



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 12:01 pm BST

PDB ID : 7OIZ / pdb_00007oiz
EMDB ID : EMD-12936
Title : Cryo-EM structure of 70S ribosome stalled with TnaC peptide
Authors : Su, T.; Kudva, R.; Becker, T.; Berninghausen, O.; Heijne, G.; Cheng, J.; Beckmann, R.
Deposited on : 2021-05-13
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.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

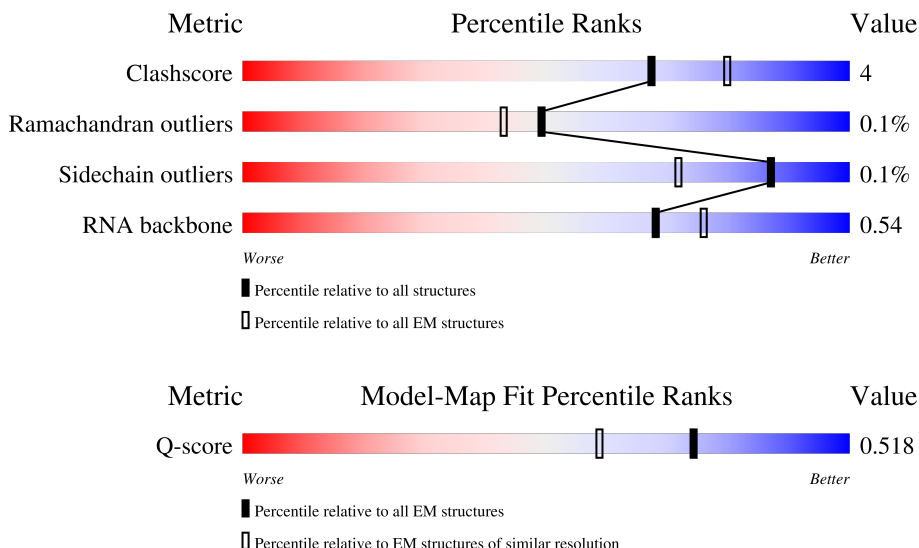
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

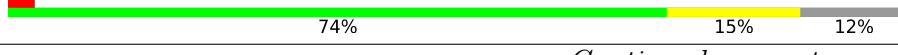
The reported resolution of this entry is 2.90 Å.

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)	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	13054 (2.40 - 3.40)

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	

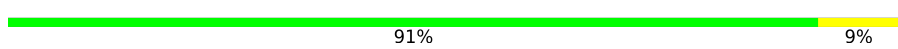
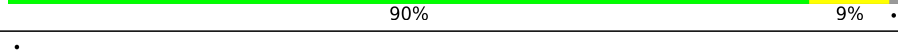
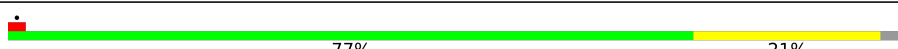
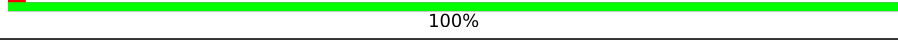
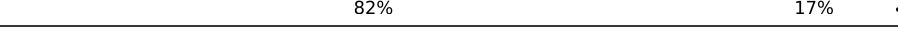
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Mol	Chain	Length	Quality of chain
4	D	206	
5	E	167	
6	F	135	
7	G	179	
8	H	130	
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	a	2753	
23	b	119	
24	c	273	
25	d	209	
26	e	201	
27	f	179	
28	g	177	

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Mol	Chain	Length	Quality of chain
29	h	149	
30	i	142	
31	j	123	
32	k	144	
33	l	136	
34	m	127	
35	n	117	
36	o	115	
37	p	118	
38	q	103	
39	r	110	
40	s	100	
41	t	104	
42	u	94	
43	v	85	
44	w	78	
45	x	63	
46	y	59	
47	z	57	
48	0	55	
49	1	46	
50	2	65	
51	3	38	
52	4	66	
53	X	6	

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Mol	Chain	Length	Quality of chain
54	7	16	94% 6%
55	V	75	65% 32%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 140295 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, fully modified isoform.

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 16S 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	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	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	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	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	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	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	6	Total	C	N	O	P	0	0
			125	56	21	42	6		

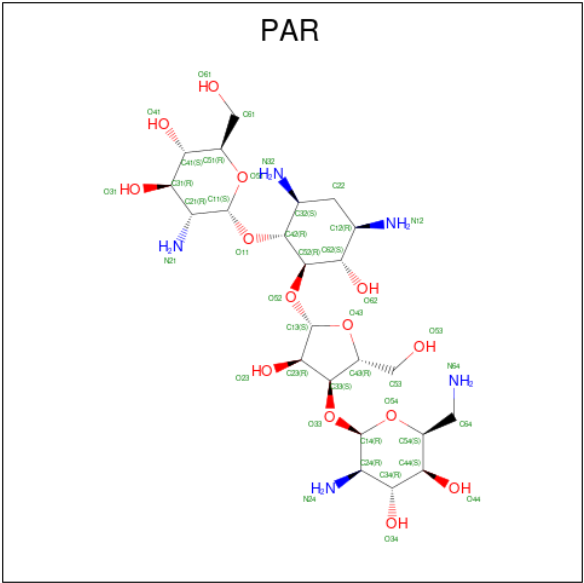
- Molecule 54 is a protein called TnaC.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	7	16	Total	C	N	O	0	0
			139	89	26	24		

- Molecule 55 is a RNA chain called tRNA.

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

- Molecule 56 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).

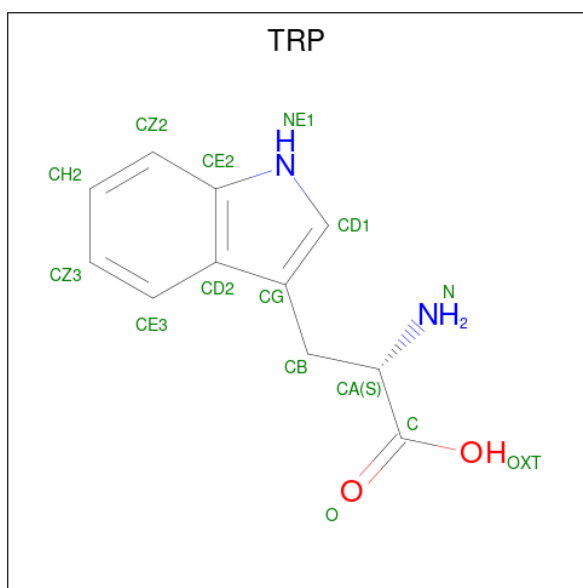


Mol	Chain	Residues	Atoms				AltConf
56	A	1	Total	C	N	O	0
			42	23	5	14	

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	A	93	Total	Mg	0
			93	93	
57	a	205	Total	Mg	0
			205	205	
57	b	5	Total	Mg	0
			5	5	
57	c	1	Total	Mg	0
			1	1	
57	k	1	Total	Mg	0
			1	1	
57	m	2	Total	Mg	0
			2	2	
57	V	1	Total	Mg	0
			1	1	

- Molecule 58 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				AltConf
58	a	1	Total	C	N	O	0
			15	11	2	2	

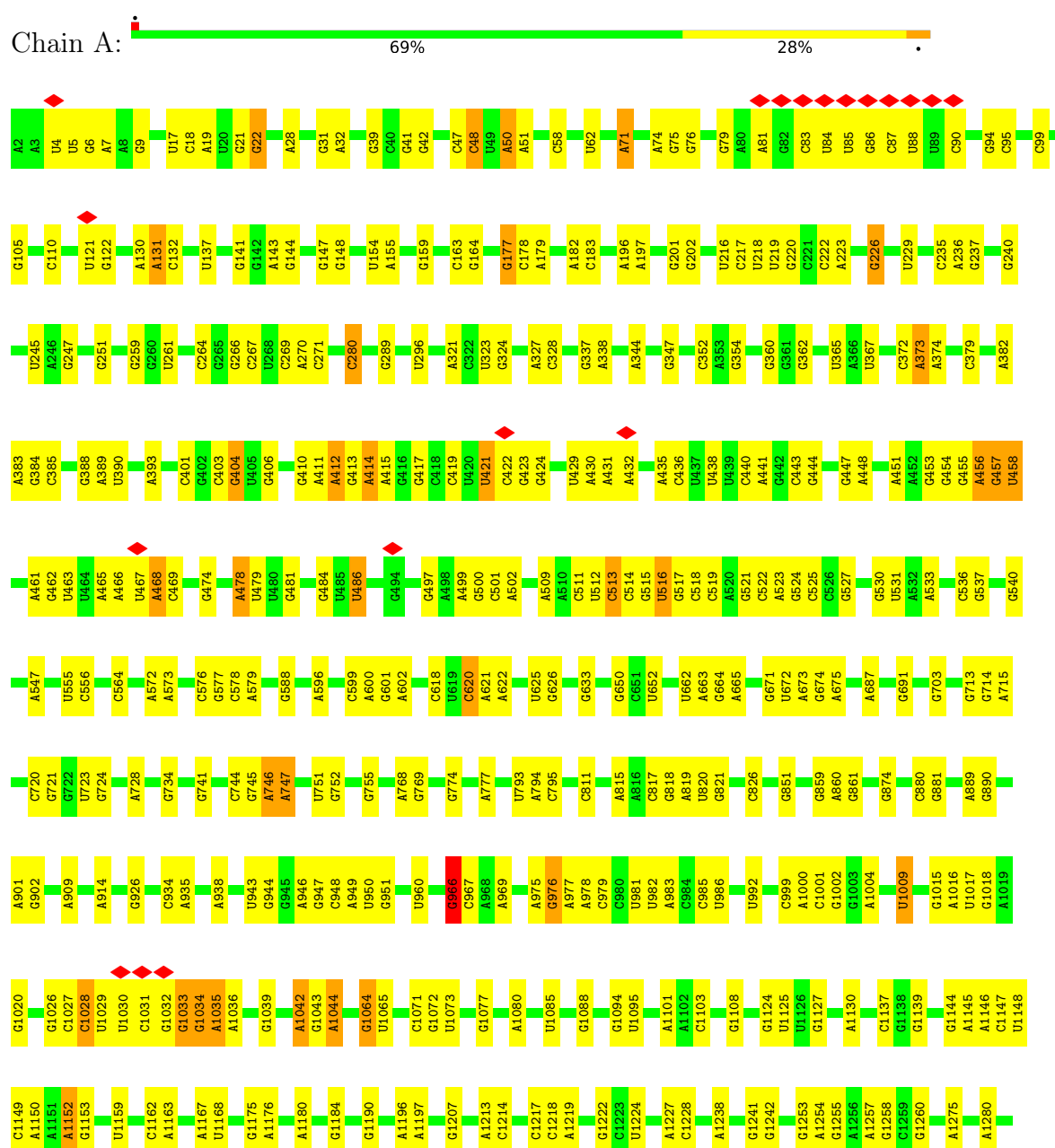
- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

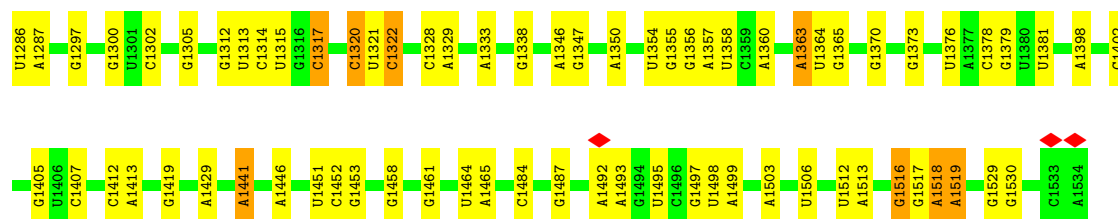
Mol	Chain	Residues	Atoms		AltConf
59	3	1	Total	Zn	0
			1	1	
59	4	1	Total	Zn	0
			1	1	

3 Residue-property plots

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.

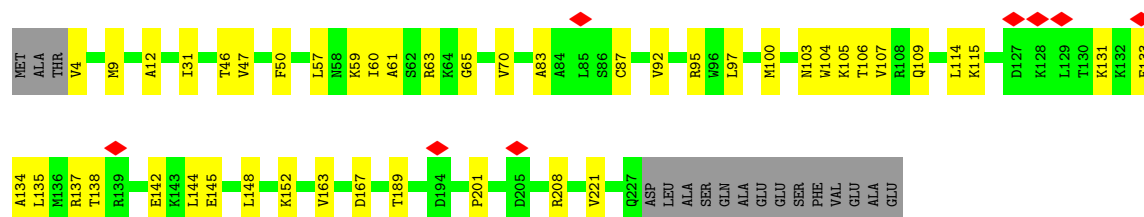
• Molecule 1: 16S rRNA





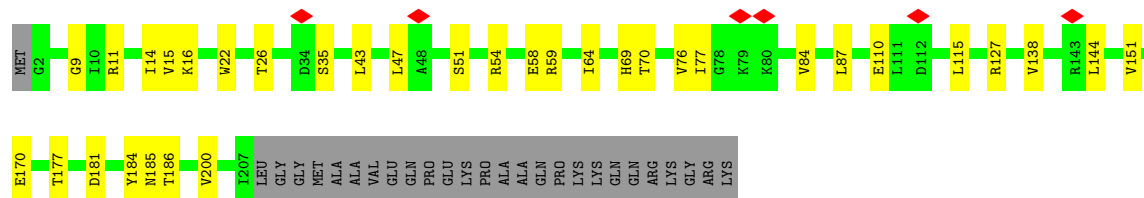
• Molecule 2: 30S ribosomal protein S2

Chain B: 74% 19% 7%



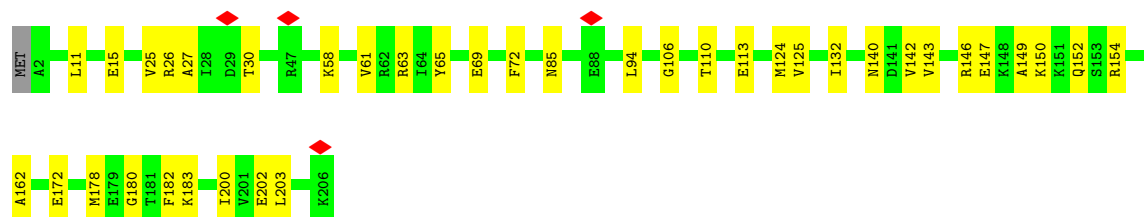
• Molecule 3: 30S ribosomal protein S3

Chain C: 74% 15% 12%



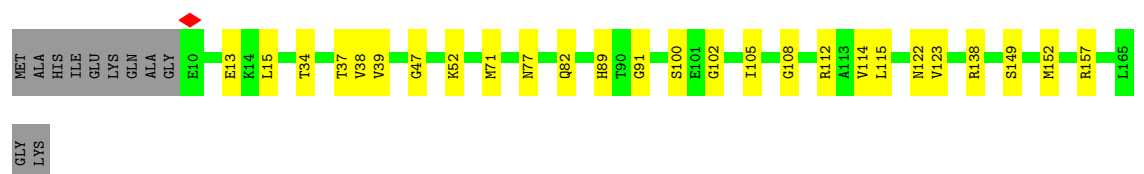
• Molecule 4: 30S ribosomal protein S4

Chain D: 81% 18%



• Molecule 5: 30S ribosomal protein S5

Chain E: 78% 16% 7%



- | | | | |
|------|------|------|------|
| MET | ALA | LYS | ALA | PRO | ILE | ARG | ALA | ARG | LYS | ARG | VAL | R13 | K14 | Q15 | V16 | S17 | V20 | I23 | I31 | I34 | L42 | T46 | G54 | K57 | Q64 | V74 | I79 | E83 | V84 | K87 | C88 | R93 | T96 | I97 | R98 | A99 | V113 | T114 | D119 | G120 |
|------|------|------|------|

V129

- Molecule 12: 30S ribosomal protein S12

Chain L:  81% 17% ..



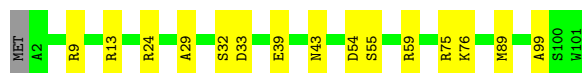
- Molecule 13: 30S ribosomal protein S13

Chain M:  90% 8% .



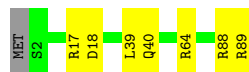
- Molecule 14: 30S ribosomal protein S14

Chain N:  84% 15% .



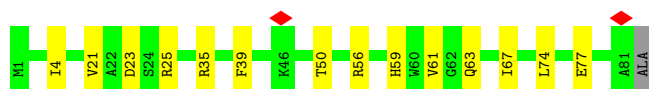
- Molecule 15: 30S ribosomal protein S15

Chain O:  91% 8% .



- Molecule 16: 30S ribosomal protein S16

Chain P:  82% 17% .



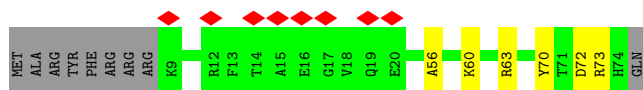
- Molecule 17: 30S ribosomal protein S17

Chain Q:  80% 14% 6%

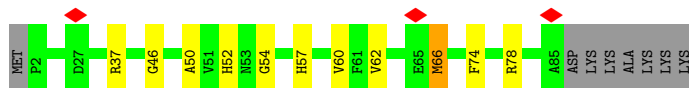
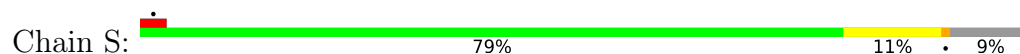


- Molecule 18: 30S ribosomal protein S18

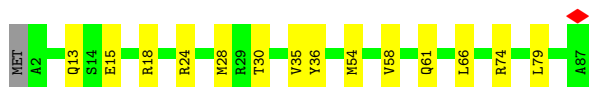
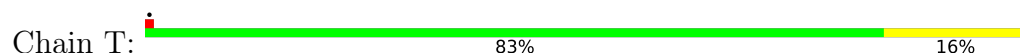
Chain R:  11% 80% 8% 12%



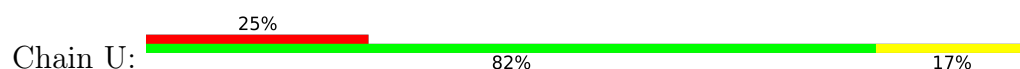
- Molecule 19: 30S ribosomal protein S19



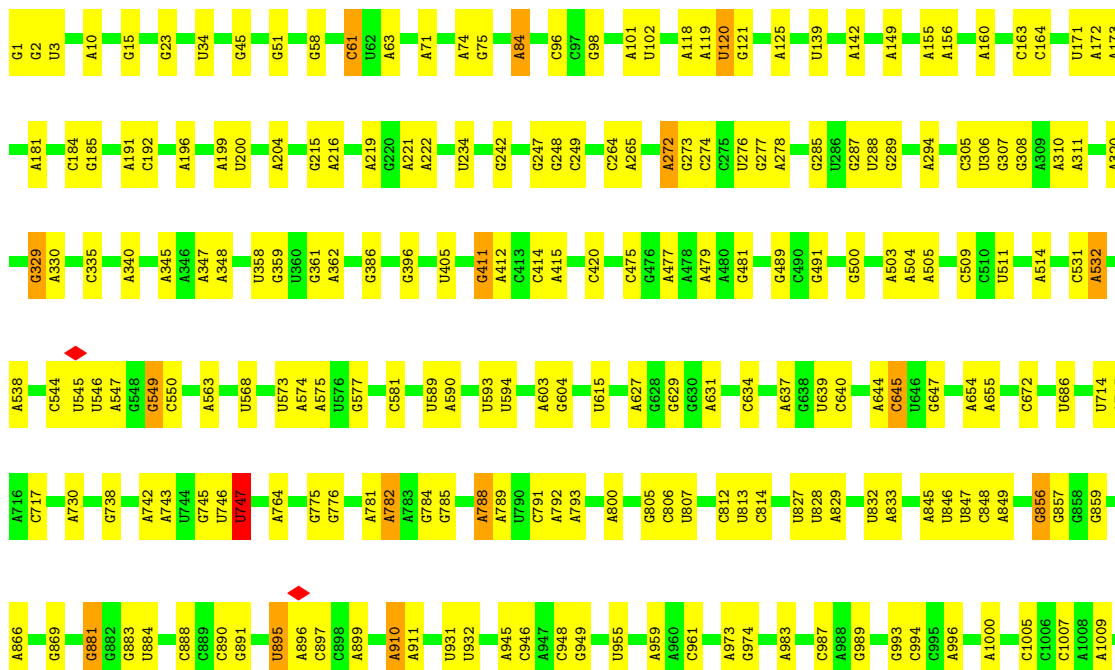
- Molecule 20: 30S ribosomal protein S20

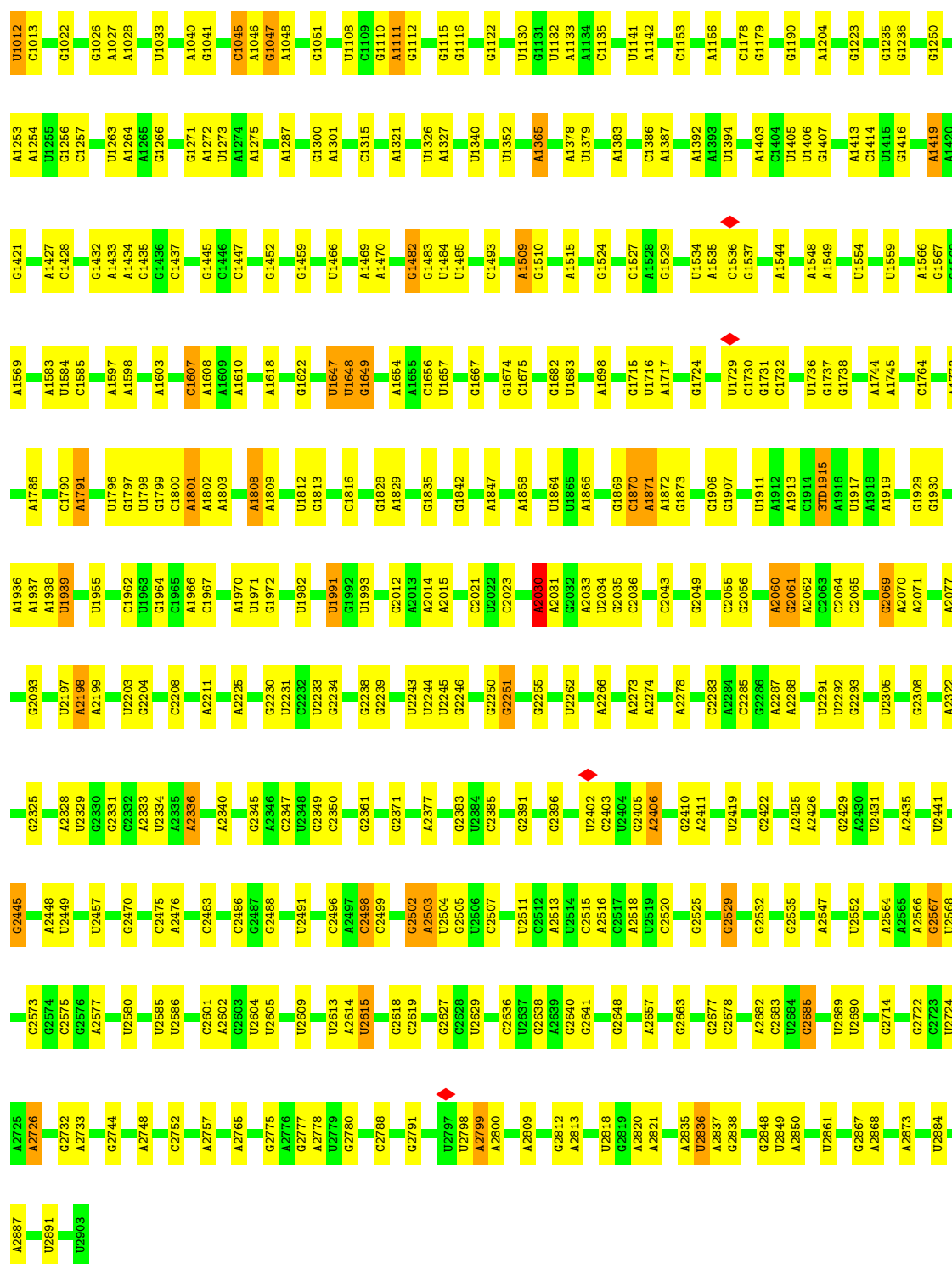


- Molecule 21: 30S ribosomal protein S21



- Molecule 22: 23S rRNA



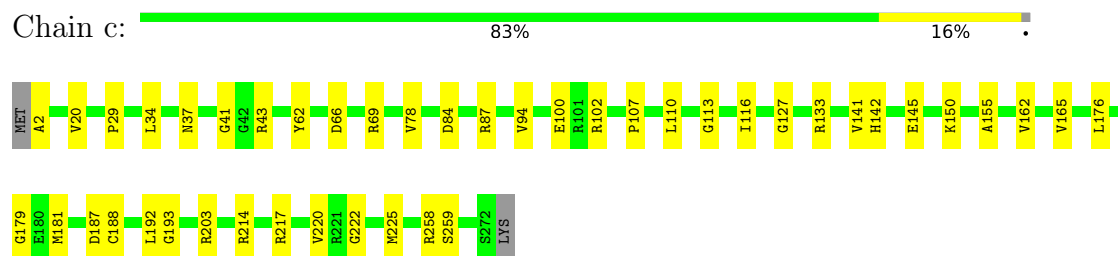


• Molecule 23: 16S rRNA

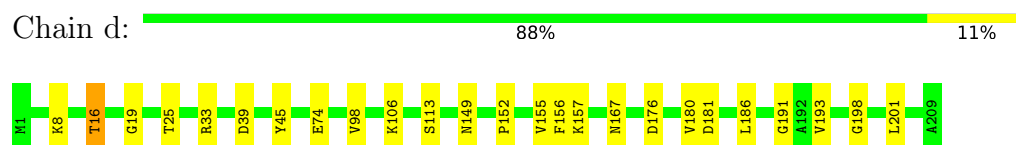
Chain b: 82% 18%



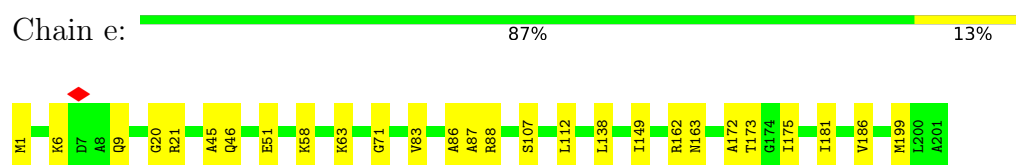
- Molecule 24: 50S ribosomal protein L2



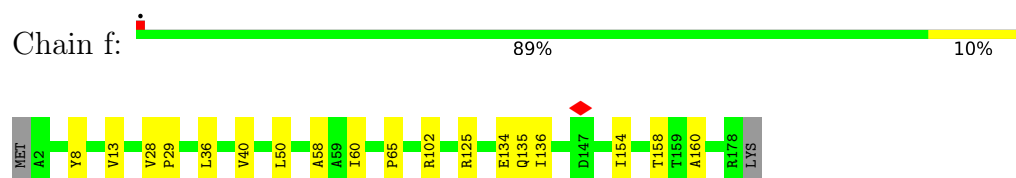
- Molecule 25: 50S ribosomal protein L3



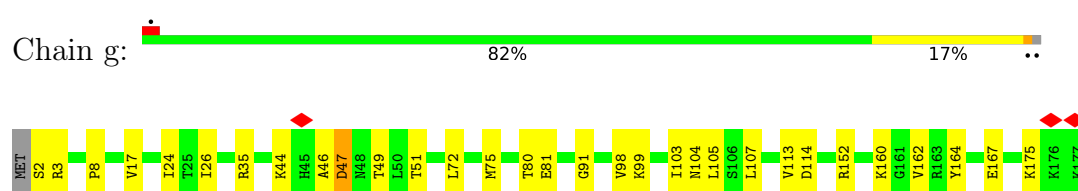
- Molecule 26: 50S ribosomal protein L4



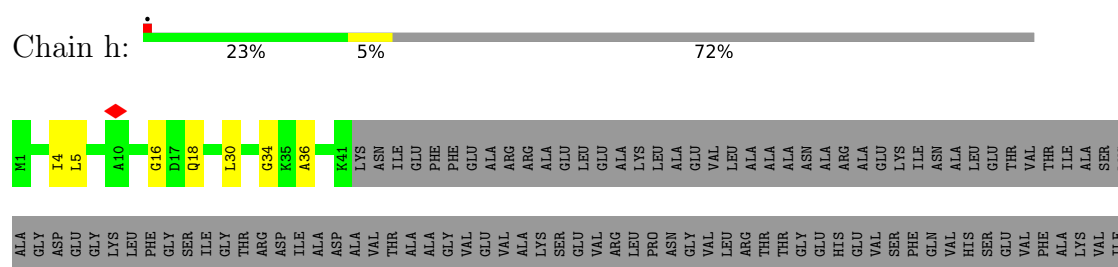
- Molecule 27: 50S ribosomal protein L5



- Molecule 28: 50S ribosomal protein L6



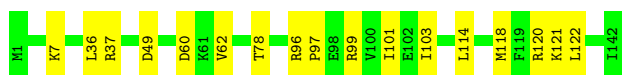
- Molecule 29: 50S ribosomal protein L9



VAL
ASN
VAL
VAL
ALA
GLU

• Molecule 30: 50S ribosomal protein L13

Chain i:  88% 12%



• Molecule 31: 50S ribosomal protein L14

Chain j:  86% 14%



• Molecule 32: 50S ribosomal protein L15

Chain k:  86% 14%



• Molecule 33: 50S ribosomal protein L16

Chain l:  82% 17%



• Molecule 34: 50S ribosomal protein L17

Chain m:  75% 18% 7%



• Molecule 35: 50S ribosomal protein L18

Chain n:  91% 9%



• Molecule 36: 50S ribosomal protein L19

Chain o:  94% 5%



- Molecule 37: 50S ribosomal protein L20

Chain p: 91% 8%



- Molecule 38: 50S ribosomal protein L21

Chain q: 84% 16%



- Molecule 39: 50S ribosomal protein L22

Chain r: 88% 12%



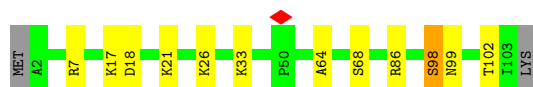
- Molecule 40: 50S ribosomal protein L23

Chain s: 82% 11% 7%



- Molecule 41: 50S ribosomal protein L24

Chain t: 87% 11% ..

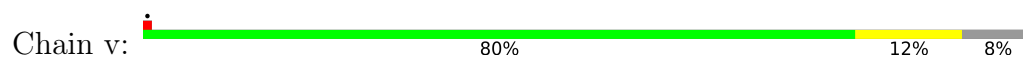


- Molecule 42: 50S ribosomal protein L25

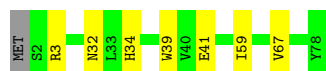
Chain u: 91% 9%



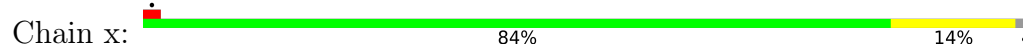
- Molecule 43: 50S ribosomal protein L27



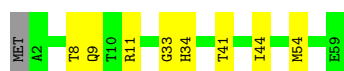
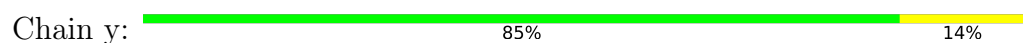
- Molecule 44: 50S ribosomal protein L28



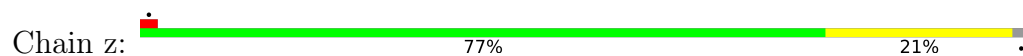
- Molecule 45: 50S ribosomal protein L29



- Molecule 46: 50S ribosomal protein L30



- Molecule 47: 50S ribosomal protein L32



- Molecule 48: 50S ribosomal protein L33



- Molecule 49: 50S ribosomal protein L34



- Molecule 50: 50S ribosomal protein L35

Chain 2:  82% 17% .



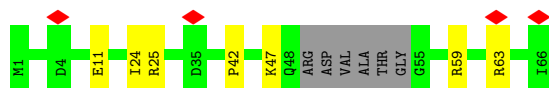
- Molecule 51: 50S ribosomal protein L36

Chain 3:  89% 11%



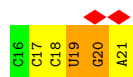
- Molecule 52: 50S ribosomal protein L31

Chain 4:  6% 80% 11% 9%

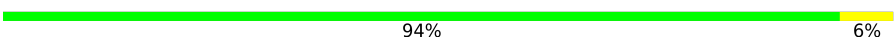


- Molecule 53: mRNA

Chain X:  17% 33% 50% 33%



- Molecule 54: TnaC

Chain 7:  94% 6%



- Molecule 55: tRNA

Chain V:  65% 32% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	459171	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	0.454	Depositor
Minimum map value	-0.258	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	398.912, 398.912, 398.912	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.084, 1.084, 1.084	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.26	0/36262	0.33	0/56561
2	B	0.25	0/1784	0.63	0/2403
3	C	0.21	0/1651	0.51	0/2225
4	D	0.24	0/1665	0.55	0/2227
5	E	0.29	0/1165	0.54	0/1568
6	F	0.34	1/858 (0.1%)	0.51	0/1160
7	G	0.26	0/1219	0.60	0/1635
8	H	0.25	0/989	0.56	0/1326
9	I	0.21	0/1034	0.51	1/1375 (0.1%)
10	J	0.27	0/796	0.60	0/1077
11	K	0.33	0/893	0.58	0/1205
12	L	0.36	0/969	0.64	0/1300
13	M	0.21	0/900	0.49	1/1204 (0.1%)
14	N	0.23	0/817	0.51	0/1088
15	O	0.24	0/722	0.44	0/964
16	P	0.24	0/653	0.48	0/877
17	Q	0.24	0/650	0.49	0/871
18	R	0.24	0/553	0.49	0/742
19	S	0.30	0/685	0.65	1/922 (0.1%)
20	T	0.26	0/676	0.49	0/895
21	U	0.19	0/597	0.50	0/792
22	a	0.42	2/65673 (0.0%)	0.39	0/102447
23	b	0.35	0/2850	0.35	0/4444
24	c	0.42	0/2121	0.56	0/2852
25	d	0.43	0/1576	0.59	0/2119
26	e	0.35	0/1571	0.54	0/2113
27	f	0.28	0/1434	0.57	0/1926
28	g	0.32	0/1343	0.70	0/1816
29	h	0.28	0/306	0.69	0/413
30	i	0.41	0/1152	0.52	0/1551
31	j	0.44	0/955	0.66	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	k	0.39	0/1062	0.55	2/1413 (0.1%)
33	l	0.48	0/1093	0.60	0/1460
34	m	0.49	0/958	0.68	0/1281
35	n	0.33	0/902	0.53	0/1209
36	o	0.40	0/929	0.57	0/1242
37	p	0.44	0/960	0.50	0/1278
38	q	0.35	0/829	0.60	0/1107
39	r	0.37	0/864	0.47	0/1156
40	s	0.32	0/744	0.62	0/994
41	t	0.29	0/787	0.60	2/1051 (0.2%)
42	u	0.36	0/766	0.55	0/1025
43	v	0.42	0/593	0.50	0/785
44	w	0.42	0/635	0.49	0/848
45	x	0.25	0/502	0.47	0/667
46	y	0.43	0/453	0.57	0/605
47	z	0.35	0/450	0.53	0/599
48	0	0.36	0/424	0.54	0/565
49	1	0.44	0/380	0.50	0/498
50	2	0.40	0/513	0.61	0/676
51	3	0.45	0/303	0.53	0/397
52	4	0.19	0/488	0.46	0/649
53	X	0.94	2/138 (1.4%)	0.41	0/212
54	7	0.34	0/143	0.78	0/193
55	V	0.25	0/1775	0.38	0/2764
All	All	0.36	5/151210 (0.0%)	0.43	7/226051 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	N	0	1
25	d	0	1
28	g	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2449	U	C5-C6	7.49	1.49	1.34
53	X	20	G	C1'-N9	-6.30	1.38	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	18	VAL	CA-CB	6.03	1.57	1.53
22	a	2449	U	C2-N3	5.51	1.48	1.37
53	X	19	U	C1'-N1	5.45	1.56	1.48

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	66	GLU	CB-CA-C	-5.68	109.51	117.23
32	k	117	THR	CA-C-N	5.57	135.34	122.31
32	k	117	THR	C-N-CA	5.57	135.34	122.31
41	t	98	SER	CA-C-N	5.19	135.35	126.32
41	t	98	SER	C-N-CA	5.19	135.35	126.32
19	S	66	MET	CB-CA-C	5.04	119.32	110.35
9	I	57	MET	CA-CB-CG	5.02	124.14	114.10

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](#)

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	A	32611	0	16429	223	0
2	B	1753	0	1780	27	0
3	C	1624	0	1696	21	0
4	D	1643	0	1707	24	0
5	E	1152	0	1196	17	0
6	F	839	0	833	12	0
7	G	1203	0	1254	17	0
8	H	979	0	1031	13	0
9	I	1022	0	1070	24	0
10	J	786	0	828	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	877	0	885	16	0
12	L	955	0	1016	21	0
13	M	891	0	952	4	0
14	N	805	0	844	12	0
15	O	714	0	734	6	0
16	P	643	0	661	10	0
17	Q	641	0	682	8	0
18	R	544	0	565	5	0
19	S	668	0	693	7	0
20	T	670	0	719	11	0
21	U	589	0	629	8	0
22	a	59130	0	29763	205	0
23	b	2549	0	1291	4	0
24	c	2082	0	2154	28	0
25	d	1566	0	1618	16	0
26	e	1552	0	1619	17	0
27	f	1410	0	1444	11	0
28	g	1323	0	1371	17	0
29	h	303	0	327	6	0
30	i	1129	0	1162	13	0
31	j	946	0	1023	9	0
32	k	1053	0	1129	12	0
33	l	1074	0	1157	17	0
34	m	945	0	989	14	0
35	n	892	0	923	6	0
36	o	917	0	962	4	0
37	p	947	0	1019	7	0
38	q	816	0	839	11	0
39	r	857	0	922	8	0
40	s	738	0	807	10	0
41	t	779	0	831	9	0
42	u	753	0	780	5	0
43	v	586	0	596	8	0
44	w	625	0	652	4	0
45	x	501	0	531	6	0
46	y	449	0	488	4	0
47	z	444	0	458	9	0
48	0	417	0	451	10	0
49	1	377	0	418	0	0
50	2	504	0	572	9	0
51	3	302	0	340	2	0
52	4	480	0	478	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	X	125	0	66	2	0
54	7	139	0	134	1	0
55	V	1609	0	812	12	0
56	A	42	0	45	2	0
57	A	93	0	0	0	0
57	V	1	0	0	0	0
57	a	205	0	0	0	0
57	b	5	0	0	0	0
57	c	1	0	0	0	0
57	k	1	0	0	0	0
57	m	2	0	0	0	0
58	a	15	0	9	0	0
59	3	1	0	0	0	0
59	4	1	0	0	0	0
All	All	140295	0	94384	869	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 4.

All (869) 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)
22:a:747:5MU:C5	22:a:747:5MU:C4	1.78	1.67
22:a:1939:5MU:C4	22:a:1939:5MU:C5	1.78	1.66
55:V:54:5MU:C5	55:V:54:5MU:C4	1.80	1.62
56:A:1601:PAR:O43	56:A:1601:PAR:C13	1.63	1.26
34:m:102:PHE:HA	34:m:108:ALA:O	1.23	1.24
47:z:29:SER:O	47:z:37:LYS:HA	1.43	1.17
9:I:24:GLY:O	9:I:60:LYS:HA	1.51	1.08
1:A:1441:A:H62	1:A:1461:G:N2	1.53	1.06
1:A:1441:A:N6	1:A:1461:G:H21	1.56	1.01
22:a:1047:G:N2	22:a:1111:A:H62	1.61	0.99
55:V:54:5MU:C4	55:V:54:5MU:C6	2.52	0.95
22:a:1047:G:H21	22:a:1111:A:H62	1.01	0.93
9:I:24:GLY:O	9:I:60:LYS:CA	2.21	0.88
22:a:1047:G:H21	22:a:1111:A:N6	1.71	0.87
34:m:102:PHE:CA	34:m:108:ALA:O	2.18	0.85
1:A:1441:A:H62	1:A:1461:G:H21	0.83	0.81
1:A:1009:U:H3	1:A:1020:G:H1	0.84	0.80
12:L:50:ARG:HB3	12:L:90:LEU:HD11	1.66	0.76
10:J:6:ILE:HB	10:J:76:ILE:HB	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:959:A:N6	33:l:82:MET:HE3	2.02	0.73
42:u:21:ARG:NH1	42:u:87:GLN:O	2.21	0.72
33:l:20:LEU:HD23	42:u:81:PRO:HG2	1.71	0.72
1:A:201:G:H1	1:A:216:U:H3	1.36	0.72
1:A:79:G:H1	1:A:90:C:H42	1.37	0.71
34:m:103:ARG:HD3	34:m:110:MET:HE3	1.73	0.71
45:x:58:ASN:HD21	45:x:63:ALA:HB3	1.54	0.71
1:A:1088:G:H21	1:A:1167:A:H61	1.38	0.70
22:a:2483:C:N3	33:l:123:LYS:NZ	2.39	0.69
1:A:454:G:H1	1:A:478:A:H61	1.38	0.69
1:A:1026:G:O6	1:A:1035:A:N1	2.25	0.69
3:C:9:GLY:HA3	14:N:89:MET:HE3	1.74	0.69
9:I:24:GLY:O	9:I:60:LYS:C	2.35	0.69
22:a:475:C:O2	22:a:479:A:N6	2.26	0.68
1:A:826:C:O2	8:H:16:ASN:ND2	2.28	0.67
24:c:222:GLY:HA2	24:c:225:MET:HG3	1.77	0.67
21:U:31:GLU:OE2	21:U:35:ARG:NH1	2.27	0.67
38:q:43:ASN:HB3	38:q:46:GLU:HB3	1.77	0.67
7:G:51:ALA:HB2	7:G:58:GLU:HB3	1.77	0.67
28:g:99:LYS:NZ	28:g:104:ASN:OD1	2.28	0.67
28:g:17:VAL:HG12	28:g:26:ILE:HG12	1.77	0.67
7:G:69:VAL:HG21	7:G:104:ILE:HD11	1.76	0.66
24:c:66:ASP:OD2	24:c:102:ARG:NH1	2.29	0.66
2:B:59:LYS:HG2	2:B:63:ARG:HH21	1.60	0.66
33:l:47:GLU:OE2	33:l:50:ARG:NH2	2.29	0.66
1:A:403:C:H2'	1:A:404:G:H8	1.61	0.65
2:B:83:ALA:O	2:B:87:CYS:HB2	1.95	0.65
21:U:13:ASP:OD1	21:U:17:ARG:NH1	2.30	0.65
30:i:96:ARG:HE	30:i:99:ARG:HG3	1.61	0.65
1:A:1028:C:N4	1:A:1033:G:O6	2.30	0.65
22:a:781:A:OP1	24:c:217:ARG:NH2	2.29	0.65
29:h:4:ILE:HG12	29:h:18:GLN:HG2	1.79	0.65
5:E:157:ARG:NH2	8:H:43:GLU:OE2	2.30	0.64
48:0:11:LEU:HB3	48:0:49:TYR:HB3	1.78	0.64
3:C:22:TRP:HB3	3:C:59:ARG:H	1.63	0.64
33:l:50:ARG:HG3	33:l:65:ILE:HD11	1.79	0.64
1:A:414:A:H62	1:A:430:A:H2	1.45	0.63
1:A:1029:U:O2	1:A:1033:G:C6	2.52	0.63
1:A:1088:G:N2	1:A:1167:A:H61	1.96	0.63
7:G:27:VAL:HG22	7:G:43:VAL:HG11	1.79	0.63
25:d:113:SER:O	25:d:167:ASN:HA	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:3:2:LYS:NZ	51:3:32:LYS:O	2.31	0.63
33:l:36:VAL:HG22	42:u:82:TYR:HB2	1.80	0.62
44:w:59:ILE:HD13	44:w:67:VAL:HG21	1.81	0.62
40:s:4:GLU:OE2	45:x:23:ARG:NH1	2.33	0.62
1:A:1029:U:C2	1:A:1033:G:O6	2.53	0.62
1:A:1072:G:H21	2:B:106:THR:HG21	1.65	0.62
26:e:1:MET:HE3	26:e:20:GLY:HA3	1.82	0.61
2:B:135:LEU:HA	2:B:138:THR:HG22	1.83	0.61
19:S:46:GLY:N	19:S:62:VAL:O	2.32	0.61
1:A:436:C:O2'	4:D:154:ARG:NH2	2.32	0.61
24:c:142:HIS:ND1	24:c:193:GLY:O	2.29	0.61
9:I:30:ILE:HG12	9:I:65:ILE:HB	1.81	0.61
1:A:1088:G:H21	1:A:1167:A:N6	1.97	0.61
2:B:12:ALA:HA	2:B:208:ARG:HE	1.65	0.61
22:a:1434:A:H2'	22:a:1435:G:H8	1.64	0.61
27:f:158:THR:HG22	27:f:160:ALA:H	1.66	0.61
1:A:261:U:OP2	20:T:74:ARG:NH2	2.34	0.61
1:A:744:C:H2'	1:A:745:G:H8	1.65	0.61
5:E:13:GLU:HG2	5:E:39:VAL:HG12	1.81	0.61
1:A:1321:U:O2'	19:S:78:ARG:NH1	2.34	0.60
22:a:61:C:OP2	45:x:47:ARG:NH2	2.34	0.60
28:g:104:ASN:ND2	28:g:114:ASP:OD1	2.33	0.60
4:D:15:GLU:OE2	4:D:63:ARG:NH1	2.34	0.60
22:a:1607:C:N4	22:a:1622:G:OP2	2.32	0.60
22:a:2683:C:OP1	36:o:51:ARG:NH2	2.34	0.60
1:A:673:A:H2'	1:A:674:G:C8	2.35	0.60
22:a:2061:G:OP1	26:e:63:LYS:NZ	2.30	0.60
24:c:2:ALA:N	24:c:20:VAL:O	2.34	0.60
33:l:29:GLY:N	33:l:104:GLU:OE2	2.27	0.60
1:A:417:G:N2	1:A:540:G:O2'	2.32	0.60
4:D:110:THR:OG1	4:D:113:GLU:OE1	2.19	0.60
33:l:106:ASP:OD1	33:l:107:GLY:N	2.35	0.60
1:A:458:U:H3	1:A:474:G:H1	1.49	0.60
1:A:1175:G:H2'	1:A:1176:A:H8	1.67	0.60
11:K:17:SER:HA	11:K:79:ILE:HA	1.82	0.60
31:j:36:GLY:N	31:j:62:VAL:O	2.30	0.60
1:A:105:G:OP2	20:T:13:GLN:NE2	2.35	0.60
46:y:8:THR:HA	46:y:34:HIS:O	2.01	0.60
1:A:515:G:H2'	1:A:516:PSU:H6	1.65	0.60
20:T:28:MET:HG3	20:T:58:VAL:HG12	1.83	0.60
22:a:2640:G:OP1	30:i:96:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:r:24:ILE:HD13	39:r:36:LEU:HD11	1.83	0.60
39:r:72:THR:HG22	39:r:73:LYS:HG3	1.82	0.60
46:y:11:ARG:HB2	46:y:54:MET:HB2	1.84	0.60
38:q:46:GLU:OE2	38:q:48:LYS:NZ	2.34	0.59
15:O:40:GLN:NE2	22:a:715:A:N3	2.50	0.59
26:e:51:GLU:OE2	26:e:88:ARG:NH2	2.35	0.59
14:N:13:ARG:NH1	14:N:54:ASP:OD1	2.34	0.59
1:A:1152:A:OP1	10:J:70:HIS:ND1	2.35	0.59
3:C:35:SER:OG	3:C:59:ARG:NH2	2.35	0.59
9:I:55:VAL:HG23	9:I:57:MET:HB3	1.85	0.59
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.83	0.59
1:A:1347:G:O6	9:I:12:ARG:NH2	2.36	0.59
22:a:857:G:OP1	43:v:78:LYS:NZ	2.36	0.59
22:a:1482:G:N3	22:a:1509:A:N1	2.51	0.59
1:A:373:A:O2'	1:A:451:A:N7	2.36	0.59
1:A:981:U:OP1	14:N:9:ARG:NH1	2.36	0.59
32:k:85:VAL:HG11	32:k:90:VAL:HG22	1.85	0.59
39:r:23:LEU:HD11	47:z:24:ALA:HB2	1.84	0.59
1:A:674:G:H2'	1:A:675:A:H8	1.66	0.59
1:A:1073:U:O2	2:B:103:ASN:ND2	2.36	0.59
52:4:11:GLU:HA	52:4:25:ARG:HA	1.84	0.59
22:a:340:A:O2'	26:e:162:ARG:NH2	2.36	0.58
22:a:1009:A:N3	22:a:1153:C:O2'	2.36	0.58
23:b:1:U:H2'	23:b:2:G:H8	1.68	0.58
15:O:88:ARG:NH2	22:a:714:U:OP2	2.36	0.58
33:l:13:HIS:O	33:l:71:LYS:NZ	2.31	0.58
4:D:172:GLU:OE2	4:D:183:LYS:NZ	2.33	0.58
30:i:62:VAL:HG11	30:i:101:ILE:HD11	1.84	0.58
34:m:67:PHE:O	34:m:71:ARG:HD2	2.03	0.58
35:n:39:VAL:HB	35:n:49:VAL:HG22	1.85	0.58
22:a:2061:G:N2	54:7:23:ARG:O	2.37	0.58
1:A:414:A:N7	1:A:430:A:N1	2.51	0.58
1:A:1071:C:H2'	1:A:1072:G:H8	1.68	0.58
7:G:15:ASP:OD1	7:G:20:SER:N	2.29	0.58
9:I:106:ARG:NH1	9:I:107:ASP:O	2.37	0.58
8:H:43:GLU:HG2	8:H:101:ILE:HD13	1.86	0.58
16:P:59:HIS:O	16:P:63:GLN:NE2	2.36	0.58
22:a:1434:A:H2'	22:a:1435:G:C8	2.38	0.58
22:a:2685:G:H21	22:a:2726:A:N6	2.02	0.58
1:A:110:C:O2'	16:P:25:ARG:O	2.22	0.57
37:p:66:ASN:OD1	37:p:70:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2848:G:O2'	22:a:2867:G:N2	2.36	0.57
1:A:1180:A:OP2	9:I:99:ARG:NH2	2.38	0.57
3:C:11:ARG:NH2	3:C:177:THR:O	2.35	0.57
24:c:78:VAL:O	24:c:113:GLY:N	2.37	0.57
29:h:5:LEU:O	29:h:16:GLY:N	2.37	0.57
22:a:1026:G:H2'	22:a:1027:A:H8	1.68	0.57
22:a:1287:A:N1	22:a:1648:U:O2'	2.36	0.57
13:M:98:ARG:HB2	13:M:100:GLN:HE22	1.70	0.57
31:j:7:MET:HB3	31:j:18:ARG:HH21	1.69	0.57
1:A:137:U:H3	1:A:226:G:H1	1.52	0.57
14:N:29:ALA:O	14:N:33:ASP:HB2	2.05	0.57
22:a:2064:C:O2'	22:a:2251:OMG:N2	2.38	0.57
1:A:412:A:H62	1:A:431:A:H2	1.49	0.57
1:A:1127:G:H1	1:A:1145:A:H61	1.53	0.57
25:d:16:THR:O	25:d:19:GLY:N	2.36	0.57
52:4:42:PRO:HB3	52:4:47:LYS:HB2	1.86	0.57
12:L:42:PRO:HB2	12:L:89:ASP:HB3	1.87	0.56
39:r:37:THR:OG1	39:r:48:LYS:NZ	2.38	0.56
41:t:86:ARG:NH2	41:t:102:THR:OG1	2.38	0.56
5:E:157:ARG:NH1	8:H:99:LEU:O	2.38	0.56
22:a:249:C:O2	50:2:12:LYS:NZ	2.33	0.56
22:a:335:C:O2	41:t:68:SER:OG	2.23	0.56
21:U:31:GLU:OE2	21:U:34:ARG:NH2	2.39	0.56
22:a:2788:C:O2'	22:a:2809:A:N3	2.36	0.56
26:e:6:LYS:O	26:e:9:GLN:NE2	2.38	0.56
17:Q:59:VAL:HG11	17:Q:75:LEU:HD22	1.87	0.56
1:A:499:A:H4'	1:A:500:G:H5'	1.86	0.56
43:v:54:GLY:O	43:v:57:HIS:N	2.39	0.56
1:A:979:C:O2	14:N:59:ARG:NH1	2.38	0.56
2:B:104:TRP:HA	2:B:107:VAL:HG12	1.87	0.56
7:G:70:ARG:NH1	7:G:97:ASN:OD1	2.37	0.56
12:L:50:ARG:HB2	12:L:90:LEU:HD21	1.87	0.56
2:B:115:LYS:NZ	2:B:152:LYS:O	2.39	0.56
26:e:21:ARG:NH1	26:e:107:SER:OG	2.39	0.56
1:A:1153:G:OP1	10:J:16:ARG:NH1	2.39	0.56
1:A:1356:G:H2'	1:A:1357:A:C8	2.40	0.56
11:K:88:GLY:O	11:K:93:ARG:NH1	2.39	0.56
1:A:404:G:H1	1:A:499:A:H62	1.54	0.55
1:A:664:G:H22	1:A:741:G:H1	1.54	0.55
9:I:88:MET:HE3	9:I:98:LEU:HD12	1.88	0.55
47:z:46:ASP:OD1	47:z:53:LYS:NZ	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:C:OP1	1:A:513:C:O2'	2.22	0.55
14:N:24:ARG:NH1	14:N:55:SER:OG	2.40	0.55
28:g:164:TYR:HB2	28:g:167:GLU:HB2	1.87	0.55
35:n:31:THR:O	35:n:102:ARG:NH2	2.37	0.55
40:s:8:LEU:O	45:x:29:ARG:NH2	2.40	0.55
1:A:401:C:O2'	1:A:621:A:N3	2.33	0.55
12:L:68:GLY:O	12:L:99:ARG:NH1	2.40	0.55
1:A:178:C:H2'	1:A:179:A:H8	1.71	0.55
4:D:125:VAL:HG22	4:D:143:VAL:HG12	1.88	0.55
11:K:64:GLN:HG3	11:K:99:ALA:HB2	1.88	0.55
11:K:84:VAL:HG11	11:K:97:ILE:HD11	1.89	0.55
22:a:1724:G:H1	22:a:1736:U:H3	1.55	0.55
22:a:320:A:N3	26:e:163:ASN:ND2	2.53	0.55
1:A:768:A:N3	1:A:1512:U:O2'	2.39	0.54
8:H:29:SER:HB3	8:H:57:PRO:HB2	1.90	0.54
32:k:78:ARG:HG3	32:k:113:ALA:HB3	1.89	0.54
24:c:133:ARG:NH2	24:c:187:ASP:OD1	2.39	0.54
5:E:15:LEU:HA	5:E:37:THR:HG22	1.87	0.54
1:A:1363:A:O2'	1:A:1365:G:N7	2.36	0.54
13:M:112:PRO:O	13:M:114:LYS:NZ	2.39	0.54
22:a:1012:U:OP2	37:p:70:ARG:NH2	2.41	0.54
1:A:751:U:OP1	15:O:17:ARG:NH2	2.41	0.54
1:A:861:G:HO2'	1:A:874:G:HO2'	1.55	0.54
22:a:568:U:O4	38:q:81:LYS:NZ	2.41	0.54
1:A:514:C:H2'	1:A:515:G:H8	1.72	0.54
22:a:1447:C:O2'	22:a:1544:A:N3	2.36	0.54
12:L:66:TYR:HD2	12:L:90:LEU:HD12	1.73	0.54
20:T:15:GLU:OE2	20:T:18:ARG:NH2	2.40	0.54
22:a:1007:C:OP1	30:i:37:ARG:NH1	2.40	0.54
9:I:130:ARG:HH21	55:V:34:G:H5''	1.73	0.54
12:L:50:ARG:CB	12:L:90:LEU:HD11	2.35	0.54
12:L:110:ARG:HB3	12:L:119:VAL:HG21	1.90	0.54
19:S:62:VAL:HA	19:S:66:MET:HE1	1.89	0.54
1:A:1124:G:N2	1:A:1125:U:O4	2.41	0.54
1:A:1355:G:H2'	1:A:1356:G:H8	1.72	0.54
22:a:1667:G:O2'	22:a:1991:U:O4	2.21	0.54
24:c:94:VAL:HG21	24:c:116:ILE:HD11	1.90	0.54
1:A:674:G:H2'	1:A:675:A:C8	2.42	0.53
1:A:1218:C:H2'	1:A:1219:A:C8	2.42	0.53
48:O:33:LYS:HE3	48:O:51:GLU:HB3	1.90	0.53
15:O:64:ARG:HH22	15:O:89:ARG:HG3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:881:G:H1	22:a:895:U:H3	1.57	0.53
24:c:69:ARG:NH1	24:c:127:GLY:O	2.40	0.53
31:j:71:ARG:HB2	31:j:75:SER:HB2	1.89	0.53
1:A:1149:C:OP2	9:I:11:ARG:NH2	2.42	0.53
4:D:150:LYS:HG2	4:D:178:MET:HE3	1.90	0.53
22:a:2293:G:H5''	35:n:94:ARG:HH12	1.73	0.53
25:d:98:VAL:HG12	25:d:180:VAL:HG13	1.91	0.53
33:l:53:MET:HE1	33:l:103:TYR:CG	2.43	0.53
38:q:55:ASP:N	38:q:55:ASP:OD1	2.41	0.53
1:A:1009:U:O2	1:A:1020:G:N2	2.29	0.53
34:m:28:LEU:HD23	34:m:48:VAL:HG21	1.91	0.53
22:a:1327:A:N6	22:a:1647:U:O2	2.41	0.53
25:d:106:LYS:NZ	25:d:176:ASP:OD1	2.42	0.53
28:g:2:SER:OG	28:g:3:ARG:N	2.42	0.53
1:A:50:A:O2'	1:A:360:G:N2	2.42	0.53
10:J:12:ALA:HB2	10:J:96:VAL:HG22	1.91	0.53
22:a:1028:A:N3	22:a:2486:C:O2'	2.39	0.53
2:B:142:GLU:HA	2:B:145:GLU:HG3	1.92	0.52
22:a:994:C:O2	38:q:10:LYS:NZ	2.42	0.52
22:a:1045:C:C2	22:a:1047:G:C2	2.97	0.52
1:A:1405:G:OP2	56:A:1601:PAR:N24	2.43	0.52
2:B:9:MET:HE1	2:B:47:VAL:HG22	1.91	0.52
35:n:29:HIS:HB3	35:n:36:TYR:HB2	1.92	0.52
5:E:38:VAL:HG11	5:E:114:VAL:HG22	1.91	0.52
1:A:71:A:H61	1:A:99:C:H1'	1.75	0.52
4:D:147:GLU:HA	4:D:150:LYS:HB2	1.92	0.52
41:t:18:ASP:HB2	41:t:21:LYS:HD3	1.91	0.52
22:a:1469:A:H2'	22:a:1470:A:C8	2.44	0.52
22:a:1744:A:H3'	22:a:1745:A:H8	1.73	0.52
23:b:5:U:OP1	23:b:61:G:O2'	2.26	0.52
1:A:720:C:O2	18:R:60:LYS:NZ	2.38	0.52
3:C:16:LYS:NZ	3:C:181:ASP:OD1	2.38	0.52
22:a:2511:U:O4	22:a:2575:C:N3	2.42	0.52
33:l:77:PRO:HG2	33:l:80:VAL:HG21	1.90	0.52
1:A:219:U:H2'	1:A:220:G:H8	1.74	0.52
1:A:625:U:H2'	1:A:626:G:H8	1.75	0.52
1:A:1148:U:O2	9:I:68:LYS:NZ	2.42	0.52
22:a:577:G:O2'	22:a:1254:A:OP1	2.28	0.52
44:w:32:ASN:OD1	44:w:34:HIS:NE2	2.42	0.52
8:H:11:LEU:HD22	8:H:75:ILE:HD11	1.92	0.52
26:e:173:THR:HA	26:e:199:MET:HE1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:r:20:VAL:HG11	39:r:44:ALA:HA	1.91	0.52
3:C:14:ILE:HG22	3:C:15:VAL:HG13	1.92	0.52
17:Q:47:HIS:HB3	17:Q:74:THR:HG22	1.92	0.52
22:a:1047:G:O2'	22:a:1110:G:N1	2.39	0.52
27:f:102:ARG:HG2	52:4:24:ILE:HG21	1.91	0.52
1:A:536:C:H2'	1:A:537:G:H8	1.75	0.51
1:A:618:C:O2	1:A:622:A:N6	2.44	0.51
4:D:72:PHE:HE1	4:D:94:LEU:HD11	1.74	0.51
6:F:38:ARG:HB3	6:F:63:ASN:HB2	1.92	0.51
7:G:74:GLU:HG2	7:G:91:VAL:HG22	1.91	0.51
22:a:160:A:N3	22:a:2208:C:O2'	2.41	0.51
22:a:807:U:OP2	32:k:41:ARG:NH2	2.43	0.51
29:h:5:LEU:O	29:h:16:GLY:CA	2.58	0.51
31:j:63:VAL:HG12	31:j:107:LEU:HD21	1.92	0.51
1:A:1064:G:O2'	1:A:1190:G:N2	2.43	0.51
4:D:58:LYS:HD3	4:D:203:LEU:HD23	1.92	0.51
6:F:47:LEU:HD13	6:F:51:ILE:HD12	1.91	0.51
9:I:65:ILE:HG21	9:I:79:ILE:HG12	1.92	0.51
11:K:31:ILE:HG12	11:K:46:THR:HG22	1.91	0.51
22:a:247:G:O6	50:2:12:LYS:NZ	2.38	0.51
22:a:1266:G:O2'	22:a:2012:G:O6	2.23	0.51
5:E:100:SER:O	5:E:122:ASN:ND2	2.42	0.51
43:v:17:GLU:O	43:v:19:LYS:NZ	2.42	0.51
1:A:946:A:H2'	1:A:947:G:C8	2.46	0.51
1:A:1241:G:H2'	1:A:1242:G:H8	1.75	0.51
32:k:108:ALA:HB3	32:k:125:LEU:HD22	1.93	0.51
44:w:39:TRP:NE1	44:w:41:GLU:OE1	2.42	0.51
1:A:454:G:H2'	1:A:455:G:H8	1.76	0.51
1:A:536:C:H2'	1:A:537:G:C8	2.46	0.51
22:a:1326:U:H2'	22:a:1327:A:H8	1.75	0.51
24:c:29:PRO:HG2	24:c:34:LEU:HD11	1.91	0.51
4:D:202:GLU:OE2	5:E:105:ILE:N	2.44	0.51
11:K:14:LYS:NZ	11:K:15:GLN:O	2.41	0.51
22:a:2848:G:HO2'	22:a:2867:G:H22	1.57	0.51
27:f:36:LEU:HD22	27:f:154:ILE:HG12	1.92	0.51
28:g:105:LEU:HB3	28:g:107:LEU:HG	1.92	0.51
37:p:58:ARG:O	37:p:62:ILE:HG12	2.10	0.51
26:e:149:ILE:HD11	26:e:172:ALA:HA	1.93	0.51
51:3:16:ILE:HD13	51:3:25:VAL:HG22	1.93	0.51
24:c:41:GLY:O	24:c:43:ARG:NH1	2.44	0.51
28:g:152:ARG:HB3	28:g:162:VAL:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:61:VAL:HG22	16:P:67:ILE:HD11	1.91	0.51
1:A:412:A:N6	1:A:431:A:C2	2.71	0.51
1:A:440:C:H2'	1:A:441:A:H8	1.76	0.51
1:A:1373:G:H5''	7:G:36:LYS:HD2	1.93	0.51
7:G:15:ASP:OD1	7:G:15:ASP:N	2.40	0.51
22:a:2619:C:H5''	25:d:157:LYS:HG2	1.93	0.51
24:c:155:ALA:HB2	24:c:162:VAL:HG23	1.92	0.51
30:i:99:ARG:O	30:i:103:ILE:HG13	2.11	0.51
1:A:28:A:O2'	1:A:296:U:OP1	2.23	0.50
1:A:691:G:O6	11:K:57:LYS:NZ	2.38	0.50
22:a:848:C:H2'	22:a:849:A:H8	1.76	0.50
22:a:1365:A:OP1	44:w:3:ARG:NH1	2.42	0.50
1:A:19:A:H5''	5:E:91:GLY:HA3	1.93	0.50
1:A:1130:A:H61	1:A:1144:G:H1'	1.77	0.50
3:C:70:THR:HG21	3:C:76:VAL:HG21	1.92	0.50
20:T:35:VAL:HG11	20:T:79:LEU:HD13	1.92	0.50
34:m:65:LEU:HD22	34:m:69:ARG:HH12	1.75	0.50
45:x:32:ALA:HB2	45:x:37:LEU:HD23	1.94	0.50
46:y:9:GLN:O	46:y:33:GLY:N	2.43	0.50
1:A:1009:U:O4	1:A:1020:G:O6	2.30	0.50
2:B:92:VAL:HG11	2:B:100:MET:HE3	1.92	0.50
22:a:2405:G:O2'	22:a:2411:A:N6	2.44	0.50
4:D:149:ALA:HA	4:D:152:GLN:HG3	1.94	0.50
24:c:176:LEU:O	24:c:179:GLY:N	2.40	0.50
22:a:1796:U:H2'	22:a:1797:G:H8	1.75	0.50
24:c:78:VAL:HG21	24:c:110:LEU:HD21	1.93	0.50
40:s:5:GLU:OE2	40:s:9:LYS:NZ	2.45	0.50
4:D:124:MET:HE3	4:D:146:ARG:HG2	1.93	0.50
28:g:35:ARG:HG2	28:g:75:MET:HE1	1.94	0.50
3:C:54:ARG:HB3	3:C:69:HIS:HB2	1.94	0.50
22:a:1799:G:OP1	24:c:258:ARG:NH1	2.36	0.50
22:a:2636:C:O2'	25:d:45:TYR:OH	2.27	0.50
27:f:134:GLU:HB3	27:f:136:ILE:HG22	1.93	0.50
39:r:22:ASP:OD1	39:r:25:ARG:NH1	2.40	0.50
41:t:98:SER:O	41:t:99:ASN:ND2	2.45	0.50
48:0:35:GLU:OE1	48:0:50:LYS:NZ	2.44	0.50
22:a:2564:A:OP1	22:a:2648:G:O2'	2.28	0.49
33:l:21:ALA:HB2	33:l:97:GLN:HB2	1.94	0.49
1:A:746:A:H2'	1:A:747:A:C8	2.47	0.49
1:A:943:U:H1'	9:I:126:GLN:HE22	1.76	0.49
1:A:1147:C:O2'	9:I:7:TYR:OH	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:12:VAL:HG22	17:Q:23:VAL:HG22	1.95	0.49
22:a:574:A:N6	22:a:2034:U:OP1	2.45	0.49
22:a:2529:G:H4'	28:g:175:LYS:HD3	1.93	0.49
3:C:26:THR:HG22	14:N:76:LYS:HE2	1.94	0.49
12:L:50:ARG:HD2	12:L:66:TYR:HE2	1.76	0.49
22:a:549:G:H2'	22:a:550:C:H6	1.76	0.49
23:b:1:U:H2'	23:b:2:G:C8	2.48	0.49
2:B:105:LYS:O	2:B:109:GLN:NE2	2.45	0.49
22:a:2618:G:H21	25:d:155:VAL:HG21	1.77	0.49
1:A:769:G:H4'	1:A:1513:A:H4'	1.94	0.49
1:A:999:C:N3	1:A:1042:A:N6	2.61	0.49
1:A:1495:U:O2'	22:a:1919:A:N1	2.42	0.49
7:G:22:LEU:HD21	7:G:66:LEU:HD22	1.95	0.49
22:a:788:A:OP1	22:a:791:C:N4	2.34	0.49
24:c:141:VAL:HG12	24:c:192:LEU:HD23	1.94	0.49
1:A:147:G:H2'	1:A:148:G:C8	2.48	0.49
22:a:1802:A:H2'	22:a:1803:A:C8	2.47	0.49
22:a:2273:A:H2'	22:a:2274:A:C8	2.48	0.49
1:A:410:G:H21	1:A:432:A:H62	1.60	0.49
2:B:60:ILE:HG13	2:B:65:GLY:HA3	1.95	0.49
5:E:102:GLY:H	5:E:122:ASN:HD21	1.61	0.49
16:P:4:ILE:HG13	16:P:21:VAL:HG22	1.94	0.49
28:g:105:LEU:HB2	28:g:113:VAL:HG23	1.95	0.49
3:C:43:LEU:O	3:C:47:LEU:HB2	2.13	0.49
21:U:7:ARG:HH12	21:U:18:ARG:HH22	1.59	0.49
22:a:1156:A:C8	37:p:51:ARG:HG2	2.48	0.49
40:s:65:GLY:HA3	40:s:77:ARG:O	2.13	0.49
1:A:373:A:H2'	1:A:374:A:H8	1.78	0.48
1:A:1346:A:OP1	9:I:122:ARG:NH1	2.43	0.48
4:D:58:LYS:NZ	4:D:69:GLU:OE1	2.45	0.48
22:a:959:A:H62	33:l:82:MET:HE3	1.75	0.48
28:g:98:VAL:HG12	28:g:103:ILE:HG12	1.95	0.48
34:m:57:THR:O	34:m:62:ASN:ND2	2.36	0.48
1:A:412:A:N6	1:A:431:A:H2	2.10	0.48
1:A:1144:G:N2	1:A:1146:A:H62	2.10	0.48
3:C:59:ARG:HG2	3:C:64:ILE:HG22	1.95	0.48
22:a:219:A:N3	22:a:234:U:O2'	2.36	0.48
47:z:43:ILE:HG22	47:z:49:TYR:HB2	1.96	0.48
1:A:522:C:H41	12:L:50:ARG:NH2	2.11	0.48
1:A:1253:G:H2'	1:A:1254:A:H8	1.78	0.48
9:I:21:ILE:HG12	9:I:63:LEU:HD22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2245:U:H5''	22:a:2246:G:H5'	1.95	0.48
26:e:181:ILE:HD13	32:k:6:LEU:HD11	1.96	0.48
1:A:1255:G:OP2	10:J:45:ARG:NH2	2.46	0.48
3:C:184:TYR:HA	3:C:200:VAL:O	2.14	0.48
3:C:185:ASN:OD1	3:C:186:THR:N	2.46	0.48
10:J:8:ILE:HB	10:J:74:VAL:HB	1.96	0.48
10:J:66:GLU:HB2	14:N:99:ALA:HB2	1.95	0.48
28:g:46:ALA:O	28:g:49:THR:OG1	2.32	0.48
48:0:7:GLU:OE2	48:0:27:LYS:NZ	2.38	0.48
1:A:269:C:H2'	1:A:270:A:H8	1.77	0.48
1:A:1255:G:O2'	1:A:1258:G:N3	2.38	0.48
25:d:39:ASP:N	25:d:39:ASP:OD1	2.46	0.48
25:d:181:ASP:HB3	25:d:186:LEU:HB2	1.95	0.48
1:A:264:C:O2'	17:Q:66:PRO:O	2.29	0.48
1:A:795:C:O2'	11:K:128:ARG:O	2.31	0.48
5:E:115:LEU:HD13	5:E:123:VAL:HG11	1.96	0.48
22:a:184:C:H2'	22:a:185:G:H8	1.78	0.48
22:a:1808:A:H3'	22:a:1809:A:C8	2.49	0.48
22:a:2722:G:O2'	34:m:3:HIS:O	2.32	0.48
52:4:59:ARG:HH22	52:4:63:ARG:HH11	1.62	0.48
5:E:108:GLY:O	5:E:112:ARG:HB2	2.14	0.48
17:Q:15:ASP:HA	17:Q:21:ILE:HG22	1.95	0.48
22:a:411:G:OP2	22:a:2406:A:O2'	2.26	0.48
22:a:2291:U:H2'	22:a:2292:U:C6	2.49	0.48
1:A:501:C:H2'	1:A:502:A:C8	2.49	0.48
22:a:993:G:N2	38:q:23:GLU:OE2	2.47	0.48
22:a:288:U:H2'	22:a:289:G:H8	1.78	0.47
45:x:10:SER:OG	45:x:13:GLU:OE1	2.22	0.47
1:A:1355:G:H2'	1:A:1356:G:C8	2.49	0.47
12:L:42:PRO:CB	12:L:89:ASP:HB3	2.44	0.47
22:a:308:G:N2	22:a:477:A:C5	2.82	0.47
30:i:36:LEU:HD11	30:i:122:LEU:HB2	1.95	0.47
48:0:38:LYS:HB2	48:0:49:TYR:CD2	2.49	0.47
1:A:714:G:H2'	1:A:715:A:C8	2.48	0.47
1:A:946:A:O2'	1:A:1333:A:N3	2.43	0.47
4:D:140:ASN:N	4:D:182:PHE:O	2.48	0.47
9:I:114:LYS:NZ	9:I:118:LEU:O	2.44	0.47
22:a:2278:A:OP1	33:l:10:ARG:NH2	2.47	0.47
22:a:856:G:H2'	22:a:857:G:C8	2.49	0.47
31:j:98:ARG:HH12	31:j:100:PHE:HE1	1.62	0.47
55:V:1:C:H2'	55:V:2:G:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:G:H2'	1:A:42:G:H8	1.79	0.47
20:T:24:ARG:NH2	20:T:61:GLN:OE1	2.47	0.47
22:a:639:U:H2'	22:a:640:C:C6	2.49	0.47
2:B:70:VAL:HB	2:B:163:VAL:HG12	1.97	0.47
22:a:1386:C:H2'	22:a:1387:A:C8	2.50	0.47
22:a:1386:C:H2'	22:a:1387:A:H8	1.79	0.47
22:a:2812:G:H2'	22:a:2813:A:C8	2.49	0.47
1:A:620:C:H1'	4:D:132:ILE:HG21	1.96	0.47
1:A:1317:C:O2	19:S:37:ARG:NH2	2.42	0.47
1:A:1356:G:H2'	1:A:1357:A:H8	1.80	0.47
3:C:77:ILE:HA	3:C:84:VAL:HG13	1.97	0.47
10:J:41:PRO:HG3	10:J:72:ARG:HH21	1.79	0.47
22:a:288:U:H2'	22:a:289:G:C8	2.50	0.47
22:a:358:U:H2'	22:a:359:G:H8	1.80	0.47
22:a:959:A:H61	33:l:82:MET:HE3	1.80	0.47
22:a:1649:G:O2'	34:m:106:ASP:OD2	2.26	0.47
22:a:1716:U:H2'	22:a:1717:A:H8	1.80	0.47
22:a:1798:U:H5''	24:c:258:ARG:HB2	1.96	0.47
25:d:152:PRO:HG3	25:d:156:PHE:CZ	2.50	0.47
53:X:20:G:H2'	53:X:21:A:C8	2.50	0.47
1:A:17:U:H2'	1:A:18:C:C6	2.50	0.47
9:I:19:VAL:HG22	9:I:65:ILE:HG12	1.97	0.47
32:k:91:ASP:HB2	32:k:94:THR:HG23	1.97	0.47
1:A:177:G:OP1	20:T:24:ARG:NH2	2.47	0.47
31:j:5:GLN:N	31:j:21:CYS:O	2.46	0.47
7:G:44:TYR:HD1	7:G:47:LEU:HD21	1.80	0.47
29:h:5:LEU:O	29:h:16:GLY:HA2	2.15	0.47
50:2:33:LEU:HD23	50:2:36:LYS:HD2	1.96	0.47
22:a:514:A:N3	22:a:581:C:O2'	2.37	0.46
26:e:83:VAL:HB	26:e:86:ALA:HB2	1.97	0.46
1:A:382:A:H2'	1:A:383:A:C8	2.49	0.46
2:B:97:LEU:HD11	2:B:148:LEU:HD11	1.97	0.46
40:s:11:LEU:HD23	40:s:11:LEU:HA	1.78	0.46
1:A:280:C:O4'	17:Q:40:ARG:NH2	2.49	0.46
1:A:745:G:H2'	1:A:746:A:C8	2.51	0.46
8:H:9:ASP:OD2	8:H:13:ARG:NH1	2.47	0.46
22:a:155:A:H2'	22:a:156:A:H8	1.79	0.46
22:a:329:G:O6	41:t:17:LYS:N	2.47	0.46
1:A:944:G:N1	1:A:1338:G:OP2	2.45	0.46
1:A:1017:U:H2'	1:A:1018:G:H8	1.80	0.46
18:R:63:ARG:HD3	18:R:70:TYR:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2887:A:N3	47:z:27:SER:OG	2.43	0.46
22:a:2243:U:H2'	22:a:2244:U:C6	2.51	0.46
22:a:2641:G:H5''	30:i:78:THR:HB	1.97	0.46
48:0:25:LYS:NZ	48:0:51:GLU:OE2	2.41	0.46
1:A:461:A:H2'	1:A:462:G:H8	1.81	0.46
1:A:671:G:O2'	6:F:79:ARG:NH2	2.49	0.46
5:E:34:THR:HG22	5:E:52:LYS:HG2	1.97	0.46
10:J:10:LEU:HD11	10:J:25:ILE:HD12	1.97	0.46
22:a:2255:G:N2	43:v:8:GLY:O	2.48	0.46
38:q:71:LYS:HD3	38:q:73:LYS:HE2	1.97	0.46
50:2:32:ILE:HG22	50:2:35:LYS:HG2	1.96	0.46
1:A:201:G:O6	1:A:216:U:O4	2.34	0.46
1:A:235:C:H2'	1:A:236:A:H8	1.80	0.46
1:A:938:A:N3	1:A:1376:U:O2'	2.42	0.46
20:T:54:MET:HE3	20:T:54:MET:HB3	1.87	0.46
22:a:155:A:H2'	22:a:156:A:C8	2.51	0.46
22:a:2419:U:H4'	48:0:22:THR:HG21	1.98	0.46
43:v:59:LEU:HD12	43:v:80:ILE:HD12	1.96	0.46
1:A:880:C:H5''	12:L:9:ARG:HH12	1.81	0.46
20:T:61:GLN:HE21	20:T:66:LEU:HD22	1.81	0.46
25:d:25:THR:OG1	25:d:191:GLY:O	2.24	0.46
1:A:946:A:H2'	1:A:947:G:H8	1.79	0.46
1:A:1032:G:H2'	1:A:1033:G:H4'	1.97	0.46
8:H:64:LYS:HG3	8:H:71:VAL:HG21	1.97	0.46
24:c:203:ARG:NH2	24:c:214:ARG:HH12	2.14	0.46
1:A:652:U:O4	1:A:752:G:O2'	2.31	0.45
1:A:744:C:H2'	1:A:745:G:C8	2.50	0.45
1:A:948:C:H2'	1:A:949:A:H8	1.81	0.45
22:a:593:U:H2'	22:a:594:U:C6	2.51	0.45
22:a:2030:6MZ:H2	22:a:2499:C:H5''	1.97	0.45
27:f:8:TYR:OH	27:f:29:PRO:O	2.27	0.45
1:A:222:C:H2'	1:A:223:A:H8	1.81	0.45
1:A:1150:A:H4'	10:J:43:PRO:HG3	1.98	0.45
1:A:1217:C:OP2	14:N:9:ARG:NH2	2.46	0.45
11:K:114:THR:O	18:R:73:ARG:NH1	2.37	0.45
22:a:1527:G:N1	22:a:1544:A:OP2	2.45	0.45
22:a:2251:OMG:HM23	22:a:2251:OMG:H1'	1.68	0.45
34:m:24:MET:HE3	34:m:44:LEU:HD13	1.98	0.45
2:B:61:ALA:HB2	2:B:221:VAL:HG23	1.97	0.45
7:G:40:GLU:HG2	7:G:44:TYR:CE2	2.51	0.45
11:K:42:LEU:HD12	11:K:79:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:203:ARG:HH22	24:c:214:ARG:HH12	1.64	0.45
34:m:101:GLY:O	34:m:110:MET:N	2.37	0.45
1:A:600:A:H5''	8:H:89:LYS:HE3	1.98	0.45
1:A:909:A:N3	1:A:1413:A:O2'	2.46	0.45
10:J:7:ARG:HB2	10:J:101:SER:HB3	1.98	0.45
25:d:113:SER:O	25:d:167:ASN:CA	2.64	0.45
42:u:14:LYS:HG2	42:u:18:ARG:HD2	1.98	0.45
1:A:21:G:H2'	1:A:22:G:C8	2.51	0.45
1:A:1222:G:OP2	1:A:1322:C:N4	2.42	0.45
1:A:1360:A:OP2	14:N:75:ARG:NH2	2.50	0.45
2:B:114:LEU:HD13	2:B:144:LEU:HB3	1.98	0.45
22:a:1812:U:H2'	22:a:1813:G:H8	1.82	0.45
22:a:2250:G:O2'	22:a:2496:C:OP1	2.22	0.45
1:A:235:C:H2'	1:A:236:A:C8	2.51	0.45
1:A:1458:G:OP1	20:T:30:THR:OG1	2.30	0.45
3:C:22:TRP:HD1	3:C:58:GLU:HA	1.80	0.45
22:a:1:G:H2'	22:a:2:G:C8	2.52	0.45
22:a:1419:A:O2'	22:a:1421:G:N7	2.47	0.45
1:A:337:G:H2'	1:A:338:A:C8	2.52	0.45
11:K:87:LYS:HB2	11:K:113:VAL:HG23	1.98	0.45
1:A:229:U:O2'	16:P:23:ASP:OD2	2.34	0.45
1:A:1224:U:O2'	1:A:1322:C:OP1	2.25	0.45
1:A:1516:2MG:N2	1:A:1519:MA6:OP2	2.49	0.45
4:D:25:VAL:HG23	4:D:26:ARG:HG3	1.98	0.45
5:E:47:GLY:HA3	5:E:71:MET:HA	1.98	0.45
22:a:84:A:N1	22:a:98:G:O2'	2.46	0.45
22:a:987:C:O2'	22:a:1000:A:N3	2.40	0.45
22:a:1796:U:H2'	22:a:1797:G:C8	2.52	0.45
32:k:123:ARG:HA	32:k:143:GLU:HB2	1.97	0.45
36:o:29:LYS:HB3	36:o:40:LEU:HD23	1.99	0.45
1:A:1017:U:H2'	1:A:1018:G:C8	2.52	0.45
1:A:1312:G:H2'	1:A:1313:U:C6	2.52	0.45
1:A:1376:U:OP2	7:G:25:LYS:NZ	2.49	0.45
12:L:29:GLN:HB3	12:L:81:LEU:HD11	1.99	0.45
22:a:1264:A:OP1	47:z:16:ARG:NH2	2.38	0.45
26:e:58:LYS:HG3	26:e:71:GLY:HA2	1.98	0.45
55:V:28:C:H2'	55:V:29:G:H8	1.81	0.45
2:B:4:VAL:HG11	2:B:50:PHE:HE2	1.82	0.45
18:R:56:ALA:O	18:R:60:LYS:HG3	2.17	0.45
30:i:114:LEU:O	30:i:118:MET:HG3	2.17	0.45
40:s:8:LEU:HD23	40:s:50:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:d:25:THR:HG21	25:d:193:VAL:HG22	1.99	0.44
50:2:16:LYS:HE3	50:2:20:GLY:HA2	1.99	0.44
1:A:466:A:H2'	1:A:468:A:H8	1.82	0.44
1:A:1464:U:H2'	1:A:1465:A:H8	1.82	0.44
2:B:46:THR:HG22	2:B:201:PRO:HB2	1.99	0.44
24:c:259:SER:O	24:c:259:SER:OG	2.34	0.44
1:A:1253:G:H2'	1:A:1254:A:C8	2.53	0.44
1:A:1320:C:H2'	1:A:1321:U:C6	2.52	0.44
2:B:133:GLU:O	2:B:137:ARG:HG2	2.18	0.44
6:F:29:ILE:HD13	6:F:64:VAL:HG11	1.99	0.44
9:I:52:LEU:HD11	9:I:63:LEU:HD11	1.98	0.44
22:a:307:G:N1	22:a:310:A:OP2	2.44	0.44
22:a:2197:U:H1'	22:a:2198:A:C8	2.52	0.44
31:j:1:MET:HE3	31:j:1:MET:HB2	1.78	0.44
22:a:549:G:H2'	22:a:550:C:C6	2.51	0.44
22:a:631:A:OP2	50:2:23:LYS:NZ	2.41	0.44
22:a:742:A:H2'	22:a:743:A:C8	2.53	0.44
22:a:2250:G:C2	33:l:83:GLY:HA3	2.52	0.44
24:c:165:VAL:HG21	24:c:181:MET:HE1	1.99	0.44
13:M:45:ILE:HD13	13:M:48:LEU:HD12	1.99	0.44
15:O:18:ASP:OD1	15:O:18:ASP:N	2.49	0.44
40:s:65:GLY:CA	40:s:77:ARG:O	2.65	0.44
12:L:87:VAL:O	12:L:88:LYS:C	2.60	0.44
22:a:2850:A:N7	22:a:2868:A:O2'	2.50	0.44
1:A:713:G:H2'	1:A:714:G:C8	2.53	0.44
1:A:1034:G:H2'	1:A:1035:A:H8	1.83	0.44
4:D:11:LEU:HD13	4:D:63:ARG:HD3	1.99	0.44
4:D:61:VAL:HG21	4:D:200:ILE:HD11	1.99	0.44
7:G:57:SER:OG	7:G:60:GLU:OE2	2.35	0.44
11:K:20:VAL:HG22	11:K:83:GLU:HB2	2.00	0.44
17:Q:6:ARG:HE	17:Q:6:ARG:HB3	1.64	0.44
22:a:276:U:H2'	22:a:277:G:C8	2.53	0.44
22:a:1432:G:H2'	22:a:1433:A:C8	2.53	0.44
43:v:23:VAL:HA	43:v:38:VAL:HG12	2.00	0.44
3:C:51:SER:HB3	3:C:115:LEU:HD11	1.98	0.44
7:G:31:MET:HE3	7:G:31:MET:HB3	1.74	0.44
1:A:384:G:H2'	1:A:385:C:C6	2.53	0.44
1:A:555:U:H2'	1:A:556:C:C6	2.53	0.44
1:A:859:G:H2'	1:A:860:A:H8	1.83	0.44
1:A:1043:G:O2'	1:A:1044:A:O5'	2.34	0.44
4:D:27:ALA:HB3	4:D:30:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:60:VAL:HG11	19:S:74:PHE:HD2	1.83	0.44
22:a:1801:A:OP2	24:c:150:LYS:NZ	2.47	0.44
32:k:20:GLY:O	32:k:21:ARG:NH1	2.41	0.44
1:A:324:G:N1	1:A:327:A:OP2	2.48	0.43
1:A:523:A:C2	12:L:88:LYS:HB3	2.53	0.43
1:A:881:G:P	12:L:9:ARG:HH22	2.40	0.43
3:C:47:LEU:HD11	3:C:87:LEU:HD11	2.00	0.43
3:C:151:VAL:HG23	3:C:200:VAL:HG22	2.00	0.43
15:O:39:LEU:HD23	15:O:39:LEU:HA	1.86	0.43
37:p:61:TRP:O	37:p:65:ILE:HG13	2.18	0.43
53:X:17:C:H2'	53:X:18:C:C6	2.52	0.43
12:L:25:GLU:OE1	12:L:59:ASN:ND2	2.50	0.43
13:M:17:ILE:HA	13:M:20:THR:HG22	2.00	0.43
16:P:39:PHE:HD1	16:P:50:THR:HG22	1.83	0.43
22:a:500:G:N1	22:a:503:A:OP2	2.46	0.43
22:a:511:U:H4'	22:a:1235:G:H4'	1.99	0.43
22:a:1469:A:H2'	22:a:1470:A:H8	1.82	0.43
41:t:7:ARG:NE	41:t:26:LYS:O	2.46	0.43
1:A:410:G:N1	1:A:431:A:OP2	2.34	0.43
1:A:578:C:O2'	1:A:728:A:N3	2.46	0.43
1:A:1162:C:H2'	1:A:1163:A:H8	1.83	0.43
22:a:1405:U:H2'	22:a:1406:U:C6	2.53	0.43
24:c:84:ASP:OD2	24:c:87:ARG:NE	2.42	0.43
27:f:40:VAL:HG11	27:f:50:LEU:HA	2.01	0.43
1:A:515:G:H2'	1:A:516:PSU:C6	2.49	0.43
21:U:21:ARG:HD2	21:U:21:ARG:HA	1.77	0.43
21:U:63:GLU:O	21:U:67:ARG:NH1	2.50	0.43
1:A:131:A:H2'	1:A:132:C:C6	2.54	0.43
22:a:910:A:H2'	22:a:911:A:C8	2.52	0.43
22:a:2371:G:O2'	48:O:46:HIS:ND1	2.38	0.43
22:a:2848:G:HO2'	22:a:2867:G:N2	2.15	0.43
30:i:60:ASP:HB3	30:i:97:PRO:HG3	2.00	0.43
55:V:23:C:H2'	55:V:24:G:C8	2.53	0.43
1:A:662:U:H2'	1:A:663:A:C8	2.54	0.43
22:a:1045:C:C2	22:a:1047:G:N2	2.87	0.43
22:a:1223:G:OP1	38:q:68:ARG:NH1	2.45	0.43
28:g:8:PRO:HB3	28:g:51:THR:HG22	1.99	0.43
1:A:217:C:H2'	1:A:218:U:C6	2.54	0.43
6:F:9:MET:HA	6:F:58:HIS:O	2.19	0.43
12:L:52:VAL:CG1	12:L:90:LEU:HD13	2.48	0.43
22:a:589:U:H2'	22:a:590:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:948:C:H2'	22:a:949:G:H8	1.84	0.43
22:a:1340:U:OP2	40:s:82:LYS:NZ	2.50	0.43
22:a:1394:U:H4'	22:a:1603:A:H4'	2.01	0.43
22:a:2567:G:H2'	22:a:2568:U:C6	2.53	0.43
22:a:2577:A:H2'	22:a:2614:A:N6	2.34	0.43
22:a:2615:U:C2	47:z:4:GLN:HA	2.53	0.43
23:b:49:C:H2'	23:b:50:A:H8	1.83	0.43
31:j:24:VAL:HG13	31:j:33:ALA:HB2	2.01	0.43
38:q:78:ARG:HB3	38:q:83:TYR:HB3	1.99	0.43
1:A:259:G:OP1	20:T:36:TYR:OH	2.29	0.43
4:D:65:TYR:CE2	4:D:94:LEU:HB3	2.53	0.43
6:F:3:HIS:HD2	6:F:65:GLU:HG3	1.83	0.43
10:J:15:HIS:HA	10:J:18:ILE:HG22	1.99	0.43
11:K:54:GLY:H	11:K:57:LYS:HE2	1.83	0.43
22:a:2014:A:H2'	22:a:2015:A:C8	2.54	0.43
24:c:37:ASN:HD22	24:c:62:TYR:HB2	1.83	0.43
24:c:107:PRO:HD2	24:c:110:LEU:HD22	2.00	0.43
27:f:60:ILE:O	27:f:102:ARG:NH2	2.52	0.43
50:2:49:MET:HE3	50:2:49:MET:HB3	1.80	0.43
1:A:270:A:H2'	1:A:271:C:C6	2.54	0.43
1:A:362:G:N2	1:A:365:U:OP2	2.51	0.43
8:H:27:MET:SD	8:H:27:MET:N	2.92	0.43
9:I:88:MET:SD	9:I:95:ARG:NE	2.87	0.43
11:K:34:ILE:HB	11:K:74:VAL:HG11	2.00	0.43
22:a:2502:G:H5''	22:a:2503:2MA:H5''	2.00	0.43
55:V:8:U:C2	55:V:15:G:O6	2.72	0.43
1:A:269:C:H2'	1:A:270:A:C8	2.54	0.43
2:B:57:LEU:HA	2:B:60:ILE:HG22	2.01	0.43
22:a:2638:G:O2'	22:a:2775:G:N2	2.44	0.43
24:c:100:GLU:OE2	24:c:102:ARG:NE	2.52	0.43
1:A:443:C:H2'	1:A:444:G:C8	2.54	0.42
1:A:447:G:N1	1:A:486:U:OP1	2.37	0.42
1:A:1328:C:H2'	1:A:1329:A:H8	1.83	0.42
1:A:1354:U:H2'	1:A:1355:G:H8	1.84	0.42
4:D:142:VAL:HA	4:D:180:GLY:O	2.19	0.42
22:a:2349:G:OP1	50:2:45:ARG:NH2	2.49	0.42
26:e:45:ALA:HA	26:e:87:ALA:O	2.19	0.42
27:f:60:ILE:HD11	27:f:135:GLN:HB2	2.00	0.42
29:h:34:GLY:O	29:h:36:ALA:N	2.51	0.42
34:m:12:ARG:O	34:m:17:ARG:NH1	2.52	0.42
1:A:715:A:H2	11:K:120:GLY:HA2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:999:C:H2'	1:A:1000:A:H8	1.84	0.42
1:A:1518:MA6:O5'	1:A:1518:MA6:H8	2.19	0.42
2:B:131:LYS:HA	2:B:134:ALA:HB3	2.01	0.42
22:a:604:G:OP2	32:k:84:LYS:NZ	2.38	0.42
22:a:1790:C:H2'	22:a:1791:A:C5	2.55	0.42
1:A:999:C:H2'	1:A:1000:A:C8	2.54	0.42
1:A:1077:G:N2	1:A:1080:A:OP2	2.47	0.42
3:C:110:GLU:HB2	3:C:144:LEU:HD12	2.00	0.42
3:C:138:VAL:HG13	3:C:170:GLU:OE2	2.18	0.42
7:G:16:PRO:HA	9:I:46:MET:HG2	2.02	0.42
8:H:66:PHE:CD2	8:H:67:GLN:HG2	2.54	0.42
16:P:59:HIS:CD2	16:P:63:GLN:HE22	2.37	0.42
22:a:120:U:H4'	22:a:121:G:H5''	2.01	0.42
28:g:24:ILE:HG21	28:g:72:LEU:HD21	2.00	0.42
28:g:80:THR:HG23	28:g:81:GLU:HG2	2.01	0.42
41:t:98:SER:O	41:t:98:SER:OG	2.35	0.42
1:A:421:U:H3	3:C:127:ARG:NH2	2.17	0.42
1:A:456:A:H3'	1:A:457:G:H8	1.83	0.42
1:A:1338:G:N3	55:V:41:C:O2'	2.52	0.42
22:a:347:A:H2'	22:a:348:A:C8	2.55	0.42
22:a:2070:A:H2'	22:a:2071:A:C8	2.55	0.42
30:i:114:LEU:HD12	30:i:114:LEU:HA	1.90	0.42
1:A:599:C:H2'	1:A:600:A:H8	1.83	0.42
1:A:976:G:OP2	1:A:1358:U:O2'	2.37	0.42
1:A:1015:G:H2'	1:A:1016:A:C8	2.54	0.42
22:a:1548:A:H2'	22:a:1549:A:C8	2.54	0.42
22:a:2331:G:O2'	22:a:2336:A:N1	2.49	0.42
22:a:2799:A:O2'	22:a:2800:A:H5''	2.20	0.42
27:f:13:VAL:HG23	27:f:28:VAL:HG11	2.01	0.42
11:K:23:ILE:HG12	11:K:96:THR:HG21	2.02	0.42
26:e:112:LEU:HD13	26:e:186:VAL:HG11	2.01	0.42
33:l:35:ALA:HB2	33:l:102:LEU:HD11	2.01	0.42
46:y:41:THR:HB	46:y:44:ILE:HG12	2.02	0.42
55:V:66:C:H2'	55:V:67:G:H8	1.83	0.42
6:F:3:HIS:CD2	6:F:65:GLU:HG3	2.54	0.42
12:L:55:VAL:HG21	12:L:80:ILE:HD11	2.01	0.42
22:a:272:A:H2'	22:a:273:G:H8	1.83	0.42
22:a:644:A:H2'	22:a:645:C:O4'	2.20	0.42
22:a:1724:G:O6	22:a:1737:G:N2	2.53	0.42
22:a:2515:C:H2'	22:a:2516:A:H8	1.85	0.42
25:d:8:LYS:O	25:d:198:GLY:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:t:33:LYS:HB3	41:t:64:ALA:HB1	2.01	0.42
1:A:1033:G:H3'	1:A:1034:G:H8	1.84	0.42
1:A:1350:A:O2'	7:G:33:ASP:OD1	2.33	0.42
18:R:72:ASP:OD1	18:R:72:ASP:N	2.53	0.42
22:a:191:A:H2'	22:a:192:C:C6	2.55	0.42
22:a:1445:G:O6	22:a:1466:U:O2	2.38	0.42
1:A:154:U:H2'	1:A:155:A:C8	2.55	0.42
1:A:513:C:H2'	1:A:514:C:C6	2.54	0.42
2:B:12:ALA:HA	2:B:208:ARG:HH21	1.85	0.42
22:a:538:A:H5''	30:i:7:LYS:HE3	2.02	0.42
22:a:2064:C:H2'	22:a:2065:C:C6	2.55	0.42
22:a:2230:G:H2'	22:a:2231:U:C6	2.55	0.42
22:a:2328:A:H2'	22:a:2329:U:C6	2.55	0.42
22:a:2677:G:H2'	22:a:2678:C:C6	2.54	0.42
24:c:145:GLU:HB2	24:c:188:CYS:HB3	2.01	0.42
25:d:8:LYS:HB2	25:d:201:LEU:HD11	2.00	0.42
32:k:103:ILE:HG23	32:k:104:GLN:HG2	2.01	0.42
43:v:19:LYS:HA	43:v:19:LYS:HD3	1.88	0.42
55:V:1:C:H2'	55:V:2:G:C8	2.55	0.42
1:A:410:G:N2	1:A:432:A:H62	2.18	0.42
1:A:454:G:H2'	1:A:455:G:C8	2.54	0.42
5:E:77:ASN:HB2	5:E:82:GLN:HE22	1.84	0.42
14:N:9:ARG:O	14:N:13:ARG:HG3	2.20	0.42
16:P:74:LEU:HA	16:P:77:GLU:HG2	2.02	0.42
22:a:832:U:H2'	22:a:833:A:C8	2.55	0.42
40:s:65:GLY:N	40:s:79:ASP:OD1	2.53	0.42
48:0:35:GLU:HA	48:0:49:TYR:O	2.20	0.42
1:A:818:G:HO2'	1:A:820:U:H6	1.66	0.41
1:A:1103:C:OP1	2:B:95:ARG:NH2	2.53	0.41
6:F:42:TRP:HB2	6:F:59:TYR:HB2	2.02	0.41
12:L:113:ALA:HB1	12:L:116:LYS:HB2	2.01	0.41
16:P:56:ARG:HA	16:P:56:ARG:HD2	1.81	0.41
38:q:57:GLY:HA2	38:q:102:SER:O	2.20	0.41
1:A:626:G:OP1	16:P:35:ARG:NH2	2.53	0.41
1:A:673:A:H2'	1:A:674:G:H8	1.83	0.41
1:A:966:2MG:HM21	9:I:129:LYS:HE2	2.03	0.41
2:B:31:ILE:HD11	2:B:189:THR:HG22	2.03	0.41
22:a:2:G:H2'	22:a:3:U:C6	2.55	0.41
22:a:793:A:OP2	22:a:2071:A:O2'	2.37	0.41
22:a:1178:C:H2'	22:a:1179:G:H8	1.85	0.41
22:a:1482:G:H2'	22:a:1483:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1870:C:O2'	22:a:1871:A:O4'	2.35	0.41
22:a:2837:A:H2'	22:a:2838:G:H8	1.85	0.41
27:f:125:ARG:HD2	27:f:125:ARG:HA	1.85	0.41
28:g:44:LYS:HE3	28:g:44:LYS:HA	2.02	0.41
37:p:86:ALA:HB2	37:p:116:ALA:HB2	2.02	0.41
1:A:524:G:H2'	1:A:525:C:C6	2.55	0.41
1:A:601:G:H2'	1:A:602:A:C8	2.56	0.41
1:A:672:U:H2'	1:A:673:A:H8	1.85	0.41
1:A:811:C:O2'	1:A:901:A:N1	2.50	0.41
1:A:1103:C:H4'	2:B:97:LEU:HD13	2.02	0.41
5:E:89:HIS:CE1	5:E:138:ARG:HD3	2.55	0.41
6:F:2:ARG:HD3	6:F:91:ARG:CZ	2.50	0.41
22:a:1315:C:O2'	22:a:1392:A:N3	2.47	0.41
22:a:1406:U:H2'	22:a:1407:G:H8	1.86	0.41
22:a:1682:G:H2'	22:a:1683:U:C6	2.55	0.41
34:m:32:GLU:HG2	34:m:115:LEU:HD12	2.01	0.41
1:A:75:G:H2'	1:A:76:G:H8	1.86	0.41
1:A:1127:G:H1	1:A:1145:A:N6	2.16	0.41
1:A:1412:C:H2'	1:A:1413:A:C8	2.56	0.41
6:F:4:TYR:HA	6:F:90:MET:O	2.20	0.41
7:G:78:ARG:NH2	7:G:154:TYR:OH	2.54	0.41
12:L:43:LYS:HG3	12:L:91:PRO:HG3	2.02	0.41
21:U:54:LYS:HB3	21:U:54:LYS:HE2	1.84	0.41
22:a:1413:A:H2'	22:a:1414:C:C6	2.54	0.41
1:A:236:A:H2'	1:A:237:G:H8	1.84	0.41
1:A:950:U:H2'	1:A:951:G:H8	1.86	0.41
1:A:1218:C:H2'	1:A:1219:A:H8	1.86	0.41
4:D:106:GLY:HA3	4:D:162:ALA:HB2	2.02	0.41
19:S:52:HIS:CE1	19:S:54:GLY:H	2.38	0.41
22:a:242:G:H5''	50:2:64:TYR:CE2	2.55	0.41
22:a:807:U:O2'	22:a:2060:A:N1	2.47	0.41
1:A:985:C:H2'	1:A:986:U:C6	2.56	0.41
1:A:1034:G:H2'	1:A:1035:A:C8	2.55	0.41
12:L:66:TYR:CD2	12:L:90:LEU:HD12	2.54	0.41
22:a:172:A:H2'	22:a:173:A:C8	2.55	0.41
22:a:184:C:H2'	22:a:185:G:C8	2.55	0.41
22:a:532:A:N7	22:a:2021:C:O2'	2.51	0.41
22:a:1791:A:N6	22:a:1828:G:O2'	2.48	0.41
36:o:27:GLU:HB2	36:o:87:LYS:HE2	2.03	0.41
38:q:61:ALA:HB2	38:q:98:ILE:HD13	2.01	0.41
39:r:88:ARG:NH1	39:r:94:ASP:OD2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:G:O2'	1:A:48:C:N4	2.54	0.41
25:d:33:ARG:NH1	25:d:74:GLU:O	2.54	0.41
28:g:91:GLY:HA3	28:g:160:LYS:HG2	2.02	0.41
30:i:49:ASP:OD1	30:i:121:LYS:NZ	2.49	0.41
47:z:28:LEU:HD23	47:z:37:LYS:HB3	2.03	0.41
55:V:66:C:H2'	55:V:67:G:C8	2.55	0.41
1:A:323:U:H2'	1:A:324:G:O4'	2.20	0.41
10:J:53:ILE:HD11	10:J:61:ALA:HB1	2.03	0.41
22:a:305:C:H2'	22:a:306:U:C6	2.55	0.41
22:a:672:C:OP2	32:k:42:SER:OG	2.37	0.41
22:a:1263:U:O2'	47:z:8:PRO:HD2	2.21	0.41
35:n:16:ARG:HD3	35:n:16:ARG:HA	1.94	0.41
41:t:21:LYS:HE2	41:t:21:LYS:HB3	1.91	0.41
1:A:966:2MG:HM22	55:V:34:G:H5'	2.03	0.41
1:A:978:A:C8	1:A:979:C:H5	2.39	0.41
4:D:85:ASN:OD1	5:E:102:GLY:HA3	2.20	0.41
8:H:28:PRO:O	8:H:33:LYS:NZ	2.38	0.41
9:I:84:THR:HG23	9:I:98:LEU:HD13	2.01	0.41
22:a:813:U:H2'	22:a:814:C:H6	1.86	0.41
22:a:1027:A:C2	22:a:2488:G:H5'	2.55	0.41
22:a:1597:A:H5''	22:a:1598:A:H5'	2.02	0.41
22:a:1864:U:OP1	22:a:2410:G:O2'	2.34	0.41
22:a:2285:C:OP2	48:0:6:ARG:NH1	2.49	0.41
29:h:30:LEU:HB3	29:h:36:ALA:HB3	2.02	0.41
35:n:77:ALA:O	35:n:80:GLU:HG2	2.21	0.41
1:A:414:A:N6	1:A:430:A:H2	2.16	0.41
1:A:1029:U:O2	1:A:1033:G:O6	2.39	0.41
22:a:414:C:H2'	22:a:415:A:C8	2.56	0.41
22:a:629:G:N3	22:a:639:U:O2'	2.52	0.41
22:a:2233:U:H2'	22:a:2234:G:C8	2.56	0.41
22:a:2262:U:OP2	43:v:19:LYS:NZ	2.51	0.41
31:j:110:GLU:HA	31:j:113:MET:HG2	2.03	0.41
37:p:95:LEU:HD23	37:p:95:LEU:HA	1.89	0.41
42:u:51:GLN:OE1	42:u:57:TYR:OH	2.32	0.41
1:A:236:A:H2'	1:A:237:G:C8	2.56	0.40
1:A:1001:C:H2'	1:A:1002:G:H8	1.86	0.40
1:A:1147:C:H2'	1:A:1148:U:C6	2.56	0.40
1:A:1314:C:H2'	1:A:1315:U:C6	2.56	0.40
14:N:39:GLU:OE2	14:N:43:ASN:ND2	2.45	0.40
22:a:782:A:N7	24:c:220:VAL:HG21	2.36	0.40
22:a:2780:G:OP2	30:i:120:ARG:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:e:138:LEU:HD23	26:e:138:LEU:HA	1.89	0.40
26:e:149:ILE:HD12	26:e:175:ILE:HG21	2.04	0.40
1:A:517:G:N2	1:A:530:G:OP1	2.48	0.40
6:F:9:MET:HG2	6:F:86:ARG:HB3	2.04	0.40
22:a:848:C:H2'	22:a:849:A:C8	2.54	0.40
22:a:1190:G:H5''	32:k:32:GLY:HA2	2.04	0.40
22:a:2532:G:O2'	22:a:2657:A:N1	2.52	0.40
22:a:2627:G:N2	22:a:2777:G:OP2	2.54	0.40
22:a:2836:U:H2'	22:a:2837:A:C8	2.56	0.40
26:e:46:GLN:HB2	26:e:86:ALA:HB1	2.03	0.40
27:f:58:ALA:HB2	27:f:65:PRO:HD3	2.03	0.40
39:r:36:LEU:HB3	39:r:48:LYS:HB2	2.02	0.40
40:s:36:LYS:HB2	40:s:36:LYS:HE3	1.69	0.40
1:A:672:U:H2'	1:A:673:A:C8	2.56	0.40
8:H:7:ILE:H	8:H:7:ILE:HD12	1.86	0.40
21:U:47:ARG:HD3	21:U:47:ARG:HA	1.77	0.40
22:a:171:U:H2'	22:a:172:A:H8	1.87	0.40
22:a:1484:U:H2'	22:a:1485:U:C6	2.57	0.40
22:a:2291:U:H2'	22:a:2292:U:H6	1.84	0.40
34:m:86:ARG:NE	34:m:117:ASP:OD2	2.41	0.40
36:o:89:ARG:HE	36:o:89:ARG:HB2	1.62	0.40
1:A:62:U:O2'	1:A:379:C:O2	2.38	0.40
1:A:1162:C:H2'	1:A:1163:A:C8	2.57	0.40
2:B:167:ASP:N	2:B:167:ASP:OD1	2.54	0.40
17:Q:81:LYS:HD2	17:Q:81:LYS:HA	1.90	0.40
22:a:1656:C:H2'	22:a:1657:U:H6	1.85	0.40
1:A:1144:G:H21	1:A:1146:A:H62	1.69	0.40
4:D:65:TYR:CD2	4:D:94:LEU:HB3	2.57	0.40
5:E:149:SER:OG	5:E:152:MET:HE3	2.21	0.40
6:F:90:MET:HE3	6:F:90:MET:HB3	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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
8	H	127/130 (98%)	119 (94%)	8 (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%)	12	39
11	K	115/129 (89%)	110 (96%)	3 (3%)	2 (2%)	7	26
12	L	121/124 (98%)	115 (95%)	4 (3%)	2 (2%)	7	26
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%)	24	54
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%)	21	51
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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	56/66 (85%)	53 (95%)	3 (5%)	0	100	100
54	7	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
All	All	5500/5925 (93%)	5301 (96%)	192 (4%)	7 (0%)	49	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%)	186 (100%)	0	100	100
3	C	170/190 (90%)	170 (100%)	0	100	100
4	D	172/173 (99%)	172 (100%)	0	100	100
5	E	119/126 (94%)	119 (100%)	0	100	100
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%)	104 (100%)	0	100	100
9	I	105/107 (98%)	105 (100%)	0	100	100
10	J	86/90 (96%)	86 (100%)	0	100	100
11	K	90/99 (91%)	89 (99%)	1 (1%)	65	88
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%)	72 (100%)	0	100	100
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	60/61 (98%)	60 (100%)	0	100	100
24	c	216/218 (99%)	216 (100%)	0	100	100
25	d	163/163 (100%)	163 (100%)	0	100	100
26	e	165/165 (100%)	165 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	107 (98%)	2 (2%)	51	80
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
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%)	38 (100%)	0	100	100
50	2	51/52 (98%)	51 (100%)	0	100	100
51	3	34/34 (100%)	34 (100%)	0	100	100
52	4	55/59 (93%)	55 (100%)	0	100	100
54	7	16/16 (100%)	16 (100%)	0	100	100
All	All	4592/4842 (95%)	4589 (100%)	3 (0%)	87	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	119	ASP
33	l	82	MET
33	l	84	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39)

such sidechains are listed below:

Mol	Chain	Res	Type
3	C	123	GLN
3	C	139	GLN
4	D	41	HIS
4	D	89	ASN
4	D	196	ASN
4	D	198	HIS
5	E	97	GLN
6	F	3	HIS
6	F	55	HIS
6	F	68	GLN
8	H	4	GLN
8	H	18	GLN
9	I	32	GLN
9	I	75	GLN
9	I	110	GLN
9	I	126	GLN
10	J	58	ASN
11	K	40	ASN
14	N	4	GLN
15	O	50	HIS
19	S	57	HIS
20	T	48	GLN
24	c	134	ASN
24	c	153	GLN
25	d	136	ASN
26	e	90	GLN
27	f	23	ASN
28	g	116	GLN
29	h	2	GLN
29	h	28	ASN
30	i	47	HIS
30	i	76	HIS
35	n	98	GLN
39	r	9	HIS
39	r	40	ASN
41	t	99	ASN
42	u	24	ASN
44	w	36	HIS
45	x	58	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1516/1519 (99%)	218 (14%)	4 (0%)
22	a	2749/2753 (99%)	363 (13%)	0
23	b	118/119 (99%)	15 (12%)	0
53	X	5/6 (83%)	1 (20%)	0
55	V	73/75 (97%)	14 (19%)	0
All	All	4461/4472 (99%)	611 (13%)	4 (0%)

All (611) 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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	1492	A
1	A	1493	A
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	1654	A
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
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

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Mol	Chain	Res	Type
22	a	1915	3TD
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	2030	6MZ
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
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

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Mol	Chain	Res	Type
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
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	2505	G
22	a	2507	C
22	a	2513	A
22	a	2518	A
22	a	2520	C

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	91	C
23	b	99	A
23	b	105	G
23	b	109	A
53	X	19	U
55	V	3	G
55	V	4	C
55	V	5	A
55	V	8	U
55	V	9	A
55	V	10	G
55	V	20	U
55	V	21	A
55	V	47	U
55	V	48	C
55	V	49	G
55	V	53	G
55	V	74	C
55	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 ⓘ

35 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	A	1407	1	18,22,23	3.39	7 (38%)	26,32,35	1.10	1 (3%)
22	5MC	a	1962	22	18,22,23	3.31	7 (38%)	26,32,35	0.99	1 (3%)
22	PSU	a	2580	22	18,21,22	1.09	2 (11%)	22,30,33	1.82	5 (22%)
22	PSU	a	1917	22	18,21,22	0.97	1 (5%)	22,30,33	1.61	4 (18%)
22	5MU	a	1939	22	19,22,23	7.09	8 (42%)	28,32,35	3.59	9 (32%)
22	3TD	a	1915	22	18,22,23	4.01	6 (33%)	22,32,35	1.75	3 (13%)
22	OMC	a	2498	22,57	19,22,23	2.75	7 (36%)	26,31,34	1.07	2 (7%)
1	MA6	A	1518	1	23,26,27	1.42	4 (17%)	34,38,41	4.19	14 (41%)
22	PSU	a	2504	22	18,21,22	1.02	2 (11%)	22,30,33	1.50	3 (13%)
1	5MC	A	967	1	18,22,23	3.51	7 (38%)	26,32,35	0.96	1 (3%)
22	OMG	a	2251	22,55	23,26,27	2.33	8 (34%)	33,38,41	2.01	9 (27%)
22	PSU	a	2604	22	18,21,22	1.05	1 (5%)	22,30,33	1.83	4 (18%)
22	6MZ	a	1618	22	22,25,26	2.66	4 (18%)	30,36,39	2.35	11 (36%)
22	2MA	a	2503	22,57	22,25,26	3.33	8 (36%)	33,37,40	1.98	8 (24%)
1	4OC	A	1402	1	20,23,24	3.01	8 (40%)	26,32,35	0.91	1 (3%)
22	PSU	a	1911	22	18,21,22	1.08	1 (5%)	22,30,33	1.79	4 (18%)
1	UR3	A	1498	1	19,22,23	2.54	6 (31%)	26,32,35	1.32	1 (3%)
1	MA6	A	1519	1	23,26,27	1.43	4 (17%)	34,38,41	4.35	13 (38%)
22	G7M	a	2069	22	23,26,27	2.74	8 (34%)	35,39,42	1.76	9 (25%)
22	2MG	a	2445	22	23,26,27	2.48	8 (34%)	32,38,41	2.30	13 (40%)
22	5MU	a	747	22	19,22,23	7.20	8 (42%)	28,32,35	3.57	10 (35%)
22	2MG	a	1835	22	23,26,27	2.46	9 (39%)	32,38,41	2.42	13 (40%)
22	PSU	a	2457	22	18,21,22	1.03	2 (11%)	22,30,33	1.92	4 (18%)
22	OMU	a	2552	22	19,22,23	2.69	6 (31%)	26,31,34	1.75	4 (15%)
22	1MG	a	745	22	22,26,27	2.68	7 (31%)	33,39,42	1.99	8 (24%)
25	MEQ	d	150	25	8,9,10	0.90	0	5,10,12	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	A	1516	1	23,26,27	2.54	9 (39%)	32,38,41	2.23	12 (37%)
22	PSU	a	955	22	18,21,22	1.04	1 (5%)	22,30,33	1.85	4 (18%)
55	5MU	V	54	55	18,21,23	5.92	8 (44%)	26,30,35	2.51	6 (23%)
1	2MG	A	966	1	23,26,27	2.69	9 (39%)	32,38,41	2.40	12 (37%)
1	2MG	A	1207	1	23,26,27	2.68	9 (39%)	32,38,41	2.41	11 (34%)
22	PSU	a	2605	22	18,21,22	1.12	2 (11%)	22,30,33	1.80	3 (13%)
1	PSU	A	516	57,1	18,21,22	0.89	1 (5%)	22,30,33	1.61	4 (18%)
22	6MZ	a	2030	22	22,25,26	2.75	4 (18%)	30,36,39	2.51	12 (40%)
22	PSU	a	746	22,57	18,21,22	1.08	2 (11%)	22,30,33	1.78	4 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
22	5MC	a	1962	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2580	22	-	0/7/25/26	0/2/2/2
22	PSU	a	1917	22	-	0/7/25/26	0/2/2/2
22	5MU	a	1939	22	-	0/7/25/26	0/2/2/2
22	3TD	a	1915	22	-	2/7/25/26	0/2/2/2
22	OMC	a	2498	22,57	-	2/9/27/28	0/2/2/2
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
22	PSU	a	2504	22	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
22	OMG	a	2251	22,55	-	1/9/27/28	0/3/3/3
22	PSU	a	2604	22	-	0/7/25/26	0/2/2/2
22	6MZ	a	1618	22	-	0/9/27/28	0/3/3/3
22	2MA	a	2503	22,57	-	1/7/25/26	0/3/3/3
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
22	PSU	a	1911	22	-	2/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	2/11/29/30	0/3/3/3
22	G7M	a	2069	22	-	2/7/25/26	0/3/3/3
22	2MG	a	2445	22	-	2/9/27/28	0/3/3/3
22	5MU	a	747	22	-	0/7/25/26	0/2/2/2
22	2MG	a	1835	22	-	0/9/27/28	0/3/3/3
22	PSU	a	2457	22	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	OMU	a	2552	22	-	0/9/27/28	0/2/2/2
22	1MG	a	745	22	-	0/7/25/26	0/3/3/3
25	MEQ	d	150	25	-	5/8/9/11	-
1	2MG	A	1516	1	-	0/9/27/28	0/3/3/3
22	PSU	a	955	22	-	0/7/25/26	0/2/2/2
55	5MU	V	54	55	-	0/7/25/26	0/2/2/2
1	2MG	A	966	1	-	2/9/27/28	0/3/3/3
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
1	PSU	A	516	57,1	-	0/7/25/26	0/2/2/2
22	6MZ	a	2030	22	-	2/9/27/28	0/3/3/3
22	PSU	a	746	22,57	-	1/7/25/26	0/2/2/2

All (184) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	747	5MU	C4-C5	20.51	1.78	1.44
22	a	1939	5MU	C4-C5	20.11	1.78	1.44
55	V	54	5MU	C5-C4	16.43	1.80	1.43
22	a	747	5MU	C6-N1	16.19	1.65	1.38
22	a	1939	5MU	C6-N1	15.81	1.65	1.38
22	a	1915	3TD	C6-C5	12.04	1.49	1.35
22	a	747	5MU	C4-N3	-11.50	1.17	1.38
55	V	54	5MU	C6-N1	11.49	1.65	1.38
22	a	2030	6MZ	C6-N6	11.32	1.46	1.34
22	a	1939	5MU	C6-C5	-11.28	1.16	1.34
22	a	1939	5MU	C4-N3	-11.12	1.18	1.38
22	a	1618	6MZ	C6-N6	11.04	1.46	1.34
22	a	747	5MU	C6-C5	-10.94	1.16	1.34
55	V	54	5MU	C4-N3	-10.93	1.19	1.38
22	a	2503	2MA	C4-N3	10.15	1.47	1.34
1	A	967	5MC	C6-C5	9.06	1.49	1.34
1	A	1407	5MC	C6-C5	8.82	1.49	1.34
22	a	1915	3TD	C2-N1	8.49	1.48	1.37
22	a	1962	5MC	C6-C5	8.24	1.48	1.34
1	A	966	2MG	C2-N3	7.71	1.46	1.31
1	A	1207	2MG	C2-N3	7.63	1.46	1.31
55	V	54	5MU	C6-C5	-7.62	1.17	1.35
1	A	1516	2MG	C2-N3	6.88	1.45	1.31
22	a	745	1MG	C2-N3	6.64	1.46	1.34
22	a	2445	2MG	C2-N3	6.63	1.44	1.31
1	A	1402	4OC	C4-N3	6.58	1.44	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1835	2MG	C2-N3	6.44	1.44	1.31
1	A	1498	UR3	C2-N1	6.42	1.47	1.38
22	a	745	1MG	C4-N3	6.39	1.49	1.34
1	A	967	5MC	C4-N3	6.37	1.44	1.34
22	a	2552	OMU	C2-N1	6.29	1.48	1.38
22	a	2069	G7M	C2-N2	6.19	1.48	1.34
22	a	1962	5MC	C4-N3	6.17	1.44	1.34
1	A	1402	4OC	C6-C5	6.14	1.49	1.35
22	a	2069	G7M	C4-N3	6.13	1.48	1.34
1	A	967	5MC	C2-N3	6.03	1.48	1.36
22	a	2503	2MA	C2-N1	5.99	1.44	1.34
22	a	2251	OMG	C4-N3	5.93	1.48	1.34
22	a	2503	2MA	C2-N3	5.90	1.44	1.34
22	a	2552	OMU	C2-N3	5.89	1.48	1.38
1	A	1407	5MC	C4-N3	5.89	1.44	1.34
22	a	1962	5MC	C2-N3	5.84	1.48	1.36
1	A	1498	UR3	C6-C5	5.84	1.48	1.35
22	a	2498	OMC	C6-C5	5.80	1.48	1.35
1	A	1407	5MC	C2-N3	5.76	1.48	1.36
1	A	1402	4OC	C2-N3	5.75	1.48	1.36
22	a	1915	3TD	C6-N1	5.69	1.45	1.36
22	a	745	1MG	C2-N2	5.65	1.44	1.34
22	a	2498	OMC	C2-N3	5.62	1.47	1.36
22	a	2552	OMU	C6-C5	5.55	1.48	1.35
1	A	1207	2MG	C2-N2	5.30	1.45	1.33
1	A	966	2MG	C4-N3	5.25	1.46	1.34
1	A	966	2MG	C2-N2	5.24	1.45	1.33
1	A	1207	2MG	C4-N3	5.20	1.46	1.34
22	a	2069	G7M	C2-N3	5.16	1.45	1.33
1	A	1516	2MG	C2-N2	5.04	1.44	1.33
22	a	2069	G7M	C5-N7	-5.01	1.33	1.39
55	V	54	5MU	C2-N3	4.97	1.46	1.38
22	a	2251	OMG	C2-N3	4.90	1.45	1.33
22	a	1835	2MG	C2-N2	4.72	1.43	1.33
22	a	2445	2MG	C2-N2	4.72	1.43	1.33
1	A	1516	2MG	C4-N3	4.65	1.45	1.34
22	a	747	5MU	C2-N3	4.63	1.46	1.38
22	a	1939	5MU	C2-N3	4.54	1.46	1.38
22	a	1835	2MG	C4-N3	4.54	1.45	1.34
22	a	2445	2MG	C4-N3	4.50	1.44	1.34
1	A	967	5MC	C6-N1	4.45	1.45	1.38
22	a	2498	OMC	C4-N4	4.39	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1498	UR3	C2-N3	4.37	1.47	1.39
22	a	1915	3TD	C2-N3	4.37	1.48	1.38
1	A	1407	5MC	C6-N1	4.36	1.45	1.38
1	A	1402	4OC	C4-N4	4.35	1.44	1.35
22	a	2503	2MA	C5-C6	4.31	1.53	1.41
1	A	967	5MC	C4-N4	4.27	1.45	1.34
1	A	1407	5MC	C4-N4	4.24	1.45	1.34
22	a	2498	OMC	C2-N1	4.23	1.49	1.40
22	a	2251	OMG	C2-N2	4.23	1.44	1.34
22	a	2498	OMC	C4-N3	4.20	1.43	1.34
22	a	1962	5MC	C4-N4	4.15	1.44	1.34
22	a	1962	5MC	C6-N1	3.99	1.44	1.38
22	a	2251	OMG	C5-N7	-3.90	1.31	1.39
1	A	967	5MC	C2-N1	3.87	1.48	1.40
1	A	1402	4OC	C2-N1	3.83	1.48	1.40
22	a	745	1MG	C5-N7	-3.68	1.31	1.39
22	a	2503	2MA	C6-N6	-3.68	1.24	1.34
1	A	1402	4OC	C5-C4	3.59	1.48	1.40
22	a	2069	G7M	C5-C6	3.54	1.53	1.43
22	a	2503	2MA	C6-N1	3.53	1.40	1.35
1	A	966	2MG	C2-N1	3.51	1.42	1.36
1	A	1407	5MC	C2-N1	3.47	1.47	1.40
1	A	1207	2MG	C2-N1	3.43	1.42	1.36
22	a	1962	5MC	C2-N1	3.37	1.47	1.40
22	a	2030	6MZ	C5-C4	-3.36	1.32	1.39
22	a	1911	PSU	C6-C5	3.26	1.39	1.35
22	a	1962	5MC	O2-C2	-3.25	1.17	1.23
22	a	2498	OMC	O2-C2	-3.22	1.17	1.23
1	A	1518	MA6	C6-N6	3.16	1.46	1.36
1	A	1519	MA6	C5-C4	-3.16	1.33	1.39
22	a	2445	2MG	C5-N7	-3.16	1.33	1.39
55	V	54	5MU	O4-C4	-3.16	1.18	1.24
22	a	1939	5MU	O2-C2	-3.14	1.17	1.23
1	A	1516	2MG	C2-N1	3.14	1.41	1.36
1	A	1519	MA6	C6-N6	3.13	1.46	1.36
1	A	1407	5MC	O2-C2	-3.11	1.17	1.23
1	A	1519	MA6	C5-N7	-3.06	1.33	1.39
22	a	1835	2MG	C5-N7	-3.05	1.33	1.39
22	a	1618	6MZ	C5-C4	-3.05	1.33	1.39
1	A	1402	4OC	O2-C2	-3.05	1.18	1.23
22	a	2445	2MG	C4-N9	-3.03	1.30	1.38
1	A	1516	2MG	C5-N7	-3.01	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1402	4OC	C6-N1	3.00	1.45	1.38
22	a	2552	OMU	O2-C2	-3.00	1.17	1.23
22	a	1835	2MG	C2-N1	2.98	1.41	1.36
22	a	1939	5MU	O4-C4	-2.98	1.17	1.23
1	A	1518	MA6	C5-N7	-2.97	1.33	1.39
1	A	1518	MA6	C5-C4	-2.96	1.33	1.39
22	a	2503	2MA	C5-N7	-2.96	1.33	1.39
22	a	2251	OMG	O6-C6	-2.95	1.18	1.23
22	a	2445	2MG	C2-N1	2.95	1.41	1.36
1	A	966	2MG	C5-N7	-2.95	1.33	1.39
22	a	747	5MU	O2-C2	-2.94	1.17	1.23
22	a	2445	2MG	O6-C6	-2.93	1.18	1.23
1	A	1516	2MG	C4-N9	-2.93	1.30	1.38
22	a	1835	2MG	C4-N9	-2.93	1.30	1.38
1	A	1207	2MG	C5-N7	-2.92	1.33	1.39
22	a	747	5MU	O4-C4	-2.90	1.18	1.23
22	a	2605	PSU	C6-C5	2.90	1.38	1.35
22	a	2552	OMU	O4-C4	-2.89	1.18	1.24
22	a	1917	PSU	C6-C5	2.89	1.38	1.35
55	V	54	5MU	C2-N1	2.88	1.43	1.38
22	a	1939	5MU	C2-N1	2.87	1.43	1.38
22	a	1835	2MG	O6-C6	-2.86	1.18	1.23
1	A	1516	2MG	O6-C6	-2.79	1.18	1.23
1	A	1519	MA6	C8-N9	-2.76	1.32	1.37
22	a	2552	OMU	C4-N3	2.76	1.43	1.38
1	A	967	5MC	O2-C2	-2.73	1.18	1.23
22	a	2069	G7M	O6-C6	-2.71	1.18	1.23
22	a	2069	G7M	C6-N1	2.71	1.43	1.38
1	A	966	2MG	O6-C6	-2.70	1.18	1.23
1	A	1207	2MG	O6-C6	-2.70	1.18	1.23
1	A	1518	MA6	C8-N9	-2.68	1.32	1.37
22	a	2030	6MZ	C8-N9	-2.65	1.32	1.37
1	A	1207	2MG	CM2-N2	2.64	1.50	1.45
22	a	745	1MG	C5-C6	2.63	1.52	1.45
22	a	2069	G7M	C2-N1	2.63	1.44	1.37
1	A	1498	UR3	C6-N1	2.60	1.44	1.38
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	1915	3TD	C4-N3	2.57	1.46	1.40
22	a	2604	PSU	C6-C5	2.57	1.38	1.35
55	V	54	5MU	O2-C2	-2.56	1.18	1.23
22	a	745	1MG	O6-C6	-2.54	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2580	PSU	O4'-C1'	-2.51	1.40	1.43
1	A	1516	2MG	CM2-N2	2.48	1.50	1.45
22	a	2030	6MZ	C5-N7	-2.46	1.34	1.39
1	A	966	2MG	CM2-N2	2.46	1.50	1.45
22	a	955	PSU	C6-C5	2.46	1.38	1.35
1	A	1498	UR3	O4-C4	-2.42	1.18	1.23
22	a	1835	2MG	CM2-N2	2.42	1.49	1.45
1	A	1498	UR3	O2-C2	-2.42	1.18	1.22
1	A	516	PSU	C6-C5	2.40	1.38	1.35
22	a	2503	2MA	C8-N7	2.36	1.36	1.31
22	a	746	PSU	C6-C5	2.34	1.38	1.35
22	a	2251	OMG	C4-N9	-2.34	1.32	1.38
22	a	2605	PSU	C4-C5	-2.34	1.37	1.44
1	A	966	2MG	C6-N1	2.33	1.43	1.38
1	A	966	2MG	C4-N9	-2.31	1.32	1.38
1	A	1207	2MG	C6-N1	2.30	1.43	1.38
22	a	746	PSU	C4-C5	-2.30	1.37	1.44
22	a	1618	6MZ	C8-N9	-2.28	1.33	1.37
22	a	1835	2MG	C6-N1	2.27	1.43	1.38
22	a	2445	2MG	CM2-N2	2.27	1.49	1.45
22	a	2504	PSU	C6-C5	2.24	1.37	1.35
1	A	1207	2MG	C4-N9	-2.23	1.32	1.38
22	a	1618	6MZ	C5-N7	-2.21	1.34	1.39
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	2457	PSU	C4-C5	-2.14	1.38	1.44
1	A	1516	2MG	C6-N1	2.14	1.42	1.38
22	a	2580	PSU	C4-C5	-2.13	1.38	1.44
22	a	745	1MG	C4-N9	-2.07	1.32	1.38
22	a	2457	PSU	O4'-C1'	-2.03	1.41	1.43
22	a	2251	OMG	C5-C6	2.02	1.51	1.44
22	a	2251	OMG	C2-N1	2.01	1.42	1.37

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1519	MA6	N1-C6-N6	-16.83	98.68	117.08
1	A	1518	MA6	N1-C6-N6	-15.82	99.78	117.08
22	a	1939	5MU	C5-C4-N3	11.32	124.98	115.31
22	a	747	5MU	C5-C4-N3	10.64	124.39	115.31
1	A	1519	MA6	C5-C6-N6	9.71	142.21	125.30
22	a	747	5MU	C5-C6-N1	-9.31	113.76	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1518	MA6	C5-C6-N6	9.22	141.36	125.30
22	a	1939	5MU	C5-C6-N1	-8.61	114.48	123.34
55	V	54	5MU	C5-C4-N3	8.14	127.02	114.84
22	a	1939	5MU	C4-N3-C2	-7.70	117.39	127.35
22	a	747	5MU	C4-N3-C2	-7.48	117.67	127.35
1	A	1518	MA6	C4-N9-C1'	-6.93	110.09	126.59
22	a	1835	2MG	C2-N3-C4	6.63	120.25	112.04
1	A	1207	2MG	C2-N3-C4	6.59	120.20	112.04
22	a	2503	2MA	C5-C4-N3	-6.52	119.86	127.19
1	A	1519	MA6	C4-N9-C1'	-6.52	111.06	126.59
1	A	966	2MG	C2-N3-C4	6.27	119.82	112.04
1	A	1518	MA6	C1'-N9-C8	6.27	141.29	127.14
22	a	2030	6MZ	C9-N6-C6	-6.21	117.52	122.87
1	A	1516	2MG	C2-N3-C4	6.18	119.70	112.04
55	V	54	5MU	C4-N3-C2	-6.15	118.46	126.58
1	A	1519	MA6	C5-C4-N3	-6.08	118.82	126.75
1	A	1519	MA6	C1'-N9-C8	5.97	140.61	127.14
22	a	2445	2MG	C2-N3-C4	5.92	119.38	112.04
22	a	745	1MG	C5-C4-N3	-5.87	118.94	128.46
1	A	1518	MA6	C5-C4-N3	-5.81	119.17	126.75
22	a	1618	6MZ	N1-C2-N3	-5.71	119.67	128.60
1	A	1519	MA6	N1-C2-N3	-5.70	119.69	128.60
22	a	1915	3TD	N1-C2-N3	5.66	120.61	116.14
22	a	2030	6MZ	N1-C2-N3	-5.46	120.06	128.60
22	a	2552	OMU	C4-N3-C2	-5.42	119.43	126.58
22	a	2251	OMG	C5-C4-N3	-5.28	119.90	128.46
22	a	1618	6MZ	C5-C4-N3	-5.17	120.01	126.75
1	A	1207	2MG	C5-C4-N3	-5.16	120.09	128.46
22	a	747	5MU	N3-C2-N1	5.13	121.70	114.89
22	a	2457	PSU	C4-N3-C2	-5.10	118.99	126.34
1	A	1518	MA6	C4-C5-C6	5.10	121.58	115.88
1	A	1518	MA6	N1-C2-N3	-5.09	120.63	128.60
1	A	966	2MG	C1'-N9-C8	-5.09	112.22	126.70
1	A	966	2MG	C5-C4-N3	-5.03	120.30	128.46
22	a	1939	5MU	O4-C4-C5	-5.01	119.10	124.90
22	a	1835	2MG	C2-N1-C6	-4.98	118.75	124.48
22	a	2030	6MZ	N9-C8-N7	-4.97	107.12	113.91
22	a	2030	6MZ	C5-C4-N3	-4.96	120.28	126.75
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	4.79	121.25	114.89
22	a	2605	PSU	C4-N3-C2	-4.77	119.46	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2604	PSU	N1-C2-N3	4.77	120.53	115.13
22	a	955	PSU	N1-C2-N3	4.76	120.53	115.13
1	A	1519	MA6	C4-C5-C6	4.76	121.20	115.88
22	a	2457	PSU	N1-C2-N3	4.74	120.50	115.13
1	A	1207	2MG	C1'-N9-C8	-4.69	113.33	126.70
22	a	2580	PSU	N1-C2-N3	4.66	120.41	115.13
22	a	2251	OMG	C2-N3-C4	4.63	120.55	112.30
22	a	2445	2MG	C2-N1-C6	-4.60	119.18	124.48
22	a	1911	PSU	C4-N3-C2	-4.60	119.71	126.34
22	a	1835	2MG	C5-C4-N3	-4.60	121.00	128.46
1	A	1516	2MG	C2-N1-C6	-4.59	119.20	124.48
1	A	1516	2MG	C5-C4-N3	-4.58	121.02	128.46
22	a	2604	PSU	C4-N3-C2	-4.58	119.73	126.34
22	a	1618	6MZ	N9-C8-N7	-4.57	107.66	113.91
22	a	1911	PSU	N1-C2-N3	4.55	120.28	115.13
22	a	746	PSU	N1-C2-N3	4.55	120.28	115.13
1	A	1207	2MG	C2-N1-C6	-4.50	119.30	124.48
22	a	2605	PSU	N1-C2-N3	4.49	120.22	115.13
22	a	955	PSU	C4-N3-C2	-4.49	119.87	126.34
22	a	2580	PSU	C4-N3-C2	-4.44	119.94	126.34
22	a	2069	G7M	C2-N3-C4	4.32	119.99	112.30
1	A	966	2MG	C2-N1-C6	-4.31	119.53	124.48
22	a	747	5MU	C5M-C5-C6	-4.29	117.12	122.85
1	A	1519	MA6	N9-C8-N7	-4.25	108.10	113.91
22	a	2445	2MG	C5-C4-N3	-4.25	121.57	128.46
1	A	516	PSU	C4-N3-C2	-4.22	120.26	126.34
22	a	1917	PSU	C4-N3-C2	-4.21	120.28	126.34
1	A	1518	MA6	N3-C4-N9	4.20	134.00	127.08
22	a	2503	2MA	N9-C8-N7	-4.20	108.17	113.91
1	A	1518	MA6	N9-C8-N7	-4.19	108.18	113.91
1	A	1519	MA6	N3-C4-N9	4.19	133.99	127.08
22	a	2552	OMU	N3-C2-N1	4.19	120.45	114.89
1	A	966	2MG	C1'-N9-C4	4.16	138.87	126.50
22	a	1618	6MZ	C9-N6-C6	-4.12	119.32	122.87
22	a	745	1MG	N9-C4-N3	4.10	134.18	125.94
22	a	1917	PSU	N1-C2-N3	4.10	119.78	115.13
22	a	745	1MG	C1'-N9-C8	-4.06	115.13	126.70
22	a	1915	3TD	C4-N3-C2	-4.05	120.22	124.61
22	a	1939	5MU	C5M-C5-C6	-4.04	117.45	122.85
22	a	2445	2MG	C1'-N9-C8	-3.94	115.48	126.70
22	a	2069	G7M	C5-C6-N1	3.90	119.93	111.79
1	A	1207	2MG	C1'-N9-C4	3.89	138.05	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	747	5MU	O4-C4-C5	-3.89	120.40	124.90
22	a	747	5MU	C6-C5-C4	3.88	121.27	118.03
22	a	2504	PSU	N1-C2-N3	3.87	119.52	115.13
22	a	2504	PSU	C4-N3-C2	-3.87	120.77	126.34
55	V	54	5MU	O4-C4-C5	-3.86	118.37	125.16
22	a	1835	2MG	C1'-N9-C8	-3.84	115.76	126.70
1	A	1519	MA6	C2-N3-C4	3.82	120.77	111.75
22	a	1835	2MG	CM2-N2-C2	-3.82	115.43	123.86
22	a	2503	2MA	N3-C4-N9	3.78	132.24	126.99
22	a	2251	OMG	C1'-N9-C8	3.73	137.30	126.70
22	a	1618	6MZ	C2-N3-C4	3.70	120.50	111.75
22	a	2251	OMG	C1'-N9-C4	-3.68	115.58	126.50
1	A	1519	MA6	C2-N1-C6	3.66	120.40	111.75
22	a	745	1MG	C2-N3-C4	3.65	120.18	111.98
22	a	2445	2MG	N9-C8-N7	-3.61	106.60	113.39
22	a	2030	6MZ	C2-N3-C4	3.60	120.26	111.75
22	a	2069	G7M	C5-C4-N3	-3.60	121.25	128.15
1	A	516	PSU	N1-C2-N3	3.59	119.20	115.13
22	a	2445	2MG	CM2-N2-C2	-3.57	115.98	123.86
1	A	1518	MA6	C2-N1-C6	3.52	120.06	111.75
22	a	1835	2MG	N9-C8-N7	-3.48	106.84	113.39
22	a	2030	6MZ	C5-N7-C8	3.47	108.44	103.51
22	a	2457	PSU	O2-C2-N1	-3.44	119.00	122.79
1	A	1516	2MG	C1'-N9-C8	-3.43	116.93	126.70
1	A	1407	5MC	C5-C6-N1	-3.41	119.83	123.34
22	a	2552	OMU	C5-C4-N3	3.40	119.93	114.84
1	A	1518	MA6	C2-N3-C4	3.36	119.70	111.75
22	a	955	PSU	O2-C2-N1	-3.32	119.14	122.79
55	V	54	5MU	C6-C5-C4	-3.31	114.99	119.52
1	A	967	5MC	C5-C6-N1	-3.29	119.95	123.34
22	a	745	1MG	C1'-N9-C4	3.29	136.26	126.50
22	a	1618	6MZ	C4-C5-C6	3.28	119.35	116.81
55	V	54	5MU	N3-C2-N1	3.25	119.20	114.89
1	A	966	2MG	N9-C4-N3	3.24	132.44	125.94
22	a	2251	OMG	C2-N1-C6	-3.23	119.20	125.10
22	a	2503	2MA	N3-C2-N1	-3.22	119.80	125.72
1	A	1207	2MG	N9-C4-N3	3.22	132.40	125.94
55	V	54	5MU	O4-C4-N3	-3.19	114.62	119.31
22	a	2069	G7M	CN7-N7-C5	3.18	130.72	126.77
1	A	1519	MA6	C5-N7-C8	3.11	107.92	103.51
1	A	966	2MG	N9-C8-N7	-3.11	107.54	113.39
22	a	1939	5MU	C6-C5-C4	3.08	120.60	118.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1207	2MG	N9-C8-N7	-3.06	107.64	113.39
1	A	1516	2MG	N9-C8-N7	-3.03	107.68	113.39
22	a	2030	6MZ	C4-C5-C6	3.02	119.15	116.81
22	a	1835	2MG	C1'-N9-C4	3.01	135.44	126.50
22	a	955	PSU	C6-N1-C2	-3.01	119.61	122.68
1	A	1518	MA6	C5-N7-C8	3.01	107.78	103.51
22	a	1618	6MZ	C5-N7-C8	3.00	107.78	103.51
22	a	2069	G7M	O6-C6-C5	-3.00	121.29	128.06
22	a	1618	6MZ	N3-C4-N9	2.99	132.00	127.08
22	a	2498	OMC	O2-C2-N3	-2.97	117.49	122.33
22	a	2251	OMG	C5-C6-N1	2.96	120.71	113.19
22	a	2445	2MG	C1'-N9-C4	2.96	135.29	126.50
22	a	2251	OMG	N9-C4-N3	2.93	131.81	125.94
22	a	1939	5MU	C5M-C5-C4	2.89	121.95	118.77
1	A	1516	2MG	CM2-N2-C2	-2.87	117.52	123.86
1	A	1516	2MG	C1'-N9-C4	2.87	135.03	126.50
22	a	2069	G7M	C2-N1-C6	-2.82	119.95	125.10
22	a	1835	2MG	C5-C6-N1	2.82	120.35	113.19
22	a	1835	2MG	O6-C6-C5	-2.80	119.18	126.60
22	a	2580	PSU	C6-N1-C2	-2.79	119.83	122.68
22	a	2503	2MA	C5-N7-C8	2.78	107.46	103.51
22	a	745	1MG	C5-C6-N1	2.78	120.27	114.91
1	A	1207	2MG	C5-C6-N1	2.77	120.24	113.19
22	a	2580	PSU	O2-C2-N1	-2.73	119.79	122.79
22	a	2445	2MG	C5-C6-N1	2.71	120.07	113.19
22	a	2251	OMG	O6-C6-C5	-2.69	119.46	126.60
22	a	2552	OMU	O4-C4-C5	-2.69	120.43	125.16
22	a	1911	PSU	O2-C2-N1	-2.68	119.83	122.79
22	a	745	1MG	N9-C8-N7	-2.68	108.35	113.39
22	a	2069	G7M	N9-C4-N3	2.66	131.27	125.94
22	a	2030	6MZ	C4-N9-C8	2.65	108.60	105.73
1	A	966	2MG	C5-C6-N1	2.64	119.91	113.19
1	A	1516	2MG	C5-C6-N1	2.64	119.89	113.19
22	a	2604	PSU	O2-C2-N1	-2.63	119.89	122.79
1	A	1518	MA6	C4-N9-C8	2.62	108.57	105.73
22	a	2030	6MZ	C4-C5-N7	-2.62	107.43	110.62
1	A	1207	2MG	O6-C6-C5	-2.60	119.69	126.60
1	A	966	2MG	O6-C6-C5	-2.59	119.72	126.60
22	a	2069	G7M	CN7-N7-C8	-2.58	120.85	124.84
22	a	747	5MU	C5M-C5-C4	2.57	121.60	118.77
22	a	2030	6MZ	N3-C4-N9	2.57	131.32	127.08
22	a	747	5MU	O4-C4-N3	-2.56	115.21	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	1618	6MZ	C4-N9-C8	2.56	108.50	105.73
1	A	516	PSU	O2-C2-N1	-2.52	120.02	122.79
22	a	747	5MU	O2-C2-N1	-2.51	119.45	122.79
22	a	2504	PSU	C6-N1-C2	-2.50	120.12	122.68
22	a	746	PSU	O2-C2-N1	-2.49	120.04	122.79
22	a	1911	PSU	C6-N1-C2	-2.49	120.14	122.68
1	A	1516	2MG	O6-C6-C5	-2.46	120.07	126.60
22	a	1962	5MC	C5-C6-N1	-2.46	120.81	123.34
22	a	1917	PSU	O2-C2-N1	-2.45	120.09	122.79
22	a	2604	PSU	C6-N1-C2	-2.44	120.19	122.68
22	a	1917	PSU	C6-N1-C2	-2.44	120.19	122.68
1	A	1207	2MG	N1-C2-N3	-2.43	120.20	123.95
22	a	2445	2MG	O6-C6-C5	-2.41	120.20	126.60
22	a	2251	OMG	N9-C8-N7	-2.40	108.86	113.39
1	A	1519	MA6	C4-N9-C8	2.40	108.33	105.73
22	a	2605	PSU	C6-N1-C2	-2.38	120.25	122.68
22	a	2445	2MG	C8-N7-C5	2.38	108.54	104.24
1	A	966	2MG	N1-C2-N3	-2.34	120.34	123.95
22	a	2580	PSU	O4'-C1'-C2'	2.34	108.44	105.14
22	a	1835	2MG	C8-N7-C5	2.32	108.44	104.24
22	a	2030	6MZ	C5-C4-N9	2.25	108.40	105.78
22	a	1835	2MG	N1-C2-N3	-2.23	120.50	123.95
1	A	1402	4OC	CM4-N4-C4	-2.22	118.11	122.45
22	a	1915	3TD	C6-C5-C4	2.22	119.75	118.22
22	a	1618	6MZ	C5-C6-N1	2.22	120.57	118.20
22	a	1835	2MG	C4-C5-N7	-2.21	107.22	110.72
22	a	746	PSU	C6-N1-C2	-2.21	120.43	122.68
22	a	1939	5MU	O4-C4-N3	-2.19	115.93	120.12
22	a	1835	2MG	N9-C4-N3	2.17	130.29	125.94
1	A	1516	2MG	N1-C2-N3	-2.15	120.63	123.95
22	a	2030	6MZ	C5-C6-N1	2.14	120.48	118.20
1	A	966	2MG	CM2-N2-C2	-2.14	119.14	123.86
1	A	516	PSU	C6-N1-C2	-2.13	120.50	122.68
22	a	2445	2MG	N1-C2-N3	-2.12	120.68	123.95
22	a	2069	G7M	N9-C8-N7	-2.12	106.97	112.21
22	a	2445	2MG	C4-C5-N7	-2.11	107.37	110.72
1	A	1207	2MG	C8-N7-C5	2.11	108.05	104.24
22	a	2503	2MA	N6-C6-N1	2.10	120.00	117.03
22	a	2445	2MG	N9-C4-N3	2.10	130.15	125.94
1	A	966	2MG	C8-N7-C5	2.10	108.03	104.24
22	a	1618	6MZ	C4-C5-N7	-2.09	108.07	110.62
1	A	1518	MA6	C6-C5-N7	-2.09	129.78	133.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2457	PSU	C6-N1-C2	-2.09	120.55	122.68
1	A	1516	2MG	N9-C4-N3	2.08	130.11	125.94
22	a	2503	2MA	C4-N9-C8	2.06	107.96	105.73
22	a	745	1MG	CM1-N1-C6	2.05	120.83	117.69
22	a	2503	2MA	C6-C5-C4	2.01	119.88	117.18
1	A	1516	2MG	C4-C5-N7	-2.00	107.55	110.72
22	a	2498	OMC	C1'-N1-C2	2.00	122.89	118.42

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.

11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	a	1939	5MU	1	0
1	A	1518	MA6	1	0
22	a	2251	OMG	2	0
22	a	2503	2MA	1	0
1	A	1519	MA6	1	0
22	a	747	5MU	1	0
1	A	1516	2MG	1	0
55	V	54	5MU	2	0
1	A	966	2MG	2	0
1	A	516	PSU	2	0
22	a	2030	6MZ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 312 ligands modelled in this entry, 310 are monoatomic - leaving 2 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	PAR	A	1601	-	45,45,45	3.33	9 (20%)	64,67,67	1.41	9 (14%)
58	TRP	a	6206	-	14,16,16	0.82	1 (7%)	20,22,22	0.92	2 (10%)

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	PAR	A	1601	-	-	10/18/94/94	0/4/4/4
58	TRP	a	6206	-	-	0/8/8/8	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	A	1601	PAR	C13-C23	-14.15	1.34	1.52
56	A	1601	PAR	O43-C13	12.32	1.63	1.41
56	A	1601	PAR	O43-C43	-6.04	1.31	1.45
56	A	1601	PAR	O51-C11	4.11	1.52	1.41
56	A	1601	PAR	C31-C21	-4.06	1.48	1.53
56	A	1601	PAR	O33-C33	-3.51	1.34	1.43
56	A	1601	PAR	O54-C14	3.48	1.50	1.41
56	A	1601	PAR	C34-C24	-3.30	1.49	1.53
56	A	1601	PAR	C33-C43	2.70	1.60	1.52
58	a	6206	TRP	OXT-C	-2.24	1.23	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	A	1601	PAR	C13-O52-C52	-4.31	107.31	117.96
56	A	1601	PAR	C14-O33-C33	-3.35	109.67	117.96
56	A	1601	PAR	C44-C34-C24	3.31	116.77	111.07
56	A	1601	PAR	C11-O51-C51	3.22	120.01	113.69
56	A	1601	PAR	C34-C44-C54	2.92	115.45	110.24
56	A	1601	PAR	O51-C51-C41	2.81	114.79	109.69
56	A	1601	PAR	O51-C11-C21	2.77	116.30	110.06
58	a	6206	TRP	OXT-C-O	-2.30	118.87	124.09
58	a	6206	TRP	OXT-C-CA	2.20	120.86	113.38
56	A	1601	PAR	C13-C23-C33	2.19	104.74	102.10
56	A	1601	PAR	C14-O54-C54	-2.04	109.69	113.69

There are no chirality outliers.

All (10) torsion outliers are listed below:

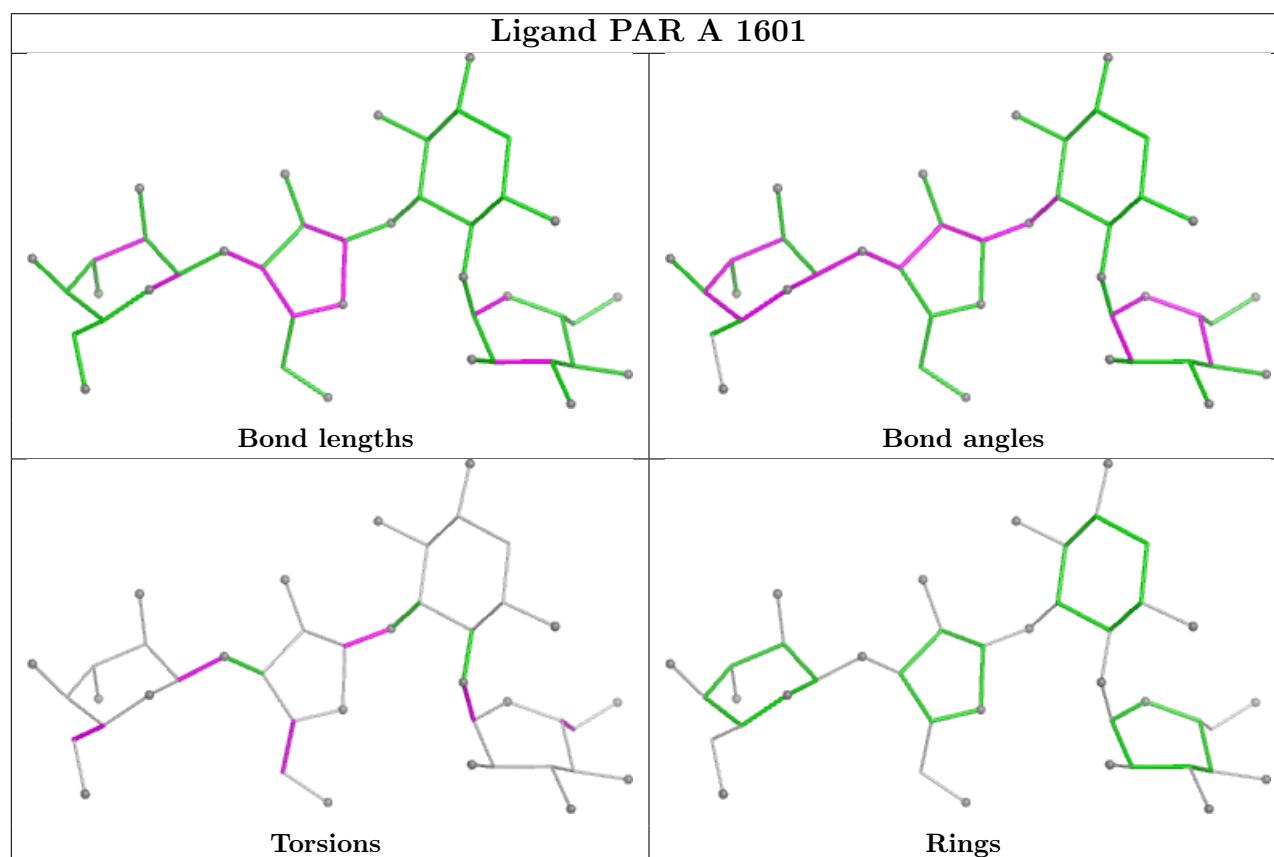
Mol	Chain	Res	Type	Atoms
56	A	1601	PAR	C23-C13-O52-C52
56	A	1601	PAR	C24-C14-O33-C33
56	A	1601	PAR	O51-C11-O11-C42
56	A	1601	PAR	O51-C51-C61-O61
56	A	1601	PAR	C33-C43-C53-O53
56	A	1601	PAR	C41-C51-C61-O61
56	A	1601	PAR	O43-C43-C53-O53
56	A	1601	PAR	O43-C13-O52-C52
56	A	1601	PAR	O54-C14-O33-C33
56	A	1601	PAR	C44-C54-C64-N64

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	A	1601	PAR	2	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	a	3
1	A	2
55	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

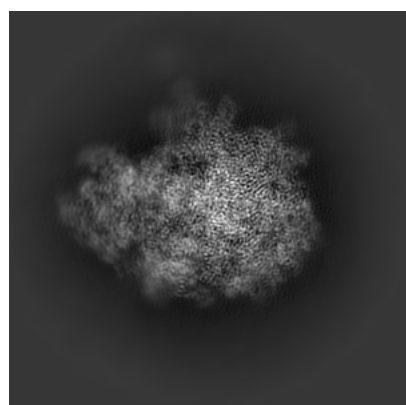
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12936. These allow visual inspection of the internal detail of the map and identification of artifacts.

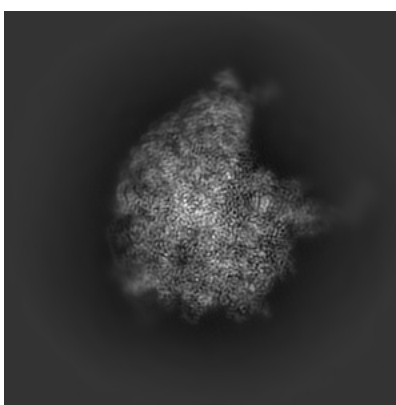
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

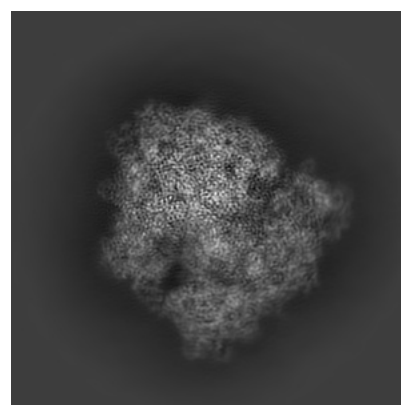
6.1.1 Primary map



X



Y

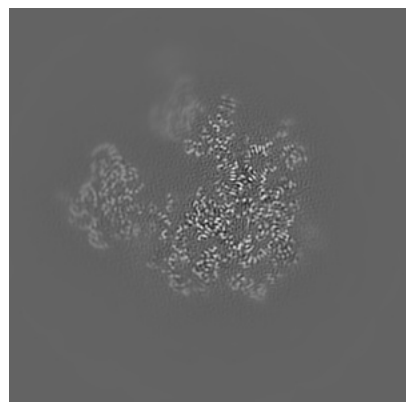


Z

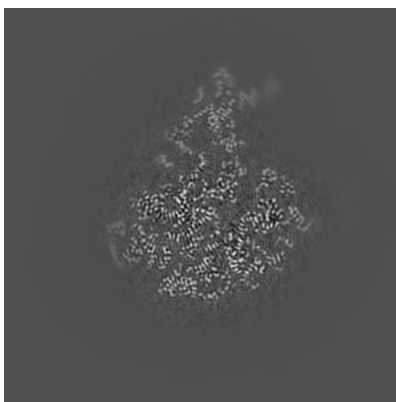
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

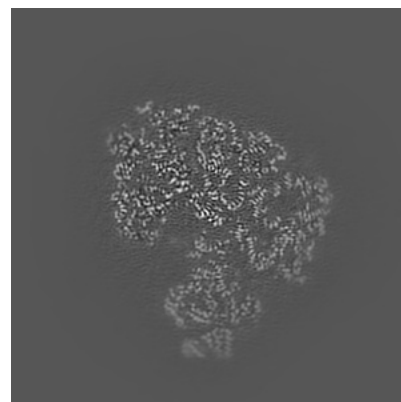
6.2.1 Primary map



X Index: 184



Y Index: 184

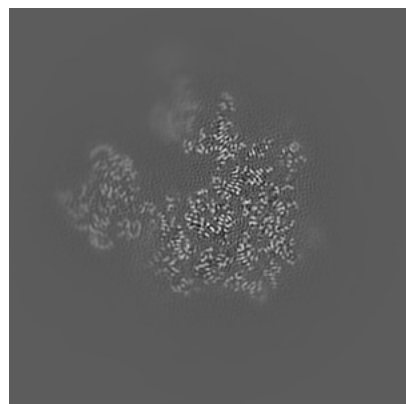


Z Index: 184

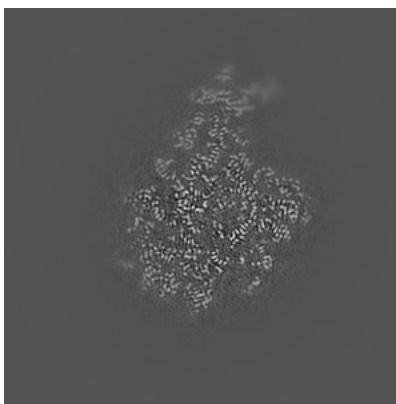
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

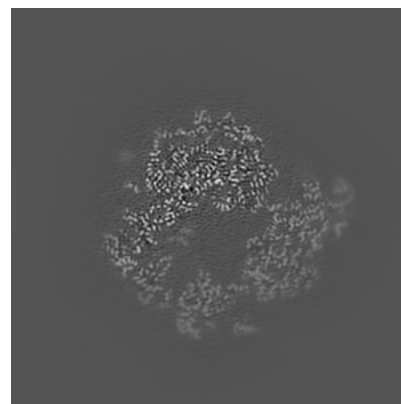
6.3.1 Primary map



X Index: 187



Y Index: 192

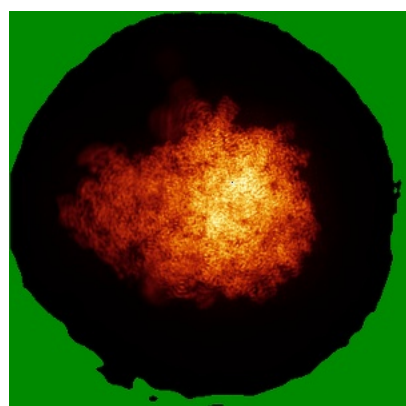


Z Index: 209

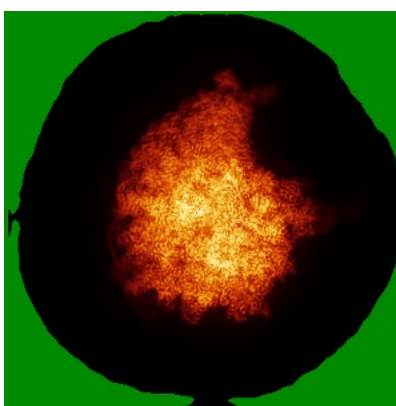
The images above show the largest variance slices of the map in three orthogonal directions.

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

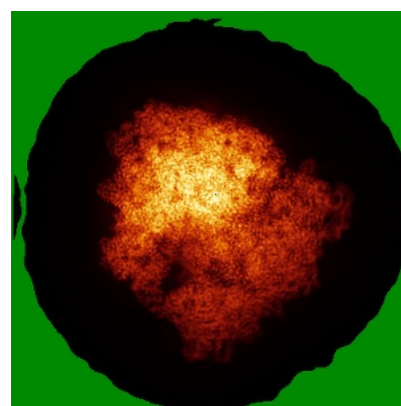
6.4.1 Primary map



X



Y

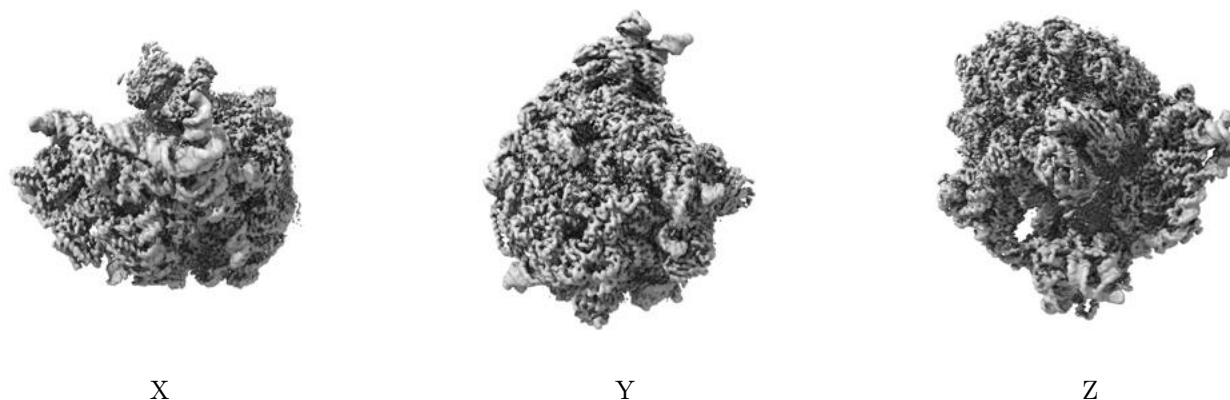


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

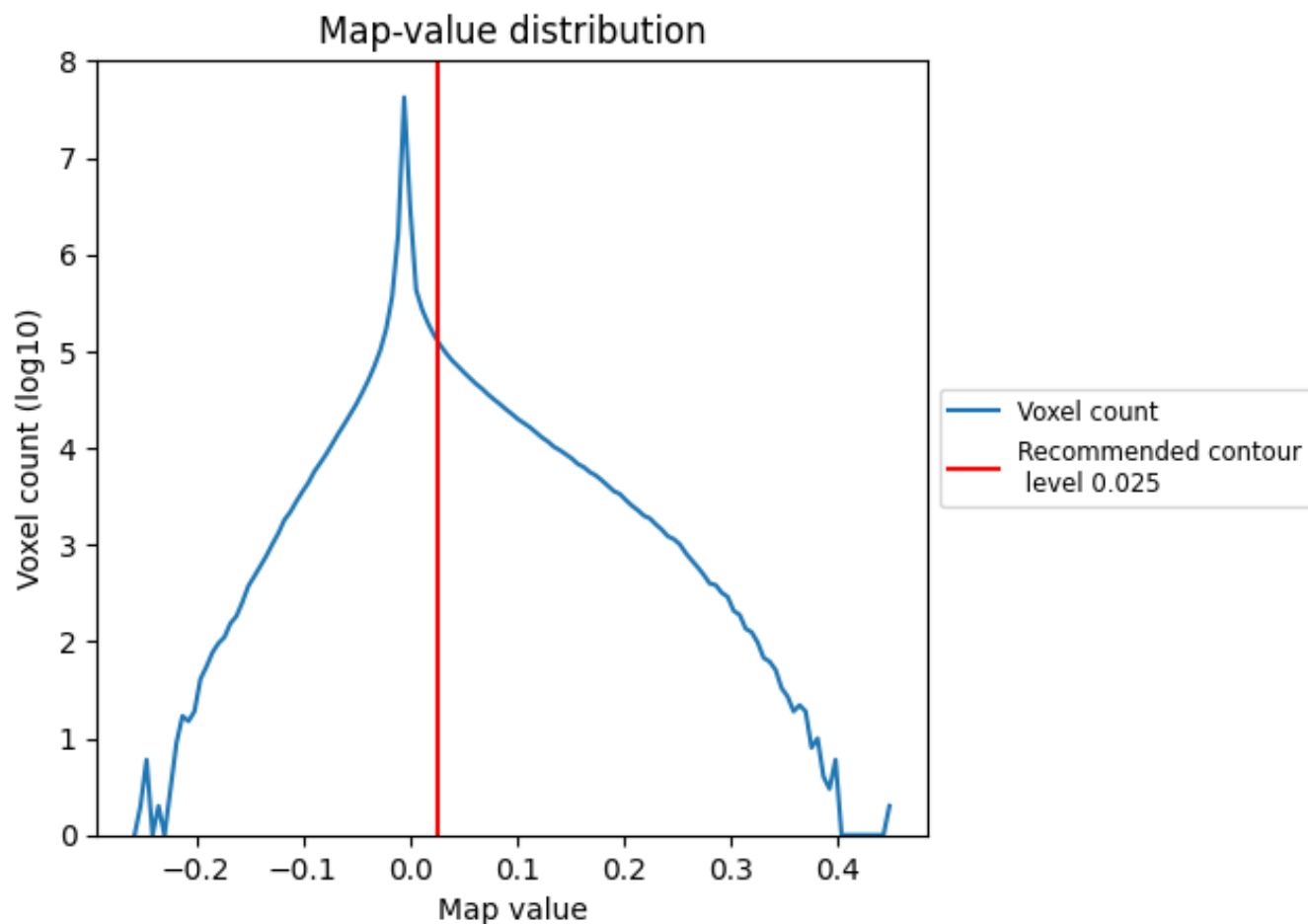
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

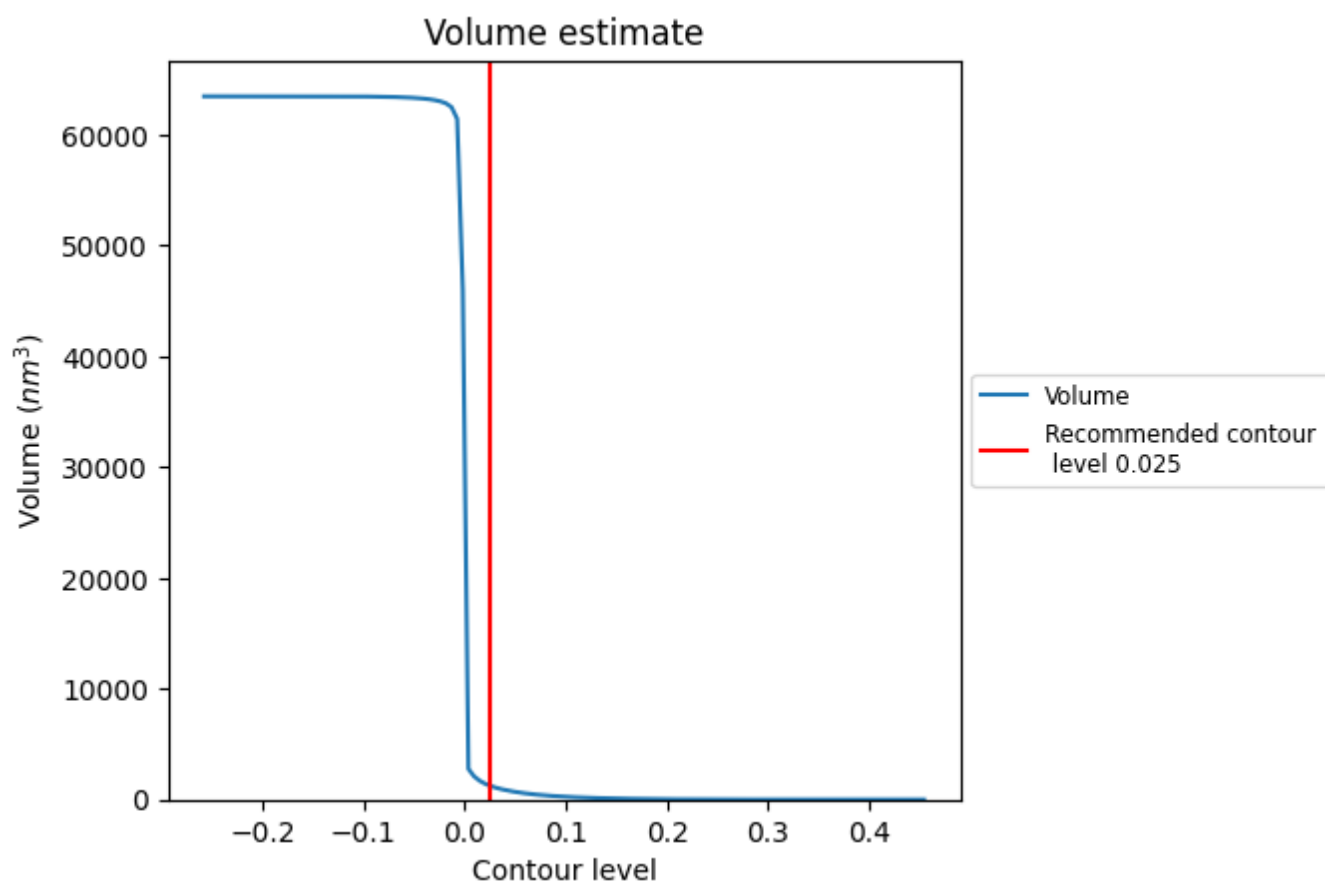
This section contains the results of statistical analysis of the map.

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.

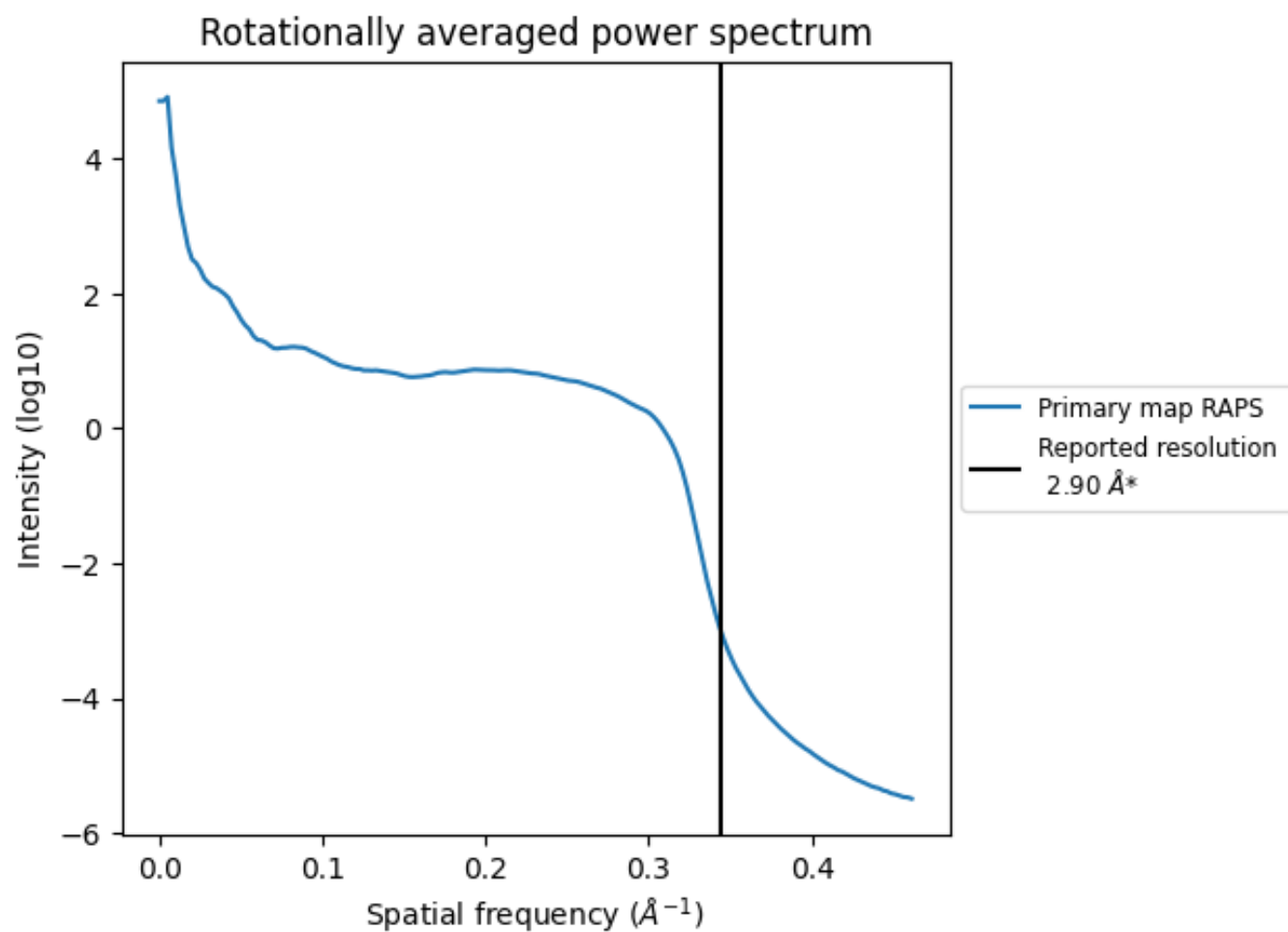
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1254 nm³; this corresponds to an approximate mass of 1133 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

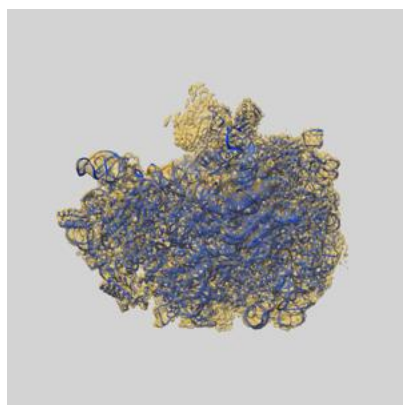
8 Fourier-Shell correlation

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

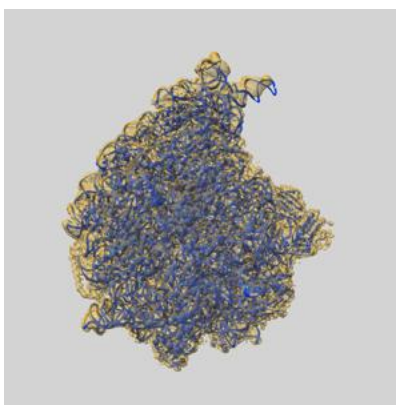
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12936 and PDB model 7OIZ. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

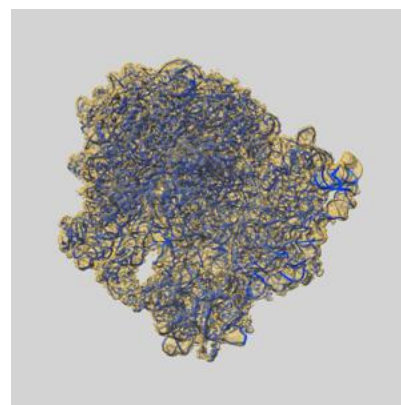
9.1 Map-model overlay [i](#)



X



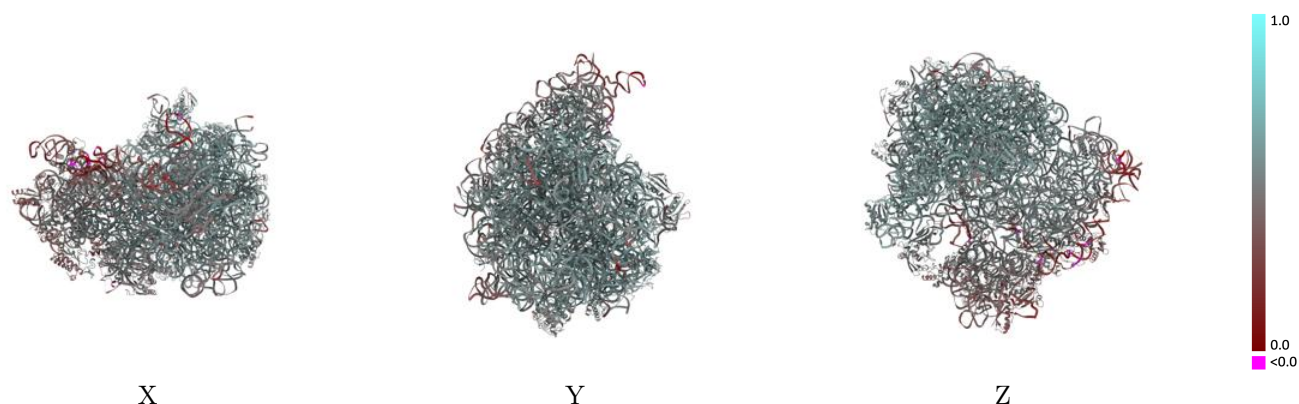
Y



Z

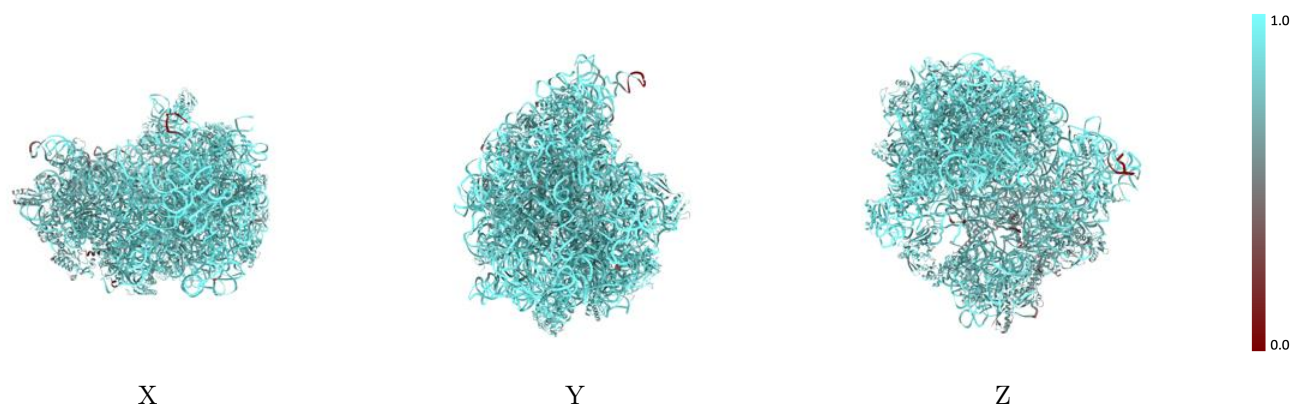
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



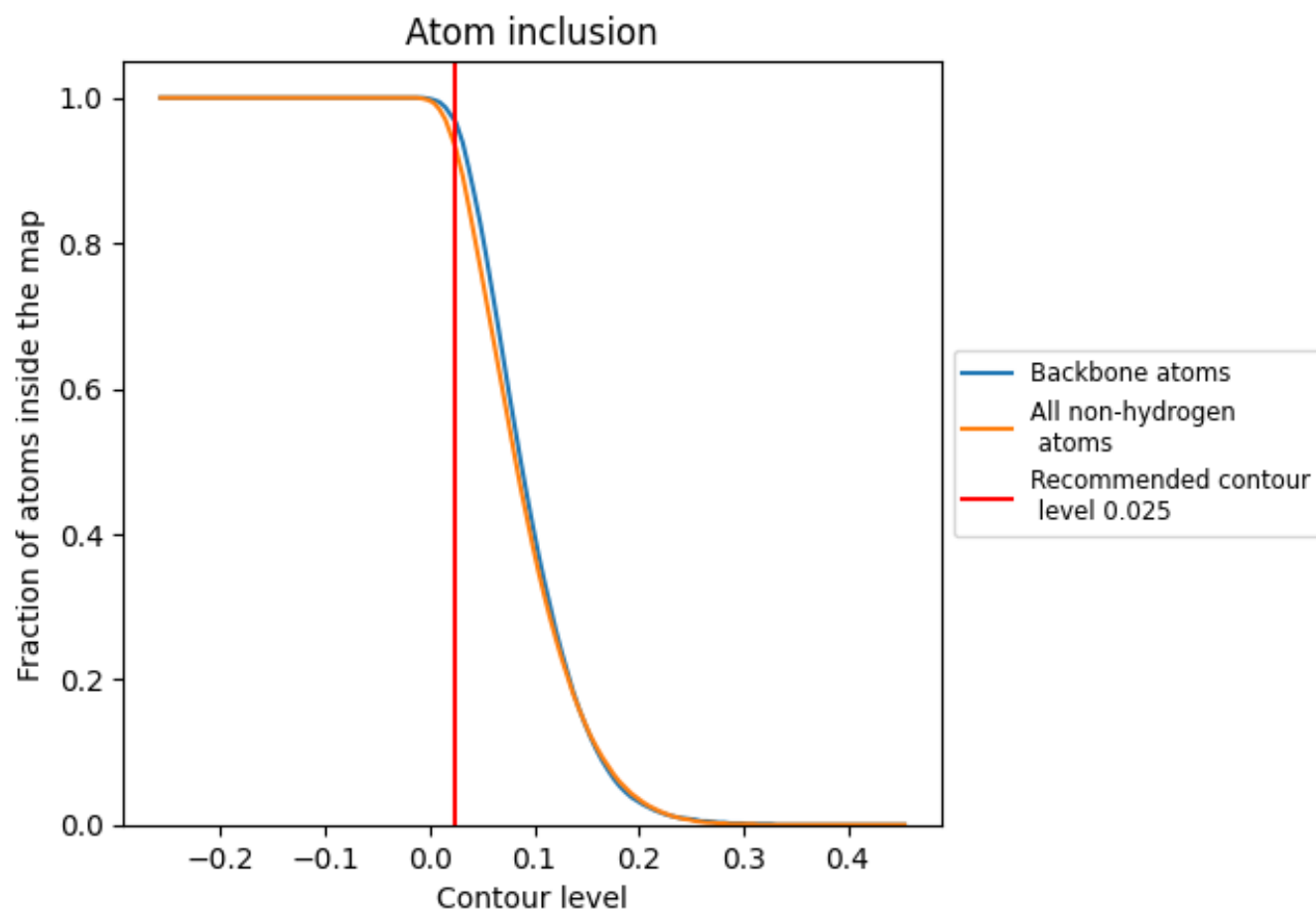
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 93% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9300	 0.5180
0	 0.9140	 0.5590
1	 0.9240	 0.5600
2	 0.9590	 0.5830
3	 0.9630	 0.5850
4	 0.7580	 0.4430
7	 0.9190	 0.5460
A	 0.9350	 0.4630
B	 0.7150	 0.4040
C	 0.7620	 0.4340
D	 0.7740	 0.4380
E	 0.8450	 0.4940
F	 0.8310	 0.4720
G	 0.7430	 0.4060
H	 0.8120	 0.4930
I	 0.7900	 0.4310
J	 0.6820	 0.3950
K	 0.8370	 0.4870
L	 0.8820	 0.5280
M	 0.8230	 0.4570
N	 0.7970	 0.4330
O	 0.8750	 0.4870
P	 0.8390	 0.4850
Q	 0.8260	 0.4940
R	 0.7780	 0.4550
S	 0.7850	 0.4220
T	 0.8730	 0.4940
U	 0.5290	 0.4060
V	 0.9180	 0.4650
X	 0.5840	 0.2900
a	 0.9800	 0.5580
b	 0.9850	 0.5490
c	 0.9460	 0.5760
d	 0.9400	 0.5720
e	 0.8740	 0.5200



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Chain	Atom inclusion	Q-score
f	 0.8550	 0.4960
g	 0.8670	 0.5020
h	 0.8330	 0.4820
i	 0.9350	 0.5740
j	 0.9370	 0.5750
k	 0.9090	 0.5520
l	 0.9290	 0.5670
m	 0.9490	 0.5720
n	 0.9080	 0.5390
o	 0.9210	 0.5740
p	 0.9500	 0.5750
q	 0.9020	 0.5550
r	 0.8850	 0.5420
s	 0.8620	 0.5170
t	 0.8720	 0.4980
u	 0.9000	 0.5430
v	 0.9460	 0.5950
w	 0.9300	 0.5610
x	 0.8410	 0.4810
y	 0.9040	 0.5470
z	 0.9230	 0.5620