



## Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 02:53 AM UTC

PDB ID : 9I89 / pdb\_00009i89  
EMDB ID : EMD-52712  
Title : Structure of the A2058-dimethylated Staphylococcus aureus 70S ribosome complexed with clincelin  
Authors : Novotna, M.; Boissier, F.; Balikova Novotna, G.; Innis, C.A.  
Deposited on : 2025-02-04  
Resolution : 3.01 Å(reported)  
Based on initial model : 9I88

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

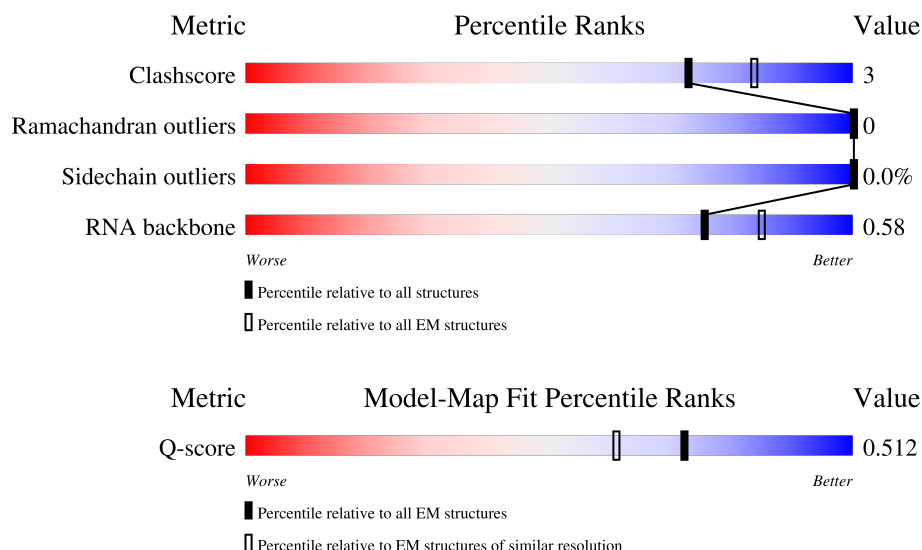
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.01 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.





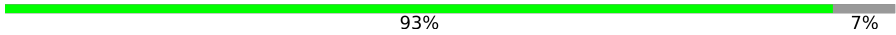





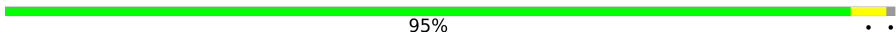

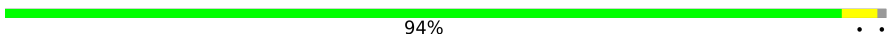


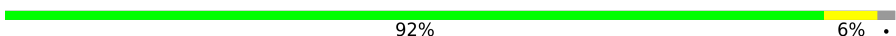

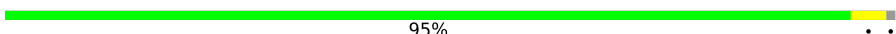

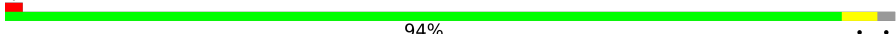



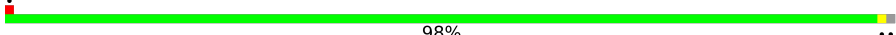



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13882 ( 2.51 - 3.51 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	62	 94% 5%
2	2	69	 84% 9% 7%
3	3	59	 88% 7% 5%




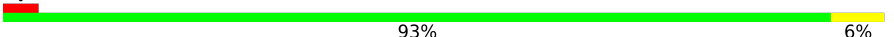






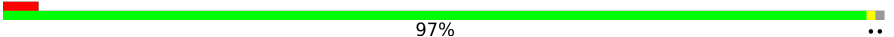
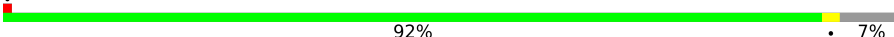


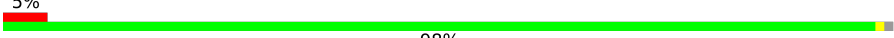








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Mol	Chain	Length	Quality of chain
4	5	57	 84%5%7%
5	6	49	 84%12%
6	7	45	 93%7%
7	8	66	 89%8%
8	9	37	 86%11%
9	B	115	 82%14%
10	C	105	 92%6%
11	D	77	 6%75%22%
12	G	277	 95%
13	H	220	 92%6%
14	I	207	 94%
15	J	179	 88%9%
16	K	178	 89%8%
17	M	145	 92%6%
18	N	122	 93%7%
19	O	146	 95%
20	P	144	 87%7%6%
21	Q	122	 94%
22	R	119	 92%7%
23	S	116	 92%6%
24	T	118	 91%8%
25	U	102	 98%
26	V	117	 82%13%5%
27	W	91	 84%14%
28	Y	217	 42%57%

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Mol	Chain	Length	Quality of chain
29	Z	94	
30	c	255	
31	d	217	
32	e	200	
33	f	166	
34	g	98	
35	i	132	
36	j	130	
37	k	102	
38	l	129	
39	m	137	
40	n	121	
41	o	61	
42	p	89	
43	q	91	
44	r	87	
45	s	80	
46	t	92	
47	u	83	
48	A	2923	
49	a	1552	
50	h	156	
51	4	84	

## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 139409 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	59	Total	C	N	O	S	0	0
			463	287	99	76	1		

- Molecule 2 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	64	Total	C	N	O	0	0
			527	324	99	104		

- Molecule 3 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	56	Total	C	N	O	0	0
			436	271	82	83		

- Molecule 4 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	53	Total	C	N	O	S	0	0
			422	256	86	75	5		

- Molecule 5 is a protein called Large ribosomal subunit protein bL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	47	Total	C	N	O	S	0	0
			394	240	78	72	4		

- Molecule 6 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	42	Total	C	N	O	S	0	0
			360	220	88	51	1		

- Molecule 7 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 8 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	36	Total	C	N	O	S	0	0
			292	184	59	44	5		

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	113	Total	C	N	O	P	0	0
			2408	1076	431	788	113		

- Molecule 10 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	99	Total	C	N	O	S	0	0
			761	480	140	139	2		

- Molecule 11 is a RNA chain called fMet-P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	77	Total	C	N	O	P	0	0
			1642	732	295	538	77		

- Molecule 12 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	273	Total	C	N	O	S	0	0
			2085	1297	413	370	5		

- Molecule 13 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	216	Total	C	N	O	S	0	0
			1637	1024	301	307	5		

- Molecule 14 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	204	Total	C	N	O	S	0	0
			1564	981	286	295	2		

- Molecule 15 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	175	Total	C	N	O	S	0	0
			1381	876	237	261	7		

- Molecule 16 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	164	Total	C	N	O	S	0	0
			1284	799	232	250	3		

- Molecule 17 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	142	Total	C	N	O	S	0	0
			1127	704	205	216	2		

- Molecule 18 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	122	Total	C	N	O	S	0	0
			920	572	174	170	4		

- Molecule 19 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	145	Total	C	N	O	S	0	0
			1090	674	214	201	1		

- Molecule 20 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	135	Total	C	N	O	S	0	0
			1081	693	205	180	3		

- Molecule 21 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	120	Total	C	N	O	S	0	0
			952	584	182	185	1		

- Molecule 22 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	118	Total	C	N	O		0	0
			914	569	173	172			

- Molecule 23 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	114	Total	C	N	O		0	0
			922	580	185	157			

- Molecule 24 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	116	Total	C	N	O	S	0	0
			943	593	189	157	4		

- Molecule 25 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	101	Total	C	N	O	S	0	0
			793	503	141	148	1		

- Molecule 26 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	111	Total	C	N	O	S	0	0
			853	532	163	155	3		

- Molecule 27 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	89	Total	C	N	O	S	0	0
			725	457	130	134	4		

- Molecule 28 is a protein called Large ribosomal subunit protein bL25.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	94	Total	C	N	O	S	0	0
			738	471	131	134	2		

- Molecule 29 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	78	Total	C	N	O	S	0	0
			597	367	116	114			

- Molecule 30 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	221	Total	C	N	O	S	0	0
			1781	1136	310	328	7		

- Molecule 31 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	202	Total	C	N	O	S	0	0
			1596	1005	300	289	2		

- Molecule 32 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	199	Total	C	N	O	S	0	0
			1617	1020	302	293	2		

- Molecule 33 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	156	Total	C	N	O	S	0	0
			1160	730	213	215	2		

- Molecule 34 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	93	Total	C	N	O	S	0	0
			773	489	136	146	2		

- Molecule 35 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	131	Total	C	N	O	S	0	0
			1032	652	183	193	4		

- Molecule 36 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	127	Total	C	N	O	S	0	0
			1008	624	201	182	1		

- Molecule 37 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	102	Total	C	N	O	S	0	0
			814	513	149	150	2		

- Molecule 38 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	118	Total	C	N	O	S	0	0
			877	542	166	166	3		

- Molecule 39 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 40 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	113	Total	C	N	O	S	0	0
			902	554	179	168	1		

- Molecule 41 is a protein called Small ribosomal subunit protein uS14B.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	60	Total	C	N	O	S	0	0
			502	317	100	80	5		

- Molecule 42 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	p	86	Total	C	N	O	S	0	0
			721	445	148	127	1		

- Molecule 43 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	q	90	Total	C	N	O	S	0	0
			712	448	132	131	1		

- Molecule 44 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	r	79	Total	C	N	O	S	0	0
			651	413	116	121	1		

- Molecule 45 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	s	63	Total	C	N	O	S	0	0
			516	330	96	87	3		

- Molecule 46 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	t	79	Total	C	N	O	S	0	0
			646	416	116	112	2		

- Molecule 47 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	u	80	Total	C	N	O	S	0	0
			606	367	119	118	2		

- Molecule 48 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	A	2808	Total	C	N	O	P	0	0
			60210	26885	11018	19499	2808		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	261	U	C	conflict	GB CP020619.1

- Molecule 49 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	a	1505	Total	C	N	O	P	0	0
			32251	14399	5898	10449	1505		

- Molecule 50 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	h	148	Total	C	N	O	S	0	0
			1180	734	226	216	4		

- Molecule 51 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	4	59	Total	C	N	O	S	0	0
			486	310	88	87	1		

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	5	1	Total	Zn	0
			1	1	
52	6	1	Total	Zn	0
			1	1	
52	9	1	Total	Zn	0
			1	1	
52	o	1	Total	Zn	0
			1	1	

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

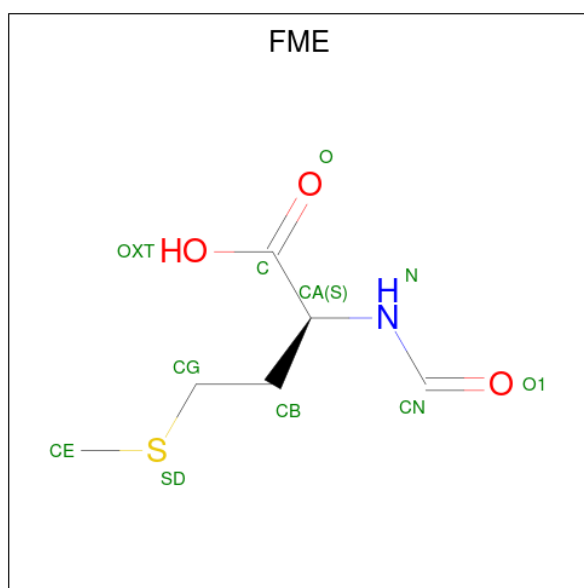
Mol	Chain	Residues	Atoms		AltConf
53	7	1	Total	Mg	0
			1	1	
53	B	7	Total	Mg	0
			7	7	
53	D	1	Total	Mg	0
			1	1	
53	G	2	Total	Mg	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
53	O	1	Total	Mg	0
			1	1	
53	t	1	Total	Mg	0
			1	1	
53	u	1	Total	Mg	0
			1	1	
53	A	306	Total	Mg	0
			306	306	
53	a	101	Total	Mg	0
			101	101	

- Molecule 54 is N-FORMYLMETHIONINE (CCD ID: FME) (formula:  $C_6H_{11}NO_3S$ ).



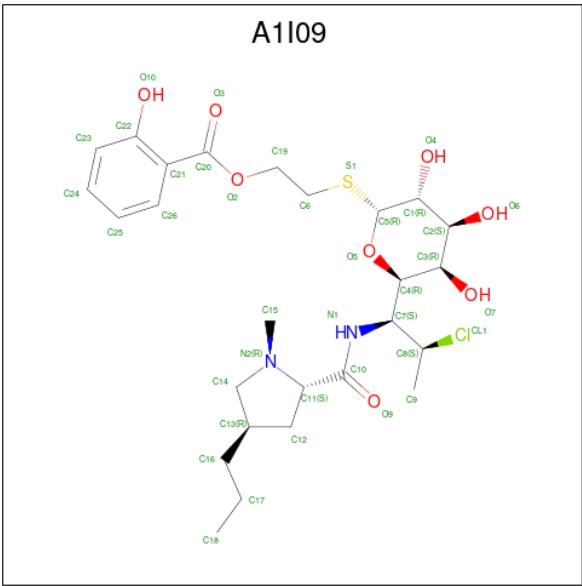
Mol	Chain	Residues	Atoms					AltConf
54	D	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 55 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
55	A	4	Total	K	0
			4	4	
55	a	1	Total	K	0
			1	1	

- Molecule 56 is Clincelin (CCD ID: A1I09) (formula:  $C_{26}H_{39}ClN_2O_8S$ ) (labeled as "Ligand of

Interest" by depositor).

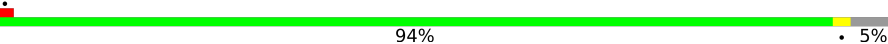


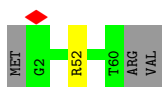
Mol	Chain	Residues	Atoms						AltConf
56	A	1	Total	C	Cl	N	O	S	0
			38	26	1	2	8	1	

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Large ribosomal subunit protein bL28

Chain 1:  94% • 5%




- Molecule 2: Large ribosomal subunit protein uL29

Chain 2:  84% 9% 7%




- Molecule 3: Large ribosomal subunit protein uL30

Chain 3:  88% 7% 5%




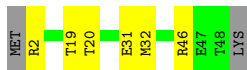
- Molecule 4: Large ribosomal subunit protein bL32

Chain 5:  84% 5% • 7%



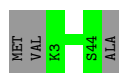
- Molecule 5: Large ribosomal subunit protein bL33A

Chain 6:  84% 12% •



- Molecule 6: Large ribosomal subunit protein bL34

Chain 7:  93% 7%




- Molecule 7: Large ribosomal subunit protein bL35

Chain 8:  89% 8% .




- Molecule 8: Large ribosomal subunit protein bL36

Chain 9:  86% 11% .



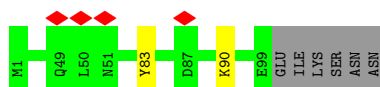
- Molecule 9: 5S ribosomal RNA

Chain B:  82% 14% . .




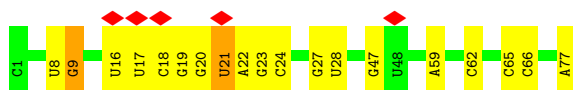
- Molecule 10: Large ribosomal subunit protein uL24

Chain C:  92% . 6%



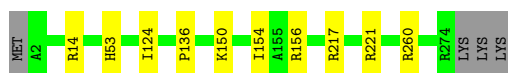
- Molecule 11: fMet-P-tRNA

Chain D:  6% 75% 22% .



- Molecule 12: Large ribosomal subunit protein uL2

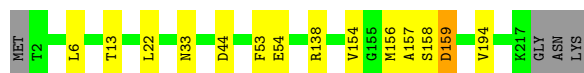
Chain G:  95% . .



- Molecule 13: Large ribosomal subunit protein uL3



Chain H:  92% 6% .




- Molecule 14: Large ribosomal subunit protein uL4

Chain I:  94% . .




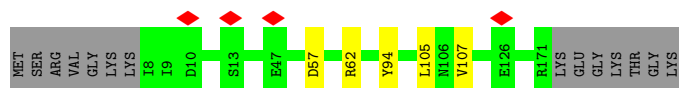
- Molecule 15: Large ribosomal subunit protein uL5

Chain J:  88% 9% . .



- Molecule 16: Large ribosomal subunit protein uL6

Chain K:  89% . 8%



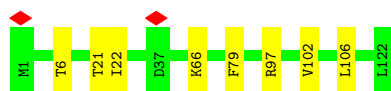
- Molecule 17: Large ribosomal subunit protein uL13

Chain M:  92% 6% .



- Molecule 18: Large ribosomal subunit protein uL14

Chain N:  93% 7%




- Molecule 19: Large ribosomal subunit protein uL15

Chain O:  95% . .



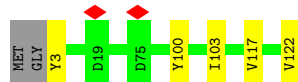
- Molecule 20: Large ribosomal subunit protein uL16

Chain P:  87% 7% 6%



- Molecule 21: Large ribosomal subunit protein bL17

Chain Q:  94% . .




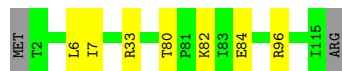
- Molecule 22: Large ribosomal subunit protein uL18

Chain R:  92% 7% .




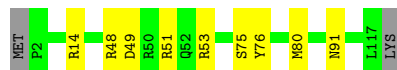
- Molecule 23: Large ribosomal subunit protein bL19

Chain S:  92% 6% .



- Molecule 24: Large ribosomal subunit protein bL20

Chain T:  91% 8% .




- Molecule 25: Large ribosomal subunit protein bL21

Chain U:  98% ..



- Molecule 26: Large ribosomal subunit protein uL22

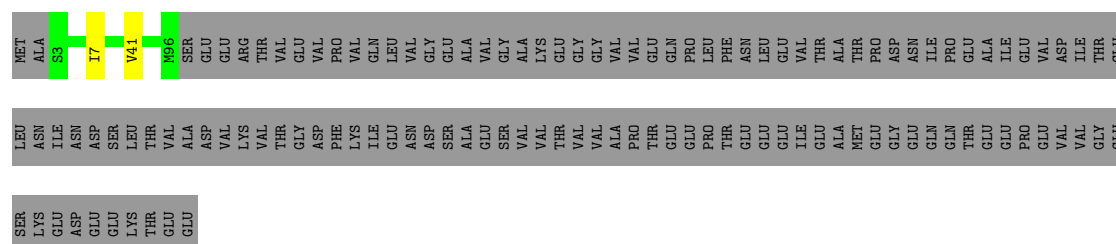
Chain V:  82% 13% 5%

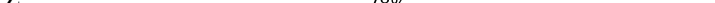


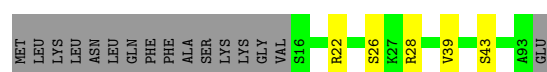
- Molecule 27: Large ribosomal subunit protein uL23

MET	E2	D5	P10	A19	K24	V29	D30	T31	R32	T45	N57	K61	R67	R76	D88	L89	F90	ASN
-----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

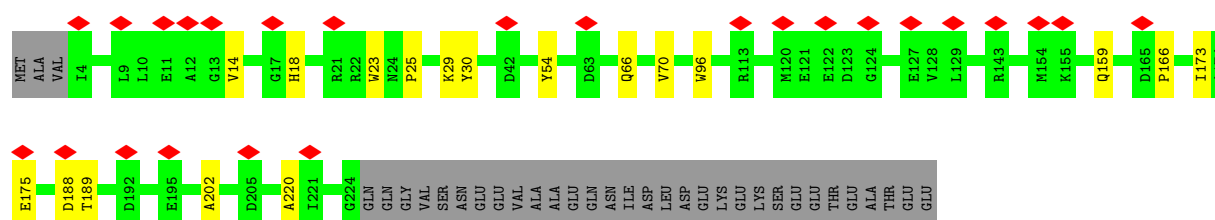
- Chain Y:  42% . 57%



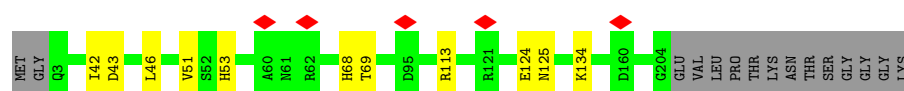
- Chain Z:  78% 5% 17%



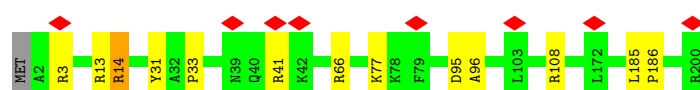
- Chain c:  10% 80% 7% 13%




- Chain d:  88% 5% 7%




- Chain e:  93% 6%




## • Molecule 33: Small ribosomal subunit protein uS5

Chain f:  88% 6% 6%


## • Molecule 34: Small ribosomal subunit protein bS6

Chain g:  89% 6% 5%


## • Molecule 35: Small ribosomal subunit protein uS8

Chain i:  90% 9% .


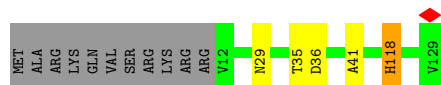
## • Molecule 36: Small ribosomal subunit protein uS9

Chain j:  90% 8% .

## • Molecule 37: Small ribosomal subunit protein uS10

Chain k:  8% 85% 15%

## • Molecule 38: Small ribosomal subunit protein uS11

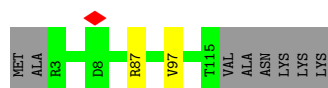
Chain l:  88% . . 9%

## • Molecule 39: Small ribosomal subunit protein uS12

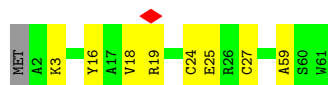
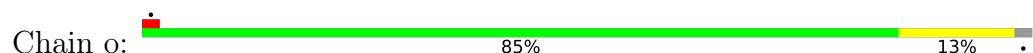
Chain m:  97% ..



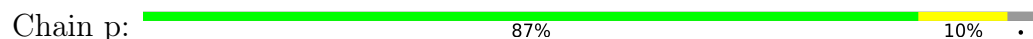
- Molecule 40: Small ribosomal subunit protein uS13



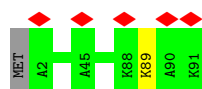
- Molecule 41: Small ribosomal subunit protein uS14B



- Molecule 42: Small ribosomal subunit protein uS15



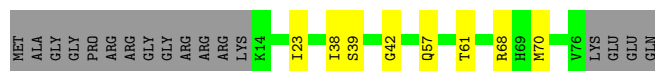
- Molecule 43: Small ribosomal subunit protein bS16



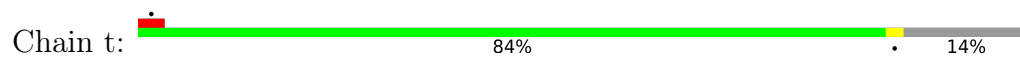
- Molecule 44: Small ribosomal subunit protein uS17



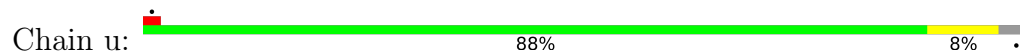
- Molecule 45: Small ribosomal subunit protein bS18



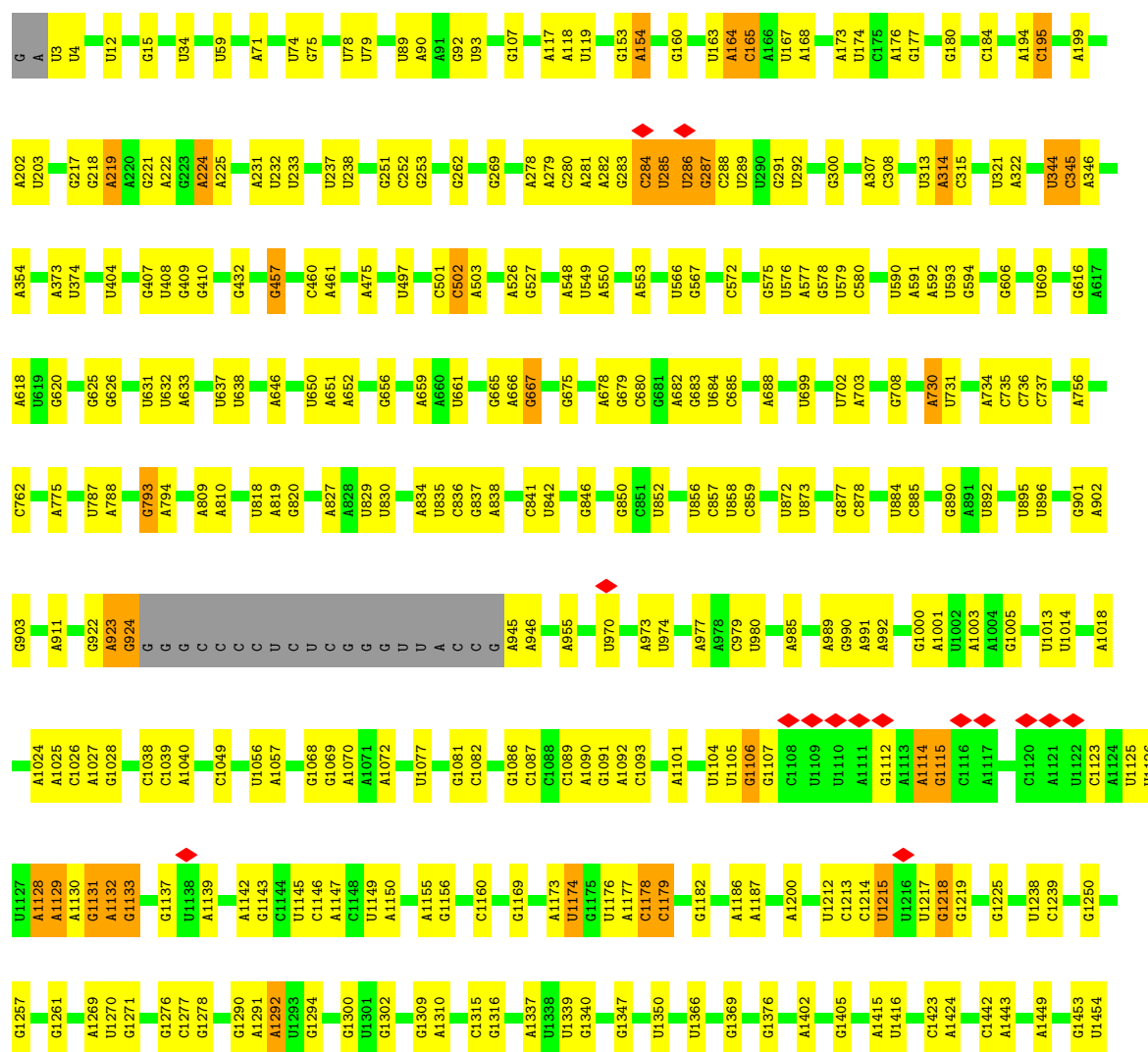
- Molecule 46: Small ribosomal subunit protein uS19



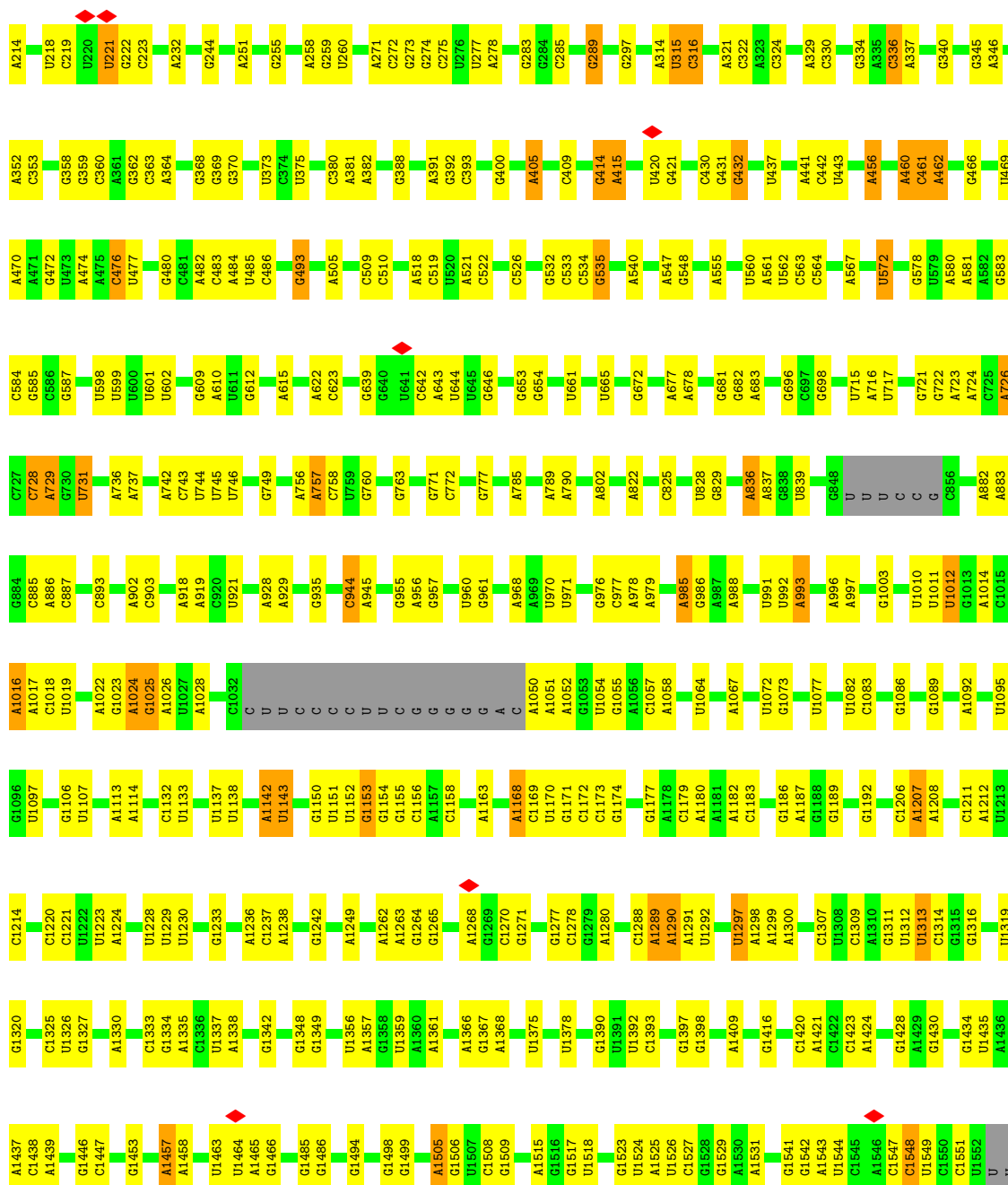
- Molecule 47: Small ribosomal subunit protein bS20



- Molecule 48: 23S ribosomal RNA

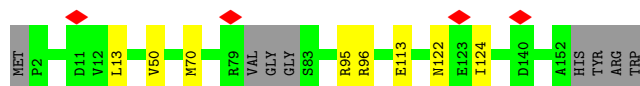






- Molecule 50: Small ribosomal subunit protein uS7

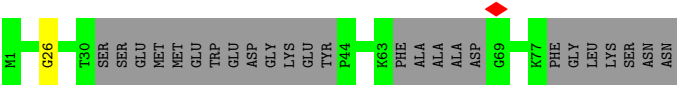
Chain h: 90% 5% 5%



- Molecule 51: Large ribosomal subunit protein bL31B

Chain 4: 69% 30%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	63589	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.013	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.003	Depositor
Map size ( $\text{\AA}$ )	365.16, 365.16, 365.16	wwPDB
Map dimensions	408, 408, 408	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.895, 0.895, 0.895	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1I09, FME, K, MG, MA6, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	1	0.34	0/469	0.48	0/625
2	2	0.30	0/528	0.48	0/703
3	3	0.36	0/438	0.52	0/590
4	5	0.36	0/429	0.45	0/571
5	6	0.33	0/399	0.49	0/535
6	7	0.43	0/364	0.50	0/474
7	8	0.37	0/526	0.57	0/690
8	9	0.38	0/295	0.50	0/388
9	B	0.39	0/2692	0.60	0/4193
10	C	0.26	0/770	0.44	0/1029
11	D	0.34	0/1834	0.61	0/2857
12	G	0.36	0/2120	0.48	0/2847
13	H	0.36	0/1661	0.56	2/2227 (0.1%)
14	I	0.35	0/1587	0.51	0/2143
15	J	0.28	0/1398	0.44	0/1877
16	K	0.23	0/1302	0.47	0/1757
17	M	0.36	0/1149	0.47	0/1549
18	N	0.33	0/927	0.45	0/1243
19	O	0.36	0/1104	0.51	0/1471
20	P	0.35	0/1105	0.47	0/1483
21	Q	0.35	0/956	0.52	0/1277
22	R	0.30	0/923	0.45	0/1234
23	S	0.32	0/934	0.45	0/1249
24	T	0.41	0/955	0.51	0/1265
25	U	0.35	0/803	0.46	0/1073
26	V	0.35	0/861	0.52	0/1159
27	W	0.34	0/733	0.51	0/978
28	Y	0.30	0/746	0.52	0/1000
29	Z	0.35	0/603	0.48	0/801
30	c	0.20	0/1808	0.43	0/2426
31	d	0.25	0/1618	0.45	0/2173
32	e	0.24	0/1647	0.48	0/2211

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	f	0.28	0/1174	0.43	0/1583
34	g	0.30	0/784	0.47	0/1052
35	i	0.30	0/1044	0.44	0/1401
36	j	0.26	0/1024	0.51	0/1374
37	k	0.25	0/826	0.46	0/1111
38	l	0.25	0/892	0.57	2/1203 (0.2%)
39	m	0.24	0/1075	0.48	0/1439
40	n	0.24	0/909	0.43	0/1218
41	o	0.28	0/512	0.48	0/678
42	p	0.29	0/730	0.48	0/975
43	q	0.25	0/723	0.43	0/971
44	r	0.25	0/659	0.51	0/881
45	s	0.30	0/525	0.40	0/704
46	t	0.21	0/663	0.38	0/889
47	u	0.28	0/606	0.49	0/810
48	A	0.47	0/67406	0.62	0/105124
49	a	0.40	0/36111	0.63	1/56310 (0.0%)
50	h	0.25	0/1195	0.51	0/1605
51	4	0.23	0/496	0.44	0/661
All	All	0.41	0/151038	0.59	5/226087 (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
1	1	0	1
4	5	0	2
12	G	0	1
14	I	0	1
15	J	0	1
23	S	0	1
31	d	0	1
32	e	0	2
36	j	0	1
37	k	0	1
50	h	0	1
All	All	0	13

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	l	118	HIS	CA-C-N	7.63	135.43	121.70
38	l	118	HIS	C-N-CA	7.63	135.43	121.70
13	H	159	ASP	CA-C-N	5.60	131.77	121.70
13	H	159	ASP	C-N-CA	5.60	131.77	121.70
49	a	893	C	N1-C1'-C2'	5.01	119.51	112.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	52	ARG	Sidechain
4	5	12	ARG	Sidechain
4	5	6	ARG	Sidechain
12	G	14	ARG	Sidechain
14	I	106	ARG	Sidechain
15	J	110	ARG	Sidechain
23	S	96	ARG	Sidechain
31	d	113	ARG	Sidechain
32	e	14	ARG	Sidechain
32	e	3	ARG	Sidechain
50	h	95	ARG	Sidechain
36	j	87	ARG	Sidechain
37	k	62	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	463	0	501	0	0
2	2	527	0	554	5	0
3	3	436	0	473	2	0
4	5	422	0	426	9	0
5	6	394	0	398	5	0
6	7	360	0	406	0	0
7	8	521	0	586	5	0
8	9	292	0	336	3	0
9	B	2408	0	1218	12	0
10	C	761	0	823	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	1642	0	833	5	0
12	G	2085	0	2192	9	0
13	H	1637	0	1680	14	0
14	I	1564	0	1611	7	0
15	J	1381	0	1435	14	0
16	K	1284	0	1301	4	0
17	M	1127	0	1117	9	0
18	N	920	0	981	6	0
19	O	1090	0	1131	6	0
20	P	1081	0	1143	7	0
21	Q	952	0	999	3	0
22	R	914	0	956	7	0
23	S	922	0	994	6	0
24	T	943	0	1014	7	0
25	U	793	0	831	1	0
26	V	853	0	914	13	0
27	W	725	0	761	9	0
28	Y	738	0	787	1	0
29	Z	597	0	607	4	0
30	c	1781	0	1844	10	0
31	d	1596	0	1659	11	0
32	e	1617	0	1646	10	0
33	f	1160	0	1223	7	0
34	g	773	0	772	4	0
35	i	1032	0	1082	9	0
36	j	1008	0	1031	7	0
37	k	814	0	863	9	0
38	l	877	0	895	4	0
39	m	1058	0	1130	2	0
40	n	902	0	950	2	0
41	o	502	0	523	6	0
42	p	721	0	751	6	0
43	q	712	0	744	1	0
44	r	651	0	689	6	0
45	s	516	0	548	6	0
46	t	646	0	653	3	0
47	u	606	0	650	7	0
48	A	60210	0	30266	298	0
49	a	32251	0	16234	260	0
50	h	1180	0	1221	4	0
51	4	486	0	488	1	0
52	5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	6	1	0	0	0	0
52	9	1	0	0	0	0
52	o	1	0	0	0	0
53	7	1	0	0	0	0
53	A	306	0	0	0	0
53	B	7	0	0	0	0
53	D	1	0	0	0	0
53	G	2	0	0	0	0
53	O	1	0	0	0	0
53	a	101	0	0	0	0
53	t	1	0	0	0	0
53	u	1	0	0	0	0
54	D	10	0	10	0	0
55	A	4	0	0	0	0
55	a	1	0	0	0	0
56	A	38	0	0	1	0
All	All	139409	0	92880	750	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 3.

All (750) 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)
48:A:1572:G:N2	48:A:1593:G:O6	2.07	0.87
24:T:48:ARG:NH1	24:T:49:ASP:OD1	2.11	0.82
33:f:157:ARG:NH2	35:i:43:GLU:OE1	2.14	0.80
25:U:67:ARG:NH1	48:A:1261:G:OP1	2.17	0.77
48:A:788:A:O2'	48:A:1703:U:OP1	2.03	0.74
48:A:2532:G:OP1	56:A:3105:A1I09:O6	2.08	0.70
49:a:189:G:O6	49:a:203:A:N6	2.25	0.70
9:B:41:C:O2	15:J:92:ARG:NH1	2.24	0.69
42:p:54:ARG:NH1	49:a:587:G:O2'	2.25	0.69
48:A:1580:A:N3	48:A:1583:G:N2	2.41	0.69
12:G:150:LYS:NZ	48:A:1828:U:OP2	2.26	0.68
48:A:314:A:N3	48:A:315:C:N4	2.43	0.67
49:a:1050:A:H2'	49:a:1051:A:C8	2.29	0.66
12:G:221:ARG:NH1	48:A:1816:A:OP2	2.28	0.66
49:a:1233:G:OP2	49:a:1333:C:N4	2.30	0.65
26:V:88:ARG:NH2	48:A:793:G:OP1	2.30	0.64
48:A:457:G:OP2	48:A:2433:C:O2'	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:40:HIS:HD1	48:A:2835:C:HO2'	1.44	0.63
49:a:1229:U:H2'	49:a:1230:U:C6	2.33	0.63
49:a:1024:A:H5'	49:a:1024:A:C8	2.32	0.63
33:f:41:ASP:OD2	33:f:43:ASN:ND2	2.32	0.63
49:a:75:A:N6	49:a:94:G:O2'	2.31	0.62
49:a:1446:G:H2'	49:a:1447:C:C6	2.34	0.62
14:I:74:ARG:HH22	48:A:2472:G:P	2.23	0.62
26:V:90:GLN:OE1	26:V:92:ARG:NH2	2.33	0.62
48:A:2354:A:H2'	48:A:2355:A:C8	2.35	0.62
49:a:456:A:OP2	49:a:493:G:N2	2.31	0.62
49:a:681:G:H2'	49:a:682:G:C8	2.35	0.61
22:R:113:ARG:NH1	48:A:2403:A:O2'	2.30	0.61
39:m:107:ARG:NH2	49:a:921:U:OP2	2.32	0.61
49:a:120:C:N4	49:a:244:G:OP2	2.30	0.61
49:a:1277:G:N2	49:a:1280:A:OP2	2.30	0.61
19:O:29:LYS:HG3	19:O:30:THR:H	1.66	0.60
24:T:53:ARG:NH2	48:A:1038:C:OP1	2.34	0.60
49:a:615:A:OP1	49:a:639:G:N2	2.31	0.60
49:a:194:G:N2	49:a:197:U:OP2	2.30	0.60
36:j:125:ARG:HE	49:a:1361:A:P	2.24	0.59
45:s:42:GLY:O	45:s:68:ARG:NH2	2.33	0.59
49:a:221:U:H1'	49:a:222:G:C8	2.37	0.59
35:i:8:ALA:O	35:i:12:THR:HG23	2.03	0.59
4:5:16:ARG:NH2	48:A:1302:G:OP1	2.34	0.59
30:c:18:HIS:ND1	30:c:188:ASP:OD2	2.36	0.59
35:i:12:THR:HG21	49:a:886:A:H1'	1.83	0.58
37:k:19:ASP:OD1	37:k:20:GLN:N	2.35	0.58
4:5:27:MET:HE1	26:V:35:ILE:HA	1.84	0.58
48:A:2355:A:H2'	48:A:2356:A:C8	2.38	0.58
19:O:41:ARG:NH2	48:A:852:U:OP2	2.36	0.58
48:A:1874:A:O2'	48:A:1875:A:H8	1.87	0.58
35:i:110:GLU:OE1	35:i:121:ARG:NH2	2.35	0.58
49:a:1017:A:H2'	49:a:1018:C:C6	2.38	0.58
22:R:56:ALA:HB3	22:R:80:ILE:HG13	1.85	0.57
48:A:1105:U:H3'	48:A:1106:G:H5''	1.86	0.57
9:B:49:G:H2'	9:B:50:A:C8	2.39	0.57
49:a:33:A:H2'	49:a:34:A:C8	2.39	0.57
49:a:721:G:H2'	49:a:722:G:C8	2.40	0.57
49:a:956:A:H2'	49:a:957:G:C8	2.40	0.57
48:A:901:G:H2'	48:A:902:A:C8	2.41	0.56
49:a:251:A:N6	49:a:289:G:O2'	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:532:G:H2'	49:a:533:C:C6	2.41	0.56
48:A:1149:U:H2'	48:A:1150:A:H8	1.71	0.56
49:a:189:G:C6	49:a:203:A:N6	2.73	0.56
31:d:134:LYS:NZ	33:f:55:GLU:OE1	2.33	0.55
33:f:69:LYS:NZ	49:a:1086:G:OP1	2.38	0.55
5:6:31:GLU:OE2	5:6:46:ARG:NE	2.39	0.55
29:Z:26:SER:O	29:Z:28:ARG:NH1	2.34	0.55
32:e:95:ASP:OD1	32:e:96:ALA:N	2.40	0.55
42:p:8:LYS:O	42:p:12:ILE:HG23	2.06	0.55
49:a:324:C:OP2	49:a:359:G:O2'	2.23	0.55
30:c:14:VAL:HG13	30:c:202:ALA:HB1	1.88	0.55
49:a:213:G:H2'	49:a:214:A:C8	2.42	0.55
49:a:722:G:H2'	49:a:723:A:C8	2.42	0.55
18:N:6:THR:HG22	48:A:1710:G:H4'	1.89	0.55
49:a:41:C:H2'	49:a:42:G:H8	1.71	0.54
48:A:1218:G:H2'	48:A:1219:G:C8	2.43	0.54
48:A:2270:U:H2'	48:A:2271:U:C6	2.43	0.54
13:H:159:ASP:OD1	48:A:1174:U:C5	2.61	0.54
49:a:723:A:H2'	49:a:724:A:C8	2.42	0.54
49:a:777:G:H4'	49:a:1525:A:H4'	1.89	0.54
12:G:217:ARG:HG3	12:G:217:ARG:HH11	1.72	0.54
27:W:31:THR:HG22	27:W:32:ARG:N	2.22	0.54
37:k:7:ARG:NH2	49:a:1138:U:OP1	2.41	0.54
49:a:1010:U:H2'	49:a:1011:U:C6	2.42	0.54
30:c:66:GLN:N	30:c:159:GLN:OE1	2.35	0.54
48:A:1442:C:H2'	48:A:1443:A:C8	2.42	0.54
48:A:2007:G:O2'	48:A:2009:U:OP2	2.22	0.54
4:5:6:ARG:NH2	48:A:2046:U:OP2	2.35	0.54
49:a:485:U:H2'	49:a:486:C:C6	2.43	0.53
15:J:107:SER:O	15:J:110:ARG:N	2.34	0.53
48:A:2318:U:H2'	48:A:2319:U:C6	2.43	0.53
49:a:414:G:H2'	49:a:415:A:H5'	1.91	0.53
48:A:631:U:H2'	48:A:632:U:C6	2.44	0.53
42:p:16:ARG:NH2	42:p:19:GLU:OE1	2.42	0.53
48:A:2612:U:O2	48:A:2612:U:H5'	2.08	0.53
2:2:38:GLU:O	2:2:39:GLU:CG	2.57	0.53
48:A:1651:C:N4	48:A:1666:A:OP2	2.38	0.53
15:J:136:LEU:HD11	15:J:146:VAL:HG21	1.91	0.53
36:j:56:VAL:O	36:j:57:THR:HG22	2.09	0.53
48:A:2091:C:H2'	48:A:2092:C:C6	2.43	0.53
48:A:620:G:O2'	48:A:1292:A:OP1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:n:97:VAL:N	49:a:1319:U:OP1	2.41	0.52
49:a:329:A:H2'	49:a:330:C:C6	2.44	0.52
49:a:388:G:N2	49:a:391:A:OP2	2.36	0.52
49:a:1434:G:H2'	49:a:1435:U:H6	1.73	0.52
15:J:134:GLU:HG3	15:J:137:ILE:HG23	1.92	0.52
49:a:956:A:H2'	49:a:957:G:H8	1.74	0.52
13:H:157:ALA:O	48:A:2080:G:H5'	2.10	0.52
48:A:2335:G:C8	48:A:2337:A:C4	2.98	0.52
49:a:222:G:H2'	49:a:223:C:C6	2.45	0.52
9:B:40:C:OP1	15:J:64:LYS:NZ	2.37	0.52
48:A:2559:G:N2	48:A:2690:G:O2'	2.42	0.52
49:a:441:A:H2'	49:a:442:C:C6	2.44	0.52
49:a:1367:G:H2'	49:a:1368:A:C8	2.45	0.52
21:Q:3:TYR:OH	48:A:2717:A:OP1	2.22	0.51
48:A:1442:C:H2'	48:A:1443:A:H8	1.73	0.51
49:a:745:U:H2'	49:a:746:U:C6	2.45	0.51
49:a:1262:A:H2'	49:a:1263:A:C8	2.45	0.51
15:J:111:VAL:HG12	15:J:113:ASP:H	1.75	0.51
48:A:1105:U:H3'	48:A:1106:G:C5'	2.40	0.51
49:a:1089:G:N2	49:a:1092:A:OP2	2.41	0.51
12:G:154:ILE:HG22	12:G:154:ILE:O	2.09	0.51
32:e:41:ARG:NH1	49:a:518:A:OP1	2.38	0.51
48:A:675:G:N2	48:A:678:A:OP2	2.40	0.51
48:A:2051:C:H2'	48:A:2052:C:C6	2.46	0.51
49:a:18:U:H2'	49:a:19:C:C6	2.46	0.51
49:a:218:U:H2'	49:a:219:C:O4'	2.10	0.51
48:A:656:G:O2'	48:A:659:A:N6	2.39	0.51
50:h:50:VAL:HG21	50:h:124:ILE:HD11	1.93	0.51
30:c:23:TRP:CZ2	30:c:25:PRO:HA	2.46	0.51
33:f:126:LYS:NZ	49:a:10:G:OP2	2.31	0.51
48:A:2231:C:H2'	48:A:2232:A:H8	1.75	0.51
48:A:291:G:H2'	48:A:292:U:C6	2.46	0.51
49:a:665:U:H3	49:a:757:A:H62	1.57	0.51
37:k:66:GLU:HB3	41:o:59:ALA:HB2	1.93	0.51
48:A:2341:A:H2'	48:A:2342:U:C6	2.46	0.51
49:a:258:A:H4'	49:a:260:U:C6	2.46	0.51
49:a:1307:C:H4'	49:a:1313:U:O4	2.11	0.50
47:u:44:ASP:OD1	47:u:45:ASN:N	2.43	0.50
48:A:684:U:H2'	48:A:685:C:C6	2.47	0.50
49:a:368:G:H2'	49:a:369:G:C8	2.46	0.50
48:A:278:A:H2'	48:A:279:A:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:1149:U:H2'	48:A:1150:A:C8	2.45	0.50
49:a:601:U:H2'	49:a:602:U:C6	2.47	0.50
49:a:1095:U:O2'	49:a:1114:A:OP2	2.27	0.50
20:P:42:ILE:HD12	20:P:97:VAL:HG21	1.92	0.50
44:r:70:SER:O	44:r:74:ARG:NH1	2.35	0.50
48:A:286:U:OP2	48:A:287:G:C8	2.64	0.50
48:A:1453:G:O2'	48:A:1630:A:N6	2.45	0.50
48:A:1509:G:C6	48:A:1510:U:C4	2.99	0.50
49:a:329:A:N7	49:a:336:C:O2'	2.44	0.50
42:p:26:GLU:OE2	42:p:77:ARG:NH1	2.41	0.50
17:M:109:MET:HE3	48:A:1182:G:H21	1.77	0.50
20:P:116:GLU:OE2	20:P:119:ARG:NH1	2.44	0.50
48:A:973:A:H2'	48:A:974:U:C6	2.47	0.50
3:3:6:ILE:HG23	3:3:54:VAL:CG1	2.41	0.50
7:8:31:HIS:CD2	7:8:32:LEU:HG	2.47	0.50
31:d:51:VAL:HG22	31:d:69:THR:HG22	1.94	0.50
48:A:92:G:H2'	48:A:93:U:C6	2.46	0.50
49:a:771:G:H2'	49:a:772:C:C6	2.46	0.50
4:5:27:MET:HE1	26:V:35:ILE:HD13	1.93	0.50
24:T:51:ARG:HD3	48:A:1200:A:C8	2.47	0.50
47:u:10:ARG:HD2	49:a:107:G:O6	2.12	0.50
48:A:89:U:H3'	48:A:90:A:H2'	1.93	0.49
48:A:163:U:O2	48:A:165:C:N4	2.42	0.49
48:A:666:A:H2'	48:A:667:G:C5'	2.42	0.49
48:A:1455:U:H4'	48:A:1457:U:C2	2.47	0.49
48:A:1823:U:H2'	48:A:1824:C:C6	2.46	0.49
49:a:1142:A:H3'	49:a:1143:U:C6	2.47	0.49
48:A:1457:U:H3'	48:A:1458:A:O4'	2.13	0.49
49:a:182:A:N7	49:a:232:A:H5'	2.27	0.49
49:a:509:C:H2'	49:a:510:C:C6	2.47	0.49
48:A:1347:G:N2	48:A:1350:U:C4	2.81	0.49
48:A:2103:U:OP2	48:A:2265:G:N2	2.41	0.49
48:A:2725:U:H2'	48:A:2726:C:C6	2.46	0.49
48:A:2824:G:H2'	48:A:2825:U:C6	2.47	0.49
49:a:213:G:H2'	49:a:214:A:H8	1.76	0.49
49:a:993:A:N3	49:a:993:A:H2'	2.27	0.49
49:a:1264:G:H2'	49:a:1265:G:H8	1.77	0.49
49:a:1485:G:H2'	49:a:1486:G:C8	2.47	0.49
48:A:1455:U:O2	48:A:1456:U:N3	2.45	0.49
12:G:260:ARG:NE	48:A:1826:G:OP1	2.39	0.49
18:N:66:LYS:HA	18:N:79:PHE:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:1025:A:OP2	48:A:1026:C:N4	2.42	0.49
48:A:1572:G:C6	48:A:1591:G:C6	3.00	0.49
49:a:1434:G:H2'	49:a:1435:U:C6	2.47	0.49
24:T:14:ARG:NH2	48:A:1290:G:OP2	2.36	0.49
37:k:15:HIS:HA	37:k:18:ILE:HG22	1.95	0.49
48:A:650:U:C5	48:A:665:G:C5	3.00	0.49
48:A:1823:U:H2'	48:A:1824:C:H6	1.77	0.49
8:9:4:ARG:NH2	48:A:2504:C:O2	2.35	0.49
49:a:828:U:H4'	49:a:829:G:OP2	2.13	0.49
14:I:39:LEU:C	14:I:39:LEU:HD23	2.38	0.49
14:I:106:ARG:HD2	48:A:661:U:OP1	2.12	0.49
24:T:91:ASN:OD1	24:T:91:ASN:C	2.56	0.49
48:A:632:U:H2'	48:A:633:A:H8	1.77	0.49
48:A:666:A:H2'	48:A:667:G:H5'	1.94	0.49
48:A:2617:A:H2'	48:A:2618:C:H6	1.78	0.49
49:a:271:A:H2'	49:a:272:C:C6	2.47	0.49
50:h:113:GLU:OE2	50:h:122:ASN:ND2	2.40	0.49
13:H:13:THR:CG2	23:S:7:ILE:HG23	2.42	0.49
37:k:32:SER:HB2	37:k:83:THR:HG23	1.95	0.49
48:A:12:U:O2	48:A:12:U:H2'	2.13	0.49
49:a:155:U:H2'	49:a:156:C:C6	2.48	0.49
49:a:578:G:C6	49:a:883:A:C2	3.01	0.49
49:a:961:G:C6	49:a:1242:G:C6	3.00	0.49
49:a:1236:A:H2'	49:a:1237:C:C5	2.48	0.49
12:G:154:ILE:O	12:G:154:ILE:CG2	2.60	0.48
30:c:166:PRO:HB3	30:c:173:ILE:CD1	2.43	0.48
48:A:923:A:N6	48:A:945:A:C8	2.81	0.48
48:A:2580:G:H5''	48:A:2581:U:OP2	2.12	0.48
49:a:99:U:HO2'	49:a:100:A:H8	1.59	0.48
49:a:189:G:C6	49:a:203:A:C6	3.01	0.48
49:a:392:G:H2'	49:a:393:C:C6	2.48	0.48
49:a:1138:U:C2	49:a:1292:U:C5	3.01	0.48
48:A:78:U:H2'	48:A:79:U:C6	2.48	0.48
48:A:1507:A:H2'	48:A:1508:C:H6	1.78	0.48
48:A:2286:G:C8	48:A:2454:C:C4	3.01	0.48
49:a:392:G:H2'	49:a:393:C:H6	1.78	0.48
8:9:7:VAL:CG1	8:9:25:VAL:HG23	2.43	0.48
41:o:16:TYR:CE1	41:o:19:ARG:HB2	2.48	0.48
48:A:194:A:H2'	48:A:195:C:C6	2.48	0.48
48:A:1238:U:H2'	48:A:1239:C:C6	2.48	0.48
48:A:1711:G:O2'	48:A:2018:U:O4	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:2293:A:H4'	48:A:2294:A:N3	2.28	0.48
49:a:68:C:H2'	49:a:69:G:C8	2.48	0.48
43:q:89:LYS:HD3	49:a:470:A:O2'	2.13	0.48
48:A:1754:C:H2'	48:A:1755:U:C6	2.49	0.48
48:A:1765:A:H2'	48:A:1766:C:C6	2.48	0.48
48:A:2334:G:H2'	48:A:2335:G:H5'	1.95	0.48
49:a:955:G:C2	49:a:956:A:C8	3.01	0.48
48:A:2500:U:C2	48:A:2501:U:C5	3.02	0.48
48:A:2782:C:HO2'	48:A:2783:U:H6	1.61	0.48
49:a:991:U:H5	49:a:992:U:HO2'	1.59	0.48
48:A:173:A:H2'	48:A:174:U:C6	2.48	0.48
48:A:278:A:H2'	48:A:279:A:H8	1.79	0.48
48:A:2406:G:H2'	48:A:2407:A:C8	2.49	0.48
15:J:159:THR:O	15:J:159:THR:HG22	2.13	0.48
26:V:39:THR:HG22	26:V:41:LYS:H	1.79	0.48
47:u:10:ARG:NE	49:a:106:G:O6	2.42	0.48
49:a:182:A:N1	49:a:184:A:C2	2.82	0.48
48:A:566:U:H2'	48:A:567:G:C8	2.49	0.48
48:A:1701:U:H2'	48:A:1702:C:H6	1.79	0.48
48:A:1782:A:H2'	48:A:1783:G:H5'	1.96	0.48
49:a:184:A:C8	49:a:185:U:C5	3.02	0.48
49:a:736:A:H2'	49:a:737:A:C8	2.49	0.48
49:a:1543:A:H2'	49:a:1544:U:C6	2.49	0.48
19:O:87:ASP:OD1	19:O:87:ASP:N	2.47	0.48
13:H:138:ARG:NH1	48:A:2024:A:OP2	2.47	0.47
48:A:1145:U:H2'	48:A:1146:C:C6	2.49	0.47
48:A:1891:U:OP1	48:A:2437:G:O2'	2.24	0.47
48:A:283:G:H3'	48:A:284:C:H4'	1.96	0.47
48:A:787:U:H2'	48:A:788:A:C8	2.48	0.47
48:A:877:G:H2'	48:A:878:C:C6	2.48	0.47
48:A:2334:G:OP2	48:A:2334:G:C8	2.67	0.47
48:A:2494:C:H2'	48:A:2495:A:O4'	2.14	0.47
49:a:1423:C:H2'	49:a:1424:A:C8	2.49	0.47
19:O:29:LYS:NZ	48:A:609:U:H5''	2.29	0.47
27:W:2:GLU:O	27:W:5:ASP:N	2.43	0.47
49:a:562:U:H2'	49:a:563:C:C6	2.50	0.47
49:a:1155:G:H2'	49:a:1156:C:C6	2.50	0.47
2:2:38:GLU:O	2:2:39:GLU:HG2	2.14	0.47
48:A:1131:G:N2	48:A:1147:A:H1'	2.29	0.47
48:A:1463:A:H2'	48:A:1465:G:N7	2.30	0.47
49:a:99:U:H2'	49:a:100:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:124:ILE:HD13	12:G:136:PRO:HD3	1.97	0.47
35:i:80:ILE:O	35:i:81:SER:OG	2.26	0.47
2:2:58:ARG:NH1	2:2:61:GLU:OE1	2.45	0.47
30:c:96:TRP:NE1	30:c:175:GLU:OE2	2.36	0.47
31:d:124:GLU:O	31:d:125:ASN:CG	2.58	0.47
47:u:6:SER:OG	49:a:106:G:N1	2.43	0.47
49:a:745:U:H2'	49:a:746:U:H6	1.79	0.47
15:J:136:LEU:CD1	15:J:146:VAL:HG21	2.45	0.47
36:j:9:ARG:NH2	49:a:1158:C:O4'	2.46	0.47
48:A:590:U:C4	48:A:1257:G:C2	3.02	0.47
48:A:979:C:H2'	48:A:980:U:C6	2.49	0.47
48:A:1104:U:C2	48:A:1106:G:O4'	2.68	0.47
13:H:156:MET:O	48:A:2079:G:H4'	2.15	0.47
16:K:94:TYR:CD2	16:K:107:VAL:HG13	2.50	0.47
47:u:10:ARG:HD2	49:a:107:G:C6	2.50	0.47
47:u:61:ALA:HB2	47:u:71:ALA:CB	2.45	0.47
48:A:280:C:H2'	48:A:281:A:H8	1.78	0.47
48:A:285:U:H4'	48:A:286:U:C6	2.50	0.47
48:A:702:U:H2'	48:A:703:A:C8	2.49	0.47
48:A:841:C:H2'	48:A:842:U:C6	2.49	0.47
48:A:1131:G:H2'	48:A:1132:A:H5''	1.96	0.47
49:a:1072:U:H2'	49:a:1073:G:H8	1.79	0.47
49:a:1168:A:C2	49:a:1192:G:C5	3.02	0.47
49:a:1325:C:H2'	49:a:1326:U:C6	2.49	0.47
49:a:1526:U:H2'	49:a:1527:C:C6	2.49	0.47
5:6:19:THR:HG22	5:6:20:THR:N	2.28	0.47
48:A:407:G:H2'	48:A:408:U:C6	2.50	0.47
49:a:363:C:C4	49:a:364:A:N7	2.82	0.47
49:a:886:A:H2'	49:a:887:C:C6	2.50	0.47
48:A:1131:G:C2'	48:A:1132:A:H5''	2.44	0.46
48:A:2372:G:N3	48:A:2408:C:H2'	2.30	0.46
49:a:988:A:C2	49:a:1330:A:C4	3.03	0.46
49:a:744:U:H2'	49:a:745:U:C6	2.49	0.46
9:B:42:G:C2	9:B:46:A:C2	3.03	0.46
11:D:20:G:H4'	11:D:21:U:OP2	2.15	0.46
26:V:82:LEU:HB2	26:V:98:LYS:HB2	1.97	0.46
28:Y:7:ILE:HG23	28:Y:41:VAL:HB	1.98	0.46
48:A:1453:G:H2'	48:A:1454:U:O4'	2.15	0.46
48:A:2584:G:H2'	48:A:2585:C:C6	2.50	0.46
48:A:2821:U:H1'	48:A:2823:G:O6	2.15	0.46
12:G:53:HIS:HA	12:G:217:ARG:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:1423:C:H2'	48:A:1424:A:C8	2.50	0.46
48:A:1580:A:O2'	48:A:1581:U:OP1	2.32	0.46
48:A:1754:C:H2'	48:A:1755:U:H6	1.79	0.46
49:a:345:G:H2'	49:a:346:A:C8	2.51	0.46
48:A:632:U:H2'	48:A:633:A:C8	2.51	0.46
48:A:830:U:H4'	48:A:1806:U:H4'	1.97	0.46
18:N:97:ARG:NH2	49:a:346:A:OP1	2.48	0.46
48:A:579:U:H2'	48:A:580:C:C6	2.51	0.46
48:A:2052:C:H2'	48:A:2053:U:C6	2.49	0.46
49:a:822:A:H5'	49:a:1523:G:H4'	1.97	0.46
33:f:106:ILE:HB	33:f:124:LEU:HD12	1.96	0.46
48:A:2431:C:H2'	48:A:2432:G:O4'	2.16	0.46
49:a:682:G:H2'	49:a:683:A:C8	2.50	0.46
49:a:742:A:H2'	49:a:743:C:C6	2.49	0.46
40:n:87:ARG:NH1	49:a:1320:G:OP1	2.49	0.46
48:A:2673:C:OP2	48:A:2759:G:O2'	2.33	0.46
49:a:1011:U:H5''	49:a:1012:U:OP2	2.15	0.46
32:e:13:ARG:CG	32:e:31:TYR:O	2.64	0.46
32:e:66:ARG:NH1	49:a:409:C:OP2	2.43	0.46
48:A:736:C:H2'	48:A:737:C:H6	1.81	0.46
48:A:2273:G:H2'	48:A:2274:A:C8	2.51	0.46
49:a:70:A:H2'	49:a:71:A:C8	2.51	0.46
49:a:653:G:C2	49:a:654:G:C8	3.03	0.46
49:a:1168:A:C2	49:a:1192:G:C4	3.03	0.46
17:M:31:SER:N	17:M:109:MET:HE1	2.31	0.46
48:A:637:U:H2'	48:A:638:U:C6	2.51	0.46
48:A:1315:C:H2'	48:A:1316:G:H8	1.80	0.46
48:A:1950:U:H2'	48:A:1951:C:C6	2.51	0.46
49:a:41:C:H2'	49:a:42:G:C8	2.49	0.46
50:h:70:MET:SD	50:h:96:ARG:HB3	2.55	0.46
14:I:41:ARG:HG3	14:I:41:ARG:HH11	1.80	0.45
48:A:1137:G:C2	48:A:1143:G:O6	2.69	0.45
49:a:1316:G:N2	49:a:1342:G:H1'	2.31	0.45
49:a:1438:C:H2'	49:a:1439:A:C8	2.51	0.45
13:H:194:VAL:HG21	23:S:6:LEU:HD21	1.97	0.45
23:S:80:THR:HG22	23:S:82:LYS:H	1.81	0.45
31:d:46:LEU:HD22	31:d:51:VAL:HG21	1.98	0.45
32:e:13:ARG:HD3	32:e:31:TYR:O	2.17	0.45
34:g:76:PHE:CD1	34:g:76:PHE:C	2.94	0.45
49:a:1548:C:H2'	49:a:1549:U:C6	2.51	0.45
47:u:45:ASN:HB3	47:u:49:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:2772:C:H2'	48:A:2773:U:C6	2.51	0.45
49:a:1138:U:O2	49:a:1291:A:H2'	2.15	0.45
48:A:307:A:C6	48:A:409:G:C6	3.04	0.45
48:A:923:A:HO2'	48:A:924:G:C5'	2.29	0.45
48:A:1489:A:H62	48:A:1504:U:H2'	1.82	0.45
48:A:1806:U:OP2	48:A:1811:A:N6	2.46	0.45
49:a:51:A:O2'	49:a:368:G:N2	2.48	0.45
4:5:40:HIS:ND1	48:A:2835:C:O2'	2.39	0.45
17:M:77:ARG:NH1	48:A:2668:A:OP1	2.46	0.45
18:N:102:VAL:HG11	18:N:106:LEU:HD12	1.98	0.45
27:W:57:ASN:OD1	27:W:76:ARG:NH1	2.49	0.45
31:d:46:LEU:HD13	31:d:51:VAL:HB	1.99	0.45
48:A:1813:A:H1'	48:A:1965:A:N6	2.31	0.45
48:A:2570:G:H2'	48:A:2571:G:C8	2.52	0.45
49:a:682:G:H2'	49:a:683:A:H8	1.82	0.45
49:a:902:A:H2'	49:a:903:C:C6	2.51	0.45
4:5:27:MET:HE2	26:V:38:LEU:HD22	1.98	0.45
17:M:77:ARG:HH12	48:A:2668:A:P	2.40	0.45
22:R:86:ASP:C	22:R:86:ASP:OD1	2.57	0.45
36:j:124:ARG:HD2	49:a:1359:U:H4'	1.98	0.45
48:A:903:G:N3	48:A:2295:A:H2'	2.32	0.45
49:a:57:U:H2'	49:a:58:G:H8	1.82	0.45
13:H:154:VAL:HG12	13:H:154:VAL:O	2.17	0.45
13:H:158:SER:OG	48:A:2599:A:N7	2.36	0.45
23:S:33:ARG:NH1	23:S:84:GLU:OE2	2.46	0.45
48:A:344:U:C2	48:A:345:C:C5	3.04	0.45
48:A:1178:C:O2'	48:A:1179:C:H5'	2.15	0.45
48:A:1870:C:H2'	48:A:1871:U:H6	1.82	0.45
49:a:609:G:H2'	49:a:610:A:H8	1.81	0.45
14:I:53:ASN:ND2	48:A:846:G:O6	2.43	0.45
32:e:14:ARG:CD	32:e:33:PRO:HD2	2.47	0.45
48:A:1013:U:H2'	48:A:1014:U:C6	2.52	0.45
48:A:1105:U:O4'	48:A:1114:A:H4'	2.16	0.45
49:a:1390:G:N2	49:a:1392:U:O4	2.44	0.45
17:M:2:ARG:N	48:A:1039:C:C2	2.85	0.45
35:i:20:VAL:HG12	35:i:20:VAL:O	2.17	0.45
48:A:2541:U:H2'	48:A:2542:C:C6	2.52	0.45
24:T:76:TYR:CZ	24:T:80:MET:HG3	2.52	0.45
35:i:55:ASP:OD1	35:i:56:LYS:N	2.49	0.45
48:A:1178:C:O2'	48:A:1179:C:C5'	2.65	0.45
48:A:1869:G:H2'	48:A:1870:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:2231:C:H2'	48:A:2232:A:C8	2.52	0.45
48:A:2810:A:H2'	48:A:2811:U:C6	2.52	0.45
48:A:2818:A:H2'	48:A:2819:C:C6	2.52	0.45
48:A:2842:G:H2'	48:A:2843:A:H5''	1.99	0.45
8:9:8:LYS:NZ	48:A:2494:C:OP1	2.43	0.44
31:d:42:ILE:O	31:d:46:LEU:HG	2.16	0.44
31:d:46:LEU:HD22	31:d:51:VAL:HB	1.98	0.44
48:A:2836:C:O2	48:A:2903:A:O2'	2.32	0.44
49:a:138:A:H2'	49:a:139:U:C6	2.51	0.44
5:6:19:THR:CG2	5:6:20:THR:N	2.80	0.44
17:M:31:SER:HA	17:M:109:MET:CE	2.47	0.44
37:k:55:VAL:HG23	37:k:56:HIS:N	2.32	0.44
48:A:2348:G:H5''	48:A:2349:A:OP2	2.17	0.44
49:a:1288:C:O2'	49:a:1290:A:C8	2.71	0.44
2:2:26:PHE:CE2	27:W:45:ILE:HD11	2.52	0.44
30:c:54:TYR:CD2	30:c:220:ALA:HB2	2.52	0.44
48:A:1680:U:H2'	48:A:1681:U:C6	2.53	0.44
48:A:2406:G:H2'	48:A:2407:A:H8	1.82	0.44
48:A:2673:C:H6	48:A:2673:C:O5'	2.01	0.44
49:a:1177:G:O2'	49:a:1180:A:N6	2.51	0.44
49:a:1524:U:H2'	49:a:1525:A:C8	2.52	0.44
13:H:44:ASP:N	13:H:44:ASP:OD1	2.47	0.44
22:R:35:ARG:HG2	22:R:35:ARG:HH11	1.82	0.44
48:A:1092:A:N7	48:A:1155:A:C6	2.85	0.44
48:A:1128:A:H2'	48:A:1129:A:C6	2.52	0.44
48:A:1277:C:H2'	48:A:1278:G:N3	2.33	0.44
48:A:1476:G:H2'	48:A:1477:U:C6	2.52	0.44
48:A:1780:G:N2	48:A:1783:G:OP2	2.40	0.44
49:a:109:C:H2'	49:a:110:G:O4'	2.18	0.44
49:a:381:A:C2	49:a:382:A:C8	3.05	0.44
30:c:70:VAL:HG12	30:c:70:VAL:O	2.18	0.44
48:A:858:U:H2'	48:A:859:C:C6	2.53	0.44
48:A:1112:G:N3	48:A:1139:A:O2'	2.47	0.44
48:A:1869:G:H2'	48:A:1870:C:H6	1.82	0.44
49:a:345:G:H2'	49:a:346:A:H8	1.82	0.44
49:a:485:U:H2'	49:a:486:C:H6	1.82	0.44
34:g:28:GLY:O	34:g:32:THR:HG23	2.18	0.44
48:A:838:A:OP2	48:A:2098:A:O2'	2.36	0.44
48:A:884:U:H2'	48:A:885:C:C6	2.52	0.44
48:A:2548:C:C2	48:A:2572:G:N2	2.86	0.44
49:a:469:U:H2'	49:a:470:A:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:1297:U:C6	49:a:1297:U:O5'	2.69	0.44
2:2:30:PHE:CZ	27:W:10:PRO:HB3	2.53	0.44
26:V:31:GLU:O	26:V:35:ILE:HG12	2.17	0.44
41:o:24:CYS:SG	41:o:25:GLU:N	2.91	0.44
45:s:38:ILE:HG22	45:s:39:SER:O	2.17	0.44
48:A:1455:U:H1'	48:A:1456:U:C2	2.52	0.44
48:A:1806:U:H5	48:A:1811:A:N7	2.16	0.44
49:a:152:A:N6	49:a:170:U:C2	2.85	0.44
9:B:39:G:H3'	9:B:40:C:H5'	2.00	0.44
26:V:99:ARG:NH1	48:A:1300:G:OP1	2.48	0.44
32:e:77:LYS:NZ	49:a:622:A:OP2	2.44	0.44
48:A:2367:A:H2'	48:A:2368:G:C8	2.52	0.44
49:a:918:A:H2'	49:a:919:A:C8	2.53	0.44
9:B:37:A:C2	9:B:42:G:N3	2.86	0.44
13:H:156:MET:SD	48:A:2598:U:O2	2.76	0.44
15:J:22:TYR:OH	15:J:165:GLU:OE2	2.29	0.44
22:R:42:ALA:HB3	22:R:80:ILE:CD1	2.48	0.44
42:p:73:LYS:NZ	49:a:760:G:OP1	2.51	0.44
48:A:2097:G:H2'	48:A:2098:A:C8	2.53	0.44
49:a:352:A:H4'	49:a:353:C:OP2	2.18	0.44
49:a:960:U:H2'	49:a:961:G:H8	1.82	0.44
41:o:24:CYS:HB3	41:o:27:CYS:O	2.18	0.43
17:M:92:GLU:OE2	17:M:95:ARG:NH2	2.51	0.43
20:P:51:ARG:HG3	20:P:66:ILE:HD11	2.00	0.43
27:W:19:ALA:HB1	27:W:24:LYS:HB2	2.00	0.43
48:A:164:A:O2'	48:A:165:C:O5'	2.36	0.43
48:A:307:A:N1	48:A:409:G:C6	2.86	0.43
48:A:526:A:N3	48:A:526:A:H2'	2.32	0.43
49:a:200:U:H2'	49:a:201:U:C6	2.53	0.43
49:a:976:G:H2'	49:a:977:C:C6	2.54	0.43
49:a:1505:A:C8	49:a:1505:A:O5'	2.71	0.43
48:A:1938:U:H4'	48:A:1939:A:OP1	2.18	0.43
48:A:1942:U:C6	48:A:1943:A:C2	3.06	0.43
49:a:547:A:H2'	49:a:548:G:C8	2.52	0.43
49:a:609:G:C6	49:a:646:G:C6	3.05	0.43
49:a:643:A:H2'	49:a:644:U:C6	2.54	0.43
48:A:1580:A:C2	48:A:1585:G:C5	3.07	0.43
49:a:561:A:H2'	49:a:562:U:C6	2.54	0.43
49:a:1082:U:H2'	49:a:1083:C:C6	2.53	0.43
36:j:49:ASP:OD1	50:h:13:LEU:HD12	2.18	0.43
36:j:97:ARG:NH2	49:a:1189:G:OP1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:o:3:LYS:NZ	49:a:1214:C:OP1	2.44	0.43
48:A:3:U:H2'	48:A:4:U:C6	2.54	0.43
48:A:287:G:C8	48:A:288:C:C2	3.06	0.43
48:A:1507:A:H2'	48:A:1508:C:C6	2.53	0.43
49:a:1054:U:H2'	49:a:1055:G:C8	2.54	0.43
9:B:60:C:C2	9:B:61:C:C5	3.07	0.43
18:N:22:ILE:HD12	48:A:1979:A:C4	2.54	0.43
32:e:14:ARG:HD2	32:e:33:PRO:HD2	2.00	0.43
48:A:625:G:H2'	48:A:626:G:C8	2.54	0.43
48:A:1269:A:H2'	48:A:1270:U:C6	2.53	0.43
48:A:2729:G:C2	48:A:2730:C:C6	3.07	0.43
49:a:715:U:H2'	49:a:716:A:H8	1.83	0.43
5:6:2:ARG:CZ	48:A:2312:C:C5	3.02	0.43
44:r:67:ARG:NH1	49:a:197:U:O2	2.52	0.43
48:A:2268:A:H2'	48:A:2269:G:C8	2.54	0.43
49:a:138:A:H2'	49:a:139:U:H6	1.84	0.43
49:a:521:A:H2'	49:a:522:C:H6	1.84	0.43
49:a:622:A:H2'	49:a:623:C:C6	2.53	0.43
49:a:1397:G:H2'	49:a:1398:G:H8	1.83	0.43
49:a:1438:C:H2'	49:a:1439:A:H8	1.83	0.43
16:K:57:ASP:O	16:K:62:ARG:NH1	2.43	0.43
16:K:94:TYR:CG	16:K:107:VAL:HG13	2.53	0.43
27:W:31:THR:O	27:W:32:ARG:HG2	2.19	0.43
37:k:85:ASP:HA	37:k:88:MET:HG2	2.00	0.43
49:a:677:A:H2'	49:a:678:A:C8	2.54	0.43
15:J:134:GLU:CG	15:J:137:ILE:HG23	2.49	0.43
48:A:1768:C:H2'	48:A:1769:C:H6	1.83	0.43
48:A:2084:G:H2'	48:A:2085:MA6:H8	2.00	0.43
49:a:944:C:C4	49:a:1356:U:C5	3.07	0.43
49:a:1153:G:H2'	49:a:1154:G:C8	2.54	0.43
49:a:1173:C:H2'	49:a:1174:G:H8	1.83	0.43
49:a:1288:C:H2'	49:a:1289:A:H5''	2.01	0.43
49:a:1416:G:O4'	49:a:1531:A:H4'	2.19	0.43
22:R:11:ARG:HD2	22:R:99:TYR:CZ	2.54	0.43
27:W:29:VAL:HG12	27:W:30:ASP:N	2.34	0.43
48:A:895:U:H2'	48:A:896:U:C6	2.54	0.43
48:A:2617:A:H2'	48:A:2618:C:C6	2.53	0.43
49:a:144:C:C2	49:a:179:A:C2	3.07	0.43
49:a:562:U:H2'	49:a:563:C:H6	1.83	0.43
37:k:56:HIS:O	37:k:56:HIS:CG	2.72	0.42
48:A:153:G:O2'	48:A:154:A:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:12:ARG:NH2	48:A:2049:U:OP2	2.51	0.42
13:H:22:LEU:C	13:H:22:LEU:HD23	2.44	0.42
27:W:61:LYS:HD3	48:A:1376:G:O6	2.18	0.42
32:e:185:LEU:HB3	32:e:186:PRO:HD2	2.01	0.42
48:A:1477:U:H2'	48:A:1478:A:C8	2.54	0.42
49:a:1171:G:C2	49:a:1172:C:C6	3.07	0.42
49:a:1508:C:H2'	49:a:1509:G:C8	2.53	0.42
15:J:102:LYS:CE	51:4:26:GLY:O	2.68	0.42
23:S:6:LEU:C	23:S:6:LEU:HD23	2.44	0.42
44:r:56:LYS:N	44:r:59:ASP:OD2	2.43	0.42
45:s:57:GLN:O	45:s:61:THR:HG23	2.19	0.42
48:A:1072:A:N6	48:A:1169:G:H2'	2.34	0.42
48:A:1129:A:H2'	48:A:1130:A:C2	2.54	0.42
49:a:209:G:C5	49:a:210:A:N6	2.87	0.42
49:a:1334:G:H2'	49:a:1335:A:C8	2.54	0.42
4:5:27:MET:CE	26:V:35:ILE:HD13	2.48	0.42
13:H:53:PHE:CG	13:H:54:GLU:N	2.87	0.42
35:i:80:ILE:HG22	35:i:81:SER:N	2.33	0.42
37:k:57:LYS:HB3	37:k:58:TYR:CD2	2.54	0.42
42:p:22:THR:O	49:a:758:C:H1'	2.19	0.42
48:A:1212:U:H2'	48:A:1213:C:C6	2.55	0.42
48:A:1829:A:H2'	48:A:1830:A:C8	2.54	0.42
48:A:2051:C:H2'	48:A:2052:C:H6	1.85	0.42
49:a:358:G:H2'	49:a:359:G:C8	2.55	0.42
49:a:1024:A:H2'	49:a:1025:G:C8	2.54	0.42
49:a:1182:A:H2'	49:a:1183:C:C6	2.55	0.42
48:A:901:G:H2'	48:A:902:A:H8	1.82	0.42
48:A:1531:U:H2'	48:A:1532:U:C6	2.54	0.42
48:A:2260:A:H2'	48:A:2261:G:C8	2.55	0.42
49:a:65:G:C5	49:a:99:U:O4	2.73	0.42
49:a:155:U:H2'	49:a:156:C:H6	1.84	0.42
49:a:612:G:C6	49:a:643:A:C6	3.07	0.42
46:t:44:PHE:CD1	46:t:44:PHE:N	2.87	0.42
48:A:221:G:H22	48:A:238:U:H4'	1.84	0.42
48:A:287:G:H3'	48:A:288:C:C6	2.54	0.42
48:A:1513:A:H2'	48:A:1514:A:C8	2.55	0.42
48:A:2342:U:H2'	48:A:2343:U:C6	2.53	0.42
49:a:315:U:H2'	49:a:316:C:C6	2.55	0.42
49:a:928:A:H2'	49:a:929:A:C8	2.54	0.42
12:G:156:ARG:NH2	48:A:1845:U:OP2	2.48	0.42
17:M:136:GLN:C	17:M:137:GLN:HG2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:g:7:MET:HE3	45:s:70:MET:CE	2.50	0.42
35:i:106:VAL:HA	35:i:126:GLU:O	2.20	0.42
48:A:153:G:O2'	48:A:154:A:H2'	2.20	0.42
48:A:460:C:H2'	48:A:461:A:C8	2.54	0.42
48:A:1583:G:N3	48:A:1583:G:H2'	2.35	0.42
48:A:2270:U:H2'	48:A:2271:U:H6	1.84	0.42
49:a:598:U:H2'	49:a:599:U:C6	2.54	0.42
48:A:224:A:C4	48:A:269:G:N7	2.87	0.42
48:A:665:G:N3	48:A:665:G:H5'	2.35	0.42
49:a:57:U:H2'	49:a:58:G:C8	2.55	0.42
49:a:70:A:H2'	49:a:71:A:H8	1.85	0.42
49:a:716:A:H2'	49:a:717:U:C6	2.54	0.42
49:a:789:A:H5'	49:a:790:A:OP2	2.20	0.42
49:a:918:A:H2'	49:a:919:A:H8	1.85	0.42
9:B:39:G:O2'	9:B:40:C:OP1	2.34	0.42
20:P:11:ARG:NH1	48:A:2305:A:OP1	2.49	0.42
38:l:118:HIS:NE2	49:a:726:A:C5	2.88	0.42
45:s:61:THR:CG2	49:a:728:C:O2'	2.68	0.42
48:A:222:A:N3	48:A:237:U:O2'	2.49	0.42
48:A:262:G:H21	48:A:666:A:H8	1.67	0.42
48:A:1423:C:H2'	48:A:1424:A:H8	1.85	0.42
48:A:2335:G:O2'	48:A:2336:A:C5	2.73	0.42
49:a:272:C:H2'	49:a:273:G:O4'	2.20	0.42
49:a:476:C:H2'	49:a:477:U:C6	2.55	0.42
49:a:1064:U:O2'	49:a:1067:A:OP2	2.35	0.42
17:M:50:ASP:O	17:M:50:ASP:CG	2.63	0.42
19:O:21:ARG:HA	48:A:856:U:H2'	2.01	0.42
29:Z:39:VAL:CG2	29:Z:43:SER:HB2	2.50	0.42
34:g:45:LYS:NZ	34:g:57:ASP:OD2	2.45	0.42
48:A:1898:C:OP2	48:A:1899:U:C4	2.72	0.42
48:A:2070:C:C2	48:A:2071:C:C5	3.08	0.42
48:A:2087:A:HO2'	48:A:2088:G:P	2.42	0.42
48:A:2091:C:H2'	48:A:2092:C:H6	1.81	0.42
48:A:2367:A:H2'	48:A:2368:G:H8	1.84	0.42
49:a:466:G:C6	49:a:484:A:C6	3.07	0.42
49:a:547:A:H2'	49:a:548:G:H8	1.84	0.42
49:a:836:A:H2'	49:a:837:A:O4'	2.20	0.42
49:a:1137:U:O2	49:a:1138:U:O2'	2.31	0.42
3:3:3:LYS:NZ	3:3:38:GLU:OE2	2.43	0.41
15:J:136:LEU:HD12	15:J:143:TYR:CB	2.50	0.41
20:P:83:MET:HE1	48:A:1000:G:C4'	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Z:22:ARG:NH1	48:A:2306:G:O6	2.50	0.41
31:d:53:HIS:CE1	31:d:68:HIS:CD2	3.08	0.41
33:f:112:ARG:NH2	33:f:116:GLU:OE2	2.53	0.41
39:m:115:LEU:HD12	39:m:115:LEU:N	2.35	0.41
48:A:890:G:O5'	48:A:890:G:H8	2.03	0.41
48:A:945:A:H2'	48:A:946:A:O4'	2.20	0.41
48:A:2084:G:O6	48:A:2085:MA6:H102	2.20	0.41
49:a:1337:U:H2'	49:a:1338:A:H8	1.85	0.41
11:D:65:C:H2'	11:D:66:C:H6	1.84	0.41
48:A:1092:A:C5	48:A:1093:C:C5	3.08	0.41
48:A:1884:G:H5''	48:A:1885:G:OP2	2.20	0.41
49:a:728:C:H5'	49:a:729:A:OP2	2.21	0.41
49:a:1457:A:N6	49:a:1458:A:N6	2.67	0.41
11:D:9:G:C2	11:D:47:G:C6	3.08	0.41
48:A:217:G:H2'	48:A:218:G:O4'	2.20	0.41
48:A:1457:U:C3'	48:A:1458:A:O4'	2.68	0.41
48:A:1800:A:N7	48:A:1856:A:H1'	2.35	0.41
48:A:2085:MA6:H102	48:A:2638:C:H42	1.85	0.41
49:a:277:U:H2'	49:a:278:A:H8	1.86	0.41
49:a:583:G:O2'	49:a:829:G:OP2	2.30	0.41
49:a:756:A:O2'	49:a:757:A:OP2	2.33	0.41
49:a:839:U:O2'	49:a:1551:C:OP1	2.35	0.41
49:a:1220:C:C2	49:a:1221:C:C5	3.08	0.41
49:a:1299:A:H2'	49:a:1300:A:O4'	2.20	0.41
7:8:12:LYS:NZ	48:A:252:C:O2	2.49	0.41
16:K:105:LEU:HB3	16:K:107:VAL:HG23	2.01	0.41
36:j:90:LEU:HD11	36:j:106:LEU:CD1	2.50	0.41
48:A:307:A:C6	48:A:308:C:C4	3.07	0.41
49:a:442:C:H2'	49:a:443:U:C6	2.55	0.41
49:a:672:G:H22	49:a:749:G:H1	1.68	0.41
49:a:1151:U:C2	49:a:1152:U:C5	3.09	0.41
29:Z:28:ARG:HG3	48:A:2383:C:H4'	2.01	0.41
44:r:9:VAL:HG21	44:r:62:LYS:HE3	2.01	0.41
46:t:44:PHE:N	46:t:44:PHE:HD1	2.18	0.41
48:A:1455:U:H4'	48:A:1457:U:N1	2.35	0.41
49:a:1428:G:C6	49:a:1494:G:C6	3.08	0.41
9:B:86:A:H3'	9:B:87:C:C5'	2.50	0.41
15:J:71:LYS:NZ	48:A:2340:C:OP2	2.40	0.41
22:R:56:ALA:HB3	22:R:80:ILE:CG1	2.51	0.41
24:T:76:TYR:CD1	24:T:76:TYR:C	2.97	0.41
26:V:10:ILE:HD13	26:V:46:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:l:29:ASN:ND2	49:a:698:G:OP2	2.44	0.41
45:s:23:ILE:O	45:s:23:ILE:HG23	2.20	0.41
48:A:160:G:H21	48:A:168:A:H2	1.68	0.41
49:a:960:U:H2'	49:a:961:G:C8	2.55	0.41
49:a:985:A:N6	49:a:1378:U:O4'	2.53	0.41
49:a:1018:C:H2'	49:a:1019:U:H6	1.84	0.41
49:a:1270:C:H3'	49:a:1271:G:H5''	2.01	0.41
49:a:1278:C:H6	49:a:1278:C:O5'	2.03	0.41
49:a:1319:U:H2'	49:a:1320:G:H8	1.86	0.41
7:8:31:HIS:CE1	48:A:2448:G:N7	2.89	0.41
14:I:177:THR:HG22	14:I:178:ALA:N	2.35	0.41
48:A:218:G:H4'	48:A:219:A:H4'	2.03	0.41
48:A:892:U:C5	48:A:977:A:N1	2.89	0.41
48:A:1213:C:H2'	48:A:1214:C:C6	2.56	0.41
48:A:1453:G:H4'	48:A:1458:A:O2'	2.21	0.41
49:a:1498:G:H2'	49:a:1499:G:C8	2.55	0.41
11:D:17:U:H5''	11:D:62:C:H5'	2.03	0.41
11:D:27:G:C5	11:D:28:U:C5	3.09	0.41
48:A:625:G:H2'	48:A:626:G:H8	1.85	0.41
48:A:734:A:H2'	48:A:735:C:C6	2.56	0.41
48:A:991:A:H2'	48:A:992:A:C8	2.56	0.41
48:A:1028:G:N3	48:A:1028:G:H2'	2.35	0.41
48:A:1105:U:H4'	48:A:1106:G:OP2	2.20	0.41
49:a:460:A:H2'	49:a:461:C:C4'	2.51	0.41
49:a:1169:C:C5	49:a:1171:G:H1'	2.56	0.41
49:a:1446:G:H2'	49:a:1447:C:H6	1.85	0.41
7:8:13:ARG:NH1	19:O:61:LEU:O	2.44	0.41
13:H:6:LEU:H	13:H:33:ASN:ND2	2.19	0.41
21:Q:103:ILE:HG23	21:Q:117:VAL:HG21	2.03	0.41
31:d:43:ASP:HA	31:d:46:LEU:HG	2.03	0.41
31:d:46:LEU:HD22	31:d:51:VAL:CG2	2.51	0.41
32:e:108:ARG:NH2	49:a:415:A:OP1	2.43	0.41
41:o:18:VAL:HG11	49:a:1327:G:H4'	2.03	0.41
44:r:14:VAL:HG13	44:r:23:ILE:CG2	2.50	0.41
48:A:688:A:N1	48:A:2396:A:O2'	2.52	0.41
48:A:2090:C:O2	48:A:2477:A:N1	2.54	0.41
48:A:2457:A:N3	48:A:2457:A:H2'	2.35	0.41
48:A:2609:G:H5'	48:A:2609:G:C8	2.56	0.41
48:A:2663:U:H2'	48:A:2664:U:C6	2.56	0.41
49:a:321:A:H2'	49:a:322:C:C6	2.56	0.41
49:a:563:C:H2'	49:a:564:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:996:A:H2'	49:a:997:A:C8	2.56	0.41
49:a:1022:A:N6	49:a:1028:A:N6	2.69	0.41
49:a:1132:C:C2	49:a:1133:U:C5	3.08	0.41
9:B:37:A:C2	9:B:42:G:C2	3.09	0.41
18:N:21:THR:HG22	18:N:22:ILE:N	2.34	0.41
30:c:29:LYS:HE3	30:c:30:TYR:CZ	2.56	0.41
38:l:36:ASP:C	38:l:36:ASP:OD1	2.64	0.41
48:A:1081:G:H2'	48:A:1082:C:C6	2.56	0.41
48:A:2482:G:H2'	48:A:2483:C:C6	2.56	0.41
48:A:2705:U:H2'	48:A:2706:A:C8	2.55	0.41
48:A:2878:U:O5'	48:A:2878:U:H6	2.04	0.41
49:a:431:G:H5'	49:a:432:G:OP2	2.21	0.41
49:a:534:C:H5''	49:a:535:G:OP2	2.20	0.41
49:a:1366:A:H2'	49:a:1367:G:C8	2.56	0.41
49:a:1526:U:H2'	49:a:1527:C:H6	1.85	0.41
5:6:32:MET:HE2	48:A:2371:U:O2'	2.21	0.40
9:B:4:G:H2'	9:B:5:G:H8	1.86	0.40
46:t:55:ARG:NH2	49:a:968:A:N7	2.69	0.40
48:A:679:G:H2'	48:A:680:C:C6	2.56	0.40
48:A:1068:G:C6	48:A:1069:G:C6	3.09	0.40
48:A:1115:G:C4	48:A:1133:G:H2'	2.56	0.40
48:A:1214:C:H3'	48:A:1215:U:C6	2.56	0.40
48:A:1701:U:H2'	48:A:1702:C:C6	2.56	0.40
49:a:39:G:H22	49:a:405:A:H5'	1.86	0.40
49:a:277:U:H2'	49:a:278:A:C8	2.57	0.40
49:a:482:A:H2'	49:a:483:C:C6	2.56	0.40
49:a:601:U:H2'	49:a:602:U:H6	1.84	0.40
49:a:731:U:O2	49:a:731:U:H2'	2.21	0.40
49:a:1051:A:H2'	49:a:1052:A:C8	2.56	0.40
49:a:1206:C:H5''	49:a:1207:A:OP2	2.21	0.40
49:a:1299:A:H2'	49:a:1300:A:C8	2.56	0.40
14:I:181:LEU:HG	14:I:186:ILE:HD11	2.03	0.40
48:A:224:A:C8	48:A:269:G:O6	2.74	0.40
48:A:280:C:H2'	48:A:281:A:C8	2.56	0.40
48:A:501:C:H3'	48:A:502:C:H5''	2.03	0.40
48:A:651:A:H2'	48:A:652:A:C8	2.57	0.40
48:A:1112:G:C4	48:A:1139:A:O2'	2.74	0.40
48:A:1570:G:H2'	48:A:1571:G:C8	2.56	0.40
49:a:108:A:C6	49:a:334:G:C6	3.09	0.40
49:a:160:A:H2'	49:a:161:A:O4'	2.21	0.40
49:a:461:C:H2'	49:a:462:A:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:470:A:C6	49:a:480:G:C6	3.08	0.40
49:a:1023:G:N2	49:a:1026:A:OP2	2.41	0.40
49:a:1186:G:H2'	49:a:1187:A:H8	1.86	0.40
49:a:1392:U:C5	49:a:1393:C:C5	3.10	0.40
13:H:13:THR:HG21	23:S:7:ILE:HG23	2.03	0.40
20:P:58:MET:O	20:P:59:LYS:C	2.64	0.40
26:V:10:ILE:HD13	26:V:46:VAL:CG1	2.52	0.40
26:V:47:ILE:HA	26:V:50:VAL:HG12	2.03	0.40
30:c:188:ASP:OD1	30:c:189:THR:N	2.53	0.40
31:d:46:LEU:HD22	31:d:51:VAL:CB	2.51	0.40
44:r:47:LYS:NZ	49:a:285:C:OP1	2.46	0.40
48:A:59:U:O2'	48:A:74:U:OP2	2.34	0.40
48:A:730:A:C8	48:A:818:U:C4	3.10	0.40
49:a:560:U:N3	49:a:561:A:N7	2.69	0.40
49:a:885:C:C4	49:a:886:A:N7	2.90	0.40
7:8:26:ARG:HG2	7:8:26:ARG:HH11	1.86	0.40
15:J:126:GLY:O	15:J:158:THR:OG1	2.31	0.40
38:l:35:THR:HG22	38:l:41:ALA:HA	2.03	0.40
48:A:345:C:H2'	48:A:346:A:H8	1.86	0.40
48:A:1086:G:C5	48:A:1087:C:C5	3.10	0.40
48:A:1806:U:C5	48:A:1811:A:N7	2.90	0.40
49:a:147:G:H2'	49:a:148:G:C8	2.56	0.40
49:a:572:U:O2	49:a:572:U:O5'	2.39	0.40
49:a:1016:A:N7	49:a:1017:A:C4	2.90	0.40
49:a:1026:A:O2'	49:a:1228:U:O2'	2.28	0.40
9:B:60:C:N3	9:B:61:C:C5	2.89	0.40
10:C:83:TYR:CD1	10:C:90:LYS:HE2	2.57	0.40
20:P:42:ILE:CD1	20:P:97:VAL:HG21	2.51	0.40
21:Q:100:TYR:O	21:Q:122:VAL:N	2.52	0.40
48:A:1000:G:H2'	48:A:1001:A:H2'	2.04	0.40
48:A:1627:G:C2	48:A:1628:A:C8	3.10	0.40
49:a:199:G:C6	49:a:200:U:C4	3.10	0.40
49:a:370:G:N2	49:a:373:U:OP2	2.53	0.40
49:a:414:G:C2'	49:a:415:A:H5'	2.51	0.40
49:a:1249:A:N7	49:a:1314:C:H1'	2.37	0.40
49:a:1420:C:H2'	49:a:1421:A:C8	2.57	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	
1	1	57/62 (92%)	57 (100%)	0	0	100	100
2	2	62/69 (90%)	62 (100%)	0	0	100	100
3	3	54/59 (92%)	54 (100%)	0	0	100	100
4	5	51/57 (90%)	50 (98%)	1 (2%)	0	100	100
5	6	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
6	7	40/45 (89%)	40 (100%)	0	0	100	100
7	8	62/66 (94%)	62 (100%)	0	0	100	100
8	9	34/37 (92%)	34 (100%)	0	0	100	100
10	C	97/105 (92%)	96 (99%)	1 (1%)	0	100	100
12	G	271/277 (98%)	265 (98%)	6 (2%)	0	100	100
13	H	214/220 (97%)	204 (95%)	10 (5%)	0	100	100
14	I	202/207 (98%)	202 (100%)	0	0	100	100
15	J	173/179 (97%)	164 (95%)	9 (5%)	0	100	100
16	K	162/178 (91%)	157 (97%)	5 (3%)	0	100	100
17	M	140/145 (97%)	137 (98%)	3 (2%)	0	100	100
18	N	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
19	O	143/146 (98%)	142 (99%)	1 (1%)	0	100	100
20	P	133/144 (92%)	132 (99%)	1 (1%)	0	100	100
21	Q	118/122 (97%)	117 (99%)	1 (1%)	0	100	100
22	R	116/119 (98%)	114 (98%)	2 (2%)	0	100	100
23	S	112/116 (97%)	112 (100%)	0	0	100	100
24	T	114/118 (97%)	114 (100%)	0	0	100	100
25	U	99/102 (97%)	96 (97%)	3 (3%)	0	100	100
26	V	109/117 (93%)	108 (99%)	1 (1%)	0	100	100
27	W	87/91 (96%)	87 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Y	92/217 (42%)	92 (100%)	0	0	100	100
29	Z	76/94 (81%)	76 (100%)	0	0	100	100
30	c	219/255 (86%)	215 (98%)	4 (2%)	0	100	100
31	d	200/217 (92%)	198 (99%)	2 (1%)	0	100	100
32	e	197/200 (98%)	197 (100%)	0	0	100	100
33	f	154/166 (93%)	153 (99%)	1 (1%)	0	100	100
34	g	91/98 (93%)	90 (99%)	1 (1%)	0	100	100
35	i	129/132 (98%)	127 (98%)	2 (2%)	0	100	100
36	j	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
37	k	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
38	l	116/129 (90%)	115 (99%)	1 (1%)	0	100	100
39	m	133/137 (97%)	131 (98%)	2 (2%)	0	100	100
40	n	111/121 (92%)	111 (100%)	0	0	100	100
41	o	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
42	p	84/89 (94%)	82 (98%)	2 (2%)	0	100	100
43	q	88/91 (97%)	88 (100%)	0	0	100	100
44	r	77/87 (88%)	75 (97%)	2 (3%)	0	100	100
45	s	61/80 (76%)	61 (100%)	0	0	100	100
46	t	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
47	u	78/83 (94%)	78 (100%)	0	0	100	100
50	h	144/156 (92%)	143 (99%)	1 (1%)	0	100	100
51	4	53/84 (63%)	51 (96%)	2 (4%)	0	100	100
All	All	5278/5773 (91%)	5199 (98%)	79 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	49/52 (94%)	49 (100%)	0	100	100
2	2	58/62 (94%)	58 (100%)	0	100	100
3	3	51/53 (96%)	51 (100%)	0	100	100
4	5	48/50 (96%)	48 (100%)	0	100	100
5	6	45/47 (96%)	45 (100%)	0	100	100
6	7	38/40 (95%)	38 (100%)	0	100	100
7	8	55/57 (96%)	55 (100%)	0	100	100
8	9	35/35 (100%)	35 (100%)	0	100	100
10	C	84/90 (93%)	84 (100%)	0	100	100
12	G	220/224 (98%)	220 (100%)	0	100	100
13	H	174/177 (98%)	174 (100%)	0	100	100
14	I	168/169 (99%)	168 (100%)	0	100	100
15	J	154/158 (98%)	154 (100%)	0	100	100
16	K	144/155 (93%)	144 (100%)	0	100	100
17	M	121/123 (98%)	121 (100%)	0	100	100
18	N	100/100 (100%)	100 (100%)	0	100	100
19	O	111/112 (99%)	111 (100%)	0	100	100
20	P	112/119 (94%)	112 (100%)	0	100	100
21	Q	101/102 (99%)	101 (100%)	0	100	100
22	R	94/95 (99%)	94 (100%)	0	100	100
23	S	100/102 (98%)	100 (100%)	0	100	100
24	T	96/98 (98%)	95 (99%)	1 (1%)	68	83
25	U	86/86 (100%)	86 (100%)	0	100	100
26	V	90/94 (96%)	90 (100%)	0	100	100
27	W	80/82 (98%)	80 (100%)	0	100	100
28	Y	83/190 (44%)	83 (100%)	0	100	100
29	Z	61/75 (81%)	61 (100%)	0	100	100
30	c	192/221 (87%)	192 (100%)	0	100	100
31	d	164/175 (94%)	164 (100%)	0	100	100
32	e	174/175 (99%)	174 (100%)	0	100	100
33	f	122/131 (93%)	122 (100%)	0	100	100
34	g	81/86 (94%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	i	112/113 (99%)	112 (100%)	0	100	100
36	j	105/107 (98%)	105 (100%)	0	100	100
37	k	91/91 (100%)	91 (100%)	0	100	100
38	l	94/104 (90%)	94 (100%)	0	100	100
39	m	117/119 (98%)	117 (100%)	0	100	100
40	n	98/104 (94%)	98 (100%)	0	100	100
41	o	52/53 (98%)	52 (100%)	0	100	100
42	p	79/81 (98%)	79 (100%)	0	100	100
43	q	76/77 (99%)	76 (100%)	0	100	100
44	r	74/82 (90%)	74 (100%)	0	100	100
45	s	56/68 (82%)	56 (100%)	0	100	100
46	t	70/80 (88%)	70 (100%)	0	100	100
47	u	67/69 (97%)	67 (100%)	0	100	100
50	h	126/132 (96%)	126 (100%)	0	100	100
51	4	55/75 (73%)	55 (100%)	0	100	100
All	All	4563/4890 (93%)	4562 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	T	75	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	4	GLN
3	3	48	ASN
4	5	19	HIS
5	6	40	ASN
7	8	31	HIS
12	G	143	ASN
13	H	50	GLN
13	H	134	HIS
13	H	146	HIS
13	H	181	GLN
15	J	135	GLN

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Mol	Chain	Res	Type
16	K	99	GLN
16	K	111	HIS
17	M	59	ASN
18	N	45	ASN
23	S	14	GLN
28	Y	13	GLN
28	Y	88	HIS
29	Z	20	ASN
29	Z	37	GLN
29	Z	58	ASN
31	d	44	ASN
31	d	53	HIS
31	d	68	HIS
31	d	99	HIS
32	e	35	GLN
32	e	36	HIS
34	g	53	ASN
35	i	18	ASN
37	k	15	HIS
37	k	20	GLN
37	k	56	HIS
46	t	57	HIS
50	h	40	GLN
50	h	130	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	D	76/77 (98%)	9 (11%)	6 (7%)
48	A	2805/2923 (95%)	326 (11%)	69 (2%)
49	a	1501/1552 (96%)	149 (9%)	0
9	B	112/115 (97%)	8 (7%)	1 (0%)
All	All	4494/4667 (96%)	492 (10%)	76 (1%)

All (492) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	B	10	U
9	B	24	C
9	B	39	G
9	B	40	C

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Mol	Chain	Res	Type
9	B	55	A
9	B	87	C
9	B	88	G
9	B	106	G
11	D	8	U
11	D	9	G
11	D	18	C
11	D	19	G
11	D	21	U
11	D	22	A
11	D	23	G
11	D	24	C
11	D	77	A
48	A	15	G
48	A	34	U
48	A	71	A
48	A	75	G
48	A	117	A
48	A	118	A
48	A	119	U
48	A	154	A
48	A	164	A
48	A	165	C
48	A	167	U
48	A	176	A
48	A	177	G
48	A	180	G
48	A	184	C
48	A	199	A
48	A	202	A
48	A	203	U
48	A	219	A
48	A	224	A
48	A	225	A
48	A	231	A
48	A	232	U
48	A	233	U
48	A	251	G
48	A	253	G
48	A	284	C
48	A	285	U
48	A	286	U

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Mol	Chain	Res	Type
48	A	287	G
48	A	289	U
48	A	300	G
48	A	314	A
48	A	321	U
48	A	322	A
48	A	344	U
48	A	345	C
48	A	354	A
48	A	373	A
48	A	374	U
48	A	404	U
48	A	410	G
48	A	432	G
48	A	457	G
48	A	497	U
48	A	502	C
48	A	503	A
48	A	527	G
48	A	549	U
48	A	550	A
48	A	553	A
48	A	572	C
48	A	575	G
48	A	576	U
48	A	577	A
48	A	578	G
48	A	591	A
48	A	592	A
48	A	593	U
48	A	594	G
48	A	606	G
48	A	616	G
48	A	618	A
48	A	646	A
48	A	667	G
48	A	682	A
48	A	683	G
48	A	699	U
48	A	730	A
48	A	731	U
48	A	762	C

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Mol	Chain	Res	Type
48	A	775	A
48	A	793	G
48	A	794	A
48	A	809	A
48	A	810	A
48	A	819	A
48	A	820	G
48	A	827	A
48	A	829	U
48	A	834	A
48	A	835	U
48	A	836	C
48	A	837	G
48	A	850	G
48	A	857	C
48	A	872	U
48	A	873	U
48	A	911	A
48	A	923	A
48	A	924	G
48	A	955	A
48	A	970	U
48	A	985	A
48	A	989	A
48	A	990	G
48	A	1003	A
48	A	1005	G
48	A	1018	A
48	A	1027	A
48	A	1040	A
48	A	1049	C
48	A	1056	U
48	A	1057	A
48	A	1070	A
48	A	1077	U
48	A	1089	C
48	A	1090	A
48	A	1091	G
48	A	1101	A
48	A	1106	G
48	A	1107	G
48	A	1114	A

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Mol	Chain	Res	Type
48	A	1115	G
48	A	1123	C
48	A	1126	U
48	A	1128	A
48	A	1129	A
48	A	1131	G
48	A	1132	A
48	A	1133	G
48	A	1156	G
48	A	1160	C
48	A	1173	A
48	A	1174	U
48	A	1176	U
48	A	1177	A
48	A	1178	C
48	A	1179	C
48	A	1186	A
48	A	1187	A
48	A	1215	U
48	A	1217	U
48	A	1218	G
48	A	1225	G
48	A	1250	G
48	A	1276	G
48	A	1291	A
48	A	1292	A
48	A	1294	G
48	A	1309	G
48	A	1310	A
48	A	1337	A
48	A	1339	U
48	A	1340	G
48	A	1366	U
48	A	1402	A
48	A	1405	G
48	A	1415	A
48	A	1416	U
48	A	1449	A
48	A	1455	U
48	A	1456	U
48	A	1457	U
48	A	1458	A

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Mol	Chain	Res	Type
48	A	1463	A
48	A	1471	A
48	A	1472	C
48	A	1490	G
48	A	1497	A
48	A	1499	U
48	A	1504	U
48	A	1511	C
48	A	1526	G
48	A	1533	A
48	A	1534	G
48	A	1536	C
48	A	1552	U
48	A	1553	A
48	A	1560	A
48	A	1569	G
48	A	1574	G
48	A	1578	A
48	A	1581	U
48	A	1583	G
48	A	1585	G
48	A	1592	A
48	A	1593	G
48	A	1594	U
48	A	1606	C
48	A	1613	G
48	A	1616	A
48	A	1625	U
48	A	1630	A
48	A	1631	G
48	A	1651	C
48	A	1652	A
48	A	1653	A
48	A	1654	A
48	A	1678	A
48	A	1679	A
48	A	1690	A
48	A	1691	G
48	A	1692	C
48	A	1718	G
48	A	1740	G
48	A	1772	G

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Mol	Chain	Res	Type
48	A	1783	G
48	A	1789	A
48	A	1790	G
48	A	1791	G
48	A	1800	A
48	A	1809	C
48	A	1818	A
48	A	1827	C
48	A	1843	U
48	A	1885	G
48	A	1893	A
48	A	1896	U
48	A	1926	A
48	A	1927	A
48	A	1928	A
48	A	1933	G
48	A	1939	A
48	A	1940	A
48	A	1941	C
48	A	1942	U
48	A	1943	A
48	A	1956	G
48	A	1957	G
48	A	1963	A
48	A	1964	A
48	A	1965	A
48	A	1982	U
48	A	1983	U
48	A	1994	C
48	A	1997	A
48	A	1998	A
48	A	1999	G
48	A	2008	A
48	A	2009	U
48	A	2019	G
48	A	2020	U
48	A	2050	A
48	A	2058	A
48	A	2059	G
48	A	2060	A
48	A	2070	C
48	A	2082	C

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Mol	Chain	Res	Type
48	A	2083	G
48	A	2087	A
48	A	2088	G
48	A	2089	A
48	A	2096	G
48	A	2225	A
48	A	2226	A
48	A	2230	G
48	A	2231	C
48	A	2238	U
48	A	2239	A
48	A	2240	U
48	A	2252	A
48	A	2265	G
48	A	2266	G
48	A	2295	A
48	A	2305	A
48	A	2310	C
48	A	2314	A
48	A	2315	A
48	A	2333	U
48	A	2334	G
48	A	2335	G
48	A	2336	A
48	A	2337	A
48	A	2338	A
48	A	2347	A
48	A	2352	G
48	A	2353	U
48	A	2354	A
48	A	2361	U
48	A	2362	A
48	A	2374	C
48	A	2377	C
48	A	2400	U
48	A	2410	G
48	A	2412	C
48	A	2417	U
48	A	2429	U
48	A	2433	C
48	A	2450	U
48	A	2455	G

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Mol	Chain	Res	Type
48	A	2456	G
48	A	2457	A
48	A	2461	A
48	A	2466	A
48	A	2468	C
48	A	2475	A
48	A	2529	G
48	A	2532	G
48	A	2545	A
48	A	2581	U
48	A	2593	A
48	A	2594	G
48	A	2600	C
48	A	2605	G
48	A	2609	G
48	A	2612	U
48	A	2613	C
48	A	2629	A
48	A	2630	G
48	A	2637	C
48	A	2638	C
48	A	2640	U
48	A	2692	A
48	A	2716	U
48	A	2718	C
48	A	2741	G
48	A	2753	U
48	A	2760	A
48	A	2762	G
48	A	2791	A
48	A	2792	A
48	A	2793	G
48	A	2796	C
48	A	2805	A
48	A	2817	A
48	A	2820	U
48	A	2821	U
48	A	2823	G
48	A	2824	G
48	A	2827	A
48	A	2863	G
48	A	2887	G

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Mol	Chain	Res	Type
48	A	2888	A
48	A	2906	G
48	A	2913	G
49	a	10	G
49	a	33	A
49	a	40	G
49	a	48	C
49	a	49	C
49	a	52	A
49	a	97	G
49	a	108	A
49	a	120	C
49	a	129	A
49	a	130	A
49	a	131	C
49	a	165	G
49	a	196	A
49	a	205	A
49	a	211	A
49	a	212	A
49	a	213	G
49	a	221	U
49	a	255	G
49	a	259	G
49	a	274	G
49	a	275	C
49	a	283	G
49	a	289	G
49	a	297	G
49	a	314	A
49	a	315	U
49	a	316	C
49	a	336	C
49	a	337	A
49	a	340	G
49	a	360	C
49	a	362	G
49	a	375	U
49	a	380	C
49	a	400	G
49	a	405	A
49	a	414	G

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Mol	Chain	Res	Type
49	a	415	A
49	a	420	U
49	a	421	G
49	a	430	C
49	a	432	G
49	a	437	U
49	a	456	A
49	a	460	A
49	a	461	C
49	a	462	A
49	a	472	G
49	a	474	A
49	a	476	C
49	a	493	G
49	a	505	A
49	a	519	C
49	a	526	C
49	a	535	G
49	a	540	A
49	a	555	A
49	a	567	A
49	a	572	U
49	a	580	A
49	a	581	A
49	a	584	C
49	a	585	G
49	a	642	C
49	a	661	U
49	a	696	G
49	a	726	A
49	a	728	C
49	a	729	A
49	a	731	U
49	a	757	A
49	a	763	G
49	a	785	A
49	a	802	A
49	a	825	C
49	a	836	A
49	a	882	A
49	a	935	G
49	a	944	C

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Mol	Chain	Res	Type
49	a	945	A
49	a	970	U
49	a	971	U
49	a	978	A
49	a	979	A
49	a	985	A
49	a	986	G
49	a	993	A
49	a	1003	G
49	a	1012	U
49	a	1014	A
49	a	1016	A
49	a	1024	A
49	a	1025	G
49	a	1057	C
49	a	1058	A
49	a	1077	U
49	a	1097	U
49	a	1106	G
49	a	1107	U
49	a	1113	A
49	a	1142	A
49	a	1143	U
49	a	1150	G
49	a	1153	G
49	a	1163	A
49	a	1168	A
49	a	1170	U
49	a	1179	C
49	a	1207	A
49	a	1208	A
49	a	1211	C
49	a	1212	A
49	a	1223	U
49	a	1224	A
49	a	1238	A
49	a	1268	A
49	a	1289	A
49	a	1290	A
49	a	1297	U
49	a	1298	A
49	a	1309	C

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Mol	Chain	Res	Type
49	a	1311	G
49	a	1312	U
49	a	1313	U
49	a	1348	G
49	a	1349	G
49	a	1357	A
49	a	1375	U
49	a	1409	A
49	a	1430	G
49	a	1437	A
49	a	1453	G
49	a	1457	A
49	a	1463	U
49	a	1464	U
49	a	1465	A
49	a	1466	G
49	a	1505	A
49	a	1506	G
49	a	1515	A
49	a	1517	G
49	a	1518	U
49	a	1529	G
49	a	1541	G
49	a	1542	G
49	a	1547	C
49	a	1548	C

All (76) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	B	39	G
11	D	8	U
11	D	9	G
11	D	16	U
11	D	21	U
11	D	23	G
11	D	59	A
48	A	107	G
48	A	176	A
48	A	184	C
48	A	195	C
48	A	202	A

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Mol	Chain	Res	Type
48	A	282	A
48	A	313	U
48	A	344	U
48	A	475	A
48	A	548	A
48	A	572	C
48	A	591	A
48	A	646	A
48	A	708	G
48	A	756	A
48	A	793	G
48	A	835	U
48	A	850	G
48	A	922	G
48	A	1024	A
48	A	1089	C
48	A	1106	G
48	A	1114	A
48	A	1125	U
48	A	1128	A
48	A	1131	G
48	A	1142	A
48	A	1177	A
48	A	1178	C
48	A	1186	A
48	A	1217	U
48	A	1271	G
48	A	1291	A
48	A	1339	U
48	A	1369	G
48	A	1456	U
48	A	1533	A
48	A	1547	C
48	A	1580	A
48	A	1592	A
48	A	1652	A
48	A	1662	A
48	A	1678	A
48	A	1691	G
48	A	1771	A
48	A	1789	A
48	A	1897	U

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Mol	Chain	Res	Type
48	A	1927	A
48	A	1938	U
48	A	1939	A
48	A	1941	C
48	A	1965	A
48	A	1982	U
48	A	2008	A
48	A	2049	U
48	A	2059	G
48	A	2238	U
48	A	2302	C
48	A	2313	A
48	A	2338	A
48	A	2353	U
48	A	2452	A
48	A	2457	A
48	A	2608	G
48	A	2629	A
48	A	2637	C
48	A	2716	U
48	A	2820	U
48	A	2887	G

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
48	MA6	A	2085	48	23,26,27	1.67	4 (17%)	33,38,41	2.88	13 (39%)

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
48	MA6	A	2085	48	-	1/11/29/30	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	A	2085	MA6	C6-N6	4.60	1.49	1.36
48	A	2085	MA6	C5-C4	-3.41	1.33	1.39
48	A	2085	MA6	C5-N7	-3.01	1.33	1.39
48	A	2085	MA6	C8-N9	-2.95	1.32	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A	2085	MA6	N1-C6-N6	-8.09	107.00	116.86
48	A	2085	MA6	C5-C4-N3	-5.57	119.04	126.72
48	A	2085	MA6	C4-C5-C6	5.38	121.47	115.91
48	A	2085	MA6	N1-C2-N3	-5.23	120.66	128.58
48	A	2085	MA6	C5-C6-N6	4.79	132.91	125.33
48	A	2085	MA6	N3-C4-N9	4.35	134.57	127.17
48	A	2085	MA6	N9-C8-N7	-4.20	107.98	113.94
48	A	2085	MA6	C2-N3-C4	3.23	119.72	111.83
48	A	2085	MA6	C4-N9-C8	3.01	108.90	105.74
48	A	2085	MA6	C2-N1-C6	2.95	119.03	111.83
48	A	2085	MA6	C6-C5-N7	-2.60	129.29	133.43
48	A	2085	MA6	C5-N7-C8	2.56	107.47	103.45
48	A	2085	MA6	C1'-N9-C8	-2.17	122.28	127.09

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
48	A	2085	MA6	C5-C6-N6-C10

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	A	2085	MA6	3	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 432 ligands modelled in this entry, 430 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	$\# Z  > 2$
54	FME	D	102	11	8,9,10	0.97	0	8,9,11	1.06	0
56	A1I09	A	3105	-	39,40,40	3.10	12 (30%)	47,56,56	1.52	9 (19%)

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
54	FME	D	102	11	-	0/7/9/11	-
56	A1I09	A	3105	-	-	3/30/62/62	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	A	3105	A1I09	C26-C21	8.91	1.53	1.39
56	A	3105	A1I09	C23-C22	8.74	1.54	1.39
56	A	3105	A1I09	C25-C24	7.23	1.54	1.38
56	A	3105	A1I09	C10-N1	6.39	1.47	1.34
56	A	3105	A1I09	C21-C22	-5.74	1.32	1.40
56	A	3105	A1I09	O2-C20	4.07	1.43	1.33
56	A	3105	A1I09	C24-C23	-3.76	1.32	1.38
56	A	3105	A1I09	C25-C26	-3.34	1.33	1.38
56	A	3105	A1I09	C21-C20	2.73	1.56	1.50
56	A	3105	A1I09	O5-C4	-2.52	1.40	1.44
56	A	3105	A1I09	O9-C10	-2.51	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	A	3105	A1I09	C6-S1	2.24	1.84	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	A	3105	A1I09	C9-C8-C7	-4.67	108.03	114.17
56	A	3105	A1I09	O2-C20-C21	3.58	119.26	112.24
56	A	3105	A1I09	C12-C13-C14	3.25	107.02	102.23
56	A	3105	A1I09	C12-C13-C16	-3.22	111.00	114.68
56	A	3105	A1I09	C17-C16-C13	-2.27	109.27	115.67
56	A	3105	A1I09	C10-C11-N2	-2.24	107.83	112.39
56	A	3105	A1I09	O5-C4-C7	2.18	110.97	105.79
56	A	3105	A1I09	C6-S1-C5	2.05	104.88	100.45
56	A	3105	A1I09	C7-N1-C10	-2.04	120.10	123.20

There are no chirality outliers.

All (3) torsion outliers are listed below:

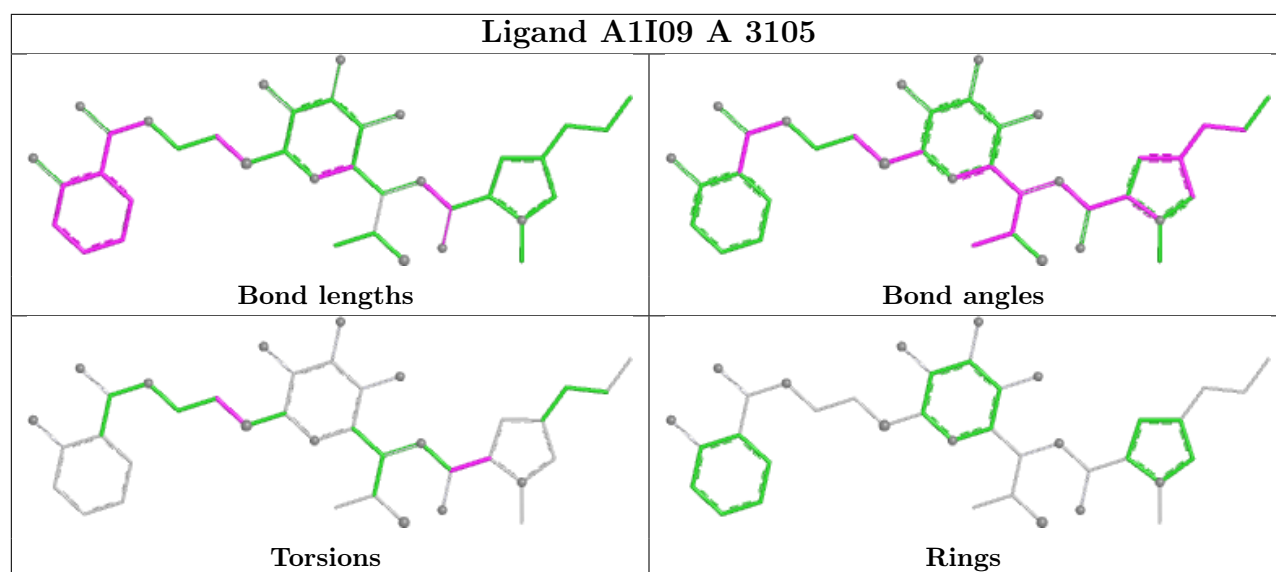
Mol	Chain	Res	Type	Atoms
56	A	3105	A1I09	N1-C10-C11-C12
56	A	3105	A1I09	O9-C10-C11-C12
56	A	3105	A1I09	C19-C6-S1-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	A	3105	A1I09	1	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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



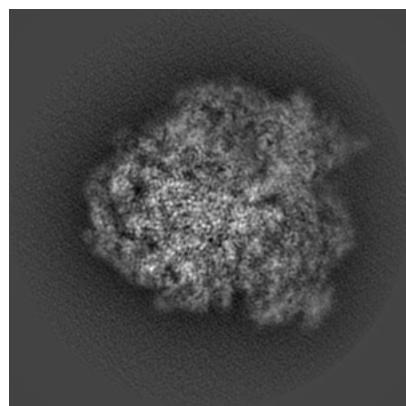
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52712. These allow visual inspection of the internal detail of the map and identification of artifacts.

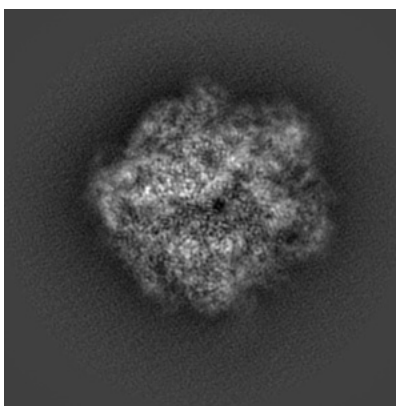
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

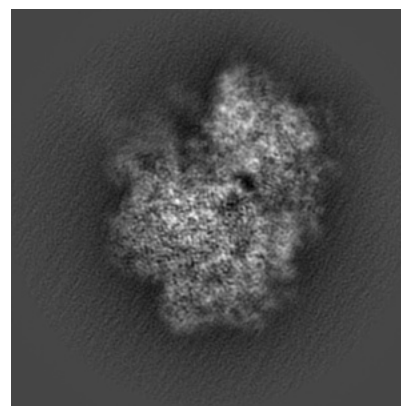
#### 6.1.1 Primary map



X

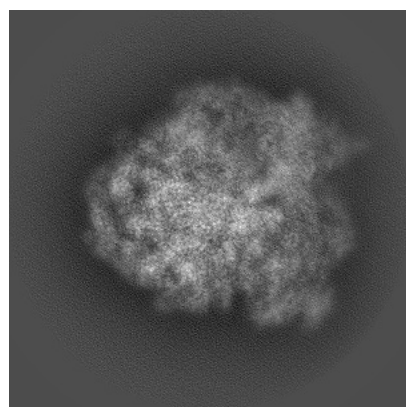


Y

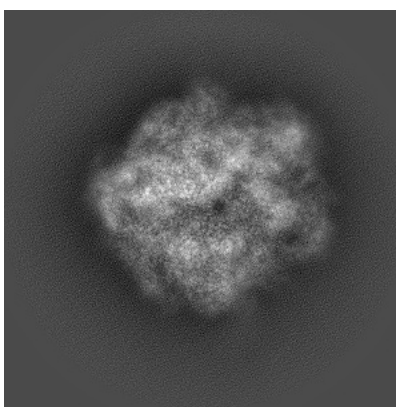


Z

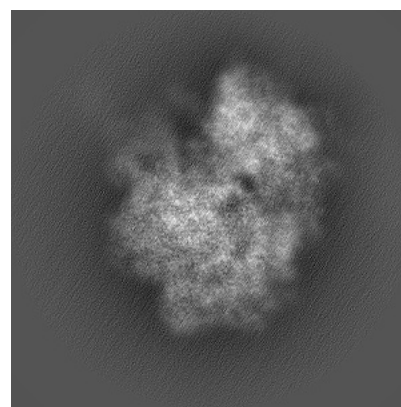
#### 6.1.2 Raw map



X



Y

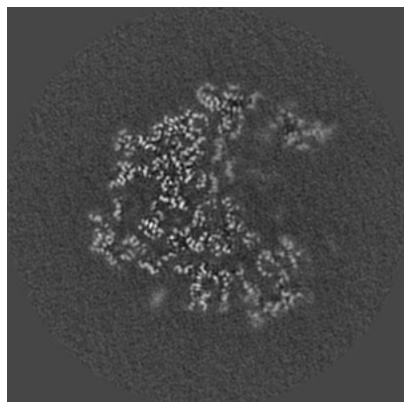


Z

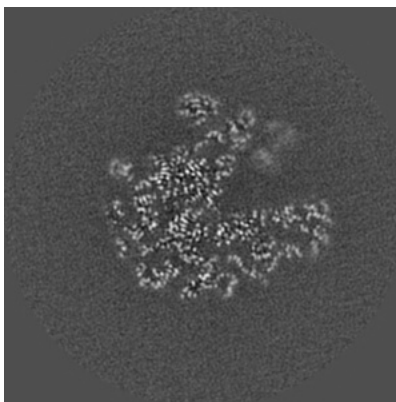
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

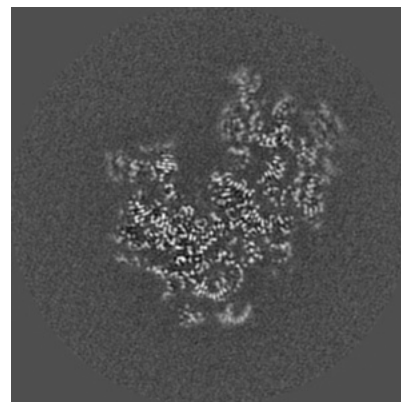
### 6.2.1 Primary map



X Index: 204

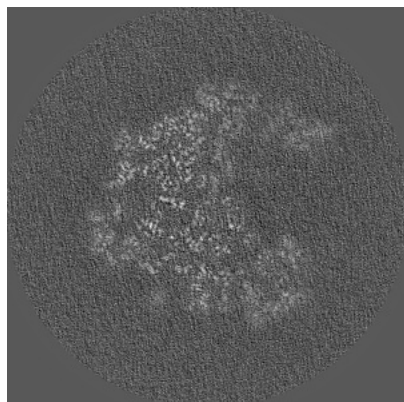


Y Index: 204

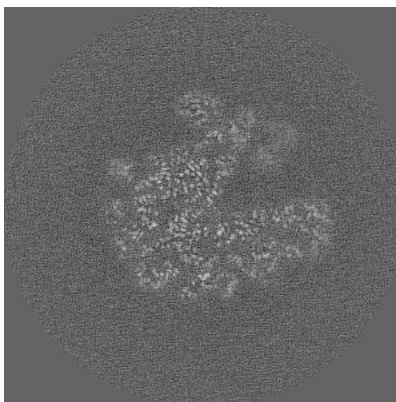


Z Index: 204

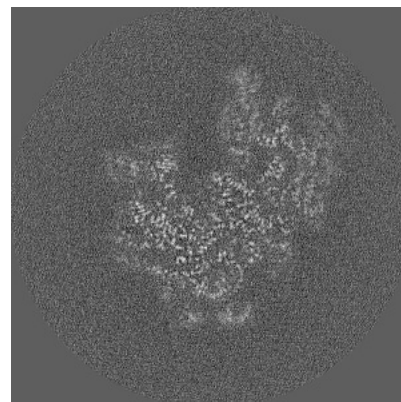
### 6.2.2 Raw map



X Index: 204



Y Index: 204

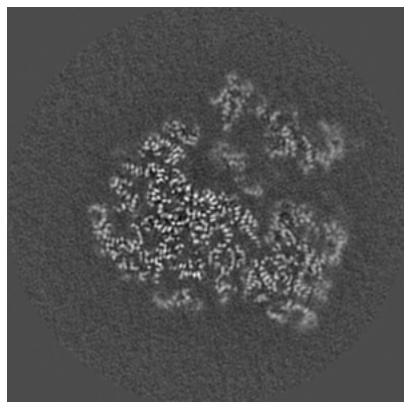


Z Index: 204

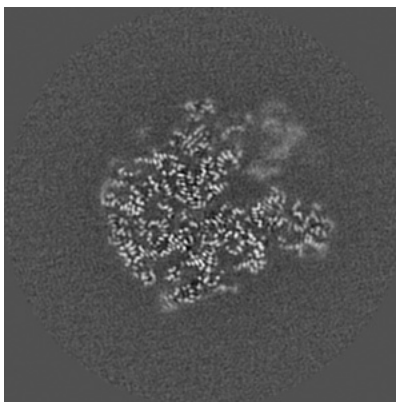
The images above show central slices of the map in three orthogonal directions.

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

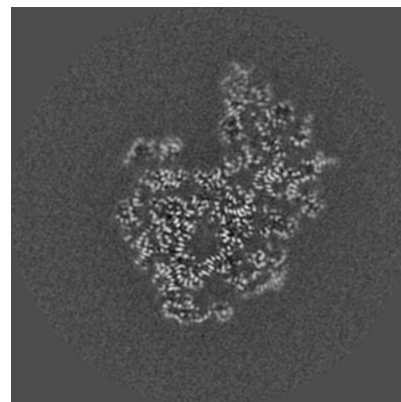
### 6.3.1 Primary map



X Index: 218

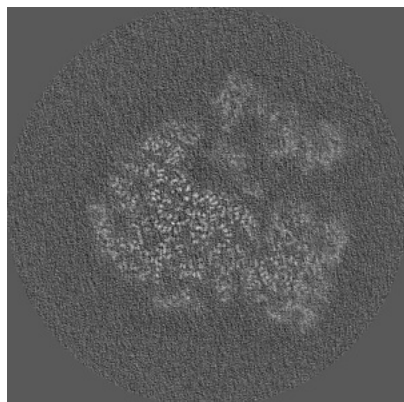


Y Index: 194

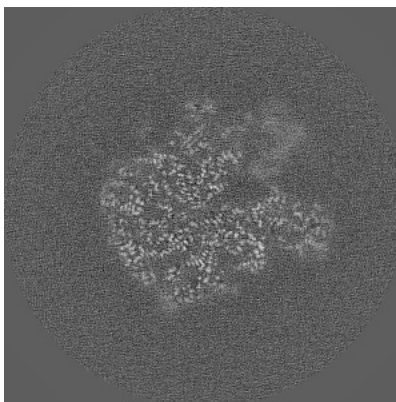


Z Index: 187

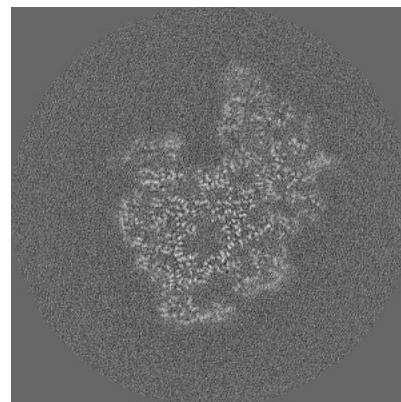
### 6.3.2 Raw map



X Index: 218



Y Index: 194



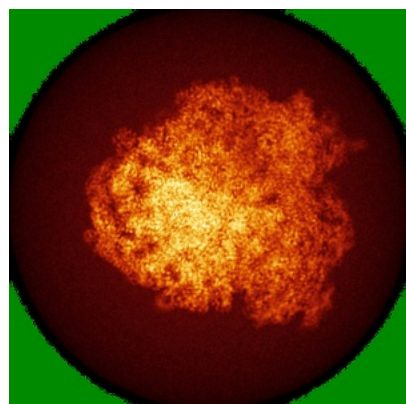
Z Index: 189

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

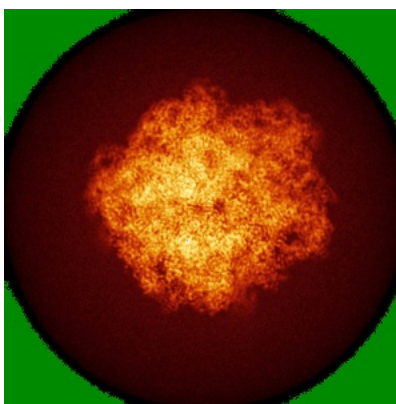


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

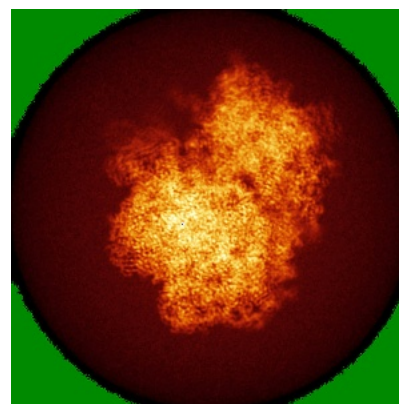
### 6.4.1 Primary map



X

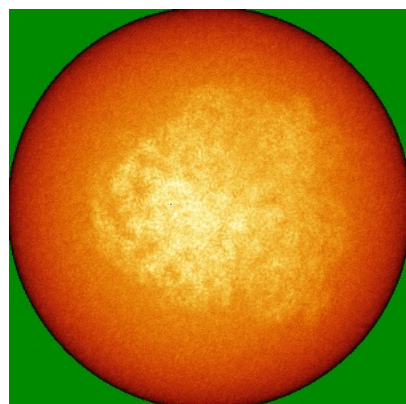


Y

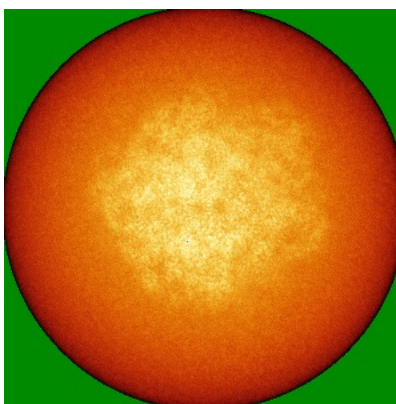


Z

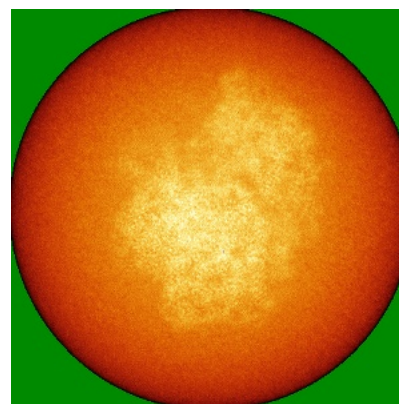
### 6.4.2 Raw map



X



Y

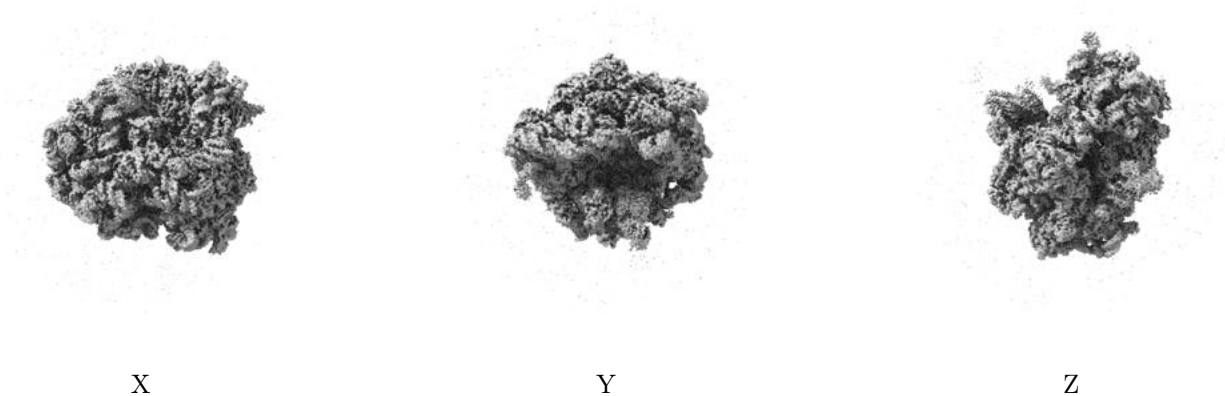


Z

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

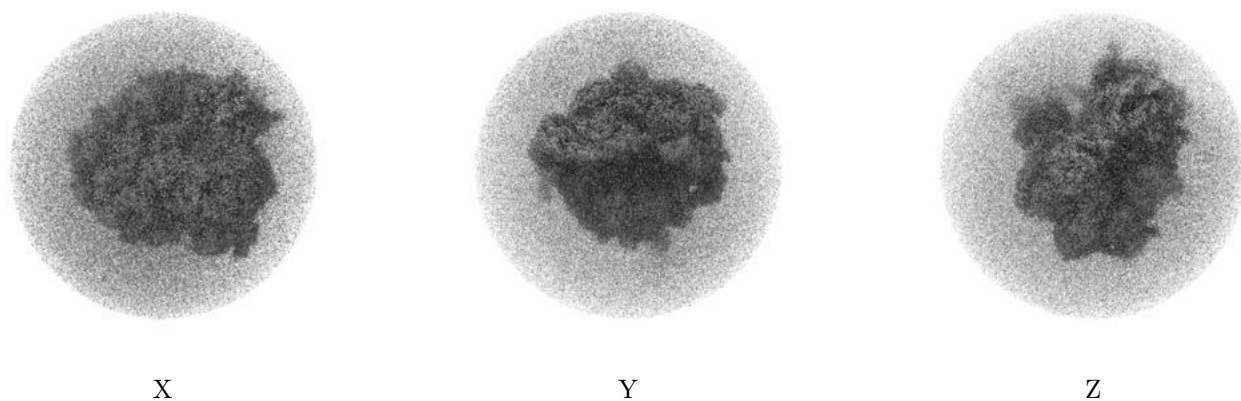
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

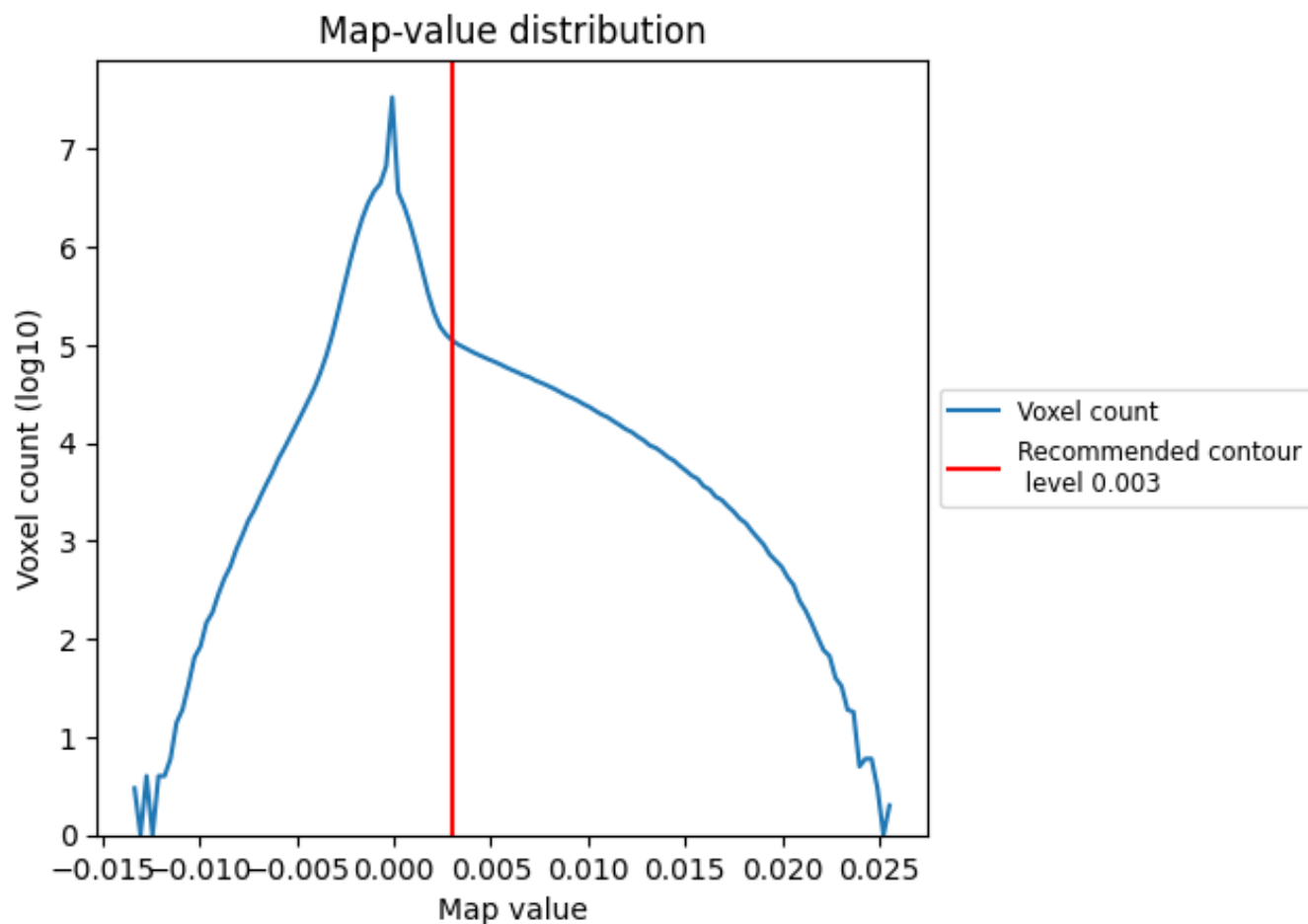
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

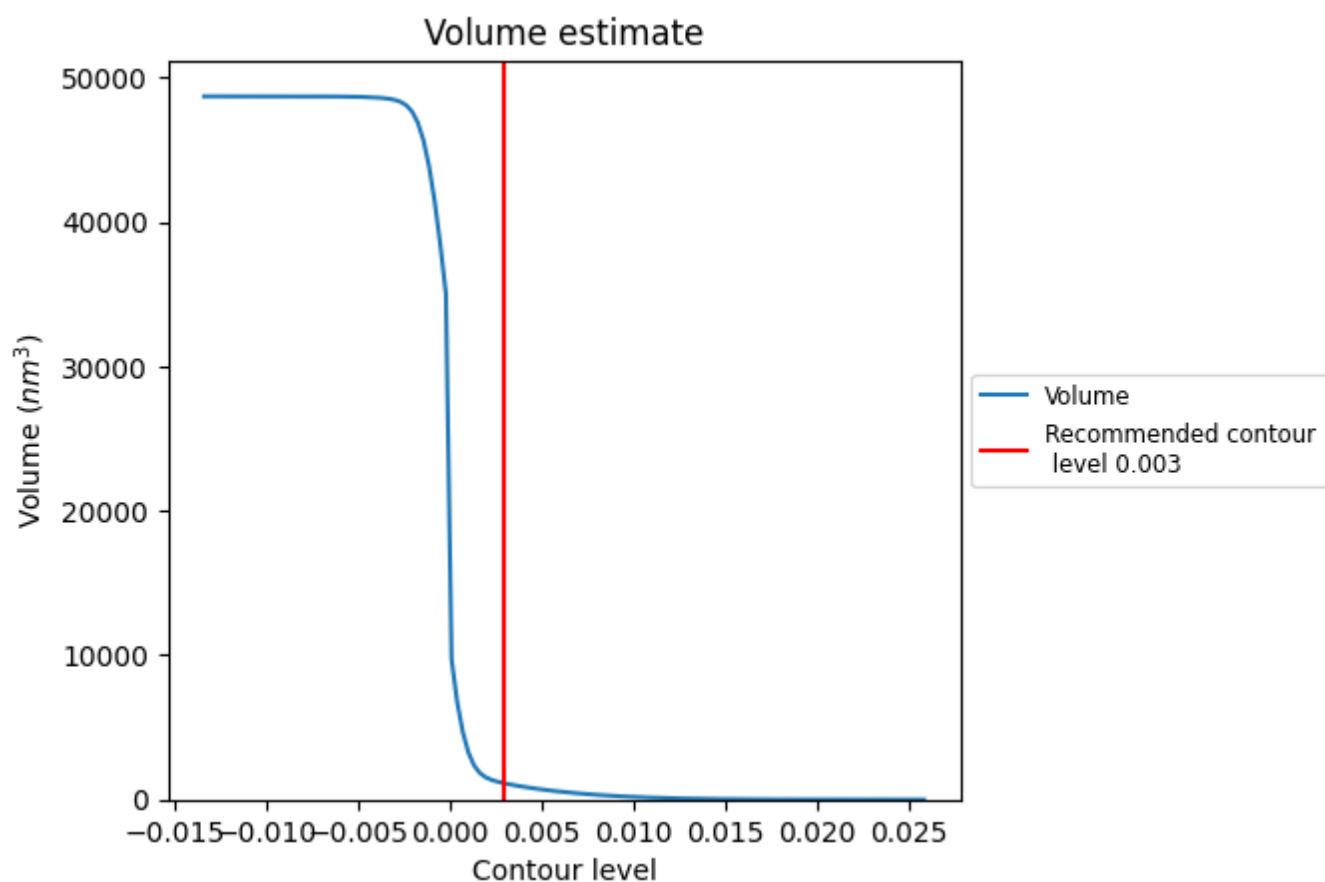
This section contains the results of statistical analysis of the map.

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



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

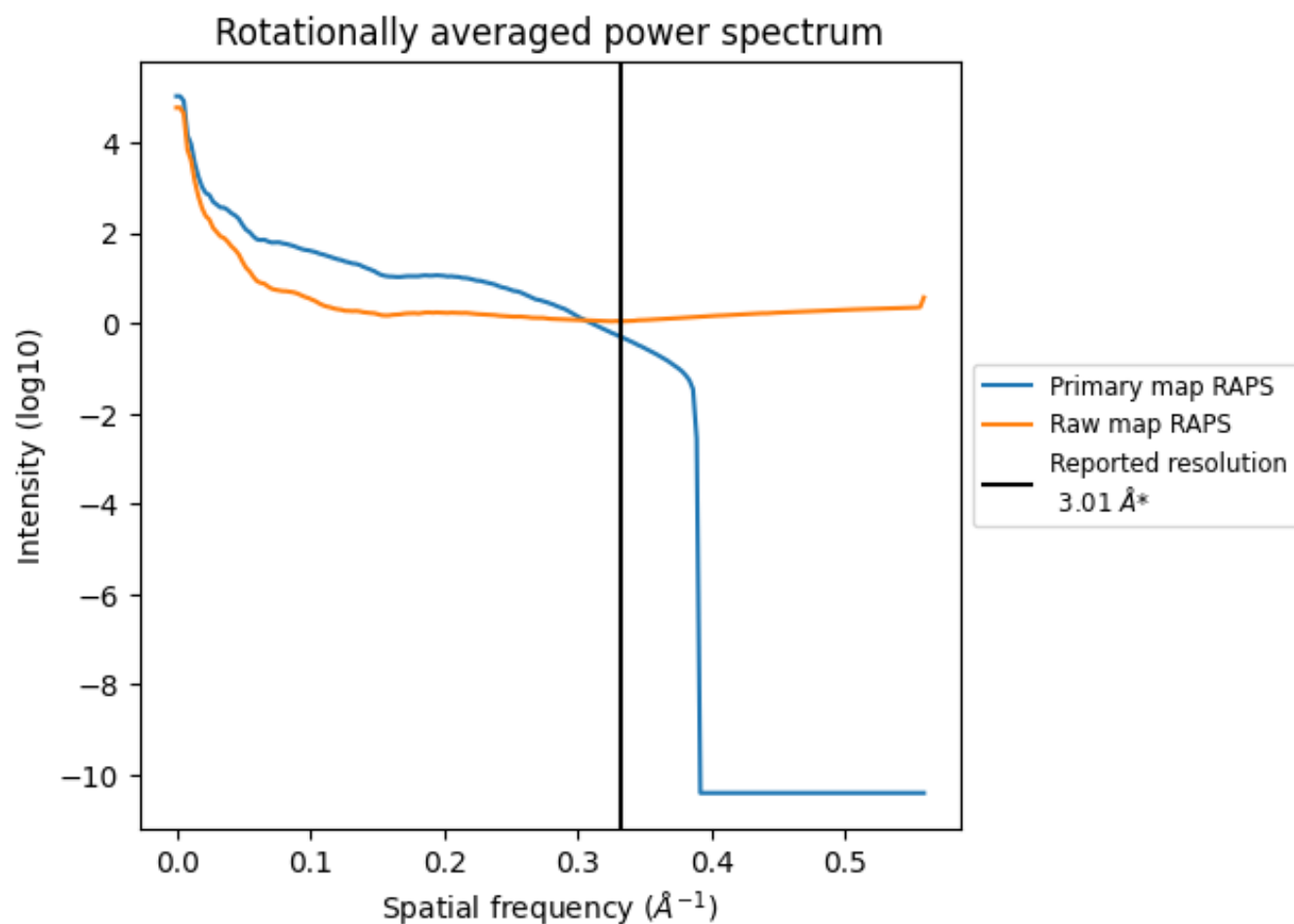
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1125 nm<sup>3</sup>; this corresponds to an approximate mass of 1016 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 ⓘ



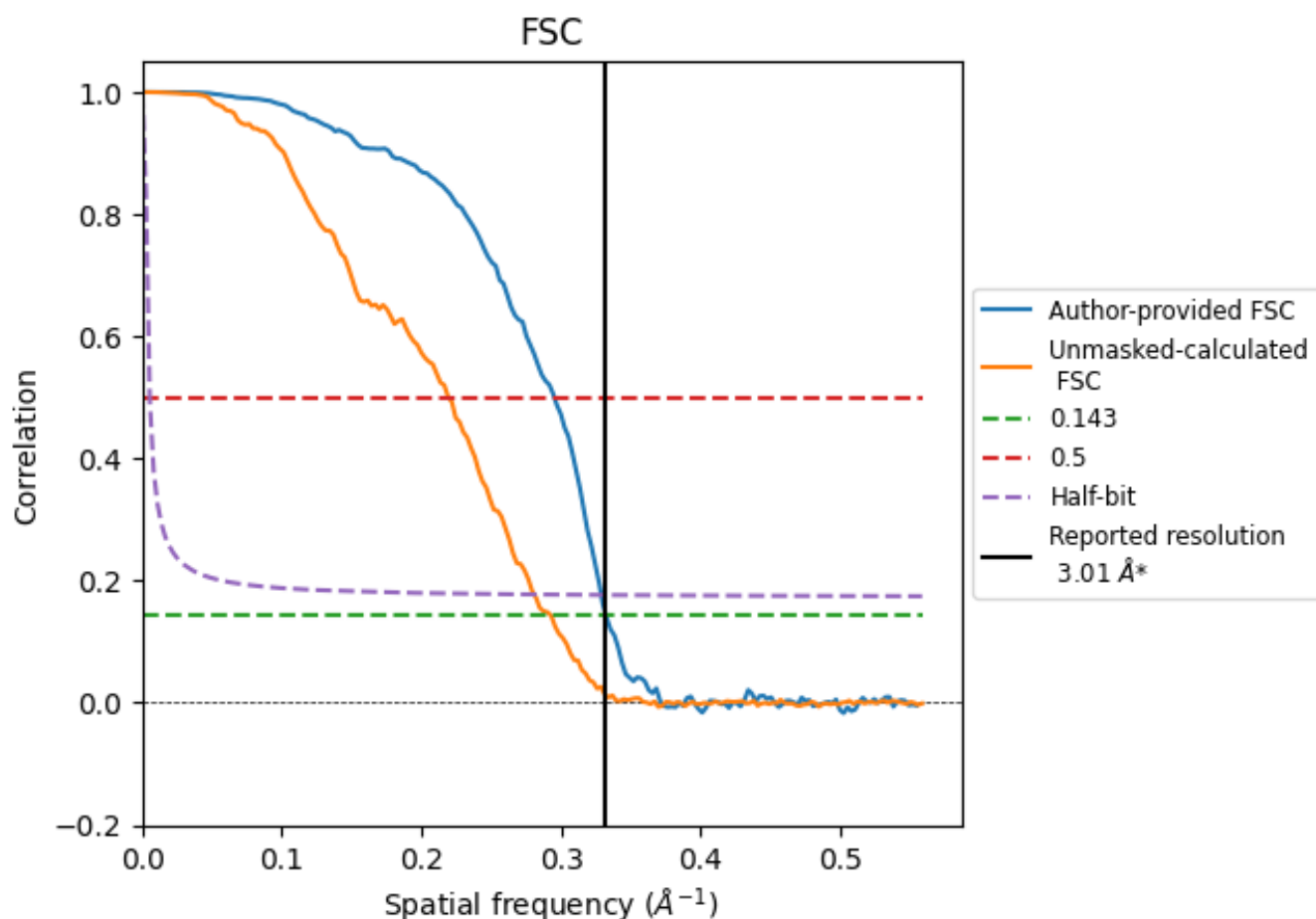
\*Reported resolution corresponds to spatial frequency of 0.332  $\text{\AA}^{-1}$



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.332  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

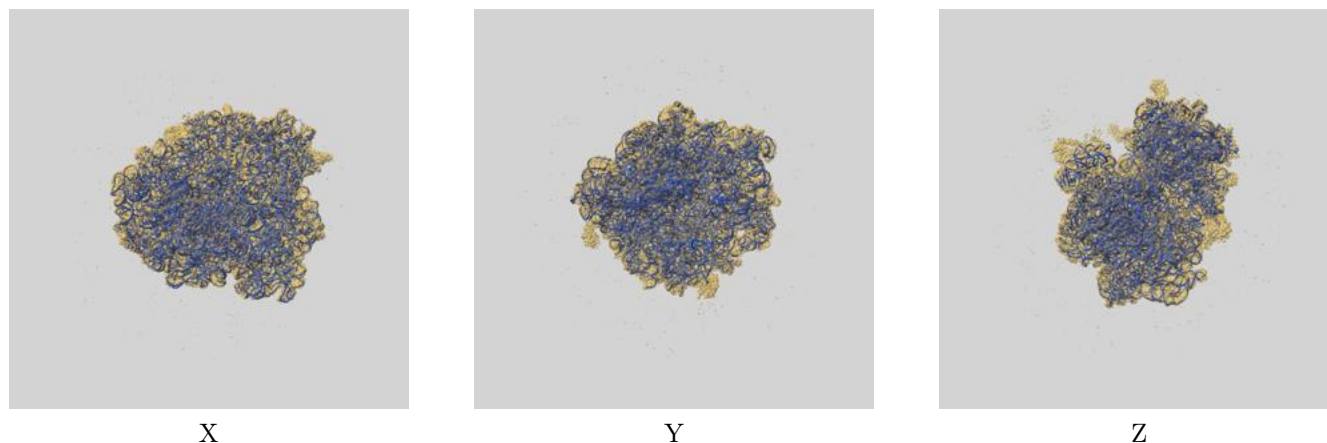
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	3.01	3.39	3.04
Unmasked-calculated*	3.42	4.56	3.56

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 3.01 by more than 10 %

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

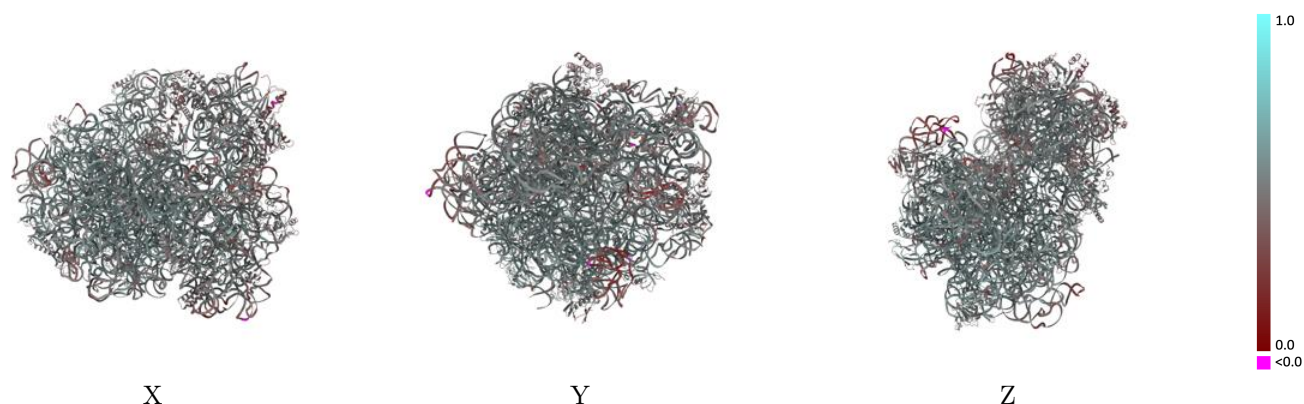
This section contains information regarding the fit between EMDB map EMD-52712 and PDB model 9I89. Per-residue inclusion information can be found in section [3](#) on page [15](#).

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



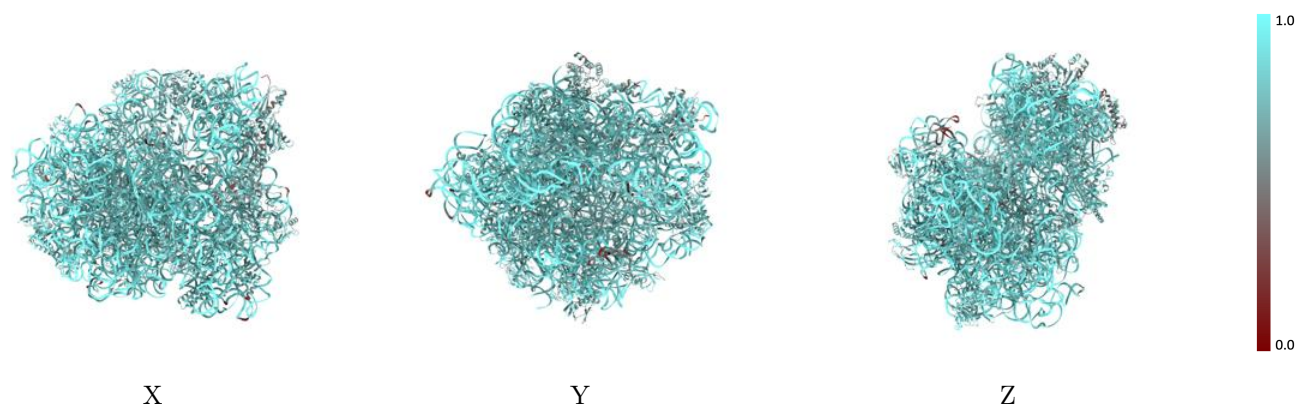
The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



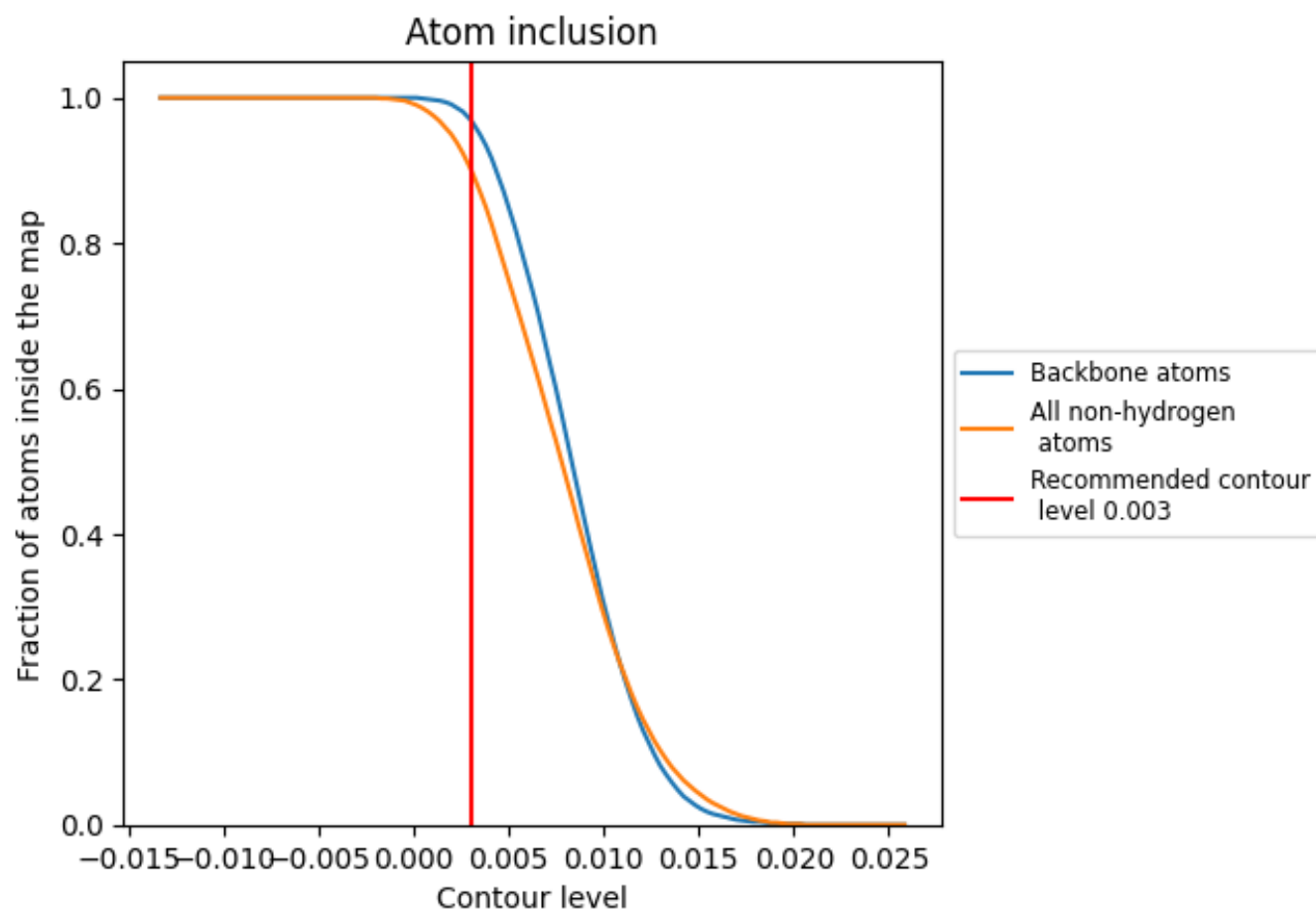
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.003).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 90% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9010	 0.5120
1	 0.8320	 0.5250
2	 0.8040	 0.4740
3	 0.8340	 0.5220
4	 0.7900	 0.4420
5	 0.8460	 0.5440
6	 0.8160	 0.5160
7	 0.8880	 0.5650
8	 0.8530	 0.5570
9	 0.8120	 0.5430
A	 0.9530	 0.5340
B	 0.9610	 0.5060
C	 0.7860	 0.4950
D	 0.8460	 0.4790
G	 0.8410	 0.5410
H	 0.8440	 0.5390
I	 0.8390	 0.5190
J	 0.7600	 0.4510
K	 0.7620	 0.4400
M	 0.8560	 0.5320
N	 0.8070	 0.5300
O	 0.8540	 0.5240
P	 0.8260	 0.5270
Q	 0.8100	 0.5200
R	 0.8080	 0.4800
S	 0.8190	 0.5180
T	 0.8570	 0.5350
U	 0.8360	 0.5250
V	 0.8390	 0.5300
W	 0.8080	 0.5000
Y	 0.8010	 0.4830
Z	 0.8460	 0.5410
a	 0.9430	 0.5000
c	 0.6050	 0.4250
d	 0.7120	 0.4630



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Chain	Atom inclusion	Q-score
e	 0.7450	 0.4530
f	 0.7700	 0.5000
g	 0.7960	 0.4780
h	 0.7570	 0.4420
i	 0.7920	 0.4860
j	 0.7690	 0.4700
k	 0.6770	 0.4190
l	 0.7730	 0.4730
m	 0.7540	 0.4850
n	 0.7660	 0.4400
o	 0.7780	 0.4910
p	 0.8130	 0.4770
q	 0.7550	 0.4590
r	 0.7860	 0.4710
s	 0.8230	 0.4950
t	 0.7600	 0.4620
u	 0.7460	 0.4320