



Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 05:23 am GMT

PDB ID : 7P3K
EMDB ID : EMD-13180
Title : Cryo-EM structure of 70S ribosome stalled with TnaC peptide (control)
Authors : Buschauer, R.; Komar, T.; Becker, T.; Berninghausen, O.; Cheng, J.; Beckmann, R.
Deposited on : 2021-07-08
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

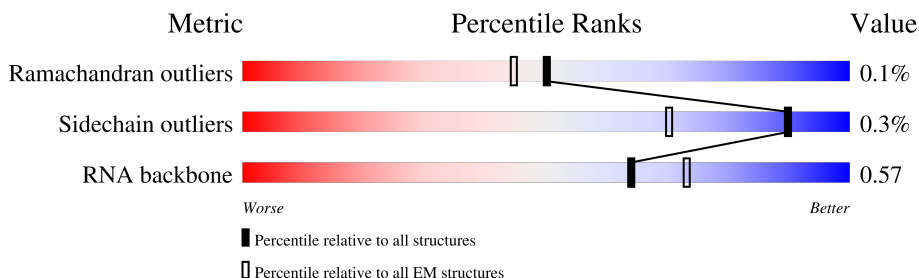
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.



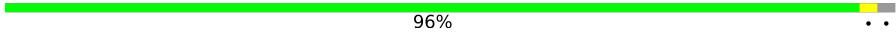
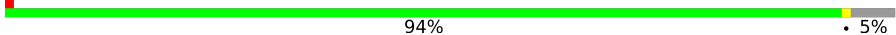

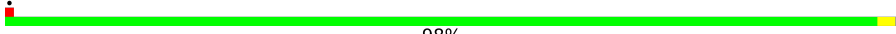


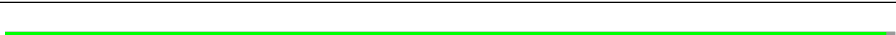
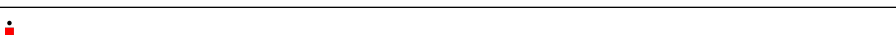
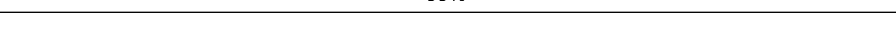
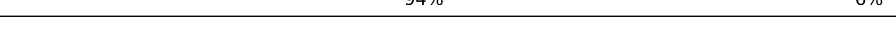
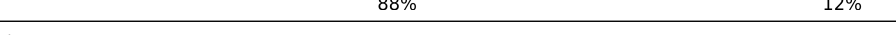
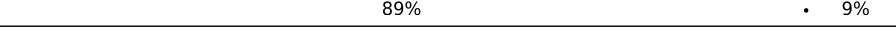
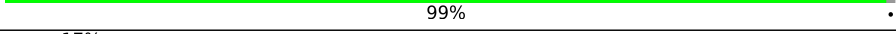
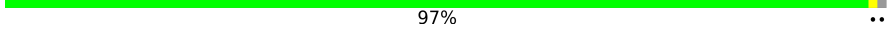


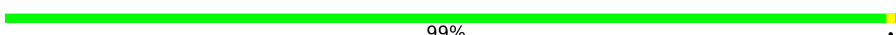
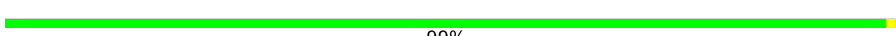





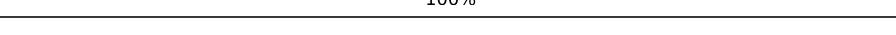
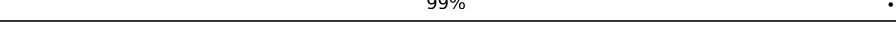
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	1519	
2	B	241	
3	C	233	
4	D	206	
5	E	167	
6	F	135	
7	G	179	
8	H	130	

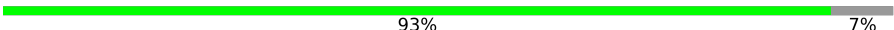
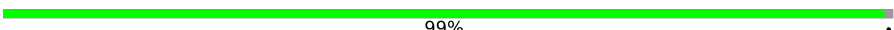
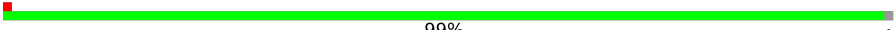
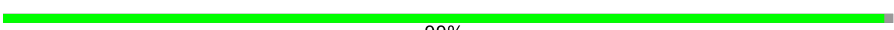








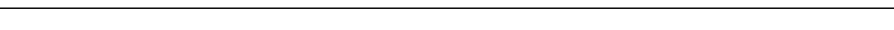
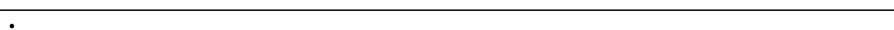
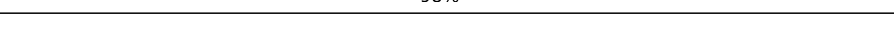

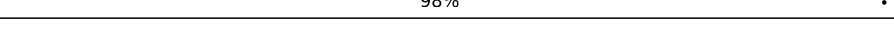
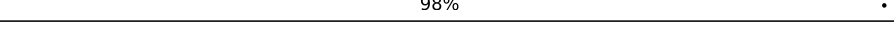
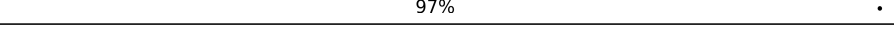


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	130	 96%
10	J	103	 94% 5%
11	K	129	 89% 9%
12	L	124	 98%
13	M	118	 97%
14	N	101	 98%
15	O	89	 99%
16	P	82	 99%
17	Q	84	 94% 6%
18	R	75	 88% 12%
19	S	92	 89% 9%
20	T	87	 99%
21	U	71	 17% 97%
22	a	2753	 85% 15%
23	b	119	 86% 14%
24	c	273	 99%
25	d	209	 99%
26	e	201	 100%
27	f	179	 99%
28	g	177	 99%
29	h	149	 28% 72%
30	i	142	 100%
31	j	123	 99%
32	k	144	 99%
33	l	136	 97%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	m	127	 93% 7%
35	n	117	 99% .
36	o	115	 99% .
37	p	118	 99% .
38	q	103	 99% .
39	r	110	 100%
40	s	100	 93% 7%
41	t	104	 97% ..
42	u	94	 100%
43	v	85	 92% 8%
44	w	78	 99% .
45	x	63	 98% .
46	y	59	 98% .
47	z	57	 98% .
48	0	55	 91% . 7%
49	1	46	 98% .
50	2	65	 98% .
51	3	38	 97% .
52	4	70	 86% 14%
53	X	3	 67% 33%
54	V	75	 73% 25% .

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 140054 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1519	Total	C	N	O	P	0	0
			32611	14551	5986	10555	1519		

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			979	616	173	184	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
			1022	634	206	179	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	98	Total	C	N	O	S	0	0
			786	493	150	142	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
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	ASP	ASN	conflict	UNP A0A6D2X4T2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	2753	Total	C	N	O	P	0	0
			59130	26384	10897	19096	2753		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
43	v	78	Total	C	N	O	S	
			586	362	116	107	1	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
48	0	51	Total	C	N	O	0	0
			417	269	76	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	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	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	X	3	Total	C	N	O	P	0	0
			60	27	9	21	3		

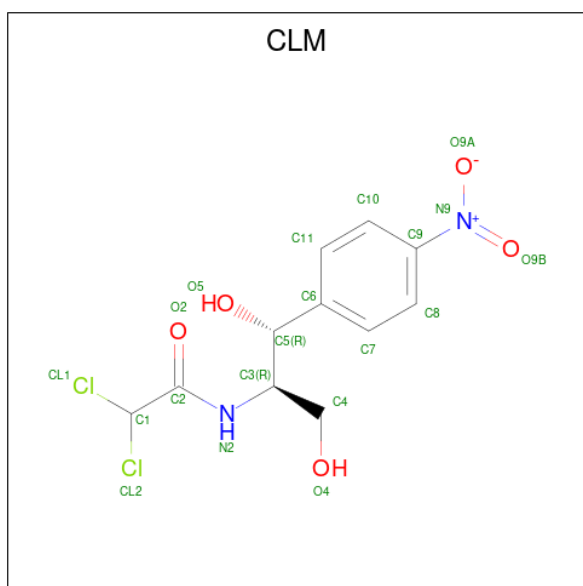
- Molecule 54 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	V	75	Total	C	N	O	P	0	0
			1609	715	292	527	75		

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	A	93	Total	Mg	0
			93	93	
55	a	206	Total	Mg	0
			206	206	
55	b	5	Total	Mg	0
			5	5	
55	c	1	Total	Mg	0
			1	1	
55	k	1	Total	Mg	0
			1	1	
55	m	1	Total	Mg	0
			1	1	
55	V	1	Total	Mg	0
			1	1	

- Molecule 56 is CHLORAMPHENICOL (three-letter code: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).



Mol	Chain	Residues	Atoms					AltConf
56	a	1	Total	C	Cl	N	O	0
			20	11	2	2	5	

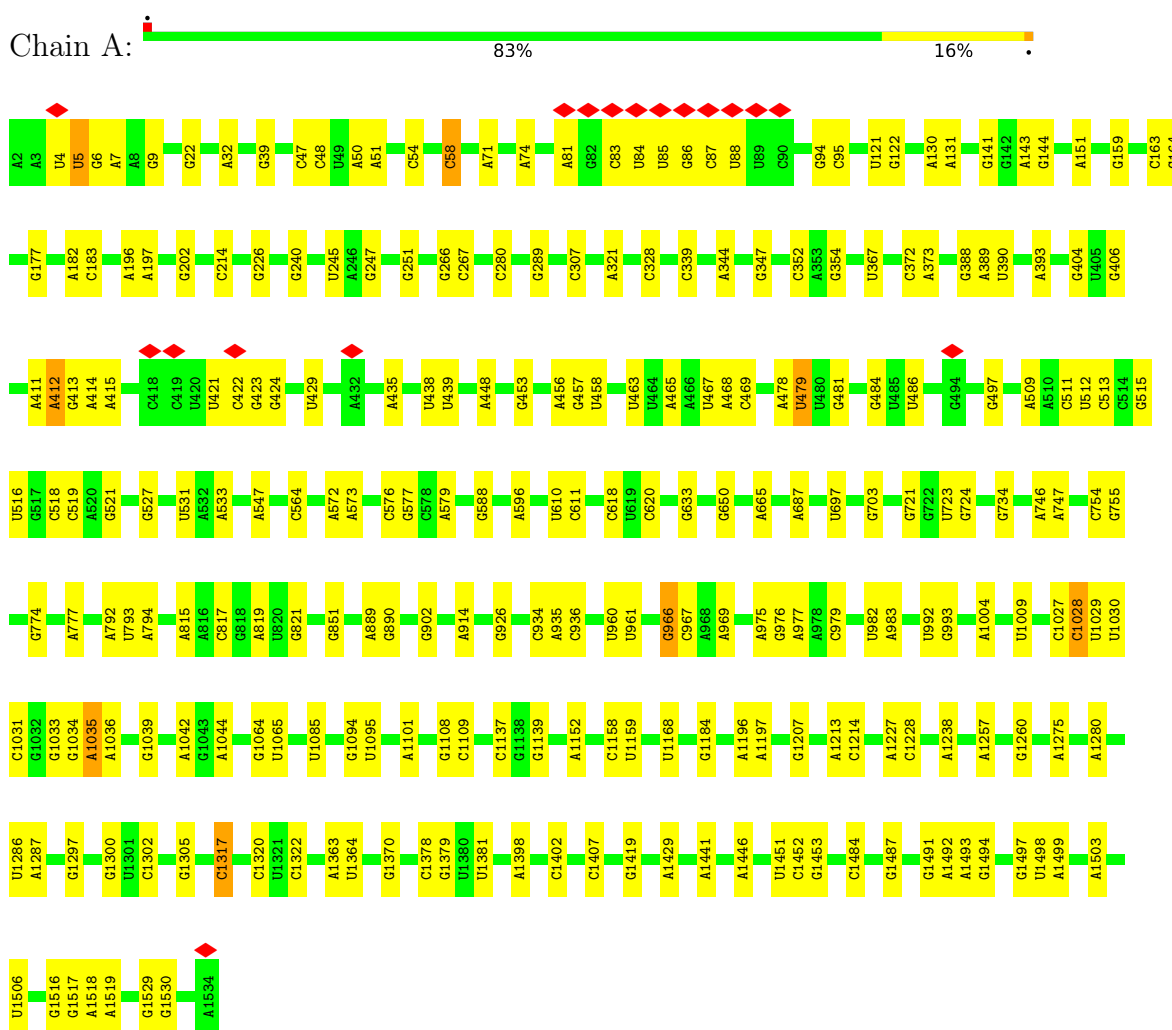
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots [i](#)

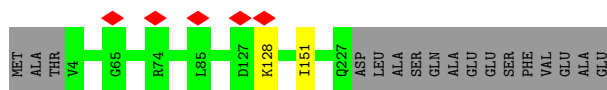
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



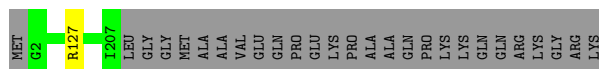
• Molecule 2: 30S ribosomal protein S2





- Molecule 3: 30S ribosomal protein S3

Chain C: 88% 12%



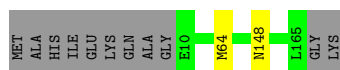
- Molecule 4: 30S ribosomal protein S4

Chain D: 100%



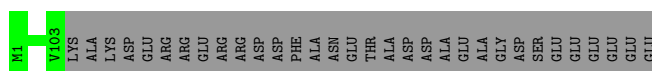
- Molecule 5: 30S ribosomal protein S5

Chain E: 92% 7%



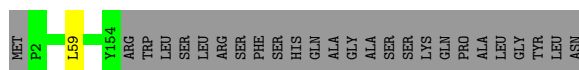
- Molecule 6: 30S ribosomal protein S6

Chain F: 76% 24%



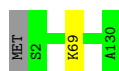
- Molecule 7: 30S ribosomal protein S7

Chain G: 85% 15%



- Molecule 8: 30S ribosomal protein S8

Chain H: 98% ..

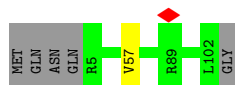


- Molecule 9: 30S ribosomal protein S9

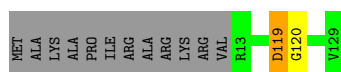
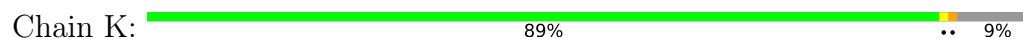
Chain I: 96% ..



- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15



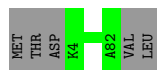
- Molecule 16: 30S ribosomal protein S16





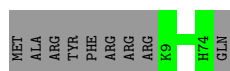
- Molecule 17: 30S ribosomal protein S17

Chain Q: 94% 6%



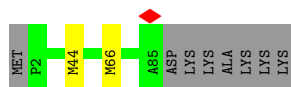
- Molecule 18: 30S ribosomal protein S18

Chain R: 88% 12%



- Molecule 19: 30S ribosomal protein S19

Chain S: 89% 9%



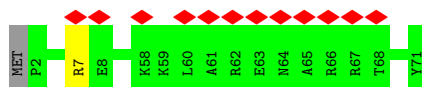
- Molecule 20: 30S ribosomal protein S20

Chain T: 99%



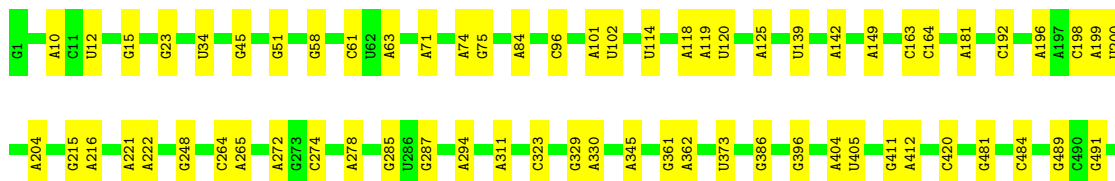
- Molecule 21: 30S ribosomal protein S21

Chain U: 17% 97%



- Molecule 22: 23S rRNA

Chain a: 85% 15%







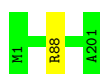
- Molecule 25: 50S ribosomal protein L3

Chain d: 99%



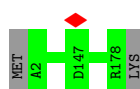
- Molecule 26: 50S ribosomal protein L4

Chain e: 100%



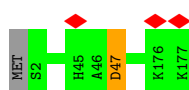
- Molecule 27: 50S ribosomal protein L5

Chain f: 99%



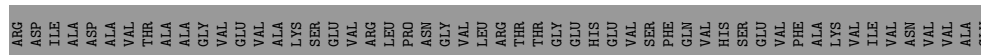
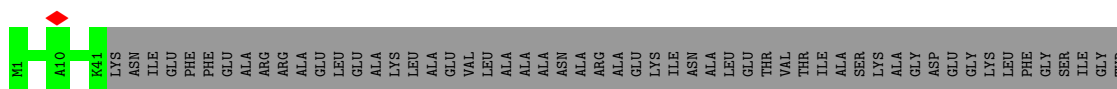
- Molecule 28: 50S ribosomal protein L6

Chain g: 99%



- Molecule 29: 50S ribosomal protein L9

Chain h: 28%



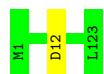
- Molecule 30: 50S ribosomal protein L13

Chain i: 100%

There are no outlier residues recorded for this chain.

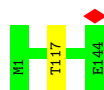
- Molecule 31: 50S ribosomal protein L14

Chain j:  99%



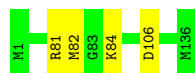
- Molecule 32: 50S ribosomal protein L15

Chain k:  99%

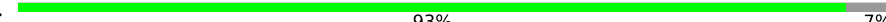


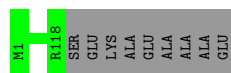
- Molecule 33: 50S ribosomal protein L16

Chain l:  97%



- Molecule 34: 50S ribosomal protein L17

Chain m:  93%



- Molecule 35: 50S ribosomal protein L18

Chain n:  99%



- Molecule 36: 50S ribosomal protein L19

Chain o:  99%



- Molecule 37: 50S ribosomal protein L20

Chain p:  99%



- Molecule 38: 50S ribosomal protein L21

Chain q:  99% .



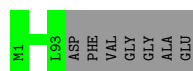
- Molecule 39: 50S ribosomal protein L22

Chain r:  100%

There are no outlier residues recorded for this chain.

- Molecule 40: 50S ribosomal protein L23

Chain s:  93% 7%



- Molecule 41: 50S ribosomal protein L24

Chain t:  97% ..



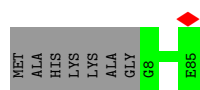
- Molecule 42: 50S ribosomal protein L25

Chain u:  100%

There are no outlier residues recorded for this chain.

- Molecule 43: 50S ribosomal protein L27

Chain v:  92% 8%



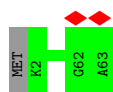
- Molecule 44: 50S ribosomal protein L28

Chain w:  99% .



- Molecule 45: 50S ribosomal protein L29

Chain x:  98% .



- Molecule 46: 50S ribosomal protein L30

Chain y:  98%




- Molecule 47: 50S ribosomal protein L32

Chain z:  98%



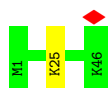
- Molecule 48: 50S ribosomal protein L33

Chain 0:  91% 7%



- Molecule 49: 50S ribosomal protein L34

Chain 1:  98%



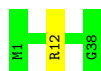
- Molecule 50: 50S ribosomal protein L35

Chain 2:  98%




- Molecule 51: 50S ribosomal protein L36

Chain 3:  97%



- Molecule 52: 50S ribosomal protein L31

Chain 4:  86% 14%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107016	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	10.529	Depositor
Minimum map value	-5.239	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.223	Depositor
Recommended contour level	0.5	Depositor
Map size (\AA)	491.4, 491.4, 491.4	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.092, 1.092, 1.092	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.55	0/36262	0.93	44/56561 (0.1%)
2	B	0.32	0/1784	0.64	1/2403 (0.0%)
3	C	0.30	0/1651	0.63	0/2225
4	D	0.34	0/1665	0.63	0/2227
5	E	0.35	0/1165	0.63	1/1568 (0.1%)
6	F	0.34	0/858	0.59	0/1160
7	G	0.34	0/1219	0.69	1/1635 (0.1%)
8	H	0.32	0/989	0.59	0/1326
9	I	0.30	0/1034	0.68	1/1375 (0.1%)
10	J	0.33	0/796	0.70	0/1077
11	K	0.36	0/893	0.65	0/1205
12	L	0.38	0/969	0.67	0/1300
13	M	0.29	0/900	0.62	0/1204
14	N	0.30	0/817	0.64	0/1088
15	O	0.31	0/722	0.59	0/964
16	P	0.31	0/653	0.62	0/877
17	Q	0.33	0/650	0.61	0/871
18	R	0.32	0/553	0.59	0/742
19	S	0.36	0/685	0.67	1/922 (0.1%)
20	T	0.31	0/676	0.52	0/895
21	U	0.31	0/597	0.64	0/792
22	a	0.90	7/65673 (0.0%)	0.98	95/102447 (0.1%)
23	b	0.74	0/2850	1.00	5/4444 (0.1%)
24	c	0.47	0/2121	0.67	1/2852 (0.0%)
25	d	0.49	0/1576	0.62	0/2119
26	e	0.42	0/1571	0.62	0/2113
27	f	0.36	0/1434	0.65	0/1926
28	g	0.39	0/1343	0.67	0/1816
29	h	0.34	0/306	0.69	0/413
30	i	0.47	0/1152	0.60	0/1551
31	j	0.48	0/955	0.74	1/1279 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	k	0.43	0/1062	0.65	1/1413 (0.1%)
33	l	0.51	0/1093	0.68	1/1460 (0.1%)
34	m	0.48	0/958	0.68	0/1281
35	n	0.40	0/902	0.65	0/1209
36	o	0.47	0/929	0.67	0/1242
37	p	0.53	0/960	0.60	0/1278
38	q	0.43	0/829	0.65	1/1107 (0.1%)
39	r	0.41	0/864	0.59	0/1156
40	s	0.38	0/744	0.61	0/994
41	t	0.35	0/787	0.65	1/1051 (0.1%)
42	u	0.42	0/766	0.60	0/1025
43	v	0.48	0/593	0.59	0/785
44	w	0.45	0/635	0.64	0/848
45	x	0.31	0/502	0.59	0/667
46	y	0.44	0/453	0.64	0/605
47	z	0.41	0/450	0.64	0/599
48	0	0.49	0/424	0.65	1/565 (0.2%)
49	1	0.46	0/380	0.72	0/498
50	2	0.43	0/513	0.67	0/676
51	3	0.52	0/303	0.62	0/397
52	4	0.28	0/488	0.55	0/649
53	X	0.83	0/65	1.07	1/98 (1.0%)
54	V	0.60	1/1797 (0.1%)	1.05	9/2798 (0.3%)
All	All	0.70	8/151016 (0.0%)	0.89	166/225778 (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
14	N	0	1
25	d	0	1
28	g	0	1
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2449	U	C5-C6	16.52	1.49	1.34
22	a	2449	U	C2-N3	15.67	1.48	1.37
54	V	1	C	OP3-P	-10.84	1.48	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2449	U	N1-C2	8.60	1.46	1.38
22	a	2449	U	N3-C4	7.51	1.45	1.38
22	a	2449	U	N1-C6	7.47	1.44	1.38
22	a	2449	U	C4-O4	-6.95	1.18	1.23
22	a	2449	U	C4-C5	5.21	1.48	1.43

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2449	U	C5-C4-O4	-11.26	119.14	125.90
22	a	2449	U	C2-N3-C4	-11.21	120.27	127.00
22	a	1313	U	C2-N1-C1'	9.96	129.66	117.70
22	a	1313	U	N3-C2-O2	-9.79	115.35	122.20
22	a	2449	U	N3-C4-C5	9.40	120.24	114.60
22	a	1313	U	N1-C2-O2	9.11	129.18	122.80
22	a	1045	C	N1-C2-O2	8.99	124.29	118.90
22	a	2902	C	N3-C2-O2	-8.89	115.68	121.90
22	a	1045	C	N3-C2-O2	-8.88	115.69	121.90
22	a	512	G	O4'-C1'-N9	8.75	115.20	108.20
22	a	1314	C	C2-N1-C1'	8.68	128.35	118.80
22	a	1045	C	C6-N1-C2	-8.20	117.02	120.30
54	V	27	C	N3-C2-O2	-8.09	116.24	121.90
22	a	2449	U	N1-C2-N3	7.90	119.64	114.90
22	a	1045	C	C2-N1-C1'	7.79	127.38	118.80
22	a	2505	G	P-O3'-C3'	7.60	128.82	119.70
1	A	961	U	N3-C2-O2	-7.35	117.06	122.20
22	a	2063	C	C2-N1-C1'	7.29	126.81	118.80
22	a	1348	C	N1-C2-O2	7.20	123.22	118.90
1	A	1028	C	N3-C2-O2	-7.07	116.95	121.90
54	V	27	C	N1-C2-O2	7.02	123.11	118.90
22	a	1963	U	N3-C2-O2	-6.92	117.36	122.20
1	A	1028	C	C6-N1-C2	-6.87	117.55	120.30
22	a	1774	C	C6-N1-C2	-6.80	117.58	120.30
1	A	214	C	C2-N1-C1'	6.64	126.11	118.80
54	V	19	G	O4'-C1'-N9	-6.58	102.94	108.20
1	A	54	C	N3-C2-O2	-6.57	117.30	121.90
23	b	17	C	N1-C2-O2	6.53	122.82	118.90
22	a	198	C	C6-N1-C2	-6.53	117.69	120.30
1	A	439	U	C2-N1-C1'	6.51	125.51	117.70
23	b	31	C	C2-N1-C1'	6.50	125.95	118.80
22	a	846	U	C2-N1-C1'	6.48	125.47	117.70
1	A	1029	U	N1-C2-O2	6.45	127.31	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	979	C	N1-C2-O2	6.43	122.76	118.90
9	I	57	MET	CA-CB-CG	6.38	124.14	113.30
22	a	1314	C	C6-N1-C1'	-6.29	113.25	120.80
22	a	1313	U	C6-N1-C1'	-6.29	112.40	121.20
1	A	979	C	C2-N1-C1'	6.28	125.71	118.80
22	a	1314	C	N1-C2-O2	6.27	122.66	118.90
1	A	993	G	C4-N9-C1'	6.26	134.65	126.50
24	c	98	ASP	CB-CG-OD1	6.25	123.93	118.30
22	a	2063	C	N1-C2-O2	6.24	122.64	118.90
1	A	618	C	N1-C2-O2	6.21	122.62	118.90
1	A	1158	C	C2-N1-C1'	6.19	125.61	118.80
22	a	2063	C	C6-N1-C2	-6.19	117.83	120.30
22	a	915	C	C2-N1-C1'	6.16	125.57	118.80
1	A	979	C	N3-C2-O2	-6.13	117.61	121.90
1	A	993	G	N3-C4-N9	6.07	129.64	126.00
22	a	1348	C	N3-C2-O2	-6.07	117.66	121.90
22	a	2585	U	O4'-C1'-N1	6.06	113.05	108.20
23	b	17	C	N3-C2-O2	-6.04	117.67	121.90
1	A	1035	A	P-O3'-C3'	5.98	126.88	119.70
1	A	479	U	N1-C2-O2	5.97	126.98	122.80
1	A	515	G	N3-C4-C5	-5.97	125.62	128.60
22	a	867	C	N1-C2-O2	5.95	122.47	118.90
22	a	1920	C	C5-C6-N1	5.95	123.98	121.00
1	A	54	C	N1-C2-O2	5.93	122.46	118.90
22	a	1774	C	C5-C6-N1	5.91	123.96	121.00
1	A	979	C	C6-N1-C2	-5.91	117.94	120.30
38	q	51	VAL	CG1-CB-CG2	-5.91	101.45	110.90
22	a	114	U	C2-N1-C1'	5.89	124.77	117.70
22	a	2683	C	N1-C2-O2	5.87	122.42	118.90
22	a	1343	G	C4-N9-C1'	5.86	134.12	126.50
22	a	12	U	N3-C2-O2	-5.86	118.10	122.20
22	a	198	C	C5-C6-N1	5.84	123.92	121.00
22	a	846	U	N1-C2-O2	5.82	126.87	122.80
54	V	44	G	C5-C6-O6	5.79	132.07	128.60
1	A	1029	U	N3-C2-O2	-5.79	118.15	122.20
22	a	2430	A	C2-N3-C4	5.79	113.49	110.60
1	A	439	U	N1-C2-O2	5.78	126.85	122.80
22	a	1956	U	N1-C2-O2	5.76	126.83	122.80
22	a	784	G	P-O3'-C3'	5.75	126.60	119.70
22	a	1788	C	C6-N1-C2	-5.74	118.00	120.30
22	a	1348	C	C2-N1-C1'	5.73	125.10	118.80
22	a	2043	C	C5-C6-N1	5.72	123.86	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	A	O4'-C1'-N9	5.70	112.76	108.20
22	a	1931	U	N1-C2-O2	5.70	126.79	122.80
22	a	1800	C	C6-N1-C2	-5.65	118.04	120.30
22	a	985	C	C2-N1-C1'	5.64	125.00	118.80
5	E	64	MET	CA-CB-CG	5.63	122.87	113.30
1	A	993	G	C8-N9-C1'	-5.62	119.70	127.00
54	V	44	G	N1-C6-O6	-5.61	116.54	119.90
1	A	610	U	N1-C2-O2	5.60	126.72	122.80
1	A	307	C	N1-C2-O2	5.59	122.25	118.90
22	a	404	A	P-O3'-C3'	5.58	126.39	119.70
22	a	783	A	C2-N3-C4	5.58	113.39	110.60
22	a	1931	U	N3-C2-O2	-5.58	118.30	122.20
22	a	1314	C	C5-C6-N1	5.56	123.78	121.00
48	0	40	ASP	CB-CG-OD1	5.56	123.30	118.30
22	a	2646	C	C5-C6-N1	5.54	123.77	121.00
22	a	1830	C	C5-C6-N1	5.53	123.77	121.00
1	A	610	U	N3-C2-O2	-5.52	118.33	122.20
1	A	439	U	N3-C2-O2	-5.52	118.34	122.20
22	a	2063	C	N3-C2-O2	-5.51	118.04	121.90
22	a	2449	U	N1-C2-O2	-5.51	118.94	122.80
54	V	3	G	N3-C4-N9	5.50	129.30	126.00
1	A	339	C	C2-N1-C1'	5.49	124.84	118.80
41	t	98	SER	C-N-CA	5.48	135.39	121.70
1	A	936	C	N1-C2-O2	5.48	122.19	118.90
19	S	66	MET	CA-CB-CG	5.47	122.60	113.30
22	a	1343	G	C8-N9-C1'	-5.47	119.89	127.00
32	k	117	THR	C-N-CA	5.45	135.34	121.70
22	a	1267	U	C2-N1-C1'	5.44	124.23	117.70
22	a	2902	C	C6-N1-C2	-5.43	118.13	120.30
22	a	867	C	N3-C2-O2	-5.42	118.10	121.90
1	A	1109	C	N1-C2-O2	5.41	122.14	118.90
22	a	1326	U	N3-C2-O2	-5.40	118.42	122.20
1	A	611	C	N1-C2-O2	5.39	122.13	118.90
22	a	2474	U	N1-C2-O2	5.39	126.57	122.80
22	a	1931	U	C2-N1-C1'	5.37	124.14	117.70
1	A	936	C	C2-N1-C1'	5.36	124.70	118.80
22	a	2666	C	N1-C2-O2	5.36	122.12	118.90
54	V	43	G	N3-C4-N9	5.35	129.21	126.00
22	a	1830	C	C6-N1-C2	-5.34	118.16	120.30
23	b	26	C	N1-C2-O2	5.33	122.10	118.90
1	A	479	U	C2-N1-C1'	5.33	124.09	117.70
7	G	59	LEU	CA-CB-CG	5.32	127.54	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	j	12	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	1317	C	N1-C2-O2	5.32	122.09	118.90
1	A	515	G	N3-C4-N9	5.31	129.19	126.00
22	a	717	C	N1-C2-O2	5.28	122.07	118.90
22	a	2072	C	C5-C6-N1	5.27	123.64	121.00
53	X	18	C	C2-N1-C1'	-5.26	113.01	118.80
22	a	1956	U	N3-C2-O2	-5.25	118.53	122.20
1	A	754	C	C2-N1-C1'	5.23	124.55	118.80
22	a	2065	C	C6-N1-C2	-5.23	118.21	120.30
1	A	1029	U	C2-N1-C1'	5.22	123.96	117.70
22	a	1314	C	C6-N1-C2	-5.22	118.21	120.30
2	B	151	ILE	CG1-CB-CG2	-5.21	99.94	111.40
1	A	58	C	C6-N1-C2	-5.20	118.22	120.30
22	a	1348	C	C6-N1-C2	-5.20	118.22	120.30
1	A	961	U	C2-N3-C4	-5.20	123.88	127.00
22	a	1313	U	C6-N1-C2	-5.20	117.88	121.00
22	a	373	U	N3-C2-O2	-5.18	118.57	122.20
33	l	106	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	515	G	C4-N9-C1'	5.17	133.22	126.50
22	a	510	C	N1-C2-O2	5.17	122.00	118.90
22	a	1197	G	C5-C6-O6	5.17	131.70	128.60
54	V	31	C	C2-N1-C1'	5.17	124.48	118.80
22	a	2752	C	N1-C2-O2	5.16	122.00	118.90
22	a	404	A	OP2-P-O3'	5.15	116.53	105.20
1	A	5	U	P-O3'-C3'	5.15	125.88	119.70
1	A	697	U	N3-C2-O2	-5.14	118.60	122.20
22	a	1352	U	N3-C2-O2	-5.14	118.60	122.20
23	b	31	C	C6-N1-C2	-5.14	118.24	120.30
22	a	1157	G	C4-N9-C1'	5.11	133.14	126.50
22	a	510	C	C2-N1-C1'	5.11	124.42	118.80
22	a	323	C	C2-N1-C1'	5.10	124.41	118.80
1	A	151	A	N1-C6-N6	-5.08	115.55	118.60
22	a	2902	C	N1-C2-N3	5.08	122.76	119.20
22	a	2474	U	N3-C2-O2	-5.07	118.65	122.20
22	a	2834	G	N3-C4-N9	5.07	129.04	126.00
22	a	2043	C	C2-N1-C1'	5.06	124.37	118.80
22	a	2582	G	N3-C4-N9	5.06	129.03	126.00
54	V	3	G	C4-N9-C1'	5.05	133.06	126.50
22	a	984	A	O4'-C1'-N9	5.05	112.24	108.20
22	a	847	U	N3-C2-O2	-5.04	118.67	122.20
22	a	2656	U	C2-N1-C1'	5.02	123.73	117.70
1	A	792	A	O4'-C1'-N9	5.02	112.21	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2043	C	C6-N1-C2	-5.01	118.30	120.30
22	a	2244	U	N3-C4-O4	5.01	122.91	119.40
22	a	484	C	C5-C6-N1	5.01	123.50	121.00
22	a	1920	C	C6-N1-C2	-5.01	118.30	120.30
22	a	192	C	C6-N1-C2	-5.00	118.30	120.30
22	a	1760	C	C6-N1-C2	-5.00	118.30	120.30
22	a	999	U	N3-C2-O2	-5.00	118.70	122.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	N	32	SER	Peptide
25	d	16	THR	Peptide
28	g	47	ASP	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	222/241 (92%)	211 (95%)	11 (5%)	0	100	100
3	C	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
4	D	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
5	E	154/167 (92%)	149 (97%)	5 (3%)	0	100	100
6	F	101/135 (75%)	98 (97%)	3 (3%)	0	100	100
7	G	151/179 (84%)	143 (95%)	8 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
9	I	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
10	J	96/103 (93%)	90 (94%)	5 (5%)	1 (1%)	13	40
11	K	115/129 (89%)	110 (96%)	3 (3%)	2 (2%)	7	27
12	L	121/124 (98%)	115 (95%)	4 (3%)	2 (2%)	7	27
13	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
14	N	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
15	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
16	P	79/82 (96%)	77 (98%)	2 (2%)	0	100	100
17	Q	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
18	R	64/75 (85%)	60 (94%)	4 (6%)	0	100	100
19	S	82/92 (89%)	75 (92%)	7 (8%)	0	100	100
20	T	84/87 (97%)	84 (100%)	0	0	100	100
21	U	68/71 (96%)	68 (100%)	0	0	100	100
24	c	269/273 (98%)	259 (96%)	10 (4%)	0	100	100
25	d	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	25	56
26	e	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
27	f	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
28	g	174/177 (98%)	157 (90%)	16 (9%)	1 (1%)	22	52
29	h	39/149 (26%)	34 (87%)	5 (13%)	0	100	100
30	i	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
31	j	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
32	k	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
33	l	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
34	m	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
35	n	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
36	o	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
37	p	115/118 (98%)	115 (100%)	0	0	100	100
38	q	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
39	r	108/110 (98%)	108 (100%)	0	0	100	100
40	s	91/100 (91%)	85 (93%)	6 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	t	100/104 (96%)	93 (93%)	7 (7%)	0	100	100
42	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
43	v	76/85 (89%)	74 (97%)	2 (3%)	0	100	100
44	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
45	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
46	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
47	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
48	0	49/55 (89%)	49 (100%)	0	0	100	100
49	1	44/46 (96%)	44 (100%)	0	0	100	100
50	2	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
51	3	36/38 (95%)	36 (100%)	0	0	100	100
52	4	56/70 (80%)	53 (95%)	3 (5%)	0	100	100
All	All	5486/5913 (93%)	5289 (96%)	190 (4%)	7 (0%)	50	77

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	g	47	ASP
10	J	57	VAL
12	L	89	ASP
25	d	149	ASN
11	K	120	GLY
11	K	119	ASP
12	L	88	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	186/199 (94%)	185 (100%)	1 (0%)	86	96
3	C	170/190 (90%)	169 (99%)	1 (1%)	84	95

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	172/173 (99%)	172 (100%)	0	100	100
5	E	119/126 (94%)	118 (99%)	1 (1%)	79	93
6	F	90/116 (78%)	90 (100%)	0	100	100
7	G	126/147 (86%)	126 (100%)	0	100	100
8	H	104/105 (99%)	103 (99%)	1 (1%)	73	91
9	I	105/107 (98%)	104 (99%)	1 (1%)	73	91
10	J	86/90 (96%)	86 (100%)	0	100	100
11	K	90/99 (91%)	89 (99%)	1 (1%)	70	90
12	L	103/104 (99%)	103 (100%)	0	100	100
13	M	93/96 (97%)	93 (100%)	0	100	100
14	N	83/84 (99%)	83 (100%)	0	100	100
15	O	76/77 (99%)	76 (100%)	0	100	100
16	P	65/65 (100%)	65 (100%)	0	100	100
17	Q	73/78 (94%)	73 (100%)	0	100	100
18	R	57/65 (88%)	57 (100%)	0	100	100
19	S	72/79 (91%)	71 (99%)	1 (1%)	62	86
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	60/61 (98%)	59 (98%)	1 (2%)	56	83
24	c	216/218 (99%)	215 (100%)	1 (0%)	86	96
25	d	163/163 (100%)	163 (100%)	0	100	100
26	e	165/165 (100%)	164 (99%)	1 (1%)	84	95
27	f	148/150 (99%)	148 (100%)	0	100	100
28	g	137/138 (99%)	137 (100%)	0	100	100
29	h	32/114 (28%)	32 (100%)	0	100	100
30	i	116/116 (100%)	116 (100%)	0	100	100
31	j	104/104 (100%)	104 (100%)	0	100	100
32	k	103/103 (100%)	103 (100%)	0	100	100
33	l	109/109 (100%)	106 (97%)	3 (3%)	38	73
34	m	98/103 (95%)	98 (100%)	0	100	100
35	n	86/87 (99%)	86 (100%)	0	100	100
36	o	99/100 (99%)	99 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	p	89/90 (99%)	89 (100%)	0	100	100
38	q	84/84 (100%)	84 (100%)	0	100	100
39	r	93/93 (100%)	93 (100%)	0	100	100
40	s	80/84 (95%)	80 (100%)	0	100	100
41	t	83/85 (98%)	83 (100%)	0	100	100
42	u	78/78 (100%)	78 (100%)	0	100	100
43	v	58/63 (92%)	58 (100%)	0	100	100
44	w	67/68 (98%)	67 (100%)	0	100	100
45	x	54/55 (98%)	54 (100%)	0	100	100
46	y	48/49 (98%)	48 (100%)	0	100	100
47	z	47/48 (98%)	47 (100%)	0	100	100
48	0	46/49 (94%)	46 (100%)	0	100	100
49	1	38/38 (100%)	37 (97%)	1 (3%)	41	74
50	2	51/52 (98%)	51 (100%)	0	100	100
51	3	34/34 (100%)	33 (97%)	1 (3%)	37	72
52	4	55/62 (89%)	55 (100%)	0	100	100
All	All	4576/4829 (95%)	4561 (100%)	15 (0%)	90	97

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	128	LYS
3	C	127	ARG
5	E	148	ASN
8	H	69	LYS
9	I	106	ARG
11	K	119	ASP
19	S	44	MET
21	U	7	ARG
24	c	214	ARG
26	e	88	ARG
33	l	81	ARG
33	l	82	MET
33	l	84	LYS
49	1	25	LYS
51	3	12	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	148	ASN
9	I	126	GLN
16	P	63	GLN
19	S	57	HIS
45	x	58	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1513/1519 (99%)	220 (14%)	4 (0%)
22	a	2745/2753 (99%)	361 (13%)	0
23	b	118/119 (99%)	14 (11%)	0
53	X	2/3 (66%)	0	0
54	V	73/75 (97%)	14 (19%)	0
All	All	4451/4469 (99%)	609 (13%)	4 (0%)

All (609) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	U
1	A	6	G
1	A	7	A
1	A	9	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	58	C
1	A	71	A
1	A	74	A
1	A	81	A
1	A	83	C
1	A	84	U
1	A	85	U
1	A	86	G
1	A	87	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	88	U
1	A	94	G
1	A	95	C
1	A	121	U
1	A	122	G
1	A	130	A
1	A	131	A
1	A	141	G
1	A	143	A
1	A	144	G
1	A	159	G
1	A	163	C
1	A	164	G
1	A	177	G
1	A	182	A
1	A	183	C
1	A	197	A
1	A	202	G
1	A	226	G
1	A	240	G
1	A	245	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	280	C
1	A	289	G
1	A	321	A
1	A	328	C
1	A	344	A
1	A	347	G
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	388	G
1	A	389	A
1	A	390	U
1	A	393	A
1	A	404	G
1	A	406	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	411	A
1	A	412	A
1	A	413	G
1	A	414	A
1	A	415	A
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	429	U
1	A	435	A
1	A	438	U
1	A	448	A
1	A	453	G
1	A	456	A
1	A	457	G
1	A	458	U
1	A	463	U
1	A	465	A
1	A	467	U
1	A	468	A
1	A	469	C
1	A	478	A
1	A	479	U
1	A	481	G
1	A	484	G
1	A	486	U
1	A	497	G
1	A	509	A
1	A	511	C
1	A	512	U
1	A	513	C
1	A	518	C
1	A	519	C
1	A	521	G
1	A	527	G
1	A	531	U
1	A	533	A
1	A	547	A
1	A	564	C
1	A	572	A
1	A	573	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	576	C
1	A	577	G
1	A	579	A
1	A	588	G
1	A	596	A
1	A	620	C
1	A	633	G
1	A	650	G
1	A	665	A
1	A	687	A
1	A	703	G
1	A	721	G
1	A	723	U
1	A	724	G
1	A	734	G
1	A	746	A
1	A	747	A
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	821	G
1	A	851	G
1	A	889	A
1	A	890	G
1	A	902	G
1	A	914	A
1	A	926	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	966	2MG
1	A	969	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	983	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	992	U
1	A	1004	A
1	A	1009	U
1	A	1027	C
1	A	1028	C
1	A	1030	U
1	A	1031	C
1	A	1033	G
1	A	1034	G
1	A	1036	A
1	A	1039	G
1	A	1042	A
1	A	1044	A
1	A	1064	G
1	A	1065	U
1	A	1085	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1108	G
1	A	1137	C
1	A	1139	G
1	A	1152	A
1	A	1159	U
1	A	1168	U
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1214	C
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1257	A
1	A	1260	G
1	A	1275	A
1	A	1280	A
1	A	1286	U
1	A	1287	A
1	A	1297	G
1	A	1300	G
1	A	1302	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1305	G
1	A	1317	C
1	A	1320	C
1	A	1322	C
1	A	1363	A
1	A	1364	U
1	A	1370	G
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1398	A
1	A	1419	G
1	A	1429	A
1	A	1441	A
1	A	1446	A
1	A	1451	U
1	A	1452	C
1	A	1453	G
1	A	1484	C
1	A	1487	G
1	A	1491	G
1	A	1492	A
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1499	A
1	A	1503	A
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
22	a	10	A
22	a	15	G
22	a	23	G
22	a	34	U
22	a	45	G
22	a	51	G
22	a	58	G
22	a	61	C
22	a	63	A
22	a	71	A
22	a	74	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	75	G
22	a	84	A
22	a	96	C
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	142	A
22	a	149	A
22	a	163	C
22	a	164	C
22	a	181	A
22	a	196	A
22	a	199	A
22	a	200	U
22	a	204	A
22	a	215	G
22	a	216	A
22	a	221	A
22	a	222	A
22	a	248	G
22	a	264	C
22	a	265	A
22	a	272	A
22	a	274	C
22	a	278	A
22	a	285	G
22	a	287	G
22	a	294	A
22	a	311	A
22	a	329	G
22	a	330	A
22	a	345	A
22	a	361	G
22	a	362	A
22	a	386	G
22	a	396	G
22	a	405	U
22	a	411	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	412	A
22	a	420	C
22	a	481	G
22	a	489	G
22	a	491	G
22	a	504	A
22	a	505	A
22	a	509	C
22	a	531	C
22	a	532	A
22	a	544	C
22	a	545	U
22	a	546	U
22	a	547	A
22	a	549	G
22	a	563	A
22	a	573	U
22	a	575	A
22	a	603	A
22	a	615	U
22	a	627	A
22	a	634	C
22	a	637	A
22	a	645	C
22	a	647	G
22	a	654	A
22	a	655	A
22	a	686	U
22	a	717	C
22	a	730	A
22	a	738	G
22	a	747	5MU
22	a	764	A
22	a	775	G
22	a	776	G
22	a	782	A
22	a	784	G
22	a	785	G
22	a	788	A
22	a	789	A
22	a	792	A
22	a	800	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	805	G
22	a	806	C
22	a	812	C
22	a	827	U
22	a	828	U
22	a	829	A
22	a	845	A
22	a	846	U
22	a	847	U
22	a	856	G
22	a	859	G
22	a	866	A
22	a	869	G
22	a	881	G
22	a	883	G
22	a	884	U
22	a	888	C
22	a	890	C
22	a	891	G
22	a	895	U
22	a	896	A
22	a	897	C
22	a	899	A
22	a	910	A
22	a	931	U
22	a	932	U
22	a	945	A
22	a	946	C
22	a	961	C
22	a	973	A
22	a	974	G
22	a	983	A
22	a	989	G
22	a	996	A
22	a	1005	C
22	a	1012	U
22	a	1013	C
22	a	1022	G
22	a	1033	U
22	a	1040	A
22	a	1041	G
22	a	1045	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	1046	A
22	a	1047	G
22	a	1048	A
22	a	1051	G
22	a	1108	U
22	a	1111	A
22	a	1112	G
22	a	1115	G
22	a	1116	G
22	a	1122	G
22	a	1130	U
22	a	1132	U
22	a	1133	A
22	a	1135	C
22	a	1141	U
22	a	1142	A
22	a	1204	A
22	a	1236	G
22	a	1250	G
22	a	1253	A
22	a	1256	G
22	a	1257	C
22	a	1271	G
22	a	1272	A
22	a	1273	U
22	a	1275	A
22	a	1300	G
22	a	1301	A
22	a	1321	A
22	a	1352	U
22	a	1365	A
22	a	1378	A
22	a	1379	U
22	a	1383	A
22	a	1403	A
22	a	1416	G
22	a	1419	A
22	a	1427	A
22	a	1428	C
22	a	1437	C
22	a	1452	G
22	a	1459	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	1482	G
22	a	1493	C
22	a	1509	A
22	a	1510	G
22	a	1515	A
22	a	1524	G
22	a	1529	G
22	a	1534	U
22	a	1535	A
22	a	1536	C
22	a	1537	G
22	a	1554	U
22	a	1559	U
22	a	1566	A
22	a	1567	G
22	a	1569	A
22	a	1583	A
22	a	1584	U
22	a	1585	C
22	a	1607	C
22	a	1608	A
22	a	1610	A
22	a	1647	U
22	a	1648	U
22	a	1649	G
22	a	1674	G
22	a	1675	C
22	a	1698	A
22	a	1715	G
22	a	1729	U
22	a	1730	C
22	a	1731	G
22	a	1732	C
22	a	1738	G
22	a	1764	C
22	a	1773	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	1829	A
22	a	1842	G
22	a	1847	A
22	a	1858	A
22	a	1866	A
22	a	1869	G
22	a	1870	C
22	a	1871	A
22	a	1872	A
22	a	1873	G
22	a	1906	G
22	a	1907	G
22	a	1913	A
22	a	1929	G
22	a	1930	G
22	a	1936	A
22	a	1937	A
22	a	1938	A
22	a	1955	U
22	a	1964	G
22	a	1966	A
22	a	1967	C
22	a	1970	A
22	a	1971	U
22	a	1972	G
22	a	1982	U
22	a	1991	U
22	a	1993	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	2049	G
22	a	2055	C
22	a	2056	G
22	a	2060	A
22	a	2061	G
22	a	2062	A
22	a	2069	G7M
22	a	2077	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	2093	G
22	a	2198	A
22	a	2199	A
22	a	2203	U
22	a	2204	G
22	a	2211	A
22	a	2225	A
22	a	2238	G
22	a	2239	G
22	a	2266	A
22	a	2283	C
22	a	2287	A
22	a	2288	A
22	a	2305	U
22	a	2308	G
22	a	2322	A
22	a	2325	G
22	a	2333	A
22	a	2334	U
22	a	2336	A
22	a	2340	A
22	a	2345	G
22	a	2347	C
22	a	2350	C
22	a	2361	G
22	a	2377	A
22	a	2383	G
22	a	2385	C
22	a	2391	G
22	a	2396	G
22	a	2402	U
22	a	2403	C
22	a	2406	A
22	a	2422	C
22	a	2425	A
22	a	2426	A
22	a	2429	G
22	a	2431	U
22	a	2435	A
22	a	2441	U
22	a	2445	2MG
22	a	2448	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	2470	G
22	a	2475	C
22	a	2476	A
22	a	2491	U
22	a	2498	OMC
22	a	2502	G
22	a	2504	PSU
22	a	2505	G
22	a	2507	C
22	a	2513	A
22	a	2518	A
22	a	2520	C
22	a	2525	G
22	a	2529	G
22	a	2535	G
22	a	2547	A
22	a	2566	A
22	a	2567	G
22	a	2573	C
22	a	2585	U
22	a	2586	U
22	a	2601	C
22	a	2602	A
22	a	2609	U
22	a	2613	U
22	a	2615	U
22	a	2629	U
22	a	2663	G
22	a	2682	A
22	a	2685	G
22	a	2689	U
22	a	2690	U
22	a	2714	G
22	a	2724	U
22	a	2726	A
22	a	2732	G
22	a	2733	A
22	a	2744	G
22	a	2748	A
22	a	2752	C
22	a	2757	A
22	a	2765	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	a	2778	A
22	a	2791	G
22	a	2798	U
22	a	2799	A
22	a	2818	U
22	a	2820	A
22	a	2821	A
22	a	2835	A
22	a	2836	U
22	a	2849	U
22	a	2861	U
22	a	2873	A
22	a	2884	U
22	a	2891	U
23	b	9	G
23	b	13	G
23	b	24	G
23	b	33	G
23	b	35	C
23	b	41	G
23	b	45	A
23	b	56	G
23	b	67	G
23	b	89	U
23	b	90	C
23	b	99	A
23	b	105	G
23	b	109	A
54	V	3	G
54	V	4	C
54	V	5	A
54	V	8	U
54	V	9	A
54	V	10	G
54	V	20	U
54	V	21	A
54	V	47	U
54	V	48	C
54	V	49	G
54	V	53	G
54	V	74	C
54	V	76	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	196	A
1	A	411	A
1	A	1035	A

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

34 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	PSU	a	1911	22	18,21,22	1.08	1 (5%)	22,30,33	1.79	4 (18%)
22	6MZ	a	1618	22	18,25,26	1.92	2 (11%)	16,36,39	2.12	3 (18%)
22	PSU	a	1917	22	18,21,22	0.98	1 (5%)	22,30,33	1.61	4 (18%)
22	OMC	a	2498	55,22	19,22,23	2.76	7 (36%)	26,31,34	1.07	1 (3%)
1	UR3	A	1498	1	19,22,23	2.54	6 (31%)	26,32,35	1.32	1 (3%)
22	PSU	a	2457	22	18,21,22	1.02	1 (5%)	22,30,33	1.92	4 (18%)
22	5MC	a	1962	22	18,22,23	3.31	7 (38%)	26,32,35	0.99	1 (3%)
1	2MG	A	966	1	18,26,27	2.23	7 (38%)	16,38,41	1.46	4 (25%)
22	G7M	a	2069	22	20,26,27	2.59	7 (35%)	17,39,42	1.19	1 (5%)
22	PSU	a	2604	22	18,21,22	1.04	1 (5%)	22,30,33	1.82	4 (18%)
22	2MG	a	1835	22	18,26,27	2.11	7 (38%)	16,38,41	1.70	4 (25%)
1	PSU	A	516	1,55	18,21,22	0.90	1 (5%)	22,30,33	1.61	4 (18%)
1	MA6	A	1519	1	18,26,27	1.09	1 (5%)	19,38,41	4.72	3 (15%)
22	OMG	a	2251	54,22	18,26,27	2.35	8 (44%)	19,38,41	1.53	4 (21%)
22	2MG	a	2445	22	18,26,27	2.09	7 (38%)	16,38,41	1.63	4 (25%)
22	PSU	a	746	55,22	18,21,22	1.08	2 (11%)	22,30,33	1.78	4 (18%)
1	2MG	A	1207	1	18,26,27	2.25	7 (38%)	16,38,41	1.44	3 (18%)
25	MEQ	d	150	25	8,9,10	0.89	0	5,10,12	0.81	0
22	1MG	a	745	22	18,26,27	2.61	5 (27%)	19,39,42	1.55	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MA6	A	1518	1	18,26,27	1.15	2 (11%)	19,38,41	4.54	3 (15%)
22	3TD	a	1915	22	18,22,23	4.01	6 (33%)	22,32,35	1.75	3 (13%)
22	5MU	a	1939	22	19,22,23	7.08	8 (42%)	28,32,35	3.59	10 (35%)
22	PSU	a	2504	22	18,21,22	1.02	2 (11%)	22,30,33	1.52	3 (13%)
1	5MC	A	1407	1	18,22,23	3.39	7 (38%)	26,32,35	1.10	1 (3%)
22	PSU	a	2605	22	18,21,22	1.13	2 (11%)	22,30,33	1.79	3 (13%)
1	2MG	A	1516	1	18,26,27	2.15	7 (38%)	16,38,41	1.49	4 (25%)
22	2MA	a	2503	55,22	17,25,26	2.11	4 (23%)	17,37,40	1.33	2 (11%)
22	5MU	a	747	22	19,22,23	7.18	8 (42%)	28,32,35	3.59	10 (35%)
22	OMU	a	2552	22	19,22,23	2.68	6 (31%)	26,31,34	1.76	4 (15%)
22	PSU	a	955	22	18,21,22	1.04	1 (5%)	22,30,33	1.84	4 (18%)
1	4OC	A	1402	1	20,23,24	3.01	8 (40%)	26,32,35	0.91	1 (3%)
22	6MZ	a	2030	22	18,25,26	1.99	2 (11%)	16,36,39	2.41	3 (18%)
22	PSU	a	2580	22	18,21,22	1.09	2 (11%)	22,30,33	1.83	5 (22%)
1	5MC	A	967	1	18,22,23	3.51	7 (38%)	26,32,35	0.96	1 (3%)

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	PSU	a	1911	22	-	2/7/25/26	0/2/2/2
22	6MZ	a	1618	22	-	0/5/27/28	0/3/3/3
22	PSU	a	1917	22	-	0/7/25/26	0/2/2/2
22	OMC	a	2498	55,22	-	2/9/27/28	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
22	PSU	a	2457	22	-	0/7/25/26	0/2/2/2
22	5MC	a	1962	22	-	0/7/25/26	0/2/2/2
1	2MG	A	966	1	-	2/5/27/28	0/3/3/3
22	G7M	a	2069	22	-	2/3/25/26	0/3/3/3
22	PSU	a	2604	22	-	0/7/25/26	0/2/2/2
22	2MG	a	1835	22	-	0/5/27/28	0/3/3/3
1	PSU	A	516	1,55	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	2/7/29/30	0/3/3/3
22	OMG	a	2251	54,22	-	1/5/27/28	0/3/3/3
22	2MG	a	2445	22	-	2/5/27/28	0/3/3/3
22	PSU	a	746	55,22	-	1/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
25	MEQ	d	150	25	-	5/8/9/11	-
22	1MG	a	745	22	-	0/3/25/26	0/3/3/3
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
22	3TD	a	1915	22	-	2/7/25/26	0/2/2/2
22	5MU	a	1939	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2504	22	-	0/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
1	2MG	A	1516	1	-	0/5/27/28	0/3/3/3
22	2MA	a	2503	55,22	-	1/3/25/26	0/3/3/3
22	5MU	a	747	22	-	0/7/25/26	0/2/2/2
22	OMU	a	2552	22	-	0/9/27/28	0/2/2/2
22	PSU	a	955	22	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
22	6MZ	a	2030	22	-	2/5/27/28	0/3/3/3
22	PSU	a	2580	22	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2

All (150) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	747	5MU	C4-C5	20.44	1.78	1.44
22	a	1939	5MU	C4-C5	20.09	1.78	1.44
22	a	747	5MU	C6-N1	16.16	1.65	1.38
22	a	1939	5MU	C6-N1	15.78	1.65	1.38
22	a	1915	3TD	C6-C5	12.07	1.49	1.35
22	a	747	5MU	C4-N3	-11.48	1.17	1.38
22	a	1939	5MU	C6-C5	-11.23	1.16	1.34
22	a	1939	5MU	C4-N3	-11.09	1.18	1.38
22	a	747	5MU	C6-C5	-10.88	1.16	1.34
1	A	967	5MC	C6-C5	9.03	1.49	1.34
1	A	1407	5MC	C6-C5	8.80	1.49	1.34
22	a	1915	3TD	C2-N1	8.47	1.48	1.37
22	a	1962	5MC	C6-C5	8.20	1.48	1.34
22	a	2030	6MZ	C6-N6	6.97	1.46	1.35
22	a	1618	6MZ	C6-N6	6.79	1.46	1.35
1	A	1402	4OC	C4-N3	6.55	1.44	1.32
22	a	745	1MG	C2-N3	6.55	1.46	1.34
1	A	1498	UR3	C2-N1	6.45	1.47	1.38
1	A	967	5MC	C4-N3	6.40	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2552	OMU	C2-N1	6.25	1.48	1.38
22	a	2503	2MA	C2-N3	6.23	1.44	1.31
22	a	2069	G7M	C2-N2	6.19	1.48	1.34
1	A	1402	4OC	C6-C5	6.16	1.49	1.35
22	a	1962	5MC	C4-N3	6.15	1.44	1.34
1	A	967	5MC	C2-N3	6.05	1.48	1.36
22	a	2552	OMU	C2-N3	5.87	1.48	1.38
1	A	1407	5MC	C4-N3	5.87	1.44	1.34
22	a	1962	5MC	C2-N3	5.85	1.48	1.36
1	A	1498	UR3	C6-C5	5.83	1.48	1.35
22	a	2498	OMC	C6-C5	5.80	1.48	1.35
1	A	1407	5MC	C2-N3	5.78	1.48	1.36
1	A	1402	4OC	C2-N3	5.76	1.48	1.36
22	a	1915	3TD	C6-N1	5.74	1.45	1.36
22	a	745	1MG	C2-N2	5.64	1.44	1.34
22	a	2498	OMC	C2-N3	5.63	1.47	1.36
22	a	2552	OMU	C6-C5	5.54	1.47	1.35
1	A	1207	2MG	C2-N2	5.29	1.45	1.33
1	A	966	2MG	C2-N2	5.23	1.45	1.33
22	a	2069	G7M	C2-N3	5.13	1.45	1.33
1	A	1516	2MG	C2-N2	5.06	1.44	1.33
22	a	745	1MG	C4-N3	5.01	1.49	1.37
22	a	2251	OMG	C2-N3	4.84	1.45	1.33
22	a	2069	G7M	C4-N3	4.74	1.48	1.37
22	a	2445	2MG	C2-N2	4.72	1.43	1.33
22	a	1835	2MG	C2-N2	4.72	1.43	1.33
22	a	747	5MU	C2-N3	4.65	1.46	1.38
22	a	1939	5MU	C2-N3	4.50	1.46	1.38
22	a	2251	OMG	C4-N3	4.50	1.48	1.37
1	A	967	5MC	C6-N1	4.48	1.45	1.38
1	A	1407	5MC	C6-N1	4.36	1.45	1.38
22	a	2498	OMC	C4-N4	4.36	1.44	1.33
1	A	1498	UR3	C2-N3	4.35	1.47	1.39
22	a	1915	3TD	C2-N3	4.34	1.48	1.38
1	A	1402	4OC	C4-N4	4.32	1.44	1.35
22	a	2498	OMC	C2-N1	4.27	1.49	1.40
1	A	1407	5MC	C4-N4	4.25	1.45	1.34
1	A	967	5MC	C4-N4	4.24	1.45	1.34
22	a	2498	OMC	C4-N3	4.23	1.43	1.34
22	a	2251	OMG	C2-N2	4.22	1.44	1.34
22	a	1962	5MC	C4-N4	4.15	1.44	1.34
22	a	1962	5MC	C6-N1	4.07	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2069	G7M	C6-N1	4.04	1.43	1.37
22	a	2503	2MA	C4-N3	4.02	1.47	1.37
1	A	967	5MC	C2-N1	3.86	1.48	1.40
1	A	966	2MG	C4-N3	3.84	1.46	1.37
1	A	1207	2MG	C4-N3	3.84	1.46	1.37
1	A	1402	4OC	C2-N1	3.83	1.48	1.40
1	A	1402	4OC	C5-C4	3.60	1.48	1.40
1	A	966	2MG	C6-N1	3.55	1.43	1.37
1	A	1407	5MC	C2-N1	3.51	1.47	1.40
1	A	966	2MG	C2-N1	3.47	1.42	1.36
1	A	1207	2MG	C6-N1	3.47	1.43	1.37
22	a	1835	2MG	C6-N1	3.46	1.43	1.37
1	A	1207	2MG	C2-N1	3.43	1.42	1.36
22	a	1962	5MC	C2-N1	3.36	1.47	1.40
1	A	1516	2MG	C6-N1	3.31	1.42	1.37
22	a	1962	5MC	O2-C2	-3.30	1.17	1.23
1	A	1516	2MG	C4-N3	3.29	1.45	1.37
22	a	2498	OMC	O2-C2	-3.27	1.17	1.23
22	a	1911	PSU	C6-C5	3.23	1.39	1.35
22	a	1835	2MG	C4-N3	3.15	1.45	1.37
1	A	1407	5MC	O2-C2	-3.15	1.17	1.23
22	a	2251	OMG	C5-C4	-3.15	1.35	1.43
22	a	1835	2MG	C5-C4	-3.10	1.35	1.43
1	A	1516	2MG	C2-N1	3.10	1.41	1.36
22	a	2030	6MZ	C5-C4	-3.10	1.32	1.40
22	a	2445	2MG	C5-C4	-3.09	1.35	1.43
22	a	2445	2MG	C4-N3	3.09	1.44	1.37
22	a	1939	5MU	O2-C2	-3.09	1.17	1.23
1	A	1402	4OC	O2-C2	-3.07	1.18	1.23
22	a	1939	5MU	O4-C4	-3.06	1.17	1.23
22	a	2069	G7M	C5-C6	3.04	1.53	1.45
1	A	1402	4OC	C6-N1	3.02	1.45	1.38
22	a	2605	PSU	C6-C5	2.97	1.38	1.35
1	A	1519	MA6	C5-C4	-2.97	1.33	1.40
22	a	2552	OMU	O2-C2	-2.95	1.17	1.23
22	a	2445	2MG	C2-N1	2.95	1.41	1.36
22	a	747	5MU	O2-C2	-2.94	1.17	1.23
22	a	1835	2MG	C2-N1	2.94	1.41	1.36
22	a	1917	PSU	C6-C5	2.93	1.38	1.35
22	a	2445	2MG	C6-N1	2.92	1.42	1.37
22	a	745	1MG	C5-C4	-2.92	1.35	1.43
22	a	747	5MU	O4-C4	-2.89	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2251	OMG	C6-N1	2.89	1.42	1.37
22	a	2503	2MA	C5-C4	-2.89	1.35	1.43
22	a	1939	5MU	C2-N1	2.87	1.43	1.38
22	a	2552	OMU	O4-C4	-2.87	1.18	1.24
22	a	1618	6MZ	C5-C4	-2.86	1.33	1.40
1	A	1516	2MG	C5-C4	-2.84	1.35	1.43
1	A	1518	MA6	C5-C4	-2.80	1.33	1.40
22	a	2552	OMU	C4-N3	2.78	1.43	1.38
1	A	967	5MC	O2-C2	-2.75	1.18	1.23
22	a	2251	OMG	O6-C6	-2.66	1.17	1.23
22	a	2069	G7M	C2-N1	2.66	1.44	1.37
1	A	1207	2MG	CM2-N2	2.65	1.50	1.45
22	a	2445	2MG	O6-C6	-2.60	1.18	1.23
1	A	1498	UR3	C6-N1	2.59	1.44	1.38
22	a	2503	2MA	C2-N1	2.58	1.44	1.36
22	a	2498	OMC	C6-N1	2.58	1.44	1.38
22	a	747	5MU	C2-N1	2.58	1.42	1.38
22	a	1835	2MG	O6-C6	-2.54	1.18	1.23
22	a	2604	PSU	C6-C5	2.53	1.38	1.35
22	a	1915	3TD	C4-N3	2.52	1.45	1.40
22	a	2580	PSU	O4'-C1'	-2.52	1.40	1.43
1	A	1516	2MG	CM2-N2	2.47	1.50	1.45
1	A	966	2MG	CM2-N2	2.46	1.50	1.45
1	A	1516	2MG	O6-C6	-2.46	1.18	1.23
1	A	516	PSU	C6-C5	2.46	1.38	1.35
1	A	1498	UR3	O2-C2	-2.46	1.18	1.22
1	A	1207	2MG	C5-C4	-2.46	1.36	1.43
22	a	955	PSU	C6-C5	2.44	1.38	1.35
22	a	2069	G7M	O6-C6	-2.42	1.18	1.23
22	a	1835	2MG	CM2-N2	2.41	1.49	1.45
1	A	1498	UR3	O4-C4	-2.40	1.18	1.23
22	a	746	PSU	C6-C5	2.39	1.38	1.35
22	a	745	1MG	O6-C6	-2.39	1.17	1.22
1	A	966	2MG	O6-C6	-2.39	1.18	1.23
1	A	966	2MG	C5-C4	-2.39	1.37	1.43
1	A	1207	2MG	O6-C6	-2.37	1.18	1.23
22	a	2605	PSU	C4-C5	-2.37	1.37	1.44
22	a	746	PSU	C4-C5	-2.32	1.37	1.44
22	a	2445	2MG	CM2-N2	2.26	1.49	1.45
22	a	2251	OMG	C5-C6	2.24	1.52	1.47
22	a	2504	PSU	C6-C5	2.22	1.37	1.35
22	a	2457	PSU	C4-C5	-2.18	1.37	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1915	3TD	O4-C4	-2.18	1.18	1.23
22	a	2504	PSU	C4-C5	-2.16	1.38	1.44
22	a	2580	PSU	C4-C5	-2.15	1.38	1.44
1	A	1518	MA6	C2-N3	2.14	1.35	1.32
22	a	2251	OMG	C2-N1	2.03	1.42	1.37

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1519	MA6	N1-C6-N6	-17.44	98.70	117.06
1	A	1518	MA6	N1-C6-N6	-16.39	99.80	117.06
22	a	1939	5MU	C5-C4-N3	11.28	124.94	115.31
22	a	747	5MU	C5-C4-N3	10.65	124.40	115.31
1	A	1518	MA6	C1'-N9-C4	-9.41	110.10	126.64
22	a	747	5MU	C5-C6-N1	-9.36	113.71	123.34
1	A	1519	MA6	C1'-N9-C4	-8.87	111.06	126.64
22	a	1939	5MU	C5-C6-N1	-8.63	114.47	123.34
22	a	1939	5MU	C4-N3-C2	-7.69	117.40	127.35
22	a	747	5MU	C4-N3-C2	-7.51	117.63	127.35
22	a	2030	6MZ	C9-N6-C6	-6.24	117.50	122.87
22	a	1618	6MZ	N3-C2-N1	-5.77	119.65	128.68
1	A	1519	MA6	N3-C2-N1	-5.73	119.72	128.68
22	a	1915	3TD	N1-C2-N3	5.71	120.64	116.14
22	a	2030	6MZ	N3-C2-N1	-5.50	120.08	128.68
22	a	2552	OMU	C4-N3-C2	-5.44	119.40	126.58
1	A	1518	MA6	N3-C2-N1	-5.15	120.63	128.68
22	a	747	5MU	N3-C2-N1	5.14	121.71	114.89
22	a	2457	PSU	C4-N3-C2	-5.10	118.99	126.34
22	a	1939	5MU	O4-C4-C5	-4.98	119.12	124.90
1	A	1498	UR3	C4-N3-C2	-4.92	119.93	124.56
22	a	746	PSU	C4-N3-C2	-4.92	119.25	126.34
22	a	1939	5MU	N3-C2-N1	4.82	121.28	114.89
22	a	2604	PSU	N1-C2-N3	4.77	120.53	115.13
22	a	2605	PSU	C4-N3-C2	-4.76	119.48	126.34
22	a	955	PSU	N1-C2-N3	4.74	120.50	115.13
22	a	2457	PSU	N1-C2-N3	4.73	120.49	115.13
22	a	2580	PSU	N1-C2-N3	4.71	120.46	115.13
22	a	1911	PSU	C4-N3-C2	-4.57	119.75	126.34
22	a	2604	PSU	C4-N3-C2	-4.57	119.76	126.34
22	a	746	PSU	N1-C2-N3	4.56	120.30	115.13
22	a	1911	PSU	N1-C2-N3	4.56	120.30	115.13
22	a	2605	PSU	N1-C2-N3	4.49	120.21	115.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	955	PSU	C4-N3-C2	-4.45	119.92	126.34
22	a	2580	PSU	C4-N3-C2	-4.45	119.93	126.34
22	a	747	5MU	C5M-C5-C6	-4.36	117.03	122.85
22	a	745	1MG	C5-C6-N1	4.29	120.35	113.90
22	a	2552	OMU	N3-C2-N1	4.20	120.47	114.89
1	A	516	PSU	C4-N3-C2	-4.20	120.29	126.34
22	a	1917	PSU	C4-N3-C2	-4.18	120.31	126.34
22	a	1618	6MZ	C9-N6-C6	-4.16	119.29	122.87
22	a	1917	PSU	N1-C2-N3	4.11	119.79	115.13
22	a	1939	5MU	C5M-C5-C6	-4.07	117.42	122.85
22	a	1915	3TD	C4-N3-C2	-4.02	120.25	124.61
22	a	2504	PSU	N1-C2-N3	3.94	119.60	115.13
22	a	747	5MU	C6-C5-C4	3.94	121.32	118.03
22	a	2504	PSU	C4-N3-C2	-3.92	120.69	126.34
22	a	1618	6MZ	C2-N1-C6	3.90	119.93	116.59
22	a	747	5MU	O4-C4-C5	-3.87	120.41	124.90
22	a	2251	OMG	C5-C6-N1	3.83	120.71	113.95
22	a	1835	2MG	CM2-N2-C2	-3.81	115.45	123.86
22	a	2030	6MZ	C2-N1-C6	3.74	119.80	116.59
22	a	2503	2MA	C5-C6-N1	3.65	120.31	114.02
22	a	1835	2MG	C5-C6-N1	3.60	120.31	113.95
1	A	516	PSU	N1-C2-N3	3.59	119.19	115.13
1	A	1207	2MG	C5-C6-N1	3.57	120.26	113.95
22	a	2445	2MG	CM2-N2-C2	-3.57	115.98	123.86
22	a	2445	2MG	C5-C6-N1	3.47	120.08	113.95
22	a	2457	PSU	O2-C2-N1	-3.43	119.02	122.79
22	a	2552	OMU	C5-C4-N3	3.42	119.95	114.84
1	A	1407	5MC	C5-C6-N1	-3.41	119.83	123.34
1	A	966	2MG	C5-C6-N1	3.39	119.93	113.95
1	A	1516	2MG	C5-C6-N1	3.35	119.87	113.95
22	a	955	PSU	O2-C2-N1	-3.33	119.12	122.79
1	A	967	5MC	C5-C6-N1	-3.30	119.94	123.34
22	a	2251	OMG	C2-N1-C6	-3.20	119.20	125.10
22	a	1939	5MU	C6-C5-C4	3.09	120.62	118.03
22	a	955	PSU	C6-N1-C2	-3.03	119.59	122.68
22	a	2498	OMC	O2-C2-N3	-2.98	117.49	122.33
22	a	1939	5MU	C5M-C5-C4	2.91	121.97	118.77
22	a	2445	2MG	C8-N7-C5	2.90	108.51	102.99
1	A	1516	2MG	CM2-N2-C2	-2.88	117.51	123.86
22	a	1835	2MG	C8-N7-C5	2.87	108.45	102.99
22	a	2580	PSU	C6-N1-C2	-2.82	119.80	122.68
22	a	2069	G7M	C2-N1-C6	-2.80	119.95	125.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2580	PSU	O2-C2-N1	-2.78	119.73	122.79
22	a	1911	PSU	O2-C2-N1	-2.73	119.78	122.79
22	a	2552	OMU	O4-C4-C5	-2.69	120.42	125.16
1	A	1207	2MG	C8-N7-C5	2.68	108.10	102.99
22	a	1835	2MG	O6-C6-C5	-2.66	119.18	124.37
1	A	966	2MG	C8-N7-C5	2.65	108.04	102.99
22	a	747	5MU	C5M-C5-C4	2.62	121.65	118.77
22	a	747	5MU	O4-C4-N3	-2.57	115.18	120.12
1	A	1516	2MG	C8-N7-C5	2.56	107.88	102.99
22	a	2604	PSU	O2-C2-N1	-2.56	119.98	122.79
22	a	2504	PSU	C6-N1-C2	-2.55	120.08	122.68
22	a	2251	OMG	O6-C6-C5	-2.53	119.43	124.37
22	a	1911	PSU	C6-N1-C2	-2.52	120.10	122.68
1	A	516	PSU	O2-C2-N1	-2.52	120.02	122.79
22	a	747	5MU	O2-C2-N1	-2.50	119.46	122.79
22	a	1917	PSU	O2-C2-N1	-2.48	120.06	122.79
22	a	1962	5MC	C5-C6-N1	-2.47	120.79	123.34
22	a	746	PSU	O2-C2-N1	-2.46	120.08	122.79
22	a	745	1MG	CM1-N1-C6	2.46	120.91	117.55
22	a	2604	PSU	C6-N1-C2	-2.45	120.18	122.68
22	a	1917	PSU	C6-N1-C2	-2.44	120.19	122.68
1	A	1207	2MG	O6-C6-C5	-2.41	119.66	124.37
22	a	745	1MG	C8-N7-C5	2.39	107.55	102.99
22	a	2605	PSU	C6-N1-C2	-2.39	120.24	122.68
1	A	966	2MG	O6-C6-C5	-2.38	119.71	124.37
22	a	2503	2MA	C8-N7-C5	2.37	107.51	102.99
22	a	2580	PSU	O4'-C1'-C2'	2.36	108.47	105.14
22	a	745	1MG	O6-C6-C5	-2.23	120.24	124.19
1	A	1402	4OC	CM4-N4-C4	-2.22	118.12	122.45
1	A	1516	2MG	O6-C6-C5	-2.21	120.05	124.37
22	a	746	PSU	C6-N1-C2	-2.20	120.43	122.68
22	a	1915	3TD	C6-C5-C4	2.20	119.74	118.22
22	a	1939	5MU	O4-C4-N3	-2.18	115.94	120.12
1	A	516	PSU	C6-N1-C2	-2.16	120.48	122.68
22	a	2251	OMG	C8-N7-C5	2.14	107.07	102.99
1	A	966	2MG	CM2-N2-C2	-2.13	119.17	123.86
22	a	2445	2MG	O6-C6-C5	-2.12	120.23	124.37
22	a	2457	PSU	C6-N1-C2	-2.11	120.52	122.68
22	a	1939	5MU	O2-C2-N1	-2.03	120.09	122.79

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	d	150	MEQ	O-C-CA-CB
22	a	2251	OMG	C1'-C2'-O2'-CM2
22	a	2445	2MG	C3'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
22	a	1915	3TD	O4'-C4'-C5'-O5'
22	a	2030	6MZ	O4'-C4'-C5'-O5'
22	a	2030	6MZ	C3'-C4'-C5'-O5'
22	a	2069	G7M	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
22	a	2069	G7M	C3'-C4'-C5'-O5'
1	A	966	2MG	C3'-C4'-C5'-O5'
22	a	1915	3TD	C3'-C4'-C5'-O5'
1	A	966	2MG	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
22	a	2445	2MG	O4'-C4'-C5'-O5'
22	a	2498	OMC	O4'-C4'-C5'-O5'
25	d	150	MEQ	N-CA-CB-CG
25	d	150	MEQ	C-CA-CB-CG
22	a	1911	PSU	O4'-C1'-C5-C4
25	d	150	MEQ	OE1-CD-CG-CB
22	a	2498	OMC	C3'-C4'-C5'-O5'
22	a	746	PSU	O4'-C1'-C5-C6
22	a	1911	PSU	O4'-C1'-C5-C6
25	d	150	MEQ	NE2-CD-CG-CB
22	a	2503	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 311 ligands modelled in this entry, 310 are monoatomic - leaving 1 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	$\# Z > 2$
56	CLM	a	6206	-	19,20,20	1.08	3 (15%)	23,27,27	1.21	2 (8%)

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
56	CLM	a	6206	-	-	4/20/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	a	6206	CLM	C1-C2	-2.90	1.48	1.53
56	a	6206	CLM	C9-N9	-2.36	1.39	1.45
56	a	6206	CLM	C6-C5	-2.06	1.48	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	a	6206	CLM	O2-C2-C1	-3.08	115.12	121.24
56	a	6206	CLM	C2-C1-CL2	-3.03	103.64	109.61

There are no chirality outliers.

All (4) torsion outliers are listed below:

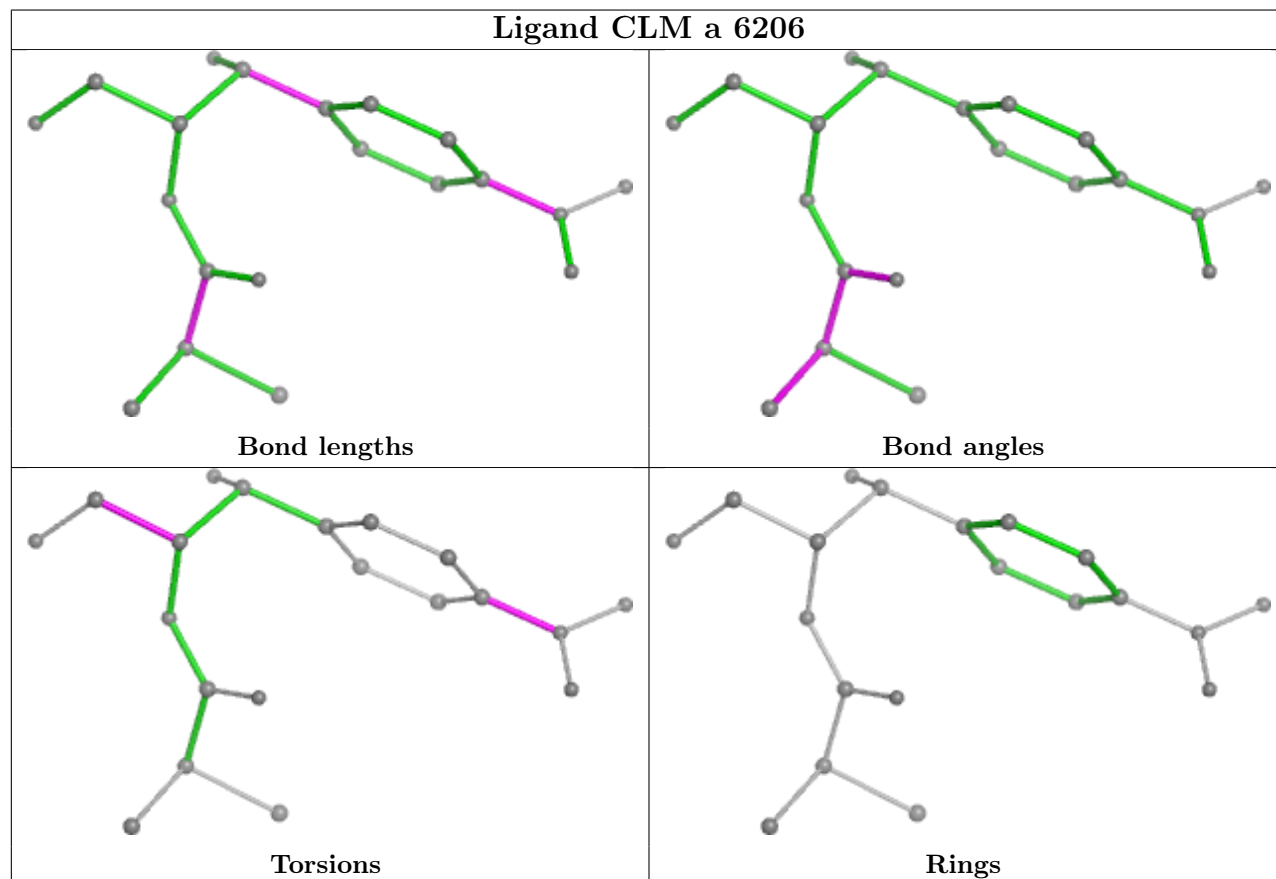
Mol	Chain	Res	Type	Atoms
56	a	6206	CLM	N2-C3-C4-O4
56	a	6206	CLM	C5-C3-C4-O4
56	a	6206	CLM	C8-C9-N9-O9B
56	a	6206	CLM	C10-C9-N9-O9B

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	3

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
1	A	2
54	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	2098:U	O3'	2191:A	P	17.56
1	A	840:C	O3'	846:G	P	17.24
1	a	1052:C	O3'	1107:G	P	17.19
1	A	204:G	O3'	214:C	P	17.13
1	a	1172:C	O3'	1177:G	P	16.62
1	V	16:C	O3'	18:G	P	6.84

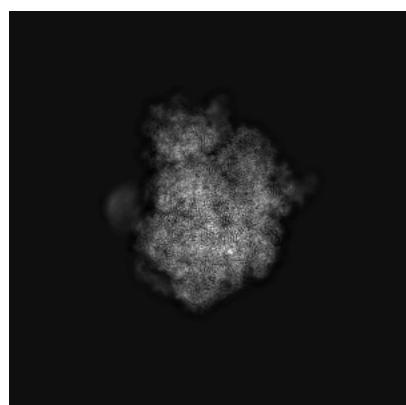
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13180. These allow visual inspection of the internal detail of the map and identification of artifacts.

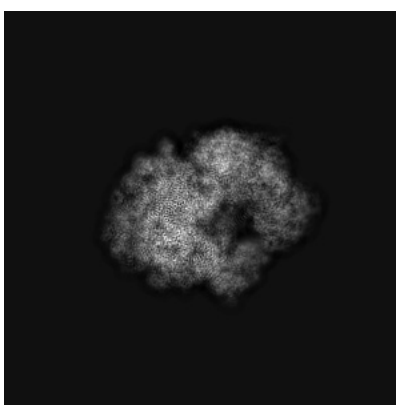
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

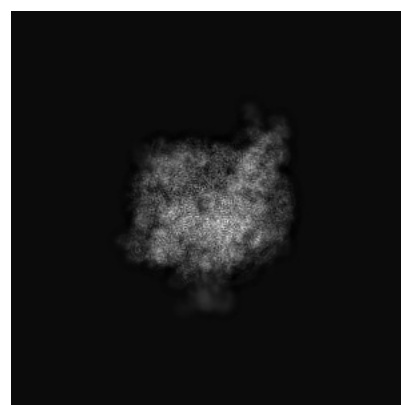
6.1.1 Primary map



X



Y

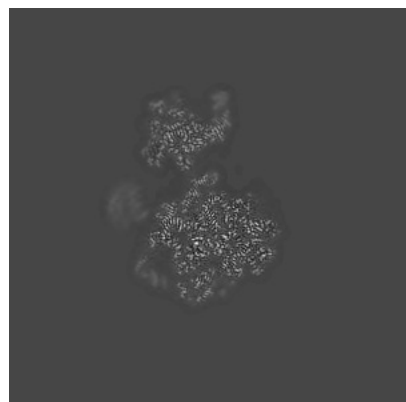


Z

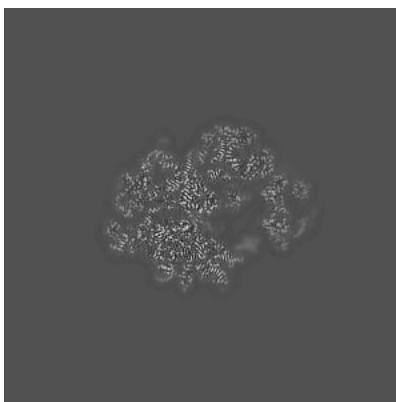
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

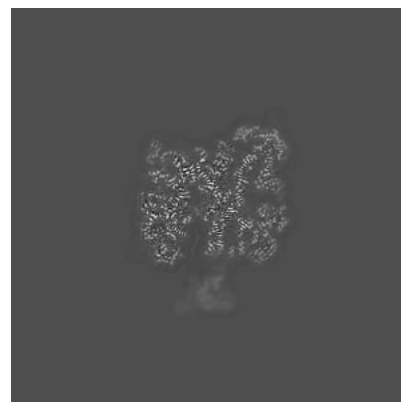
6.2.1 Primary map



X Index: 225



Y Index: 225

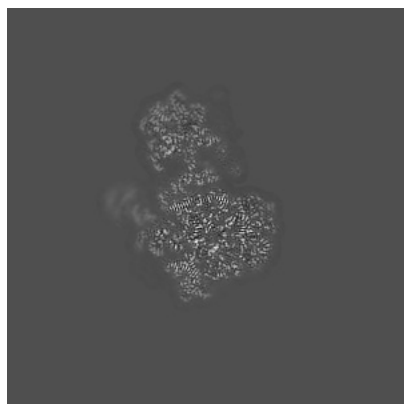


Z Index: 225

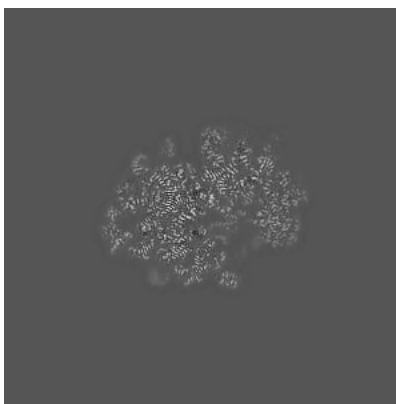
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

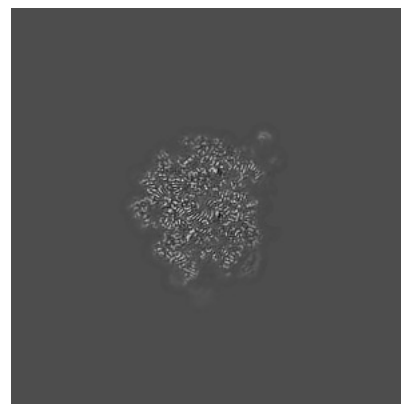
6.3.1 Primary map



X Index: 234



Y Index: 211

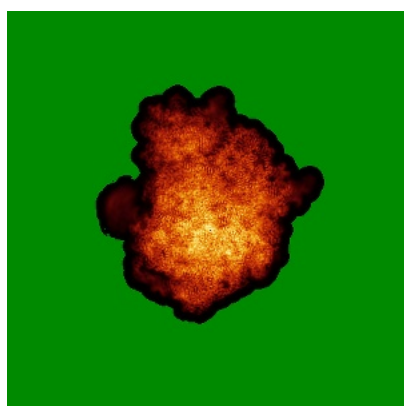


Z Index: 201

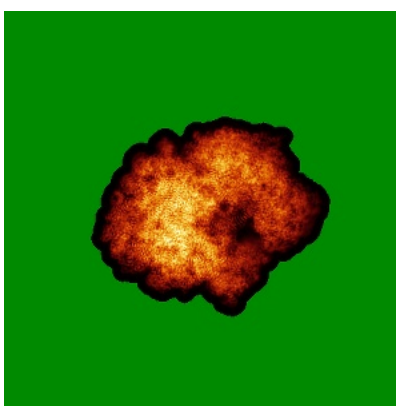
The images above show the largest variance slices of the map in three orthogonal directions.

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

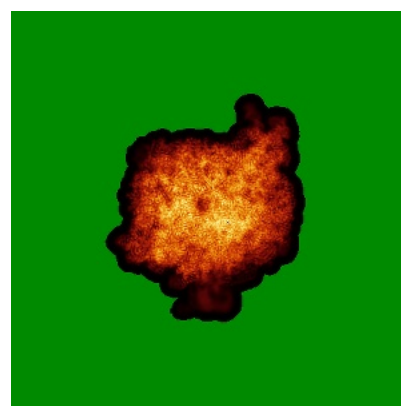
6.4.1 Primary map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

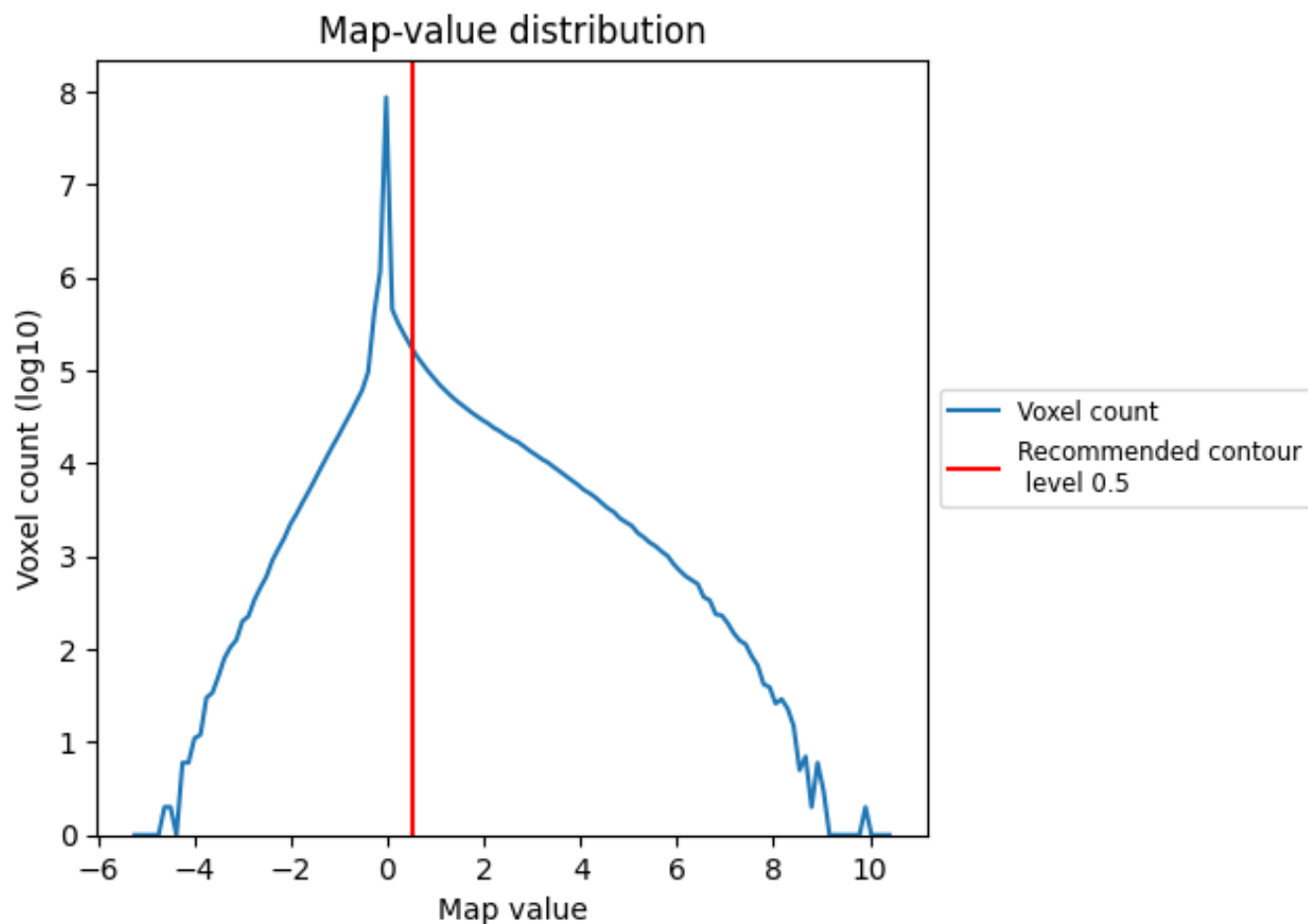
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

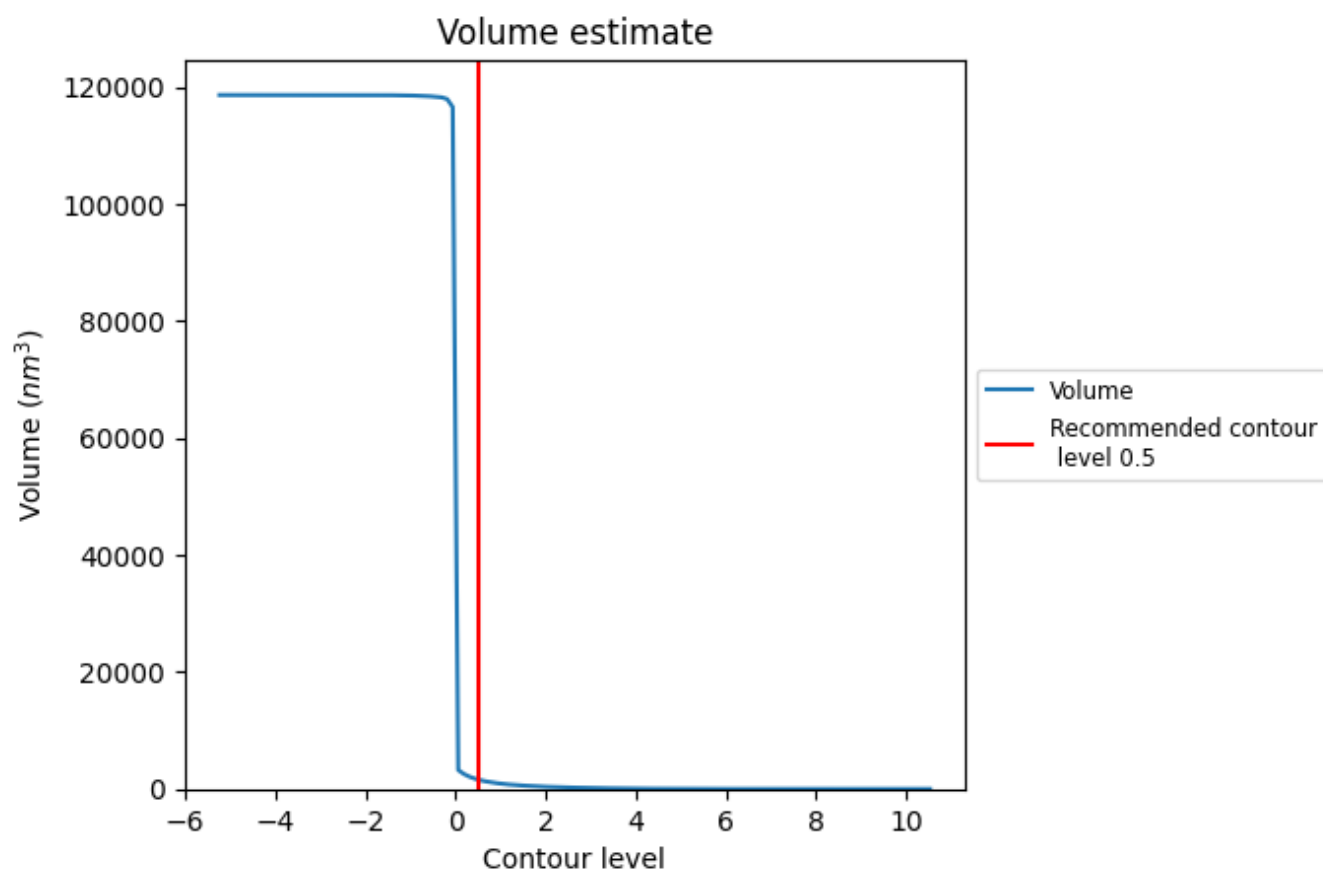
This section contains the results of statistical analysis of the map.

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.

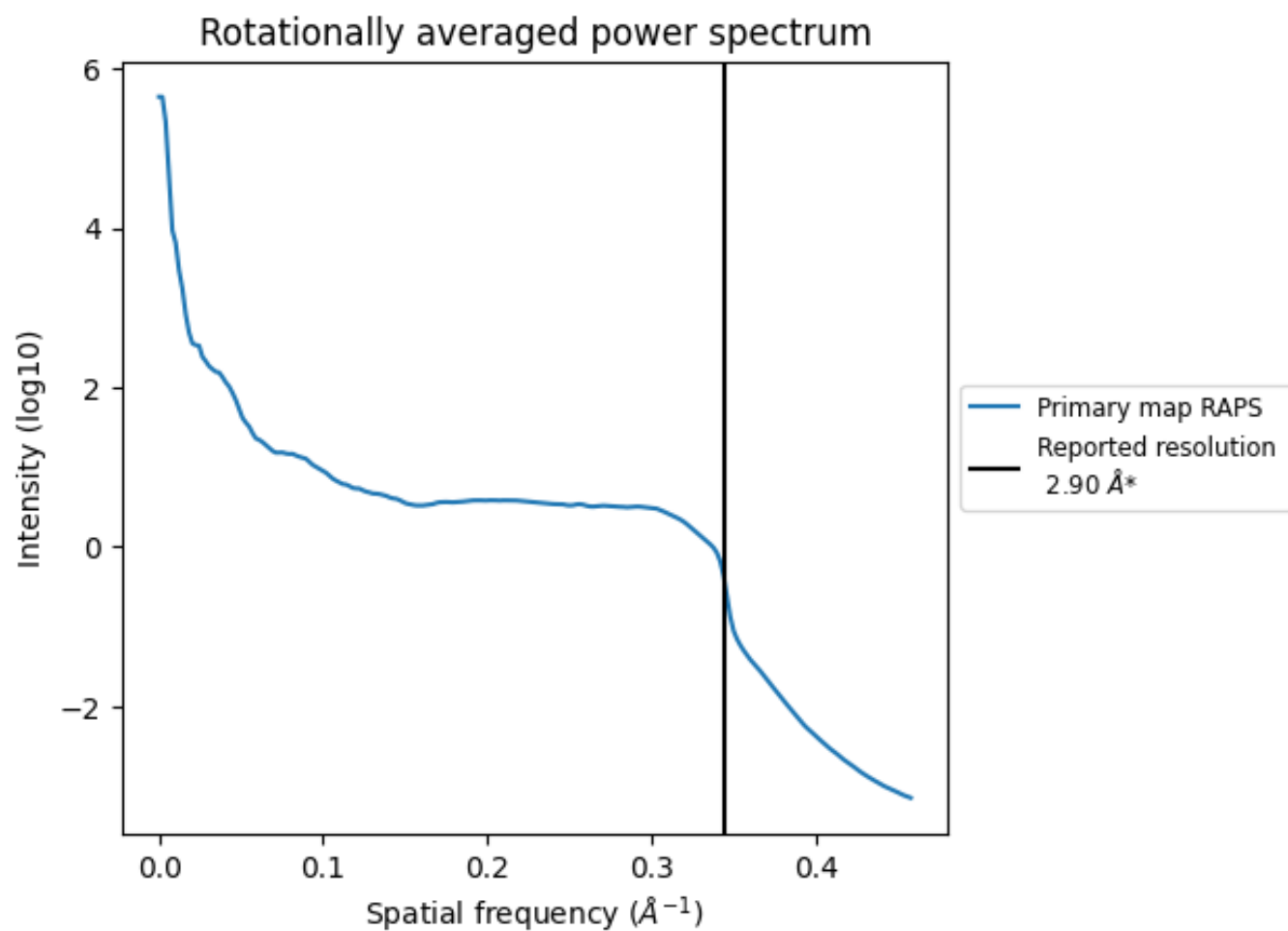
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1602 nm^3 ; this corresponds to an approximate mass of 1447 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

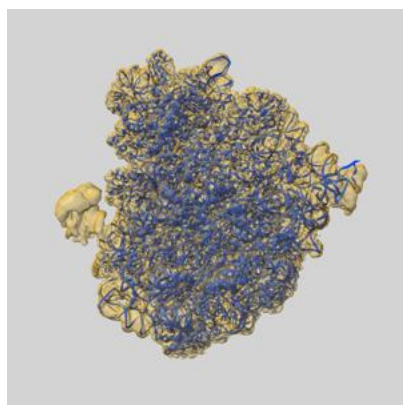
8 Fourier-Shell correlation ⓘ

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

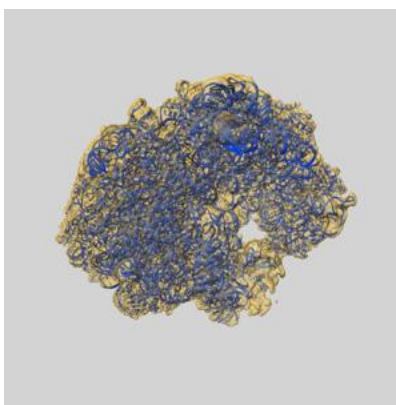
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13180 and PDB model 7P3K. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

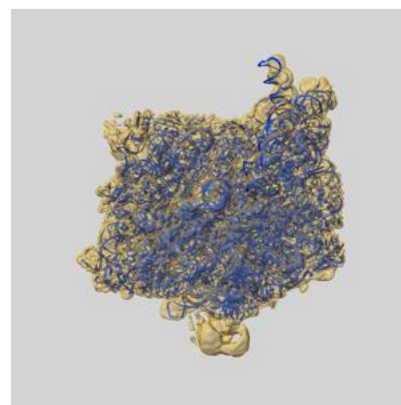
9.1 Map-model overlay [i](#)



X



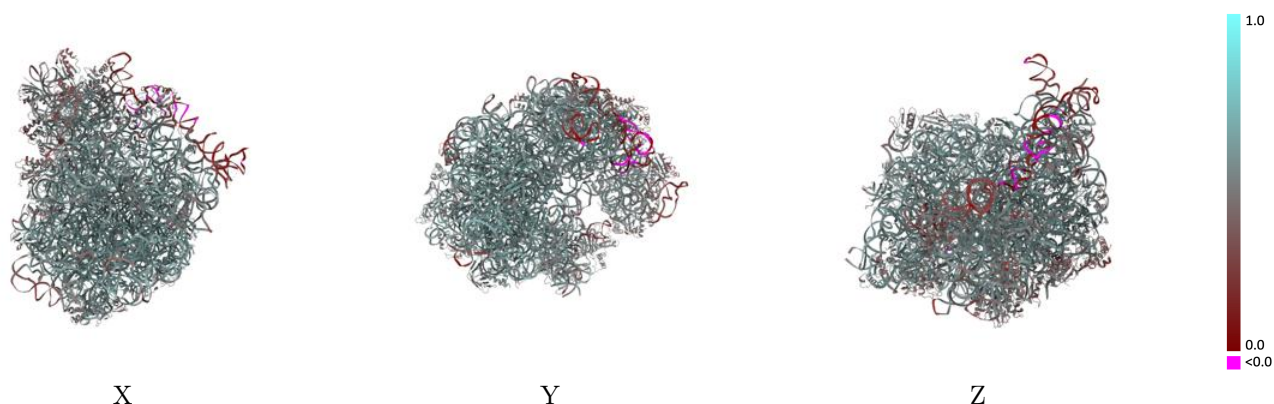
Y



Z

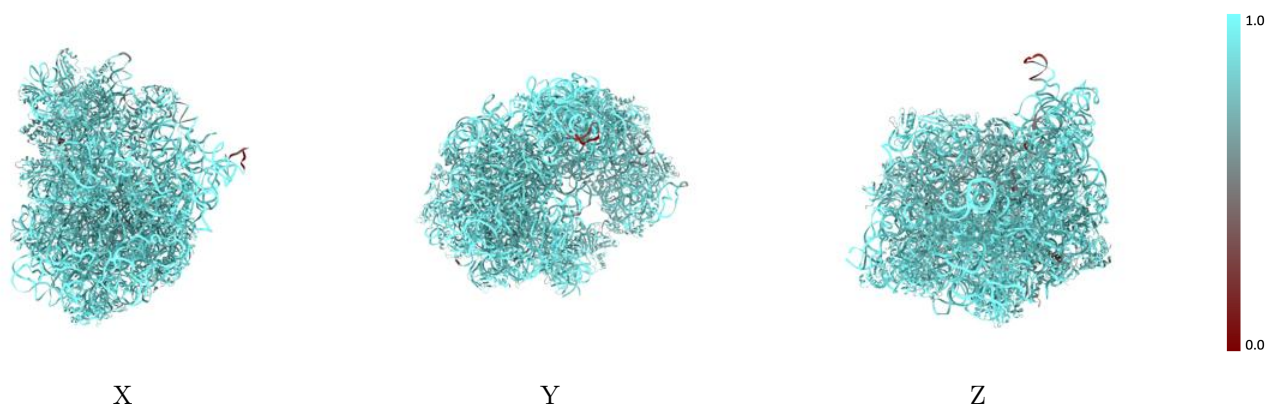
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



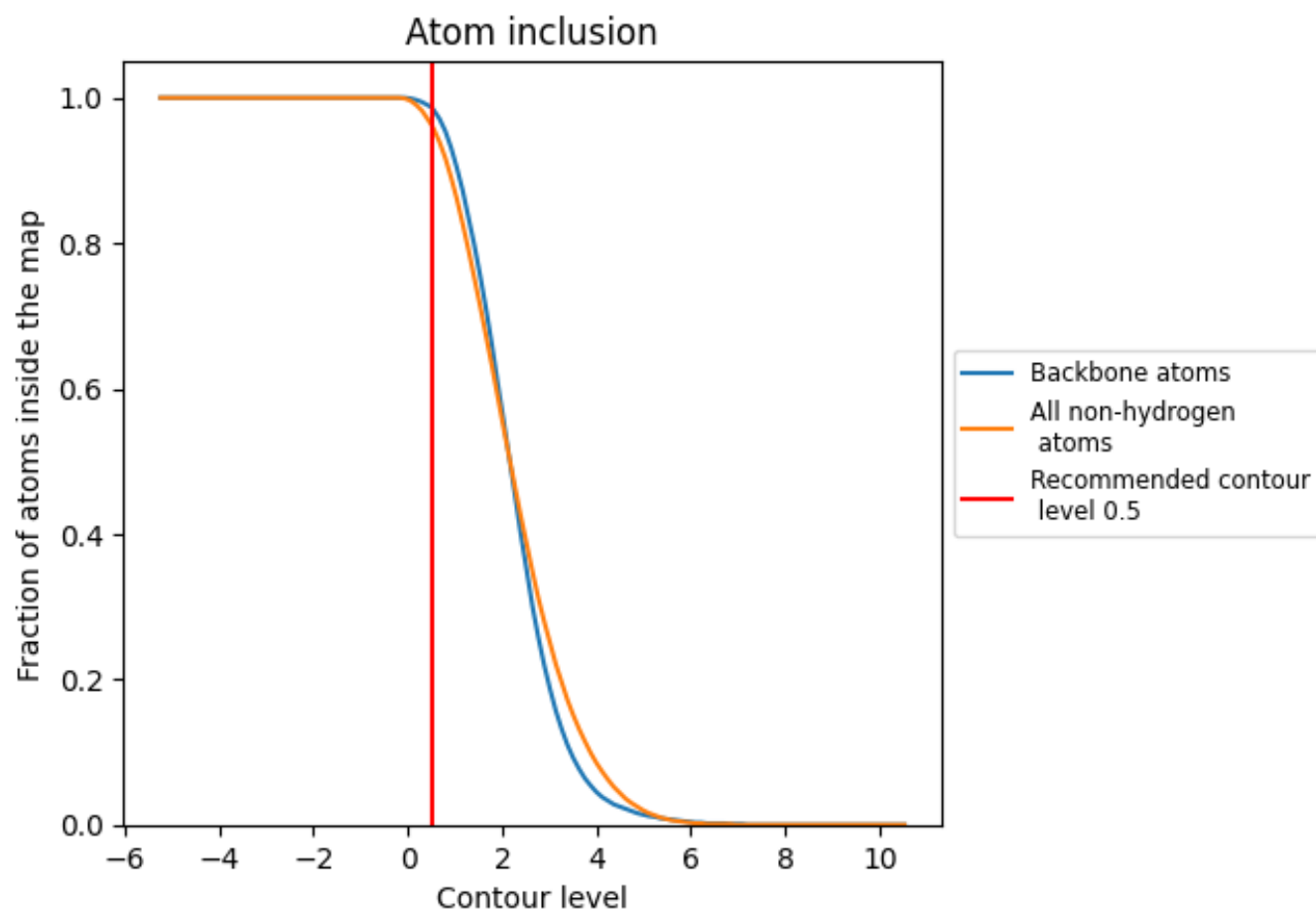
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9630	 0.5410
0	 0.9120	 0.5240
1	 0.9720	 0.5840
2	 0.9860	 0.5940
3	 0.9630	 0.5600
4	 0.8880	 0.4190
A	 0.9670	 0.5100
B	 0.8050	 0.4120
C	 0.9070	 0.4750
D	 0.9130	 0.4830
E	 0.9290	 0.5200
F	 0.8980	 0.4690
G	 0.8750	 0.4400
H	 0.9320	 0.5240
I	 0.9110	 0.4750
J	 0.8580	 0.4280
K	 0.9120	 0.4920
L	 0.9250	 0.5240
M	 0.9010	 0.4780
N	 0.9220	 0.4750
O	 0.9320	 0.5100
P	 0.9420	 0.5250
Q	 0.9170	 0.5050
R	 0.9080	 0.4740
S	 0.8940	 0.4600
T	 0.9360	 0.5150
U	 0.6490	 0.3730
V	 0.9370	 0.4680
X	 0.9830	 0.5720
a	 0.9930	 0.5820
b	 0.9930	 0.5590
c	 0.9660	 0.5780
d	 0.9510	 0.5640
e	 0.9340	 0.5250
f	 0.9070	 0.4850



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g	 0.8920	 0.4650
h	 0.8500	 0.4610
i	 0.9530	 0.5480
j	 0.9380	 0.5590
k	 0.9480	 0.5520
l	 0.9450	 0.5560
m	 0.9750	 0.5750
n	 0.9430	 0.5280
o	 0.9260	 0.5530
p	 0.9690	 0.5690
q	 0.9310	 0.5410
r	 0.9280	 0.5360
s	 0.9150	 0.5090
t	 0.9100	 0.4920
u	 0.9040	 0.5230
v	 0.9490	 0.5660
w	 0.9570	 0.5610
x	 0.9140	 0.4800
y	 0.9270	 0.5420
z	 0.9320	 0.5480