



Full wwPDB EM Validation Report ⓘ

May 21, 2026 – 11:31 am BST

PDB ID : 30RA / pdb_000030ra
EMDB ID : EMD-57974
Title : E. coli 70S ribosome with peptidyl-tRNA, mRNA and Hsp15
Authors : Larsson, D.S.D.; Akbar, S.; Selmer, M.
Deposited on : 2026-05-10
Resolution : 2.78 Å (reported)
Based on initial models : 8CGJ, ., 7K00, 8CF1

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

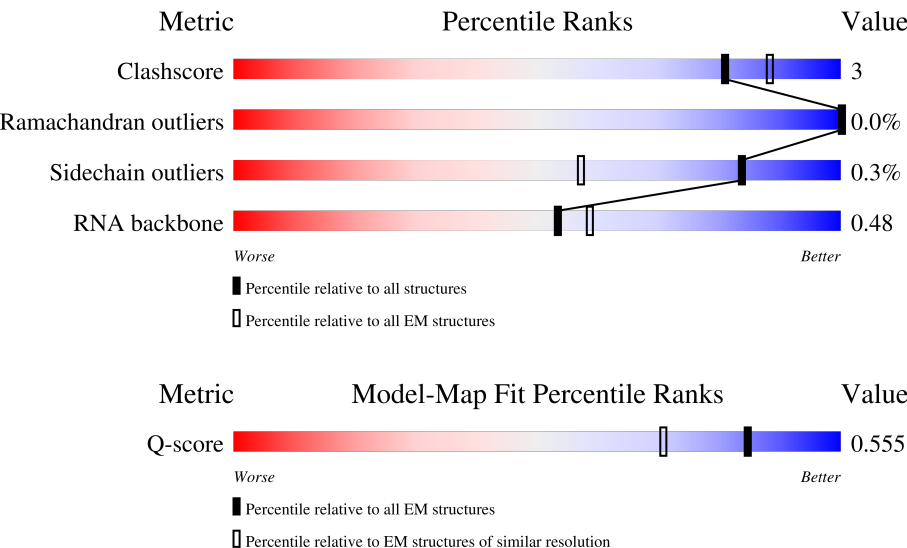
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.78 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	10754 (2.28 - 3.28)

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

Mol	Chain	Length	Quality of chain
1	0	55	<div> <div style="width: 89%;"></div> <div style="width: 7%;"></div> </div>
2	1	46	<div> <div style="width: 100%;"></div> </div>
3	2	65	<div> <div style="width: 88%;"></div> <div style="width: 9%;"></div> </div>



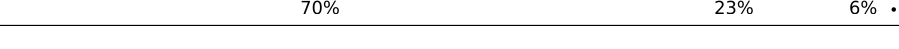
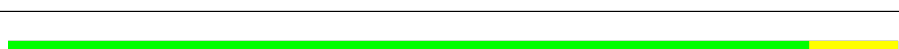
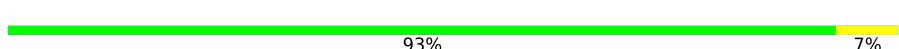


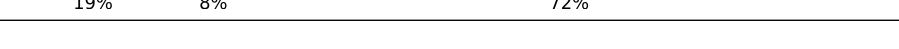
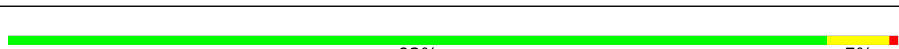


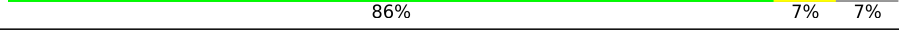
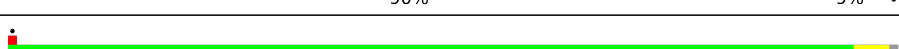
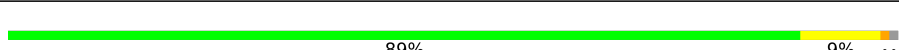

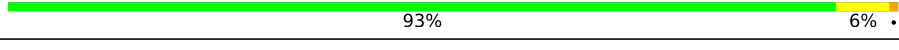
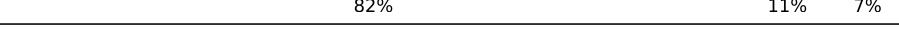







Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	A	1542	
7	B	241	
8	C	233	
9	D	206	
10	E	167	
11	F	135	
12	G	179	
13	H	130	
14	I	130	
15	J	103	
16	K	129	
17	L	124	
18	M	118	
19	N	101	
20	O	89	
21	P	82	
22	Q	84	
23	R	75	
24	S	92	
25	T	87	
26	U	71	
27	V	142	
28	X	3	



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	Z	77	
30	a	2904	
31	b	120	
32	c	273	
33	d	209	
34	e	201	
35	f	179	
36	g	177	
37	h	149	
38	i	142	
39	j	123	
40	k	144	
41	l	136	
42	m	127	
43	n	117	
44	o	115	
45	p	118	
46	q	103	
47	r	110	
48	s	100	
49	t	104	
50	u	94	
51	v	85	
52	w	78	
53	x	63	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	y	59	 88% 10%
55	z	57	 89% 9%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 230884 atoms, of which 89881 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	51	Total	C	H	N	O	0	0
			858	269	441	76	72		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1	46	Total	C	H	N	O	S	0	0
			788	228	411	90	57	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2	64	Total	C	H	N	O	S	0	0
			1065	323	561	105	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
4	3	38	Total	C	H	N	O	S	0	0
			639	185	337	65	48	4		

- Molecule 5 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4	60	Total	C	H	N	O	S	0	0
			948	299	468	90	85	6		

- Molecule 6 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	A	1518	Total	C	H	N	O	P	0	0
			47455	14542	14865	5981	10549	1518		

- Molecule 7 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	B	224	Total	C	H	N	O	S	0	0
			3504	1109	1751	315	321	8		

- Molecule 8 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	C	206	Total	C	H	N	O	S	0	0
			3293	1028	1669	305	288	3		

- Molecule 9 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	D	205	Total	C	H	N	O	S	0	0
			3322	1026	1679	315	298	4		

- Molecule 10 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	E	156	Total	C	H	N	O	S	0	0
			2329	717	1177	217	212	6		

- Molecule 11 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	F	103	Total	C	H	N	O	S	0	0
			1653	530	814	151	151	7		

- Molecule 12 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	G	153	Total	C	H	N	O	S	0	0
			2437	750	1234	231	218	4		

- Molecule 13 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	H	129	Total	C	H	N	O	S	0	0
			1994	616	1015	173	184	6		

- Molecule 14 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	I	127	Total	C	H	N	O	S	0	0
			2075	634	1053	206	179	3		

- Molecule 15 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	J	98	Total	C	H	N	O	S	0	0
			1601	493	815	150	142	1		

- Molecule 16 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	K	117	Total	C	H	N	O	S	0	0
			1742	540	865	173	161	3		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	L	123	Total	C	H	N	O	S	0	0
			1951	591	994	196	165	5		

- Molecule 18 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	M	115	Total	C	H	N	O	S	0	0
			1826	552	935	179	157	3		

- Molecule 19 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	N	100	Total	C	H	N	O	S	0	0
			1637	499	832	164	139	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	O	88	Total	C	H	N	O	S	0	0
			1430	439	716	144	130	1		

- Molecule 21 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	P	81	Total	C	H	N	O	S	0	0
			1295	403	652	127	112	1		

- Molecule 22 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	Q	79	Total	C	H	N	O	S	0	0
			1309	406	668	120	112	3		

- Molecule 23 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	R	66	Total	C	H	N	O	S	0	0
			1094	345	550	102	96	1		

- Molecule 24 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	S	84	Total	C	H	N	O	S	0	0
			1345	427	677	127	112	2		

- Molecule 25 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	T	86	Total	C	H	N	O	S	0	0
			1380	414	710	138	115	3		

- Molecule 26 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	U	70	Total	C	H	N	O	S	0	0
			1209	366	620	125	97	1		

- Molecule 27 is a protein called Heat shock protein 15.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	V	129	Total	C	H	N	O	S	0	0
			2119	655	1066	204	191	3		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	-8	MET	-	initiating methionine	UNP P0ACG8
V	-7	HIS	-	expression tag	UNP P0ACG8
V	-6	HIS	-	expression tag	UNP P0ACG8
V	-5	HIS	-	expression tag	UNP P0ACG8
V	-4	HIS	-	expression tag	UNP P0ACG8
V	-3	HIS	-	expression tag	UNP P0ACG8
V	-2	HIS	-	expression tag	UNP P0ACG8
V	-1	GLY	-	expression tag	UNP P0ACG8
V	0	SER	-	expression tag	UNP P0ACG8
V	1	GLY	-	expression tag	UNP P0ACG8

- Molecule 28 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	X	3	Total	C	H	N	O	P	0	0
			95	29	30	13	20	3		

- Molecule 29 is a RNA chain called tRNA Asp.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	Z	73	Total	C	H	N	O	P	0	0
			2271	693	714	275	516	73		

- Molecule 30 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	a	2753	Total	C	H	N	O	P	0	0
			86112	26384	26982	10897	19096	2753		

- Molecule 31 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	b	119	Total	C	H	N	O	P	0	0
			3720	1135	1171	466	829	119		

- Molecule 32 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	c	271	Total	C	H	N	O	S	0	0
			4196	1288	2114	423	364	7		

- Molecule 33 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	d	209	Total	C	H	N	O	S	0	0
			3152	980	1586	288	294	4		

- Molecule 34 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	e	201	Total	C	H	N	O	S	0	0
			3142	974	1590	283	290	5		

- Molecule 35 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	f	177	Total	C	H	N	O	S	0	0
			2831	899	1421	249	256	6		

- Molecule 36 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	g	176	Total	C	H	N	O	S	0	0
			2670	832	1347	243	246	2		

- Molecule 37 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	h	41	Total	C	H	N	O	S	0	0
			627	194	324	54	54	1		

- Molecule 38 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	i	142	Total	C	H	N	O	S	0	0
			2266	714	1137	212	199	4		

- Molecule 39 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	j	123	Total	C	H	N	O	S	0	0
			1954	593	1008	181	166	6		

- Molecule 40 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	k	144	Total	C	H	N	O	S	0	0
			2164	654	1111	207	190	2		

- Molecule 41 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	l	136	Total	C	H	N	O	S	0	0
			2217	686	1142	205	177	7		

- Molecule 42 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	m	118	Total	C	H	N	O	S	0	0
			1916	585	971	194	161	5		

- Molecule 43 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	n	116	Total	C	H	N	O		0	0
			1800	552	908	178	162			

- Molecule 44 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	o	114	Total	C	H	N	O	S	0	0
			1864	574	947	179	163	1		

- Molecule 45 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	p	117	Total	C	H	N	O		0	0
			1955	604	1008	192	151			

- Molecule 46 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	q	103	Total	C	H	N	O	S	0	0
			1641	516	825	153	145	2		

- Molecule 47 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	r	110	Total	C	H	N	O	S	0	0
			1761	532	904	166	156	3		

- Molecule 48 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	s	93	Total	C	H	N	O	S	0	0
			1533	466	795	139	131	2		

- Molecule 49 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	102	Total	C	H	N	O	0	0
			1602	492	823	146	141		

- Molecule 50 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	u	94	Total	C	H	N	O	S	0	0
			1523	479	770	137	134	3		

- Molecule 51 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	v	78	Total	C	H	N	O	S	0	0
			1172	362	586	116	107	1		

- Molecule 52 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	w	77	Total	C	H	N	O	S	0	0
			1263	388	638	129	106	2		

- Molecule 53 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	x	62	Total	C	H	N	O	S	0	0
			1027	308	526	98	94	1		

- Molecule 54 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	y	58	Total	C	H	N	O	S	0	0
			928	281	479	87	79	2		

- Molecule 55 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	z	56	Total	C	H	N	O	S	0	0
			887	269	443	94	80	1		

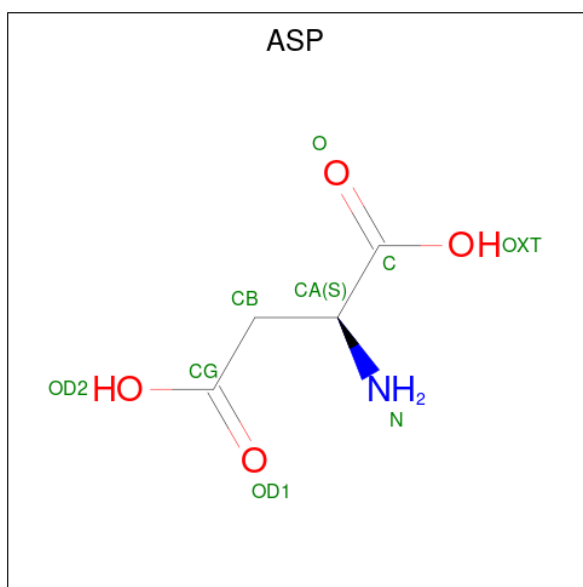
- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	3	1	Total	Zn	0
			1	1	
56	4	1	Total	Zn	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
57	A	71	Total	Mg	0
			71	71	
57	N	1	Total	Mg	0
			1	1	
57	a	201	Total	Mg	0
			201	201	
57	b	5	Total	Mg	0
			5	5	
57	c	1	Total	Mg	0
			1	1	
57	d	1	Total	Mg	0
			1	1	
57	z	1	Total	Mg	0
			1	1	

- Molecule 58 is ASPARTIC ACID (CCD ID: ASP) (formula: C₄H₇NO₄).




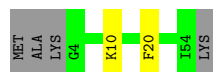
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
58	Z	1	14	4	6	1	3	0

3 Residue-property plots [i](#)

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

- Molecule 1: Large ribosomal subunit protein bL33

Chain 0:  89% 7%




- Molecule 2: Large ribosomal subunit protein bL34

Chain 1:  100%



- Molecule 3: Large ribosomal subunit protein bL35

Chain 2:  88% 9%



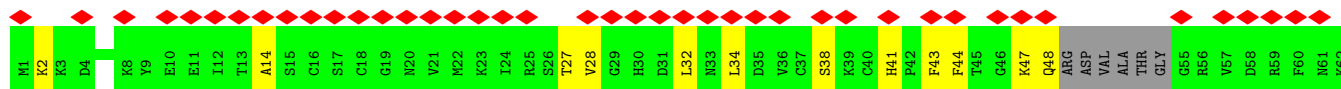
- Molecule 4: Large ribosomal subunit protein bL36A

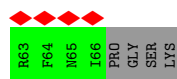
Chain 3:  92% 8%



- Molecule 5: Large ribosomal subunit protein bL31

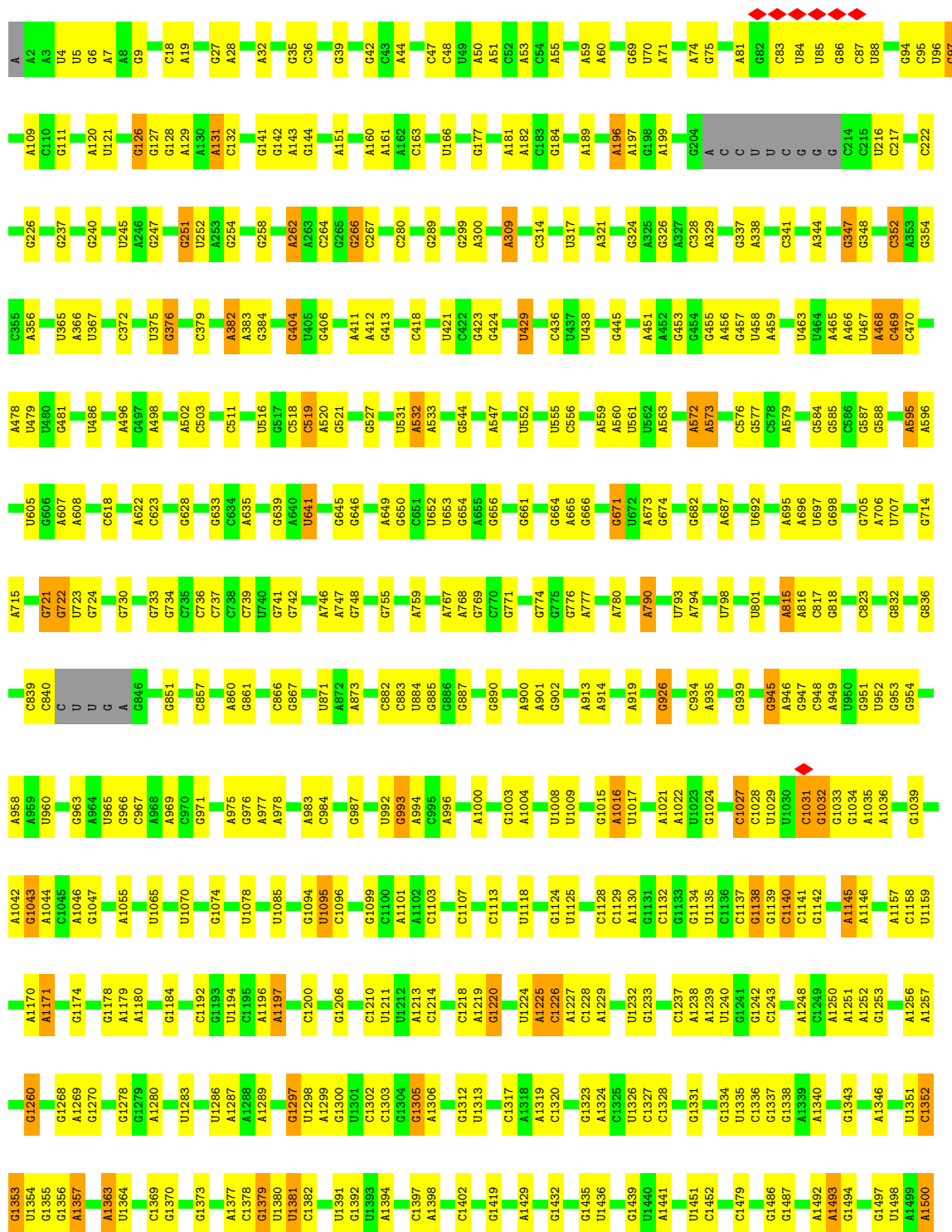
Chain 4:  66% 69% 17% 14%





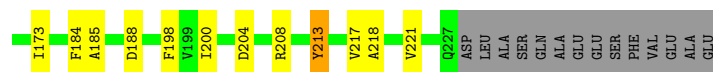
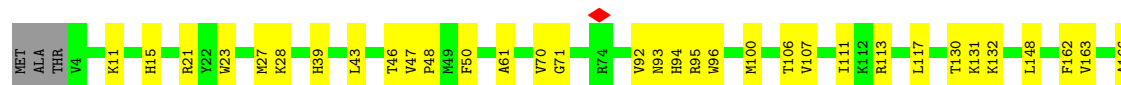
• Molecule 6: 16S rRNA

Chain A: 66% 29%

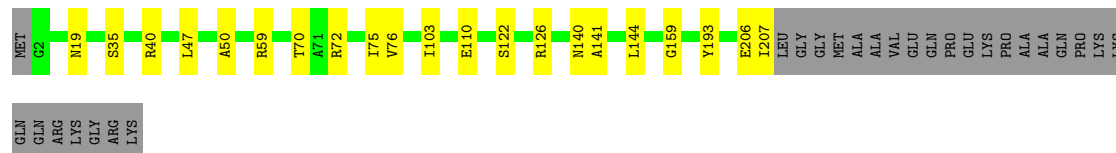




- Molecule 7: Small ribosomal subunit protein uS2



- Molecule 8: Small ribosomal subunit protein uS3



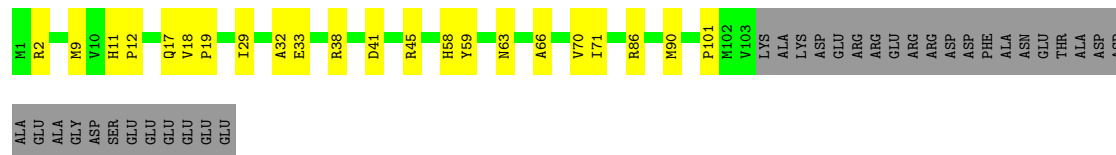
- Molecule 9: Small ribosomal subunit protein uS4



- Molecule 10: Small ribosomal subunit protein uS5

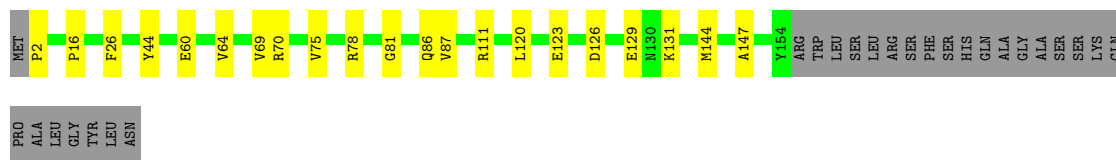


- Molecule 11: Small ribosomal subunit protein bS6, fully modified isoform



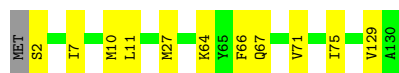
- Molecule 12: Small ribosomal subunit protein uS7

Chain G:  74% 12% 15%




- Molecule 13: Small ribosomal subunit protein uS8

Chain H:  91% 8%



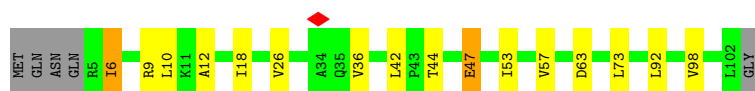
- Molecule 14: Small ribosomal subunit protein uS9

Chain I:  88% 9%




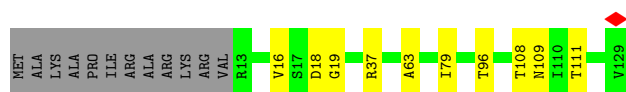
- Molecule 15: Small ribosomal subunit protein uS10

Chain J:  80% 14% 5%




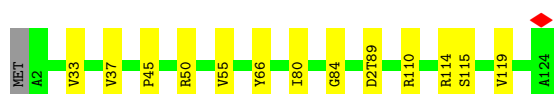
- Molecule 16: Small ribosomal subunit protein uS11

Chain K:  83% 8% 9%



- Molecule 17: Small ribosomal subunit protein uS12

Chain L:  89% 10%



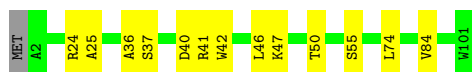
- Molecule 18: Small ribosomal subunit protein uS13

Chain M:  91% 7%



- Molecule 19: Small ribosomal subunit protein uS14

Chain N: 86% 13% .



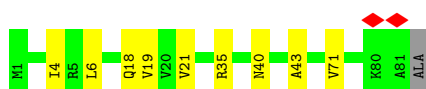
- Molecule 20: Small ribosomal subunit protein uS15

Chain O: 91% 8% .



- Molecule 21: Small ribosomal subunit protein bS16

Chain P: 88% 11% .



- Molecule 22: Small ribosomal subunit protein uS17

Chain Q: 85% 10% 6%



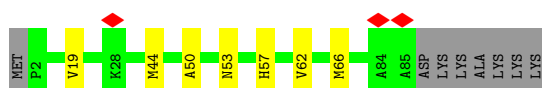
- Molecule 23: Small ribosomal subunit protein bS18

Chain R: 80% 7% 12%



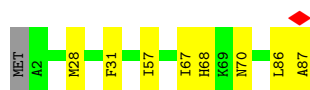
- Molecule 24: Small ribosomal subunit protein uS19

Chain S: 84% 8% 9%

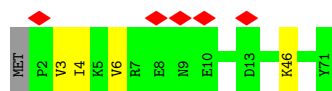
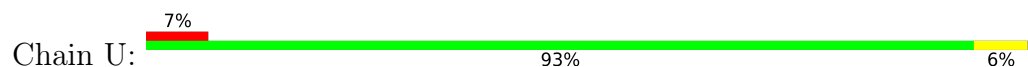


- Molecule 25: Small ribosomal subunit protein bS20

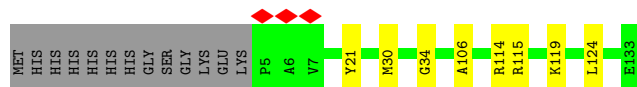
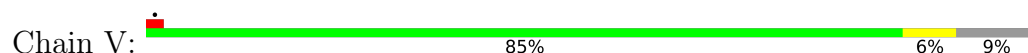
Chain T: 90% 9% .



- Molecule 26: Small ribosomal subunit protein bS21



- Molecule 27: Heat shock protein 15



- Molecule 28: mRNA

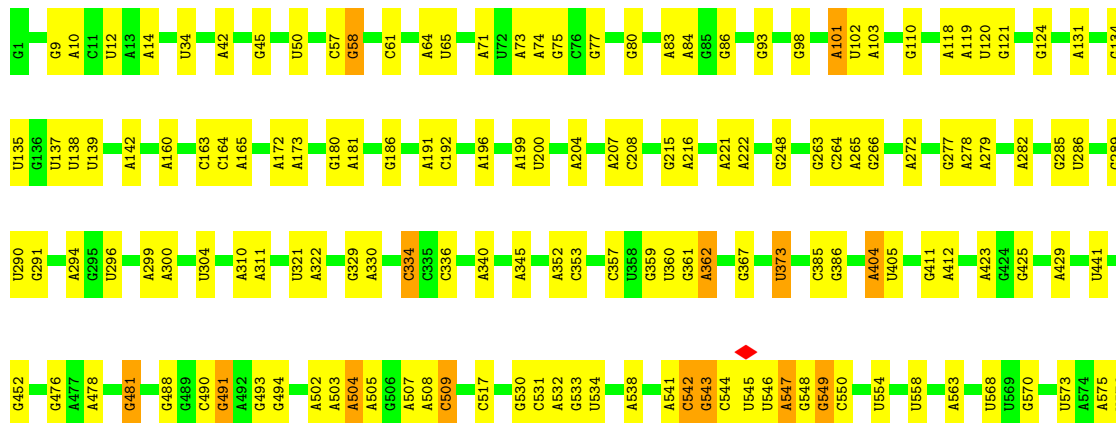


There are no outlier residues recorded for this chain.

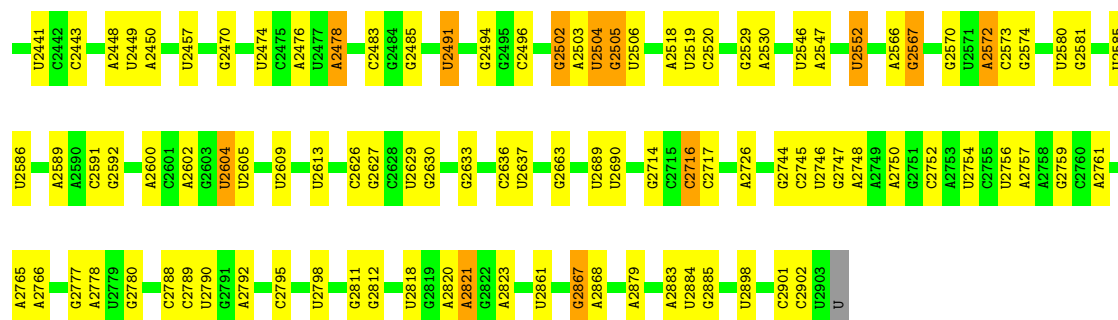
- Molecule 29: tRNA Asp



- Molecule 30: 23S rRNA

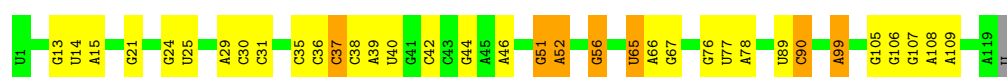






• Molecule 31: 5S rRNA

Chain b: 70% 23% 6% .



• Molecule 32: Large ribosomal subunit protein uL2

Chain c: 93% 6% .



• Molecule 33: Large ribosomal subunit protein uL3

Chain d: 90% 10%



• Molecule 34: Large ribosomal subunit protein uL4

Chain e: 93% 7%



• Molecule 35: Large ribosomal subunit protein uL5

Chain f: 84% 15% .

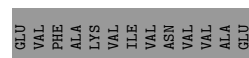
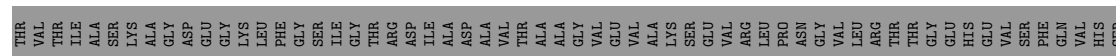
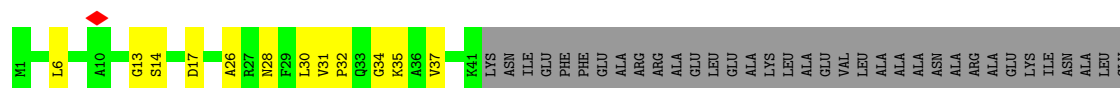


• Molecule 36: Large ribosomal subunit protein uL6

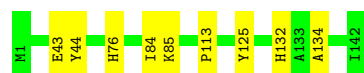
Chain g: 87% 12% .



- Molecule 37: Large ribosomal subunit protein bL9



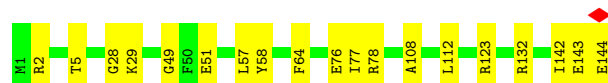
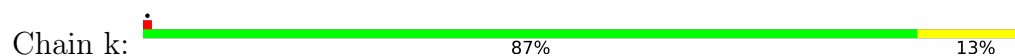
- Molecule 38: Large ribosomal subunit protein uL13



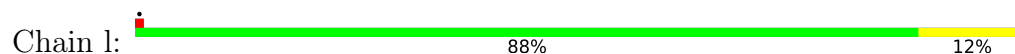
- Molecule 39: Large ribosomal subunit protein uL14



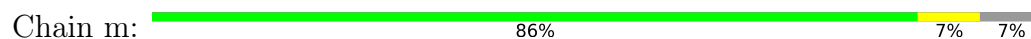
- Molecule 40: Large ribosomal subunit protein uL15



- Molecule 41: Large ribosomal subunit protein uL16



- Molecule 42: Large ribosomal subunit protein bL17





- Molecule 43: Large ribosomal subunit protein uL18

Chain n: 90% 9% ..



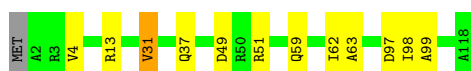
- Molecule 44: Large ribosomal subunit protein bL19

Chain o: 95% ..



- Molecule 45: Large ribosomal subunit protein bL20

Chain p: 89% 9% ..



- Molecule 46: Large ribosomal subunit protein bL21

Chain q: 87% 13% ..



- Molecule 47: Large ribosomal subunit protein uL22

Chain r: 93% 6% ..



- Molecule 48: Large ribosomal subunit protein uL23

Chain s: 82% 11% 7% ..



- Molecule 49: Large ribosomal subunit protein uL24

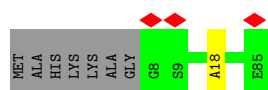
Chain t: 84% 13% ..



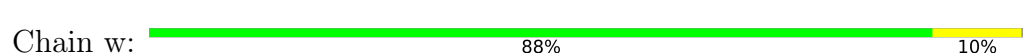
- Molecule 50: Large ribosomal subunit protein bL25



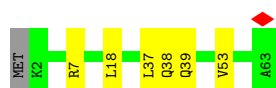
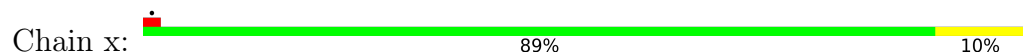
- Molecule 51: Large ribosomal subunit protein bL27



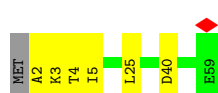
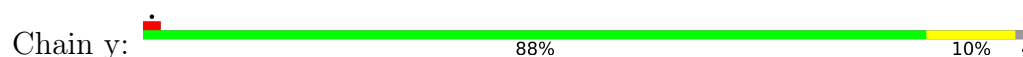
- Molecule 52: Large ribosomal subunit protein bL28



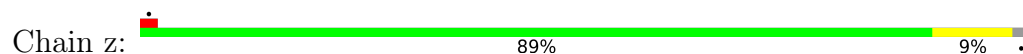
- Molecule 53: Large ribosomal subunit protein uL29



- Molecule 54: Large ribosomal subunit protein uL30



- Molecule 55: Large ribosomal subunit protein bL32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	41043	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32.3	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.342	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	411.36, 411.36, 411.36	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8034375, 0.8034375, 0.8034375	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3TD, 2MG, UR3, 2MA, 5MU, OMG, MG, 1MG, 4D4, 4OC, MA6, 6MZ, OMC, MEQ, PSU, 5MC, IAS, G7M, H2U, OMU, MS6, ZN, D2T

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.59	0/424	0.99	0/565
2	1	0.72	0/380	1.12	0/498
3	2	0.72	0/513	1.22	0/676
4	3	0.67	0/303	1.15	0/397
5	4	0.56	0/488	1.08	3/649 (0.5%)
6	A	0.59	1/36211 (0.0%)	0.97	53/56481 (0.1%)
7	B	0.50	0/1784	1.06	3/2403 (0.1%)
8	C	0.54	0/1651	1.00	0/2225
9	D	0.53	0/1665	1.04	0/2227
10	E	0.55	0/1165	1.02	1/1568 (0.1%)
11	F	0.51	0/858	1.00	0/1160
12	G	0.53	0/1219	1.05	0/1635
13	H	0.54	0/989	1.01	0/1326
14	I	0.57	0/1034	1.09	1/1375 (0.1%)
15	J	0.61	0/796	1.16	1/1077 (0.1%)
16	K	0.55	0/884	0.95	0/1191
17	L	0.61	0/960	1.13	0/1286
18	M	0.55	0/900	1.09	1/1204 (0.1%)
19	N	0.55	0/817	1.05	0/1088
20	O	0.57	0/722	1.10	0/964
21	P	0.52	0/653	1.00	0/877
22	Q	0.57	0/650	1.14	2/871 (0.2%)
23	R	0.52	0/553	1.11	1/742 (0.1%)
24	S	0.55	0/685	1.01	1/922 (0.1%)
25	T	0.54	0/676	1.10	0/895
26	U	0.49	0/597	1.08	0/792
27	V	0.49	0/1070	0.96	0/1435
28	X	0.70	0/72	0.83	0/110
29	Z	0.58	0/1737	0.84	0/2704
30	a	0.61	0/65651	1.03	146/102413 (0.1%)
31	b	0.59	0/2850	0.95	3/4444 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.66	1/2121 (0.0%)	1.10	0/2852
33	d	0.63	0/1576	1.06	3/2119 (0.1%)
34	e	0.60	0/1571	1.04	0/2113
35	f	0.51	0/1434	1.04	0/1926
36	g	0.55	0/1343	1.04	0/1816
37	h	0.57	0/306	1.16	1/413 (0.2%)
38	i	0.61	0/1152	1.04	0/1551
39	j	0.66	0/955	1.13	1/1279 (0.1%)
40	k	0.66	0/1062	1.13	0/1413
41	l	0.60	0/1073	1.05	0/1433
42	m	0.68	1/958 (0.1%)	1.14	0/1281
43	n	0.57	0/902	1.08	0/1209
44	o	0.62	0/929	1.01	0/1242
45	p	0.69	0/960	1.12	3/1278 (0.2%)
46	q	0.60	0/829	1.07	2/1107 (0.2%)
47	r	0.67	0/864	1.12	3/1156 (0.3%)
48	s	0.55	0/744	1.02	0/994
49	t	0.60	0/787	1.06	0/1051
50	u	0.55	0/766	1.02	0/1025
51	v	0.64	0/593	1.08	0/785
52	w	0.65	0/635	1.13	0/848
53	x	0.53	0/502	1.10	1/667 (0.1%)
54	y	0.61	0/453	1.12	0/605
55	z	0.71	0/450	1.09	0/599
All	All	0.59	3/151922 (0.0%)	1.02	230/226962 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	I	0	1
32	c	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1498	UR3	O3'-P	5.34	1.61	1.56
42	m	3	HIS	CG-CD2	-5.09	1.30	1.35
32	c	53	HIS	CG-CD2	-5.08	1.30	1.35

All (230) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	781	A	O3'-P-O5'	-7.76	92.36	104.00
30	a	2060	A	O3'-P-O5'	-7.73	92.40	104.00
30	a	859	G	O3'-P-O5'	-7.70	92.44	104.00
30	a	2066	C	O3'-P-O5'	-7.70	92.46	104.00
30	a	1810	A	O3'-P-O5'	-7.58	92.63	104.00
6	A	196	A	C1'-C2'-O2'	7.57	119.75	108.40
30	a	1212	G	O3'-P-O5'	-7.49	92.77	104.00
30	a	1269	A	O3'-P-O5'	-7.37	92.95	104.00
30	a	1408	G	O3'-P-O5'	-7.35	92.98	104.00
30	a	124	G	O3'-P-O5'	-7.34	93.00	104.00
30	a	385	C	O3'-P-O5'	-7.25	93.13	104.00
6	A	587	G	O3'-P-O5'	-7.24	93.14	104.00
30	a	2519	U	O3'-P-O5'	-7.22	93.16	104.00
30	a	310	A	O3'-P-O5'	-7.21	93.19	104.00
6	A	53	A	O3'-P-O5'	-7.06	93.41	104.00
6	A	883	C	O3'-P-O5'	-7.02	93.47	104.00
30	a	727	A	O3'-P-O5'	-6.88	93.68	104.00
39	j	58	LEU	CA-C-O	-6.85	113.84	121.51
30	a	504	A	O3'-P-O5'	-6.82	93.78	104.00
6	A	181	A	O3'-P-O5'	-6.79	93.81	104.00
30	a	1957	C	O3'-P-O5'	-6.76	93.86	104.00
30	a	134	G	O3'-P-O5'	-6.69	93.96	104.00
30	a	1131	G	O3'-P-O5'	-6.66	94.01	104.00
30	a	1252	G	O3'-P-O5'	-6.66	94.02	104.00
30	a	1190	G	C4'-C3'-C2'	-6.65	95.95	102.60
30	a	1672	A	O3'-P-O5'	-6.64	94.03	104.00
30	a	14	A	O3'-P-O5'	-6.58	94.13	104.00
30	a	1971	U	O3'-P-O5'	-6.56	94.15	104.00
46	q	72	VAL	N-CA-CB	-6.56	102.33	111.25
30	a	404	A	C2'-C3'-O3'	6.52	119.28	109.50
30	a	45	G	O3'-P-O5'	-6.48	94.29	104.00
30	a	204	A	O3'-P-O5'	-6.46	94.31	104.00
22	Q	7	THR	CA-CB-OG1	-6.44	99.93	109.60
30	a	1152	C	O3'-P-O5'	-6.44	94.34	104.00
30	a	1135	C	C4'-C3'-O3'	-6.42	103.37	113.00
30	a	334	C	O3'-P-O5'	-6.41	94.39	104.00
30	a	821	A	C2'-C3'-O3'	-6.41	104.09	113.70
30	a	2589	A	O3'-P-O5'	-6.40	94.41	104.00
6	A	348	G	O3'-P-O5'	-6.39	94.42	104.00
30	a	818	G	O3'-P-O5'	-6.37	94.45	104.00
30	a	1664	A	O3'-P-O5'	-6.37	94.45	104.00
30	a	684	G	O3'-P-O5'	-6.35	94.47	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1354	U	O3'-P-O5'	-6.34	94.49	104.00
5	4	43	PHE	N-CA-CB	6.31	119.39	110.12
31	b	14	U	O3'-P-O5'	-6.29	94.56	104.00
30	a	743	A	O3'-P-O5'	-6.27	94.60	104.00
6	A	1232	U	O3'-P-O5'	-6.26	94.61	104.00
6	A	563	A	O3'-P-O5'	-6.26	94.61	104.00
30	a	1261	C	O3'-P-O5'	-6.25	94.62	104.00
6	A	573	A	C4'-C3'-O3'	-6.25	103.62	113.00
6	A	883	C	C4'-C3'-O3'	-6.25	103.63	113.00
30	a	2581	G	O3'-P-O5'	-6.24	94.64	104.00
6	A	790	A	O3'-P-O5'	-6.22	94.66	104.00
30	a	83	A	C2'-C3'-O3'	-6.19	104.41	113.70
30	a	478	A	O3'-P-O5'	-6.18	94.73	104.00
30	a	1258	U	O3'-P-O5'	-6.16	94.76	104.00
46	q	73	LYS	N-CA-CB	6.14	120.29	110.16
14	I	124	ARG	CB-CA-C	-6.13	99.68	108.88
30	a	2761	A	O3'-P-O5'	-6.13	94.81	104.00
6	A	652	U	C2'-C3'-O3'	6.12	118.67	109.50
6	A	1377	A	O3'-P-O5'	-6.11	94.84	104.00
6	A	196	A	C3'-C2'-O2'	6.08	119.82	110.70
30	a	1331	G	O3'-P-O5'	-6.08	94.89	104.00
30	a	998	C	O3'-P-O5'	-6.07	94.89	104.00
30	a	1326	U	O3'-P-O5'	-6.05	94.93	104.00
6	A	585	G	O3'-P-O5'	-6.04	94.93	104.00
30	a	121	G	O3'-P-O5'	-6.04	94.94	104.00
30	a	83	A	O3'-P-O5'	-6.04	94.94	104.00
30	a	2017	U	C2'-C3'-O3'	-6.03	104.65	113.70
30	a	2094	A	O3'-P-O5'	-6.01	94.98	104.00
30	a	1452	G	O3'-P-O5'	-5.97	95.04	104.00
30	a	1543	G	O3'-P-O5'	-5.95	95.07	104.00
6	A	1500	A	O3'-P-O5'	-5.94	95.09	104.00
30	a	1246	A	O3'-P-O5'	-5.93	95.11	104.00
30	a	1136	G	C4'-C3'-C2'	-5.92	96.68	102.60
30	a	1272	A	O3'-P-O5'	-5.90	95.14	104.00
30	a	1643	G	O3'-P-O5'	-5.89	95.16	104.00
30	a	2049	G	O3'-P-O5'	-5.89	95.17	104.00
30	a	517	C	O3'-P-O5'	-5.88	95.18	104.00
6	A	1355	G	O3'-P-O5'	-5.87	95.20	104.00
30	a	1187	G	O3'-P-O5'	-5.84	95.24	104.00
6	A	730	G	O3'-P-O5'	-5.83	95.25	104.00
18	M	105	ASN	CB-CA-C	-5.82	104.06	111.86
30	a	2336	A	O3'-P-O5'	-5.82	95.27	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	p	13	ARG	CB-CA-C	-5.82	101.74	110.88
30	a	775	G	O3'-P-O5'	-5.82	95.27	104.00
30	a	1790	C	C2'-C3'-O3'	-5.80	105.00	113.70
31	b	65	U	O3'-P-O5'	-5.79	95.31	104.00
30	a	916	G	O3'-P-O5'	-5.79	95.31	104.00
30	a	1895	C	O3'-P-O5'	-5.79	95.32	104.00
30	a	1757	A	C4'-C3'-O3'	-5.76	104.36	113.00
30	a	1162	G	O3'-P-O5'	-5.75	95.38	104.00
30	a	373	U	O3'-P-O5'	-5.74	95.39	104.00
30	a	180	G	O3'-P-O5'	-5.74	95.39	104.00
30	a	781	A	C4'-C3'-O3'	-5.74	104.40	113.00
30	a	1016	G	O3'-P-O5'	-5.73	95.41	104.00
22	Q	34	TYR	N-CA-CB	-5.72	101.71	110.12
6	A	1357	A	C2'-C3'-O3'	-5.72	105.12	113.70
47	r	110	ARG	CD-NE-CZ	5.72	132.40	124.40
30	a	2519	U	C1'-C2'-O2'	-5.70	103.25	111.80
30	a	2051	A	O3'-P-O5'	-5.70	95.45	104.00
30	a	2600	A	O3'-P-O5'	-5.70	95.45	104.00
30	a	1135	C	C2'-C3'-O3'	5.68	122.23	113.70
30	a	1778	U	O3'-P-O5'	-5.68	95.48	104.00
6	A	126	G	O3'-P-O5'	-5.68	95.48	104.00
30	a	1598	A	O3'-P-O5'	-5.67	95.50	104.00
47	r	95	ARG	N-CA-CB	5.65	118.27	109.97
30	a	1398	C	O3'-P-O5'	-5.64	95.53	104.00
6	A	1352	C	O3'-P-O5'	-5.64	95.54	104.00
30	a	321	U	O3'-P-O5'	-5.64	95.54	104.00
6	A	816	A	O3'-P-O5'	-5.62	95.57	104.00
30	a	2423	U	O3'-P-O5'	-5.62	95.57	104.00
30	a	9	G	O3'-P-O5'	-5.60	95.60	104.00
30	a	2074	U	O3'-P-O5'	-5.60	95.60	104.00
6	A	579	A	O3'-P-O5'	-5.59	95.61	104.00
30	a	1168	G	O3'-P-O5'	-5.59	95.61	104.00
30	a	1759	A	O3'-P-O5'	-5.59	95.62	104.00
30	a	1664	A	C4'-C3'-O3'	-5.56	104.66	113.00
30	a	2572	A	O3'-P-O5'	-5.56	95.66	104.00
30	a	1482	G	O3'-P-O5'	-5.55	95.67	104.00
33	d	12	THR	CA-C-O	-5.55	115.47	121.36
6	A	1237	C	OP2-P-O3'	-5.55	91.36	108.00
30	a	2879	A	O3'-P-O5'	-5.54	95.68	104.00
6	A	866	C	O3'-P-O5'	-5.54	95.69	104.00
30	a	2210	U	O3'-P-O5'	-5.52	95.72	104.00
30	a	2020	A	C4'-C3'-O3'	-5.50	104.74	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	1566	A	O3'-P-O5'	-5.50	95.75	104.00
30	a	1565	C	O3'-P-O5'	-5.49	95.76	104.00
47	r	59	GLU	CB-CA-C	-5.48	101.70	110.79
30	a	652	U	O3'-P-O5'	-5.47	95.80	104.00
30	a	763	G	C4'-C3'-O3'	-5.46	104.81	113.00
30	a	1816	C	O3'-P-O5'	-5.46	95.82	104.00
30	a	1909	C	O3'-P-O5'	-5.45	95.82	104.00
30	a	2546	U	O3'-P-O5'	-5.44	95.84	104.00
6	A	1278	G	O3'-P-O5'	-5.40	95.90	104.00
30	a	554	U	O3'-P-O5'	-5.38	95.93	104.00
30	a	1436	G	O3'-P-O5'	-5.38	95.94	104.00
30	a	2633	G	O3'-P-O5'	-5.38	95.94	104.00
30	a	2386	A	O3'-P-O5'	-5.37	95.95	104.00
30	a	2717	C	O3'-P-O5'	-5.36	95.97	104.00
30	a	1453	A	O3'-P-O5'	-5.35	95.97	104.00
6	A	1107	C	O3'-P-O5'	-5.35	95.98	104.00
30	a	2754	U	O3'-P-O5'	-5.34	95.99	104.00
30	a	1240	U	C4'-C3'-O3'	-5.34	104.99	113.00
30	a	1710	G	O3'-P-O5'	-5.34	95.99	104.00
6	A	1297	G	C1'-O4'-C4'	-5.33	104.37	109.70
6	A	1523	G	O3'-P-O5'	-5.33	96.00	104.00
30	a	429	A	O3'-P-O5'	-5.33	96.00	104.00
30	a	1983	G	O3'-P-O5'	-5.33	96.01	104.00
30	a	2821	A	O3'-P-O5'	-5.32	96.02	104.00
6	A	1192	C	O3'-P-O5'	-5.32	96.03	104.00
45	p	13	ARG	N-CA-CB	5.32	117.72	110.01
30	a	2867	G	O3'-P-O5'	-5.31	96.04	104.00
30	a	296	U	O3'-P-O5'	-5.30	96.05	104.00
30	a	662	G	O3'-P-O5'	-5.30	96.05	104.00
30	a	1610	A	C2'-C3'-O3'	5.30	117.45	109.50
30	a	491	G	O3'-P-O5'	-5.30	96.05	104.00
30	a	1630	A	C4'-C3'-C2'	-5.29	97.31	102.60
30	a	2496	C	O3'-P-O5'	-5.29	96.06	104.00
10	E	31	PHE	CA-CB-CG	-5.28	108.52	113.80
30	a	488	G	O3'-P-O5'	-5.28	96.08	104.00
30	a	2287	A	O3'-P-O5'	-5.28	96.08	104.00
30	a	1278	C	O3'-P-O5'	-5.27	96.10	104.00
6	A	1145	A	C1'-O4'-C4'	-5.27	104.43	109.70
6	A	746	A	O3'-P-O5'	-5.26	96.11	104.00
6	A	1129	C	O3'-P-O5'	-5.25	96.12	104.00
53	x	38	GLN	N-CA-C	-5.25	105.95	112.93
6	A	314	C	O3'-P-O5'	-5.25	96.12	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	2272	U	C2'-C3'-O3'	-5.25	105.83	113.70
30	a	1237	A	O3'-P-O5'	-5.25	96.13	104.00
45	p	31	VAL	N-CA-CB	-5.24	104.13	111.25
24	S	53	ASN	N-CA-C	-5.24	106.67	113.16
6	A	913	A	O3'-P-O5'	-5.23	96.15	104.00
30	a	822	G	O3'-P-O5'	-5.23	96.15	104.00
30	a	1154	G	C2'-C3'-O3'	-5.23	105.85	113.70
5	4	41	HIS	CA-C-N	5.23	124.85	119.05
5	4	41	HIS	C-N-CA	5.23	124.85	119.05
30	a	336	C	O3'-P-O5'	-5.22	96.17	104.00
6	A	771	G	O3'-P-O5'	-5.21	96.19	104.00
6	A	1369	C	O3'-P-O5'	-5.20	96.20	104.00
6	A	379	C	O3'-P-O5'	-5.20	96.20	104.00
30	a	1344	U	O3'-P-O5'	-5.20	96.20	104.00
6	A	356	A	C4'-C3'-C2'	-5.19	97.41	102.60
6	A	455	G	O3'-P-O5'	-5.18	96.22	104.00
6	A	595	A	O3'-P-O5'	-5.18	96.22	104.00
6	A	1055	A	O3'-P-O5'	-5.18	96.23	104.00
30	a	299	A	O3'-P-O5'	-5.18	96.23	104.00
30	a	1485	U	O3'-P-O5'	-5.18	96.23	104.00
7	B	213	TYR	N-CA-CB	5.18	118.98	110.39
30	a	840	C	O3'-P-O5'	-5.18	96.24	104.00
33	d	141	ARG	CB-CA-C	-5.18	102.63	111.02
6	A	561	U	O3'-P-O5'	-5.17	96.24	104.00
30	a	2777	G	O3'-P-O5'	-5.17	96.24	104.00
30	a	2245	U	C4'-C3'-O3'	-5.17	105.24	113.00
30	a	576	U	O3'-P-O5'	-5.17	96.25	104.00
33	d	157	LYS	N-CA-CB	5.17	117.63	110.04
30	a	1959	G	O3'-P-O5'	-5.16	96.26	104.00
30	a	1293	C	O3'-P-O5'	-5.16	96.26	104.00
30	a	1693	U	O3'-P-O5'	-5.15	96.27	104.00
30	a	1843	C	O3'-P-O5'	-5.15	96.27	104.00
30	a	137	U	O3'-P-O5'	-5.15	96.27	104.00
7	B	21	ARG	CB-CA-C	-5.14	102.27	110.79
31	b	77	U	O3'-P-O5'	-5.14	96.30	104.00
30	a	1823	G	C4'-C3'-C2'	-5.13	97.47	102.60
30	a	509	C	C4'-C3'-O3'	-5.13	105.30	113.00
7	B	162	PHE	CA-CB-CG	-5.13	108.67	113.80
30	a	2483	C	O3'-P-O5'	-5.13	96.31	104.00
30	a	1696	G	O3'-P-O5'	-5.10	96.34	104.00
6	A	97	G	O3'-P-O5'	-5.10	96.35	104.00
30	a	1254	A	C4'-C3'-O3'	-5.10	105.35	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	h	13	GLY	N-CA-C	5.10	117.93	110.38
30	a	2502	G	C4'-C3'-O3'	-5.10	105.35	113.00
30	a	2016	U	C2'-C3'-O3'	-5.10	106.06	113.70
6	A	347	G	O3'-P-O5'	-5.09	96.36	104.00
6	A	1225	A	C2'-C3'-O3'	-5.09	106.06	113.70
30	a	1611	C	O3'-P-O5'	-5.09	96.37	104.00
6	A	722	G	O3'-P-O5'	-5.08	96.38	104.00
30	a	542	C	O3'-P-O5'	-5.07	96.39	104.00
6	A	1043	G	O3'-P-O5'	-5.07	96.40	104.00
6	A	1197	A	O3'-P-O5'	-5.07	96.40	104.00
30	a	1355	G	O3'-P-O5'	-5.05	96.42	104.00
6	A	815	A	O3'-P-O5'	-5.04	96.43	104.00
15	J	47	GLU	CB-CA-C	5.04	118.36	110.19
30	a	2485	G	O3'-P-O5'	-5.04	96.44	104.00
30	a	73	A	O3'-P-O5'	-5.02	96.47	104.00
6	A	1194	U	O3'-P-O5'	-5.02	96.47	104.00
23	R	25	ASP	CA-CB-CG	5.02	117.62	112.60
30	a	452	G	O3'-P-O5'	-5.01	96.49	104.00
6	A	900	A	O3'-P-O5'	-5.01	96.49	104.00
30	a	589	U	O3'-P-O5'	-5.01	96.49	104.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	I	122	ARG	Sidechain
32	c	189	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	417	441	451	1	0
2	1	377	411	418	0	0
3	2	504	561	572	5	0
4	3	302	337	340	2	0
5	4	480	468	478	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	32590	14865	16421	115	0
7	B	1753	1751	1780	27	0
8	C	1624	1669	1696	14	0
9	D	1643	1679	1707	11	0
10	E	1152	1177	1196	5	0
11	F	839	814	833	15	0
12	G	1203	1234	1254	16	0
13	H	979	1015	1031	8	0
14	I	1022	1053	1070	7	0
15	J	786	815	828	11	0
16	K	877	865	883	8	0
17	L	957	994	1015	7	0
18	M	891	935	952	6	0
19	N	805	832	844	8	0
20	O	714	716	734	4	0
21	P	643	652	661	5	0
22	Q	641	668	682	6	0
23	R	544	550	565	4	0
24	S	668	677	693	3	0
25	T	670	710	719	4	0
26	U	589	620	629	4	0
27	V	1053	1066	1084	6	0
28	X	65	30	34	0	0
29	Z	1557	714	789	9	0
30	a	59130	26982	29769	161	0
31	b	2549	1171	1291	14	0
32	c	2082	2114	2154	9	0
33	d	1566	1586	1618	10	0
34	e	1552	1590	1619	9	0
35	f	1410	1421	1444	18	0
36	g	1323	1347	1371	11	0
37	h	303	324	327	9	0
38	i	1129	1137	1162	6	0
39	j	946	1008	1023	7	0
40	k	1053	1111	1129	14	0
41	l	1075	1142	1145	13	0
42	m	945	971	989	4	0
43	n	892	908	923	7	0
44	o	917	947	962	4	0
45	p	947	1008	1019	9	0
46	q	816	825	839	9	0
47	r	857	904	922	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	s	738	795	807	6	0
49	t	779	823	831	11	0
50	u	753	770	780	6	0
51	v	586	586	596	1	0
52	w	625	638	652	5	0
53	x	501	526	531	3	0
54	y	449	479	488	4	0
55	z	444	443	458	4	0
56	3	1	0	0	0	0
56	4	1	0	0	0	0
57	A	71	0	0	0	0
57	N	1	0	0	0	0
57	a	201	0	0	0	0
57	b	5	0	0	0	0
57	c	1	0	0	0	0
57	d	1	0	0	0	0
57	z	1	0	0	0	0
58	Z	8	6	3	1	0
All	All	141003	89881	95211	599	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 (599) 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)
7:B:166:ALA:HB2	7:B:185:ALA:HB1	1.75	0.67
15:J:57:VAL:HG12	15:J:57:VAL:O	1.94	0.66
30:a:568:U:H1'	30:a:2030:6MZ:H9C1	1.76	0.66
35:f:126:GLY:HA2	35:f:163:ASP:HA	1.78	0.66
48:s:92:ASN:O	48:s:93:LEU:C	2.39	0.65
6:A:697:U:H5''	27:V:34:GLY:O	1.97	0.65
6:A:945:G:C2	6:A:946:A:C8	2.85	0.64
6:A:946:A:H2'	6:A:947:G:C8	2.32	0.64
30:a:2327:A:H2'	30:a:2328:A:C8	2.33	0.63
6:A:127:G:H4'	22:Q:6:ARG:NH1	2.14	0.63
6:A:823:C:HO2'	13:H:2:SER:N	1.97	0.63
6:A:309:A:O2'	6:A:607:A:N1	2.30	0.62
29:Z:76:A:O3'	58:Z:101:ASP:C	2.43	0.62
30:a:2395:C:H2'	30:a:2396:G:O4'	2.01	0.61
35:f:44:ILE:HD11	35:f:85:ILE:HG12	1.80	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2020:A:H5'	55:z:9:THR:CG2	2.31	0.61
13:H:11:LEU:HD22	13:H:75:ILE:HD11	1.83	0.61
6:A:404:G:N7	9:D:2:ALA:HB3	2.14	0.61
5:4:47:LYS:O	5:4:48:GLN:C	2.43	0.61
48:s:61:LEU:HD12	48:s:61:LEU:C	2.26	0.60
15:J:42:LEU:HD22	15:J:73:LEU:HD23	1.82	0.60
31:b:29:A:C2	31:b:30:C:C2	2.90	0.60
41:l:20:LEU:HD13	50:u:81:PRO:HG2	1.84	0.60
41:l:53:MET:HE1	41:l:103:TYR:CD2	2.37	0.60
30:a:1266:G:O2'	30:a:2012:G:O6	2.18	0.60
48:s:71:GLY:O	48:s:72:GLN:HG2	2.03	0.59
29:Z:56:C:O2'	35:f:75:ALA:N	2.36	0.59
32:c:107:PRO:HD2	32:c:110:LEU:HD22	1.84	0.59
35:f:38:MET:HE2	35:f:150:ARG:HB2	1.84	0.59
41:l:66:ARG:NH1	41:l:104:GLU:OE2	2.35	0.59
6:A:1251:A:H2'	6:A:1252:A:O4'	2.03	0.58
37:h:34:GLY:O	37:h:35:LYS:HB2	2.03	0.58
49:t:12:ILE:CG2	49:t:80:ALA:HB2	2.34	0.58
40:k:77:ILE:CD1	40:k:108:ALA:HB1	2.34	0.58
6:A:19:A:O2'	6:A:572:A:N1	2.37	0.58
23:R:26:ILE:HD11	23:R:67:LEU:HB3	1.84	0.58
48:s:88:LYS:HB2	48:s:91:GLN:HE22	1.68	0.58
24:S:50:ALA:HB1	24:S:57:HIS:HB3	1.86	0.58
6:A:160:A:H2'	6:A:161:A:O4'	2.04	0.58
43:n:82:ALA:HB3	43:n:115:LEU:HD21	1.85	0.57
6:A:948:C:OP1	18:M:108:THR:HG22	2.04	0.57
30:a:2291:U:H2'	30:a:2292:U:C6	2.38	0.57
6:A:404:G:N7	9:D:2:ALA:CB	2.67	0.57
15:J:12:ALA:HB3	15:J:18:ILE:HG12	1.86	0.57
6:A:1103:C:O2	7:B:106:THR:HG21	2.04	0.57
4:3:16:ILE:HD13	4:3:25:VAL:HG22	1.86	0.57
30:a:897:C:H2'	30:a:898:C:C6	2.40	0.56
6:A:635:A:O2'	22:Q:6:ARG:NH1	2.39	0.56
19:N:37:SER:HB3	19:N:40:ASP:CG	2.31	0.56
29:Z:21:A:H61	29:Z:46:G:H2'	1.71	0.56
7:B:50:PHE:HD1	7:B:200:ILE:HG21	1.71	0.56
30:a:290:U:H2'	30:a:291:G:O4'	2.05	0.56
23:R:73:ARG:O	23:R:74:HIS:C	2.49	0.56
8:C:110:GLU:HB2	8:C:144:LEU:HD12	1.86	0.56
16:K:108:THR:O	26:U:6:VAL:N	2.39	0.55
35:f:38:MET:HE3	35:f:152:LEU:HD11	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:j:58:LEU:HA	39:j:89:ASN:HD22	1.72	0.55
30:a:263:G:H2'	30:a:264:C:O4'	2.07	0.55
6:A:1226:C:H2'	18:M:102:THR:HB	1.89	0.55
13:H:66:PHE:CD2	13:H:67:GLN:HG2	2.41	0.55
29:Z:18:G:O2'	29:Z:57:G:N2	2.39	0.55
6:A:860:A:H2'	6:A:861:G:O4'	2.07	0.55
11:F:66:ALA:HB3	11:F:71:ILE:HD11	1.89	0.55
13:H:7:ILE:O	13:H:11:LEU:HG	2.07	0.55
30:a:548:G:H2'	30:a:549:G:H1'	1.88	0.55
30:a:1870:C:O2'	30:a:1871:A:O4'	2.24	0.55
30:a:2756:U:H1'	30:a:2757:A:H5''	1.88	0.55
33:d:35:THR:HG22	33:d:73:VAL:HG21	1.88	0.54
8:C:206:GLU:O	8:C:207:ILE:C	2.50	0.54
11:F:66:ALA:HB1	11:F:70:VAL:HG11	1.89	0.54
40:k:123:ARG:HA	40:k:143:GLU:HB2	1.89	0.54
6:A:1305:G:N2	6:A:1331:G:H1'	2.22	0.54
40:k:77:ILE:HD13	40:k:108:ALA:HB1	1.88	0.54
17:L:110:ARG:HB3	17:L:119:VAL:HG21	1.90	0.54
31:b:24:G:N7	31:b:56:G:H2'	2.22	0.54
6:A:382:A:H2'	6:A:383:A:C8	2.43	0.54
30:a:2328:A:H2'	30:a:2329:U:C6	2.43	0.54
8:C:70:THR:HG21	8:C:76:VAL:CG2	2.38	0.54
36:g:89:LEU:HD22	36:g:162:VAL:HG22	1.90	0.54
6:A:404:G:O2'	6:A:498:A:N1	2.38	0.54
38:i:76:HIS:CE1	38:i:85:LYS:HB2	2.43	0.54
6:A:1027:C:C4	6:A:1028:C:C4	2.96	0.54
38:i:43:GLU:O	38:i:44:TYR:C	2.51	0.54
6:A:1530:G:N7	26:U:46:LYS:NZ	2.55	0.53
12:G:75:VAL:HG11	12:G:86:GLN:HB3	1.90	0.53
30:a:2038:G:H2'	30:a:2039:U:O4'	2.07	0.53
44:o:100:LEU:HD11	44:o:110:ILE:HD11	1.88	0.53
16:K:18:ASP:OD2	16:K:37:ARG:NH1	2.41	0.53
30:a:2271:G:OP1	51:v:18:ALA:HB1	2.09	0.53
32:c:29:PRO:HG2	32:c:34:LEU:HD11	1.90	0.53
30:a:1607:C:H4'	30:a:1608:A:O5'	2.08	0.53
49:t:12:ILE:HG21	49:t:80:ALA:HB2	1.90	0.53
30:a:930:G:H1'	54:y:25:LEU:HD11	1.89	0.53
20:O:18:ASP:OD1	20:O:19:ALA:N	2.42	0.53
37:h:34:GLY:O	37:h:35:LYS:CB	2.56	0.53
49:t:45:HIS:ND1	49:t:58:ILE:HG12	2.23	0.53
14:I:57:MET:HE1	14:I:90:TYR:CZ	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1778:U:H2'	30:a:1784:A:N6	2.24	0.53
6:A:254:G:H21	22:Q:18:GLU:HG3	1.74	0.53
7:B:130:THR:O	7:B:131:LYS:HB3	2.09	0.52
30:a:549:G:H2'	30:a:550:C:C6	2.44	0.52
40:k:78:ARG:HH21	40:k:78:ARG:HG3	1.74	0.52
27:V:21:TYR:CE1	27:V:30:MET:HG3	2.44	0.52
41:l:78:LEU:HD23	41:l:79:ALA:N	2.24	0.52
6:A:502:A:H2'	6:A:503:C:O4'	2.09	0.52
30:a:2065:C:H4'	30:a:2251:OMG:HM22	1.92	0.52
7:B:166:ALA:HB1	7:B:173:ILE:HD11	1.91	0.52
30:a:84:A:N1	30:a:98:G:O2'	2.36	0.52
6:A:451:A:H61	6:A:481:G:H5'	1.73	0.52
14:I:6:TYR:O	14:I:20:PHE:HA	2.09	0.52
21:P:18:GLN:OE1	21:P:35:ARG:NE	2.32	0.52
30:a:543:G:H8	30:a:543:G:H5''	1.73	0.52
30:a:644:A:H2'	30:a:645:C:O4'	2.09	0.52
12:G:129:GLU:HB2	12:G:131:LYS:HG2	1.90	0.52
6:A:780:A:C2	6:A:801:U:C5	2.98	0.52
30:a:896:A:H3'	30:a:897:C:H4'	1.91	0.52
6:A:552:U:O3'	17:L:84:GLY:HA3	2.10	0.52
36:g:23:VAL:HG22	36:g:36:THR:HG22	1.92	0.51
5:4:2:LYS:HE3	31:b:40:U:H2'	1.92	0.51
6:A:467:U:H3'	6:A:468:A:H5''	1.91	0.51
7:B:47:VAL:N	7:B:48:PRO:HD2	2.25	0.51
12:G:123:GLU:HA	12:G:126:ASP:OD2	2.09	0.51
43:n:41:ALA:HB2	43:n:48:LEU:HD21	1.92	0.51
8:C:76:VAL:HG11	8:C:103:ILE:HD12	1.91	0.51
45:p:97:ASP:OD2	46:q:13:ARG:NE	2.43	0.51
52:w:10:LYS:HE3	52:w:54:LYS:HD2	1.91	0.51
25:T:31:PHE:CD2	25:T:57:ILE:HD13	2.45	0.51
6:A:1269:A:H1'	6:A:1326:U:H1'	1.93	0.51
33:d:121:THR:HB	33:d:127:PHE:CD2	2.46	0.51
20:O:42:HIS:C	20:O:42:HIS:CD2	2.89	0.51
36:g:95:ARG:HD2	36:g:128:GLN:NE2	2.26	0.51
40:k:2:ARG:H	40:k:5:THR:HG1	1.57	0.51
46:q:5:PHE:HB3	46:q:59:ILE:HD12	1.93	0.51
12:G:75:VAL:HG21	12:G:144:MET:HB3	1.93	0.51
22:Q:58:VAL:HB	22:Q:80:GLU:HB2	1.93	0.51
6:A:502:A:OP1	17:L:115:SER:HB3	2.11	0.51
49:t:14:LEU:HD11	49:t:71:ALA:HB2	1.93	0.51
6:A:951:G:C6	6:A:952:U:C4	3.00	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:35:GLU:OE2	9:D:45:LYS:HE2	2.11	0.50
42:m:28:LEU:HD23	42:m:48:VAL:HG21	1.93	0.50
3:2:45:ARG:N	3:2:46:PRO:HD2	2.26	0.50
7:B:96:TRP:CZ2	7:B:100:MET:HB3	2.46	0.50
11:F:18:VAL:HB	11:F:19:PRO:HD3	1.93	0.50
30:a:1853:A:N1	30:a:2087:G:H1'	2.26	0.50
30:a:547:A:H4'	30:a:548:G:O4'	2.11	0.50
30:a:580:U:O3'	45:p:31:VAL:HG13	2.11	0.50
6:A:337:G:H2'	6:A:338:A:C8	2.47	0.50
30:a:1421:G:C2	30:a:1422:G:C8	2.99	0.50
30:a:1544:A:H2'	30:a:1545:A:C8	2.47	0.50
30:a:2006:C:O2'	30:a:2823:A:N3	2.44	0.50
6:A:993:G:H2'	6:A:993:G:N3	2.27	0.50
30:a:1042:G:C6	30:a:1043:C:C4	3.00	0.50
30:a:1111:A:N3	30:a:1112:G:H1'	2.26	0.50
6:A:1352:C:H2'	6:A:1353:G:C8	2.47	0.50
30:a:1338:G:O2'	30:a:1393:A:N1	2.37	0.50
30:a:2636:C:H2'	30:a:2637:U:C6	2.46	0.50
50:u:48:MET:SD	50:u:86:LEU:HG	2.51	0.50
7:B:188:ASP:HB2	7:B:204:ASP:OD2	2.12	0.49
7:B:61:ALA:HB2	7:B:221:VAL:HG23	1.93	0.49
7:B:111:ILE:HG12	7:B:148:LEU:HD13	1.95	0.49
14:I:10:GLY:HA3	14:I:78:ALA:O	2.12	0.49
34:e:149:ILE:HG22	34:e:192:ALA:HB1	1.94	0.49
44:o:22:PRO:HD3	44:o:50:ILE:HD12	1.94	0.49
23:R:71:THR:HG23	23:R:74:HIS:H	1.76	0.49
30:a:1182:G:H2'	30:a:1183:U:O4'	2.12	0.49
30:a:1225:G:OP1	46:q:71:LYS:NZ	2.43	0.49
43:n:12:THR:O	43:n:13:ARG:C	2.55	0.49
6:A:1078:U:C2	10:E:90:THR:HG21	2.47	0.49
7:B:23:TRP:CG	7:B:39:HIS:HE2	2.30	0.49
15:J:26:VAL:HG23	15:J:36:VAL:HG21	1.94	0.49
6:A:109:A:H2'	6:A:326:G:N2	2.28	0.49
9:D:35:GLU:OE2	9:D:45:LYS:CE	2.61	0.49
16:K:19:GLY:HA3	16:K:79:ILE:HD13	1.95	0.49
24:S:62:VAL:HA	24:S:66:MET:HE2	1.95	0.49
30:a:2898:U:O2	38:i:134:ALA:HB1	2.12	0.49
8:C:50:ALA:HA	8:C:75:ILE:HD11	1.95	0.49
3:2:54:ASP:HB3	40:k:57:LEU:HD22	1.95	0.49
6:A:721:G:H4'	6:A:722:G:O4'	2.12	0.49
30:a:984:A:N3	30:a:984:A:H2'	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1405:U:H2'	30:a:1406:U:C6	2.48	0.49
18:M:107:ARG:O	18:M:108:THR:C	2.56	0.48
46:q:74:ILE:N	46:q:74:ILE:HD12	2.28	0.48
48:s:49:LYS:HD3	48:s:50:LEU:HD23	1.94	0.48
6:A:1435:G:H2'	6:A:1436:U:C6	2.48	0.48
30:a:570:G:H2'	30:a:2030:6MZ:N7	2.28	0.48
54:y:2:ALA:O	54:y:3:LYS:C	2.56	0.48
6:A:466:A:C2	6:A:468:A:C4	3.02	0.48
6:A:1379:G:N7	12:G:2:PRO:N	2.61	0.48
30:a:2491:U:H5''	30:a:2570:G:H5''	1.94	0.48
38:i:84:ILE:HG23	38:i:84:ILE:O	2.13	0.48
39:j:70:ARG:HG2	39:j:76:VAL:HG22	1.95	0.48
41:l:53:MET:HE1	41:l:103:TYR:CG	2.49	0.48
36:g:42:GLU:HB3	36:g:44:LYS:HE2	1.96	0.48
30:a:624:C:O2'	30:a:657:U:OP1	2.30	0.48
30:a:657:U:H2'	30:a:658:U:C6	2.48	0.48
49:t:86:ARG:O	49:t:93:VAL:HG22	2.13	0.48
53:x:37:LEU:HG	53:x:39:GLN:O	2.14	0.48
6:A:1158:C:O2'	7:B:132:LYS:NZ	2.42	0.48
6:A:1225:A:H2'	6:A:1225:A:N3	2.27	0.48
31:b:42:C:C6	35:f:66:LEU:HB2	2.49	0.48
6:A:706:A:C6	6:A:707:U:C4	3.02	0.48
7:B:92:VAL:HG21	7:B:96:TRP:HE3	1.79	0.48
21:P:4:ILE:HG22	21:P:71:VAL:HG11	1.96	0.48
35:f:44:ILE:HD11	35:f:85:ILE:HG23	1.95	0.47
6:A:1356:G:H2'	6:A:1357:A:C8	2.49	0.47
35:f:151:GLY:C	35:f:152:LEU:HD12	2.39	0.47
43:n:49:VAL:HG21	43:n:82:ALA:HA	1.96	0.47
6:A:299:G:H2'	6:A:300:A:C8	2.49	0.47
21:P:6:LEU:CD2	21:P:19:VAL:HG22	2.45	0.47
6:A:126:G:OP1	6:A:605:U:O2'	2.24	0.47
7:B:70:VAL:HB	7:B:163:VAL:HG22	1.96	0.47
8:C:159:GLY:HA2	8:C:193:TYR:CG	2.49	0.47
53:x:18:LEU:HB2	53:x:53:VAL:HG11	1.96	0.47
6:A:1351:U:H2'	6:A:1352:C:C6	2.49	0.47
8:C:35:SER:OG	8:C:59:ARG:NH2	2.48	0.47
11:F:101:PRO:HG2	23:R:25:ASP:HB2	1.96	0.47
30:a:481:G:C4	30:a:507:A:C2	3.03	0.47
7:B:213:TYR:O	7:B:217:VAL:HG23	2.15	0.47
30:a:1678:A:H2'	30:a:1679:A:O4'	2.15	0.47
7:B:148:LEU:HD12	7:B:148:LEU:O	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:126:ASP:HB2	12:G:131:LYS:HG3	1.97	0.46
30:a:77:G:O3'	53:x:7:ARG:NH2	2.48	0.46
6:A:698:G:O5'	6:A:698:G:H8	1.98	0.46
6:A:1178:G:H3'	14:I:99:ARG:HH12	1.80	0.46
30:a:1020:A:N1	30:a:1141:U:O2'	2.37	0.46
6:A:469:C:H2'	6:A:470:C:O4'	2.15	0.46
9:D:124:MET:HE3	9:D:146:ARG:HG2	1.98	0.46
30:a:322:A:OP2	34:e:163:ASN:HB2	2.16	0.46
30:a:534:U:O2'	45:p:49:ASP:OD2	2.33	0.46
6:A:131:A:H2'	6:A:132:C:C6	2.50	0.46
11:F:11:HIS:ND1	11:F:12:PRO:HD2	2.30	0.46
25:T:86:LEU:O	25:T:87:ALA:C	2.58	0.46
30:a:172:A:H2'	30:a:173:A:C8	2.50	0.46
30:a:493:G:H2'	30:a:494:G:O4'	2.15	0.46
33:d:110:THR:CG2	33:d:202:ILE:HB	2.45	0.46
37:h:26:ALA:HA	37:h:30:LEU:HB2	1.96	0.46
40:k:49:GLY:O	40:k:51:GLU:HG3	2.15	0.46
6:A:429:U:H3'	9:D:9:LEU:HD12	1.98	0.46
30:a:494:G:H4'	47:r:6:LYS:HB2	1.97	0.46
30:a:2032:G:C8	33:d:150:MEQ:HE3	2.50	0.46
43:n:53:THR:HB	43:n:65:THR:HB	1.97	0.46
30:a:340:A:O2'	34:e:162:ARG:NH1	2.48	0.46
30:a:1799:G:N2	30:a:1818:U:O2'	2.48	0.46
41:l:53:MET:HE1	41:l:103:TYR:CE2	2.50	0.46
42:m:38:LEU:N	42:m:39:PRO:HD2	2.30	0.46
6:A:769:G:H4'	6:A:1513:A:H4'	1.98	0.46
19:N:42:TRP:O	19:N:46:LEU:HD12	2.16	0.46
30:a:1327:A:H2'	30:a:1328:A:O4'	2.16	0.46
11:F:29:ILE:HG23	11:F:66:ALA:HB2	1.97	0.46
32:c:37:ASN:HB2	32:c:62:TYR:HB2	1.98	0.46
34:e:23:PHE:CD1	34:e:111:GLU:HG3	2.50	0.46
6:A:1391:U:H2'	6:A:1392:G:C8	2.51	0.46
30:a:700:G:H2'	30:a:701:G:O4'	2.16	0.46
30:a:1046:A:H3'	30:a:1047:G:H5''	1.97	0.46
30:a:1425:G:H2'	30:a:1426:G:O4'	2.15	0.46
30:a:2228:G:H2'	30:a:2229:U:C6	2.51	0.46
30:a:2788:C:H2'	30:a:2789:C:C6	2.51	0.46
52:w:74:ARG:NH2	52:w:76:GLU:OE2	2.48	0.46
5:4:38:SER:O	5:4:44:PHE:HB3	2.16	0.46
11:F:32:ALA:O	11:F:33:GLU:C	2.59	0.46
30:a:2811:G:H2'	30:a:2812:G:O4'	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:j:58:LEU:HD11	39:j:86:LEU:HD22	1.97	0.46
54:y:5:ILE:HD11	54:y:40:ASP:HB2	1.98	0.46
6:A:1328:C:H5''	18:M:28:THR:HG21	1.97	0.45
29:Z:21:A:H62	29:Z:47:U:C1'	2.29	0.45
30:a:594:U:H2'	30:a:595:C:C6	2.50	0.45
30:a:1932:A:H2'	30:a:1933:G:O4'	2.15	0.45
31:b:65:U:C4	31:b:108:A:C4	3.04	0.45
34:e:168:ASP:OD2	34:e:170:ARG:NE	2.49	0.45
35:f:41:GLY:HA2	35:f:44:ILE:HD13	1.98	0.45
5:4:14:ALA:HB1	5:4:34:LEU:HD11	1.98	0.45
15:J:53:ILE:CG2	15:J:63:ASP:HB2	2.46	0.45
16:K:16:VAL:O	16:K:79:ILE:HA	2.17	0.45
1:0:10:LYS:HE2	1:0:20:PHE:CD1	2.50	0.45
6:A:1138:G:H2'	6:A:1140:C:H5'	1.99	0.45
6:A:867:G:O2'	6:A:873:A:N1	2.47	0.45
6:A:1351:U:H2'	6:A:1352:C:H6	1.82	0.45
9:D:95:GLU:HA	9:D:100:ASN:HD22	1.81	0.45
10:E:156:LYS:HA	13:H:66:PHE:CG	2.51	0.45
30:a:2505:G:N2	30:a:2506:U:O4	2.49	0.45
37:h:31:VAL:HB	37:h:32:PRO:HD3	1.98	0.45
30:a:548:G:H2'	30:a:549:G:C1'	2.46	0.45
6:A:736:C:H2'	6:A:737:C:C6	2.51	0.45
7:B:71:GLY:O	7:B:93:ASN:HA	2.16	0.45
11:F:38:ARG:HB3	11:F:63:ASN:HD22	1.80	0.45
13:H:75:ILE:HG13	13:H:129:VAL:HG22	1.98	0.45
19:N:24:ARG:NH1	19:N:55:SER:OG	2.48	0.45
30:a:1263:U:O2'	55:z:8:PRO:HD2	2.17	0.45
33:d:110:THR:HG22	33:d:202:ILE:HB	1.98	0.45
12:G:78:ARG:HD3	12:G:87:VAL:HG21	1.97	0.45
27:V:114:ARG:O	27:V:115:ARG:C	2.60	0.45
31:b:29:A:C6	31:b:30:C:C4	3.05	0.45
37:h:6:LEU:CD2	37:h:37:VAL:HG23	2.47	0.45
30:a:568:U:O4	46:q:81:LYS:NZ	2.50	0.45
30:a:829:A:N7	30:a:2247:A:O2'	2.43	0.45
30:a:857:G:H2'	30:a:858:G:O4'	2.17	0.45
30:a:2063:C:O2	30:a:2450:A:N1	2.49	0.45
30:a:2585:U:O2	30:a:2585:U:O4'	2.33	0.45
40:k:76:GLU:C	40:k:77:ILE:HD12	2.41	0.45
21:P:4:ILE:HG12	21:P:21:VAL:HG22	1.99	0.45
30:a:1980:G:O2'	30:a:1982:U:OP2	2.35	0.45
12:G:75:VAL:CG1	12:G:86:GLN:HB3	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:30:C:C4	31:b:31:C:C2	3.05	0.44
6:A:1486:G:H2'	6:A:1487:G:O4'	2.16	0.44
13:H:10:MET:HG3	13:H:27:MET:SD	2.57	0.44
29:Z:63:C:H2'	29:Z:64:G:O4'	2.17	0.44
6:A:1141:C:H2'	6:A:1142:G:H8	1.83	0.44
11:F:9:MET:HE3	11:F:86:ARG:HB3	1.99	0.44
12:G:60:GLU:O	12:G:64:VAL:HG23	2.18	0.44
12:G:147:ALA:HB1	27:V:106:ALA:CB	2.47	0.44
6:A:1225:A:C2	6:A:1226:C:C4	3.05	0.44
8:C:140:ASN:O	8:C:141:ALA:C	2.60	0.44
13:H:64:LYS:HE2	13:H:71:VAL:HG21	1.98	0.44
30:a:352:A:H2'	30:a:353:C:O4'	2.17	0.44
30:a:675:A:N3	30:a:2443:C:O2'	2.46	0.44
30:a:1754:A:N1	30:a:2716:C:O2'	2.36	0.44
15:J:9:ARG:HG2	15:J:73:LEU:HD21	2.00	0.44
19:N:36:ALA:HB3	19:N:41:ARG:HH11	1.83	0.44
24:S:19:VAL:HG21	24:S:44:MET:HG2	2.00	0.44
31:b:37:C:C5	31:b:38:C:C5	3.06	0.44
41:l:36:VAL:CG2	41:l:129:THR:HG23	2.47	0.44
52:w:13:VAL:CG2	52:w:29:PHE:HB2	2.48	0.44
6:A:251:G:C6	6:A:266:G:C6	3.05	0.44
16:K:109:ASN:HA	26:U:4:ILE:O	2.18	0.44
17:L:50:ARG:HB3	17:L:66:TYR:HE1	1.82	0.44
30:a:1720:U:H2'	30:a:1721:G:O4'	2.18	0.44
36:g:19:ILE:HG12	36:g:24:ILE:HD12	1.99	0.44
6:A:622:A:C8	6:A:623:C:C6	3.05	0.44
6:A:714:G:H2'	6:A:715:A:C8	2.52	0.44
30:a:1019:U:OP1	30:a:1035:U:O2'	2.21	0.44
30:a:2091:C:O3'	52:w:56:MET:HE1	2.18	0.44
31:b:106:G:H2'	31:b:107:G:O4'	2.18	0.44
32:c:79:GLU:OE2	32:c:101:ARG:NE	2.51	0.44
6:A:901:A:O2'	6:A:1513:A:OP1	2.29	0.44
6:A:1260:G:H4'	6:A:1283:U:O2'	2.18	0.44
9:D:102:VAL:HG13	9:D:107:PHE:HB2	1.98	0.44
11:F:9:MET:HA	11:F:58:HIS:O	2.18	0.44
11:F:41:ASP:OD1	11:F:58:HIS:NE2	2.50	0.44
12:G:111:ARG:NH1	12:G:126:ASP:OD2	2.51	0.44
30:a:927:A:H2'	30:a:928:A:C8	2.51	0.44
30:a:1261:C:C2'	30:a:1262:A:O5'	2.66	0.44
30:a:1641:A:H2'	30:a:1642:G:O4'	2.18	0.44
31:b:76:G:OP1	50:u:9:ARG:NH1	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:359:G:H2'	30:a:360:U:O4'	2.18	0.43
30:a:1115:G:O2'	30:a:1116:G:O5'	2.29	0.43
30:a:1469:A:H2'	30:a:1470:A:C8	2.53	0.43
30:a:2040:G:H2'	30:a:2041:U:O4'	2.17	0.43
49:t:13:VAL:HG21	49:t:39:ILE:HG21	1.99	0.43
6:A:109:A:C6	6:A:326:G:C6	3.05	0.43
6:A:664:G:H22	6:A:741:G:H1	1.66	0.43
6:A:1508:A:H2'	6:A:1509:C:O4'	2.18	0.43
12:G:16:PRO:HD2	12:G:44:TYR:OH	2.19	0.43
19:N:47:LYS:O	19:N:50:THR:OG1	2.35	0.43
30:a:1904:G:O2'	30:a:1928:A:N1	2.49	0.43
40:k:64:PHE:CD1	40:k:64:PHE:C	2.96	0.43
14:I:45:ARG:O	14:I:46:MET:C	2.60	0.43
20:O:29:VAL:HG11	20:O:67:LEU:HD21	2.01	0.43
30:a:373:U:O2'	30:a:423:A:H1'	2.19	0.43
30:a:558:U:OP1	38:i:113:PRO:HD2	2.18	0.43
30:a:674:G:H5''	34:e:71:GLY:H	1.83	0.43
30:a:878:A:H2'	30:a:879:G:O4'	2.18	0.43
35:f:108:VAL:HB	35:f:109:PRO:HD3	2.00	0.43
54:y:25:LEU:C	54:y:25:LEU:HD13	2.42	0.43
8:C:70:THR:HG22	8:C:72:ARG:H	1.84	0.43
30:a:2626:C:H2'	30:a:2627:G:O4'	2.17	0.43
35:f:73:SER:OG	35:f:81:GLN:N	2.51	0.43
5:4:28:VAL:HG21	5:4:32:LEU:HD21	2.00	0.43
19:N:74:LEU:HD12	19:N:84:VAL:HG21	2.00	0.43
30:a:972:A:H8	30:a:972:A:O5'	2.00	0.43
30:a:1545:A:H2'	30:a:1546:G:O4'	2.19	0.43
30:a:2305:U:H1'	35:f:151:GLY:HA3	2.01	0.43
49:t:22:ARG:CZ	49:t:73:PHE:CE2	3.02	0.43
7:B:184:PHE:CE2	7:B:198:PHE:CD2	3.07	0.43
20:O:43:PHE:CE2	20:O:56:LEU:HD22	2.54	0.43
30:a:747:5MU:O2	30:a:2014:A:H1'	2.18	0.43
30:a:1021:A:H3'	30:a:1021:A:N3	2.33	0.43
30:a:1680:U:H2'	30:a:1681:G:O4'	2.18	0.43
6:A:1218:C:H2'	6:A:1219:A:C8	2.54	0.43
30:a:1798:U:H5'	32:c:257:THR:OG1	2.19	0.43
6:A:1242:G:C6	6:A:1243:C:C4	3.06	0.43
6:A:1268:G:H2'	6:A:1269:A:C8	2.54	0.43
7:B:15:HIS:HB3	7:B:43:LEU:HD11	2.01	0.43
9:D:105:MET:HE1	9:D:143:VAL:HB	2.00	0.43
30:a:541:A:H2'	30:a:542:C:O4'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1028:A:N6	30:a:1125:G:H2'	2.34	0.43
35:f:177:PHE:O	35:f:178:ARG:C	2.62	0.43
22:Q:27:ARG:HG3	22:Q:40:ARG:HB2	2.01	0.43
30:a:1370:C:H2'	30:a:1371:G:O4'	2.19	0.43
30:a:1414:C:H2'	30:a:1415:U:O4'	2.17	0.43
30:a:1509:A:H2'	30:a:1510:G:H8	1.83	0.43
30:a:1995:U:H3'	30:a:1996:C:H2'	2.00	0.43
37:h:32:PRO:HA	52:w:39:TRP:CD1	2.53	0.43
41:l:74:THR:HA	41:l:88:ASN:O	2.19	0.43
55:z:43:ILE:HG22	55:z:49:TYR:HB2	2.01	0.43
6:A:1219:A:H2'	6:A:1220:G:C8	2.54	0.43
30:a:645:C:O2'	30:a:646:U:H5''	2.19	0.43
30:a:766:U:H2'	30:a:767:U:C6	2.54	0.43
30:a:861:A:C2	30:a:917:A:C4	3.06	0.43
35:f:40:VAL:HG12	35:f:50:LEU:HD13	2.00	0.43
41:l:36:VAL:HG21	41:l:129:THR:HG23	2.01	0.43
6:A:945:G:N1	6:A:1337:G:C2	2.87	0.42
9:D:168:PRO:HB3	9:D:170:TRP:CZ3	2.53	0.42
25:T:68:HIS:CD2	25:T:70:ASN:HD22	2.36	0.42
29:Z:55:U:O2'	29:Z:57:G:N7	2.44	0.42
30:a:2766:A:N3	30:a:2766:A:H2'	2.34	0.42
48:s:2:ILE:HD13	48:s:42:GLU:HA	2.00	0.42
6:A:1493:A:H2'	6:A:1494:G:H5'	2.01	0.42
8:C:70:THR:HG21	8:C:76:VAL:HG23	2.01	0.42
10:E:150:PRO:O	10:E:164:ILE:HD11	2.18	0.42
30:a:1020:A:C2	30:a:1141:U:C2	3.07	0.42
30:a:1443:U:H2'	30:a:1444:G:C8	2.54	0.42
30:a:1810:A:O5'	30:a:1810:A:H8	2.03	0.42
30:a:2273:A:H2'	30:a:2274:A:C8	2.53	0.42
30:a:2552:OMU:H6	30:a:2552:OMU:O5'	2.19	0.42
33:d:122:VAL:HG21	33:d:129:THR:HG22	2.01	0.42
37:h:28:ASN:O	37:h:32:PRO:HD2	2.19	0.42
42:m:49:GLU:N	42:m:50:PRO:CD	2.83	0.42
50:u:75:GLN:HB2	50:u:92:VAL:HG23	2.01	0.42
6:A:1179:A:H5''	14:I:104:VAL:HG12	2.00	0.42
30:a:1199:U:H1'	45:p:4:VAL:HG22	2.00	0.42
6:A:60:A:OP1	6:A:111:G:N2	2.51	0.42
6:A:237:G:H5''	22:Q:27:ARG:CZ	2.50	0.42
15:J:10:LEU:N	15:J:10:LEU:HD22	2.34	0.42
30:a:784:G:H5'	30:a:785:G:OP1	2.20	0.42
30:a:813:U:H2'	30:a:814:C:C6	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1313:U:O2	30:a:1313:U:C2'	2.67	0.42
36:g:30:ASN:HB3	36:g:79:VAL:HA	2.01	0.42
30:a:1450:G:C6	30:a:1451:C:N4	2.87	0.42
30:a:2321:U:O2	30:a:2321:U:C2'	2.67	0.42
39:j:43:ILE:CD1	39:j:52:VAL:HB	2.49	0.42
43:n:68:LYS:HD3	43:n:101:GLY:HA2	2.01	0.42
6:A:963:G:H21	15:J:57:VAL:CG2	2.31	0.42
12:G:26:PHE:HZ	12:G:120:LEU:HD11	1.84	0.42
16:K:16:VAL:O	16:K:79:ILE:HG12	2.19	0.42
30:a:191:A:H2'	30:a:192:C:C6	2.55	0.42
30:a:207:A:H2'	30:a:208:C:O4'	2.20	0.42
30:a:627:A:N1	30:a:636:G:O2'	2.49	0.42
30:a:631:A:N3	30:a:2415:G:O2'	2.45	0.42
33:d:135:GLY:O	33:d:136:ASN:C	2.61	0.42
35:f:142:ASP:O	35:f:146:VAL:HG23	2.20	0.42
40:k:143:GLU:O	40:k:144:GLU:C	2.62	0.42
45:p:98:ILE:O	45:p:99:ALA:C	2.63	0.42
12:G:69:VAL:O	12:G:70:ARG:C	2.63	0.42
12:G:86:GLN:HG3	12:G:144:MET:HE1	2.01	0.42
30:a:1156:A:C8	45:p:51:ARG:HG2	2.55	0.42
31:b:51:G:C6	31:b:52:A:C6	3.08	0.42
43:n:53:THR:HB	43:n:65:THR:CG2	2.50	0.42
6:A:375:U:C4	6:A:376:G:N7	2.88	0.42
6:A:1015:G:C6	6:A:1016:A:C6	3.08	0.42
32:c:145:GLU:HB2	32:c:188:CYS:HB3	2.02	0.42
33:d:62:LYS:N	33:d:63:PRO:CD	2.83	0.42
35:f:35:THR:HA	35:f:89:VAL:O	2.20	0.42
7:B:92:VAL:HG21	7:B:96:TRP:CE3	2.55	0.42
30:a:720:U:H2'	30:a:721:A:C8	2.55	0.42
34:e:58:LYS:HA	34:e:59:PRO:HD3	1.94	0.42
50:u:40:ILE:HD12	50:u:42:LEU:HD21	2.01	0.42
15:J:57:VAL:O	15:J:57:VAL:CG1	2.62	0.42
30:a:1593:A:H2'	30:a:1594:U:O4'	2.19	0.42
30:a:2520:C:C6	30:a:2567:G:H1'	2.54	0.42
36:g:76:VAL:O	36:g:80:THR:HG23	2.20	0.42
40:k:112:LEU:C	40:k:112:LEU:HD23	2.44	0.42
6:A:645:G:C2	6:A:646:G:C8	3.08	0.41
7:B:43:LEU:HA	7:B:46:THR:HB	2.03	0.41
8:C:122:SER:HB2	8:C:126:ARG:HH12	1.85	0.41
30:a:1528:A:H2'	30:a:1529:G:O4'	2.19	0.41
35:f:146:VAL:HG11	35:f:149:VAL:HG22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:26:HIS:NE2	3:2:48:ALA:HB2	2.35	0.41
6:A:35:G:H2'	6:A:36:C:C6	2.55	0.41
6:A:673:A:H2'	6:A:674:G:C8	2.55	0.41
6:A:949:A:C4	6:A:1233:G:N2	2.88	0.41
6:A:1402:4OC:O2	6:A:1500:A:N1	2.54	0.41
16:K:111:THR:CG2	26:U:3:VAL:HG12	2.50	0.41
30:a:956:G:O6	41:l:14:LYS:HE3	2.19	0.41
30:a:1009:A:O4'	45:p:59:GLN:HG3	2.20	0.41
47:r:4:ILE:HG12	47:r:106:VAL:HG22	2.01	0.41
47:r:109:ASP:OD1	47:r:110:ARG:N	2.53	0.41
6:A:519:C:H2'	6:A:520:A:O4'	2.20	0.41
6:A:926:G:H4'	27:V:119:LYS:CD	2.51	0.41
8:C:47:LEU:HD22	8:C:76:VAL:HG22	2.02	0.41
10:E:161:VAL:CG1	10:E:165:LEU:HD12	2.50	0.41
30:a:476:G:H4'	30:a:502:A:N1	2.35	0.41
30:a:1252:G:H1	45:p:37:GLN:HE21	1.67	0.41
30:a:1872:A:C5	30:a:1873:G:H1'	2.56	0.41
6:A:352:C:H5''	6:A:352:C:H6	1.86	0.41
7:B:27:MET:O	7:B:28:LYS:C	2.64	0.41
7:B:94:HIS:O	7:B:95:ARG:C	2.63	0.41
21:P:40:ASN:HB3	21:P:43:ALA:HB2	2.03	0.41
25:T:28:MET:HE1	25:T:67:ILE:HG21	2.03	0.41
30:a:1039:A:H2'	30:a:1040:A:O4'	2.20	0.41
30:a:2591:C:H2'	30:a:2592:G:C8	2.55	0.41
30:a:2747:G:C2	30:a:2756:U:C5	3.08	0.41
31:b:39:A:O2'	31:b:46:A:N1	2.50	0.41
36:g:30:ASN:OD1	36:g:30:ASN:O	2.37	0.41
39:j:40:LYS:HE3	39:j:89:ASN:HD21	1.86	0.41
3:2:32:ILE:HG21	30:a:2391:G:OP2	2.20	0.41
6:A:767:A:H2'	6:A:768:A:O4'	2.21	0.41
8:C:19:ASN:O	8:C:40:ARG:NH2	2.54	0.41
30:a:279:A:H1'	30:a:362:A:O2'	2.21	0.41
34:e:1:MET:HB3	34:e:14:VAL:O	2.20	0.41
37:h:14:SER:O	37:h:17:ASP:OD1	2.38	0.41
40:k:132:ARG:HG3	40:k:142:ILE:HD12	2.01	0.41
3:2:13:ARG:HD2	40:k:58:TYR:O	2.20	0.41
6:A:131:A:O2'	6:A:262:A:N3	2.46	0.41
6:A:532:A:C6	8:C:193:TYR:CE1	3.07	0.41
6:A:607:A:H2'	6:A:608:A:C8	2.56	0.41
6:A:695:A:H2'	6:A:696:A:C8	2.56	0.41
11:F:17:GLN:N	11:F:17:GLN:OE1	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:64:A:C6	30:a:65:U:C4	3.09	0.41
30:a:1746:A:H2'	30:a:1747:U:C6	2.55	0.41
32:c:247:PRO:HD2	32:c:248:TRP:CE3	2.55	0.41
6:A:1305:G:O2'	6:A:1331:G:N2	2.54	0.41
7:B:100:MET:HA	7:B:107:VAL:HG21	2.02	0.41
29:Z:21:A:C2	29:Z:46:G:C2	3.09	0.41
29:Z:23:A:H2'	29:Z:24:A:C8	2.56	0.41
30:a:1288:G:C4	30:a:1327:A:C2	3.08	0.41
30:a:1509:A:C2	30:a:1510:G:C4	3.08	0.41
32:c:31:ALA:N	32:c:32:PRO:CD	2.83	0.41
46:q:93:PHE:CD1	46:q:93:PHE:C	2.98	0.41
5:4:27:THR:O	5:4:28:VAL:C	2.63	0.41
30:a:300:A:H2'	30:a:334:C:H1'	2.02	0.41
30:a:588:U:H2'	30:a:589:U:C6	2.55	0.41
30:a:1939:5MU:OP1	30:a:2604:PSU:O2'	2.33	0.41
37:h:6:LEU:HD22	37:h:37:VAL:HG23	2.02	0.41
46:q:5:PHE:HE1	46:q:14:VAL:HG11	1.86	0.41
6:A:705:G:C5	6:A:706:A:C8	3.09	0.41
6:A:1170:A:H2'	6:A:1171:A:O4'	2.21	0.41
6:A:1323:G:H2'	6:A:1324:A:C8	2.56	0.41
7:B:113:ARG:HH22	7:B:117:LEU:HD13	1.85	0.41
16:K:63:ALA:HB1	16:K:96:THR:OG1	2.20	0.41
17:L:114:ARG:HB3	17:L:119:VAL:O	2.20	0.41
19:N:37:SER:O	19:N:40:ASP:N	2.53	0.41
30:a:2331:G:O2'	30:a:2336:A:N1	2.41	0.41
33:d:48:ILE:HG12	33:d:84:LEU:HD21	2.02	0.41
36:g:94:TYR:HA	36:g:106:SER:O	2.20	0.41
39:j:25:LEU:HD12	39:j:38:ILE:HG22	2.03	0.41
39:j:40:LYS:NZ	39:j:89:ASN:HD21	2.18	0.41
41:l:135:VAL:CG1	50:u:57:TYR:CD2	3.04	0.41
49:t:71:ALA:HB3	49:t:80:ALA:HB1	2.03	0.41
6:A:142:G:C2	6:A:222:C:C2	3.09	0.41
6:A:736:C:H4'	11:F:90:MET:HG2	2.03	0.41
6:A:739:C:P	11:F:2:ARG:HH22	2.44	0.41
7:B:11:LYS:O	7:B:208:ARG:NH2	2.52	0.41
15:J:6:ILE:HD13	15:J:6:ILE:HA	2.00	0.41
30:a:880:G:N2	30:a:898:C:C2	2.89	0.41
30:a:1320:C:N3	30:a:1331:G:O6	2.53	0.41
30:a:2745:C:C4	30:a:2746:U:C4	3.09	0.41
31:b:90:C:H5''	41:l:18:ARG:HG2	2.02	0.41
40:k:28:GLY:O	40:k:29:LYS:C	2.61	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:p:62:ILE:O	45:p:63:ALA:C	2.62	0.41
49:t:85:PHE:CE1	49:t:94:ARG:HG2	2.56	0.41
6:A:544:G:OP2	9:D:63:ARG:NH2	2.54	0.40
6:A:946:A:H2'	6:A:947:G:H8	1.82	0.40
6:A:953:G:C6	6:A:954:G:C4	3.09	0.40
7:B:217:VAL:O	7:B:218:ALA:C	2.64	0.40
12:G:81:GLY:HA3	27:V:124:LEU:HG	2.02	0.40
17:L:33:VAL:C	17:L:55:VAL:HG23	2.46	0.40
30:a:1042:G:C5	30:a:1043:C:C5	3.08	0.40
30:a:1444:G:H2'	30:a:1445:G:H8	1.86	0.40
33:d:142:VAL:HB	33:d:143:PRO:HD2	2.02	0.40
36:g:105:LEU:HD11	36:g:131:ILE:HD11	2.02	0.40
4:3:2:LYS:NZ	30:a:2478:A:OP2	2.38	0.40
6:A:18:C:OP1	10:E:132:ASN:ND2	2.49	0.40
18:M:69:LEU:O	18:M:72:GLU:N	2.54	0.40
30:a:1444:G:H2'	30:a:1445:G:C8	2.56	0.40
30:a:1754:A:C8	44:o:94:LYS:CE	3.04	0.40
36:g:12:PRO:HD2	36:g:15:VAL:HG21	2.02	0.40
6:A:1381:U:C5	6:A:1382:C:C5	3.09	0.40
15:J:92:LEU:HD13	15:J:98:VAL:HG21	2.04	0.40
18:M:69:LEU:O	18:M:70:ARG:C	2.63	0.40
30:a:441:U:O2	34:e:41:GLN:NE2	2.54	0.40
30:a:608:A:H2'	30:a:609:A:C8	2.56	0.40
30:a:1562:U:H2'	30:a:1563:U:O4'	2.21	0.40
31:b:78:A:C2	31:b:99:A:C4	3.09	0.40
32:c:247:PRO:HD2	32:c:248:TRP:CZ3	2.56	0.40
35:f:60:ILE:HG13	35:f:141:ILE:HD11	2.03	0.40
42:m:67:PHE:O	42:m:71:ARG:HD2	2.21	0.40
46:q:71:LYS:HG2	46:q:90:ARG:CG	2.52	0.40
49:t:71:ALA:CB	49:t:80:ALA:HB1	2.52	0.40
6:A:27:G:H2'	6:A:28:A:O4'	2.21	0.40
6:A:216:U:H2'	6:A:217:C:C6	2.56	0.40
6:A:555:U:H2'	6:A:556:C:C6	2.57	0.40
6:A:671:G:N2	6:A:736:C:C2	2.89	0.40
6:A:1095:U:H2'	6:A:1096:C:O4'	2.21	0.40
11:F:45:ARG:HD3	11:F:59:TYR:CD1	2.56	0.40
19:N:24:ARG:O	19:N:25:ALA:C	2.64	0.40
30:a:57:C:H2'	30:a:58:G:O4'	2.21	0.40
30:a:1538:G:C2	30:a:1539:U:C2	3.09	0.40
38:i:125:TYR:OH	38:i:132:HIS:NE2	2.43	0.40
47:r:23:LEU:HD21	55:z:22:LEU:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:t:29:LEU:N	49:t:29:LEU:HD12	2.36	0.40
6:A:595:A:C2	6:A:641:U:C2	3.09	0.40
6:A:1031:C:H4'	6:A:1032:G:C2	2.56	0.40
6:A:1180:A:OP2	14:I:99:ARG:NH2	2.54	0.40
6:A:1363:A:N3	6:A:1363:A:H2'	2.37	0.40
17:L:55:VAL:HG21	17:L:80:ILE:HD11	2.03	0.40
30:a:101:A:N3	30:a:101:A:H2'	2.36	0.40
41:l:66:ARG:HB2	41:l:101:VAL:O	2.22	0.40
44:o:100:LEU:CD1	44:o:110:ILE:HD11	2.50	0.40
46:q:34:GLU:OE1	46:q:60:LYS:HG2	2.22	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	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
2	1	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
3	2	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	7	23
4	3	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
5	4	56/70 (80%)	49 (88%)	7 (12%)	0	100	100
7	B	222/241 (92%)	207 (93%)	15 (7%)	0	100	100
8	C	204/233 (88%)	189 (93%)	15 (7%)	0	100	100
9	D	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
10	E	154/167 (92%)	150 (97%)	4 (3%)	0	100	100
11	F	101/135 (75%)	92 (91%)	9 (9%)	0	100	100
12	G	151/179 (84%)	145 (96%)	6 (4%)	0	100	100
13	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	I	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
15	J	96/103 (93%)	89 (93%)	7 (7%)	0	100	100
16	K	113/129 (88%)	104 (92%)	9 (8%)	0	100	100
17	L	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
18	M	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
19	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
20	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
21	P	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
22	Q	77/84 (92%)	68 (88%)	9 (12%)	0	100	100
23	R	64/75 (85%)	60 (94%)	4 (6%)	0	100	100
24	S	82/92 (89%)	76 (93%)	6 (7%)	0	100	100
25	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
26	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
27	V	127/142 (89%)	124 (98%)	3 (2%)	0	100	100
32	c	269/273 (98%)	254 (94%)	15 (6%)	0	100	100
33	d	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
34	e	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
35	f	175/179 (98%)	162 (93%)	13 (7%)	0	100	100
36	g	174/177 (98%)	161 (92%)	13 (8%)	0	100	100
37	h	39/149 (26%)	33 (85%)	6 (15%)	0	100	100
38	i	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
39	j	121/123 (98%)	113 (93%)	8 (7%)	0	100	100
40	k	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
41	l	132/136 (97%)	130 (98%)	2 (2%)	0	100	100
42	m	116/127 (91%)	106 (91%)	10 (9%)	0	100	100
43	n	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
44	o	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
45	p	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
46	q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
47	r	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
48	s	91/100 (91%)	89 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	t	100/104 (96%)	96 (96%)	4 (4%)	0	100	100
50	u	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
51	v	76/85 (89%)	73 (96%)	3 (4%)	0	100	100
52	w	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
53	x	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
54	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
55	z	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
All	All	5608/6055 (93%)	5334 (95%)	273 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	32	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	46 (100%)	0	100	100
2	1	38/38 (100%)	38 (100%)	0	100	100
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	55/62 (89%)	55 (100%)	0	100	100
7	B	186/199 (94%)	186 (100%)	0	100	100
8	C	170/190 (90%)	170 (100%)	0	100	100
9	D	172/173 (99%)	170 (99%)	2 (1%)	63	84
10	E	119/126 (94%)	119 (100%)	0	100	100
11	F	90/116 (78%)	90 (100%)	0	100	100
12	G	126/147 (86%)	126 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	H	104/105 (99%)	104 (100%)	0	100	100
14	I	105/107 (98%)	105 (100%)	0	100	100
15	J	86/90 (96%)	83 (96%)	3 (4%)	32	64
16	K	89/98 (91%)	89 (100%)	0	100	100
17	L	102/103 (99%)	100 (98%)	2 (2%)	48	77
18	M	93/96 (97%)	93 (100%)	0	100	100
19	N	83/84 (99%)	83 (100%)	0	100	100
20	O	76/77 (99%)	76 (100%)	0	100	100
21	P	65/65 (100%)	65 (100%)	0	100	100
22	Q	73/78 (94%)	73 (100%)	0	100	100
23	R	57/65 (88%)	57 (100%)	0	100	100
24	S	72/79 (91%)	72 (100%)	0	100	100
25	T	65/66 (98%)	65 (100%)	0	100	100
26	U	60/61 (98%)	60 (100%)	0	100	100
27	V	110/121 (91%)	110 (100%)	0	100	100
32	c	216/218 (99%)	216 (100%)	0	100	100
33	d	163/163 (100%)	163 (100%)	0	100	100
34	e	165/165 (100%)	165 (100%)	0	100	100
35	f	148/150 (99%)	148 (100%)	0	100	100
36	g	137/138 (99%)	135 (98%)	2 (2%)	57	81
37	h	32/114 (28%)	32 (100%)	0	100	100
38	i	116/116 (100%)	116 (100%)	0	100	100
39	j	104/104 (100%)	103 (99%)	1 (1%)	68	86
40	k	103/103 (100%)	103 (100%)	0	100	100
41	l	107/107 (100%)	107 (100%)	0	100	100
42	m	98/103 (95%)	98 (100%)	0	100	100
43	n	86/87 (99%)	86 (100%)	0	100	100
44	o	99/100 (99%)	99 (100%)	0	100	100
45	p	89/90 (99%)	89 (100%)	0	100	100
46	q	84/84 (100%)	84 (100%)	0	100	100
47	r	93/93 (100%)	93 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	s	80/84 (95%)	80 (100%)	0	100	100
49	t	83/85 (98%)	82 (99%)	1 (1%)	63	84
50	u	78/78 (100%)	78 (100%)	0	100	100
51	v	58/63 (92%)	58 (100%)	0	100	100
52	w	67/68 (98%)	67 (100%)	0	100	100
53	x	54/55 (98%)	54 (100%)	0	100	100
54	y	48/49 (98%)	47 (98%)	1 (2%)	47	76
55	z	47/48 (98%)	47 (100%)	0	100	100
All	All	4682/4946 (95%)	4670 (100%)	12 (0%)	84	94

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	D	185	LYS
9	D	188	ARG
15	J	6	ILE
15	J	44	THR
15	J	47	GLU
17	L	37	VAL
17	L	45	PRO
36	g	3	ARG
36	g	102	VAL
39	j	58	LEU
49	t	39	ILE
54	y	4	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
7	B	94	HIS
8	C	190	HIS
11	F	37	HIS
11	F	55	HIS
11	F	63	ASN
12	G	68	ASN
13	H	4	GLN
14	I	5	GLN
14	I	32	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	I	50	GLN
14	I	81	HIS
16	K	15	GLN
16	K	38	GLN
16	K	81	ASN
17	L	6	GLN
17	L	46	ASN
17	L	112	GLN
18	M	8	ASN
18	M	14	HIS
18	M	52	GLN
18	M	105	ASN
19	N	43	ASN
21	P	9	HIS
21	P	26	ASN
21	P	63	GLN
23	R	52	GLN
24	S	14	HIS
24	S	52	HIS
25	T	3	ASN
25	T	20	HIS
25	T	70	ASN
25	T	84	ASN
26	U	64	ASN
27	V	41	GLN
27	V	52	ASN
27	V	105	ASN
27	V	129	HIS
32	c	25	HIS
32	c	37	ASN
32	c	243	HIS
35	f	27	GLN
36	g	30	ASN
36	g	48	ASN
36	g	88	GLN
36	g	128	GLN
37	h	2	GLN
38	i	80	HIS
38	i	128	ASN
38	i	138	GLN
39	j	9	ASN
39	j	89	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	l	13	HIS
42	m	9	GLN
43	n	19	GLN
43	n	29	HIS
44	o	12	GLN
44	o	52	ASN
45	p	37	GLN
45	p	81	ASN
46	q	6	GLN
47	r	40	ASN
48	s	91	GLN
48	s	92	ASN
49	t	40	ASN
50	u	49	ASN
50	u	87	GLN
51	v	12	ASN
52	w	6	GLN
52	w	36	HIS
53	x	27	ASN
53	x	31	GLN
53	x	38	GLN
53	x	39	GLN
53	x	58	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	X	2/3 (66%)	0	0
29	Z	71/77 (92%)	18 (25%)	1 (1%)
30	a	2749/2904 (94%)	390 (14%)	0
31	b	118/120 (98%)	18 (15%)	0
6	A	1515/1542 (98%)	319 (21%)	33 (2%)
All	All	4455/4646 (95%)	745 (16%)	34 (0%)

All (745) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	4	U
6	A	5	U
6	A	6	G
6	A	7	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	9	G
6	A	32	A
6	A	39	G
6	A	42	G
6	A	44	A
6	A	47	C
6	A	48	C
6	A	50	A
6	A	51	A
6	A	55	A
6	A	59	A
6	A	69	G
6	A	70	U
6	A	71	A
6	A	74	A
6	A	75	G
6	A	81	A
6	A	83	C
6	A	84	U
6	A	85	U
6	A	86	G
6	A	87	C
6	A	88	U
6	A	94	G
6	A	95	C
6	A	96	U
6	A	97	G
6	A	120	A
6	A	121	U
6	A	128	G
6	A	129	A
6	A	131	A
6	A	141	G
6	A	143	A
6	A	144	G
6	A	151	A
6	A	163	C
6	A	166	U
6	A	177	G
6	A	182	A
6	A	184	G
6	A	189	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	197	A
6	A	226	G
6	A	240	G
6	A	245	U
6	A	247	G
6	A	251	G
6	A	252	U
6	A	258	G
6	A	262	A
6	A	264	C
6	A	266	G
6	A	267	C
6	A	280	C
6	A	289	G
6	A	309	A
6	A	317	U
6	A	321	A
6	A	324	G
6	A	328	C
6	A	329	A
6	A	341	C
6	A	344	A
6	A	347	G
6	A	352	C
6	A	354	G
6	A	365	U
6	A	366	A
6	A	367	U
6	A	372	C
6	A	376	G
6	A	382	A
6	A	384	G
6	A	404	G
6	A	406	G
6	A	411	A
6	A	412	A
6	A	413	G
6	A	418	C
6	A	421	U
6	A	423	G
6	A	424	G
6	A	429	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	436	C
6	A	445	G
6	A	453	G
6	A	456	A
6	A	457	G
6	A	458	U
6	A	459	A
6	A	463	U
6	A	465	A
6	A	468	A
6	A	469	C
6	A	478	A
6	A	479	U
6	A	486	U
6	A	496	A
6	A	511	C
6	A	518	C
6	A	519	C
6	A	521	G
6	A	531	U
6	A	532	A
6	A	533	A
6	A	547	A
6	A	559	A
6	A	560	A
6	A	572	A
6	A	573	A
6	A	576	C
6	A	577	G
6	A	584	G
6	A	588	G
6	A	596	A
6	A	618	C
6	A	628	G
6	A	633	G
6	A	639	G
6	A	649	A
6	A	650	G
6	A	653	U
6	A	654	G
6	A	656	G
6	A	661	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	665	A
6	A	666	G
6	A	671	G
6	A	682	G
6	A	687	A
6	A	692	U
6	A	721	G
6	A	723	U
6	A	724	G
6	A	733	G
6	A	734	G
6	A	742	G
6	A	747	A
6	A	748	G
6	A	755	G
6	A	759	A
6	A	774	G
6	A	777	A
6	A	790	A
6	A	793	U
6	A	794	A
6	A	798	U
6	A	815	A
6	A	817	C
6	A	818	G
6	A	832	G
6	A	836	G
6	A	839	C
6	A	840	C
6	A	851	G
6	A	857	C
6	A	871	U
6	A	882	C
6	A	884	U
6	A	885	G
6	A	887	G
6	A	890	G
6	A	902	G
6	A	914	A
6	A	919	A
6	A	926	G
6	A	934	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	935	A
6	A	939	G
6	A	945	G
6	A	958	A
6	A	960	U
6	A	965	U
6	A	966	2MG
6	A	969	A
6	A	971	G
6	A	975	A
6	A	976	G
6	A	977	A
6	A	978	A
6	A	983	A
6	A	984	C
6	A	987	G
6	A	992	U
6	A	993	G
6	A	994	A
6	A	996	A
6	A	1000	A
6	A	1003	G
6	A	1004	A
6	A	1008	U
6	A	1009	U
6	A	1016	A
6	A	1017	U
6	A	1021	A
6	A	1022	A
6	A	1024	G
6	A	1027	C
6	A	1029	U
6	A	1031	C
6	A	1032	G
6	A	1033	G
6	A	1034	G
6	A	1035	A
6	A	1036	A
6	A	1039	G
6	A	1042	A
6	A	1043	G
6	A	1044	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	1046	A
6	A	1065	U
6	A	1070	U
6	A	1074	G
6	A	1085	U
6	A	1094	G
6	A	1095	U
6	A	1099	G
6	A	1101	A
6	A	1113	C
6	A	1118	U
6	A	1124	G
6	A	1125	U
6	A	1128	C
6	A	1130	A
6	A	1132	C
6	A	1134	G
6	A	1135	U
6	A	1137	C
6	A	1138	G
6	A	1139	G
6	A	1140	C
6	A	1145	A
6	A	1146	A
6	A	1157	A
6	A	1159	U
6	A	1171	A
6	A	1174	G
6	A	1184	G
6	A	1196	A
6	A	1197	A
6	A	1200	C
6	A	1206	G
6	A	1210	C
6	A	1211	U
6	A	1213	A
6	A	1214	C
6	A	1220	G
6	A	1224	U
6	A	1226	C
6	A	1227	A
6	A	1228	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	1229	A
6	A	1238	A
6	A	1239	A
6	A	1240	U
6	A	1248	A
6	A	1250	A
6	A	1253	G
6	A	1256	A
6	A	1257	A
6	A	1260	G
6	A	1270	G
6	A	1280	A
6	A	1286	U
6	A	1287	A
6	A	1289	A
6	A	1297	G
6	A	1298	U
6	A	1299	A
6	A	1300	G
6	A	1302	C
6	A	1303	C
6	A	1305	G
6	A	1306	A
6	A	1312	G
6	A	1313	U
6	A	1317	C
6	A	1320	C
6	A	1327	C
6	A	1334	G
6	A	1335	U
6	A	1336	C
6	A	1338	G
6	A	1340	A
6	A	1346	A
6	A	1353	G
6	A	1363	A
6	A	1364	U
6	A	1370	G
6	A	1373	G
6	A	1378	C
6	A	1379	G
6	A	1380	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	1381	U
6	A	1394	A
6	A	1397	C
6	A	1398	A
6	A	1419	G
6	A	1429	A
6	A	1432	G
6	A	1439	G
6	A	1441	A
6	A	1451	U
6	A	1452	C
6	A	1479	C
6	A	1492	A
6	A	1493	A
6	A	1497	G
6	A	1503	A
6	A	1505	G
6	A	1506	U
6	A	1517	G
6	A	1529	G
6	A	1530	G
29	Z	6	G
29	Z	8	U
29	Z	9	A
29	Z	19	U
29	Z	21	A
29	Z	43	G
29	Z	46	G
29	Z	47	U
29	Z	48	C
29	Z	49	G
29	Z	50	C
29	Z	56	C
29	Z	57	G
29	Z	58	A
29	Z	65	U
29	Z	68	G
29	Z	70	U
29	Z	76	A
30	a	10	A
30	a	12	U
30	a	34	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	42	A
30	a	50	U
30	a	58	G
30	a	61	C
30	a	71	A
30	a	74	A
30	a	75	G
30	a	80	G
30	a	86	G
30	a	93	G
30	a	101	A
30	a	102	U
30	a	103	A
30	a	110	G
30	a	118	A
30	a	119	A
30	a	120	U
30	a	131	A
30	a	135	U
30	a	138	U
30	a	139	U
30	a	142	A
30	a	160	A
30	a	163	C
30	a	164	C
30	a	165	A
30	a	181	A
30	a	186	G
30	a	196	A
30	a	199	A
30	a	200	U
30	a	215	G
30	a	216	A
30	a	221	A
30	a	222	A
30	a	248	G
30	a	265	A
30	a	266	G
30	a	272	A
30	a	277	G
30	a	278	A
30	a	282	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	285	G
30	a	286	U
30	a	289	G
30	a	294	A
30	a	304	U
30	a	311	A
30	a	329	G
30	a	330	A
30	a	345	A
30	a	357	C
30	a	361	G
30	a	362	A
30	a	367	G
30	a	386	G
30	a	404	A
30	a	405	U
30	a	411	G
30	a	412	A
30	a	425	G
30	a	481	G
30	a	490	C
30	a	491	G
30	a	503	A
30	a	504	A
30	a	505	A
30	a	508	A
30	a	509	C
30	a	530	G
30	a	531	C
30	a	532	A
30	a	533	G
30	a	538	A
30	a	543	G
30	a	544	C
30	a	545	U
30	a	546	U
30	a	547	A
30	a	549	G
30	a	563	A
30	a	573	U
30	a	575	A
30	a	592	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	603	A
30	a	614	A
30	a	615	U
30	a	627	A
30	a	637	A
30	a	645	C
30	a	647	G
30	a	653	U
30	a	654	A
30	a	655	A
30	a	664	G
30	a	686	U
30	a	711	G
30	a	717	C
30	a	721	A
30	a	730	A
30	a	738	G
30	a	747	5MU
30	a	764	A
30	a	765	C
30	a	775	G
30	a	776	G
30	a	777	G
30	a	782	A
30	a	784	G
30	a	785	G
30	a	792	A
30	a	805	G
30	a	812	C
30	a	822	G
30	a	827	U
30	a	828	U
30	a	846	U
30	a	847	U
30	a	856	G
30	a	859	G
30	a	869	G
30	a	881	G
30	a	883	G
30	a	884	U
30	a	888	C
30	a	890	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	891	G
30	a	896	A
30	a	897	C
30	a	898	C
30	a	905	A
30	a	910	A
30	a	914	G
30	a	915	C
30	a	931	U
30	a	932	U
30	a	946	C
30	a	961	C
30	a	974	G
30	a	983	A
30	a	984	A
30	a	985	C
30	a	990	A
30	a	996	A
30	a	1009	A
30	a	1012	U
30	a	1013	C
30	a	1022	G
30	a	1026	G
30	a	1033	U
30	a	1040	A
30	a	1045	C
30	a	1046	A
30	a	1047	G
30	a	1048	A
30	a	1051	G
30	a	1052	C
30	a	1108	U
30	a	1109	C
30	a	1110	G
30	a	1111	A
30	a	1112	G
30	a	1115	G
30	a	1116	G
30	a	1122	G
30	a	1130	U
30	a	1132	U
30	a	1135	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	1136	G
30	a	1141	U
30	a	1142	A
30	a	1169	A
30	a	1171	G
30	a	1178	C
30	a	1181	U
30	a	1187	G
30	a	1253	A
30	a	1256	G
30	a	1259	G
30	a	1271	G
30	a	1272	A
30	a	1275	A
30	a	1300	G
30	a	1301	A
30	a	1302	A
30	a	1303	G
30	a	1321	A
30	a	1343	G
30	a	1344	U
30	a	1345	C
30	a	1352	U
30	a	1365	A
30	a	1379	U
30	a	1383	A
30	a	1386	C
30	a	1407	G
30	a	1411	U
30	a	1416	G
30	a	1417	C
30	a	1427	A
30	a	1428	C
30	a	1437	C
30	a	1452	G
30	a	1453	A
30	a	1478	G
30	a	1482	G
30	a	1483	G
30	a	1486	U
30	a	1490	A
30	a	1493	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	1509	A
30	a	1515	A
30	a	1529	G
30	a	1534	U
30	a	1535	A
30	a	1536	C
30	a	1537	G
30	a	1554	U
30	a	1569	A
30	a	1578	U
30	a	1583	A
30	a	1584	U
30	a	1585	C
30	a	1586	A
30	a	1590	A
30	a	1608	A
30	a	1609	A
30	a	1610	A
30	a	1630	A
30	a	1647	U
30	a	1648	U
30	a	1649	G
30	a	1674	G
30	a	1677	A
30	a	1715	G
30	a	1729	U
30	a	1730	C
30	a	1731	G
30	a	1732	C
30	a	1736	U
30	a	1738	G
30	a	1750	G
30	a	1764	C
30	a	1773	A
30	a	1782	U
30	a	1791	A
30	a	1800	C
30	a	1801	A
30	a	1807	G
30	a	1808	A
30	a	1816	C
30	a	1829	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	1839	G
30	a	1847	A
30	a	1848	A
30	a	1862	G
30	a	1870	C
30	a	1871	A
30	a	1873	G
30	a	1876	A
30	a	1906	G
30	a	1907	G
30	a	1910	G
30	a	1912	A
30	a	1913	A
30	a	1929	G
30	a	1930	G
30	a	1937	A
30	a	1938	A
30	a	1955	U
30	a	1965	C
30	a	1966	A
30	a	1967	C
30	a	1970	A
30	a	1971	U
30	a	1972	G
30	a	1991	U
30	a	1992	G
30	a	1993	U
30	a	2023	C
30	a	2027	G
30	a	2031	A
30	a	2033	A
30	a	2043	C
30	a	2055	C
30	a	2056	G
30	a	2060	A
30	a	2061	G
30	a	2062	A
30	a	2069	G7M
30	a	2093	G
30	a	2098	U
30	a	2198	A
30	a	2203	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	2204	G
30	a	2211	A
30	a	2223	G
30	a	2225	A
30	a	2238	G
30	a	2239	G
30	a	2268	A
30	a	2273	A
30	a	2275	C
30	a	2276	G
30	a	2278	A
30	a	2282	G
30	a	2283	C
30	a	2287	A
30	a	2294	G
30	a	2305	U
30	a	2307	G
30	a	2308	G
30	a	2312	U
30	a	2322	A
30	a	2325	G
30	a	2333	A
30	a	2335	A
30	a	2340	A
30	a	2347	C
30	a	2350	C
30	a	2361	G
30	a	2383	G
30	a	2385	C
30	a	2402	U
30	a	2406	A
30	a	2424	C
30	a	2425	A
30	a	2429	G
30	a	2430	A
30	a	2431	U
30	a	2434	A
30	a	2435	A
30	a	2441	U
30	a	2448	A
30	a	2470	G
30	a	2474	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	2476	A
30	a	2478	A
30	a	2491	U
30	a	2494	G
30	a	2502	G
30	a	2504	PSU
30	a	2505	G
30	a	2518	A
30	a	2529	G
30	a	2530	A
30	a	2547	A
30	a	2566	A
30	a	2567	G
30	a	2572	A
30	a	2573	C
30	a	2574	G
30	a	2586	U
30	a	2602	A
30	a	2609	U
30	a	2613	U
30	a	2629	U
30	a	2630	G
30	a	2663	G
30	a	2689	U
30	a	2690	U
30	a	2714	G
30	a	2716	C
30	a	2726	A
30	a	2744	G
30	a	2748	A
30	a	2750	A
30	a	2752	C
30	a	2759	G
30	a	2765	A
30	a	2778	A
30	a	2780	G
30	a	2790	U
30	a	2792	A
30	a	2795	C
30	a	2798	U
30	a	2818	U
30	a	2820	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	2821	A
30	a	2861	U
30	a	2867	G
30	a	2868	A
30	a	2883	A
30	a	2884	U
30	a	2885	G
30	a	2901	C
30	a	2902	C
31	b	13	G
31	b	15	A
31	b	21	G
31	b	25	U
31	b	35	C
31	b	36	C
31	b	37	C
31	b	44	G
31	b	51	G
31	b	52	A
31	b	56	G
31	b	66	A
31	b	67	G
31	b	89	U
31	b	90	C
31	b	99	A
31	b	105	G
31	b	109	A

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	4	U
6	A	47	C
6	A	69	G
6	A	70	U
6	A	94	G
6	A	196	A
6	A	199	A
6	A	251	G
6	A	365	U
6	A	438	U
6	A	468	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	532	A
6	A	533	A
6	A	559	A
6	A	641	U
6	A	776	G
6	A	793	U
6	A	884	U
6	A	983	A
6	A	1034	G
6	A	1035	A
6	A	1047	G
6	A	1124	G
6	A	1145	A
6	A	1210	C
6	A	1239	A
6	A	1297	G
6	A	1298	U
6	A	1319	A
6	A	1320	C
6	A	1343	G
6	A	1492	A
6	A	1505	G
29	Z	47	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	IAS	K	119	16	6,7,8	0.94	0	6,8,10	0.92	0
30	OMU	a	2552	30	19,22,23	0.64	0	26,31,34	0.70	1 (3%)
30	PSU	a	2580	30	18,21,22	1.00	2 (11%)	22,30,33	0.73	1 (4%)
30	OMC	a	2498	57,30	19,22,23	0.50	0	26,31,34	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PSU	a	2605	30	18,21,22	0.72	1 (5%)	22,30,33	1.08	2 (9%)
30	3TD	a	1915	30	18,22,23	0.90	1 (5%)	22,32,35	0.65	0
41	4D4	l	81	41	9,11,12	0.49	0	8,13,15	0.96	1 (12%)
33	MEQ	d	150	33	8,9,10	0.53	0	5,10,12	0.71	0
30	2MG	a	1835	30	23,26,27	0.42	0	32,38,41	0.47	0
30	H2U	a	2449	30	18,21,22	0.62	1 (5%)	21,30,33	1.09	3 (14%)
30	G7M	a	2069	57,30	23,26,27	0.78	1 (4%)	35,39,42	0.79	1 (2%)
6	2MG	A	1207	6	23,26,27	0.34	0	32,38,41	0.55	0
30	PSU	a	2457	30	18,21,22	1.06	2 (11%)	22,30,33	0.63	0
6	MA6	A	1519	6	23,26,27	0.35	0	34,38,41	0.75	1 (2%)
41	MS6	l	82	41	5,7,8	0.27	0	2,7,9	0.11	0
30	5MU	a	1939	30	19,22,23	0.47	0	28,32,35	0.69	1 (3%)
6	5MC	A	967	6	18,22,23	0.34	0	26,32,35	0.69	1 (3%)
30	PSU	a	2504	30	18,21,22	0.72	1 (5%)	22,30,33	1.15	1 (4%)
30	1MG	a	745	30	22,26,27	0.70	1 (4%)	33,39,42	0.75	2 (6%)
30	2MG	a	2445	30	23,26,27	0.54	0	32,38,41	0.49	0
6	4OC	A	1402	6	20,23,24	0.33	0	26,32,35	0.57	0
6	G7M	A	527	6	23,26,27	0.77	1 (4%)	35,39,42	0.72	1 (2%)
6	PSU	A	516	57,6	18,21,22	0.84	1 (5%)	22,30,33	0.76	1 (4%)
6	UR3	A	1498	6	19,22,23	0.59	0	26,32,35	0.84	0
6	2MG	A	966	6	23,26,27	0.35	0	32,38,41	0.46	0
6	MA6	A	1518	6	23,26,27	0.31	0	34,38,41	0.73	1 (2%)
6	2MG	A	1516	6	23,26,27	0.36	0	32,38,41	0.52	0
30	PSU	a	955	30	18,21,22	0.95	1 (5%)	22,30,33	0.90	1 (4%)
30	PSU	a	746	57,30	18,21,22	0.92	2 (11%)	22,30,33	0.71	0
30	5MU	a	747	30	19,22,23	0.55	0	28,32,35	0.66	0
30	6MZ	a	2030	30	22,25,26	0.68	0	30,36,39	0.76	0
6	5MC	A	1407	6	18,22,23	0.30	0	26,32,35	0.70	0
30	PSU	a	1917	30	18,21,22	0.96	1 (5%)	22,30,33	0.71	0
30	PSU	a	1911	30	18,21,22	0.79	1 (5%)	22,30,33	0.64	0
30	6MZ	a	1618	30	22,25,26	0.65	0	30,36,39	0.69	0
30	PSU	a	2604	30	18,21,22	1.00	2 (11%)	22,30,33	0.85	1 (4%)
30	OMG	a	2251	29,30	23,26,27	0.40	0	33,38,41	0.62	0
30	2MA	a	2503	57,30	22,25,26	0.85	2 (9%)	33,37,40	1.13	2 (6%)
30	5MC	a	1962	30	18,22,23	0.41	0	26,32,35	0.56	1 (3%)
17	D2T	L	89	17	7,9,10	0.95	0	6,11,13	2.40	3 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	IAS	K	119	16	-	0/7/7/8	-
30	OMU	a	2552	30	-	2/9/27/28	0/2/2/2
30	PSU	a	2580	30	-	0/7/25/26	0/2/2/2
30	OMC	a	2498	57,30	-	0/9/27/28	0/2/2/2
30	PSU	a	2605	30	-	0/7/25/26	0/2/2/2
30	3TD	a	1915	30	-	0/7/25/26	0/2/2/2
41	4D4	l	81	41	-	2/11/12/14	-
33	MEQ	d	150	33	-	3/8/9/11	-
30	2MG	a	1835	30	-	0/9/27/28	0/3/3/3
30	H2U	a	2449	30	-	0/7/38/39	0/2/2/2
30	G7M	a	2069	57,30	-	2/7/25/26	0/3/3/3
6	2MG	A	1207	6	-	1/9/27/28	0/3/3/3
30	PSU	a	2457	30	-	0/7/25/26	0/2/2/2
6	MA6	A	1519	6	-	3/11/29/30	0/3/3/3
41	MS6	l	82	41	-	0/4/6/8	-
30	5MU	a	1939	30	-	0/7/25/26	0/2/2/2
6	5MC	A	967	6	-	0/7/25/26	0/2/2/2
30	PSU	a	2504	30	-	2/7/25/26	0/2/2/2
30	1MG	a	745	30	-	0/7/25/26	0/3/3/3
30	2MG	a	2445	30	-	1/9/27/28	0/3/3/3
6	4OC	A	1402	6	-	1/9/29/30	0/2/2/2
6	G7M	A	527	6	-	0/7/25/26	0/3/3/3
6	PSU	A	516	57,6	-	0/7/25/26	0/2/2/2
6	UR3	A	1498	6	-	0/7/25/26	0/2/2/2
6	2MG	A	966	6	-	1/9/27/28	0/3/3/3
6	MA6	A	1518	6	-	0/11/29/30	0/3/3/3
6	2MG	A	1516	6	-	0/9/27/28	0/3/3/3
30	PSU	a	955	30	-	0/7/25/26	0/2/2/2
30	PSU	a	746	57,30	-	4/7/25/26	0/2/2/2
30	5MU	a	747	30	-	0/7/25/26	0/2/2/2
30	6MZ	a	2030	30	-	2/9/27/28	0/3/3/3
6	5MC	A	1407	6	-	0/7/25/26	0/2/2/2
30	PSU	a	1917	30	-	0/7/25/26	0/2/2/2
30	PSU	a	1911	30	-	0/7/25/26	0/2/2/2
30	6MZ	a	1618	30	-	0/9/27/28	0/3/3/3
30	PSU	a	2604	30	-	0/7/25/26	0/2/2/2
30	OMG	a	2251	29,30	-	0/9/27/28	0/3/3/3
30	2MA	a	2503	57,30	-	1/7/25/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	5MC	a	1962	30	-	0/7/25/26	0/2/2/2
17	D2T	L	89	17	-	2/7/12/14	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	1915	3TD	C6-C5	3.47	1.39	1.35
30	a	1917	PSU	C6-C5	3.08	1.38	1.35
6	A	516	PSU	C6-C5	3.04	1.38	1.35
30	a	2457	PSU	C4-C5	-2.90	1.35	1.44
30	a	1911	PSU	C6-C5	2.76	1.38	1.35
30	a	746	PSU	C6-C5	2.67	1.38	1.35
30	a	2604	PSU	C4-C5	-2.63	1.36	1.44
30	a	955	PSU	C6-C5	2.59	1.38	1.35
30	a	2604	PSU	C6-C5	2.57	1.38	1.35
30	a	2580	PSU	C6-C5	2.44	1.38	1.35
30	a	2605	PSU	C6-C5	2.38	1.38	1.35
30	a	2504	PSU	C6-C5	2.33	1.38	1.35
6	A	527	G7M	C8-N7	2.29	1.37	1.33
30	a	2457	PSU	C6-C5	2.28	1.38	1.35
30	a	2503	2MA	C6-N1	2.21	1.38	1.35
30	a	2449	H2U	C2-N3	-2.15	1.34	1.38
30	a	2503	2MA	C6-N6	-2.12	1.28	1.34
30	a	2069	G7M	C5-C6	-2.11	1.36	1.43
30	a	745	1MG	C5-C6	-2.09	1.40	1.45
30	a	746	PSU	C4-C5	-2.05	1.38	1.44
30	a	2580	PSU	C4-C5	-2.05	1.38	1.44

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	L	89	D2T	CB-CA-N	4.02	117.67	109.10
30	a	2503	2MA	C5-C4-N3	-3.23	123.56	127.19
30	a	2604	PSU	C2'-C3'-C4'	-2.99	96.82	102.64
30	a	2504	PSU	C2'-C3'-C4'	-2.98	96.85	102.64
30	a	2449	H2U	N3-C2-N1	2.98	119.80	116.65
30	a	2552	OMU	C2'-C1'-N1	-2.67	109.04	114.22
6	A	1519	MA6	C2-N1-C6	2.66	118.04	111.75
30	a	2605	PSU	C2'-C3'-C4'	-2.65	97.50	102.64
17	L	89	D2T	OD1-CG-CB	-2.64	116.91	122.44
6	A	1518	MA6	C2-N1-C6	2.64	117.98	111.75
30	a	2503	2MA	CM2-C2-N1	2.63	121.25	117.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	745	1MG	CM1-N1-C2	-2.55	118.07	120.72
17	L	89	D2T	O-C-CA	-2.50	118.22	124.78
30	a	2069	G7M	N9-C8-N7	-2.48	106.06	112.21
30	a	2449	H2U	C4-N3-C2	-2.47	123.74	125.79
30	a	2449	H2U	O2-C2-N1	-2.42	120.07	123.11
41	l	81	4D4	O-C-CA	-2.41	118.46	124.78
30	a	955	PSU	C2'-C3'-C4'	-2.38	98.02	102.64
30	a	2580	PSU	C3'-C2'-C1'	2.37	104.40	101.64
30	a	2605	PSU	C5-C6-N1	-2.25	118.73	122.11
30	a	1939	5MU	O3'-C3'-C2'	-2.17	104.79	111.82
6	A	516	PSU	C3'-C2'-C1'	2.14	104.12	101.64
30	a	745	1MG	C2-N1-C6	2.11	122.66	120.95
6	A	967	5MC	O3'-C3'-C4'	-2.04	105.14	111.05
6	A	527	G7M	N9-C8-N7	-2.04	107.16	112.21
30	a	1962	5MC	C5-C6-N1	-2.02	121.26	123.34

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	d	150	MEQ	C-CA-CB-CG
33	d	150	MEQ	CG-CD-NE2-CE
30	a	746	PSU	C2'-C1'-C5-C4
30	a	746	PSU	C2'-C1'-C5-C6
30	a	2030	6MZ	O4'-C4'-C5'-O5'
30	a	2030	6MZ	C3'-C4'-C5'-O5'
30	a	2504	PSU	C3'-C4'-C5'-O5'
30	a	2504	PSU	O4'-C4'-C5'-O5'
6	A	1519	MA6	O4'-C4'-C5'-O5'
33	d	150	MEQ	OE1-CD-NE2-CE
6	A	1519	MA6	C3'-C4'-C5'-O5'
6	A	1519	MA6	C5-C6-N6-C10
30	a	2552	OMU	C1'-C2'-O2'-CM2
17	L	89	D2T	CG-CB-SB-CB1
30	a	2552	OMU	C3'-C2'-O2'-CM2
6	A	1207	2MG	O4'-C4'-C5'-O5'
30	a	2069	G7M	C4'-C5'-O5'-P
30	a	2503	2MA	O4'-C4'-C5'-O5'
30	a	746	PSU	O4'-C1'-C5-C4
6	A	1402	4OC	O4'-C4'-C5'-O5'
30	a	746	PSU	O4'-C1'-C5-C6
6	A	966	2MG	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	a	2069	G7M	O4'-C4'-C5'-O5'
30	a	2445	2MG	C3'-C4'-C5'-O5'
17	L	89	D2T	SB-CB-CG-OD1
41	l	81	4D4	O-C-CA-CB
41	l	81	4D4	NH1-CZ-NE-CD

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	a	2552	OMU	1	0
33	d	150	MEQ	1	0
30	a	1939	5MU	1	0
6	A	1402	4OC	1	0
30	a	747	5MU	1	0
30	a	2030	6MZ	2	0
30	a	2604	PSU	1	0
30	a	2251	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 284 ligands modelled in this entry, 283 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	ASP	Z	101	-	6,7,8	0.99	0	5,8,10	1.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	ASP	Z	101	-	-	2/5/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	Z	101	ASP	CA-CB-CG-OD1
58	Z	101	ASP	CA-CB-CG-OD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	Z	101	ASP	1	0

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.

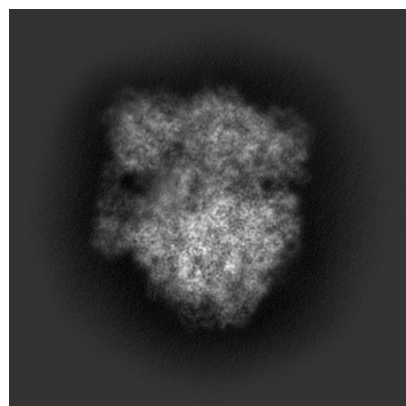
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57974. These allow visual inspection of the internal detail of the map and identification of artifacts.

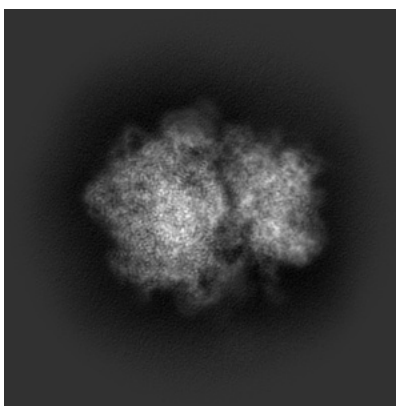
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

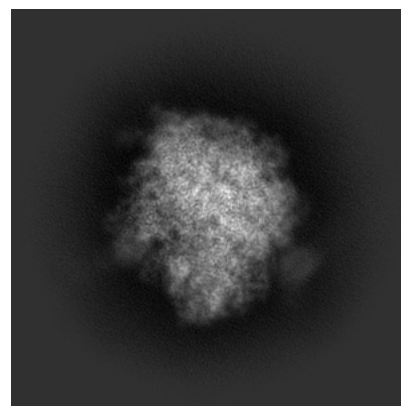
6.1.1 Primary map



X

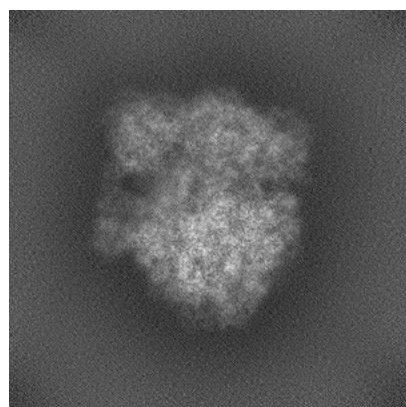


Y

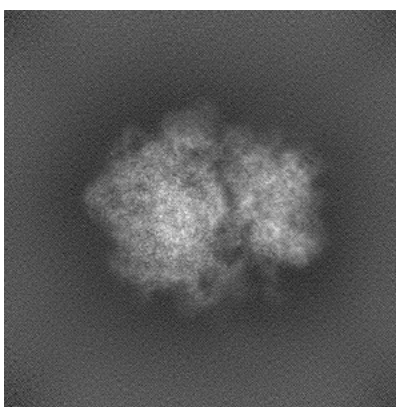


Z

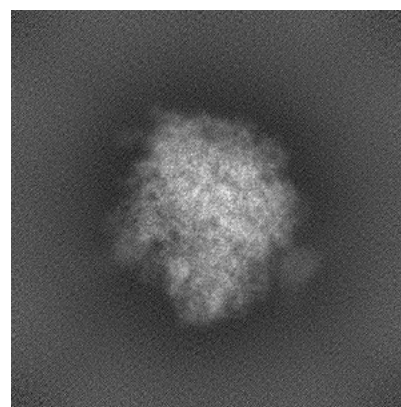
6.1.2 Raw map



X



Y

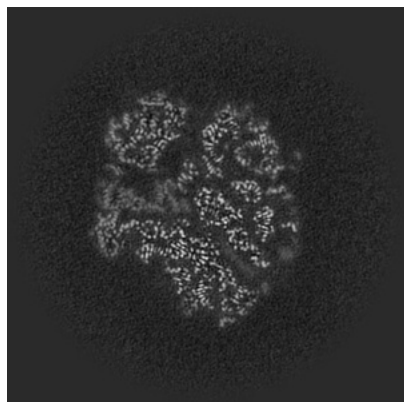


Z

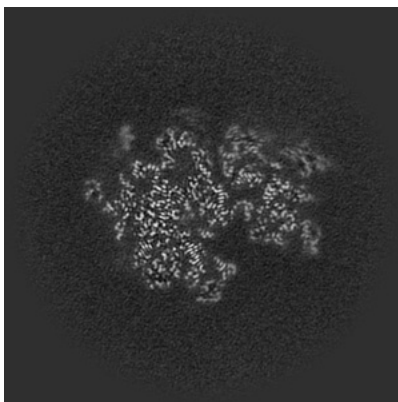
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

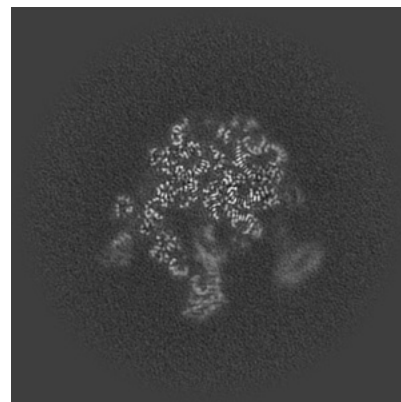
6.2.1 Primary map



X Index: 256

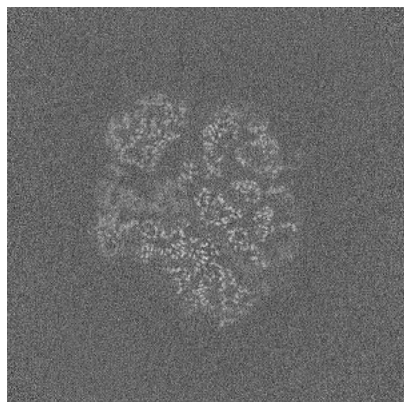


Y Index: 256

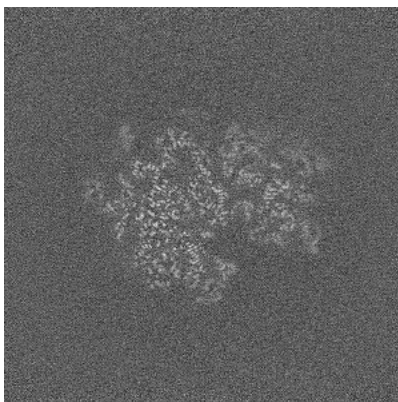


Z Index: 256

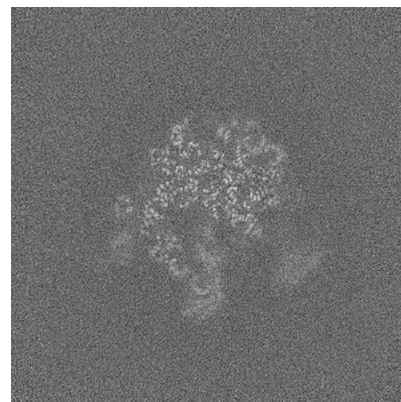
6.2.2 Raw map



X Index: 256



Y Index: 256

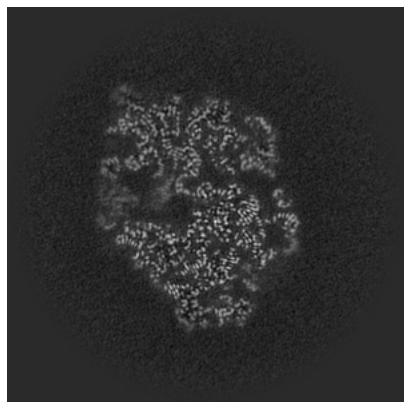


Z Index: 256

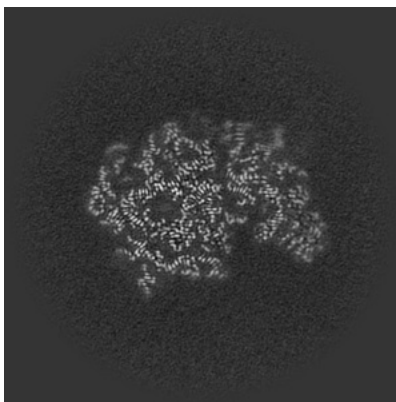
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

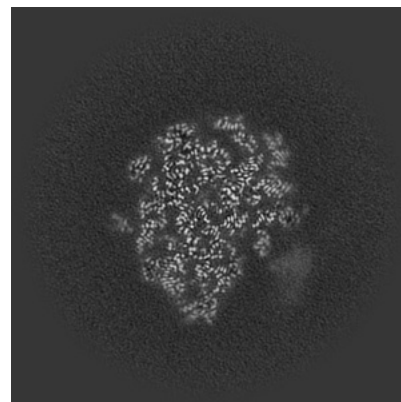
6.3.1 Primary map



X Index: 269

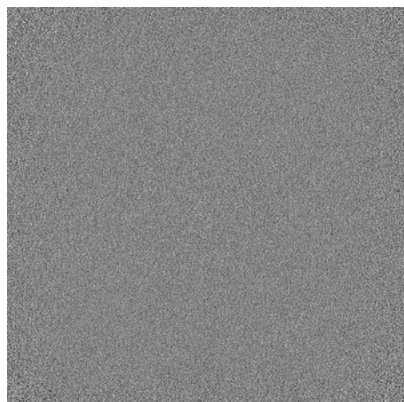


Y Index: 278

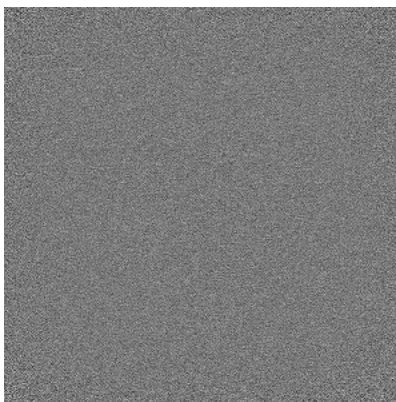


Z Index: 221

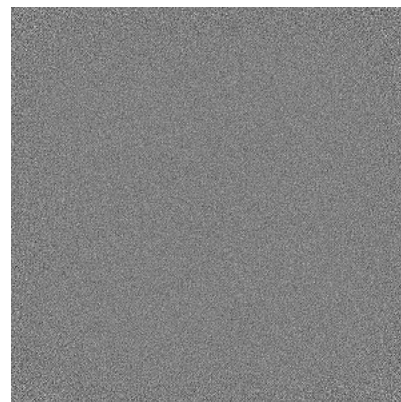
6.3.2 Raw map



X Index: 0



Y Index: 0

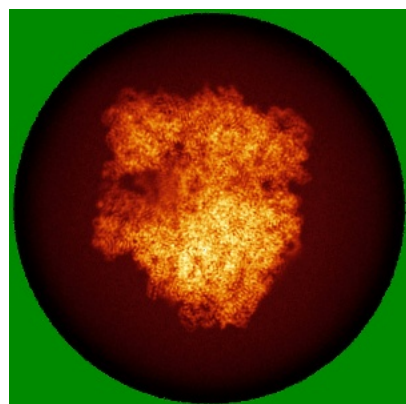


Z Index: 0

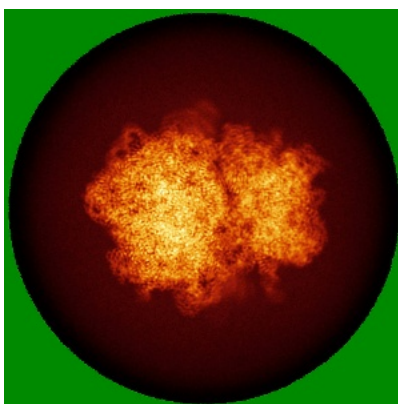
The images above show the largest variance slices of the map in three orthogonal directions.

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

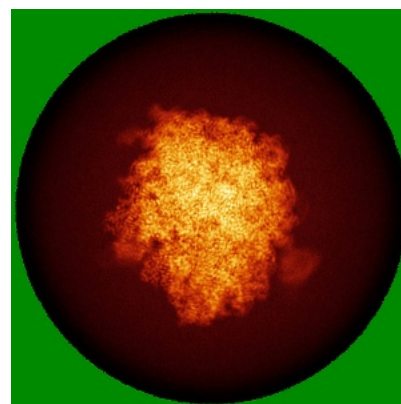
6.4.1 Primary map



X

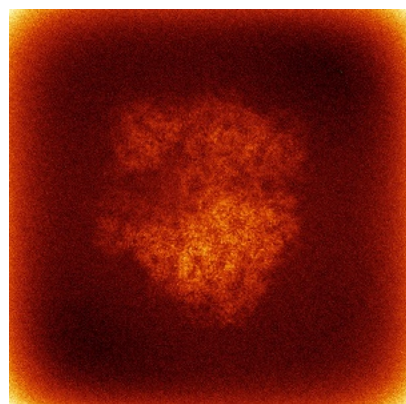


Y

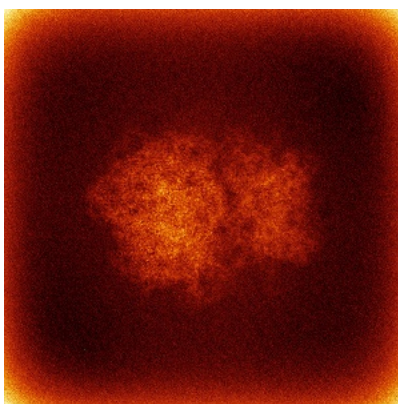


Z

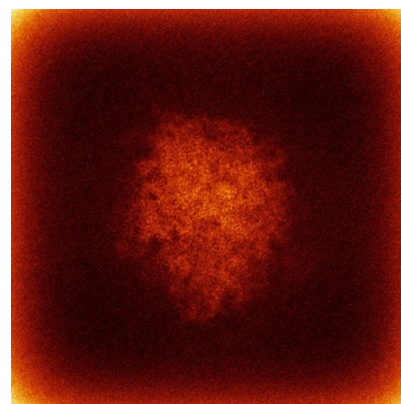
6.4.2 Raw map



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



X



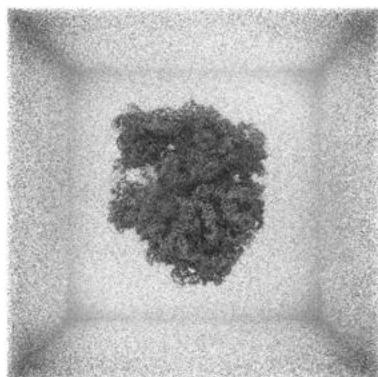
Y



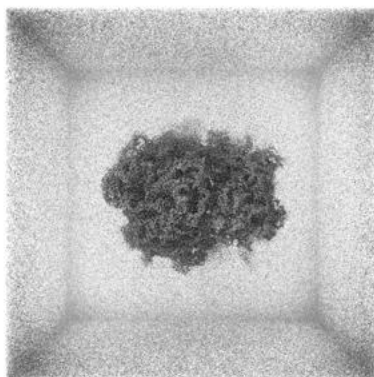
Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

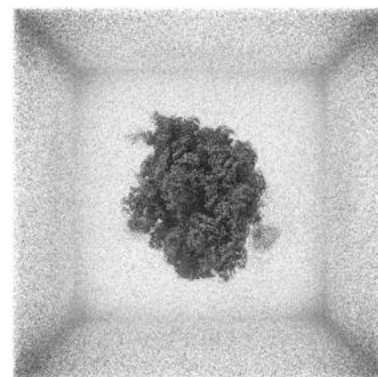
6.5.2 Raw map



X



Y



Z

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.

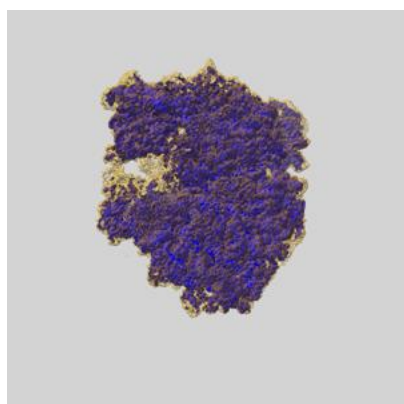
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

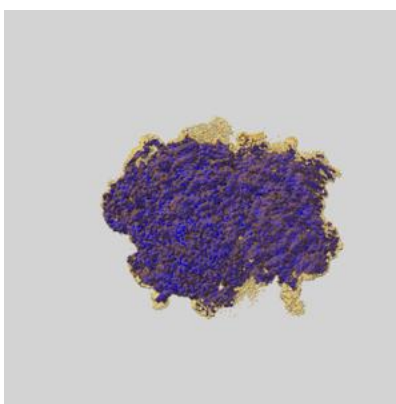
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

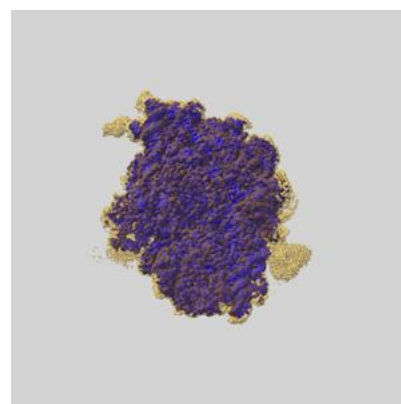
6.6.1 emd_57974_msk_1.map [i](#)



X

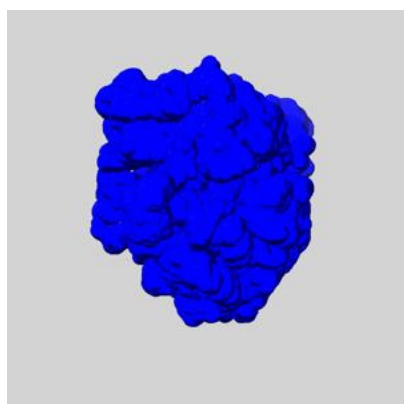


Y

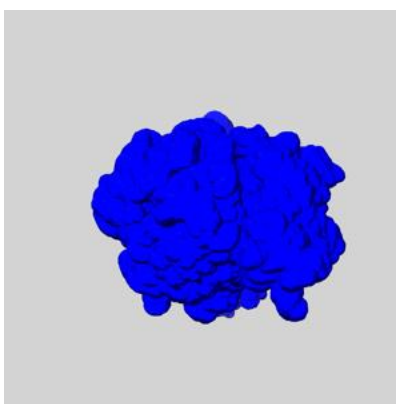


Z

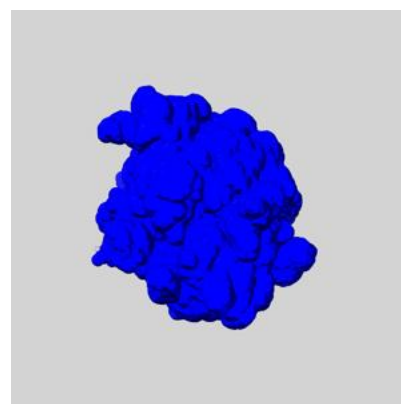
6.6.2 emd_57974_msk_2.map [i](#)



X



Y

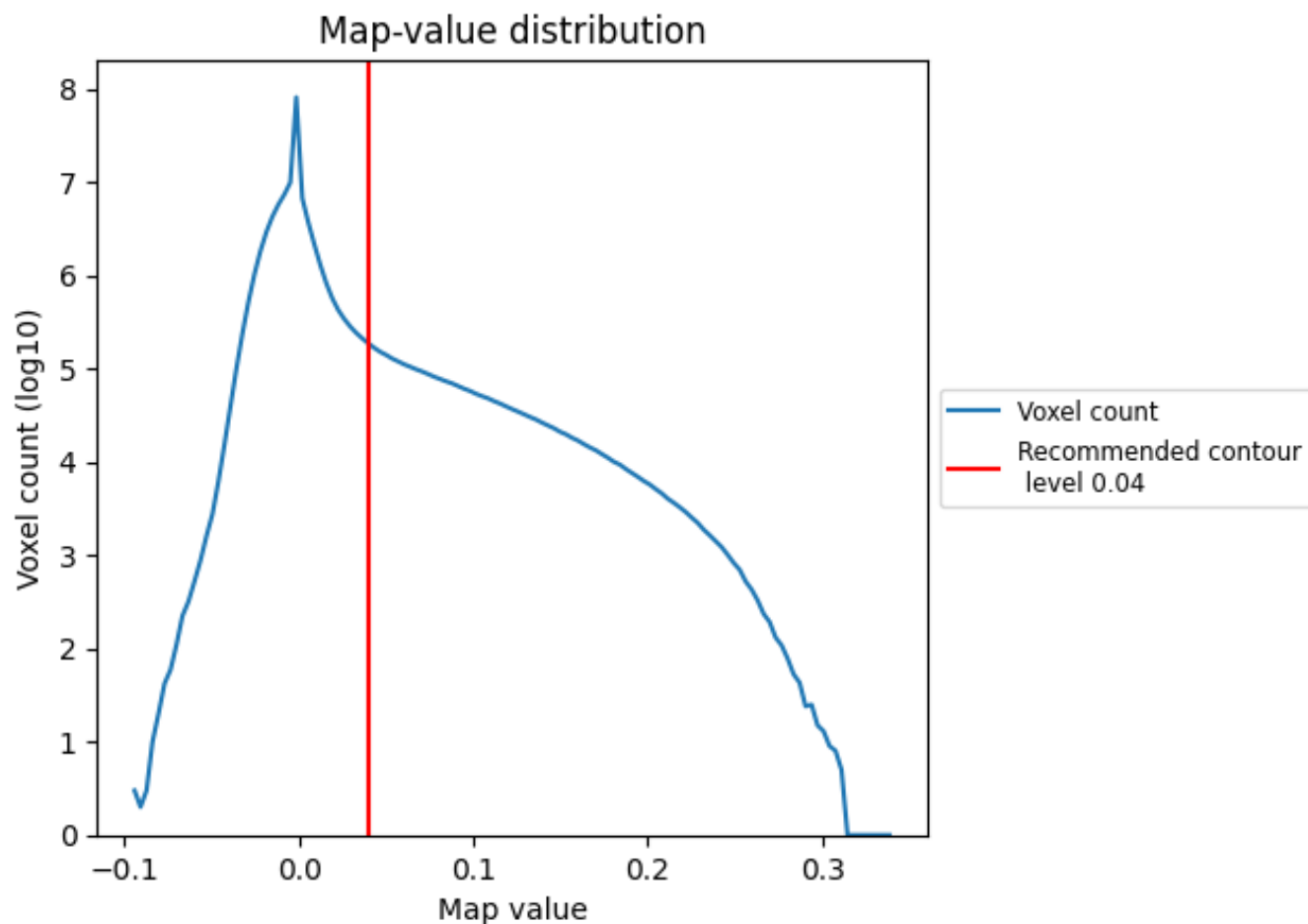


Z

7 Map analysis [i](#)

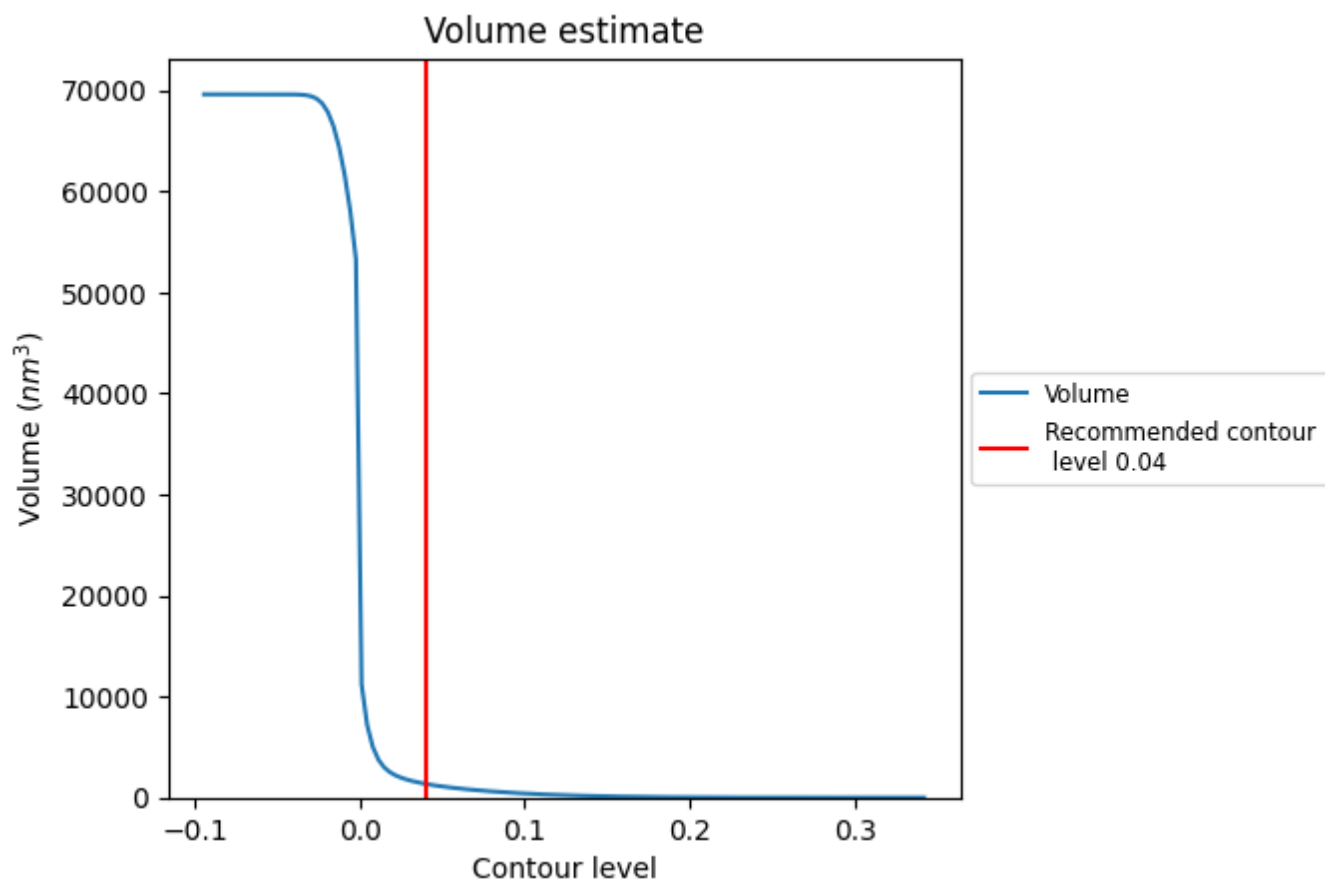
This section contains the results of statistical analysis of the map.

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.

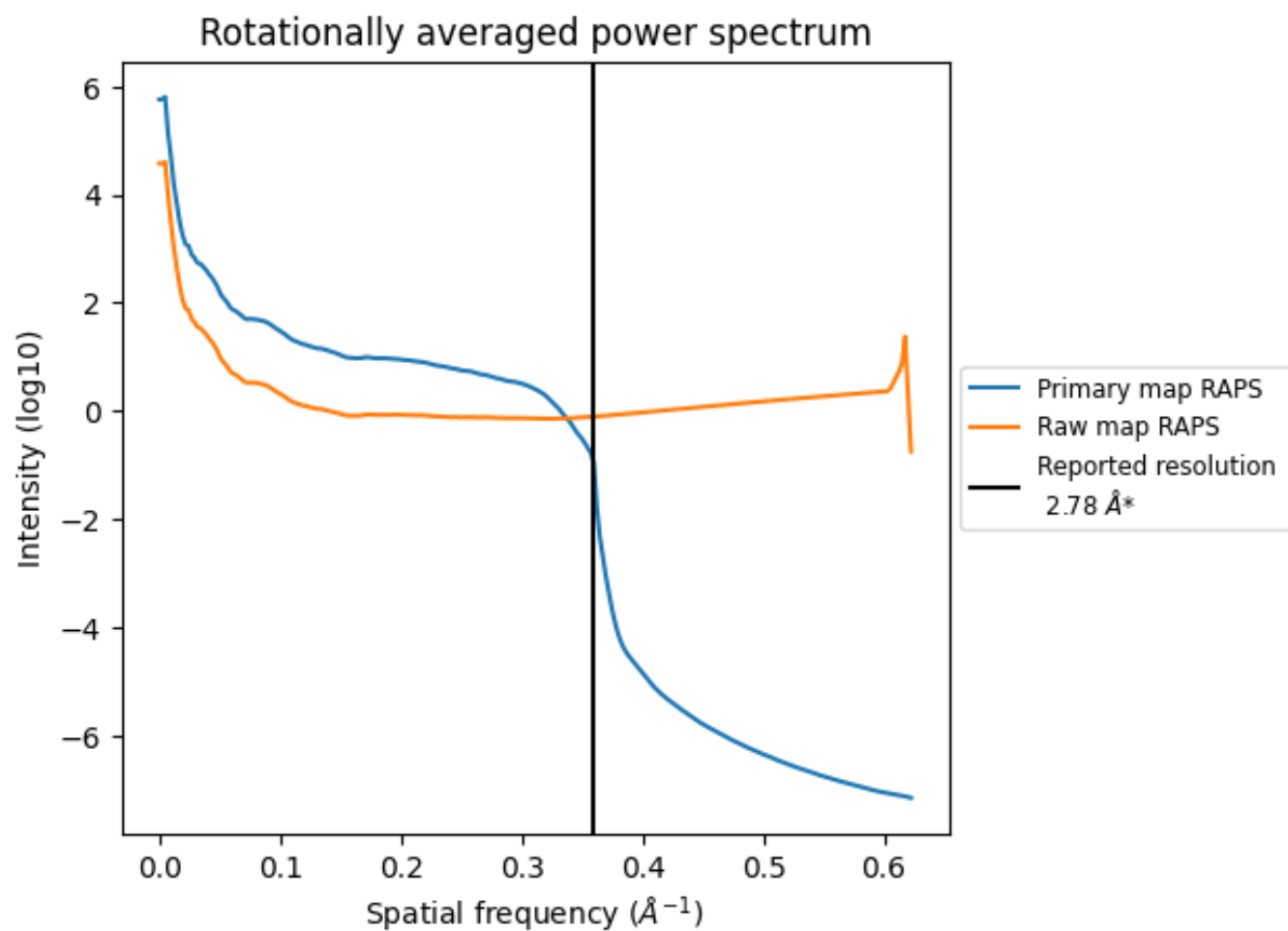
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1353 nm³; this corresponds to an approximate mass of 1222 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

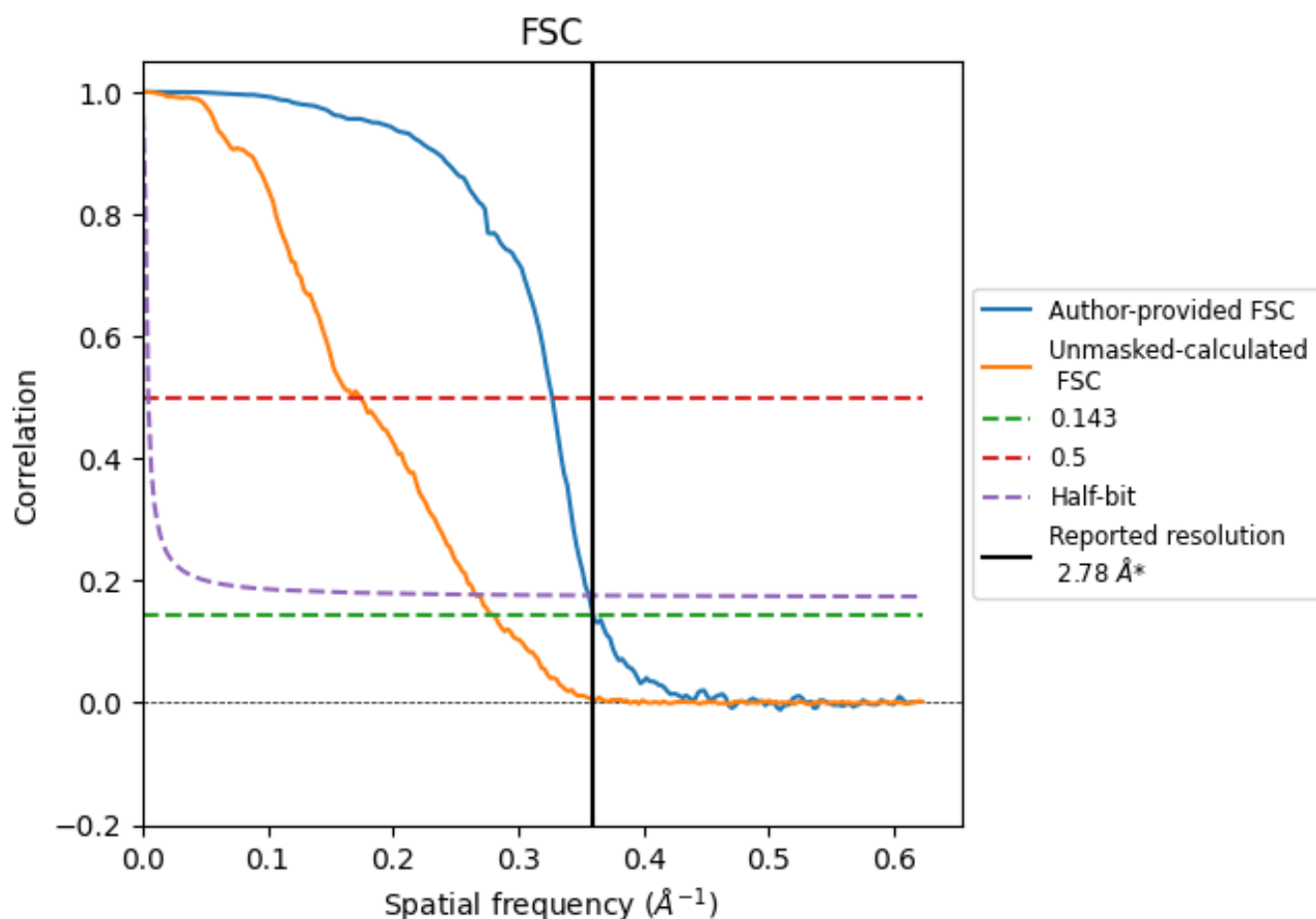


*Reported resolution corresponds to spatial frequency of 0.360 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.360 \AA^{-1}

8.2 Resolution estimates [i](#)

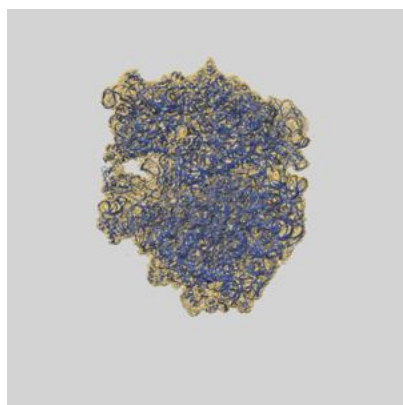
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	2.78	3.06	2.81
Unmasked-calculated*	3.57	5.75	3.76

*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 3.57 differs from the reported value 2.78 by more than 10 %

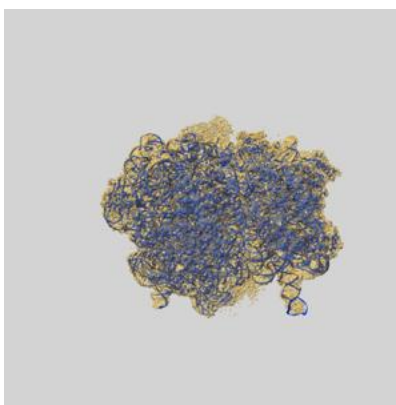
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-57974 and PDB model 30RA. Per-residue inclusion information can be found in section [3](#) on page [16](#).

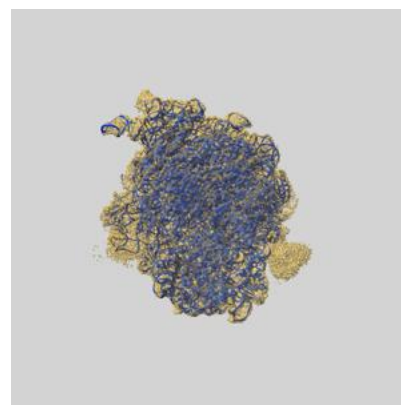
9.1 Map-model overlay [i](#)



X



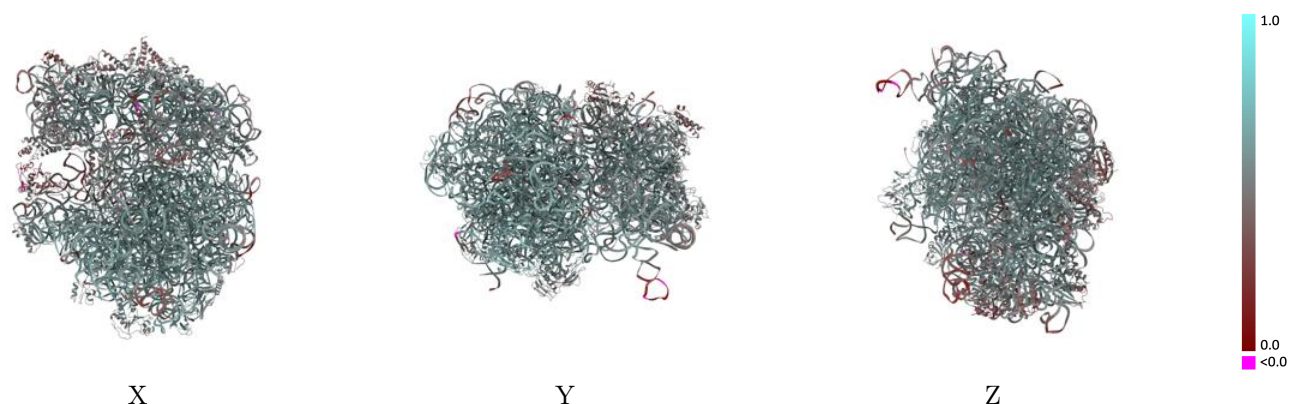
Y



Z

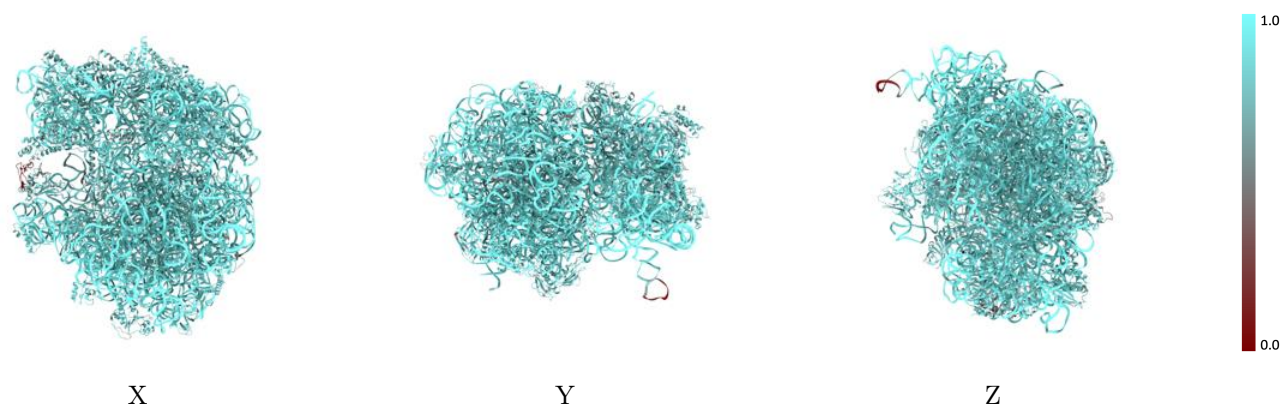
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



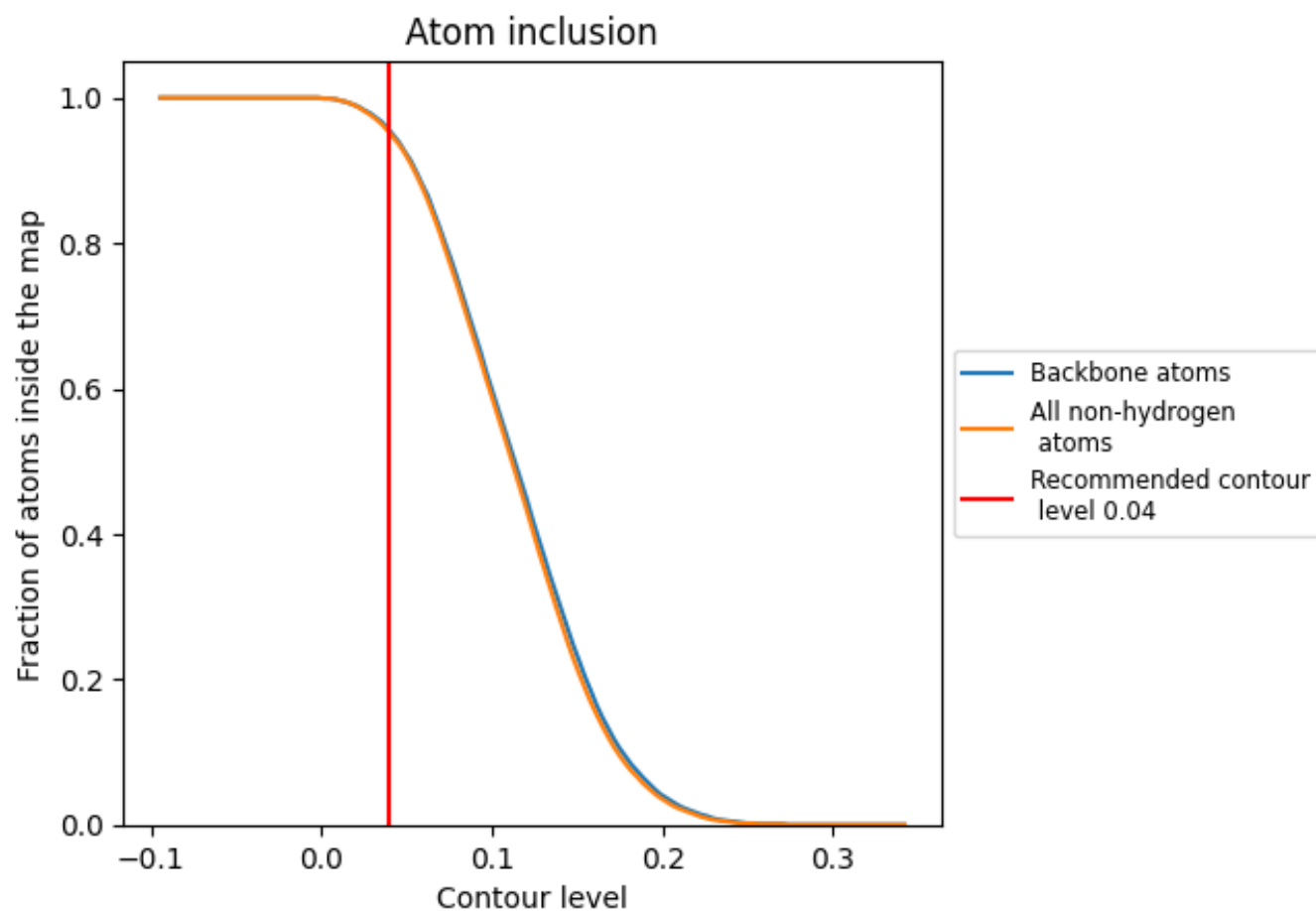
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9520	 0.5550
0	 0.9090	 0.5680
1	 0.9690	 0.6030
2	 0.9720	 0.6080
3	 0.9390	 0.5820
4	 0.2650	 0.2340
A	 0.9840	 0.5440
B	 0.8400	 0.4340
C	 0.8870	 0.5230
D	 0.8810	 0.5030
E	 0.9230	 0.5460
F	 0.7970	 0.3880
G	 0.8490	 0.4870
H	 0.9040	 0.5350
I	 0.8940	 0.4970
J	 0.8410	 0.4560
K	 0.8820	 0.4900
L	 0.9020	 0.5470
M	 0.8550	 0.4550
N	 0.9070	 0.5200
O	 0.8880	 0.5080
P	 0.9230	 0.5520
Q	 0.8900	 0.5190
R	 0.8220	 0.4090
S	 0.8470	 0.4690
T	 0.9070	 0.5390
U	 0.7120	 0.3590
V	 0.7940	 0.4860
X	 0.9230	 0.5870
Z	 0.9220	 0.4140
a	 0.9910	 0.5890
b	 0.9840	 0.5390
c	 0.9590	 0.5990
d	 0.9450	 0.5890
e	 0.9170	 0.5610



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	 0.7570	 0.3470
g	 0.8580	 0.5020
h	 0.8130	 0.4860
i	 0.9520	 0.5880
j	 0.9280	 0.5750
k	 0.9410	 0.5780
l	 0.9330	 0.5810
m	 0.9790	 0.6040
n	 0.9080	 0.5240
o	 0.9090	 0.5780
p	 0.9730	 0.6020
q	 0.9270	 0.5780
r	 0.9290	 0.5770
s	 0.8920	 0.5520
t	 0.8880	 0.5440
u	 0.8900	 0.5530
v	 0.9230	 0.5820
w	 0.9370	 0.5810
x	 0.8960	 0.5300
y	 0.9340	 0.5760
z	 0.9510	 0.5930