



Full wwPDB EM Validation Report ⓘ

Jun 21, 2026 – 07:56 am BST

PDB ID : 8PHJ / pdb_00008phj
EMDB ID : EMD-17667
Title : cA4-bound Cami1 in complex with 70S ribosome
Authors : Tamulaitiene, G.; Mogila, I.; Sasnauskas, G.; Tamulaitis, G.
Deposited on : 2023-06-20
Resolution : 3.67 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

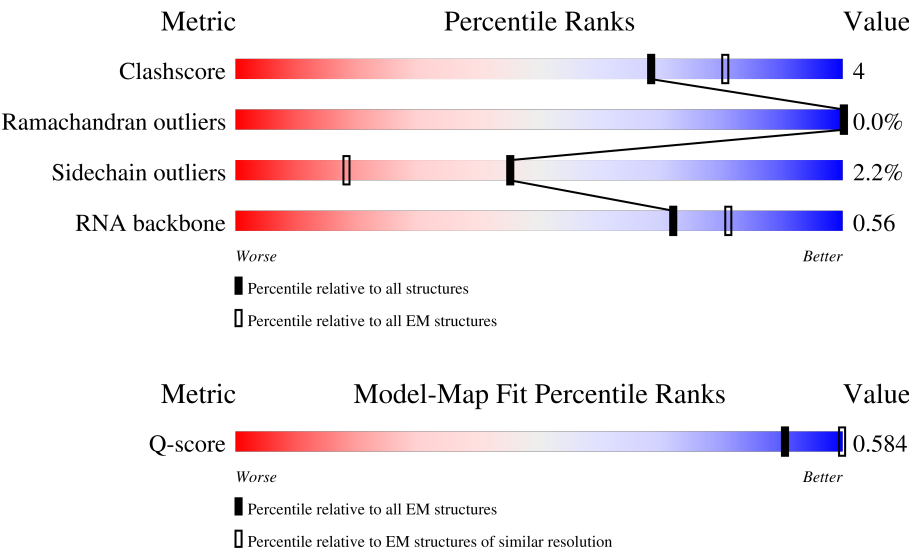
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.67 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	11424 (3.17 - 4.17)

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

Mol	Chain	Length	Quality of chain
1	0	55	
2	1	46	
3	2	65	

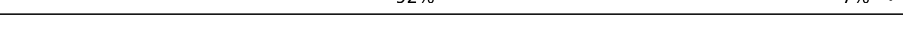
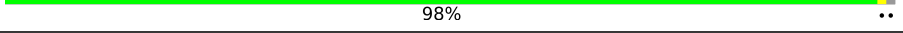
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Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	5	165	
7	6	142	
8	7	77	
8	8	77	
9	9	31	
10	A	1542	
11	B	241	
12	C	233	
13	D	206	
14	E	167	
15	F	135	
16	G	179	
17	H	130	
18	I	130	
19	J	103	
20	K	129	
21	L	124	
22	M	118	
23	N	101	
24	O	89	
25	P	82	
26	Q	84	
27	R	75	

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Mol	Chain	Length	Quality of chain
28	S	92	 82% 8% 10%
29	T	87	 90% 7% ..
30	U	71	 86% 13% .
31	W	120	 36% 15% 49%
32	X	406	 73% 21% . 5%
32	Y	406	 76% 16% 8%
33	a	2904	 79% 18% ..
34	b	120	 85% 12% ..
35	c	273	 91% 8% .
36	d	209	 85% 14% .
37	e	201	 90% 9% .
38	f	179	 80% 18% ..
39	g	177	 84% 14% ..
40	h	149	 11% 71% 26% .
41	i	142	 92% 7% .
42	j	123	 89% 11%
43	k	144	 85% 14% .
44	l	136	 79% 21%
45	m	127	 83% 9% . 7%
46	n	117	 88% 10% ..
47	o	115	 90% 9% .
48	p	118	 98% ..
49	q	103	 92% 6% .
50	r	110	 93% 6% .
51	s	100	 84% 9% 7%

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Mol	Chain	Length	Quality of chain
52	t	104	 78% 15% 7%
53	u	94	 84% 16%
54	v	85	 87% 9%
55	w	78	 90% 8% ..
56	x	63	 81% 14% 5%
57	y	59	 85% 8% . .
58	z	57	 77% 19% .
59	Z	4	 25% 25% 50%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 152518 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

- Molecule 5 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	121	Total	C	N	O	S	0	0
			907	577	161	166	3		

- Molecule 7 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	134	Total	C	N	O	S	0	0
			968	613	167	182	6		

- Molecule 8 is a RNA chain called fMet-tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
8	7	76	Total	C	N	O	P	S	0	0
			1625	726	294	528	76	1		
8	8	77	Total	C	N	O	P	S	0	0
			1642	735	297	533	76	1		

- Molecule 9 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	3	Total	C	N	O	P	0	0
			65	29	12	21	3		

- Molecule 10 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	1503	Total	C	N	O	P	0	0
			32276	14402	5932	10439	1503		

- Molecule 11 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 12 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 15 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	152	Total	C	N	O	S	0	0
			1185	738	227	216	4		

- Molecule 17 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 20 is a protein called Small ribosomal subunit protein uS11.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 21 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L	123	Total	C	N	O	S	0	0
			949	585	195	165	4		

- Molecule 22 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 23 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 24 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 25 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 26 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 27 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 28 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 29 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 30 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 31 is a protein called Large ribosomal subunit protein bL12.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	W	61	Total	C	N	O	0	0
			402	251	71	80		

- Molecule 32 is a protein called CRISPR-associated protein, APE2256 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	X	384	Total	C	N	O	S	0	0
			2984	1905	531	538	10		
32	Y	375	Total	C	N	O	S	0	0
			2912	1852	517	533	10		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	2	ALA	PRO	engineered mutation	UNP D3RW14
X	11	ALA	SER	engineered mutation	UNP D3RW14
X	343	ALA	HIS	engineered mutation	UNP D3RW14
X	382	GLY	-	expression tag	UNP D3RW14

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Chain	Residue	Modelled	Actual	Comment	Reference
X	383	GLU	-	expression tag	UNP D3RW14
X	384	GLY	-	expression tag	UNP D3RW14
X	385	TRP	-	expression tag	UNP D3RW14
X	386	SER	-	expression tag	UNP D3RW14
X	387	HIS	-	expression tag	UNP D3RW14
X	388	PRO	-	expression tag	UNP D3RW14
X	389	GLN	-	expression tag	UNP D3RW14
X	390	PHE	-	expression tag	UNP D3RW14
X	391	GLU	-	expression tag	UNP D3RW14
X	392	LYS	-	expression tag	UNP D3RW14
X	393	GLY	-	expression tag	UNP D3RW14
X	394	VAL	-	expression tag	UNP D3RW14
X	395	GLU	-	expression tag	UNP D3RW14
X	396	GLY	-	expression tag	UNP D3RW14
X	397	HIS	-	expression tag	UNP D3RW14
X	398	HIS	-	expression tag	UNP D3RW14
X	399	HIS	-	expression tag	UNP D3RW14
X	400	HIS	-	expression tag	UNP D3RW14
X	401	HIS	-	expression tag	UNP D3RW14
X	402	HIS	-	expression tag	UNP D3RW14
X	403	HIS	-	expression tag	UNP D3RW14
X	404	HIS	-	expression tag	UNP D3RW14
X	405	HIS	-	expression tag	UNP D3RW14
X	406	HIS	-	expression tag	UNP D3RW14
Y	2	ALA	PRO	engineered mutation	UNP D3RW14
Y	11	ALA	SER	engineered mutation	UNP D3RW14
Y	343	ALA	HIS	engineered mutation	UNP D3RW14
Y	382	GLY	-	expression tag	UNP D3RW14
Y	383	GLU	-	expression tag	UNP D3RW14
Y	384	GLY	-	expression tag	UNP D3RW14
Y	385	TRP	-	expression tag	UNP D3RW14
Y	386	SER	-	expression tag	UNP D3RW14
Y	387	HIS	-	expression tag	UNP D3RW14
Y	388	PRO	-	expression tag	UNP D3RW14
Y	389	GLN	-	expression tag	UNP D3RW14
Y	390	PHE	-	expression tag	UNP D3RW14
Y	391	GLU	-	expression tag	UNP D3RW14
Y	392	LYS	-	expression tag	UNP D3RW14
Y	393	GLY	-	expression tag	UNP D3RW14
Y	394	VAL	-	expression tag	UNP D3RW14
Y	395	GLU	-	expression tag	UNP D3RW14
Y	396	GLY	-	expression tag	UNP D3RW14

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	397	HIS	-	expression tag	UNP D3RW14
Y	398	HIS	-	expression tag	UNP D3RW14
Y	399	HIS	-	expression tag	UNP D3RW14
Y	400	HIS	-	expression tag	UNP D3RW14
Y	401	HIS	-	expression tag	UNP D3RW14
Y	402	HIS	-	expression tag	UNP D3RW14
Y	403	HIS	-	expression tag	UNP D3RW14
Y	404	HIS	-	expression tag	UNP D3RW14
Y	405	HIS	-	expression tag	UNP D3RW14
Y	406	HIS	-	expression tag	UNP D3RW14

- Molecule 33 is a RNA chain called 23S rRNA (2862-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	2862	Total	C	N	O	P	0	0
			61456	27423	11310	19861	2862		

- Molecule 34 is a RNA chain called 5S rRNA.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 37 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 38 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	174	Total	C	N	O	S	0	0
			1301	819	239	241	2		

- Molecule 40 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	145	Total	C	N	O	S	0	0
			1079	682	192	204	1		

- Molecule 41 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 42 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 43 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 44 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 45 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 46 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 47 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 48 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 49 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 50 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 51 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 52 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	t	97	Total	C	N	O	0	0
			742	469	139	134		

- Molecule 53 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 54 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	v	77	Total	C	N	O	S	0	0
			582	360	115	106	1		

- Molecule 55 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 56 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	60	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 57 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	y	57	Total	C	N	O	S	0	0
			440	275	85	78	2		

- Molecule 58 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 59 is a RNA chain called Cyclic tetraadenosine monophosphate (cA4).

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Z	4	Total	C	N	O	P	0	0
			88	40	20	24	4		

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
60	3	1	Total	Zn	0
			1	1	
60	4	1	Total	Zn	0
			1	1	

- Molecule 61 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
61	A	79	Total	Mg	0
			79	79	
61	a	156	Total	Mg	0
			156	156	
61	b	4	Total	Mg	0
			4	4	
61	c	1	Total	Mg	0
			1	1	
61	z	1	Total	Mg	0
			1	1	

3 Residue-property plots [i](#)

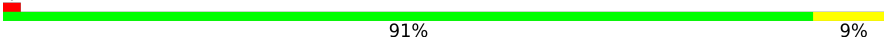
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

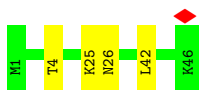
- Molecule 1: Large ribosomal subunit protein bL33

Chain 0: 



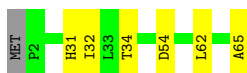
- Molecule 2: Large ribosomal subunit protein bL34

Chain 1: 



- Molecule 3: Large ribosomal subunit protein bL35

Chain 2: 



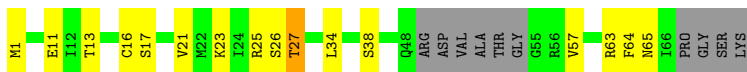
- Molecule 4: Large ribosomal subunit protein bL36A

Chain 3: 

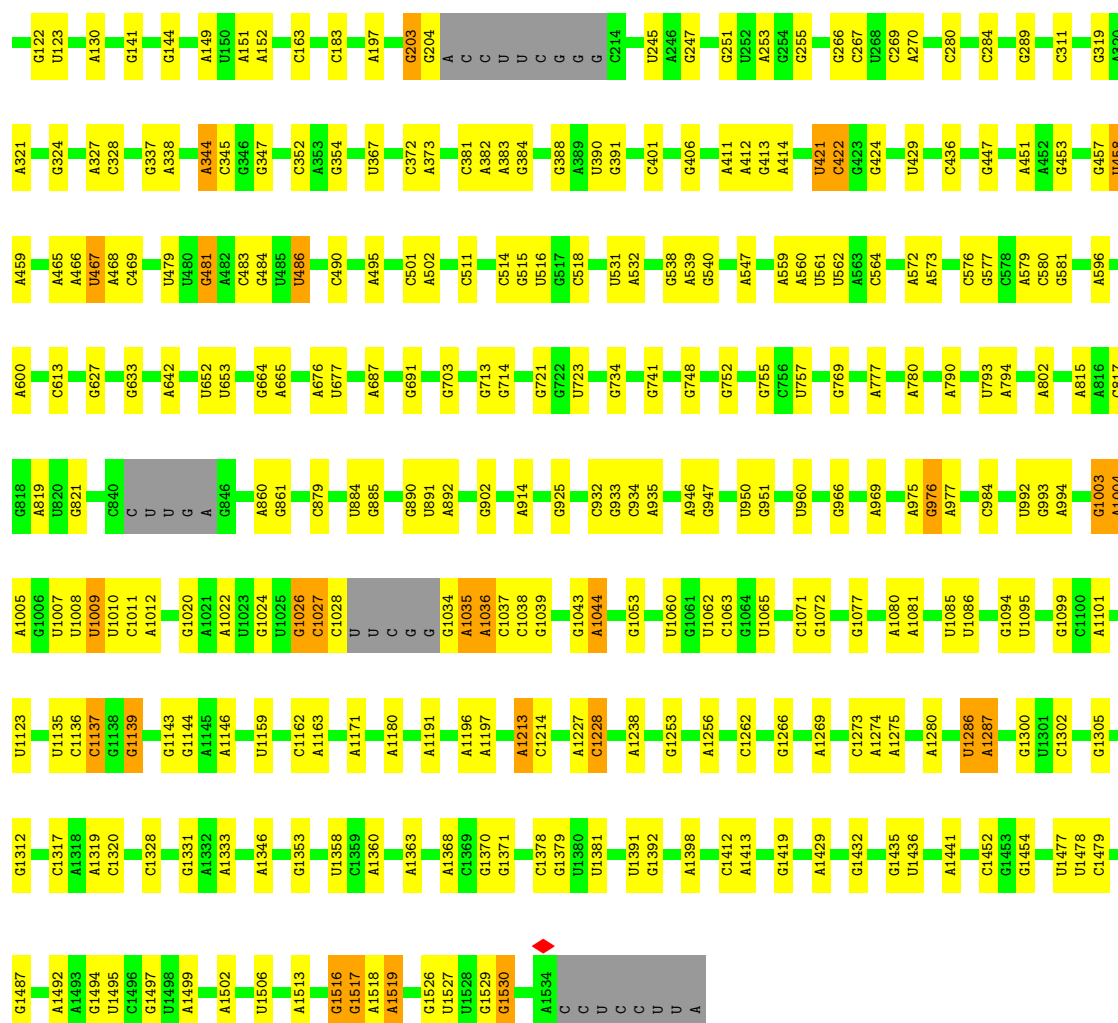


- Molecule 5: Large ribosomal subunit protein bL31A

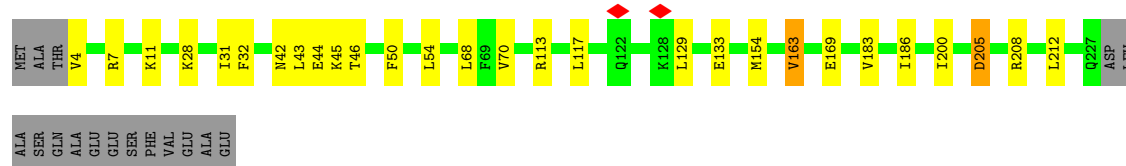
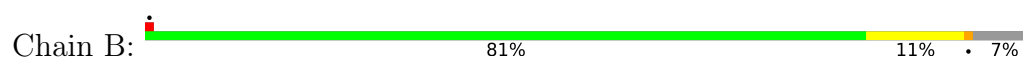
Chain 4: 



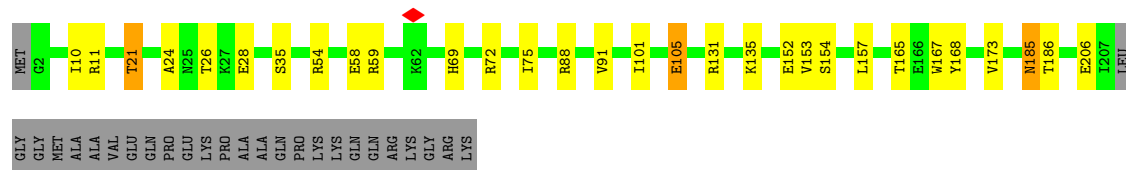
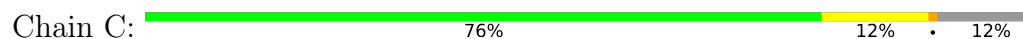
- Molecule 6: Large ribosomal subunit protein uL10



- Molecule 11: Small ribosomal subunit protein uS2



- Molecule 12: Small ribosomal subunit protein uS3



- Molecule 13: Small ribosomal subunit protein uS4

Chain D:  92% 8%



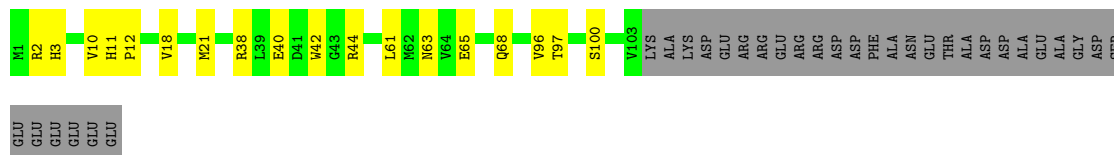
- Molecule 14: Small ribosomal subunit protein uS5

Chain E:  81% 11% 7%



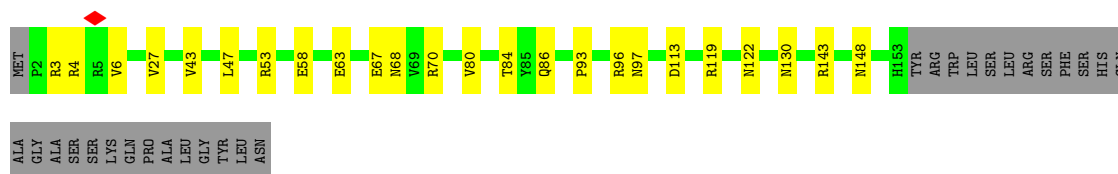
- Molecule 15: Small ribosomal subunit protein bS6, fully modified isoform

Chain F:  63% 13% 24%



- Molecule 16: Small ribosomal subunit protein uS7

Chain G:  72% 13% 15%



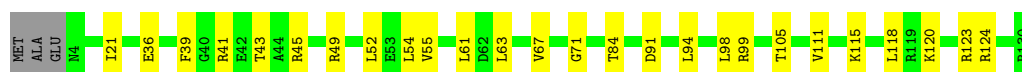
- Molecule 17: Small ribosomal subunit protein uS8

Chain H:  92% 8%



- Molecule 18: Small ribosomal subunit protein uS9

Chain I:  78% 20%



- Molecule 19: Small ribosomal subunit protein uS10

Chain J:  80% 16% 5%



- Molecule 20: Small ribosomal subunit protein uS11

Chain K:  77% 13% 9%



- Molecule 21: Small ribosomal subunit protein uS12

Chain L:  87% 10% 3%



- Molecule 22: Small ribosomal subunit protein uS13

Chain M:  82% 14% 4%



- Molecule 23: Small ribosomal subunit protein uS14

Chain N:  90% 9% 1%



- Molecule 24: Small ribosomal subunit protein uS15

Chain O:  90% 9% 1%



- Molecule 25: Small ribosomal subunit protein bS16

Chain P:  91% 7% 2%



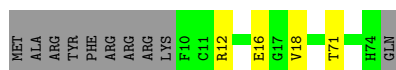
- Molecule 26: Small ribosomal subunit protein uS17

Chain Q:  82% 10% • 6%



- Molecule 27: Small ribosomal subunit protein bS18

Chain R:  81% 5% 13%



- Molecule 28: Small ribosomal subunit protein uS19

Chain S:  82% 8% • 10%



- Molecule 29: Small ribosomal subunit protein bS20

Chain T:  90% 7% • •



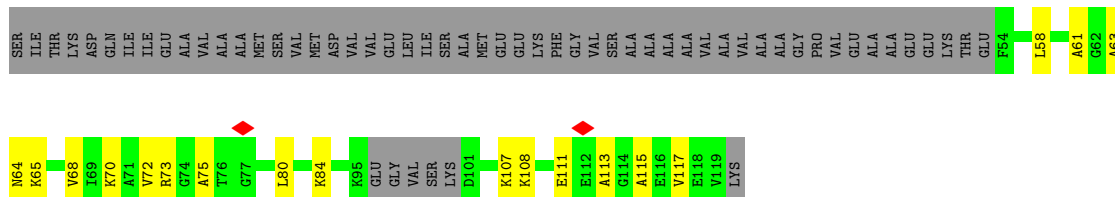
- Molecule 30: Small ribosomal subunit protein bS21

Chain U:  86% 13% •



- Molecule 31: Large ribosomal subunit protein bL12

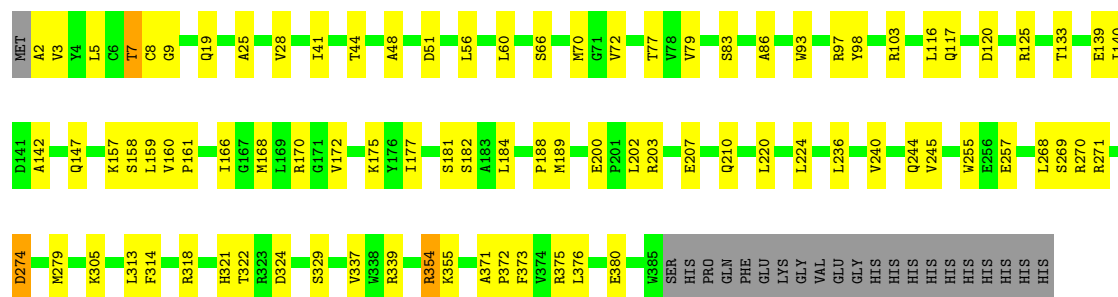
Chain W:  36% 15% 49%



- Molecule 32: CRISPR-associated protein, APE2256 family

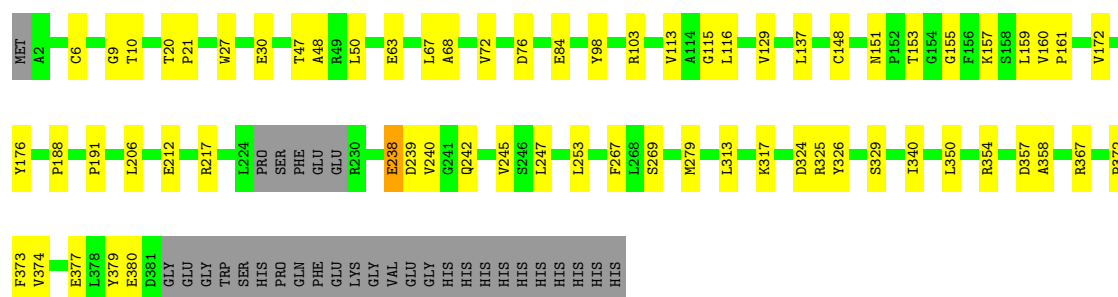
Chain X:  73% 21% • 5%





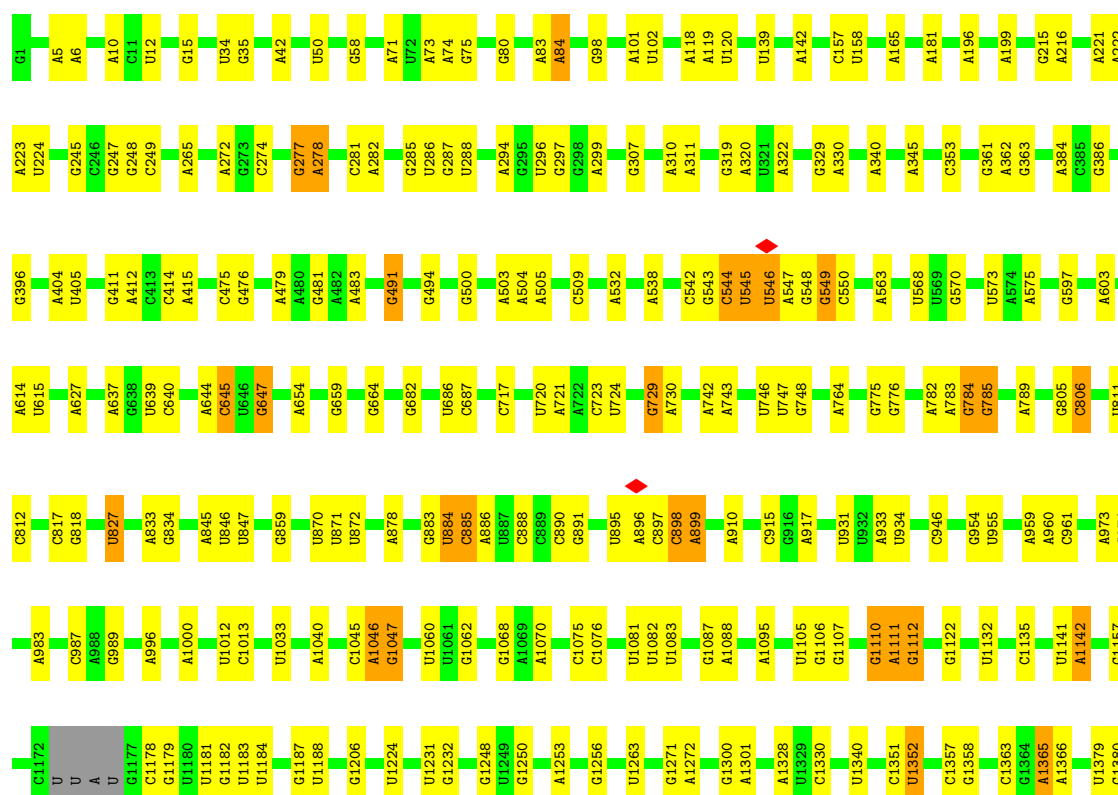
- Molecule 32: CRISPR-associated protein, APE2256 family

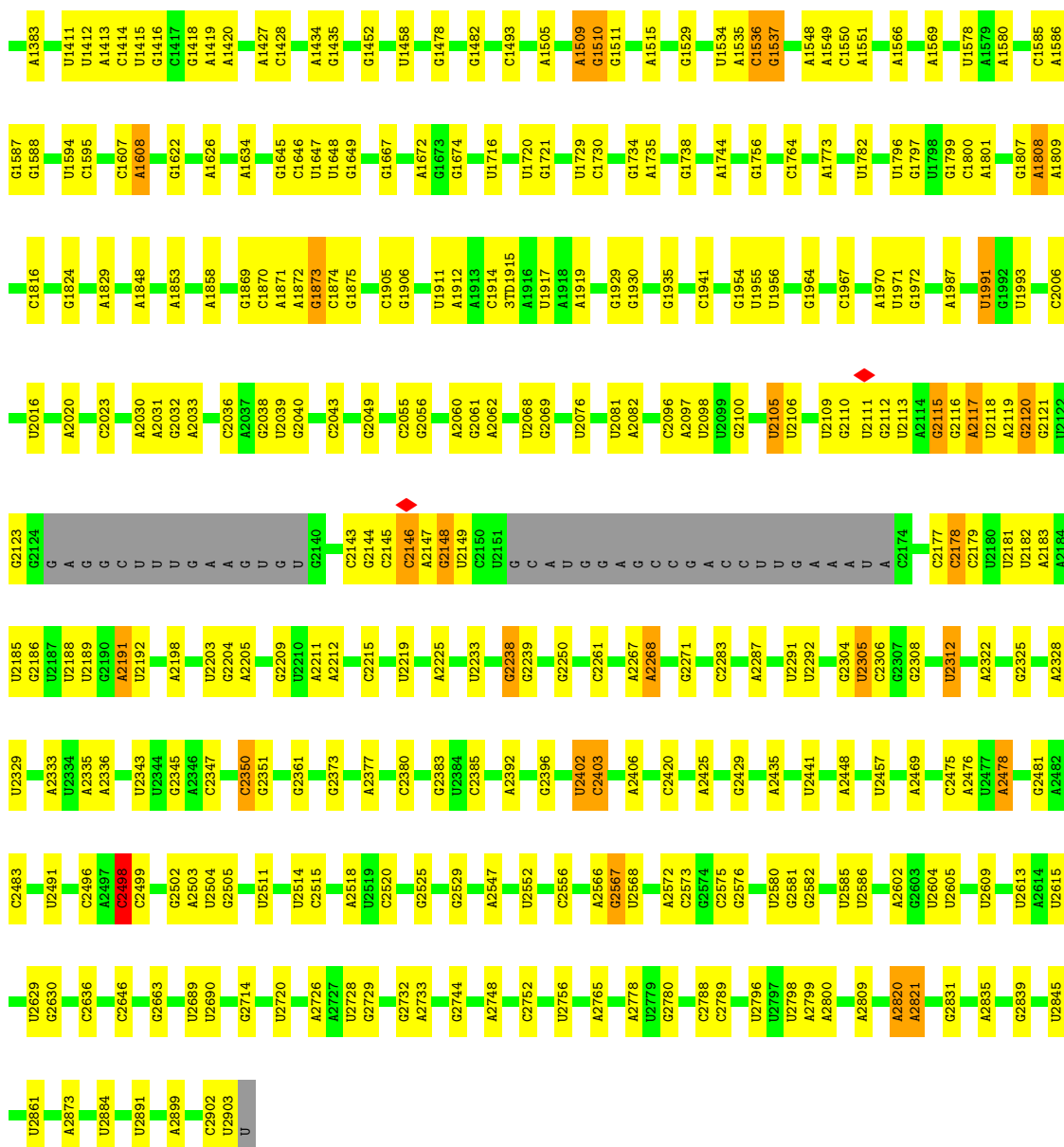
Chain Y: 76% 16% 8%



- Molecule 33: 23S rRNA (2862-MER)

Chain a: 79% 18% 3%





- Molecule 34: 5S rRNA

Chain b: 85% 12% ..



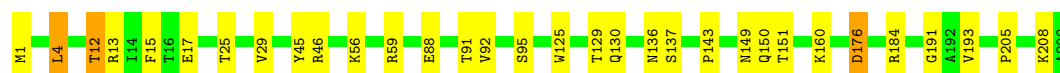
- Molecule 35: Large ribosomal subunit protein uL2

Chain c: 91% 8% .



- Molecule 36: Large ribosomal subunit protein uL3

Chain d:  85% 14%



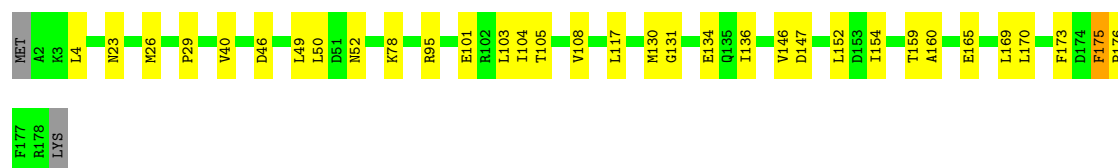
- Molecule 37: Large ribosomal subunit protein uL4

Chain e:  90% 9%



- Molecule 38: Large ribosomal subunit protein uL5

Chain f:  80% 18%



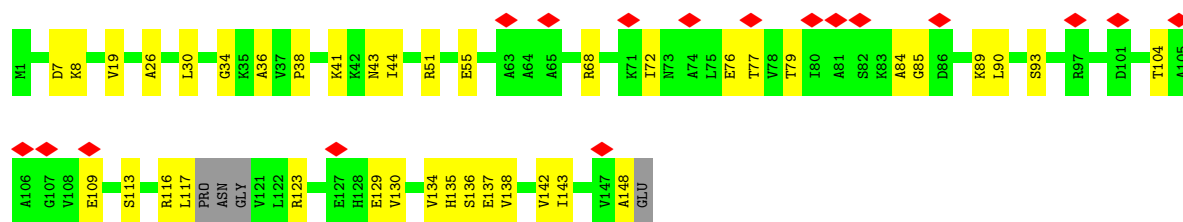
- Molecule 39: Large ribosomal subunit protein uL6

Chain g:  84% 14%



- Molecule 40: Large ribosomal subunit protein bL9

Chain h:  11% 71% 26%



- Molecule 41: Large ribosomal subunit protein uL13

Chain i:  92% 7%



- Molecule 42: Large ribosomal subunit protein uL14

Chain j:  89% 11%



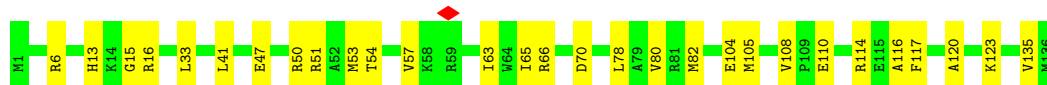
- Molecule 43: Large ribosomal subunit protein uL15

Chain k:  85% 14%



- Molecule 44: Large ribosomal subunit protein uL16

Chain l:  79% 21%



- Molecule 45: Large ribosomal subunit protein bL17

Chain m:  83% 9% 7%



- Molecule 46: Large ribosomal subunit protein uL18

Chain n:  88% 10%



- Molecule 47: Large ribosomal subunit protein bL19

Chain o:  90% 9%

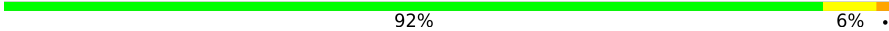


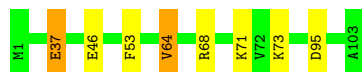
- Molecule 48: Large ribosomal subunit protein bL20

Chain p:  98%

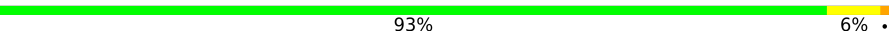


- Molecule 49: Large ribosomal subunit protein bL21

Chain q:  92% 6% .



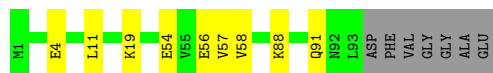
- Molecule 50: Large ribosomal subunit protein uL22

Chain r:  93% 6% .



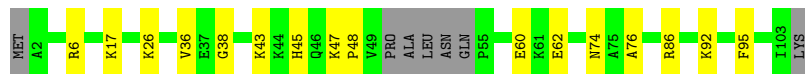
- Molecule 51: Large ribosomal subunit protein uL23

Chain s:  84% 9% 7%



- Molecule 52: Large ribosomal subunit protein uL24

Chain t:  78% 15% 7%



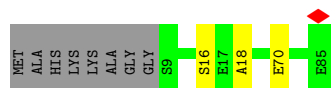
- Molecule 53: Large ribosomal subunit protein bL25

Chain u:  84% 16%



- Molecule 54: Large ribosomal subunit protein bL27

Chain v:  87% 9% .

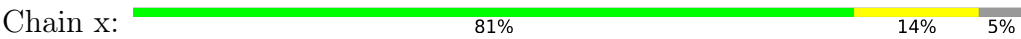


- Molecule 55: Large ribosomal subunit protein bL28

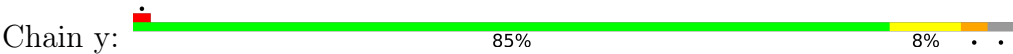
Chain w:  90% 8% ..



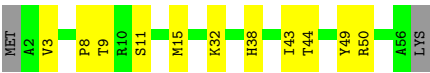
- Molecule 56: Large ribosomal subunit protein uL29



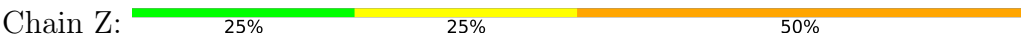
• Molecule 57: Large ribosomal subunit protein uL30



• Molecule 58: Large ribosomal subunit protein bL32



• Molecule 59: Cyclic tetraadenosine monophosphate (cA4)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	158387	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	33.264	Depositor
Minimum map value	-14.170	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2	Depositor
Map size ($\text{\AA}$)	448.0, 448.0, 448.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.12, 1.12, 1.12	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.23	0/424	0.28	0/565
2	1	0.27	0/380	0.30	0/498
3	2	0.25	0/513	0.30	0/676
4	3	0.25	0/303	0.27	0/397
5	4	0.12	0/488	0.24	0/649
6	5	0.10	0/916	0.24	0/1232
7	6	0.11	0/982	0.32	0/1328
8	7	0.16	0/1701	0.20	0/2649
8	8	0.15	0/1720	0.23	0/2679
9	9	0.17	0/72	0.18	0/110
10	A	0.25	0/35860	0.24	0/55930
11	B	0.14	0/1784	0.27	0/2403
12	C	0.20	0/1651	0.26	0/2225
13	D	0.19	0/1665	0.23	0/2227
14	E	0.22	0/1165	0.28	0/1568
15	F	0.17	0/858	0.27	0/1160
16	G	0.15	0/1200	0.25	0/1610
17	H	0.21	0/989	0.29	0/1326
18	I	0.17	0/1034	0.26	0/1375
19	J	0.18	0/796	0.31	0/1077
20	K	0.18	0/884	0.25	0/1191
21	L	0.21	0/963	0.27	0/1293
22	M	0.16	0/900	0.23	0/1204
23	N	0.19	0/817	0.22	0/1088
24	O	0.18	0/722	0.22	0/964
25	P	0.22	0/653	0.30	0/877
26	Q	0.19	0/650	0.26	0/871
27	R	0.19	0/544	0.23	0/731
28	S	0.16	0/680	0.25	0/915
29	T	0.19	0/676	0.21	0/895
30	U	0.14	0/597	0.22	0/792

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	W	0.11	0/401	0.25	0/541
32	X	0.23	0/3049	0.30	0/4143
32	Y	0.24	0/2972	0.30	0/4039
33	a	0.29	0/68253	0.27	0/106469
34	b	0.23	0/2850	0.22	0/4444
35	c	0.25	0/2121	0.31	0/2852
36	d	0.25	0/1576	0.30	0/2119
37	e	0.21	0/1571	0.29	0/2113
38	f	0.15	0/1434	0.24	0/1926
39	g	0.18	0/1321	0.26	0/1790
40	h	0.12	0/1088	0.29	0/1468
41	i	0.24	0/1152	0.27	0/1551
42	j	0.24	0/955	0.31	0/1279
43	k	0.23	0/1052	0.28	0/1401
44	l	0.24	0/1093	0.31	0/1460
45	m	0.25	0/958	0.31	0/1281
46	n	0.19	0/902	0.28	0/1209
47	o	0.23	0/929	0.26	0/1242
48	p	0.26	0/960	0.28	0/1278
49	q	0.21	0/829	0.30	0/1107
50	r	0.23	0/864	0.27	0/1156
51	s	0.21	0/744	0.29	0/994
52	t	0.18	0/748	0.27	0/994
53	u	0.21	0/766	0.26	0/1025
54	v	0.24	0/589	0.31	0/780
55	w	0.24	0/635	0.27	0/848
56	x	0.17	0/492	0.25	0/655
57	y	0.22	0/444	0.26	0/594
58	z	0.25	0/440	0.31	0/588
59	Z	0.38	0/99	0.41	0/152
All	All	0.25	0/163874	0.27	0/244003

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	417	0	451	4	0
2	1	377	0	418	3	0
3	2	504	0	572	4	0
4	3	302	0	340	7	0
5	4	480	0	478	11	0
6	5	907	0	935	14	0
7	6	968	0	1009	28	0
8	7	1625	0	833	12	0
8	8	1642	0	845	15	0
9	9	65	0	33	1	0
10	A	32276	0	16264	113	0
11	B	1753	0	1780	16	0
12	C	1624	0	1696	18	0
13	D	1643	0	1707	10	0
14	E	1152	0	1196	11	0
15	F	839	0	833	11	0
16	G	1185	0	1234	15	0
17	H	979	0	1031	6	0
18	I	1022	0	1070	13	0
19	J	786	0	828	9	0
20	K	877	0	884	16	0
21	L	949	0	998	9	0
22	M	891	0	952	12	0
23	N	805	0	844	7	0
24	O	714	0	734	4	0
25	P	643	0	661	3	0
26	Q	641	0	682	8	0
27	R	535	0	552	2	0
28	S	663	0	688	5	0
29	T	670	0	719	6	0
30	U	589	0	629	8	0
31	W	402	0	402	13	0
32	X	2984	0	2973	65	0
32	Y	2912	0	2886	44	0
33	a	61456	0	30938	213	0
34	b	2549	0	1291	8	0
35	c	2082	0	2154	13	0
36	d	1566	0	1618	26	0
37	e	1552	0	1619	12	0
38	f	1410	0	1444	23	0
39	g	1301	0	1343	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	h	1079	0	1123	31	0
41	i	1129	0	1162	9	0
42	j	946	0	1023	7	0
43	k	1043	0	1123	12	0
44	l	1074	0	1157	19	0
45	m	945	0	989	7	0
46	n	892	0	923	10	0
47	o	917	0	962	10	0
48	p	947	0	1019	0	0
49	q	816	0	839	5	0
50	r	857	0	922	5	0
51	s	738	0	807	6	0
52	t	742	0	794	10	0
53	u	753	0	780	7	0
54	v	582	0	593	2	0
55	w	625	0	652	5	0
56	x	491	0	523	4	0
57	y	440	0	472	4	0
58	z	434	0	445	7	0
59	Z	88	0	44	2	0
60	3	1	0	0	0	0
60	4	1	0	0	0	0
61	A	79	0	0	0	0
61	a	156	0	0	0	0
61	b	4	0	0	0	0
61	c	1	0	0	0	0
61	z	1	0	0	0	0
All	All	152518	0	104916	855	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (855) 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)
33:a:1047:G:HO2'	33:a:1110:G:H1	1.03	0.95
40:h:117:LEU:HD23	40:h:130:VAL:HG23	1.48	0.94
10:A:1009:U:H3	10:A:1020:G:H1	1.22	0.83
51:s:56:GLU:HG3	51:s:57:VAL:HG23	1.66	0.78
20:K:74:VAL:HG12	20:K:74:VAL:O	1.81	0.78
33:a:659:G:H4'	37:e:95:LYS:HG2	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:O:33:THR:O	24:O:37:ASN:ND2	2.20	0.75
14:E:90:THR:OG1	14:E:91:GLY:N	2.18	0.75
51:s:54:GLU:H	51:s:91:GLN:HG2	1.50	0.74
7:6:13:VAL:HG12	7:6:24:VAL:CG2	2.18	0.73
38:f:40:VAL:HG11	38:f:50:LEU:HD13	1.71	0.73
33:a:2831:G:OP2	36:d:59:ARG:NH1	2.21	0.72
29:T:39:ILE:HD11	29:T:83:ILE:HG12	1.71	0.71
56:x:16:THR:O	56:x:20:ASN:ND2	2.24	0.71
33:a:2483:C:N3	44:l:123:LYS:NZ	2.39	0.70
35:c:107:PRO:HD2	35:c:110:LEU:HD22	1.74	0.70
7:6:13:VAL:CG1	7:6:24:VAL:HG21	2.22	0.70
33:a:2115:G:N7	33:a:2117:A:O2'	2.24	0.70
39:g:104:ASN:ND2	39:g:114:ASP:OD1	2.23	0.69
10:A:203:G:O2'	10:A:465:A:N1	2.25	0.69
33:a:543:G:H1	33:a:550:C:H42	1.40	0.69
31:W:68:VAL:CG2	31:W:115:ALA:HB2	2.23	0.69
11:B:32:PHE:HB2	11:B:42:ASN:HB2	1.74	0.69
37:e:21:ARG:HD3	37:e:106:LYS:HB3	1.75	0.68
32:X:210:GLN:OE1	32:X:255:TRP:NE1	2.25	0.68
33:a:2305:U:H5''	38:f:131:GLY:HA3	1.76	0.68
31:W:63:ALA:O	32:Y:242:GLN:NE2	2.27	0.67
40:h:134:VAL:HG13	40:h:138:VAL:HB	1.76	0.67
10:A:481:G:O2'	10:A:483:C:N4	2.27	0.67
32:Y:72:VAL:O	32:Y:103:ARG:NH1	2.26	0.67
32:Y:116:LEU:HD11	32:Y:159:LEU:HD21	1.76	0.67
7:6:100:LYS:HB2	7:6:141:GLU:HB2	1.77	0.67
10:A:932:C:H5''	16:G:4:ARG:HE	1.59	0.67
40:h:38:PRO:O	40:h:43:ASN:ND2	2.27	0.66
32:X:157:LYS:NZ	32:Y:153:THR:O	2.28	0.66
10:A:627:G:OP1	25:P:51:ARG:NH2	2.29	0.66
31:W:107:LYS:HG3	31:W:117:VAL:HG11	1.77	0.66
32:X:375:ARG:NE	32:Y:377:GLU:OE1	2.25	0.66
2:1:25:LYS:NZ	2:1:26:ASN:OD1	2.29	0.66
36:d:184:ARG:NH2	47:o:7:GLN:OE1	2.28	0.66
22:M:110:LYS:O	22:M:114:LYS:NZ	2.29	0.65
8:7:7:G:OP1	8:7:16:C:N4	2.29	0.65
53:u:20:LEU:HD21	53:u:41:GLU:HG2	1.78	0.65
15:F:11:HIS:HD2	15:F:12:PRO:HD2	1.60	0.65
33:a:83:A:OP1	52:t:92:LYS:NZ	2.29	0.65
38:f:29:PRO:HB2	38:f:169:LEU:HD22	1.79	0.65
4:3:2:LYS:NZ	4:3:32:LYS:O	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:35:SER:OG	12:C:59:ARG:NH2	2.29	0.65
28:S:50:ALA:HB1	28:S:57:HIS:HB3	1.79	0.65
33:a:1869:G:N2	33:a:1872:A:OP2	2.29	0.65
44:l:53:MET:HG3	44:l:120:ALA:HB2	1.79	0.65
56:x:6:LEU:HD11	56:x:53:VAL:HG22	1.77	0.65
7:6:56:PRO:HG2	7:6:72:LYS:HB2	1.79	0.64
7:6:13:VAL:CG1	7:6:24:VAL:CG2	2.75	0.64
39:g:60:ASP:OD1	39:g:60:ASP:N	2.24	0.64
40:h:117:LEU:HD23	40:h:130:VAL:CG2	2.26	0.64
15:F:2:ARG:HE	15:F:68:GLN:HE21	1.46	0.63
11:B:113:ARG:HH21	11:B:117:LEU:HD21	1.63	0.63
33:a:494:G:H4'	50:r:6:LYS:HB2	1.80	0.63
18:I:41:ARG:NH1	18:I:43:THR:OG1	2.32	0.63
8:7:38:A:OP1	32:X:355:LYS:NZ	2.31	0.63
32:X:83:SER:HA	32:X:116:LEU:HD23	1.80	0.63
47:o:2:SER:OG	47:o:3:ASN:N	2.32	0.63
13:D:159:LEU:HD21	13:D:175:ALA:HB1	1.80	0.63
40:h:113:SER:O	40:h:116:ARG:NH1	2.26	0.62
33:a:2120:G:N2	33:a:2178:C:O2	2.28	0.62
33:a:2720:U:H5''	47:o:53:ARG:HH21	1.64	0.62
40:h:134:VAL:CG1	40:h:138:VAL:HB	2.29	0.62
14:E:34:THR:HG22	14:E:52:LYS:HG3	1.82	0.62
4:3:25:VAL:HB	4:3:35:GLN:HG2	1.81	0.62
40:h:84:ALA:HA	40:h:90:LEU:HA	1.82	0.62
49:q:71:LYS:HD3	49:q:73:LYS:HE2	1.79	0.62
7:6:73:THR:OG1	7:6:113:LYS:NZ	2.33	0.62
33:a:568:U:H1'	33:a:2030:6MZ:H9C1	1.80	0.62
33:a:1105:U:H2'	33:a:1106:G:H8	1.64	0.62
33:a:546:U:H2'	33:a:548:G:H1'	1.81	0.62
33:a:1045:C:O2	33:a:1111:A:N6	2.33	0.62
10:A:1213:A:H4'	32:Y:367:ARG:HH12	1.64	0.61
36:d:149:ASN:OD1	36:d:150:MEQ:N	2.32	0.61
10:A:664:G:H22	10:A:741:G:H1	1.48	0.61
46:n:31:THR:HG22	46:n:34:HIS:H	1.66	0.61
7:6:13:VAL:HG11	7:6:24:VAL:HG21	1.82	0.61
51:s:4:GLU:OE2	56:x:23:ARG:NH1	2.33	0.61
16:G:67:GLU:OE2	16:G:68:ASN:ND2	2.33	0.61
16:G:113:ASP:OD2	16:G:122:ASN:ND2	2.34	0.61
32:X:318:ARG:HG2	32:X:322:THR:HG21	1.81	0.61
33:a:2032:G:H21	36:d:151:THR:HG23	1.64	0.61
33:a:2469:A:N6	33:a:2481:G:O2'	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:13:GLU:OE2	14:E:68:ARG:NH2	2.33	0.61
33:a:2820:A:O2'	33:a:2821:A:OP1	2.17	0.60
7:6:55:ILE:HD11	7:6:71:THR:HB	1.82	0.60
18:I:39:PHE:O	18:I:45:ARG:NH1	2.34	0.60
7:6:31:GLN:H	7:6:31:GLN:NE2	1.99	0.60
24:O:18:ASP:OD1	24:O:19:ALA:N	2.34	0.60
40:h:76:GLU:O	40:h:77:THR:HG23	2.02	0.60
40:h:117:LEU:CD2	40:h:130:VAL:HG23	2.28	0.60
33:a:2343:U:HO2'	33:a:2373:G:HO2'	1.48	0.60
33:a:2720:U:H5''	47:o:53:ARG:NH2	2.17	0.60
42:j:38:ILE:HD11	42:j:112:PHE:HZ	1.66	0.60
4:3:19:ARG:NE	33:a:2756:U:OP2	2.32	0.59
14:E:115:LEU:HD13	14:E:123:VAL:HG11	1.84	0.59
32:Y:116:LEU:HD21	32:Y:159:LEU:HD11	1.83	0.59
10:A:1005:A:OP2	10:A:1024:G:N2	2.35	0.59
38:f:160:ALA:HB1	38:f:165:GLU:HB2	1.84	0.59
14:E:13:GLU:HG2	14:E:39:VAL:HG22	1.84	0.59
17:H:50:LYS:NZ	17:H:60:GLU:OE1	2.35	0.59
36:d:1:MET:HB3	36:d:205:PRO:HG2	1.84	0.59
32:Y:239:ASP:N	32:Y:239:ASP:OD1	2.35	0.59
43:k:78:ARG:HG2	43:k:113:ALA:HB3	1.85	0.59
53:u:45:ASP:O	53:u:49:ASN:ND2	2.34	0.59
10:A:1266:G:N2	10:A:1269:A:OP2	2.33	0.59
18:I:21:ILE:HD11	18:I:61:LEU:HD13	1.85	0.59
10:A:344:A:H5''	10:A:345:C:H5	1.66	0.59
19:J:59:LYS:HE2	19:J:62:ARG:NH2	2.18	0.59
7:6:31:GLN:H	7:6:31:GLN:HE21	1.51	0.59
29:T:3:ASN:OD1	29:T:3:ASN:N	2.36	0.59
33:a:84:A:OP1	52:t:6:ARG:NH1	2.35	0.59
38:f:104:ILE:HG23	38:f:105:THR:HG23	1.85	0.59
46:n:31:THR:HG23	46:n:33:ARG:H	1.68	0.59
16:G:93:PRO:HA	16:G:96:ARG:HD2	1.84	0.59
33:a:2377:A:O2'	46:n:117:PHE:O	2.21	0.59
39:g:2:SER:OG	39:g:3:ARG:N	2.35	0.58
41:i:140:LEU:HG	41:i:142:ILE:HG13	1.84	0.58
21:L:55:VAL:HG11	21:L:80:ILE:HD11	1.85	0.58
32:X:207:GLU:OE1	32:X:375:ARG:NH2	2.31	0.58
43:k:127:VAL:HG21	43:k:142:ILE:HD13	1.84	0.58
10:A:1060:U:OP1	23:N:85:ARG:NH2	2.28	0.58
16:G:70:ARG:NH1	16:G:97:ASN:OD1	2.35	0.58
36:d:46:ARG:NH2	36:d:88:GLU:O	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:k:108:ALA:HB3	43:k:125:LEU:HD22	1.85	0.58
51:s:56:GLU:OE1	51:s:88:LYS:NZ	2.24	0.58
33:a:1607:C:N4	33:a:1622:G:OP2	2.28	0.58
52:t:43:LYS:HG2	52:t:60:GLU:HG2	1.85	0.58
32:X:313:LEU:HD23	32:X:329:SER:HB3	1.84	0.58
33:a:1248:G:OP1	37:e:44:ARG:NH1	2.33	0.57
32:X:188:PRO:HG2	32:Y:129:VAL:HG21	1.86	0.57
33:a:2205:A:H61	33:a:2219:U:H3	1.53	0.57
6:5:119:PRO:HG2	6:5:122:GLN:HB2	1.85	0.57
20:K:74:VAL:O	20:K:74:VAL:CG1	2.51	0.57
55:w:43:GLU:OE1	55:w:45:ARG:NH2	2.35	0.57
8:8:42:C:H4'	16:G:143:ARG:HD2	1.85	0.57
31:W:68:VAL:HG22	31:W:115:ALA:HB2	1.85	0.57
8:7:37:U:O2'	32:X:354:ARG:NH1	2.35	0.57
11:B:43:LEU:HA	11:B:46:THR:HG22	1.87	0.57
33:a:6:A:O2'	41:i:135:GLN:NE2	2.37	0.57
33:a:2799:A:O2'	33:a:2800:A:H5''	2.04	0.57
10:A:76:G:H1	10:A:93:U:H3	1.51	0.56
10:A:933:G:O6	16:G:3:ARG:NH2	2.36	0.56
10:A:1086:U:H3	10:A:1099:G:H22	1.53	0.56
7:6:13:VAL:HG12	7:6:24:VAL:HG21	1.85	0.56
40:h:76:GLU:O	40:h:77:THR:CG2	2.54	0.56
11:B:4:VAL:HG11	11:B:212:LEU:HD21	1.85	0.56
15:F:12:PRO:O	15:F:44:ARG:NH2	2.37	0.56
23:N:27:LEU:HD21	23:N:47:LYS:HG2	1.87	0.56
20:K:38:GLN:H	20:K:38:GLN:NE2	2.04	0.56
36:d:25:THR:OG1	36:d:191:GLY:O	2.24	0.56
1:0:5:ILE:HG21	1:0:28:ARG:HH22	1.71	0.56
5:4:63:ARG:NH1	10:A:1312:G:OP2	2.39	0.56
19:J:6:ILE:HB	19:J:76:ILE:HB	1.87	0.56
33:a:544:C:O2	33:a:549:G:N1	2.37	0.56
10:A:1494:G:O2'	33:a:1912:A:O2'	2.23	0.56
33:a:2146:C:H4'	33:a:2147:A:C8	2.40	0.56
32:X:177:ILE:HB	32:X:184:LEU:HD23	1.88	0.56
39:g:12:PRO:HD2	39:g:15:VAL:HG21	1.87	0.56
7:6:28:LEU:HA	7:6:31:GLN:NE2	2.21	0.55
33:a:1434:A:H2'	33:a:1435:G:C8	2.40	0.55
32:Y:317:LYS:HB3	32:Y:325:ARG:HG2	1.88	0.55
36:d:12:THR:OG1	36:d:13:ARG:N	2.40	0.55
32:X:19:GLN:N	32:X:19:GLN:OE1	2.39	0.55
32:X:236:LEU:HD11	32:Y:191:PRO:HG2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:21:THR:HG23	12:C:58:GLU:HG2	1.88	0.55
15:F:18:VAL:HA	15:F:21:MET:HE2	1.89	0.55
31:W:58:LEU:HD11	31:W:61:ALA:HB2	1.88	0.55
32:X:25:ALA:O	32:X:28:VAL:HG12	2.07	0.55
33:a:2291:U:OP1	33:a:2380:C:O2'	2.23	0.55
10:A:677:U:H3	10:A:713:G:H22	1.55	0.55
38:f:134:GLU:HG2	38:f:136:ILE:H	1.71	0.55
39:g:22:GLN:OE1	39:g:55:ARG:NH2	2.40	0.55
33:a:500:G:N1	33:a:503:A:OP2	2.40	0.55
33:a:287:G:H1	33:a:353:C:H42	1.54	0.55
8:8:7:G:OP1	8:8:16:C:N4	2.39	0.55
17:H:11:LEU:HD22	17:H:75:ILE:HD11	1.89	0.55
14:E:38:VAL:HG11	14:E:114:VAL:HG22	1.89	0.54
58:z:43:ILE:HG22	58:z:49:TYR:HB2	1.89	0.54
10:A:946:A:O2'	10:A:1333:A:N3	2.38	0.54
35:c:167:ARG:HG3	35:c:172:VAL:HG12	1.89	0.54
51:s:11:LEU:O	56:x:29:ARG:NH2	2.40	0.54
21:L:110:ARG:NH1	21:L:112:GLN:O	2.41	0.54
16:G:63:GLU:OE2	16:G:70:ARG:NH2	2.40	0.54
33:a:2511:U:O2'	36:d:143:PRO:O	2.24	0.54
12:C:91:VAL:HG11	12:C:101:ILE:HD11	1.89	0.54
18:I:123:ARG:NH1	18:I:124:ARG:O	2.41	0.54
20:K:38:GLN:H	20:K:38:GLN:HE21	1.54	0.54
32:X:375:ARG:HE	32:Y:377:GLU:CD	2.16	0.54
7:6:17:MET:SD	7:6:17:MET:N	2.81	0.54
10:A:1077:G:N2	10:A:1080:A:OP2	2.40	0.54
32:X:2:ALA:HA	32:X:147:GLN:HG2	1.90	0.54
33:a:475:C:O2	33:a:479:A:N6	2.36	0.54
38:f:52:ASN:ND2	38:f:147:ASP:OD2	2.40	0.54
8:7:19:G:N2	8:7:58:A:O2'	2.40	0.54
35:c:146:MET:HE2	35:c:154:LEU:HD21	1.88	0.54
10:A:1026:G:O2'	10:A:1027:C:OP1	2.26	0.53
16:G:27:VAL:HG22	16:G:43:VAL:HG11	1.90	0.53
33:a:2032:G:C5	36:d:150:MEQ:HE3	2.43	0.53
46:n:83:LEU:HD11	46:n:114:GLY:HA3	1.90	0.53
5:4:16:CYS:SG	5:4:17:SER:N	2.82	0.53
11:B:11:LYS:O	11:B:208:ARG:NH2	2.42	0.53
12:C:185:ASN:HD22	12:C:186:THR:H	1.56	0.53
32:Y:148:CYS:HB2	32:Y:172:VAL:HG11	1.90	0.53
33:a:1509:A:HO2'	33:a:1510:G:H8	1.55	0.53
32:X:125:ARG:HB2	32:Y:188:PRO:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:G:53:ARG:HH12	16:G:122:ASN:HA	1.74	0.53
33:a:1181:U:H2'	33:a:1182:G:C8	2.43	0.53
8:8:34:U:H4'	16:G:84:THR:HG21	1.91	0.53
10:A:1530:G:O6	30:U:46:LYS:NZ	2.42	0.53
37:e:188:MET:HE3	37:e:193:VAL:HG22	1.90	0.53
44:l:47:GLU:OE2	44:l:51:ARG:NH1	2.42	0.53
8:7:39:A:O2'	10:A:790:A:OP1	2.27	0.53
32:X:170:ARG:NH1	32:X:257:GLU:OE2	2.25	0.53
33:a:277:G:H4'	33:a:278:A:O5'	2.08	0.53
32:Y:279:MET:HE1	32:Y:324:ASP:HB3	1.91	0.52
6:5:12:VAL:HG13	6:5:63:ALA:HB2	1.90	0.52
32:X:48:ALA:O	32:X:98:TYR:OH	2.23	0.52
33:a:1797:G:HO2'	35:c:257:THR:HG1	1.57	0.52
12:C:72:ARG:HD3	12:C:75:ILE:HD12	1.91	0.52
43:k:55:MET:HE3	43:k:59:ARG:HB3	1.91	0.52
5:4:11:GLU:HA	5:4:25:ARG:HA	1.92	0.52
29:T:44:LYS:HD3	29:T:87:ALA:HA	1.91	0.52
6:5:73:LYS:HA	6:5:76:PHE:HE2	1.74	0.52
8:8:26:C:H2'	8:8:27:G:H8	1.74	0.52
7:6:11:LEU:HD23	7:6:24:VAL:HG22	1.90	0.52
8:8:26:C:H2'	8:8:27:G:C8	2.44	0.52
32:X:5:LEU:HD23	32:X:79:VAL:HB	1.91	0.52
49:q:46:GLU:OE1	49:q:46:GLU:N	2.41	0.52
10:A:1180:A:OP2	18:I:99:ARG:NH2	2.42	0.52
33:a:84:A:N1	33:a:98:G:O2'	2.37	0.52
34:b:66:A:N6	34:b:107:G:H2'	2.24	0.52
16:G:86:GLN:HB2	16:G:148:ASN:ND2	2.25	0.52
3:2:62:LEU:HB3	3:2:65:ALA:HB2	1.92	0.52
10:A:1028:C:H1'	10:A:1034:G:C2	2.44	0.52
22:M:77:ILE:HG22	22:M:81:MET:HE2	1.91	0.52
36:d:149:ASN:CG	36:d:150:MEQ:H	2.18	0.52
4:3:4:ARG:NH2	4:3:35:GLN:OE1	2.43	0.51
19:J:26:VAL:HG13	19:J:36:VAL:HG21	1.92	0.51
33:a:476:G:N1	33:a:479:A:OP2	2.40	0.51
33:a:2343:U:O2'	33:a:2373:G:O2'	2.26	0.51
41:i:18:VAL:HG22	41:i:140:LEU:HB3	1.92	0.51
10:A:1139:G:O6	10:A:1143:G:N2	2.43	0.51
20:K:35:THR:HG22	20:K:41:ALA:HA	1.91	0.51
31:W:84:LYS:NZ	32:Y:238:GLU:OE1	2.43	0.51
38:f:4:LEU:HD12	38:f:173:PHE:HD2	1.75	0.51
32:X:72:VAL:O	32:X:103:ARG:NE	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:l:57:VAL:HG13	44:l:108:VAL:HG11	1.92	0.51
33:a:878:A:N6	33:a:899:A:O2'	2.44	0.51
10:A:1081:A:H5'	14:E:23:LYS:HD3	1.91	0.51
25:P:40:ASN:HB3	25:P:43:ALA:HB2	1.92	0.51
32:Y:6:CYS:HA	32:Y:151:ASN:HB3	1.93	0.51
32:Y:206:LEU:HD22	32:Y:247:LEU:HD21	1.93	0.51
32:Y:313:LEU:HD23	32:Y:329:SER:HB3	1.93	0.51
33:a:1365:A:OP1	55:w:3:ARG:NH1	2.40	0.51
43:k:82:LEU:HD13	43:k:90:VAL:HG21	1.93	0.51
53:u:77:VAL:HG12	53:u:89:ILE:HG23	1.92	0.51
4:3:10:LEU:HD23	4:3:35:GLN:HE22	1.75	0.51
10:A:1526:G:OP2	30:U:42:THR:OG1	2.28	0.51
11:B:205:ASP:OD1	11:B:205:ASP:N	2.41	0.51
12:C:168:TYR:OH	14:E:55:GLU:OE2	2.26	0.51
22:M:29:ARG:O	22:M:33:ILE:HG22	2.09	0.51
33:a:1796:U:H2'	33:a:1797:G:C8	2.46	0.51
33:a:2335:A:OP1	46:n:13:ARG:NH1	2.44	0.51
33:a:320:A:N3	37:e:163:ASN:ND2	2.55	0.51
10:A:1494:G:HO2'	33:a:1912:A:HO2'	1.55	0.51
32:X:168:MET:HE2	32:X:189:MET:HA	1.92	0.51
32:Y:10:THR:O	32:Y:10:THR:OG1	2.28	0.51
33:a:2498:OMC:HM22	33:a:2499:C:H5'	1.91	0.51
4:3:16:ILE:HD13	4:3:25:VAL:HG22	1.93	0.51
11:B:28:LYS:O	11:B:31:ILE:HG22	2.11	0.51
15:F:38:ARG:HB3	15:F:63:ASN:HB2	1.93	0.51
32:X:279:MET:HE1	32:X:324:ASP:HB3	1.92	0.51
33:a:973:A:H5'	33:a:1188:U:H1'	1.93	0.51
6:5:8:LYS:HG2	6:5:59:LEU:HD11	1.93	0.50
10:A:1003:G:N2	10:A:1005:A:H5'	2.26	0.50
10:A:381:C:H2'	10:A:382:A:O4'	2.11	0.50
16:G:47:LEU:HB3	16:G:58:GLU:HG2	1.92	0.50
19:J:18:ILE:O	19:J:22:THR:OG1	2.26	0.50
7:6:56:PRO:HD3	7:6:75:PRO:HD3	1.93	0.50
40:h:76:GLU:C	40:h:77:THR:HG23	2.37	0.50
10:A:401:C:OP2	13:D:70:ARG:NH1	2.44	0.50
23:N:46:LEU:HD12	28:S:13:LEU:HD13	1.94	0.50
33:a:2267:A:H5''	33:a:2268:A:H5'	1.93	0.50
10:A:1062:U:H2'	10:A:1063:C:C6	2.47	0.50
33:a:1363:C:O2'	33:a:1809:A:N3	2.44	0.50
34:b:36:C:N4	34:b:49:C:O2	2.45	0.50
36:d:176:ASP:OD1	36:d:176:ASP:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:7:ARG:O	11:B:11:LYS:HG3	2.12	0.50
32:Y:9:GLY:HA3	32:Y:155:GLY:H	1.77	0.50
32:Y:84:GLU:HG3	32:Y:115:GLY:H	1.76	0.50
40:h:135:HIS:CG	40:h:136:SER:N	2.80	0.50
32:Y:217:ARG:HG2	32:Y:245:VAL:HG23	1.94	0.49
46:n:95:SER:O	46:n:95:SER:OG	2.28	0.49
38:f:130:MET:HE3	38:f:154:ILE:HD12	1.94	0.49
32:Y:137:LEU:HD11	32:Y:253:LEU:HD11	1.94	0.49
33:a:645:C:H2'	33:a:647:G:C8	2.47	0.49
10:A:691:G:O6	20:K:57:LYS:NZ	2.42	0.49
19:J:66:GLU:HB2	23:N:99:ALA:HB2	1.92	0.49
36:d:136:ASN:OD1	36:d:137:SER:N	2.45	0.49
26:Q:51:ASN:OD1	26:Q:51:ASN:N	2.44	0.49
39:g:4:VAL:O	39:g:69:ARG:HG2	2.12	0.49
33:a:870:U:OP1	44:l:6:ARG:NH2	2.46	0.49
33:a:1412:U:H2'	33:a:1413:A:C8	2.48	0.49
10:A:538:G:H5''	21:L:111:LYS:HB2	1.95	0.49
12:C:105:GLU:CD	12:C:105:GLU:H	2.20	0.49
32:X:41:ILE:O	32:X:44:THR:OG1	2.30	0.49
33:a:1224:U:OP2	49:q:68:ARG:NH2	2.46	0.49
33:a:1853:A:N3	33:a:2233:U:O2'	2.39	0.49
14:E:45:ARG:HG2	14:E:73:ASN:HB3	1.94	0.49
3:2:54:ASP:HB3	43:k:57:LEU:HD22	1.94	0.49
5:4:13:THR:HG22	5:4:23:LYS:HG2	1.95	0.49
10:A:421:U:H5'	10:A:422:C:C5	2.47	0.49
10:A:713:G:H2'	10:A:714:G:C8	2.48	0.49
32:X:70:MET:HE3	32:X:175:LYS:HD2	1.95	0.49
33:a:2636:C:O2'	36:d:45:TYR:OH	2.22	0.49
38:f:46:ASP:HB2	38:f:49:LEU:HD13	1.93	0.49
10:A:1123:U:O2'	19:J:39:PRO:O	2.31	0.49
18:I:91:ASP:HB3	18:I:94:LEU:HD13	1.95	0.49
33:a:2182:U:H2'	33:a:2183:A:C8	2.47	0.49
36:d:15:PHE:H	47:o:12:GLN:HE22	1.60	0.49
7:6:22:PRO:N	7:6:23:PRO:HD2	2.28	0.48
12:C:21:THR:O	12:C:21:THR:OG1	2.27	0.48
18:I:84:THR:HG23	18:I:98:LEU:HD13	1.95	0.48
33:a:720:U:H2'	33:a:721:A:C8	2.48	0.48
33:a:1068:G:N2	33:a:1095:A:O2'	2.41	0.48
33:a:1734:G:H2'	33:a:1735:A:H8	1.78	0.48
36:d:4:LEU:HD23	36:d:29:VAL:HG11	1.95	0.48
8:8:9:G:O2'	8:8:46:G:N3	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:255:G:OP1	26:Q:71:LYS:NZ	2.46	0.48
33:a:827:U:O2'	33:a:2068:U:C2	2.64	0.48
33:a:2839:G:N2	45:m:91:ALA:O	2.42	0.48
38:f:4:LEU:HD23	38:f:101:GLU:HB2	1.95	0.48
40:h:68:ARG:NH2	40:h:109:GLU:O	2.46	0.48
44:l:53:MET:HE3	44:l:117:PHE:HE1	1.78	0.48
10:A:1144:G:N2	10:A:1146:A:H62	2.11	0.48
11:B:129:LEU:HB3	11:B:133:GLU:HB2	1.95	0.48
6:5:8:LYS:NZ	33:a:1047:G:OP1	2.46	0.48
10:A:1071:C:H2'	10:A:1072:G:C8	2.48	0.48
26:Q:19:LYS:NZ	26:Q:49:GLU:OE1	2.45	0.48
33:a:277:G:H1'	33:a:278:A:C5	2.48	0.48
33:a:817:C:H2'	33:a:818:G:O4'	2.14	0.48
33:a:1594:U:H2'	33:a:1595:C:C6	2.49	0.48
33:a:1645:G:H5''	33:a:1646:C:H5'	1.94	0.48
20:K:16:VAL:HG23	20:K:79:ILE:HG12	1.95	0.48
21:L:59:ASN:C	21:L:59:ASN:HD22	2.22	0.48
40:h:26:ALA:HA	40:h:30:LEU:HB2	1.96	0.48
43:k:79:LEU:HA	43:k:82:LEU:HD23	1.95	0.48
10:A:1412:C:H2'	10:A:1413:A:C8	2.48	0.48
29:T:20:HIS:O	29:T:24:ARG:HG2	2.14	0.48
34:b:28:C:OP1	46:n:31:THR:HG21	2.12	0.48
16:G:113:ASP:HB2	16:G:119:ARG:HG3	1.96	0.48
32:Y:350:LEU:O	32:Y:354:ARG:HG2	2.13	0.48
33:a:784:G:H5'	33:a:785:G:OP1	2.13	0.48
10:A:652:U:O4	10:A:752:G:O2'	2.30	0.48
33:a:960:A:H61	44:l:82:MET:HE2	1.79	0.48
37:e:125:SER:O	37:e:137:LYS:NZ	2.46	0.48
10:A:390:U:H2'	10:A:391:G:C8	2.49	0.48
13:D:188:ARG:NH2	13:D:195:ILE:O	2.47	0.48
31:W:73:ARG:HH21	31:W:80:LEU:N	2.11	0.48
46:n:53:THR:O	46:n:59:ALA:HB2	2.14	0.48
10:A:925:G:H1'	10:A:1502:A:C4	2.48	0.47
33:a:2845:U:H5''	47:o:52:ASN:O	2.14	0.47
6:5:56:ARG:HA	33:a:1107:G:OP1	2.14	0.47
44:l:66:ARG:NH1	44:l:104:GLU:OE2	2.47	0.47
10:A:382:A:H2'	10:A:383:A:C8	2.48	0.47
10:A:613:C:OP1	13:D:81:ARG:NH1	2.45	0.47
10:A:1144:G:H21	10:A:1146:A:H62	1.61	0.47
32:X:8:CYS:SG	32:X:9:GLY:N	2.87	0.47
42:j:40:LYS:HE3	42:j:57:VAL:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:l:33:LEU:HD13	44:l:117:PHE:HB3	1.96	0.47
1:0:40:ASP:HB3	1:0:43:VAL:HG22	1.95	0.47
20:K:74:VAL:HG11	20:K:79:ILE:HD12	1.95	0.47
32:X:305:LYS:HB3	32:X:305:LYS:HE2	1.65	0.47
10:A:151:A:H2'	10:A:152:A:O4'	2.15	0.47
28:S:11:ILE:HD12	28:S:38:SER:OG	2.14	0.47
7:6:101:ILE:O	7:6:141:GLU:N	2.47	0.47
10:A:73:C:O2'	10:A:74:A:H8	1.97	0.47
19:J:52:LEU:HD21	19:J:59:LYS:HD2	1.96	0.47
20:K:94:GLU:CD	20:K:94:GLU:H	2.22	0.47
32:Y:63:GLU:OE1	32:Y:63:GLU:N	2.27	0.47
33:a:917:A:H5''	33:a:2268:A:H61	1.80	0.47
40:h:7:ASP:OD1	40:h:8:LYS:N	2.46	0.47
10:A:501:C:H2'	10:A:502:A:C8	2.50	0.47
10:A:1527:U:H5	30:U:42:THR:HG21	1.79	0.47
32:X:271:ARG:HH21	32:X:339:ARG:CZ	2.28	0.47
36:d:17:GLU:OE1	36:d:17:GLU:N	2.43	0.47
21:L:54:ARG:NH1	21:L:62:GLU:OE2	2.48	0.47
33:a:806:C:OP2	43:k:41:ARG:NH2	2.43	0.47
33:a:2788:C:H2'	33:a:2789:C:C6	2.50	0.47
4:3:32:LYS:HE2	33:a:2478:A:H5'	1.96	0.47
25:P:12:LYS:HG2	25:P:13:LYS:HG2	1.97	0.47
47:o:88:ARG:NH2	47:o:110:ILE:O	2.40	0.47
10:A:560:A:H4'	10:A:561:U:H5''	1.97	0.46
14:E:153:VAL:O	14:E:157:ARG:HG3	2.15	0.46
33:a:1365:A:OP1	55:w:28:ARG:NH2	2.48	0.46
35:c:76:ALA:HB1	35:c:94:VAL:HG22	1.97	0.46
8:8:22:A:N6	8:8:48:U:O2'	2.41	0.46
33:a:2304:G:H22	33:a:2312:U:H3	1.64	0.46
2:1:4:THR:HG22	33:a:687:C:H1'	1.97	0.46
10:A:860:A:H2'	10:A:861:G:O4'	2.15	0.46
32:X:28:VAL:HG11	32:X:86:ALA:HB1	1.96	0.46
52:t:17:LYS:HE2	52:t:17:LYS:HB3	1.79	0.46
32:Y:357:ASP:OD1	32:Y:358:ALA:N	2.49	0.46
33:a:987:C:O2'	33:a:1000:A:N3	2.47	0.46
33:a:2514:U:H2'	33:a:2515:C:C6	2.50	0.46
38:f:136:ILE:HD11	38:f:146:VAL:HG11	1.97	0.46
40:h:43:ASN:OD1	40:h:44:ILE:N	2.48	0.46
8:8:33:4OC:O5'	8:8:33:4OC:H6	2.16	0.46
10:A:1517:G:N3	33:a:1919:A:O2'	2.42	0.46
13:D:35:GLU:O	13:D:45:LYS:NZ	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:h:41:LYS:O	40:h:44:ILE:HG22	2.15	0.46
40:h:85:GLY:N	40:h:89:LYS:O	2.46	0.46
8:7:21:H2U:H2'	8:7:22:A:H5''	1.97	0.46
10:A:757:U:O2'	10:A:879:C:O2	2.33	0.46
22:M:89:LEU:O	22:M:93:ARG:HG2	2.16	0.46
32:X:271:ARG:HH21	32:X:339:ARG:NH1	2.14	0.46
10:A:1136:C:OP2	10:A:1137:C:N4	2.47	0.46
32:X:240:VAL:HG12	32:X:244:GLN:HB2	1.98	0.46
36:d:25:THR:HG21	36:d:193:VAL:HG22	1.98	0.46
36:d:129:THR:HG22	36:d:130:GLN:O	2.16	0.46
38:f:103:LEU:HD21	38:f:130:MET:HE1	1.98	0.46
42:j:105:ARG:NH1	47:o:34:GLU:OE2	2.48	0.46
57:y:31:ARG:HG2	57:y:34:HIS:HB2	1.97	0.46
58:z:32:LYS:NZ	58:z:50:ARG:O	2.48	0.46
6:5:64:VAL:HG22	6:5:69:PHE:HB2	1.97	0.46
7:6:113:LYS:HB3	7:6:117:MET:HE3	1.98	0.46
33:a:597:G:O2'	43:k:11:GLY:O	2.29	0.46
33:a:2039:U:H2'	33:a:2040:G:C8	2.50	0.46
33:a:2732:G:OP1	36:d:208:LYS:NZ	2.45	0.46
34:b:66:A:H61	34:b:107:G:H2'	1.81	0.46
37:e:171:ASP:OD1	37:e:171:ASP:N	2.39	0.46
40:h:68:ARG:O	40:h:72:ILE:HG12	2.16	0.46
10:A:1273:C:H2'	10:A:1274:A:O4'	2.16	0.46
33:a:491:G:O6	50:r:49:LYS:NZ	2.45	0.46
32:X:270:ARG:HH11	32:X:372:PRO:HD2	1.80	0.46
32:Y:20:THR:HB	32:Y:21:PRO:HD3	1.98	0.46
32:Y:113:VAL:HB	32:Y:116:LEU:HD22	1.98	0.46
33:a:1872:A:C5	33:a:1873:G:H1'	2.50	0.46
33:a:2096:C:H2'	33:a:2097:A:C8	2.51	0.46
35:c:120:VAL:HG23	35:c:121:ASP:OD1	2.16	0.46
52:t:86:ARG:HG3	52:t:95:PHE:CE1	2.51	0.46
27:R:16:GLU:HG3	27:R:18:VAL:HG23	1.98	0.45
33:a:157:C:H2'	33:a:158:U:O4'	2.15	0.45
33:a:1111:A:N3	33:a:1112:G:H1'	2.30	0.45
33:a:1231:U:H2'	33:a:1232:G:H8	1.81	0.45
10:A:600:A:OP1	17:H:89:LYS:HG2	2.15	0.45
33:a:274:C:H42	33:a:363:G:H1	1.64	0.45
8:8:9:G:O2'	8:8:10:G:N7	2.39	0.45
33:a:247:G:OP2	33:a:249:C:N4	2.49	0.45
33:a:783:A:O2'	33:a:785:G:OP1	2.30	0.45
39:g:164:TYR:HB2	39:g:167:GLU:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:57:VAL:HG13	28:S:42:PRO:HB3	1.97	0.45
33:a:2820:A:N3	33:a:2820:A:H2'	2.31	0.45
37:e:165:HIS:CE1	37:e:166:LYS:HG3	2.51	0.45
7:6:86:ILE:HD13	7:6:138:LEU:HD21	1.98	0.45
10:A:344:A:H5''	10:A:345:C:C5	2.49	0.45
32:X:5:LEU:HD21	32:X:139:GLU:HG2	1.98	0.45
5:4:26:SER:OG	5:4:27:THR:N	2.49	0.45
8:8:19:G:H22	8:8:58:A:HO2'	1.60	0.45
32:X:117:GLN:HE22	32:X:120:ASP:HB3	1.82	0.45
33:a:5:A:H2'	33:a:6:A:C8	2.52	0.45
33:a:2030:6MZ:C2	33:a:2499:C:H5''	2.47	0.45
44:l:50:ARG:HD3	44:l:65:ILE:HD11	1.97	0.45
53:u:9:ARG:HG2	53:u:41:GLU:HG3	1.97	0.45
1:0:6:ARG:HG2	1:0:24:THR:HB	1.99	0.45
10:A:769:G:H4'	10:A:1513:A:H4'	1.99	0.45
10:A:1477:U:H2'	10:A:1478:U:C6	2.52	0.45
30:U:5:LYS:HE3	30:U:5:LYS:HB3	1.85	0.45
33:a:1587:G:H2'	33:a:1588:G:H8	1.81	0.45
50:r:37:THR:HG23	50:r:38:TYR:CD2	2.51	0.45
57:y:28:GLY:HA3	57:y:38:ARG:HH21	1.81	0.45
10:A:1043:G:O2'	10:A:1044:A:O5'	2.35	0.45
18:I:36:GLU:OE2	18:I:49:ARG:NH2	2.50	0.45
22:M:44:LYS:HB2	22:M:44:LYS:HE3	1.83	0.45
33:a:1667:G:O2'	33:a:1991:U:O4	2.29	0.45
33:a:2016:U:H1'	58:z:3:VAL:HG21	1.99	0.45
33:a:2143:C:H2'	33:a:2144:G:O4'	2.17	0.45
33:a:2147:A:C5	33:a:2148:G:H1'	2.51	0.45
33:a:2328:A:H2'	33:a:2329:U:C6	2.52	0.45
11:B:50:PHE:O	11:B:54:LEU:HG	2.17	0.45
32:X:158:SER:HB3	32:Y:176:TYR:CD2	2.52	0.45
32:X:270:ARG:NH1	32:X:371:ALA:O	2.50	0.45
36:d:125:TRP:CD1	36:d:160:LYS:HB3	2.52	0.45
40:h:84:ALA:HB3	40:h:148:ALA:HB2	1.99	0.45
10:A:1007:U:H3	10:A:1022:A:H61	1.65	0.45
32:X:324:ASP:OD1	32:X:324:ASP:N	2.50	0.45
33:a:1510:G:H2'	33:a:1511:G:C8	2.52	0.45
33:a:1808:A:H3'	33:a:1809:A:C8	2.52	0.45
33:a:2392:A:H2	43:k:55:MET:HE2	1.82	0.45
34:b:54:G:H21	38:f:26:MET:HE3	1.82	0.45
38:f:108:VAL:HG11	38:f:176:PRO:HG2	1.99	0.45
44:l:110:GLU:O	44:l:114:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:X:354:ARG:O	32:X:354:ARG:NE	2.45	0.44
33:a:58:G:O2'	33:a:73:A:N1	2.50	0.44
33:a:1328:A:H2'	33:a:1330:C:C5	2.52	0.44
33:a:2839:G:O2'	45:m:49:GLU:OE1	2.28	0.44
18:I:115:LYS:HB2	18:I:118:LEU:HD12	1.99	0.44
34:b:79:G:N7	53:u:14:LYS:NZ	2.65	0.44
44:l:15:GLY:O	44:l:16:ARG:NH1	2.44	0.44
52:t:47:LYS:HD3	52:t:48:PRO:HD2	2.00	0.44
10:A:67:C:H2'	10:A:68:G:C8	2.52	0.44
30:U:29:LEU:O	30:U:33:ARG:HG2	2.18	0.44
31:W:72:VAL:HA	31:W:75:ALA:HB3	1.99	0.44
32:X:159:LEU:HA	32:X:159:LEU:HD23	1.76	0.44
32:X:207:GLU:CD	32:X:375:ARG:HH22	2.19	0.44
7:6:8:TYR:HE1	7:6:60:THR:HG23	1.82	0.44
10:A:451:A:H61	10:A:481:G:H5'	1.83	0.44
15:F:3:HIS:NE2	15:F:65:GLU:OE1	2.50	0.44
20:K:81:ASN:OD1	20:K:81:ASN:N	2.50	0.44
32:X:181:SER:OG	32:X:182:SER:N	2.51	0.44
33:a:414:C:H2'	33:a:415:A:C8	2.52	0.44
33:a:1340:U:OP1	51:s:19:LYS:NZ	2.47	0.44
58:z:11:SER:O	58:z:15:MET:HG3	2.18	0.44
3:2:34:THR:OG1	33:a:2420:C:OP1	2.24	0.44
5:4:65:ASN:OD1	5:4:65:ASN:N	2.50	0.44
10:A:1360:A:OP2	23:N:75:ARG:NH2	2.50	0.44
32:X:56:LEU:HD23	32:X:60:LEU:HD12	1.99	0.44
32:X:375:ARG:HG2	32:X:376:LEU:N	2.33	0.44
33:a:1141:U:H4'	33:a:1142:A:O4'	2.18	0.44
44:l:70:ASP:OD1	44:l:70:ASP:N	2.48	0.44
20:K:67:ALA:HB2	20:K:96:THR:HG23	1.99	0.44
31:W:61:ALA:O	31:W:65:LYS:HG2	2.17	0.44
33:a:538:A:H5''	41:i:7:LYS:HE3	2.00	0.44
10:A:324:G:N1	10:A:327:A:OP2	2.51	0.44
10:A:1035:A:H1'	10:A:1036:A:O5'	2.18	0.44
10:A:1071:C:H2'	10:A:1072:G:H8	1.82	0.44
21:L:68:GLY:O	21:L:99:ARG:NH1	2.49	0.44
32:X:93:TRP:O	32:X:97:ARG:HG3	2.18	0.44
32:Y:267:PHE:HB3	32:Y:373:PHE:HB3	1.99	0.44
40:h:104:THR:HG22	40:h:109:GLU:HA	1.99	0.44
45:m:69:ARG:O	45:m:70:THR:OG1	2.34	0.44
3:2:31:HIS:CD2	3:2:32:ILE:HG13	2.53	0.44
8:7:20:G:H5''	8:7:21:H2U:HN3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:X:380:GLU:HG2	32:Y:372:PRO:HB3	1.99	0.44
33:a:2209:G:H1	33:a:2215:C:H42	1.65	0.44
41:i:92:MET:HE3	41:i:92:MET:HB3	1.94	0.44
44:l:50:ARG:O	44:l:54:THR:HG23	2.18	0.44
5:4:1:MET:HE1	38:f:95:ARG:HD2	2.00	0.43
11:B:70:VAL:HG12	11:B:169:GLU:HG2	1.99	0.43
33:a:1954:G:O2'	33:a:1956:U:O4	2.30	0.43
5:4:64:PHE:CG	28:S:9:PRO:HD3	2.53	0.43
14:E:81:LEU:HB2	14:E:98:PRO:HG3	2.00	0.43
15:F:68:GLN:H	15:F:68:GLN:CD	2.26	0.43
19:J:25:ILE:HG12	19:J:90:LEU:HD23	1.99	0.43
20:K:111:THR:HG23	30:U:3:VAL:HG22	2.01	0.43
32:X:274:ASP:OD1	32:X:274:ASP:N	2.47	0.43
33:a:296:U:H2'	33:a:297:G:C8	2.52	0.43
33:a:742:A:H2'	33:a:743:A:C8	2.53	0.43
33:a:811:U:H2'	43:k:21:ARG:HA	2.00	0.43
40:h:30:LEU:HB3	40:h:36:ALA:HB3	2.00	0.43
10:A:466:A:H4'	10:A:467:U:H5	1.83	0.43
10:A:1435:G:H2'	10:A:1436:U:C6	2.53	0.43
13:D:62:ARG:NH1	13:D:69:GLU:HB2	2.34	0.43
20:K:16:VAL:HG22	20:K:77:TYR:HB3	2.00	0.43
32:Y:326:TYR:HD2	32:Y:340:ILE:HG12	1.82	0.43
33:a:644:A:H2'	33:a:645:C:O4'	2.18	0.43
33:a:2261:C:C6	54:v:16:SER:HB3	2.53	0.43
33:a:2728:U:HO2'	33:a:2729:G:H8	1.65	0.43
33:a:2780:G:OP2	41:i:120:ARG:HD3	2.18	0.43
39:g:20:ASN:OD1	39:g:20:ASN:N	2.50	0.43
40:h:51:ARG:NH1	40:h:55:GLU:OE2	2.51	0.43
6:5:61:ARG:HB2	6:5:73:LYS:HD2	2.00	0.43
10:A:1011:C:H2'	10:A:1012:A:H8	1.84	0.43
33:a:1824:G:O3'	35:c:247:PRO:HD3	2.17	0.43
33:a:2796:U:H3	33:a:2799:A:N6	2.16	0.43
7:6:15:ALA:HB2	7:6:53:LEU:H	1.82	0.43
10:A:77:A:H2'	10:A:78:A:C8	2.53	0.43
10:A:676:A:H5''	20:K:115:PRO:HB3	2.00	0.43
10:A:1035:A:O2'	10:A:1036:A:H5''	2.19	0.43
10:A:1038:C:H2'	10:A:1039:G:C8	2.53	0.43
22:M:11:ASP:HA	22:M:45:ILE:HB	2.00	0.43
31:W:70:LYS:NZ	32:Y:212:GLU:O	2.51	0.43
32:Y:379:TYR:O	32:Y:379:TYR:CG	2.70	0.43
33:a:570:G:H2'	33:a:2030:6MZ:N7	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:1187:G:N2	33:a:1188:U:O4	2.52	0.43
33:a:1874:C:H2'	33:a:1875:G:O4'	2.19	0.43
33:a:2096:C:H2'	33:a:2097:A:H8	1.84	0.43
50:r:4:ILE:HD11	50:r:6:LYS:HE3	2.01	0.43
11:B:42:ASN:HD21	11:B:44:GLU:HB3	1.83	0.43
24:O:64:ARG:HH22	24:O:89:ARG:C	2.26	0.43
21:L:73:ASN:HD22	32:X:142:ALA:HB1	1.82	0.43
33:a:12:U:O2	33:a:12:U:H2'	2.16	0.43
33:a:299:A:N3	33:a:319:G:O2'	2.50	0.43
33:a:1060:U:C2	33:a:1062:G:H5'	2.54	0.43
33:a:1183:U:H2'	33:a:1184:U:C6	2.54	0.43
33:a:1434:A:H2'	33:a:1435:G:H8	1.81	0.43
33:a:1799:G:OP1	35:c:258:ARG:NH1	2.41	0.43
8:7:33:4OC:H6	8:7:33:4OC:O5'	2.18	0.43
27:R:12:ARG:O	27:R:16:GLU:HG2	2.19	0.43
32:X:220:LEU:HD13	32:X:245:VAL:HG21	2.00	0.43
33:a:548:G:H2'	33:a:549:G:C4	2.54	0.43
33:a:2581:G:OP2	33:a:2581:G:N2	2.48	0.43
39:g:155:GLU:HG3	39:g:157:TYR:H	1.83	0.43
57:y:8:THR:HG23	57:y:35:THR:HB	2.01	0.43
32:X:158:SER:O	32:X:161:PRO:HD2	2.19	0.43
33:a:989:G:OP2	57:y:12:SER:HB2	2.19	0.43
33:a:1366:A:OP1	55:w:2:SER:OG	2.29	0.43
33:a:1536:C:H4'	33:a:1537:G:N3	2.34	0.43
33:a:1797:G:O2'	35:c:257:THR:OG1	2.29	0.43
33:a:2402:U:HO2'	33:a:2403:C:P	2.42	0.43
6:5:73:LYS:HE2	6:5:73:LYS:HB3	1.91	0.43
8:8:66:C:H2'	8:8:67:C:C6	2.54	0.43
32:Y:269:SER:HB3	32:Y:373:PHE:CE2	2.54	0.43
33:a:538:A:H4'	41:i:7:LYS:HG2	2.00	0.43
33:a:1720:U:H2'	33:a:1721:G:O4'	2.19	0.43
33:a:2032:G:C4	36:d:150:MEQ:HE3	2.54	0.43
40:h:68:ARG:HB2	40:h:134:VAL:HG21	2.01	0.43
40:h:135:HIS:CG	40:h:136:SER:H	2.36	0.43
7:6:19:ASN:C	7:6:21:SER:H	2.26	0.42
10:A:1527:U:OP2	30:U:42:THR:HG23	2.18	0.42
33:a:639:U:H2'	33:a:640:C:C6	2.54	0.42
33:a:1418:G:H1'	33:a:1580:A:H61	1.84	0.42
33:a:2796:U:H3	33:a:2799:A:H61	1.67	0.42
40:h:135:HIS:CD2	40:h:137:GLU:H	2.37	0.42
59:Z:3:A:N3	59:Z:3:A:H2'	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:35:C:H42	9:9:19:G:H1	1.67	0.42
15:F:40:GLU:OE1	15:F:100:SER:OG	2.21	0.42
32:X:160:VAL:HG12	32:Y:161:PRO:HG3	2.01	0.42
32:X:200:GLU:OE2	32:X:203:ARG:NH2	2.41	0.42
33:a:1351:C:H2'	33:a:1352:U:O4'	2.19	0.42
33:a:1915:3TD:H6	33:a:1915:3TD:O5'	2.18	0.42
33:a:1935:G:H1'	33:a:1964:G:N2	2.34	0.42
33:a:2552:OMU:H6	33:a:2552:OMU:O5'	2.19	0.42
34:b:49:C:H2'	34:b:50:A:C8	2.54	0.42
35:c:41:GLY:O	35:c:43:ARG:NH1	2.52	0.42
36:d:56:LYS:HB2	36:d:59:ARG:HB2	2.02	0.42
45:m:51:LEU:HD13	45:m:51:LEU:HA	1.84	0.42
8:8:20:G:H5''	8:8:21:H2U:HN3	1.85	0.42
10:A:950:U:H2'	10:A:951:G:C8	2.54	0.42
10:A:1010:U:H2'	10:A:1011:C:C6	2.54	0.42
11:B:186:ILE:HD13	11:B:200:ILE:HB	2.02	0.42
17:H:96:MET:HE3	17:H:130:ALA:HB1	2.01	0.42
22:M:48:LEU:HD22	22:M:52:GLN:HG2	2.01	0.42
32:X:3:VAL:HA	32:X:77:THR:O	2.20	0.42
33:a:1047:G:HO2'	33:a:1110:G:N2	2.16	0.42
37:e:119:ILE:HD11	37:e:141:MET:HE2	2.01	0.42
7:6:106:LEU:HB3	7:6:126:THR:HG23	2.02	0.42
8:8:11:A:H2'	8:8:12:G:C8	2.55	0.42
12:C:152:GLU:HG3	12:C:167:TRP:HB3	2.01	0.42
19:J:40:ILE:HB	19:J:73:LEU:HB3	2.01	0.42
21:L:49:LEU:HD23	21:L:49:LEU:HA	1.93	0.42
32:X:161:PRO:HG3	32:Y:160:VAL:HG12	2.02	0.42
32:X:268:LEU:HD11	32:X:376:LEU:HD13	2.01	0.42
33:a:307:G:N1	33:a:310:A:OP2	2.51	0.42
33:a:884:U:O4	33:a:885:C:N4	2.52	0.42
33:a:2250:G:O2'	33:a:2496:C:OP1	2.34	0.42
33:a:2902:C:H2'	33:a:2903:U:O4'	2.20	0.42
33:a:320:A:H2'	37:e:131:THR:HG21	2.00	0.42
33:a:1105:U:H2'	33:a:1106:G:C8	2.50	0.42
35:c:145:GLU:HB2	35:c:188:CYS:HB3	2.01	0.42
39:g:19:ILE:HG12	39:g:24:ILE:HD12	2.01	0.42
10:A:337:G:H2'	10:A:338:A:C8	2.54	0.42
11:B:42:ASN:OD1	11:B:45:LYS:HG3	2.19	0.42
26:Q:47:HIS:NE2	26:Q:49:GLU:HG2	2.35	0.42
32:Y:48:ALA:O	32:Y:98:TYR:OH	2.23	0.42
32:Y:157:LYS:HB2	59:Z:4:A:OP1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:l:41:LEU:HD23	44:l:41:LEU:HA	1.87	0.42
8:7:26:C:H2'	8:7:27:G:O4'	2.19	0.42
10:A:642:A:C5	17:H:107:SER:HA	2.55	0.42
32:X:279:MET:HE2	32:X:279:MET:HB3	1.81	0.42
33:a:1357:C:H2'	33:a:1358:G:O4'	2.20	0.42
52:t:38:GLY:H	52:t:62:GLU:CD	2.28	0.42
7:6:97:LYS:HD3	7:6:139:VAL:HG11	2.01	0.42
10:A:458:U:H2'	10:A:459:A:C8	2.55	0.42
10:A:1371:G:O3'	18:I:71:GLY:HA3	2.20	0.42
26:Q:68:SER:HB3	26:Q:71:LYS:HB2	2.00	0.42
33:a:2109:U:N3	33:a:2110:G:O6	2.52	0.42
45:m:35:LYS:HB2	45:m:112:TYR:CE1	2.55	0.42
8:8:61:U:H5''	8:8:62:C:H5	1.85	0.42
10:A:253:A:O2'	26:Q:17:MET:SD	2.78	0.42
10:A:1162:C:H2'	10:A:1163:A:C8	2.55	0.42
12:C:26:THR:HG23	23:N:76:LYS:HD2	2.01	0.42
13:D:197:GLU:OE1	13:D:197:GLU:N	2.42	0.42
31:W:64:ASN:HD22	31:W:113:ALA:HB1	1.84	0.42
33:a:1414:C:H2'	33:a:1415:U:O4'	2.20	0.42
33:a:2191:A:H2'	33:a:2192:U:C6	2.55	0.42
8:8:47:A:H5'	8:8:48:U:OP2	2.20	0.42
10:A:96:U:H2'	10:A:97:G:C8	2.55	0.42
18:I:120:LYS:HB2	18:I:123:ARG:HB3	2.02	0.42
33:a:245:G:O2'	33:a:384:A:N1	2.45	0.42
33:a:2081:U:H2'	33:a:2082:A:C8	2.55	0.42
33:a:2081:U:H2'	33:a:2082:A:H8	1.84	0.42
33:a:2105:U:H2'	33:a:2106:U:O4'	2.19	0.42
33:a:2567:G:H2'	33:a:2568:U:C6	2.54	0.42
6:5:111:ALA:HB3	6:5:118:ILE:HB	2.02	0.41
10:A:946:A:H2'	10:A:947:G:C8	2.55	0.41
12:C:88:ARG:HA	12:C:91:VAL:HG12	2.02	0.41
12:C:153:VAL:HG12	12:C:157:LEU:HD21	2.01	0.41
20:K:13:ARG:HA	20:K:13:ARG:HH11	1.85	0.41
33:a:2271:G:OP1	54:v:18:ALA:HB1	2.20	0.41
38:f:23:ASN:OD1	38:f:23:ASN:N	2.53	0.41
55:w:59:ILE:HG12	55:w:67:VAL:HG21	2.02	0.41
8:7:63:C:H2'	8:7:64:G:H8	1.85	0.41
10:A:976:G:OP2	10:A:1358:U:O2'	2.36	0.41
10:A:1516:2MG:N2	10:A:1519:MA6:OP2	2.41	0.41
21:L:67:ILE:HD13	21:L:74:LEU:HD12	2.02	0.41
22:M:49:SER:HB3	22:M:52:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:T:57:ILE:HD12	29:T:57:ILE:HA	1.92	0.41
42:j:23:LYS:HB2	42:j:23:LYS:HE2	1.92	0.41
42:j:121:GLU:OE1	47:o:65:SER:OG	2.38	0.41
44:l:54:THR:HG22	44:l:63:ILE:HD12	2.02	0.41
44:l:57:VAL:HG21	44:l:105:MET:SD	2.60	0.41
6:5:97:LYS:HE3	6:5:123:ILE:HB	2.01	0.41
10:A:490:C:OP1	13:D:146:ARG:NH2	2.45	0.41
10:A:1495:U:O2'	33:a:1919:A:N1	2.44	0.41
12:C:131:ARG:O	12:C:135:LYS:HG3	2.21	0.41
12:C:154:SER:HB3	12:C:165:THR:HG23	2.02	0.41
26:Q:57:ASP:OD1	26:Q:57:ASP:N	2.53	0.41
26:Q:68:SER:OG	26:Q:69:LYS:N	2.53	0.41
31:W:68:VAL:HG22	31:W:115:ALA:CB	2.50	0.41
33:a:2020:A:H5'	58:z:9:THR:CG2	2.51	0.41
38:f:78:LYS:HB2	38:f:78:LYS:HE2	1.86	0.41
6:5:8:LYS:HZ2	33:a:1046:A:HO2'	1.58	0.41
7:6:14:ALA:HB1	7:6:17:MET:HE2	2.01	0.41
7:6:36:MET:HE2	7:6:40:LYS:HD2	2.03	0.41
10:A:447:G:N1	10:A:486:U:OP2	2.43	0.41
10:A:539:A:H2'	10:A:540:G:C8	2.55	0.41
10:A:1286:U:H2'	10:A:1287:A:H5'	2.02	0.41
10:A:1478:U:H2'	10:A:1479:C:C6	2.54	0.41
24:O:18:ASP:HB3	24:O:21:ASP:HB2	2.02	0.41
33:a:2076:U:OP2	33:a:2238:G:N2	2.43	0.41
40:h:79:THR:O	40:h:79:THR:HG23	2.20	0.41
43:k:55:MET:O	43:k:60:ARG:NH1	2.52	0.41
46:n:16:ARG:HD3	46:n:16:ARG:HA	1.88	0.41
10:A:1143:G:H2'	10:A:1144:G:H8	1.85	0.41
10:A:1328:C:H5''	22:M:28:THR:HG21	2.02	0.41
10:A:1391:U:H2'	10:A:1392:G:C8	2.55	0.41
15:F:11:HIS:HD2	15:F:12:PRO:CD	2.32	0.41
33:a:729:G:C6	35:c:207:LYS:HB2	2.55	0.41
33:a:1263:U:O2'	58:z:8:PRO:HD2	2.20	0.41
33:a:2305:U:H2'	33:a:2306:C:C6	2.55	0.41
40:h:34:GLY:O	40:h:36:ALA:N	2.54	0.41
40:h:129:GLU:OE2	40:h:143:ILE:HG12	2.21	0.41
41:i:115:GLY:HA2	41:i:118:MET:HE3	2.03	0.41
58:z:38:HIS:HB3	58:z:44:THR:HG22	2.02	0.41
6:5:120:ALA:O	6:5:123:ILE:HG13	2.20	0.41
10:A:8:A:N7	13:D:206:LYS:HA	2.36	0.41
10:A:1003:G:H21	10:A:1005:A:H5'	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:I:54:LEU:HD23	18:I:98:LEU:HD23	2.02	0.41
32:Y:27:TRP:O	32:Y:30:GLU:HG2	2.20	0.41
33:a:322:A:H5'	33:a:340:A:H1'	2.02	0.41
33:a:483:A:C8	52:t:45:HIS:HD2	2.37	0.41
33:a:1178:C:H2'	33:a:1179:G:H8	1.85	0.41
33:a:2575:C:H5'	36:d:149:ASN:HB2	2.02	0.41
33:a:2720:U:OP1	47:o:53:ARG:NH2	2.53	0.41
39:g:86:LYS:HB2	39:g:86:LYS:HE3	1.83	0.41
10:A:58:C:O2'	10:A:388:G:N7	2.44	0.41
10:A:1036:A:H2'	10:A:1037:C:O4'	2.20	0.41
13:D:124:MET:SD	13:D:146:ARG:HG3	2.61	0.41
15:F:11:HIS:CD2	15:F:12:PRO:HD2	2.49	0.41
33:a:933:A:H5'	33:a:934:U:OP2	2.21	0.41
33:a:1081:U:H2'	33:a:1082:U:C6	2.55	0.41
42:j:24:VAL:HG12	42:j:30:ARG:HD3	2.02	0.41
2:1:26:ASN:CG	33:a:682:G:H5'	2.46	0.41
10:A:514:C:H2'	10:A:515:G:C8	2.56	0.41
10:A:1135:U:H2'	10:A:1137:C:C5	2.56	0.41
11:B:70:VAL:O	11:B:163:VAL:HA	2.20	0.41
18:I:52:LEU:HD11	18:I:63:LEU:HD11	2.01	0.41
32:X:140:ILE:HD13	32:X:172:VAL:HG21	2.02	0.41
33:a:886:A:H2	33:a:890:C:H5	1.69	0.41
33:a:1075:C:H2'	33:a:1076:C:C6	2.55	0.41
33:a:1550:C:H2'	33:a:1551:A:C8	2.56	0.41
33:a:1734:G:H2'	33:a:1735:A:C8	2.54	0.41
33:a:2097:A:H2'	33:a:2098:U:C6	2.56	0.41
35:c:29:PRO:HG2	35:c:34:LEU:HD11	2.01	0.41
38:f:130:MET:HE2	38:f:130:MET:HB3	1.94	0.41
38:f:175:PHE:HA	38:f:176:PRO:HD3	1.92	0.41
40:h:93:SER:HB3	40:h:123:ARG:NH1	2.36	0.41
44:l:105:MET:HE1	44:l:116:ALA:HB3	2.03	0.41
49:q:64:VAL:HG22	49:q:95:ASP:O	2.20	0.41
1:0:5:ILE:CG2	1:0:28:ARG:HH12	2.34	0.41
5:4:16:CYS:HA	5:4:34:LEU:HB2	2.03	0.41
12:C:54:ARG:HB3	12:C:69:HIS:HB2	2.02	0.41
30:U:54:LYS:HG3	30:U:55:ARG:N	2.36	0.41
31:W:108:LYS:O	31:W:111:GLU:HG2	2.21	0.41
32:X:51:ASP:N	32:X:51:ASP:OD1	2.53	0.41
32:X:268:LEU:HD23	32:X:337:VAL:HB	2.01	0.41
32:X:305:LYS:HG2	32:X:314:PHE:CD1	2.55	0.41
32:Y:67:LEU:HD23	32:Y:67:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:549:G:H2'	33:a:550:C:C6	2.55	0.41
33:a:833:A:H2'	33:a:834:G:C8	2.56	0.41
33:a:1672:A:C2	33:a:2582:G:H5'	2.56	0.41
33:a:2038:G:H2'	33:a:2039:U:O4'	2.21	0.41
33:a:2100:G:H1	33:a:2189:U:H3	1.69	0.41
33:a:2291:U:H2'	33:a:2292:U:C6	2.56	0.41
33:a:2572:A:N7	36:d:150:MEQ:HB3	2.36	0.41
34:b:35:C:N3	34:b:36:C:H1'	2.36	0.41
39:g:30:ASN:HB3	39:g:79:VAL:HA	2.03	0.41
52:t:74:ASN:C	52:t:76:ALA:H	2.29	0.41
5:4:38:SER:HB3	38:f:105:THR:HA	2.02	0.41
23:N:10:GLU:HG3	23:N:63:ARG:HD2	2.02	0.41
40:h:117:LEU:CD2	40:h:130:VAL:CG2	2.95	0.41
42:j:38:ILE:HD11	42:j:112:PHE:CZ	2.51	0.41
10:A:780:A:H5''	20:K:125:LYS:HD3	2.03	0.40
10:A:1004:A:H2'	10:A:1005:A:O4'	2.21	0.40
11:B:68:LEU:HD13	11:B:154:MET:HE1	2.02	0.40
12:C:10:ILE:HG23	12:C:11:ARG:HG3	2.03	0.40
12:C:24:ALA:HB1	12:C:28:GLU:HG2	2.02	0.40
12:C:206:GLU:OE1	12:C:206:GLU:N	2.33	0.40
29:T:39:ILE:HD13	29:T:39:ILE:HA	1.88	0.40
32:X:66:SER:O	32:X:70:MET:HG3	2.20	0.40
32:X:184:LEU:HD23	32:X:184:LEU:HA	1.94	0.40
32:X:202:LEU:HD21	32:X:224:LEU:HD21	2.03	0.40
33:a:542:C:H2'	33:a:543:G:C8	2.56	0.40
33:a:1548:A:H2'	33:a:1549:A:C8	2.56	0.40
37:e:1:MET:HB3	37:e:14:VAL:HG23	2.02	0.40
37:e:63:LYS:HB2	37:e:63:LYS:HE2	1.88	0.40
38:f:170:LEU:O	38:f:175:PHE:HB2	2.22	0.40
46:n:31:THR:CG2	46:n:34:HIS:H	2.30	0.40
52:t:26:LYS:HD3	52:t:26:LYS:HA	1.96	0.40
53:u:75:GLN:HB2	53:u:92:VAL:HG23	2.03	0.40
10:A:123:U:OP1	10:A:311:C:O2'	2.33	0.40
10:A:580:C:H2'	10:A:581:G:O4'	2.21	0.40
10:A:891:U:H2'	10:A:892:A:H8	1.86	0.40
17:H:39:VAL:O	17:H:43:GLU:HG2	2.21	0.40
22:M:19:LEU:HD13	22:M:33:ILE:HD13	2.03	0.40
33:a:544:C:O3'	33:a:545:U:H2'	2.21	0.40
33:a:723:C:H2'	33:a:724:U:O4'	2.22	0.40
33:a:2120:G:H2'	33:a:2121:G:C8	2.56	0.40
53:u:6:ALA:HB1	53:u:40:ILE:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:120:ALA:HA	6:5:123:ILE:HD11	2.03	0.40
7:6:28:LEU:HB3	7:6:33:VAL:HG22	2.02	0.40
10:A:269:C:H2'	10:A:270:A:C8	2.56	0.40
10:A:1305:G:N2	10:A:1331:G:H1'	2.36	0.40
32:X:133:THR:HG23	32:X:166:ILE:HD11	2.03	0.40
33:a:871:U:H2'	33:a:872:U:C6	2.57	0.40
33:a:959:A:H2'	33:a:960:A:C8	2.57	0.40
36:d:4:LEU:HD12	36:d:4:LEU:HA	1.98	0.40
38:f:4:LEU:HD12	38:f:173:PHE:CD2	2.56	0.40
45:m:69:ARG:C	45:m:71:ARG:H	2.29	0.40
49:q:37:GLU:HG3	49:q:53:PHE:CE1	2.56	0.40
16:G:130:ASN:OD1	16:G:130:ASN:N	2.54	0.40
32:X:269:SER:HB3	32:X:373:PHE:CE2	2.56	0.40
32:Y:50:LEU:HD22	32:Y:68:ALA:HB2	2.03	0.40
33:a:898:C:H2'	33:a:899:A:O4'	2.22	0.40
33:a:954:G:H5''	44:l:13:HIS:CG	2.57	0.40
33:a:2350:C:H2'	33:a:2351:G:O4'	2.21	0.40
41:i:110:PRO:O	41:i:115:GLY:HA3	2.22	0.40
45:m:33:ILE:HG13	45:m:114:GLU:HB3	2.03	0.40
7:6:95:LYS:HD2	33:a:1076:C:O3'	2.22	0.40
8:7:69:C:H2'	8:7:70:C:O4'	2.22	0.40
10:A:1011:C:H2'	10:A:1012:A:C8	2.57	0.40
10:A:1228:C:OP2	22:M:110:LYS:NZ	2.36	0.40
15:F:42:TRP:HZ2	15:F:61:LEU:HD22	1.85	0.40
22:M:27:LYS:HB2	22:M:27:LYS:HE2	1.89	0.40
32:X:7:THR:HG22	32:X:8:CYS:H	1.86	0.40
32:Y:380:GLU:H	32:Y:380:GLU:HG2	1.69	0.40
33:a:1607:C:H4'	33:a:1608:A:O5'	2.21	0.40
50:r:80:PRO:O	50:r:100:THR:OG1	2.30	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%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	54 (96%)	2 (4%)	0	100	100
6	5	113/165 (68%)	111 (98%)	2 (2%)	0	100	100
7	6	132/142 (93%)	123 (93%)	9 (7%)	0	100	100
11	B	222/241 (92%)	211 (95%)	11 (5%)	0	100	100
12	C	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
13	D	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
14	E	154/167 (92%)	149 (97%)	4 (3%)	1 (1%)	21	52
15	F	101/135 (75%)	97 (96%)	4 (4%)	0	100	100
16	G	150/179 (84%)	145 (97%)	5 (3%)	0	100	100
17	H	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
18	I	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
19	J	96/103 (93%)	90 (94%)	6 (6%)	0	100	100
20	K	113/129 (88%)	109 (96%)	4 (4%)	0	100	100
21	L	121/124 (98%)	115 (95%)	6 (5%)	0	100	100
22	M	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
23	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
24	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
25	P	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
26	Q	77/84 (92%)	73 (95%)	4 (5%)	0	100	100
27	R	63/75 (84%)	62 (98%)	1 (2%)	0	100	100
28	S	81/92 (88%)	79 (98%)	2 (2%)	0	100	100
29	T	84/87 (97%)	84 (100%)	0	0	100	100
30	U	68/71 (96%)	68 (100%)	0	0	100	100
31	W	57/120 (48%)	54 (95%)	3 (5%)	0	100	100
32	X	382/406 (94%)	363 (95%)	19 (5%)	0	100	100
32	Y	371/406 (91%)	351 (95%)	20 (5%)	0	100	100
35	c	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
36	d	206/209 (99%)	199 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	e	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
38	f	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
39	g	172/177 (97%)	163 (95%)	9 (5%)	0	100	100
40	h	141/149 (95%)	129 (92%)	12 (8%)	0	100	100
41	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
42	j	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
43	k	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
44	l	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
45	m	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
46	n	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
47	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
48	p	115/118 (98%)	115 (100%)	0	0	100	100
49	q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
50	r	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
51	s	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
52	t	93/104 (89%)	88 (95%)	5 (5%)	0	100	100
53	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
54	v	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
55	w	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
56	x	58/63 (92%)	56 (97%)	2 (3%)	0	100	100
57	y	55/59 (93%)	54 (98%)	1 (2%)	0	100	100
58	z	53/57 (93%)	53 (100%)	0	0	100	100
All	All	6623/7152 (93%)	6396 (97%)	226 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	E	90	THR

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%)	45 (98%)	1 (2%)	45	62
2	1	38/38 (100%)	37 (97%)	1 (3%)	40	59
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%)	53 (96%)	2 (4%)	31	54
6	5	90/123 (73%)	89 (99%)	1 (1%)	65	72
7	6	101/110 (92%)	99 (98%)	2 (2%)	48	64
11	B	186/199 (94%)	183 (98%)	3 (2%)	55	67
12	C	170/190 (90%)	166 (98%)	4 (2%)	43	61
13	D	172/173 (99%)	170 (99%)	2 (1%)	63	71
14	E	119/126 (94%)	117 (98%)	2 (2%)	53	67
15	F	90/116 (78%)	87 (97%)	3 (3%)	33	55
16	G	124/147 (84%)	122 (98%)	2 (2%)	55	67
17	H	104/105 (99%)	104 (100%)	0	100	100
18	I	105/107 (98%)	101 (96%)	4 (4%)	29	52
19	J	86/90 (96%)	85 (99%)	1 (1%)	63	71
20	K	89/98 (91%)	87 (98%)	2 (2%)	45	62
21	L	101/104 (97%)	98 (97%)	3 (3%)	36	57
22	M	93/96 (97%)	91 (98%)	2 (2%)	45	62
23	N	83/84 (99%)	83 (100%)	0	100	100
24	O	76/77 (99%)	75 (99%)	1 (1%)	61	70
25	P	65/65 (100%)	64 (98%)	1 (2%)	57	68
26	Q	73/78 (94%)	70 (96%)	3 (4%)	27	51
27	R	56/65 (86%)	55 (98%)	1 (2%)	51	66
28	S	72/79 (91%)	70 (97%)	2 (3%)	38	58
29	T	65/66 (98%)	63 (97%)	2 (3%)	35	56
30	U	60/61 (98%)	59 (98%)	1 (2%)	53	67
31	W	33/84 (39%)	33 (100%)	0	100	100
32	X	305/339 (90%)	301 (99%)	4 (1%)	61	70
32	Y	299/339 (88%)	294 (98%)	5 (2%)	53	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	c	216/218 (99%)	212 (98%)	4 (2%)	50	65
36	d	163/163 (100%)	157 (96%)	6 (4%)	30	53
37	e	165/165 (100%)	161 (98%)	4 (2%)	43	61
38	f	148/150 (99%)	144 (97%)	4 (3%)	39	58
39	g	134/138 (97%)	128 (96%)	6 (4%)	24	49
40	h	110/114 (96%)	108 (98%)	2 (2%)	51	66
41	i	116/116 (100%)	114 (98%)	2 (2%)	53	67
42	j	104/104 (100%)	99 (95%)	5 (5%)	23	48
43	k	102/103 (99%)	98 (96%)	4 (4%)	28	52
44	l	109/109 (100%)	106 (97%)	3 (3%)	38	58
45	m	98/103 (95%)	95 (97%)	3 (3%)	35	56
46	n	86/87 (99%)	83 (96%)	3 (4%)	32	54
47	o	99/100 (99%)	99 (100%)	0	100	100
48	p	89/90 (99%)	88 (99%)	1 (1%)	65	72
49	q	84/84 (100%)	82 (98%)	2 (2%)	43	61
50	r	93/93 (100%)	91 (98%)	2 (2%)	45	62
51	s	80/84 (95%)	79 (99%)	1 (1%)	61	70
52	t	79/85 (93%)	78 (99%)	1 (1%)	61	70
53	u	78/78 (100%)	75 (96%)	3 (4%)	29	52
54	v	58/63 (92%)	57 (98%)	1 (2%)	53	67
55	w	67/68 (98%)	66 (98%)	1 (2%)	57	68
56	x	54/55 (98%)	51 (94%)	3 (6%)	19	45
57	y	47/49 (96%)	45 (96%)	2 (4%)	26	50
58	z	46/48 (96%)	46 (100%)	0	100	100
All	All	5466/5823 (94%)	5348 (98%)	118 (2%)	45	62

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	54	ILE
2	1	42	LEU
5	4	21	VAL
5	4	27	THR
6	5	77	VAL

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Mol	Chain	Res	Type
7	6	31	GLN
7	6	55	ILE
11	B	163	VAL
11	B	183	VAL
11	B	205	ASP
12	C	21	THR
12	C	105	GLU
12	C	173	VAL
12	C	185	ASN
13	D	85	ASN
13	D	184	ARG
14	E	90	THR
14	E	131	THR
15	F	10	VAL
15	F	96	VAL
15	F	97	THR
16	G	6	VAL
16	G	80	VAL
18	I	55	VAL
18	I	67	VAL
18	I	105	THR
18	I	111	VAL
19	J	57	VAL
20	K	38	GLN
20	K	108	THR
21	L	35	THR
21	L	55	VAL
21	L	59	ASN
22	M	33	ILE
22	M	102	THR
24	O	75	VAL
25	P	52	LEU
26	Q	42	THR
26	Q	51	ASN
26	Q	57	ASP
27	R	71	THR
28	S	11	ILE
28	S	48	THR
29	T	3	ASN
29	T	57	ILE
30	U	6	VAL
32	X	7	THR

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Mol	Chain	Res	Type
32	X	274	ASP
32	X	321	HIS
32	X	354	ARG
32	Y	47	THR
32	Y	76	ASP
32	Y	238	GLU
32	Y	240	VAL
32	Y	374	VAL
35	c	82	GLU
35	c	121	ASP
35	c	162	VAL
35	c	195	VAL
36	d	4	LEU
36	d	12	THR
36	d	91	THR
36	d	92	VAL
36	d	95	SER
36	d	176	ASP
37	e	72	SER
37	e	95	LYS
37	e	119	ILE
37	e	140	ASP
38	f	117	LEU
38	f	152	LEU
38	f	159	THR
38	f	175	PHE
39	g	9	VAL
39	g	17	VAL
39	g	60	ASP
39	g	84	THR
39	g	127	THR
39	g	169	VAL
40	h	19	VAL
40	h	142	VAL
41	i	84	ILE
41	i	135	GLN
42	j	10	VAL
42	j	28	SER
42	j	58	LEU
42	j	76	VAL
42	j	104	THR
43	k	42	SER

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Mol	Chain	Res	Type
43	k	67	THR
43	k	85	VAL
43	k	94	THR
44	l	78	LEU
44	l	80	VAL
44	l	135	VAL
45	m	15	SER
45	m	51	LEU
45	m	116	VAL
46	n	2	ASP
46	n	28	VAL
46	n	31	THR
48	p	117	LEU
49	q	37	GLU
49	q	64	VAL
50	r	4	ILE
50	r	29	VAL
51	s	58	VAL
52	t	36	VAL
53	u	62	THR
53	u	65	VAL
53	u	66	ASP
54	v	70	GLU
55	w	2	SER
56	x	42	LEU
56	x	55	THR
56	x	56	LEU
57	y	8	THR
57	y	35	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	45	GLN
3	2	28	ASN
5	4	48	GLN
6	5	4	ASN
7	6	31	GLN
11	B	177	ASN
12	C	100	GLN
12	C	102	ASN
12	C	185	ASN

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Mol	Chain	Res	Type
13	D	40	GLN
13	D	41	HIS
13	D	152	GLN
14	E	97	GLN
15	F	11	HIS
15	F	37	HIS
16	G	52	GLN
16	G	68	ASN
17	H	4	GLN
20	K	38	GLN
21	L	5	ASN
25	P	9	HIS
29	T	61	GLN
30	U	64	ASN
31	W	64	ASN
32	X	122	HIS
32	X	143	ASN
32	X	300	GLN
32	X	353	ASN
32	Y	321	HIS
35	c	25	HIS
35	c	53	HIS
35	c	143	ASN
36	d	32	ASN
36	d	49	GLN
36	d	173	GLN
37	e	165	HIS
40	h	33	GLN
40	h	66	ASN
40	h	135	HIS
41	i	76	HIS
41	i	135	GLN
42	j	5	GLN
42	j	82	ASN
43	k	104	GLN
44	l	60	GLN
45	m	31	HIS
46	n	100	HIS
47	o	12	GLN
47	o	52	ASN
47	o	66	ASN
48	p	44	GLN

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Mol	Chain	Res	Type
48	p	81	ASN
49	q	12	HIS
50	r	9	HIS
54	v	76	ASN
55	w	34	HIS
58	z	6	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	1498/1542 (97%)	180 (12%)	3 (0%)
33	a	2858/2904 (98%)	326 (11%)	0
34	b	118/120 (98%)	10 (8%)	0
59	Z	3/4 (75%)	3 (100%)	0
8	7	75/77 (97%)	22 (29%)	0
8	8	77/77 (100%)	22 (28%)	1 (1%)
9	9	2/31 (6%)	0	0
All	All	4631/4755 (97%)	563 (12%)	4 (0%)

All (563) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	4	G
8	7	8	4SU
8	7	9	G
8	7	14	A
8	7	16	C
8	7	17	C
8	7	18	U
8	7	19	G
8	7	20	G
8	7	21	H2U
8	7	22	A
8	7	23	G
8	7	46	G
8	7	47	A
8	7	48	U
8	7	50	G
8	7	56	PSU
8	7	59	A
8	7	62	C

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Mol	Chain	Res	Type
8	7	65	G
8	7	70	C
8	7	77	A
8	8	2	G
8	8	4	G
8	8	8	4SU
8	8	9	G
8	8	14	A
8	8	17	C
8	8	18	U
8	8	19	G
8	8	20	G
8	8	21	H2U
8	8	22	A
8	8	23	G
8	8	45	A
8	8	47	A
8	8	48	U
8	8	50	G
8	8	56	PSU
8	8	62	C
8	8	65	G
8	8	70	C
8	8	76	C
8	8	77	A
10	A	4	U
10	A	5	U
10	A	6	G
10	A	7	A
10	A	9	G
10	A	22	G
10	A	32	A
10	A	39	G
10	A	47	C
10	A	48	C
10	A	50	A
10	A	51	A
10	A	54	C
10	A	63	C
10	A	71	A
10	A	74	A
10	A	75	G

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Mol	Chain	Res	Type
10	A	93	U
10	A	94	G
10	A	116	A
10	A	122	G
10	A	130	A
10	A	141	G
10	A	144	G
10	A	149	A
10	A	163	C
10	A	183	C
10	A	197	A
10	A	203	G
10	A	204	G
10	A	245	U
10	A	247	G
10	A	251	G
10	A	266	G
10	A	267	C
10	A	280	C
10	A	284	C
10	A	289	G
10	A	319	G
10	A	321	A
10	A	328	C
10	A	344	A
10	A	347	G
10	A	352	C
10	A	354	G
10	A	367	U
10	A	372	C
10	A	373	A
10	A	384	G
10	A	406	G
10	A	411	A
10	A	412	A
10	A	413	G
10	A	414	A
10	A	421	U
10	A	422	C
10	A	424	G
10	A	429	U
10	A	436	C

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Mol	Chain	Res	Type
10	A	453	G
10	A	457	G
10	A	458	U
10	A	467	U
10	A	468	A
10	A	469	C
10	A	479	U
10	A	481	G
10	A	484	G
10	A	486	U
10	A	495	A
10	A	511	C
10	A	518	C
10	A	531	U
10	A	532	A
10	A	547	A
10	A	559	A
10	A	562	U
10	A	564	C
10	A	572	A
10	A	573	A
10	A	576	C
10	A	577	G
10	A	579	A
10	A	596	A
10	A	633	G
10	A	653	U
10	A	665	A
10	A	687	A
10	A	703	G
10	A	721	G
10	A	723	U
10	A	734	G
10	A	748	G
10	A	755	G
10	A	777	A
10	A	793	U
10	A	794	A
10	A	802	A
10	A	815	A
10	A	817	C
10	A	819	A

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Mol	Chain	Res	Type
10	A	821	G
10	A	884	U
10	A	885	G
10	A	890	G
10	A	902	G
10	A	914	A
10	A	934	C
10	A	935	A
10	A	960	U
10	A	966	2MG
10	A	969	A
10	A	975	A
10	A	976	G
10	A	977	A
10	A	984	C
10	A	992	U
10	A	993	G
10	A	994	A
10	A	1003	G
10	A	1004	A
10	A	1008	U
10	A	1009	U
10	A	1027	C
10	A	1035	A
10	A	1036	A
10	A	1044	A
10	A	1053	G
10	A	1065	U
10	A	1085	U
10	A	1094	G
10	A	1095	U
10	A	1101	A
10	A	1137	C
10	A	1139	G
10	A	1159	U
10	A	1171	A
10	A	1191	A
10	A	1196	A
10	A	1197	A
10	A	1213	A
10	A	1214	C
10	A	1227	A

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Mol	Chain	Res	Type
10	A	1228	C
10	A	1238	A
10	A	1253	G
10	A	1256	A
10	A	1262	C
10	A	1275	A
10	A	1280	A
10	A	1286	U
10	A	1287	A
10	A	1300	G
10	A	1302	C
10	A	1317	C
10	A	1319	A
10	A	1320	C
10	A	1346	A
10	A	1353	G
10	A	1363	A
10	A	1368	A
10	A	1370	G
10	A	1378	C
10	A	1379	G
10	A	1381	U
10	A	1398	A
10	A	1419	G
10	A	1429	A
10	A	1432	G
10	A	1441	A
10	A	1452	C
10	A	1454	G
10	A	1487	G
10	A	1492	A
10	A	1497	G
10	A	1499	A
10	A	1506	U
10	A	1517	G
10	A	1529	G
10	A	1530	G
33	a	10	A
33	a	15	G
33	a	34	U
33	a	35	G
33	a	42	A

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Mol	Chain	Res	Type
33	a	50	U
33	a	71	A
33	a	74	A
33	a	75	G
33	a	80	G
33	a	84	A
33	a	101	A
33	a	102	U
33	a	118	A
33	a	119	A
33	a	120	U
33	a	139	U
33	a	142	A
33	a	165	A
33	a	181	A
33	a	196	A
33	a	199	A
33	a	215	G
33	a	216	A
33	a	221	A
33	a	222	A
33	a	223	A
33	a	224	U
33	a	248	G
33	a	265	A
33	a	272	A
33	a	277	G
33	a	278	A
33	a	281	C
33	a	282	A
33	a	285	G
33	a	286	U
33	a	288	U
33	a	294	A
33	a	311	A
33	a	329	G
33	a	330	A
33	a	345	A
33	a	361	G
33	a	362	A
33	a	386	G
33	a	396	G

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Mol	Chain	Res	Type
33	a	404	A
33	a	405	U
33	a	411	G
33	a	412	A
33	a	481	G
33	a	491	G
33	a	504	A
33	a	505	A
33	a	509	C
33	a	532	A
33	a	544	C
33	a	545	U
33	a	546	U
33	a	547	A
33	a	549	G
33	a	563	A
33	a	573	U
33	a	575	A
33	a	603	A
33	a	614	A
33	a	615	U
33	a	627	A
33	a	637	A
33	a	645	C
33	a	647	G
33	a	654	A
33	a	664	G
33	a	686	U
33	a	717	C
33	a	729	G
33	a	730	A
33	a	747	5MU
33	a	748	G
33	a	764	A
33	a	775	G
33	a	776	G
33	a	782	A
33	a	784	G
33	a	785	G
33	a	789	A
33	a	805	G
33	a	806	C

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Mol	Chain	Res	Type
33	a	812	C
33	a	827	U
33	a	845	A
33	a	846	U
33	a	847	U
33	a	859	G
33	a	883	G
33	a	884	U
33	a	885	C
33	a	888	C
33	a	891	G
33	a	895	U
33	a	896	A
33	a	897	C
33	a	898	C
33	a	899	A
33	a	910	A
33	a	915	C
33	a	931	U
33	a	946	C
33	a	961	C
33	a	974	G
33	a	983	A
33	a	996	A
33	a	1012	U
33	a	1013	C
33	a	1033	U
33	a	1040	A
33	a	1046	A
33	a	1047	G
33	a	1070	A
33	a	1083	U
33	a	1087	G
33	a	1088	A
33	a	1110	G
33	a	1111	A
33	a	1112	G
33	a	1122	G
33	a	1132	U
33	a	1135	C
33	a	1142	A
33	a	1157	G

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Mol	Chain	Res	Type
33	a	1206	G
33	a	1250	G
33	a	1253	A
33	a	1256	G
33	a	1271	G
33	a	1272	A
33	a	1300	G
33	a	1301	A
33	a	1352	U
33	a	1365	A
33	a	1379	U
33	a	1380	G
33	a	1383	A
33	a	1411	U
33	a	1416	G
33	a	1419	A
33	a	1420	A
33	a	1427	A
33	a	1428	C
33	a	1452	G
33	a	1458	U
33	a	1478	G
33	a	1482	G
33	a	1493	C
33	a	1505	A
33	a	1509	A
33	a	1510	G
33	a	1515	A
33	a	1529	G
33	a	1534	U
33	a	1535	A
33	a	1536	C
33	a	1537	G
33	a	1566	A
33	a	1569	A
33	a	1578	U
33	a	1585	C
33	a	1586	A
33	a	1608	A
33	a	1626	A
33	a	1634	A
33	a	1647	U

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Mol	Chain	Res	Type
33	a	1648	U
33	a	1649	G
33	a	1674	G
33	a	1716	U
33	a	1729	U
33	a	1730	C
33	a	1738	G
33	a	1744	A
33	a	1756	G
33	a	1764	C
33	a	1773	A
33	a	1782	U
33	a	1800	C
33	a	1801	A
33	a	1807	G
33	a	1808	A
33	a	1816	C
33	a	1829	A
33	a	1848	A
33	a	1858	A
33	a	1870	C
33	a	1871	A
33	a	1873	G
33	a	1905	C
33	a	1906	G
33	a	1914	C
33	a	1929	G
33	a	1930	G
33	a	1941	C
33	a	1955	U
33	a	1967	C
33	a	1970	A
33	a	1971	U
33	a	1972	G
33	a	1987	A
33	a	1991	U
33	a	1993	U
33	a	2006	C
33	a	2023	C
33	a	2031	A
33	a	2033	A
33	a	2036	C

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Mol	Chain	Res	Type
33	a	2043	C
33	a	2049	G
33	a	2055	C
33	a	2056	G
33	a	2060	A
33	a	2061	G
33	a	2062	A
33	a	2069	G7M
33	a	2105	U
33	a	2111	U
33	a	2112	G
33	a	2113	U
33	a	2115	G
33	a	2116	G
33	a	2117	A
33	a	2118	U
33	a	2119	A
33	a	2120	G
33	a	2123	G
33	a	2145	C
33	a	2146	C
33	a	2148	G
33	a	2149	U
33	a	2177	C
33	a	2178	C
33	a	2179	C
33	a	2181	U
33	a	2185	U
33	a	2186	G
33	a	2188	U
33	a	2191	A
33	a	2198	A
33	a	2203	U
33	a	2204	G
33	a	2211	A
33	a	2212	A
33	a	2225	A
33	a	2238	G
33	a	2239	G
33	a	2268	A
33	a	2283	C
33	a	2287	A

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Mol	Chain	Res	Type
33	a	2305	U
33	a	2308	G
33	a	2312	U
33	a	2322	A
33	a	2325	G
33	a	2333	A
33	a	2336	A
33	a	2345	G
33	a	2347	C
33	a	2350	C
33	a	2361	G
33	a	2383	G
33	a	2385	C
33	a	2396	G
33	a	2402	U
33	a	2403	C
33	a	2406	A
33	a	2425	A
33	a	2429	G
33	a	2435	A
33	a	2441	U
33	a	2448	A
33	a	2475	C
33	a	2476	A
33	a	2478	A
33	a	2491	U
33	a	2498	OMC
33	a	2502	G
33	a	2505	G
33	a	2518	A
33	a	2520	C
33	a	2525	G
33	a	2529	G
33	a	2547	A
33	a	2556	C
33	a	2566	A
33	a	2567	G
33	a	2573	C
33	a	2576	G
33	a	2585	U
33	a	2586	U
33	a	2602	A

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Mol	Chain	Res	Type
33	a	2609	U
33	a	2613	U
33	a	2615	U
33	a	2629	U
33	a	2630	G
33	a	2646	C
33	a	2663	G
33	a	2689	U
33	a	2690	U
33	a	2714	G
33	a	2726	A
33	a	2733	A
33	a	2744	G
33	a	2748	A
33	a	2752	C
33	a	2765	A
33	a	2778	A
33	a	2798	U
33	a	2809	A
33	a	2820	A
33	a	2821	A
33	a	2835	A
33	a	2861	U
33	a	2873	A
33	a	2884	U
33	a	2891	U
33	a	2899	A
34	b	35	C
34	b	36	C
34	b	45	A
34	b	56	G
34	b	67	G
34	b	89	U
34	b	90	C
34	b	99	A
34	b	105	G
34	b	109	A
59	Z	2	A
59	Z	3	A
59	Z	4	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	8	1	C
10	A	4	U
10	A	1026	G
10	A	1035	A

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

47 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	$\# Z > 2$
8	4OC	8	33	8	20,23,24	0.36	0	26,32,35	0.66	0
10	PSU	A	516	10	18,21,22	0.65	0	22,30,33	0.93	1 (4%)
33	2MG	a	1835	33	23,26,27	0.44	0	32,38,41	0.48	0
33	PSU	a	2504	33	18,21,22	0.65	0	22,30,33	1.00	1 (4%)
10	4OC	A	1402	10	20,23,24	0.34	0	26,32,35	0.58	0
33	PSU	a	746	61,33	18,21,22	0.77	0	22,30,33	0.82	1 (4%)
10	2MG	A	1516	10	23,26,27	1.33	4 (17%)	32,38,41	2.36	9 (28%)
10	G7M	A	527	10	23,26,27	0.44	0	35,39,42	0.66	0
8	4SU	8	8	8	18,21,22	0.36	0	26,30,33	1.16	2 (7%)
8	5MU	7	55	8	19,22,23	0.36	0	28,32,35	0.52	0
33	5MC	a	1962	33	18,22,23	0.37	0	26,32,35	0.75	0
33	6MZ	a	1618	33	22,25,26	0.37	0	30,36,39	0.57	0
33	OMC	a	2498	61,33	19,22,23	0.64	0	26,31,34	0.83	1 (3%)
10	MA6	A	1519	10	23,26,27	0.39	0	34,38,41	0.82	1 (2%)
33	PSU	a	955	33	18,21,22	0.69	0	22,30,33	1.03	1 (4%)
33	PSU	a	2605	33	18,21,22	0.68	0	22,30,33	1.04	1 (4%)
33	H2U	a	2449	33	18,21,22	0.41	0	21,30,33	0.57	0
8	H2U	8	21	8	18,21,22	0.58	0	21,30,33	0.81	1 (4%)
8	PSU	7	56	8	18,21,22	0.60	0	22,30,33	0.98	1 (4%)
33	PSU	a	2580	33	18,21,22	0.72	0	22,30,33	0.93	1 (4%)
33	PSU	a	2457	33	18,21,22	0.70	0	22,30,33	0.98	1 (4%)
33	6MZ	a	2030	33	22,25,26	0.38	0	30,36,39	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	H2U	7	21	8	18,21,22	0.58	0	21,30,33	0.82	1 (4%)
36	MEQ	d	150	36	8,9,10	0.82	0	5,10,12	0.41	0
33	OMU	a	2552	33	19,22,23	0.39	0	26,31,34	0.46	0
10	5MC	A	1407	10	18,22,23	0.36	0	26,32,35	0.78	0
33	2MG	a	2445	33	23,26,27	0.49	0	32,38,41	0.46	0
33	PSU	a	1911	33	18,21,22	0.62	0	22,30,33	0.95	1 (4%)
8	4OC	7	33	8	20,23,24	0.34	0	26,32,35	0.54	0
33	5MU	a	1939	33	19,22,23	0.40	0	28,32,35	0.57	0
33	G7M	a	2069	33	23,26,27	0.44	0	35,39,42	0.60	0
33	5MU	a	747	33	19,22,23	0.36	0	28,32,35	0.45	0
10	2MG	A	966	10	23,26,27	0.47	0	32,38,41	0.49	0
10	MA6	A	1518	10	23,26,27	0.38	0	34,38,41	0.79	1 (2%)
8	PSU	8	56	8	18,21,22	0.60	0	22,30,33	0.98	1 (4%)
33	3TD	a	1915	33	19,22,23	0.58	0	21,32,35	0.86	0
10	2MG	A	1207	10	23,26,27	0.48	0	32,38,41	0.51	0
8	4SU	7	8	8	18,21,22	0.37	0	26,30,33	1.19	2 (7%)
33	OMG	a	2251	8,33	23,26,27	0.60	0	33,38,41	0.45	0
33	PSU	a	1917	33	18,21,22	0.65	0	22,30,33	0.96	1 (4%)
33	PSU	a	2604	33	18,21,22	0.67	0	22,30,33	1.08	1 (4%)
10	5MC	A	967	10	18,22,23	0.37	0	26,32,35	0.70	0
33	1MG	a	745	33	22,26,27	0.56	0	33,39,42	0.59	0
8	5MU	8	55	8	19,22,23	0.37	0	28,32,35	0.51	0
20	IAS	K	119	20	6,7,8	1.03	0	6,8,10	1.31	1 (16%)
33	2MA	a	2503	61,33	22,25,26	1.29	3 (13%)	33,37,40	0.98	1 (3%)
10	UR3	A	1498	10	19,22,23	0.39	0	26,32,35	0.63	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
8	4OC	8	33	8	-	0/9/29/30	0/2/2/2
10	PSU	A	516	10	-	0/7/25/26	0/2/2/2
33	2MG	a	1835	33	-	0/9/27/28	0/3/3/3
33	PSU	a	2504	33	-	2/7/25/26	0/2/2/2
10	4OC	A	1402	10	-	0/9/29/30	0/2/2/2
33	PSU	a	746	61,33	-	4/7/25/26	0/2/2/2
10	2MG	A	1516	10	-	0/9/27/28	0/3/3/3
10	G7M	A	527	10	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	4SU	8	8	8	-	0/7/25/26	0/2/2/2
8	5MU	7	55	8	-	0/7/25/26	0/2/2/2
33	5MC	a	1962	33	-	4/7/25/26	0/2/2/2
33	6MZ	a	1618	33	-	0/9/27/28	0/3/3/3
33	OMC	a	2498	61,33	-	2/9/27/28	0/2/2/2
10	MA6	A	1519	10	-	0/11/29/30	0/3/3/3
33	PSU	a	955	33	-	0/7/25/26	0/2/2/2
33	PSU	a	2605	33	-	0/7/25/26	0/2/2/2
33	H2U	a	2449	33	-	0/7/38/39	0/2/2/2
8	H2U	8	21	8	-	5/7/38/39	0/2/2/2
8	PSU	7	56	8	-	1/7/25/26	0/2/2/2
33	PSU	a	2580	33	-	0/7/25/26	0/2/2/2
33	PSU	a	2457	33	-	0/7/25/26	0/2/2/2
33	6MZ	a	2030	33	-	2/9/27/28	0/3/3/3
8	H2U	7	21	8	-	5/7/38/39	0/2/2/2
36	MEQ	d	150	36	-	3/8/9/11	-
33	OMU	a	2552	33	-	0/9/27/28	0/2/2/2
10	5MC	A	1407	10	-	0/7/25/26	0/2/2/2
33	2MG	a	2445	33	-	0/9/27/28	0/3/3/3
33	PSU	a	1911	33	-	0/7/25/26	0/2/2/2
8	4OC	7	33	8	-	0/9/29/30	0/2/2/2
33	5MU	a	1939	33	-	0/7/25/26	0/2/2/2
33	G7M	a	2069	33	-	2/7/25/26	0/3/3/3
33	5MU	a	747	33	-	0/7/25/26	0/2/2/2
10	2MG	A	966	10	-	2/9/27/28	0/3/3/3
10	MA6	A	1518	10	-	0/11/29/30	0/3/3/3
8	PSU	8	56	8	-	1/7/25/26	0/2/2/2
33	3TD	a	1915	33	-	0/7/25/26	0/2/2/2
10	2MG	A	1207	10	-	0/9/27/28	0/3/3/3
8	4SU	7	8	8	-	0/7/25/26	0/2/2/2
33	OMG	a	2251	8,33	-	1/9/27/28	0/3/3/3
33	PSU	a	1917	33	-	0/7/25/26	0/2/2/2
33	PSU	a	2604	33	-	0/7/25/26	0/2/2/2
10	5MC	A	967	10	-	0/7/25/26	0/2/2/2
33	1MG	a	745	33	-	0/7/25/26	0/3/3/3
8	5MU	8	55	8	-	0/7/25/26	0/2/2/2
20	IAS	K	119	20	-	1/7/7/8	-
33	2MA	a	2503	61,33	-	2/7/25/26	0/3/3/3
10	UR3	A	1498	10	-	0/7/25/26	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	a	2503	2MA	C2-N1	3.70	1.40	1.34
33	a	2503	2MA	C6-N1	3.18	1.39	1.35
10	A	1516	2MG	C6-N1	-2.96	1.33	1.38
33	a	2503	2MA	C6-N6	-2.67	1.27	1.34
10	A	1516	2MG	C5-C4	2.50	1.45	1.38
10	A	1516	2MG	C5-N7	-2.40	1.34	1.39
10	A	1516	2MG	C4-N9	-2.31	1.32	1.38

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1516	2MG	C2-N3-C4	7.41	121.23	112.04
10	A	1516	2MG	C5-C4-N3	-5.80	119.05	128.46
10	A	1516	2MG	N9-C4-N3	4.08	134.13	125.94
10	A	1516	2MG	C2'-C1'-N9	-3.93	102.08	113.22
8	7	8	4SU	C4-N3-C2	-3.72	123.73	127.34
10	A	1516	2MG	C6-C5-N7	3.70	137.13	130.25
8	8	8	4SU	C4-N3-C2	-3.67	123.77	127.34
10	A	1519	MA6	C2-N1-C6	3.46	119.92	111.75
10	A	1518	MA6	C2-N1-C6	3.45	119.89	111.75
10	A	1516	2MG	C4-C5-N7	-2.74	106.38	110.72
20	K	119	IAS	OD1-CG-CB	-2.56	117.96	125.43
33	a	955	PSU	C6-C5-C4	2.55	119.98	118.20
33	a	2604	PSU	C6-C5-C4	2.54	119.97	118.20
33	a	2503	2MA	C5-C4-N3	-2.54	124.34	127.19
8	7	8	4SU	C5-C4-N3	2.52	117.03	114.69
33	a	2457	PSU	C6-C5-C4	2.46	119.92	118.20
10	A	516	PSU	C6-C5-C4	2.46	119.92	118.20
33	a	2605	PSU	C6-C5-C4	2.44	119.90	118.20
8	7	56	PSU	C6-C5-C4	2.43	119.90	118.20
33	a	746	PSU	C6-C5-C4	2.43	119.90	118.20
33	a	1917	PSU	C6-C5-C4	2.42	119.89	118.20
8	8	8	4SU	C5-C4-N3	2.42	116.94	114.69
33	a	2580	PSU	C6-C5-C4	2.42	119.89	118.20
10	A	1516	2MG	C2-N1-C6	-2.41	121.70	124.48
8	8	56	PSU	C6-C5-C4	2.40	119.88	118.20
33	a	1911	PSU	C6-C5-C4	2.39	119.87	118.20
10	A	1516	2MG	O6-C6-C5	-2.32	120.45	126.60
33	a	2504	PSU	C6-C5-C4	2.31	119.82	118.20
33	a	2498	OMC	C1'-N1-C2	2.22	123.37	118.42
10	A	1516	2MG	C5-C6-N1	2.20	118.77	113.19
8	7	21	H2U	O4'-C1'-N1	2.19	112.28	109.30
8	8	21	H2U	O4'-C1'-N1	2.12	112.19	109.30

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	7	21	H2U	O4'-C1'-N1-C2
8	7	21	H2U	O4'-C1'-N1-C6
8	8	21	H2U	O4'-C1'-N1-C2
8	8	21	H2U	O4'-C1'-N1-C6
36	d	150	MEQ	N-CA-CB-CG
33	a	746	PSU	C2'-C1'-C5-C4
33	a	746	PSU	C2'-C1'-C5-C6
33	a	2251	OMG	C1'-C2'-O2'-CM2
33	a	2030	6MZ	O4'-C4'-C5'-O5'
8	7	21	H2U	O4'-C4'-C5'-O5'
8	8	56	PSU	C4'-C5'-O5'-P
33	a	2498	OMC	O4'-C4'-C5'-O5'
33	a	2030	6MZ	C3'-C4'-C5'-O5'
8	7	56	PSU	C4'-C5'-O5'-P
8	7	21	H2U	C3'-C4'-C5'-O5'
8	8	21	H2U	O4'-C4'-C5'-O5'
10	A	966	2MG	C3'-C4'-C5'-O5'
33	a	2504	PSU	O4'-C4'-C5'-O5'
33	a	1962	5MC	C2'-C1'-N1-C6
36	d	150	MEQ	OE1-CD-CG-CB
8	7	21	H2U	C4'-C5'-O5'-P
8	8	21	H2U	C4'-C5'-O5'-P
33	a	1962	5MC	O4'-C1'-N1-C6
20	K	119	IAS	CA-CB-CG-OD1
33	a	2498	OMC	C3'-C4'-C5'-O5'
36	d	150	MEQ	NE2-CD-CG-CB
33	a	746	PSU	O4'-C1'-C5-C4
8	8	21	H2U	C3'-C4'-C5'-O5'
10	A	966	2MG	O4'-C4'-C5'-O5'
33	a	1962	5MC	O4'-C1'-N1-C2
33	a	2504	PSU	C3'-C4'-C5'-O5'
33	a	746	PSU	O4'-C1'-C5-C6
33	a	1962	5MC	C2'-C1'-N1-C2
33	a	2503	2MA	C4'-C5'-O5'-P
33	a	2503	2MA	O4'-C4'-C5'-O5'
33	a	2069	G7M	O4'-C4'-C5'-O5'
33	a	2069	G7M	C4'-C5'-O5'-P

There are no ring outliers.

11 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	8	33	4OC	1	0
10	A	1516	2MG	1	0
33	a	2498	OMC	1	0
10	A	1519	MA6	1	0
8	8	21	H2U	1	0
33	a	2030	6MZ	3	0
8	7	21	H2U	2	0
36	d	150	MEQ	5	0
33	a	2552	OMU	1	0
8	7	33	4OC	1	0
33	a	1915	3TD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 243 ligands modelled in this entry, 243 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

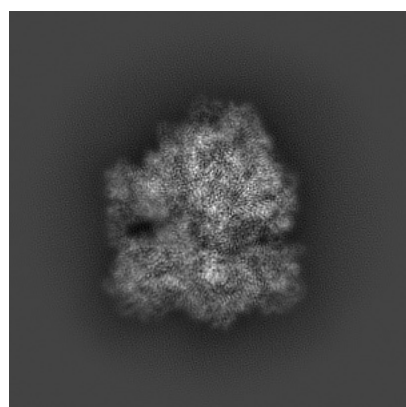
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17667. These allow visual inspection of the internal detail of the map and identification of artifacts.

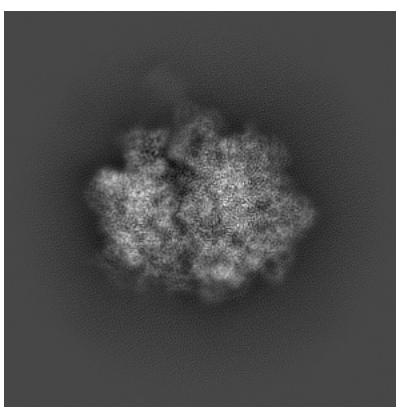
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

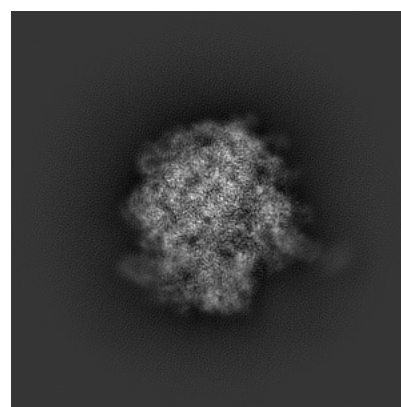
6.1.1 Primary map



X



Y

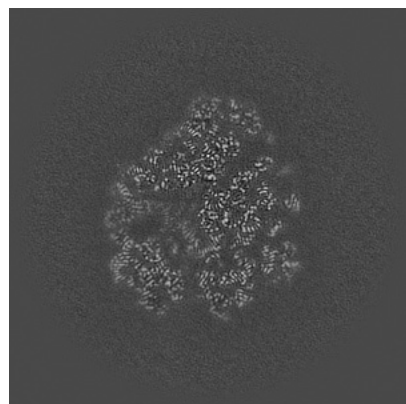


Z

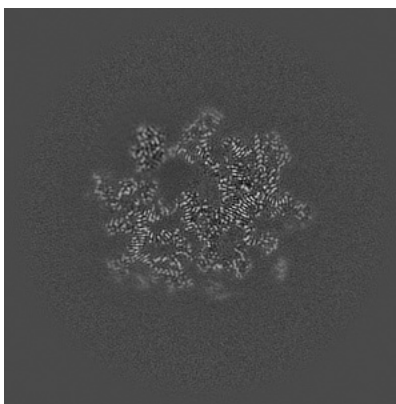
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

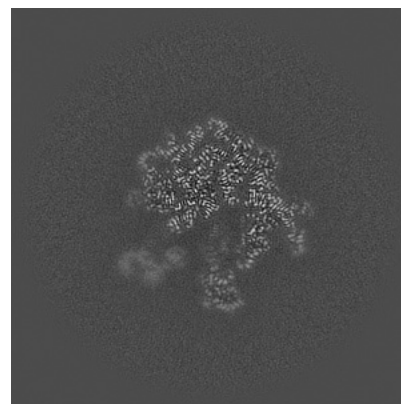
6.2.1 Primary map



X Index: 200



Y Index: 200

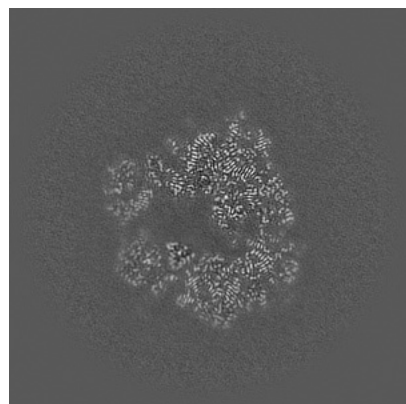


Z Index: 200

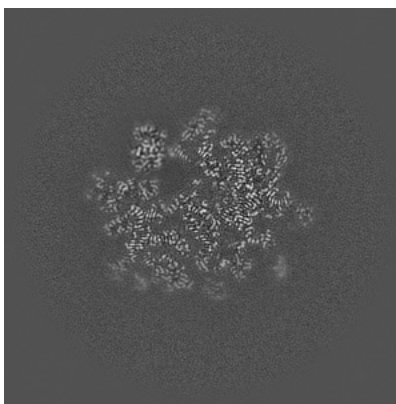
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

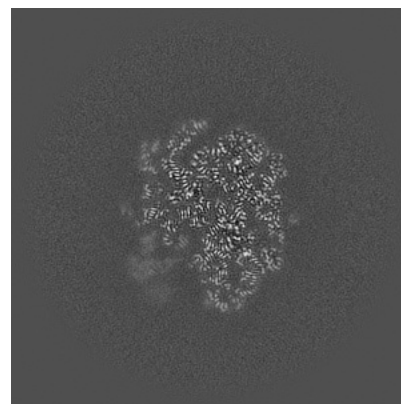
6.3.1 Primary map



X Index: 218



Y Index: 202

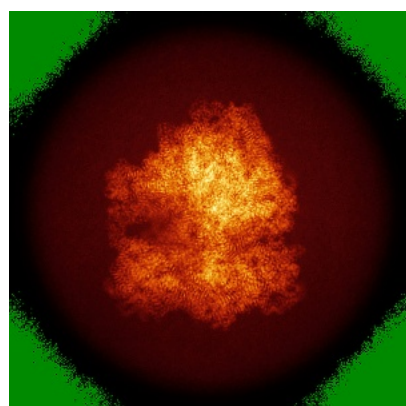


Z Index: 222

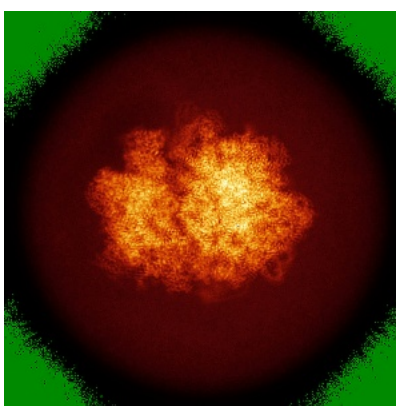
The images above show the largest variance slices of the map in three orthogonal directions.

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

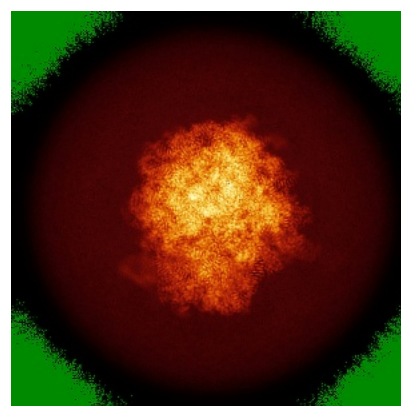
6.4.1 Primary map



X



Y

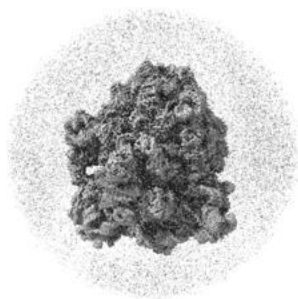


Z

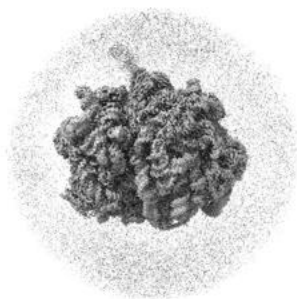
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

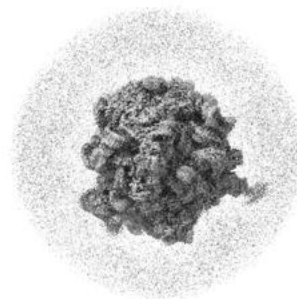
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

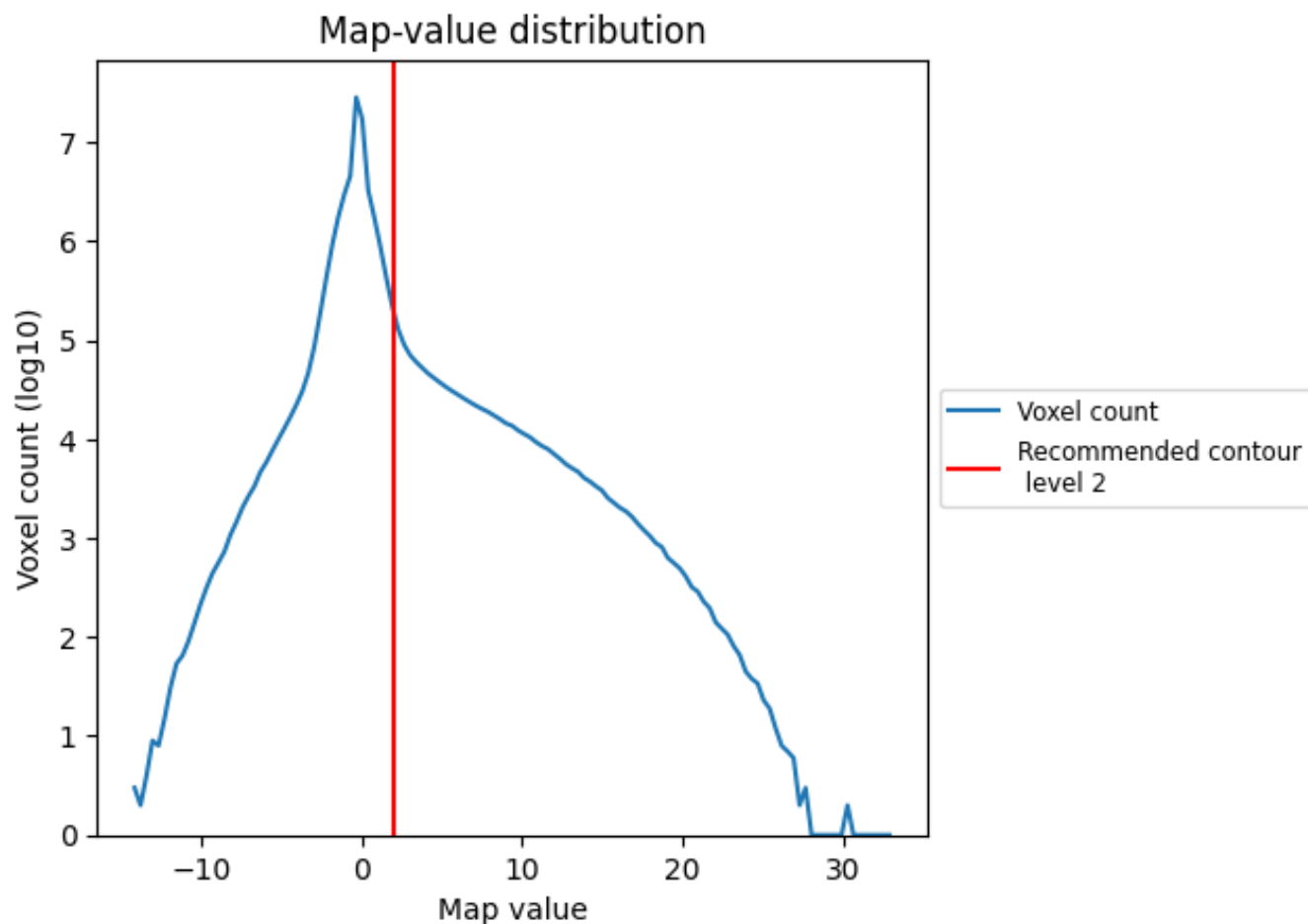
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

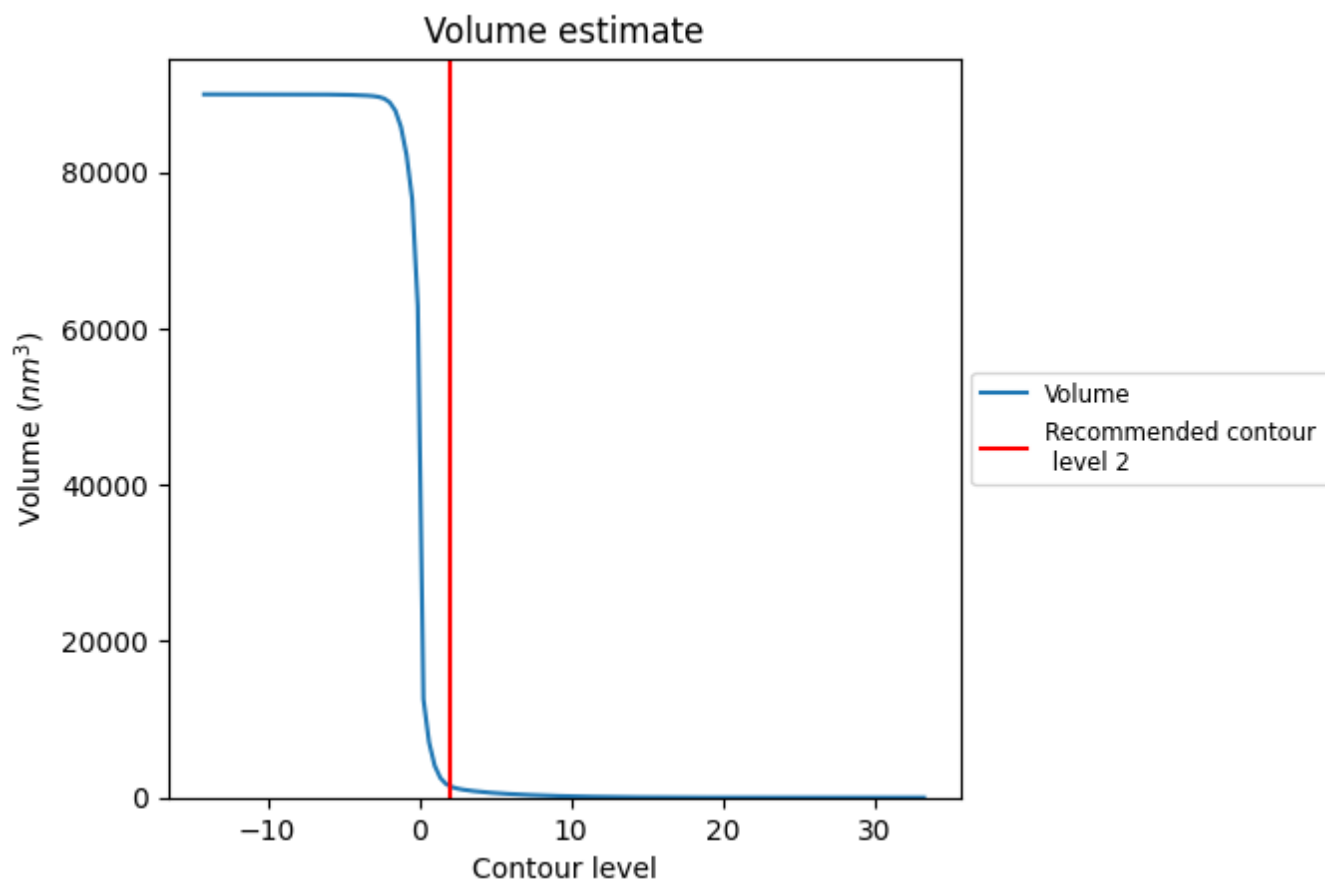
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

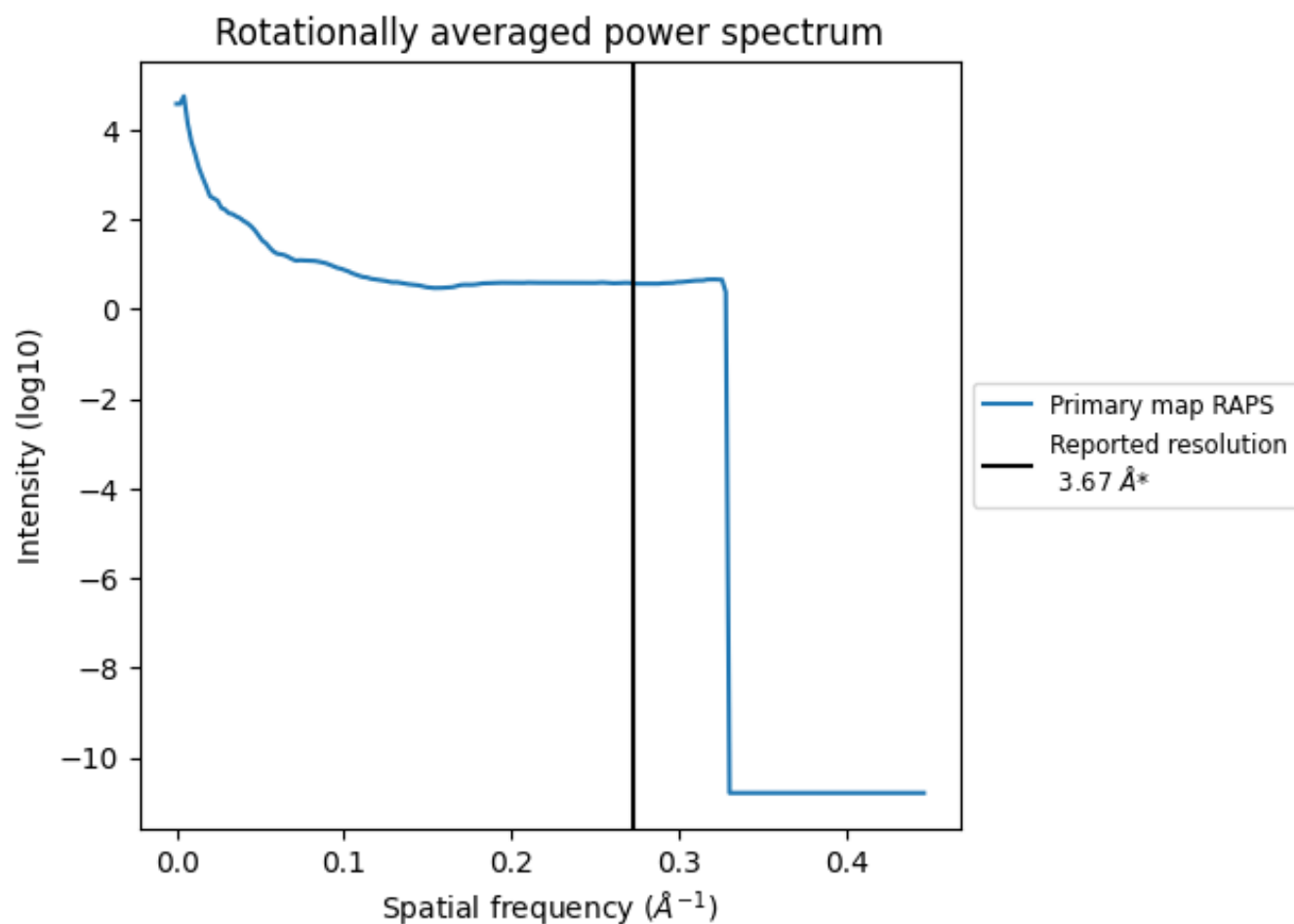
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1507 nm^3 ; this corresponds to an approximate mass of 1361 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.272 Å⁻¹

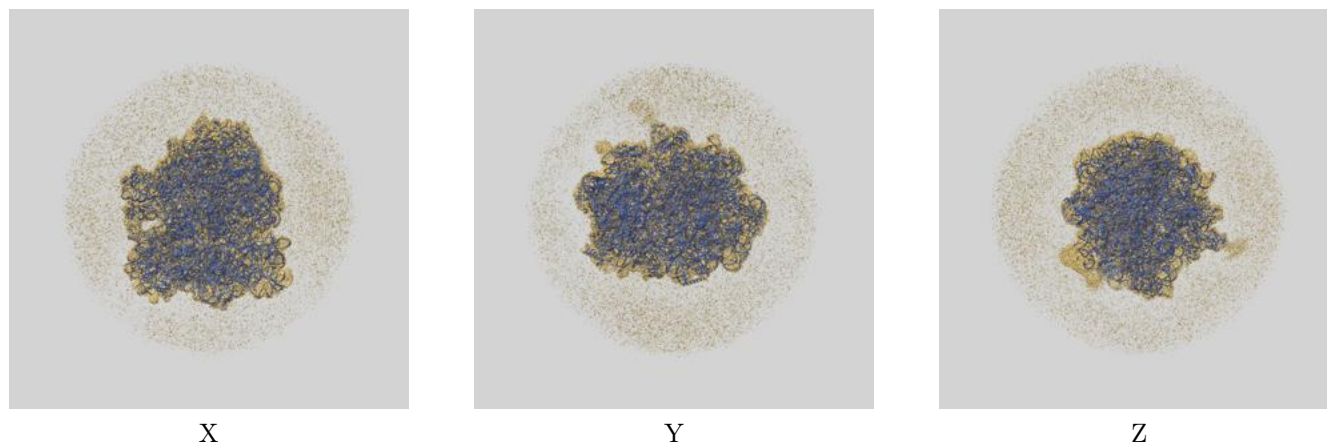
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

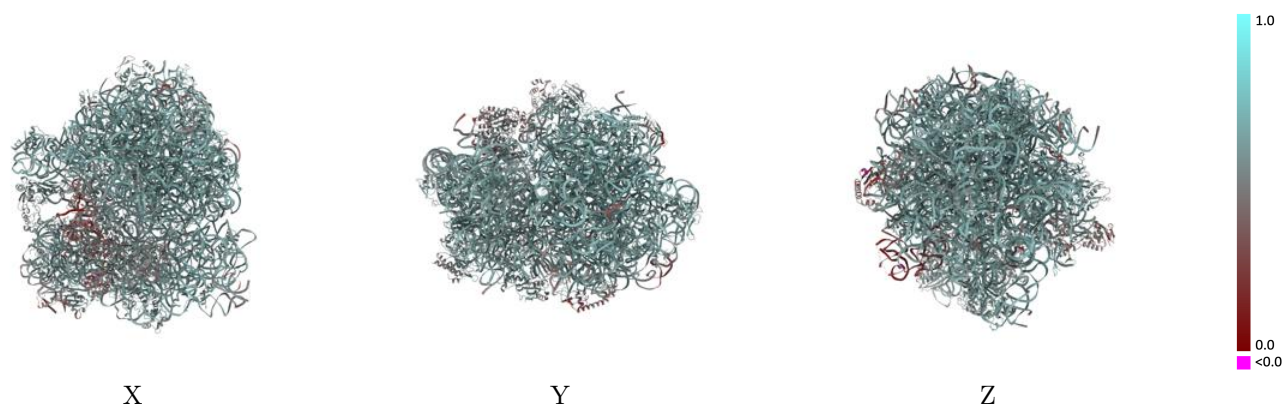
This section contains information regarding the fit between EMDB map EMD-17667 and PDB model 8PHJ. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



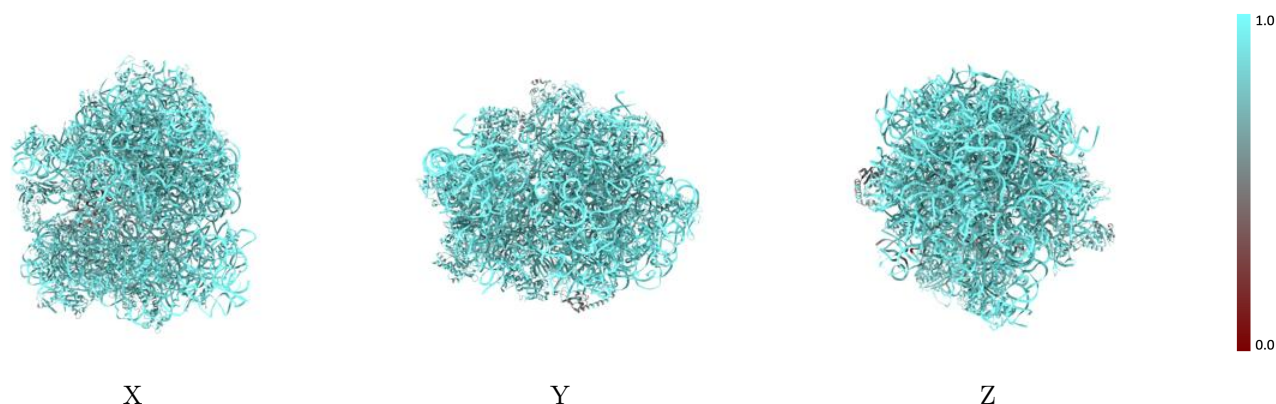
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



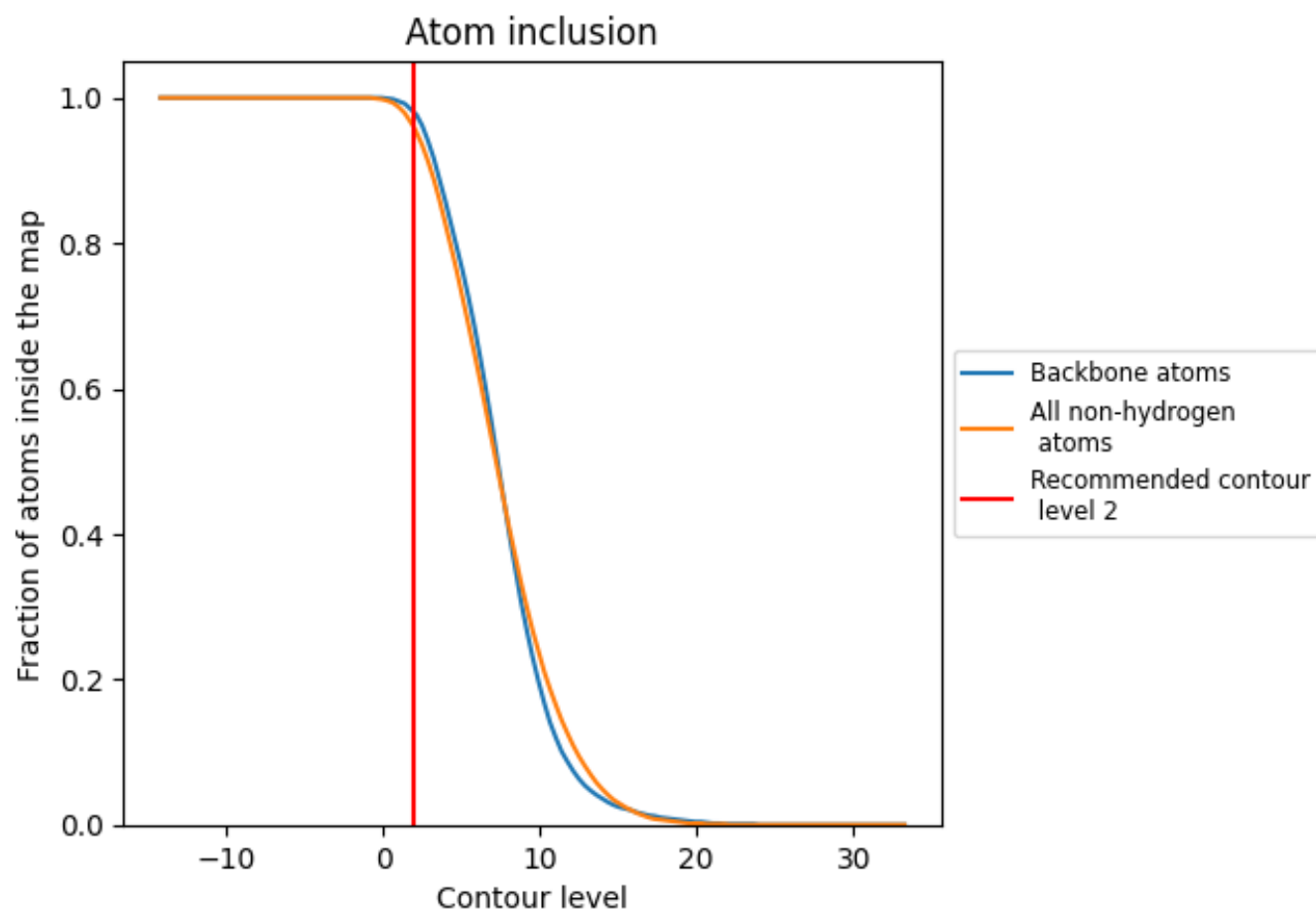
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9590	 0.5840
0	 0.9310	 0.5990
1	 0.9690	 0.6370
2	 0.9900	 0.6380
3	 0.9630	 0.6130
4	 0.8920	 0.5190
5	 0.7130	 0.3780
6	 0.7240	 0.3250
7	 0.6370	 0.4920
8	 0.7150	 0.2620
9	 0.9690	 0.6100
A	 0.9930	 0.6020
B	 0.8570	 0.5190
C	 0.9260	 0.5740
D	 0.9360	 0.5740
E	 0.9500	 0.5960
F	 0.9120	 0.5440
G	 0.8830	 0.5330
H	 0.9500	 0.5980
I	 0.9380	 0.5710
J	 0.8700	 0.5200
K	 0.9320	 0.5790
L	 0.9390	 0.6010
M	 0.9200	 0.5630
N	 0.9560	 0.5860
O	 0.9320	 0.5770
P	 0.9500	 0.5940
Q	 0.9340	 0.5770
R	 0.9320	 0.5720
S	 0.9370	 0.5720
T	 0.9470	 0.5820
U	 0.7870	 0.5150
W	 0.8450	 0.3380
X	 0.8920	 0.4820
Y	 0.9270	 0.4780



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Chain	Atom inclusion	Q-score
Z	 0.9660	 0.5170
a	 0.9880	 0.6050
b	 0.9920	 0.5990
c	 0.9700	 0.6280
d	 0.9600	 0.6160
e	 0.9470	 0.5880
f	 0.8910	 0.5390
g	 0.9230	 0.5530
h	 0.6830	 0.4230
i	 0.9660	 0.6160
j	 0.9520	 0.6170
k	 0.9670	 0.6080
l	 0.9560	 0.6220
m	 0.9810	 0.6280
n	 0.9550	 0.5820
o	 0.9390	 0.6070
p	 0.9850	 0.6330
q	 0.9510	 0.6080
r	 0.9510	 0.6130
s	 0.9280	 0.5830
t	 0.9450	 0.5810
u	 0.9400	 0.5960
v	 0.9560	 0.6200
w	 0.9670	 0.6180
x	 0.9270	 0.5570
y	 0.9440	 0.6070
z	 0.9740	 0.6220