21:r:98:LYS:HE3	2.34	0.43
32:a:586:A:N1	32:a:809:G:O2'	2.51	0.43
32:a:1021:A:N3	32:a:1021:A:H3'	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:Y:33:U:N3	55:Y:36:U:OP2	2.43	0.43
29:z:4:GLN:HA	32:a:2615:U:C2	2.54	0.42
32:a:861:A:C2	32:a:917:A:C4	3.06	0.42
33:A:337:G:H2'	33:A:338:A:C8	2.54	0.42
12:i:114:LEU:HG	12:i:118:MET:HE3	1.99	0.42
32:a:247:G:H4'	32:a:386:G:C5	2.53	0.42
32:a:1421:G:C2	32:a:1422:G:C8	3.07	0.42
4:3:34:LYS:NZ	32:a:2743:U:OP1	2.50	0.42
28:y:26:GLY:O	32:a:929:U:H1'	2.18	0.42
32:a:723:C:H2'	32:a:724:U:O4'	2.19	0.42
2:1:39:ARG:NH2	32:a:468:G:N7	2.56	0.42
32:a:2756:U:H1'	32:a:2757:A:H5''	2.02	0.42
32:a:716:A:N6	32:a:717:C:C4	2.87	0.42
32:a:1028:A:N6	32:a:1125:G:H2'	2.35	0.42
32:a:2331:G:O2'	32:a:2336:A:N1	2.44	0.42
41:B:94:HIS:O	41:B:95:ARG:C	2.62	0.42
46:O:25:THR:HG21	46:O:70:LEU:HB2	2.02	0.42
32:a:603:A:N1	32:a:625:G:O2'	2.51	0.42
33:A:946:A:H2'	33:A:947:G:C8	2.55	0.42
33:A:1073:U:O2'	41:B:103:ASN:ND2	2.52	0.42
33:A:1516:2MG:HM21	33:A:1519:A:N7	2.34	0.42
6:c:107:PRO:HD2	6:c:110:LEU:HD22	2.02	0.42
12:i:120:ARG:HD3	32:a:2780:G:OP2	2.20	0.42
33:A:1309:G:N7	37:M:98:ARG:NH2	2.68	0.42
43:E:38:VAL:HG11	43:E:114:VAL:HG22	2.02	0.42
6:c:31:ALA:N	6:c:32:PRO:CD	2.83	0.42
32:a:12:U:O2	32:a:12:U:C2'	2.67	0.42
32:a:1846:G:C6	32:a:1847:A:C6	3.07	0.42
32:a:1932:A:H2'	32:a:1933:G:O4'	2.20	0.42
33:A:721:G:H4'	33:A:722:G:O4'	2.19	0.42
10:g:26:ILE:HG22	10:g:79:VAL:HG21	2.01	0.41
32:a:1735:A:H2'	32:a:1736:U:O4'	2.20	0.41
33:A:409:U:H2'	33:A:410:G:O4'	2.20	0.41
32:a:57:C:H2'	32:a:58:G:O4'	2.20	0.41
32:a:1039:A:H2'	32:a:1040:A:O4'	2.21	0.41
33:A:629:A:H2'	33:A:630:A:O4'	2.20	0.41
32:a:654:A:H2'	32:a:654:A:N3	2.34	0.41
32:a:1125:G:C6	32:a:1126:A:N6	2.89	0.41
42:D:168:PRO:HG2	42:D:171:LEU:HD12	2.01	0.41
5:b:41:G:N2	32:a:2339:C:O3'	2.52	0.41
32:a:715:A:C6	32:a:716:A:C6	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1853:A:N1	32:a:2087:G:H1'	2.35	0.41
31:4:13:THR:HG23	31:4:21:VAL:HG13	2.02	0.41
19:p:58:ARG:HA	19:p:61:TRP:CE3	2.56	0.41
32:a:2788:C:O2'	32:a:2809:A:N3	2.48	0.41
33:A:868:C:H2'	33:A:869:G:O4'	2.21	0.41
24:u:28:ALA:HB3	24:u:40:ILE:HG13	2.03	0.41
32:a:2627:G:O2'	32:a:2781:A:N1	2.43	0.41
33:A:1412:C:H2'	33:A:1413:A:C8	2.56	0.41
32:a:55:G:O2'	32:a:127:A:N1	2.48	0.41
32:a:207:A:H2'	32:a:208:C:O4'	2.20	0.41
32:a:374:A:C2	32:a:401:A:C4	3.09	0.41
2:1:3:ARG:HH12	32:a:752:A:P	2.43	0.41
3:2:12:LYS:NZ	32:a:249:C:O2	2.44	0.41
32:a:1269:A:O5'	32:a:1269:A:H8	2.04	0.41
33:A:61:G:H2'	33:A:62:U:O4'	2.21	0.41
33:A:918:A:H2'	33:A:919:A:O4'	2.20	0.41
41:B:28:LYS:N	41:B:29:PRO:CD	2.84	0.41
44:F:90:MET:HE1	49:R:23:TYR:CZ	2.56	0.41
7:d:12:THR:HG22	7:d:13:ARG:H	1.85	0.40
32:a:747:5MU:O2	32:a:2014:A:H1'	2.21	0.40
32:a:2512:C:H2'	32:a:2513:A:O4'	2.21	0.40
6:c:178:SER:OG	32:a:1799:G:N7	2.50	0.40
7:d:8:LYS:NZ	7:d:195:GLY:O	2.52	0.40
9:f:108:VAL:N	9:f:109:PRO:HD2	2.37	0.40
15:l:96:ILE:HG21	15:l:126:ILE:CD1	2.51	0.40
32:a:1209:U:O2'	32:a:1237:A:N1	2.51	0.40
32:a:1320:C:N3	32:a:1331:G:O6	2.54	0.40
33:A:1328:C:H5''	37:M:28:THR:HG21	2.03	0.40
32:a:1115:G:O2'	32:a:1116:G:O5'	2.34	0.40
32:a:722:A:H2'	32:a:723:C:O4'	2.22	0.40
32:a:1370:C:H2'	32:a:1371:G:O4'	2.21	0.40
52:K:67:ALA:HB2	52:K:96:THR:HG23	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	1 (2%)	1 (2%)	7	11
4	3	36/38 (95%)	36 (100%)	0	0	100	100
6	c	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
7	d	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
8	e	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
9	f	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
10	g	174/177 (98%)	167 (96%)	6 (3%)	1 (1%)	21	32
11	h	39/149 (26%)	35 (90%)	4 (10%)	0	100	100
12	i	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
13	j	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
14	k	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	18	28
15	l	132/136 (97%)	129 (98%)	3 (2%)	0	100	100
16	m	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
17	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
18	o	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
19	p	115/118 (98%)	115 (100%)	0	0	100	100
20	q	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
21	r	108/110 (98%)	107 (99%)	0	1 (1%)	14	22
22	s	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
23	t	100/104 (96%)	92 (92%)	7 (7%)	1 (1%)	12	20
24	u	92/94 (98%)	88 (96%)	3 (3%)	1 (1%)	11	18
25	v	76/85 (89%)	74 (97%)	2 (3%)	0	100	100
26	w	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
27	x	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
28	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
29	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
31	4	46/70 (66%)	43 (94%)	2 (4%)	1 (2%)	5	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	C	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
35	I	125/130 (96%)	116 (93%)	9 (7%)	0	100	100
36	J	96/103 (93%)	88 (92%)	5 (5%)	3 (3%)	3	3
37	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
38	N	98/101 (97%)	98 (100%)	0	0	100	100
39	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100
40	G	151/179 (84%)	142 (94%)	6 (4%)	3 (2%)	6	7
41	B	222/241 (92%)	212 (96%)	10 (4%)	0	100	100
42	D	203/206 (98%)	197 (97%)	4 (2%)	2 (1%)	12	20
43	E	154/167 (92%)	148 (96%)	6 (4%)	0	100	100
44	F	101/135 (75%)	97 (96%)	3 (3%)	1 (1%)	12	20
45	H	127/130 (98%)	119 (94%)	7 (6%)	1 (1%)	16	25
46	O	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
47	P	79/82 (96%)	69 (87%)	8 (10%)	2 (2%)	4	5
48	Q	77/84 (92%)	72 (94%)	5 (6%)	0	100	100
49	R	64/75 (85%)	61 (95%)	3 (5%)	0	100	100
50	T	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
51	U	68/71 (96%)	67 (98%)	0	1 (2%)	8	12
52	K	113/129 (88%)	109 (96%)	4 (4%)	0	100	100
53	L	120/124 (97%)	116 (97%)	4 (3%)	0	100	100
All	All	5471/5913 (92%)	5269 (96%)	182 (3%)	20 (0%)	31	43

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
40	G	6	VAL
40	G	57	SER
42	D	10	LYS
42	D	98	LEU
24	u	58	SER
36	J	57	VAL
47	P	51	ARG
51	U	3	VAL
36	J	27	GLU
44	F	33	GLU

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Mol	Chain	Res	Type
47	P	80	LYS
14	k	29	LYS
21	r	12	SER
31	4	4	ASP
10	g	176	LYS
3	2	28	ASN
23	t	39	ILE
36	J	36	VAL
40	G	16	PRO
45	H	75	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	43 (94%)	3 (6%)	15	27
2	1	38/38 (100%)	38 (100%)	0	100	100
3	2	51/52 (98%)	49 (96%)	2 (4%)	28	48
4	3	34/34 (100%)	33 (97%)	1 (3%)	37	60
6	c	216/218 (99%)	211 (98%)	5 (2%)	44	66
7	d	163/163 (100%)	160 (98%)	3 (2%)	51	73
8	e	165/165 (100%)	163 (99%)	2 (1%)	63	81
9	f	148/150 (99%)	142 (96%)	6 (4%)	27	46
10	g	137/138 (99%)	130 (95%)	7 (5%)	21	37
11	h	32/114 (28%)	28 (88%)	4 (12%)	4	6
12	i	116/116 (100%)	115 (99%)	1 (1%)	70	85
13	j	104/104 (100%)	100 (96%)	4 (4%)	29	49
14	k	103/103 (100%)	101 (98%)	2 (2%)	50	71
15	l	107/107 (100%)	105 (98%)	2 (2%)	50	71
16	m	98/103 (95%)	96 (98%)	2 (2%)	48	70
17	n	86/87 (99%)	84 (98%)	2 (2%)	44	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	o	99/100 (99%)	99 (100%)	0	100	100
19	p	89/90 (99%)	88 (99%)	1 (1%)	65	82
20	q	84/84 (100%)	82 (98%)	2 (2%)	43	65
21	r	93/93 (100%)	92 (99%)	1 (1%)	65	82
22	s	80/84 (95%)	80 (100%)	0	100	100
23	t	83/85 (98%)	78 (94%)	5 (6%)	17	31
24	u	78/78 (100%)	76 (97%)	2 (3%)	40	63
25	v	59/63 (94%)	59 (100%)	0	100	100
26	w	67/68 (98%)	65 (97%)	2 (3%)	36	58
27	x	54/55 (98%)	48 (89%)	6 (11%)	6	9
28	y	48/49 (98%)	48 (100%)	0	100	100
29	z	47/48 (98%)	47 (100%)	0	100	100
31	4	44/62 (71%)	39 (89%)	5 (11%)	5	8
34	C	170/190 (90%)	165 (97%)	5 (3%)	37	60
35	I	105/107 (98%)	103 (98%)	2 (2%)	50	71
36	J	86/90 (96%)	82 (95%)	4 (5%)	23	41
37	M	93/96 (97%)	90 (97%)	3 (3%)	34	56
38	N	83/84 (99%)	83 (100%)	0	100	100
39	S	72/79 (91%)	69 (96%)	3 (4%)	26	45
40	G	126/147 (86%)	119 (94%)	7 (6%)	19	33
41	B	186/199 (94%)	181 (97%)	5 (3%)	39	62
42	D	172/173 (99%)	160 (93%)	12 (7%)	14	24
43	E	119/126 (94%)	118 (99%)	1 (1%)	73	86
44	F	90/116 (78%)	89 (99%)	1 (1%)	65	82
45	H	104/105 (99%)	99 (95%)	5 (5%)	23	40
46	O	76/77 (99%)	76 (100%)	0	100	100
47	P	65/65 (100%)	64 (98%)	1 (2%)	57	77
48	Q	73/78 (94%)	71 (97%)	2 (3%)	39	62
49	R	57/65 (88%)	56 (98%)	1 (2%)	51	73
50	T	65/66 (98%)	64 (98%)	1 (2%)	57	77
51	U	60/61 (98%)	56 (93%)	4 (7%)	15	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
52	K	89/98 (91%)	87 (98%)	2 (2%)	45 67
53	L	102/103 (99%)	100 (98%)	2 (2%)	48 70
All	All	4562/4825 (94%)	4431 (97%)	131 (3%)	38 60

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	5	ILE
1	0	27	LYS
1	0	54	ILE
3	2	31	HIS
3	2	57	LEU
4	3	36	ARG
6	c	4	VAL
6	c	37	ASN
6	c	162	VAL
6	c	182	ARG
6	c	184	VAL
7	d	1	MET
7	d	12	THR
7	d	157	LYS
8	e	55	SER
8	e	80	SER
9	f	42	GLU
9	f	48	LYS
9	f	50	LEU
9	f	117	LEU
9	f	140	GLU
9	f	150	ARG
10	g	3	ARG
10	g	20	ASN
10	g	43	VAL
10	g	89	LEU
10	g	90	VAL
10	g	103	ILE
10	g	155	GLU
11	h	9	VAL
11	h	21	VAL
11	h	37	VAL
11	h	41	LYS
12	i	5	THR

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Mol	Chain	Res	Type
13	j	1	MET
13	j	76	VAL
13	j	93	GLN
13	j	99	ILE
14	k	112	LEU
14	k	129	LYS
15	l	51	ARG
15	l	135	VAL
16	m	6	SER
16	m	51	LEU
17	n	2	ASP
17	n	20	GLU
19	p	112	LYS
20	q	47	VAL
20	q	70	GLU
21	r	72	THR
23	t	15	THR
23	t	24	LYS
23	t	54	GLN
23	t	74	ASN
23	t	81	ASP
24	u	34	LYS
24	u	61	LEU
26	w	16	ASN
26	w	71	LEU
27	x	6	LEU
27	x	8	GLU
27	x	14	LEU
27	x	16	THR
27	x	24	GLU
27	x	56	LEU
31	4	8	LYS
31	4	20	ASN
31	4	36	VAL
31	4	47	LYS
31	4	48	GLN
34	C	107	ARG
34	C	147	LYS
34	C	170	GLU
34	C	178	LEU
34	C	206	GLU
35	I	85	ARG

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Mol	Chain	Res	Type
35	I	89	GLU
36	J	30	LYS
36	J	77	VAL
36	J	83	THR
36	J	88	MET
37	M	16	VAL
37	M	27	LYS
37	M	113	ARG
39	S	13	LEU
39	S	15	LEU
39	S	43	ASN
40	G	17	LYS
40	G	18	PHE
40	G	25	LYS
40	G	30	LEU
40	G	50	LEU
40	G	136	LYS
40	G	144	MET
41	B	63	ARG
41	B	73	LYS
41	B	89	GLN
41	B	93	ASN
41	B	161	LEU
42	D	8	LYS
42	D	11	LEU
42	D	14	ARG
42	D	21	LEU
42	D	45	LYS
42	D	48	LEU
42	D	116	GLN
42	D	128	ARG
42	D	131	ASN
42	D	138	SER
42	D	183	LYS
42	D	202	GLU
43	E	26	LYS
44	F	102	MET
45	H	54	ASP
45	H	56	LYS
45	H	60	GLU
45	H	89	LYS
45	H	117	ARG

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Mol	Chain	Res	Type
47	P	1	MET
48	Q	20	SER
48	Q	74	THR
49	R	10	PHE
50	T	40	GLU
51	U	8	GLU
51	U	21	ARG
51	U	49	LYS
51	U	58	LYS
52	K	89	PRO
52	K	94	GLU
53	L	55	VAL
53	L	111	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
3	2	31	HIS
6	c	37	ASN
6	c	90	ASN
6	c	197	ASN
8	e	94	GLN
8	e	115	GLN
9	f	37	ASN
9	f	63	GLN
9	f	81	GLN
10	g	30	ASN
12	i	47	HIS
12	i	80	HIS
12	i	128	ASN
13	j	3	GLN
13	j	89	ASN
14	k	104	GLN
15	l	13	HIS
15	l	60	GLN
18	o	10	GLN
18	o	12	GLN
18	o	66	ASN
19	p	52	GLN
21	r	9	HIS
21	r	40	ASN
22	s	48	GLN

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Mol	Chain	Res	Type
23	t	27	ASN
23	t	46	GLN
23	t	53	ASN
23	t	54	GLN
23	t	74	ASN
24	u	49	ASN
26	w	6	GLN
26	w	20	HIS
26	w	36	HIS
27	x	27	ASN
27	x	58	ASN
28	y	9	GLN
29	z	6	ASN
34	C	140	ASN
35	I	31	ASN
35	I	32	GLN
35	I	110	GLN
36	J	35	GLN
38	N	35	ASN
40	G	68	ASN
40	G	148	ASN
41	B	89	GLN
41	B	93	ASN
41	B	103	ASN
41	B	177	ASN
42	D	40	GLN
42	D	152	GLN
42	D	196	ASN
43	E	82	GLN
43	E	97	GLN
43	E	148	ASN
44	F	3	HIS
44	F	46	GLN
45	H	21	ASN
46	O	35	GLN
47	P	40	ASN
47	P	59	HIS
48	Q	9	GLN
50	T	52	ASN
50	T	84	ASN
51	U	64	ASN
52	K	118	HIS

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Mol	Chain	Res	Type
53	L	5	ASN
53	L	112	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	X	9/10 (90%)	1 (11%)	0
32	a	2733/2903 (94%)	303 (11%)	0
33	A	1516/1534 (98%)	206 (13%)	31 (2%)
5	b	118/120 (98%)	9 (7%)	0
54	Z	69/85 (81%)	17 (24%)	4 (5%)
55	Y	68/76 (89%)	13 (19%)	4 (5%)
All	All	4513/4728 (95%)	549 (12%)	39 (0%)

All (549) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	b	25	U
5	b	36	C
5	b	44	G
5	b	56	G
5	b	67	G
5	b	89	U
5	b	90	C
5	b	99	A
5	b	109	A
30	X	14	U
32	a	10	A
32	a	12	U
32	a	34	U
32	a	58	G
32	a	71	A
32	a	74	A
32	a	75	G
32	a	101	A
32	a	102	U
32	a	118	A
32	a	119	A
32	a	120	U
32	a	125	A
32	a	126	A

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Mol	Chain	Res	Type
32	a	131	A
32	a	139	U
32	a	142	A
32	a	165	A
32	a	181	A
32	a	196	A
32	a	199	A
32	a	200	U
32	a	215	G
32	a	216	A
32	a	221	A
32	a	222	A
32	a	233	A
32	a	248	G
32	a	272	A
32	a	276	U
32	a	277	G
32	a	278	A
32	a	289	G
32	a	311	A
32	a	329	G
32	a	330	A
32	a	345	A
32	a	353	C
32	a	356	G
32	a	361	G
32	a	386	G
32	a	404	A
32	a	405	U
32	a	411	G
32	a	412	A
32	a	425	G
32	a	451	U
32	a	456	C
32	a	481	G
32	a	491	G
32	a	503	A
32	a	504	A
32	a	505	A
32	a	509	C
32	a	530	G
32	a	532	A

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Mol	Chain	Res	Type
32	a	533	G
32	a	538	A
32	a	545	U
32	a	546	U
32	a	547	A
32	a	548	G
32	a	549	G
32	a	563	A
32	a	573	U
32	a	575	A
32	a	586	A
32	a	592	A
32	a	603	A
32	a	614	A
32	a	615	U
32	a	627	A
32	a	637	A
32	a	645	C
32	a	647	G
32	a	653	U
32	a	654	A
32	a	655	A
32	a	664	G
32	a	686	U
32	a	713	G
32	a	717	C
32	a	718	A
32	a	730	A
32	a	738	G
32	a	747	5MU
32	a	764	A
32	a	765	C
32	a	775	G
32	a	776	G
32	a	782	A
32	a	784	G
32	a	785	G
32	a	805	G
32	a	812	C
32	a	827	U
32	a	828	U
32	a	846	U

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Mol	Chain	Res	Type
32	a	847	U
32	a	858	G
32	a	859	G
32	a	880	G
32	a	881	G
32	a	899	A
32	a	900	A
32	a	907	G
32	a	910	A
32	a	914	G
32	a	915	C
32	a	927	A
32	a	931	U
32	a	934	U
32	a	946	C
32	a	961	C
32	a	974	G
32	a	983	A
32	a	984	A
32	a	985	C
32	a	996	A
32	a	1012	U
32	a	1013	C
32	a	1022	G
32	a	1025	G
32	a	1026	G
32	a	1033	U
32	a	1040	A
32	a	1045	C
32	a	1046	A
32	a	1047	G
32	a	1109	C
32	a	1110	G
32	a	1111	A
32	a	1112	G
32	a	1116	G
32	a	1122	G
32	a	1128	G
32	a	1129	A
32	a	1132	U
32	a	1133	A
32	a	1134	A

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Mol	Chain	Res	Type
32	a	1135	C
32	a	1142	A
32	a	1143	A
32	a	1171	G
32	a	1172	C
32	a	1187	G
32	a	1253	A
32	a	1256	G
32	a	1271	G
32	a	1272	A
32	a	1294	U
32	a	1300	G
32	a	1301	A
32	a	1352	U
32	a	1365	A
32	a	1379	U
32	a	1383	A
32	a	1386	C
32	a	1409	U
32	a	1416	G
32	a	1417	C
32	a	1427	A
32	a	1428	C
32	a	1434	A
32	a	1435	G
32	a	1452	G
32	a	1453	A
32	a	1459	G
32	a	1482	G
32	a	1493	C
32	a	1508	A
32	a	1509	A
32	a	1510	G
32	a	1515	A
32	a	1529	G
32	a	1535	A
32	a	1536	C
32	a	1537	G
32	a	1569	A
32	a	1578	U
32	a	1583	A
32	a	1584	U

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Mol	Chain	Res	Type
32	a	1585	C
32	a	1586	A
32	a	1608	A
32	a	1609	A
32	a	1647	U
32	a	1648	U
32	a	1649	G
32	a	1674	G
32	a	1715	G
32	a	1729	U
32	a	1730	C
32	a	1731	G
32	a	1732	C
32	a	1738	G
32	a	1764	C
32	a	1773	A
32	a	1782	U
32	a	1800	C
32	a	1801	A
32	a	1808	A
32	a	1816	C
32	a	1829	A
32	a	1839	G
32	a	1848	A
32	a	1858	A
32	a	1870	C
32	a	1871	A
32	a	1907	G
32	a	1910	G
32	a	1925	C
32	a	1926	U
32	a	1930	G
32	a	1937	A
32	a	1938	A
32	a	1955	U
32	a	1967	C
32	a	1970	A
32	a	1971	U
32	a	1972	G
32	a	1987	A
32	a	1991	U
32	a	1993	U

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Mol	Chain	Res	Type
32	a	2023	C
32	a	2027	G
32	a	2031	A
32	a	2033	A
32	a	2043	C
32	a	2055	C
32	a	2056	G
32	a	2060	A
32	a	2061	G
32	a	2062	A
32	a	2069	G7M
32	a	2198	A
32	a	2203	U
32	a	2204	G
32	a	2211	A
32	a	2225	A
32	a	2238	G
32	a	2239	G
32	a	2268	A
32	a	2283	C
32	a	2287	A
32	a	2303	G
32	a	2305	U
32	a	2308	G
32	a	2310	C
32	a	2312	U
32	a	2322	A
32	a	2325	G
32	a	2333	A
32	a	2335	A
32	a	2347	C
32	a	2361	G
32	a	2372	U
32	a	2383	G
32	a	2385	C
32	a	2396	G
32	a	2402	U
32	a	2406	A
32	a	2425	A
32	a	2429	G
32	a	2430	A
32	a	2435	A

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Mol	Chain	Res	Type
32	a	2441	U
32	a	2448	A
32	a	2464	G
32	a	2476	A
32	a	2478	A
32	a	2502	G
32	a	2505	G
32	a	2518	A
32	a	2525	G
32	a	2529	G
32	a	2547	A
32	a	2566	A
32	a	2567	G
32	a	2573	C
32	a	2602	A
32	a	2609	U
32	a	2613	U
32	a	2629	U
32	a	2663	G
32	a	2682	A
32	a	2689	U
32	a	2690	U
32	a	2714	G
32	a	2724	U
32	a	2726	A
32	a	2744	G
32	a	2748	A
32	a	2757	A
32	a	2765	A
32	a	2778	A
32	a	2791	G
32	a	2798	U
32	a	2800	A
32	a	2820	A
32	a	2821	A
32	a	2884	U
32	a	2885	G
33	A	4	U
33	A	5	U
33	A	7	A
33	A	9	G
33	A	22	G

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Mol	Chain	Res	Type
33	A	32	A
33	A	39	G
33	A	44	A
33	A	47	C
33	A	48	C
33	A	51	A
33	A	70	U
33	A	71	A
33	A	72	A
33	A	75	G
33	A	83	C
33	A	84	U
33	A	85	U
33	A	86	G
33	A	87	C
33	A	88	U
33	A	94	G
33	A	95	C
33	A	119	A
33	A	120	A
33	A	122	G
33	A	131	A
33	A	142	G
33	A	144	G
33	A	159	G
33	A	163	C
33	A	164	G
33	A	182	A
33	A	197	A
33	A	226	G
33	A	240	G
33	A	245	U
33	A	247	G
33	A	251	G
33	A	266	G
33	A	267	C
33	A	289	G
33	A	321	A
33	A	328	C
33	A	329	A
33	A	345	C
33	A	347	G

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Mol	Chain	Res	Type
33	A	348	G
33	A	352	C
33	A	354	G
33	A	367	U
33	A	372	C
33	A	376	G
33	A	391	G
33	A	392	C
33	A	406	G
33	A	412	A
33	A	413	G
33	A	414	A
33	A	417	G
33	A	421	U
33	A	422	C
33	A	423	G
33	A	424	G
33	A	429	U
33	A	430	A
33	A	438	U
33	A	439	U
33	A	446	G
33	A	451	A
33	A	453	G
33	A	456	A
33	A	457	G
33	A	458	U
33	A	467	U
33	A	468	A
33	A	481	G
33	A	484	G
33	A	485	U
33	A	486	U
33	A	511	C
33	A	513	C
33	A	518	C
33	A	530	G
33	A	531	U
33	A	532	A
33	A	533	A
33	A	542	G
33	A	547	A

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Mol	Chain	Res	Type
33	A	559	A
33	A	572	A
33	A	573	A
33	A	576	C
33	A	577	G
33	A	579	A
33	A	587	G
33	A	588	G
33	A	596	A
33	A	633	G
33	A	642	A
33	A	650	G
33	A	653	U
33	A	654	G
33	A	656	G
33	A	661	G
33	A	665	A
33	A	723	U
33	A	724	G
33	A	734	G
33	A	748	G
33	A	755	G
33	A	777	A
33	A	793	U
33	A	794	A
33	A	815	A
33	A	817	C
33	A	851	G
33	A	857	C
33	A	874	G
33	A	887	G
33	A	890	G
33	A	914	A
33	A	926	G
33	A	934	C
33	A	935	A
33	A	936	C
33	A	958	A
33	A	960	U
33	A	966	2MG
33	A	969	A
33	A	975	A

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Mol	Chain	Res	Type
33	A	976	G
33	A	977	A
33	A	978	A
33	A	984	C
33	A	992	U
33	A	993	G
33	A	994	A
33	A	996	A
33	A	1003	G
33	A	1004	A
33	A	1005	A
33	A	1008	U
33	A	1009	U
33	A	1027	C
33	A	1028	C
33	A	1031	C
33	A	1033	G
33	A	1034	G
33	A	1036	A
33	A	1044	A
33	A	1065	U
33	A	1085	U
33	A	1094	G
33	A	1095	U
33	A	1101	A
33	A	1132	C
33	A	1137	C
33	A	1138	G
33	A	1139	G
33	A	1159	U
33	A	1169	A
33	A	1171	A
33	A	1184	G
33	A	1187	G
33	A	1196	A
33	A	1197	A
33	A	1213	A
33	A	1225	A
33	A	1226	C
33	A	1227	A
33	A	1238	A
33	A	1256	A

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Mol	Chain	Res	Type
33	A	1260	G
33	A	1280	A
33	A	1287	A
33	A	1300	G
33	A	1302	C
33	A	1317	C
33	A	1320	C
33	A	1335	U
33	A	1336	C
33	A	1338	G
33	A	1340	A
33	A	1346	A
33	A	1353	G
33	A	1363	A
33	A	1364	U
33	A	1368	A
33	A	1370	G
33	A	1378	C
33	A	1379	G
33	A	1397	C
33	A	1419	G
33	A	1441	A
33	A	1451	U
33	A	1453	G
33	A	1492	A
33	A	1497	G
33	A	1503	A
33	A	1505	G
33	A	1506	U
33	A	1517	G
33	A	1529	G
33	A	1530	G
33	A	1534	A
54	Z	4	G
54	Z	5	A
54	Z	6	A
54	Z	7	G
54	Z	8	U
54	Z	19	G
54	Z	23	A
54	Z	24	C
54	Z	38	MIA

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Mol	Chain	Res	Type
54	Z	43	A
54	Z	44	C
54	Z	45	C
54	Z	46	G
54	Z	47	U
54	Z	58	G
54	Z	70	C
54	Z	85	A
55	Y	9	A
55	Y	14	A
55	Y	18	G
55	Y	46	G
55	Y	47	U
55	Y	48	C
55	Y	49	G
55	Y	53	G
55	Y	54	U
55	Y	60	U
55	Y	61	C
55	Y	63	A
55	Y	76	A

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
33	A	7	A
33	A	70	U
33	A	83	C
33	A	86	G
33	A	94	G
33	A	119	A
33	A	199	A
33	A	367	U
33	A	412	A
33	A	429	U
33	A	438	U
33	A	485	U
33	A	530	G
33	A	532	A
33	A	587	G
33	A	641	U
33	A	653	U

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Mol	Chain	Res	Type
33	A	733	G
33	A	776	G
33	A	793	U
33	A	858	G
33	A	992	U
33	A	1008	U
33	A	1035	A
33	A	1045	C
33	A	1046	A
33	A	1109	C
33	A	1124	G
33	A	1225	A
33	A	1335	U
33	A	1447	A
54	Z	6	A
54	Z	7	G
54	Z	22	G
54	Z	44	C
55	Y	7	U
55	Y	13	C
55	Y	46	G
55	Y	60	U

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

46 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	$\# Z > 2$
32	PSU	a	2605	32	18,21,22	0.96	1 (5%)	22,30,33	0.91	1 (4%)
32	2MG	a	2445	32	23,26,27	0.59	0	32,38,41	0.46	0
33	2MG	A	1516	33	23,26,27	0.48	0	32,38,41	0.52	0
32	PSU	a	2457	32	18,21,22	1.03	1 (5%)	22,30,33	0.69	0
15	4D4	l	81	15	9,11,12	0.59	0	8,13,15	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	MIA	Z	38	54	28,31,32	0.50	0	40,44,47	2.63	1 (2%)
32	PSU	a	2604	32	18,21,22	1.02	1 (5%)	22,30,33	0.83	0
53	D2T	L	89	53	7,9,10	0.94	0	6,11,13	1.74	3 (50%)
56	YFQ	5	3	56	3,6,7	0.69	0	0,6,8	-	-
33	5MC	A	1407	33	18,22,23	0.32	0	26,32,35	0.74	0
32	6MZ	a	1618	32	22,25,26	0.56	1 (4%)	30,36,39	0.62	0
32	5MC	a	1962	32	18,22,23	0.43	0	26,32,35	0.73	0
32	H2U	a	2449	32	18,21,22	0.73	1 (5%)	21,30,33	0.87	2 (9%)
32	PSU	a	1917	32	18,21,22	0.93	1 (5%)	22,30,33	0.63	0
32	2MG	a	1835	32	23,26,27	0.35	0	32,38,41	0.44	0
52	IAS	K	119	52	6,7,8	0.87	0	6,8,10	0.95	0
32	PSU	a	955	32	18,21,22	0.90	1 (5%)	22,30,33	0.68	0
7	MEQ	d	150	7	8,9,10	0.54	0	5,10,12	0.85	0
32	PSU	a	2504	32	18,21,22	0.96	1 (5%)	22,30,33	0.75	0
33	4OC	A	1402	33	20,23,24	0.39	0	26,32,35	0.64	0
32	5MU	a	1939	32	19,22,23	0.49	0	28,32,35	0.36	0
33	G7M	A	527	33	23,26,27	0.71	1 (4%)	35,39,42	0.68	0
55	MKX	Y	37	55	31,33,35	0.50	0	42,49,54	1.27	5 (11%)
33	5MC	A	967	33	18,22,23	0.36	0	26,32,35	0.61	0
56	YFZ	5	5	56	11,11,12	0.42	0	9,13,15	0.69	0
33	2MG	A	1207	33	23,26,27	0.42	0	32,38,41	0.43	0
33	UR3	A	1498	33	19,22,23	0.34	0	26,32,35	0.71	1 (3%)
32	1MG	a	745	32	22,26,27	0.83	1 (4%)	33,39,42	0.42	0
32	OMC	a	2498	32,58	19,22,23	0.47	0	26,31,34	0.58	0
32	PSU	a	2580	32,58	18,21,22	1.04	1 (5%)	22,30,33	0.73	0
32	OMU	a	2552	32	19,22,23	0.34	0	26,31,34	0.46	0
56	YF5	5	1	56	15,17,18	0.48	0	16,21,23	0.88	0
32	6MZ	a	2030	32	22,25,26	0.78	2 (9%)	30,36,39	0.70	0
56	ORD	5	4	56	6,7,8	0.51	0	2,7,9	0.29	0
32	G7M	a	2069	32	23,26,27	0.73	1 (4%)	35,39,42	0.68	1 (2%)
33	2MG	A	966	33	23,26,27	0.47	0	32,38,41	0.40	0
15	MS6	l	82	15	5,7,8	0.38	0	2,7,9	0.07	0
32	PSU	a	746	32,58	18,21,22	0.98	1 (5%)	22,30,33	0.60	0
32	PSU	a	1911	32	18,21,22	0.92	1 (5%)	22,30,33	0.65	0
32	2MA	a	2503	32,58	22,25,26	1.14	4 (18%)	33,37,40	1.10	3 (9%)
32	OMG	a	2251	32,55	23,26,27	0.38	0	33,38,41	0.43	0
33	PSU	A	516	33,58	18,21,22	1.02	1 (5%)	22,30,33	0.77	1 (4%)
32	5MU	a	747	32	19,22,23	0.35	0	28,32,35	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	DAL	5	2	56	3,4,5	0.57	0	2,4,6	1.06	0
56	YFQ	5	6	56	3,6,7	0.74	0	0,6,8	-	-
32	3TD	a	1915	32	18,22,23	0.96	1 (5%)	22,32,35	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PSU	a	2605	32	-	0/7/25/26	0/2/2/2
32	2MG	a	2445	32	-	0/9/27/28	0/3/3/3
33	2MG	A	1516	33	-	0/9/27/28	0/3/3/3
32	PSU	a	2457	32	-	0/7/25/26	0/2/2/2
15	4D4	l	81	15	-	3/11/12/14	-
54	MIA	Z	38	54	-	2/15/33/34	0/3/3/3
32	PSU	a	2604	32	-	0/7/25/26	0/2/2/2
53	D2T	L	89	53	-	3/7/12/14	-
56	YFQ	5	3	56	-	0/2/5/7	-
33	5MC	A	1407	33	-	0/7/25/26	0/2/2/2
32	6MZ	a	1618	32	-	0/9/27/28	0/3/3/3
32	5MC	a	1962	32	-	2/7/25/26	0/2/2/2
32	H2U	a	2449	32	-	0/7/38/39	0/2/2/2
32	PSU	a	1917	32	-	0/7/25/26	0/2/2/2
32	2MG	a	1835	32	-	0/9/27/28	0/3/3/3
52	IAS	K	119	52	-	0/7/7/8	-
32	PSU	a	955	32	-	0/7/25/26	0/2/2/2
7	MEQ	d	150	7	-	2/8/9/11	-
32	PSU	a	2504	32	-	0/7/25/26	0/2/2/2
33	4OC	A	1402	33	-	0/9/29/30	0/2/2/2
32	5MU	a	1939	32	-	0/7/25/26	0/2/2/2
33	G7M	A	527	33	-	1/7/25/26	0/3/3/3
55	MKX	Y	37	55	-	4/14/48/50	0/4/4/4
33	5MC	A	967	33	-	0/7/25/26	0/2/2/2
56	YFZ	5	5	56	-	3/13/13/14	-
33	2MG	A	1207	33	-	0/9/27/28	0/3/3/3
33	UR3	A	1498	33	-	0/7/25/26	0/2/2/2
32	1MG	a	745	32	-	0/7/25/26	0/3/3/3
32	OMC	a	2498	32,58	-	0/9/27/28	0/2/2/2
32	PSU	a	2580	32,58	-	0/7/25/26	0/2/2/2
32	OMU	a	2552	32	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	YF5	5	1	56	-	4/19/21/23	-
32	6MZ	a	2030	32	-	1/9/27/28	0/3/3/3
56	ORD	5	4	56	-	2/5/6/8	-
32	G7M	a	2069	32	-	2/7/25/26	0/3/3/3
33	2MG	A	966	33	-	0/9/27/28	0/3/3/3
15	MS6	l	82	15	-	1/4/6/8	-
32	PSU	a	746	32,58	-	1/7/25/26	0/2/2/2
32	PSU	a	1911	32	-	0/7/25/26	0/2/2/2
32	2MA	a	2503	32,58	-	2/7/25/26	0/3/3/3
32	OMG	a	2251	32,55	-	0/9/27/28	0/3/3/3
33	PSU	A	516	33,58	-	0/7/25/26	0/2/2/2
32	5MU	a	747	32	-	0/7/25/26	0/2/2/2
56	DAL	5	2	56	-	0/0/2/4	-
56	YFQ	5	6	56	-	0/2/5/7	-
32	3TD	a	1915	32	-	2/7/25/26	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	516	PSU	C6-C5	3.96	1.39	1.35
32	a	1915	3TD	C6-C5	3.64	1.39	1.35
32	a	2604	PSU	C6-C5	3.62	1.39	1.35
32	a	1917	PSU	C6-C5	3.59	1.39	1.35
32	a	1911	PSU	C6-C5	3.58	1.39	1.35
32	a	2580	PSU	C6-C5	3.58	1.39	1.35
32	a	2457	PSU	C6-C5	3.51	1.39	1.35
32	a	746	PSU	C6-C5	3.42	1.39	1.35
32	a	2605	PSU	C6-C5	3.12	1.39	1.35
32	a	2504	PSU	C6-C5	3.11	1.38	1.35
32	a	955	PSU	C6-C5	2.87	1.38	1.35
33	A	527	G7M	C8-N7	2.68	1.37	1.33
32	a	2503	2MA	C6-N1	2.47	1.38	1.35
32	a	2503	2MA	C6-N6	-2.42	1.28	1.34
32	a	745	1MG	C1'-N9	-2.31	1.40	1.47
32	a	2069	G7M	C8-N7	2.27	1.37	1.33
32	a	2503	2MA	C2-N1	2.25	1.38	1.34
32	a	2030	6MZ	C8-N9	-2.18	1.33	1.37
32	a	2503	2MA	C2-N3	2.15	1.37	1.34
32	a	2030	6MZ	C1'-N9	-2.14	1.40	1.46
32	a	1618	6MZ	C6-N6	2.09	1.36	1.34
32	a	2449	H2U	C2-N3	-2.08	1.34	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	Z	38	MIA	C11-S10-C2	16.06	114.26	102.27
55	Y	37	MKX	C14-C12-N11	-3.48	109.76	113.75
55	Y	37	MKX	C2-N1-C6	3.16	119.21	111.75
32	a	2503	2MA	CM2-C2-N1	3.05	121.92	117.15
55	Y	37	MKX	C13-N6-C10	-2.95	108.47	111.28
55	Y	37	MKX	C6-N6-C10	2.86	126.69	123.20
32	a	2503	2MA	N3-C2-N1	-2.62	120.90	125.72
32	a	2503	2MA	C5-C4-N3	-2.62	124.25	127.19
53	L	89	D2T	OD1-CG-CB	-2.51	117.18	122.44
33	A	516	PSU	C3'-C2'-C1'	2.47	104.51	101.64
55	Y	37	MKX	C14-C12-C13	2.38	115.44	109.52
32	a	2449	H2U	N3-C2-N1	2.33	119.12	116.65
53	L	89	D2T	OD2-CG-CB	2.18	117.86	113.15
53	L	89	D2T	O-C-CA	-2.15	119.14	124.78
32	a	2605	PSU	C2'-C3'-C4'	-2.12	98.52	102.64
32	a	2069	G7M	N9-C8-N7	-2.11	106.98	112.21
32	a	2449	H2U	O2-C2-N1	-2.08	120.50	123.11
33	A	1498	UR3	C6-N1-C2	-2.04	119.96	121.79

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	L	89	D2T	O-C-CA-CB
55	Y	37	MKX	C5-C6-N6-C10
55	Y	37	MKX	C5-C6-N6-C13
55	Y	37	MKX	N1-C6-N6-C10
55	Y	37	MKX	N1-C6-N6-C13
32	a	1915	3TD	O4'-C1'-C5-C4
32	a	1915	3TD	O4'-C1'-C5-C6
56	5	4	ORD	O-C-CA-CB
56	5	5	YFZ	CD-CE-CZ-OH
56	5	5	YFZ	N-CE-CZ-OH
54	Z	38	MIA	O4'-C4'-C5'-O5'
54	Z	38	MIA	C3'-C4'-C5'-O5'
56	5	1	YF5	CZ-CZ1-CZ2-NZ3
7	d	150	MEQ	NE2-CD-CG-CB
7	d	150	MEQ	OE1-CD-CG-CB
56	5	1	YF5	CE-CZ-CZ1-CZ2
56	5	4	ORD	C-CA-CB-CG
15	l	81	4D4	NH1-CZ-NE-CD

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Mol	Chain	Res	Type	Atoms
56	5	1	YF5	NZ6-CZ4-NZ3-CZ2
56	5	1	YF5	NZ5-CZ4-NZ3-CZ2
56	5	5	YFZ	O-C-CA-CB
32	a	2069	G7M	C4'-C5'-O5'-P
15	l	81	4D4	CG-CD-NE-CZ
53	L	89	D2T	SB-CB-CG-OD2
32	a	2030	6MZ	O4'-C4'-C5'-O5'
32	a	1962	5MC	O4'-C1'-N1-C6
53	L	89	D2T	CG-CB-SB-CB1
32	a	746	PSU	O4'-C1'-C5-C6
15	l	82	MS6	CB-CG-SD-CE
32	a	2503	2MA	O4'-C1'-N9-C8
32	a	2069	G7M	O4'-C4'-C5'-O5'
32	a	2503	2MA	O4'-C4'-C5'-O5'
32	a	1962	5MC	C2'-C1'-N1-C6
15	l	81	4D4	O-C-CA-CB
33	A	527	G7M	C4'-C5'-O5'-P

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	A	1516	2MG	1	0
32	a	2604	PSU	1	0
33	A	1402	4OC	1	0
32	a	1939	5MU	1	0
55	Y	37	MKX	1	0
56	5	5	YFZ	1	0
32	a	2030	6MZ	2	0
32	a	747	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 311 ligands modelled in this entry, 311 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.

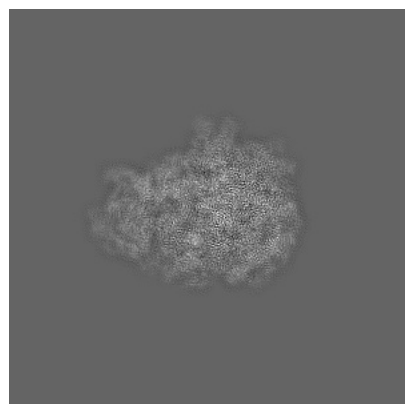
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19004. These allow visual inspection of the internal detail of the map and identification of artifacts.

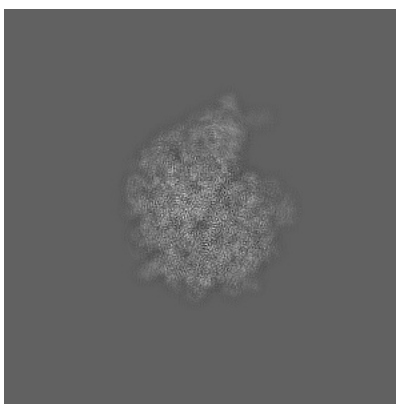
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

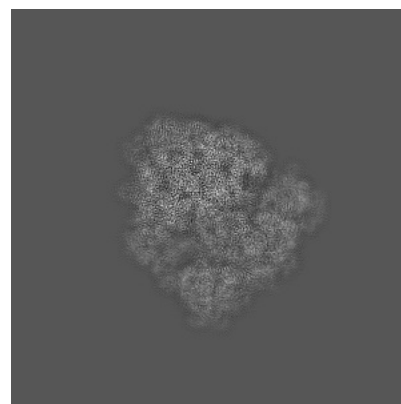
6.1.1 Primary map



X

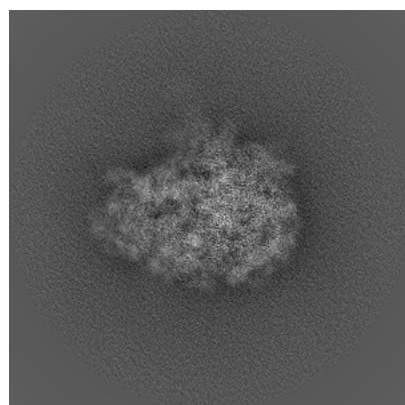


Y

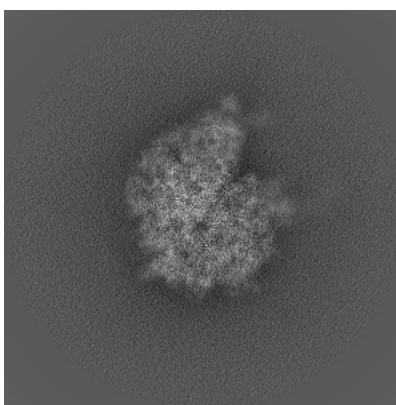


Z

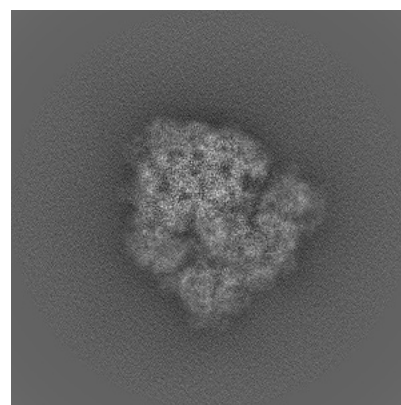
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 300

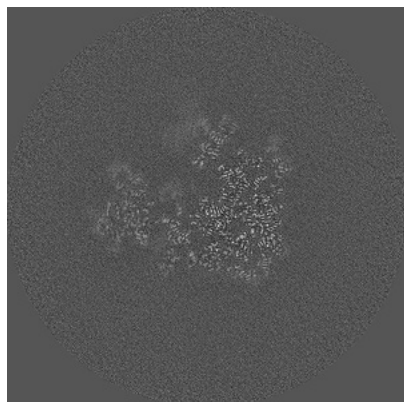


Y Index: 300

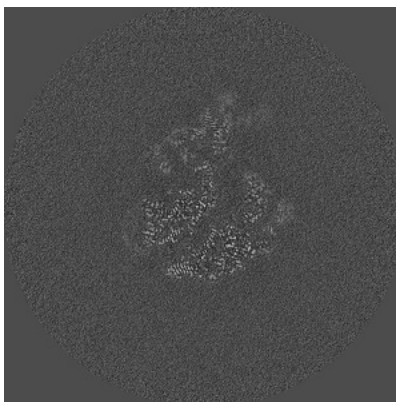


Z Index: 300

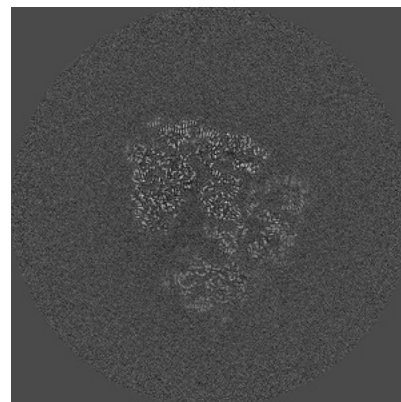
6.2.2 Raw map



X Index: 300



Y Index: 300

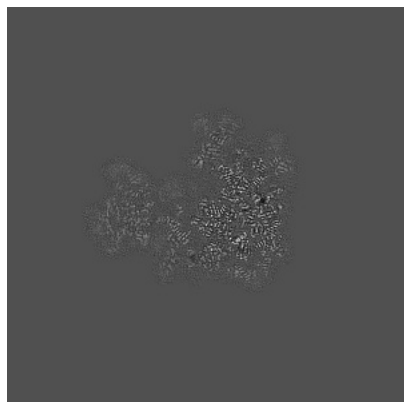


Z Index: 300

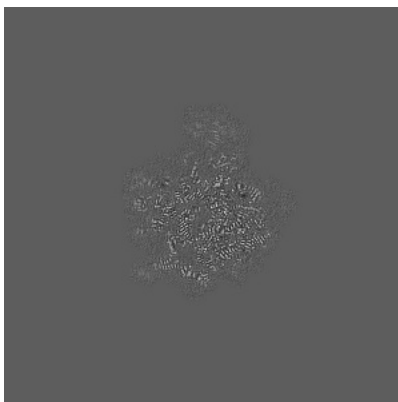
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

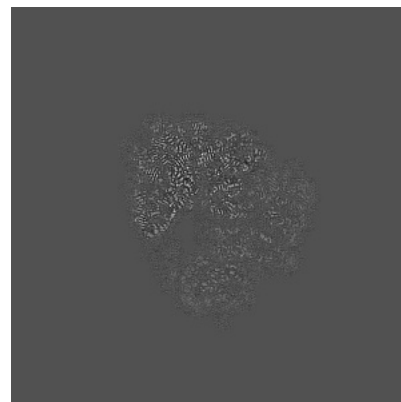
6.3.1 Primary map



X Index: 299

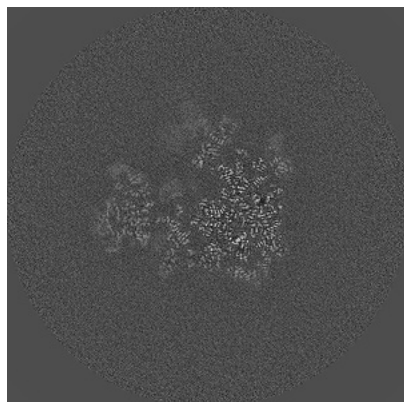


Y Index: 345

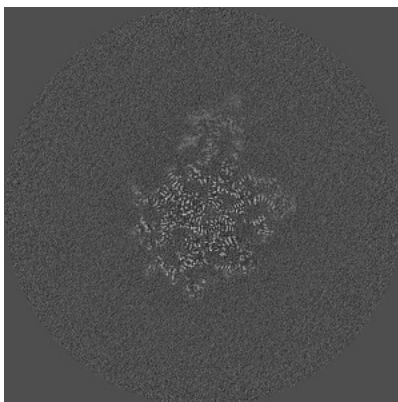


Z Index: 308

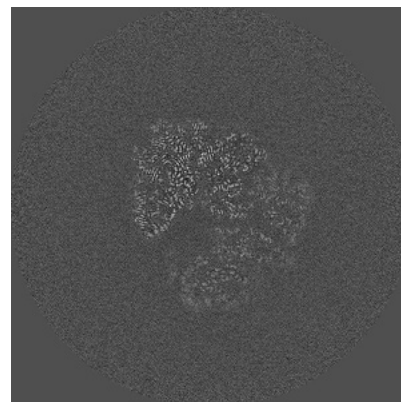
6.3.2 Raw map



X Index: 299



Y Index: 327

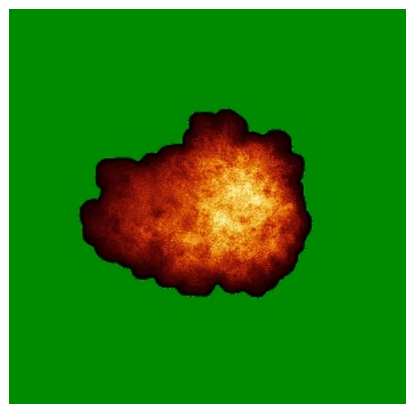


Z Index: 308

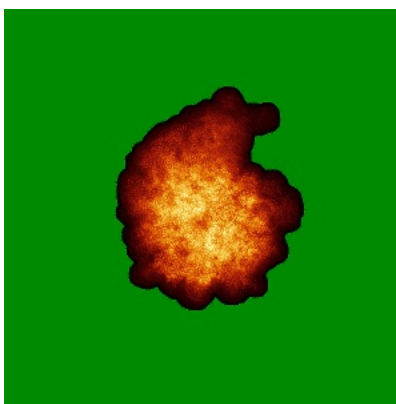
The images above show the largest variance slices of the map in three orthogonal directions.

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

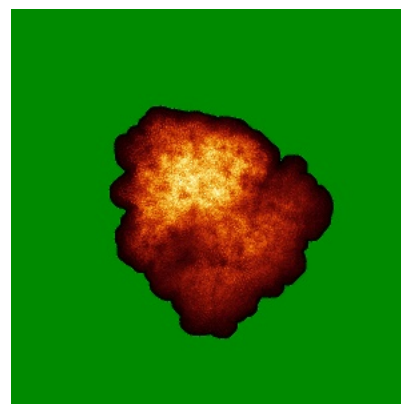
6.4.1 Primary map



X

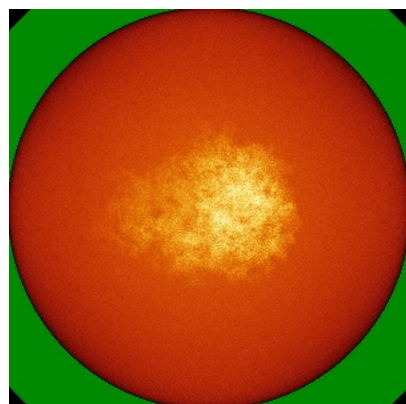


Y

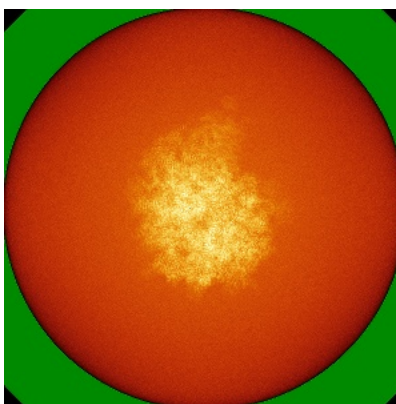


Z

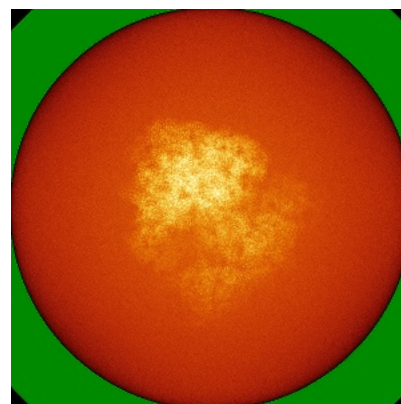
6.4.2 Raw map



X



Y

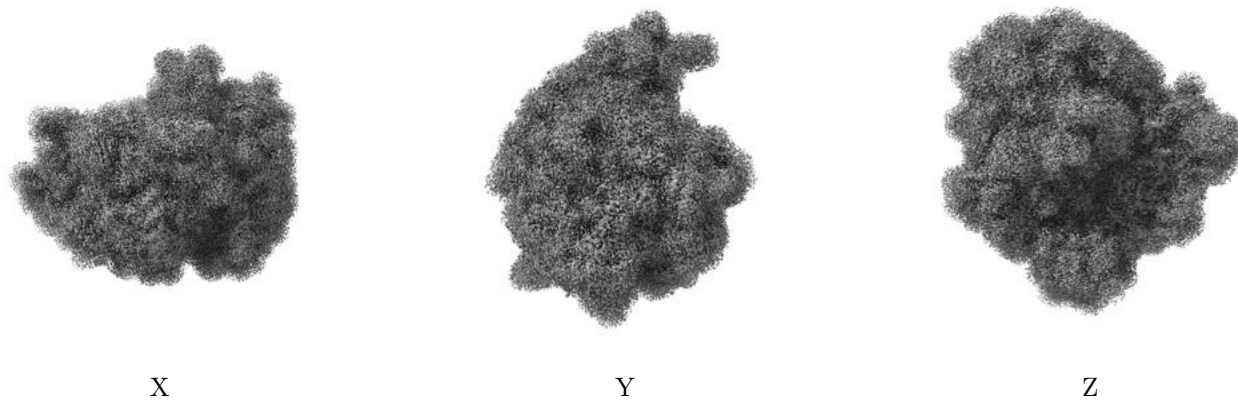


Z

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

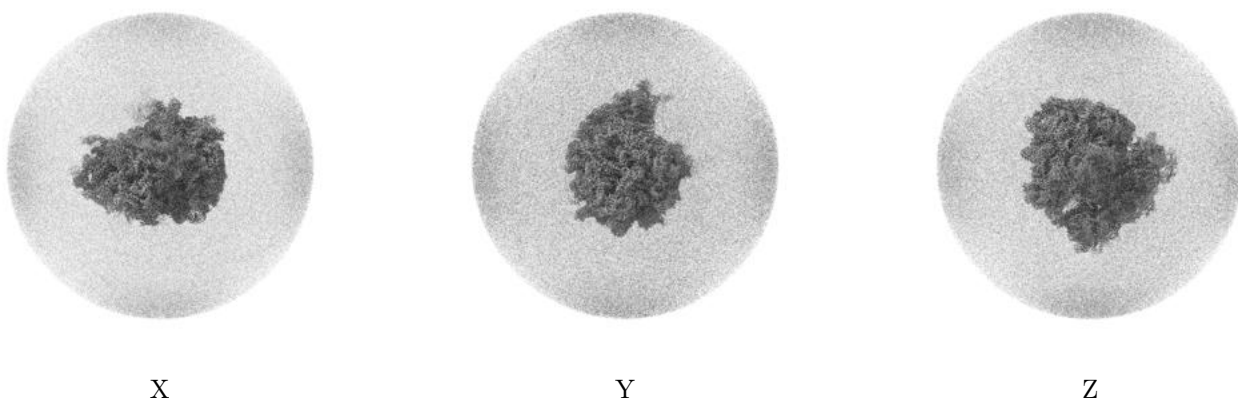
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

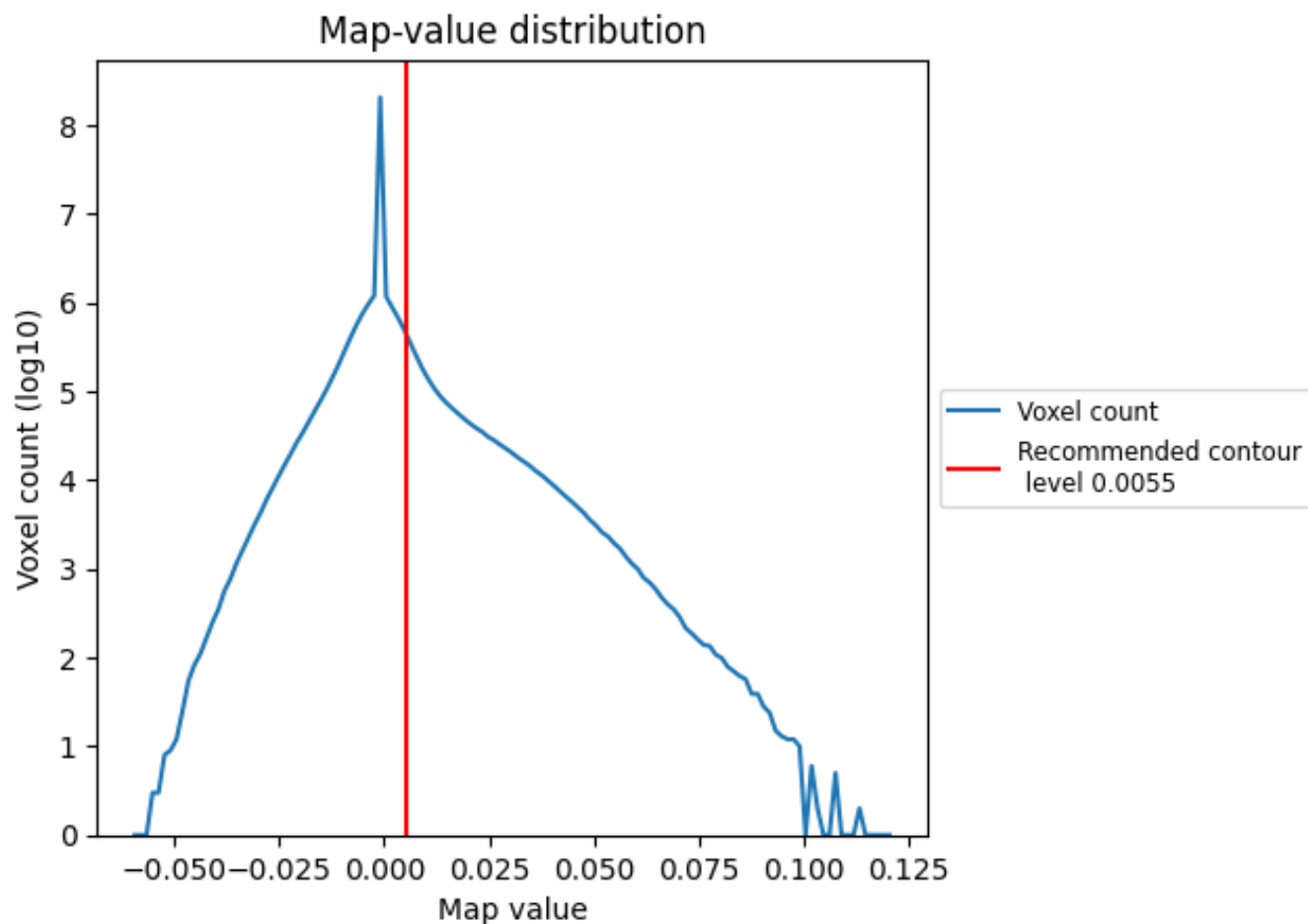
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

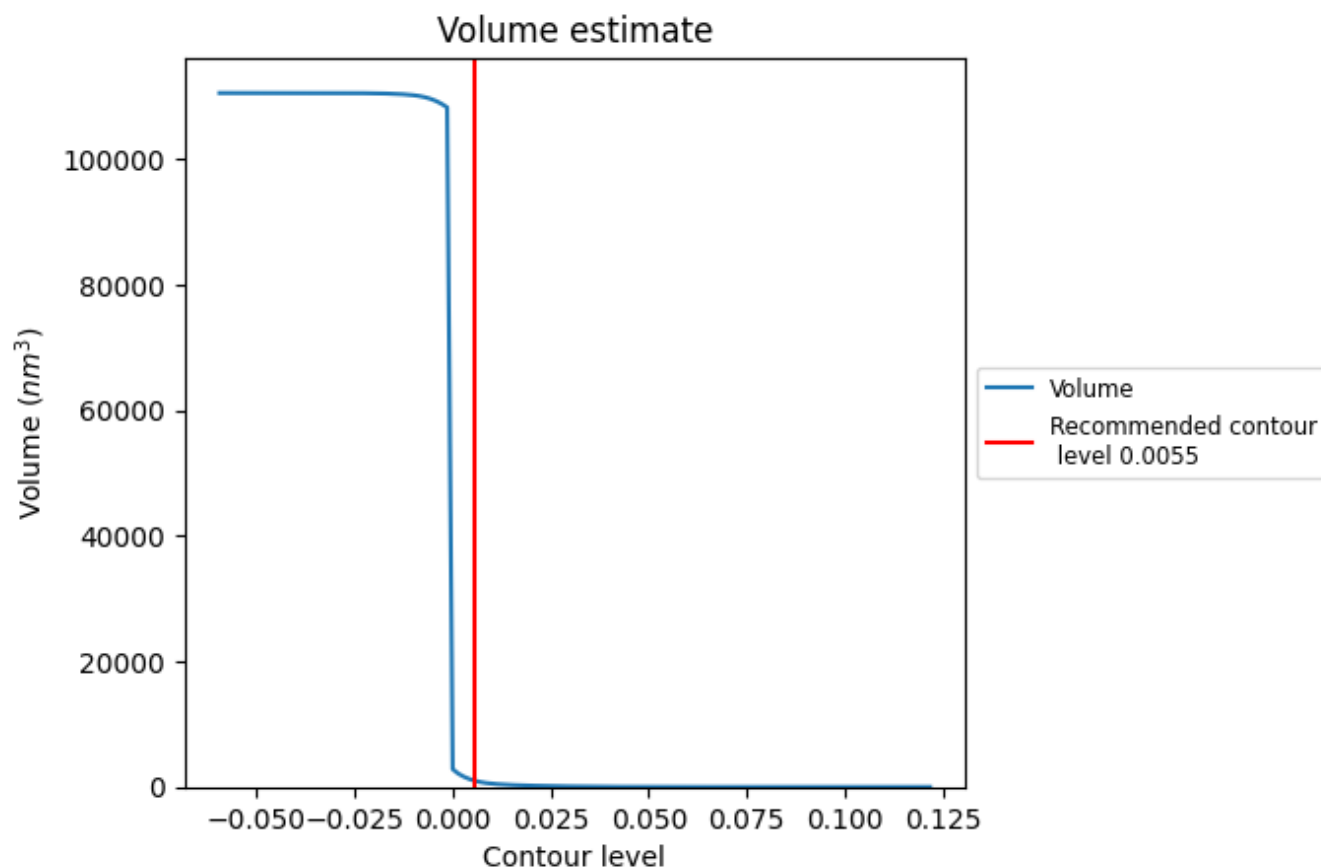
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

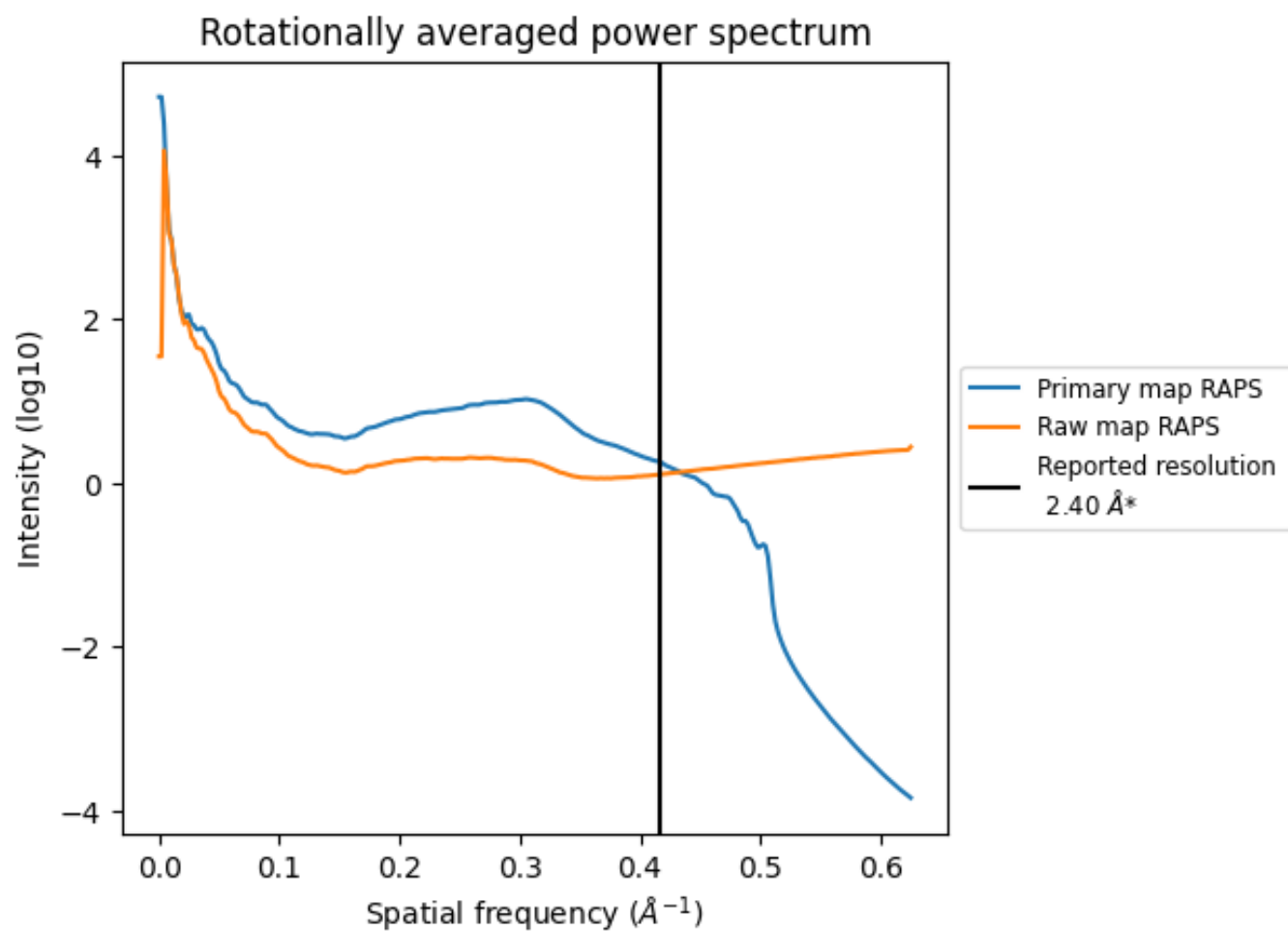
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1026 nm^3 ; this corresponds to an approximate mass of 927 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](#)

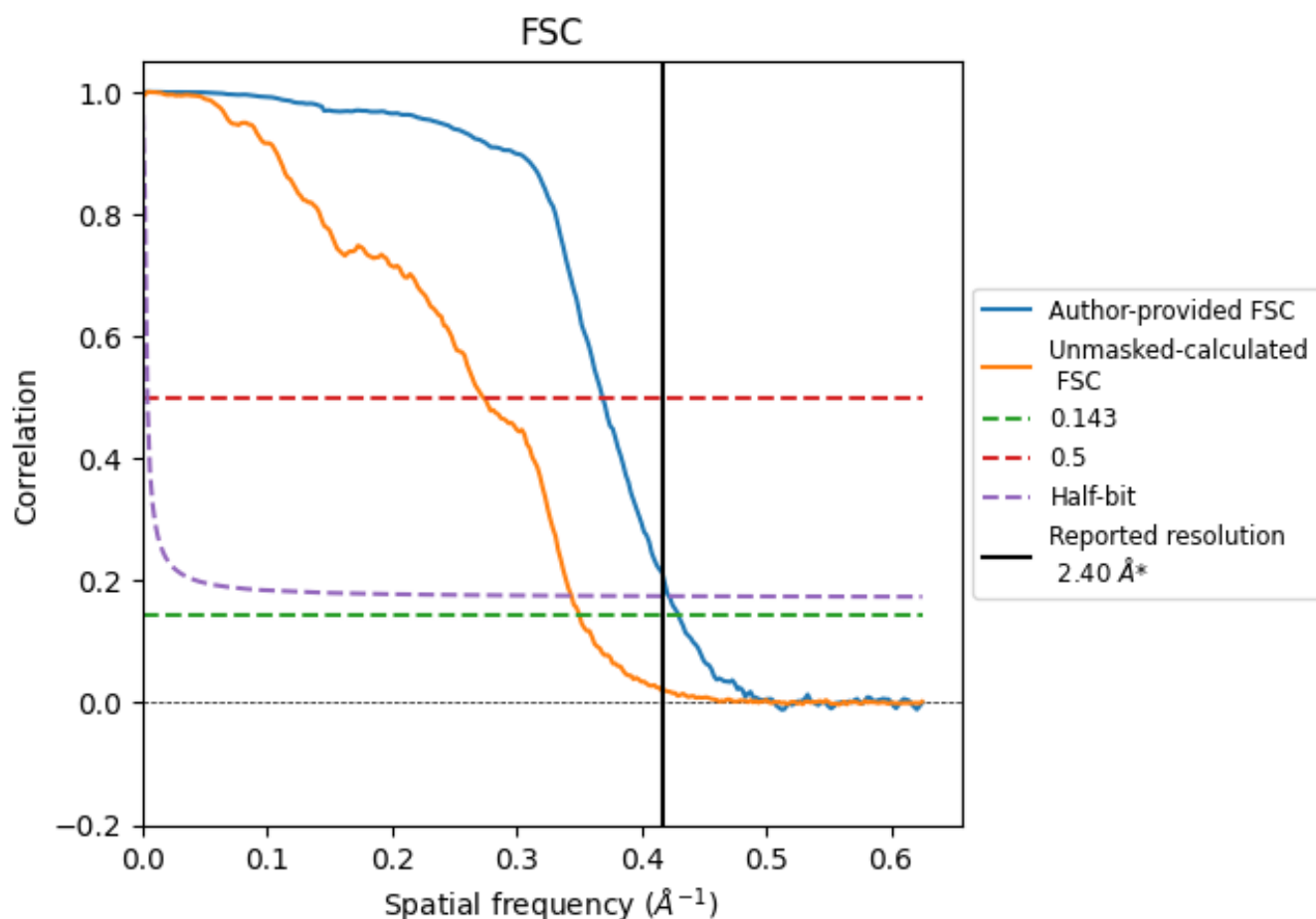


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

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

8.2 Resolution estimates [i](#)

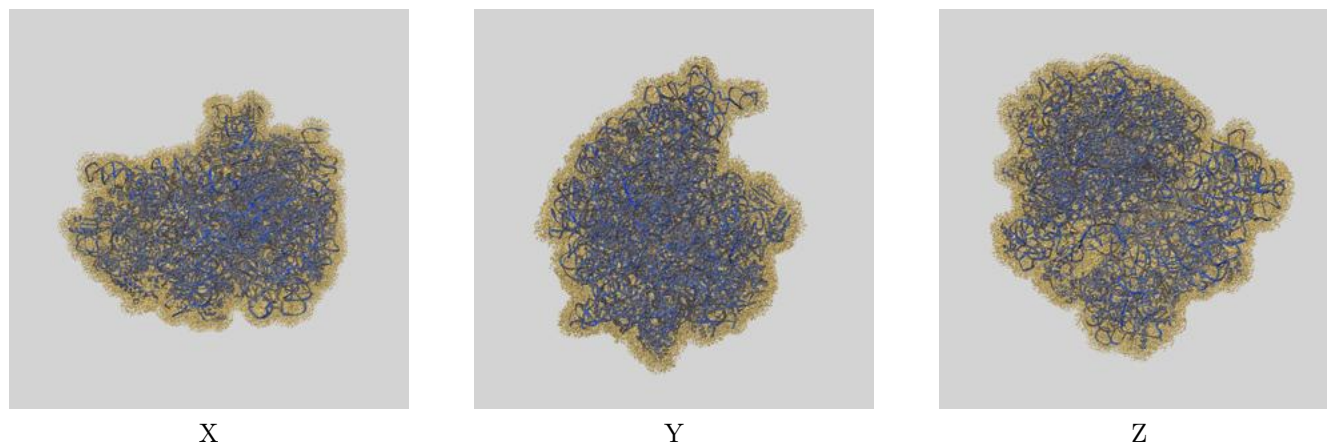
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.33	2.71	2.37
Unmasked-calculated*	2.85	3.66	2.91

*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 2.85 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

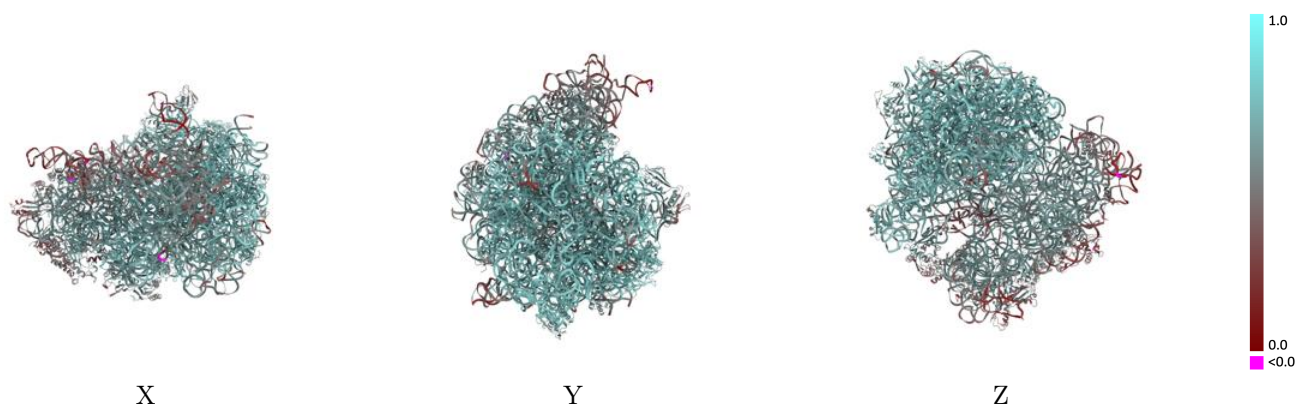
This section contains information regarding the fit between EMDB map EMD-19004 and PDB model 8R8M. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



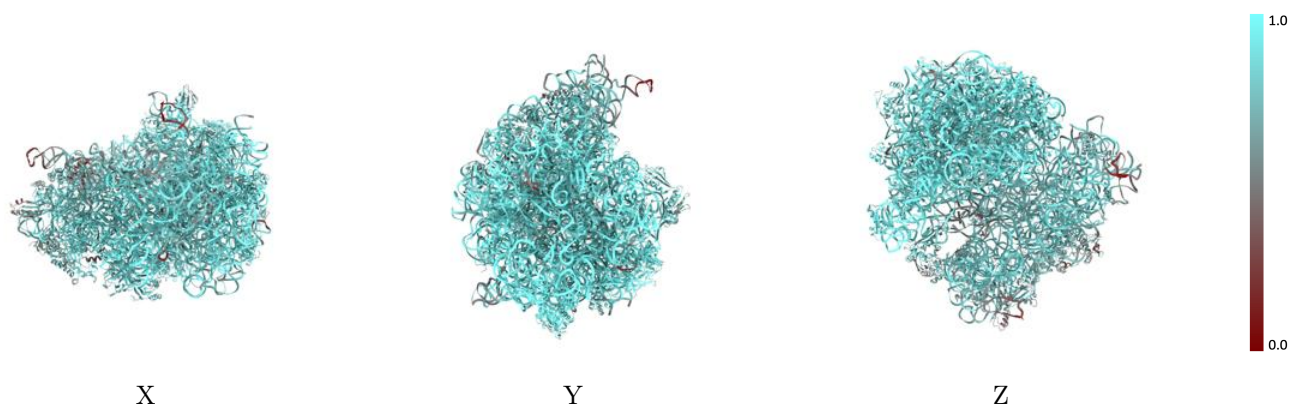
The images above show the 3D surface view of the map at the recommended contour level 0.0055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



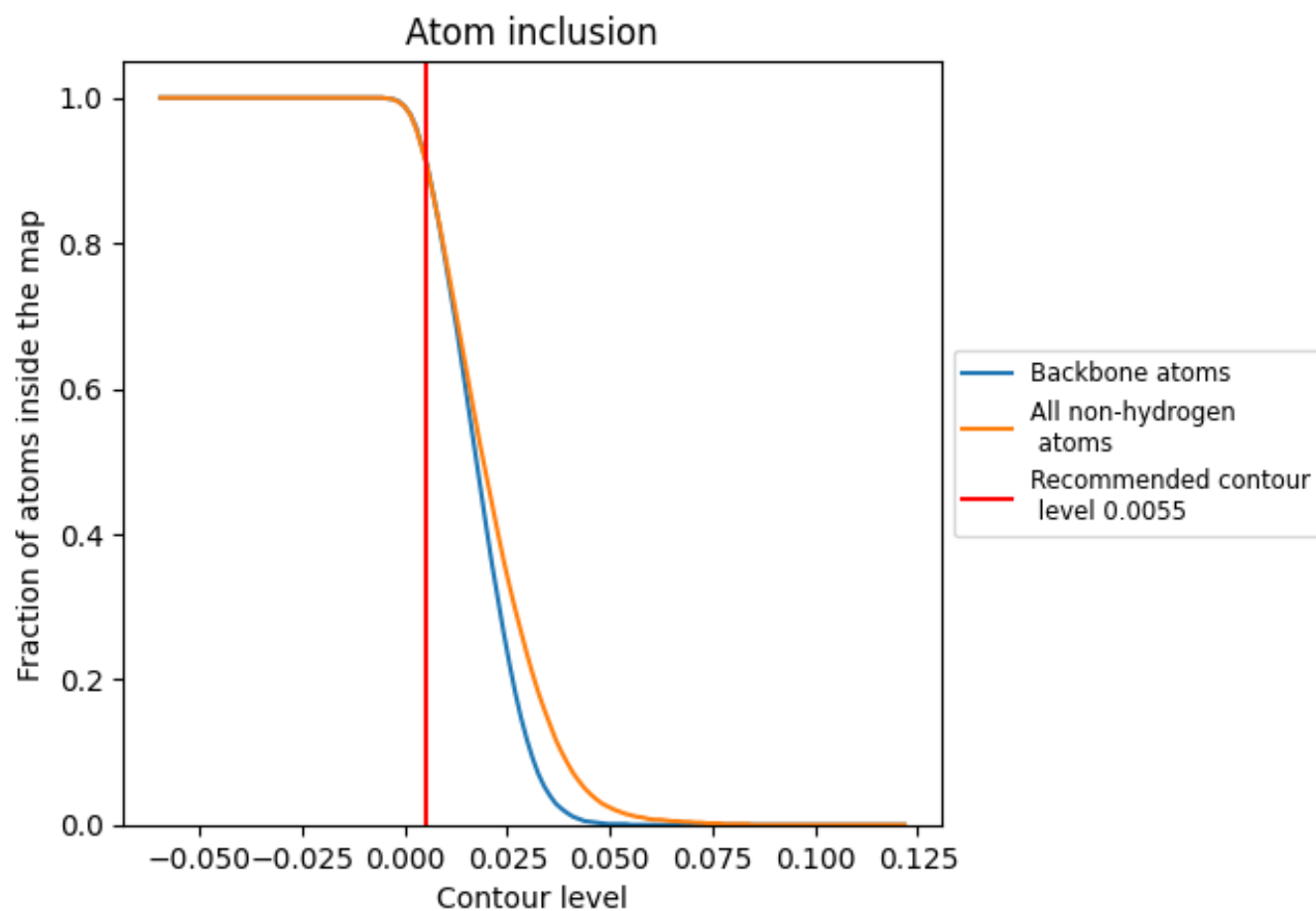
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0055).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% 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 (0.0055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9070	 0.6340
0	 0.9220	 0.6630
1	 0.9660	 0.7440
2	 0.9840	 0.7460
3	 0.9590	 0.6940
4	 0.6600	 0.4360
5	 0.8450	 0.6110
A	 0.8880	 0.5800
B	 0.7300	 0.4900
C	 0.8050	 0.5490
D	 0.5960	 0.4130
E	 0.9050	 0.6350
F	 0.8070	 0.5400
G	 0.5400	 0.3760
H	 0.9080	 0.6370
I	 0.7320	 0.4850
J	 0.6690	 0.4580
K	 0.9070	 0.6280
L	 0.8090	 0.5610
M	 0.7240	 0.4800
N	 0.8270	 0.5580
O	 0.8990	 0.6270
P	 0.7840	 0.5240
Q	 0.8030	 0.5460
R	 0.8720	 0.6070
S	 0.7820	 0.5170
T	 0.7420	 0.4910
U	 0.7140	 0.5150
X	 0.9290	 0.6400
Y	 0.5450	 0.3590
Z	 0.7640	 0.4840
a	 0.9680	 0.6930
b	 0.9550	 0.6490
c	 0.9740	 0.7310
d	 0.9630	 0.7180



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Chain	Atom inclusion	Q-score
e	 0.9260	 0.6840
f	 0.7690	 0.5140
g	 0.8030	 0.5500
h	 0.8470	 0.5870
i	 0.9650	 0.7220
j	 0.9600	 0.7070
k	 0.9530	 0.7080
l	 0.9530	 0.7050
m	 0.9860	 0.7430
n	 0.9180	 0.6390
o	 0.9080	 0.6720
p	 0.9840	 0.7490
q	 0.9330	 0.6940
r	 0.9510	 0.7180
s	 0.9110	 0.6700
t	 0.9020	 0.6430
u	 0.9080	 0.6460
v	 0.9340	 0.7050
w	 0.9480	 0.6970
x	 0.8730	 0.6260
y	 0.9430	 0.7030
z	 0.9390	 0.7070