Full wwPDB EM Validation Report ⓘ

Mar 2, 2024 – 08:13 pm GMT

PDB ID	:	8RD8
EMDB ID	:	EMD-19067
Title	:	Cryo-EM structure of P. urativorans 70S ribosome in complex with hibernation factors Balon and RaiA (structure 1).
Authors	:	Helena-Bueno, K.; Rybak, M.Y.; Gagnon, M.G.; Hill, C.H.; Melnikov, S.V.
Deposited on	:	2023-12-07
Resolution	:	2.62 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:

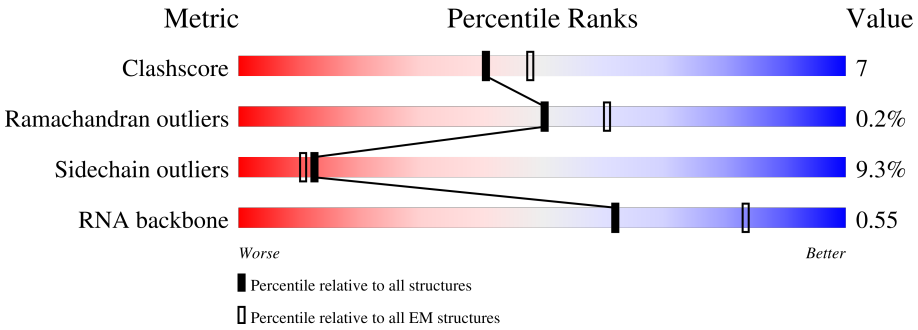
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.62 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	B	369	21% 66% 27% 5%
2	F	128	65% 62% 30% 5%
3	H	396	41% 31% 13% 54%
4	C1	166	13% 22% 8% 70%
5	Z2	2882	60% 30% 6%
6	R3	76	13% 62% 11% 26%
7	A4	269	65% 59% 23% 13%

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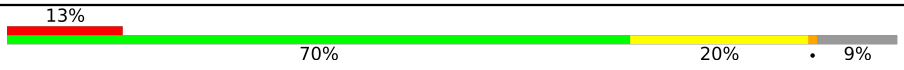
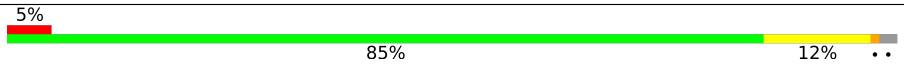
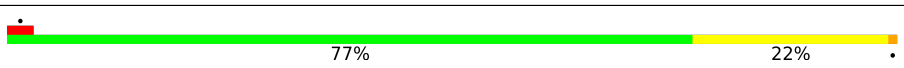
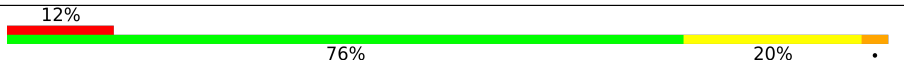
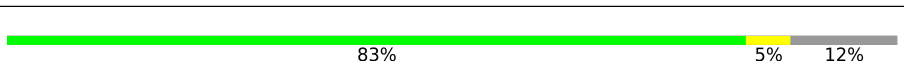
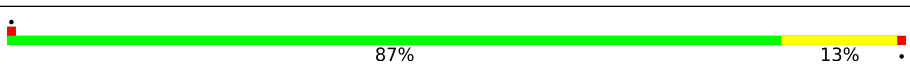
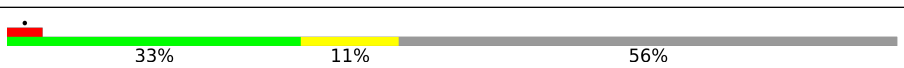
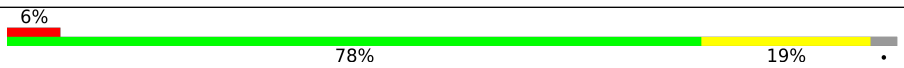
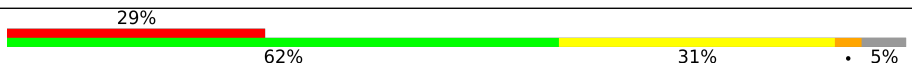
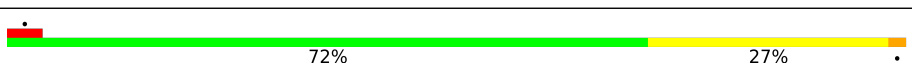
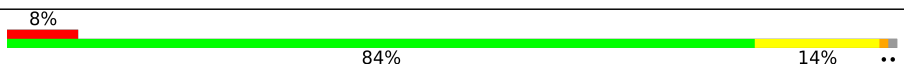
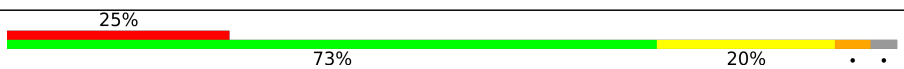
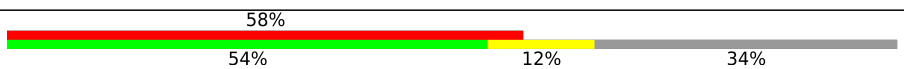
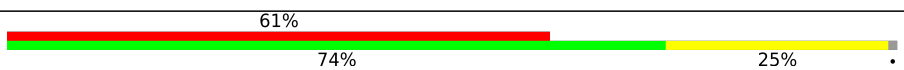
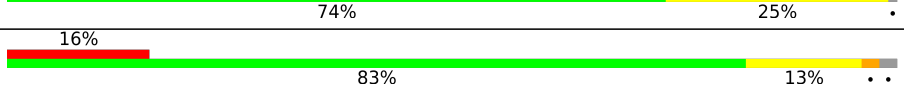
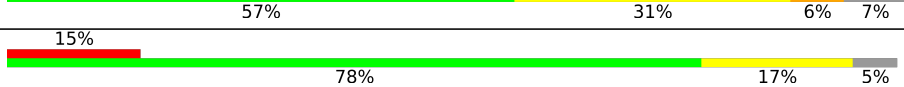
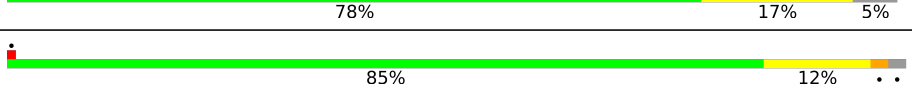
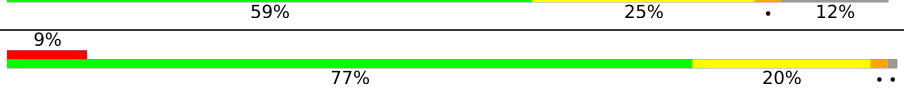
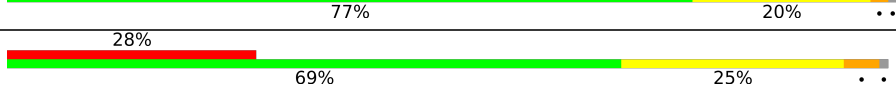
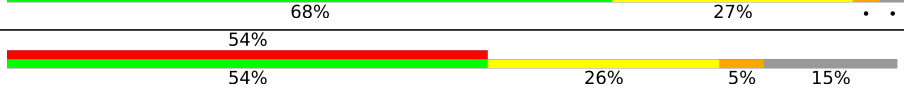
Mol	Chain	Length	Quality of chain
8	E5	171	
9	L6	124	
10	F7	178	
11	D8	115	
12	E9	200	
13	aA	60	
14	MB	119	
15	UC	219	
16	WD	78	
17	XE	65	
18	RF	109	
19	FG	134	
20	VH	85	
21	TI	105	
22	fJ	93	
23	HK	101	
24	OL	88	
25	MM	118	
26	iN	1590	
27	PO	118	
28	SP	91	
29	BQ	132	
30	GR	177	
31	GS	157	
32	CT	241	

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Mol	Chain	Length	Quality of chain
33	KU	129	29% 57% 27% 5% 12%
34	NV	71	41% 61% 18% 20%
35	YW	59	76% 15% 5%
36	IX	142	82% 15%
37	JY	103	68% 55% 32% 8%
38	QZ	91	20% 55% 27% 13%
39	Ba	44	91% 9%
40	Qb	103	10% 87% 13%
41	Nc	116	12% 97%
42	Kd	146	95%
43	Je	122	98%
44	Af	212	92% 7%
45	Lg	137	93% 7%
46	dh	65	92% 6%
47	Oi	130	84% 5% 12%
48	Pj	89	20% 89% 9%
49	bk	51	86% 10%
50	Cl	274	96%
51	Dm	213	47% 96%
52	Sn	116	6% 68% 8% 24%
53	To	88	25% 98%
54	ep	38	97%
55	D	126	30% 61% 20% 17%

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 141222 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 Methyl-accepting chemotaxis protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	360	2812	1748	495	560	9	0	0

- Molecule 2 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	125	974	607	190	176	1	0	0

- Molecule 3 is a protein called Elongation factor Tu.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	184	1404	876	251	269	8	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C1	49	374	244	64	65	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	Z2	2705	58043	25910	10660	18768	2705	0	0

- Molecule 6 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	R3	56	457	290	80	87	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A4	233	Total	C	N	O	S	0	0
			1816	1147	327	335	7		

- Molecule 8 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E5	156	Total	C	N	O	S	0	0
			1151	716	218	211	6		

- Molecule 9 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L6	122	Total	C	N	O	S	0	0
			946	583	193	165	5		

- Molecule 10 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F7	177	Total	C	N	O	S	0	0
			1362	873	237	246	6		

- Molecule 11 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D8	115	Total	C	N	O	P	0	0
			2446	1093	436	802	115		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D8	85	U	-	variant	GB 930356181
D8	88	A	C	variant	GB 930356181

- Molecule 12 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E9	199	Total	C	N	O	S	0	0
			1537	966	282	284	5		

- Molecule 13 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	aA	53	Total	C	N	O	S	0	0
			442	264	100	75	3		

- Molecule 14 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	MB	119	Total	C	N	O	S	0	0
			947	587	188	164	8		

- Molecule 15 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	UC	97	Total	C	N	O	S	0	0
			760	485	138	136	1		

- Molecule 16 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	WD	76	Total	C	N	O	S	0	0
			618	383	131	101	3		

- Molecule 17 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	XE	62	Total	C	N	O	S	0	0
			502	307	99	95	1		

- Molecule 18 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	RF	109	Total	C	N	O	S	0	0
			834	521	159	151	3		

- Molecule 19 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	FG	102	Total	C	N	O	S	0	0
			849	535	154	158	2		

- Molecule 20 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	VH	84	Total 626	C 389	N 124	O 110	S 3	0	0

- Molecule 21 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	TI	102	Total 784	C 487	N 149	O 148	0	0

- Molecule 22 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	fJ	61	Total 493	C 313	N 85	O 94	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	HK	100	Total 811	C 498	N 162	O 144	S 7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	OL	86	Total 694	C 427	N 137	O 128	S 2	0	0

- Molecule 25 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	MM	110	Total 858	C 528	N 172	O 155	S 3	0	0

- Molecule 26 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	iN	1503	Total 32246	C 14388	N 5917	O 10438	P 1503	0	0

- Molecule 27 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	PO	116	Total	C	N	O	S	0	0
			935	586	199	148	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SP	80	Total	C	N	O	S	0	0
			637	405	121	108	3		

- Molecule 29 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BQ	131	Total	C	N	O	S	0	0
			974	602	179	187	6		

- Molecule 30 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	GR	175	Total	C	N	O	S	0	0
			1357	848	248	259	2		

- Molecule 31 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	GS	152	Total	C	N	O	S	0	0
			1190	738	230	215	7		

- Molecule 32 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	CT	204	Total	C	N	O	S	0	0
			1609	1011	301	290	7		

- Molecule 33 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	KU	114	Total	C	N	O	S	0	0
			836	518	162	155	1		

- Molecule 34 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	NV	57	Total	C	N	O	S	0	0
			472	299	95	77	1		

- Molecule 35 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	YW	56	Total	C	N	O	S	0	0
			438	272	88	76	2		

- Molecule 36 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	IX	142	Total	C	N	O	S	0	0
			1108	710	198	197	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	JY	99	Total	C	N	O	S	0	0
			784	487	149	145	3		

- Molecule 38 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	QZ	79	Total	C	N	O	S	0	0
			632	395	119	116	2		

- Molecule 39 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ba	44	Total	C	N	O	S	0	0
			369	227	89	51	2		

- Molecule 40 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Qb	103	Total	C	N	O	S	0	0
			827	524	153	148	2		

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	Nc	113	Total 852	C 530	N 170	O 152	0	0

- Molecule 42 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Kd	144	Total 1062	C 656	N 206	O 197	S 3	1	0

- Molecule 43 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Je	122	Total 937	C 585	N 181	O 166	S 5	0	0

- Molecule 44 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Af	211	Total 1548	C 954	N 292	O 296	S 6	0	0

- Molecule 45 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lg	137	Total 1093	C 697	N 210	O 179	S 7	0	0

- Molecule 46 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	dh	64	Total 519	C 326	N 107	O 82	S 4	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
47	Oi	115	Total 917	C 572	N 184	O 161	0	0

- Molecule 48 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Pj	81	Total	C	N	O	S	0	0
			648	409	126	111	2		

- Molecule 49 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	bk	49	Total	C	N	O	S	0	0
			394	254	68	69	3		

- Molecule 50 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Cl	272	Total	C	N	O	S	0	0
			2107	1305	432	364	6		

- Molecule 51 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Dm	212	Total	C	N	O	S	0	0
			1688	1058	318	309	3		

- Molecule 52 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Sn	88	Total	C	N	O	S	0	0
			698	446	126	124	2		

- Molecule 53 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	To	86	Total	C	N	O	S	0	0
			675	410	144	119	2		

- Molecule 54 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	ep	38	Total	C	N	O	S	0	0
			298	182	66	46	4		

- Molecule 55 is a protein called 30S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	D	105	Total	C	N	O	S	0	0
			830	509	155	160	6		

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

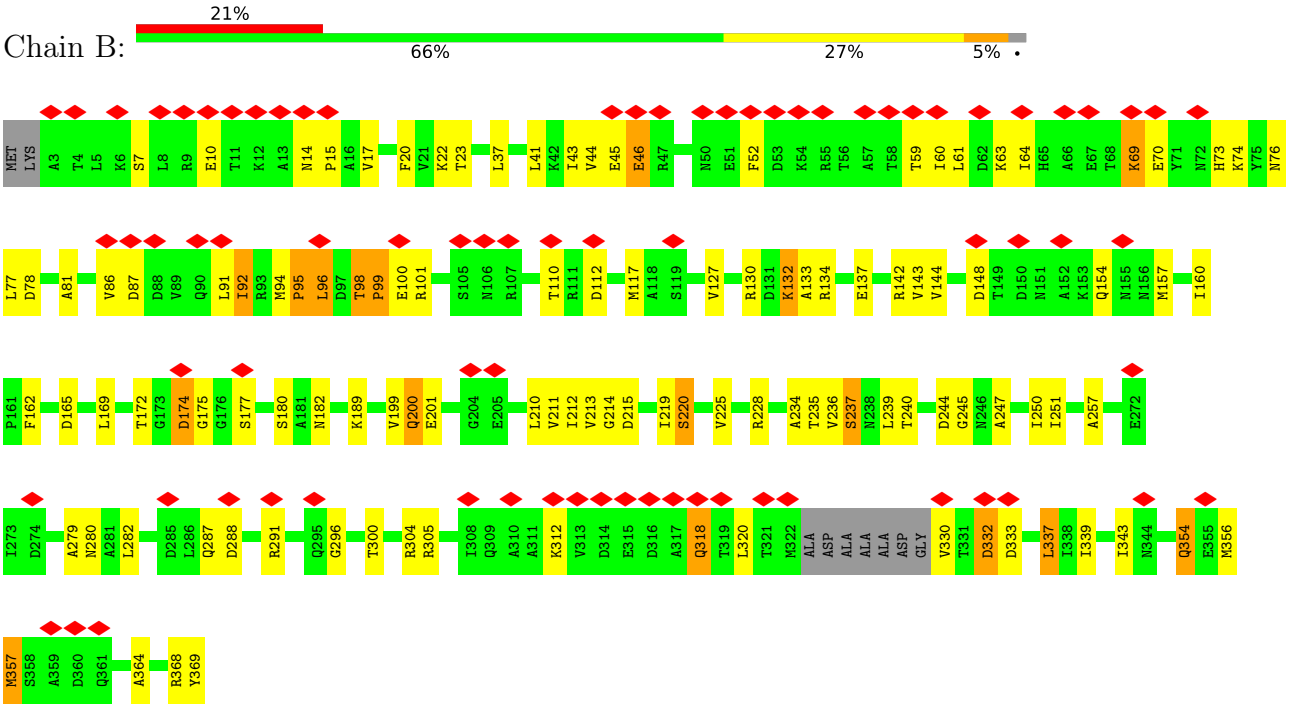
Mol	Chain	Residues	Atoms		AltConf
56	Z2	2	Total	Mg	0
			2	2	

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.

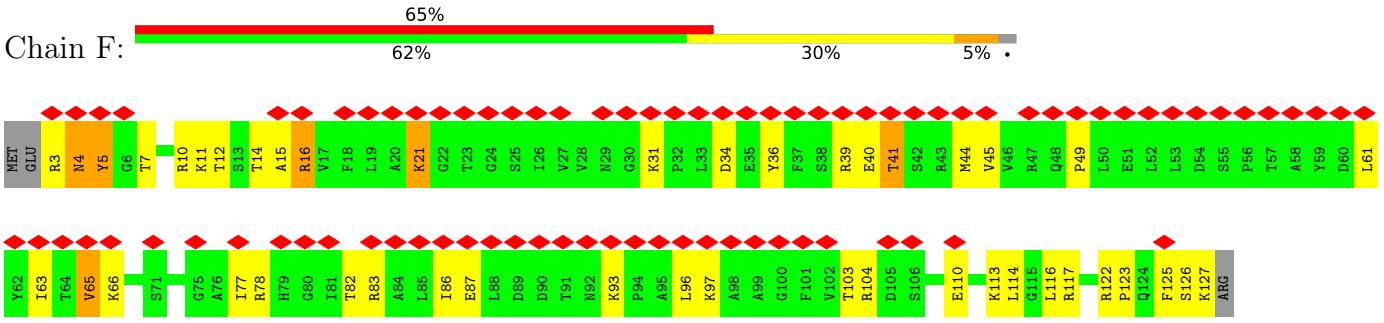
• Molecule 1: Methyl-accepting chemotaxis protein

Chain B:



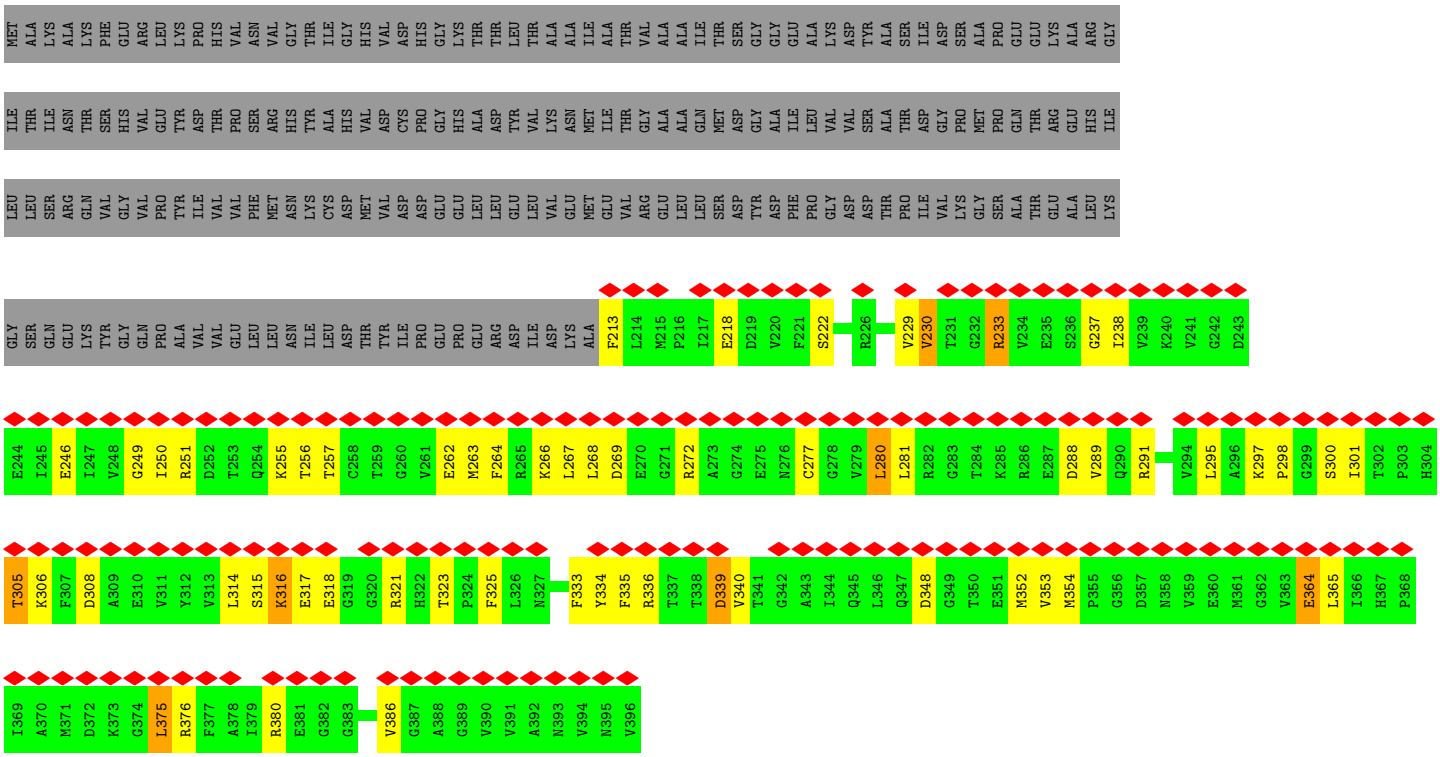
• Molecule 2: Small ribosomal subunit protein uS9

Chain F:



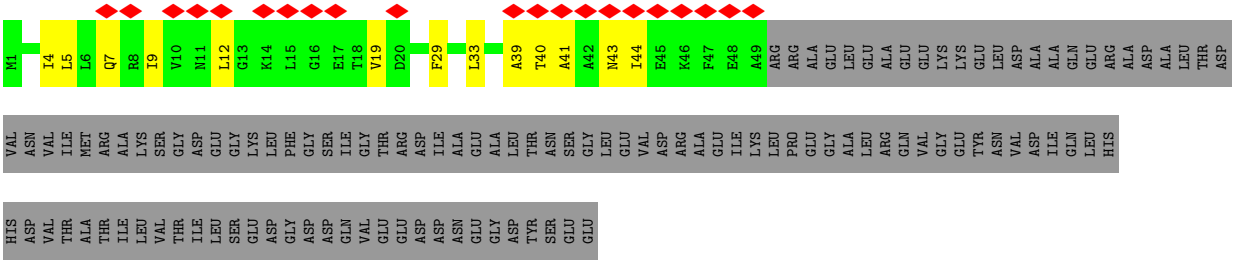
• Molecule 3: Elongation factor Tu

Chain H:



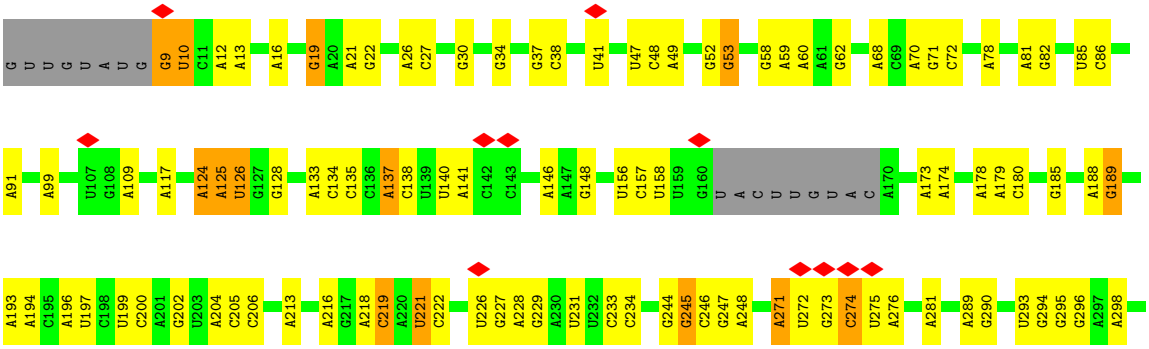
• Molecule 4: Large ribosomal subunit protein bL9

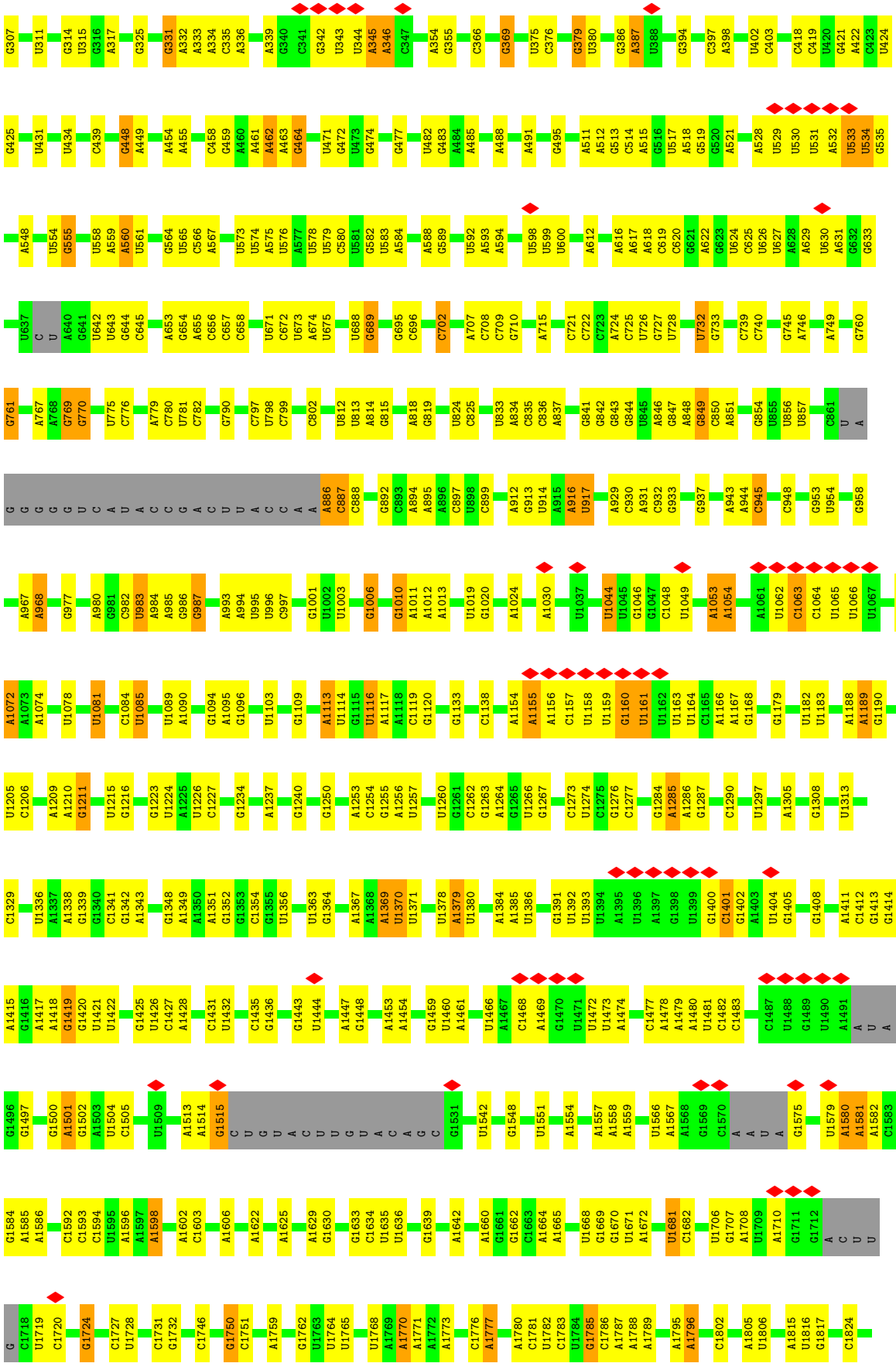
Chain C1:

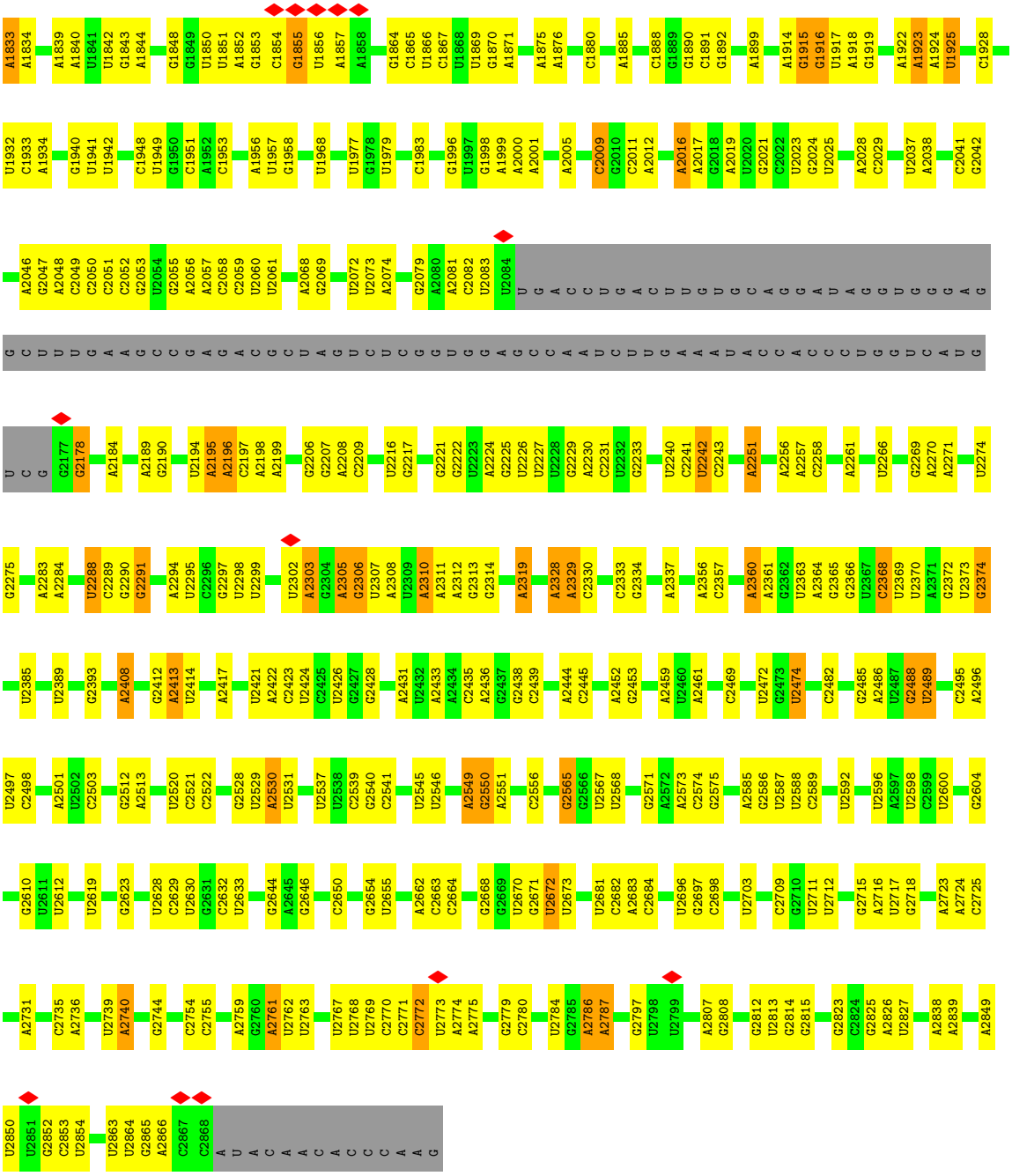


• Molecule 5: 23S rRNA

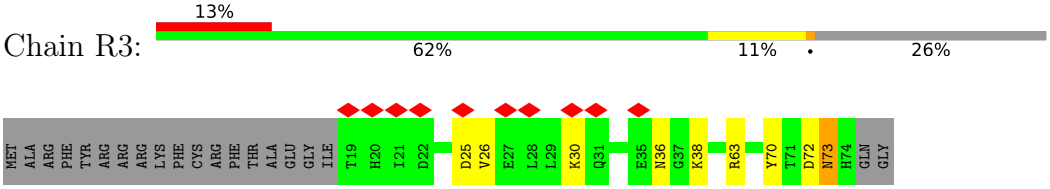
Chain Z2:



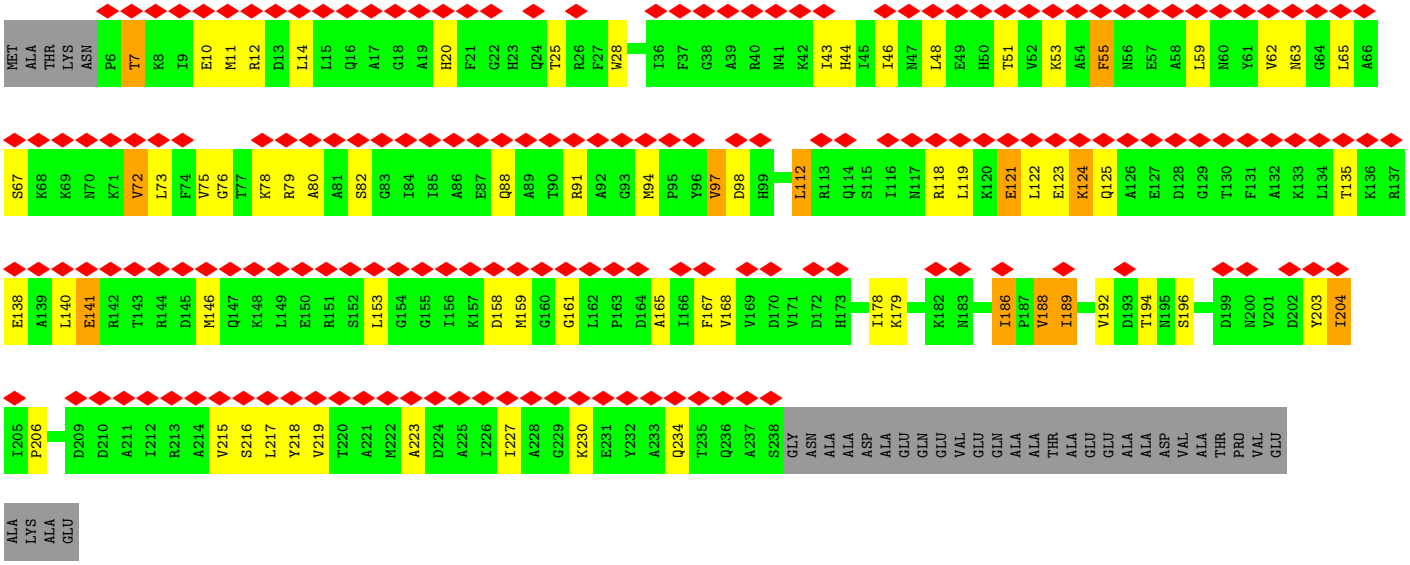




• Molecule 6: Small ribosomal subunit protein bS18

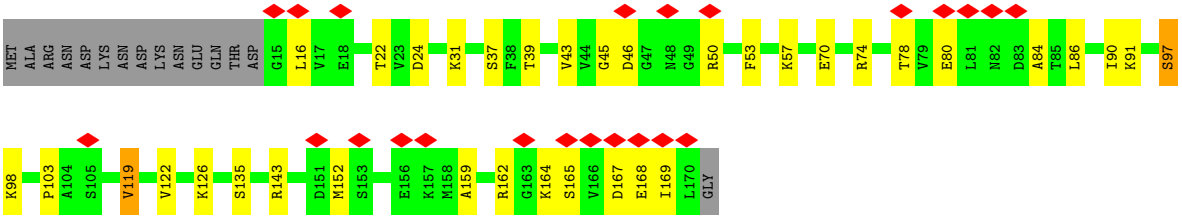


• Molecule 7: Small ribosomal subunit protein uS2



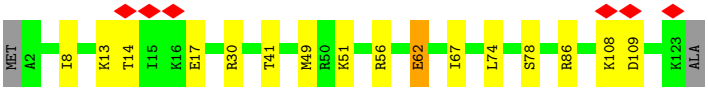
• Molecule 8: Small ribosomal subunit protein uS5

Chain E5:



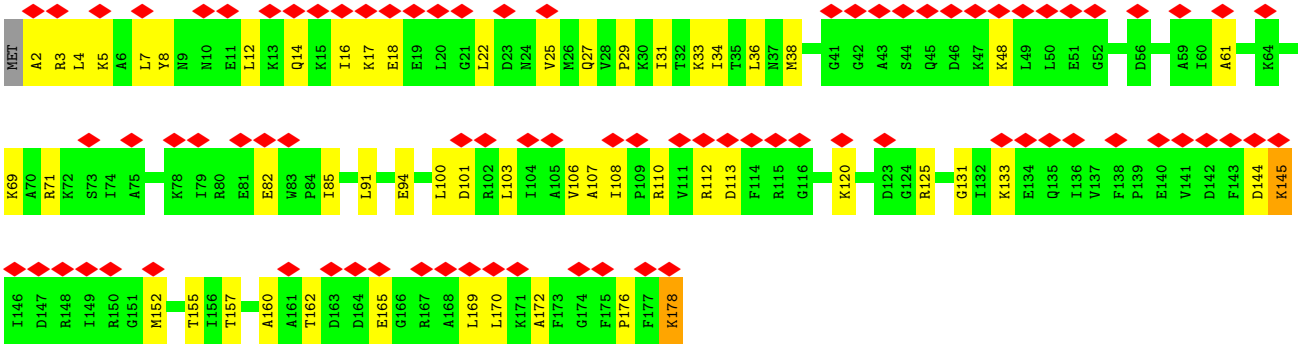
• Molecule 9: Small ribosomal subunit protein uS12

Chain L6:



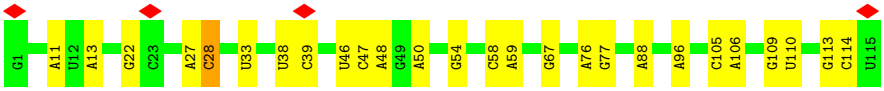
• Molecule 10: Large ribosomal subunit protein uL5

Chain F7:



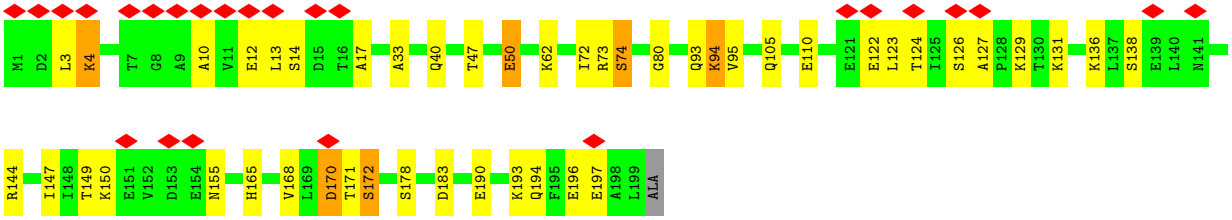
• Molecule 11: 5S rRNA

Chain D8:



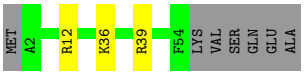
• Molecule 12: Large ribosomal subunit protein uL4

Chain E9:



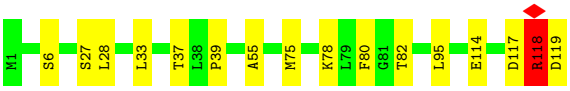
• Molecule 13: Large ribosomal subunit protein bL32

Chain aA:



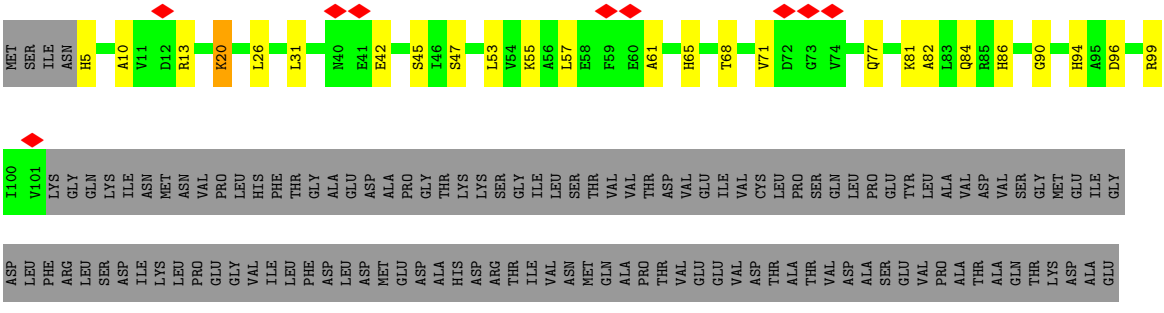
• Molecule 14: Large ribosomal subunit protein bL17

Chain MB:



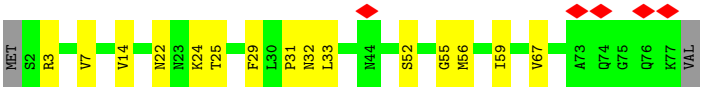
• Molecule 15: Large ribosomal subunit protein bL25

Chain UC:



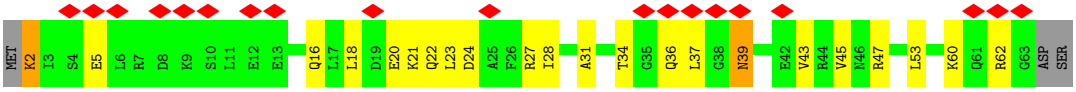
• Molecule 16: Large ribosomal subunit protein bL28

Chain WD:



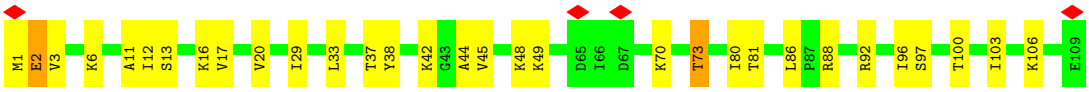
• Molecule 17: Large ribosomal subunit protein uL29

Chain XE:



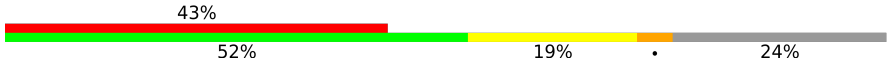
• Molecule 18: Large ribosomal subunit protein uL22

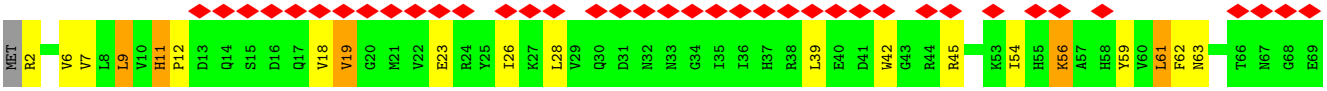
Chain RF:

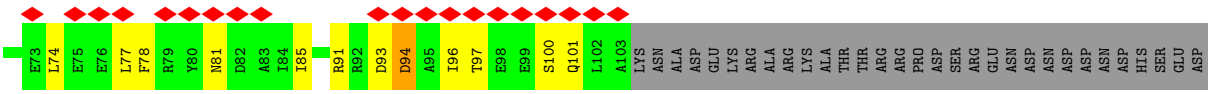


• Molecule 19: Small ribosomal subunit protein bS6

Chain FG:

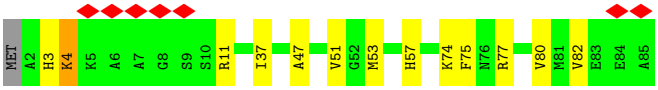






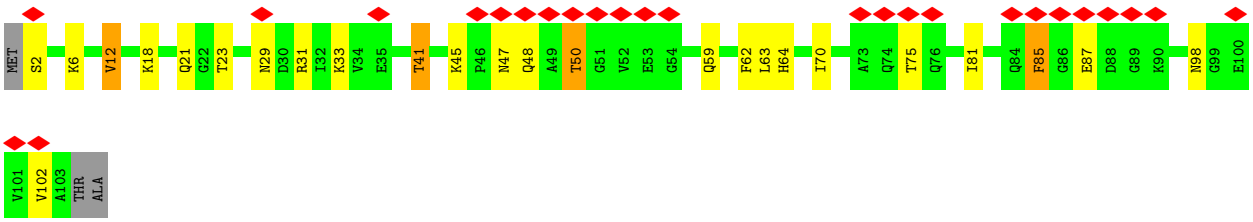
• Molecule 20: Large ribosomal subunit protein bL27

Chain VH:



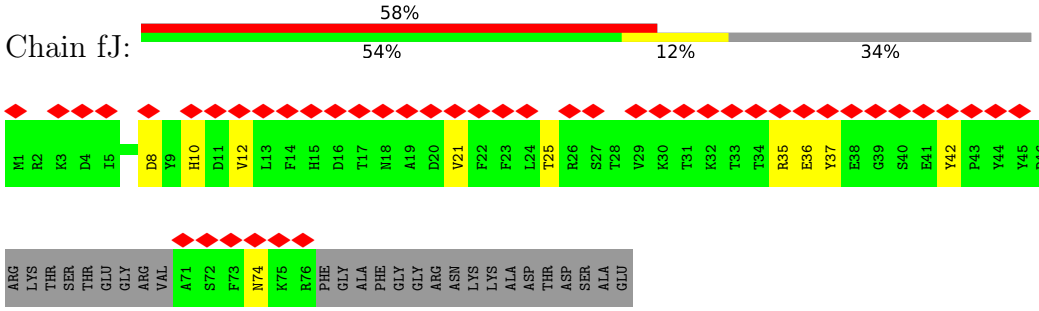
• Molecule 21: Large ribosomal subunit protein uL24

Chain TI:



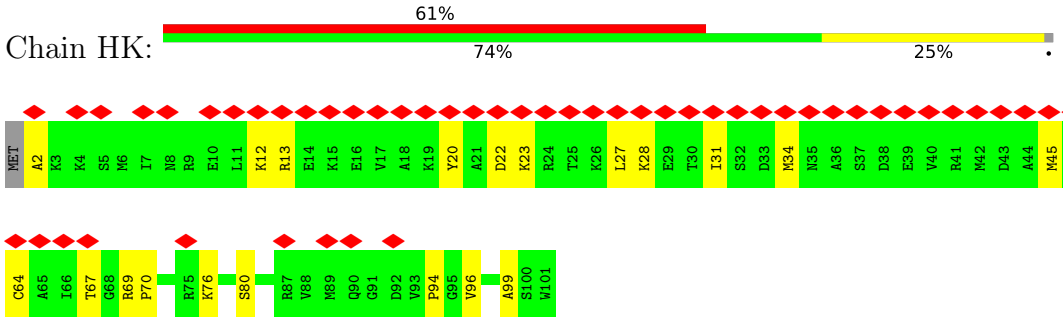
• Molecule 22: Large ribosomal subunit protein bL31B

Chain fJ:



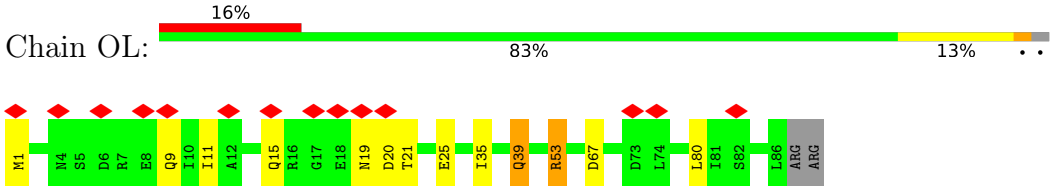
• Molecule 23: Small ribosomal subunit protein uS14

Chain HK:



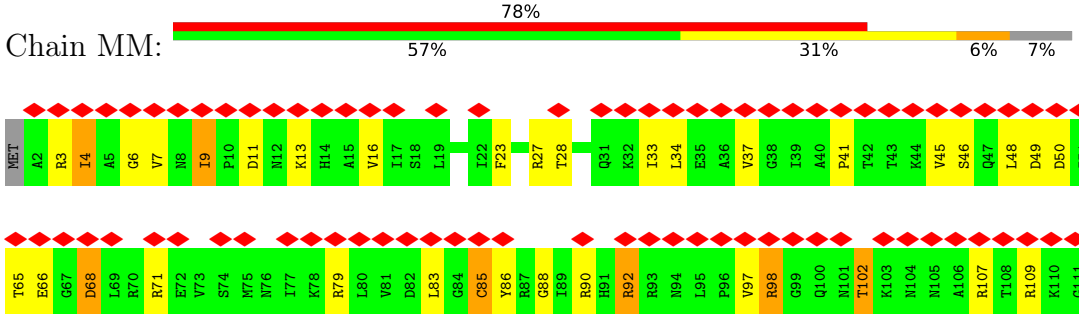
• Molecule 24: Small ribosomal subunit protein uS15

Chain OL:



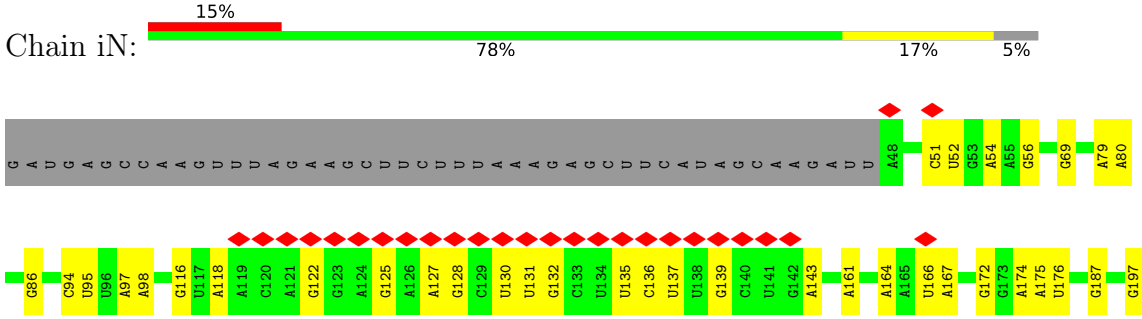
• Molecule 25: Small ribosomal subunit protein uS13

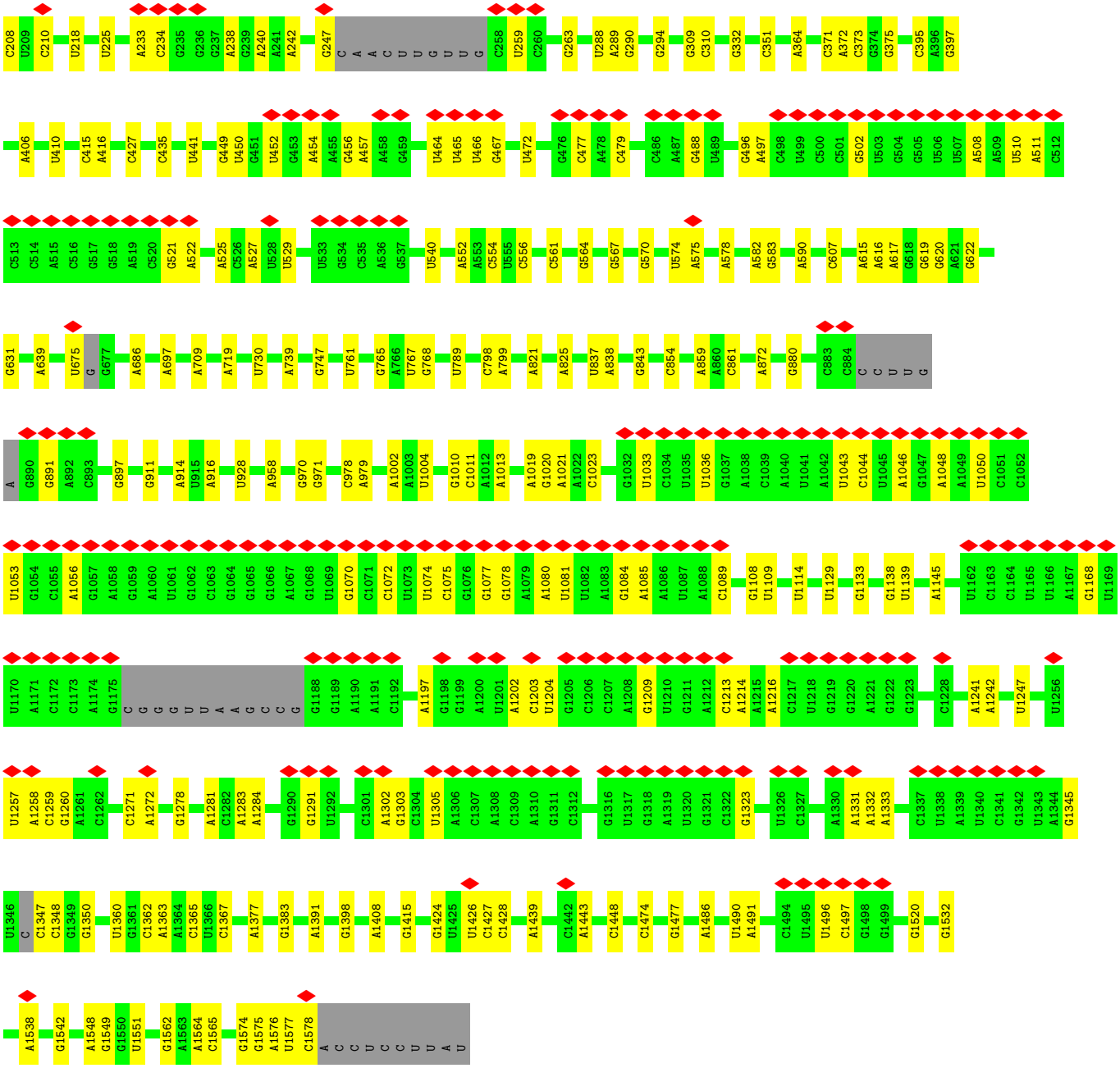
Chain MM:



• Molecule 26: 16S rRNA

Chain iN:



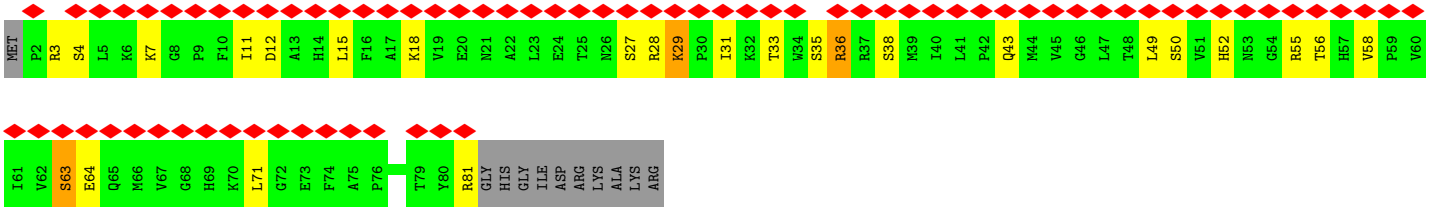


• Molecule 27: Large ribosomal subunit protein bL20

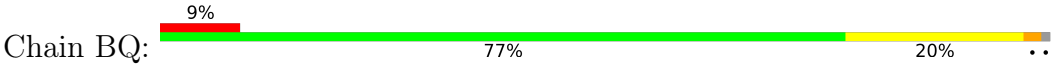
Chain PO:

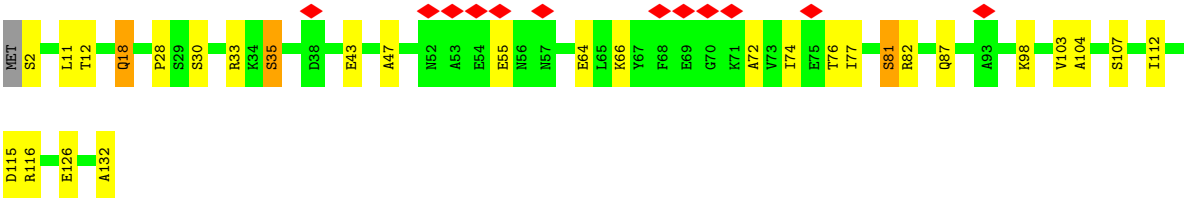
• Molecule 28: Small ribosomal subunit protein uS19

Chain SP:

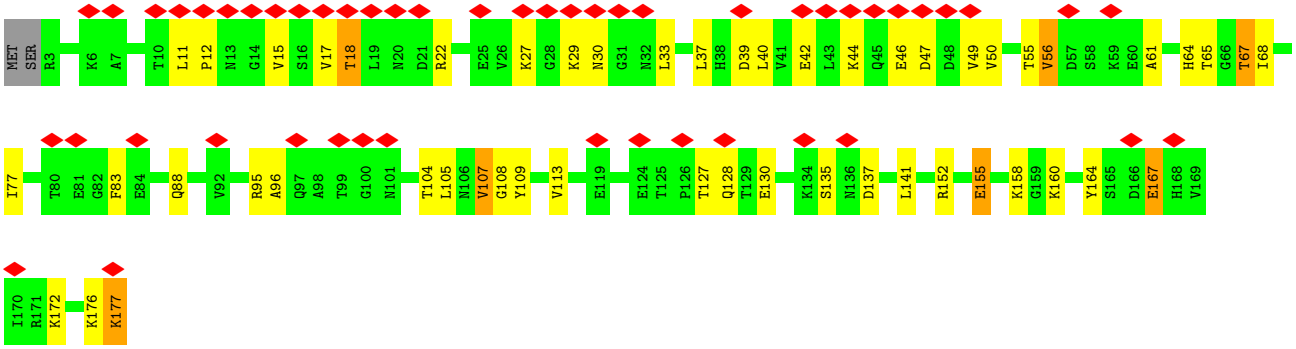


• Molecule 29: Small ribosomal subunit protein uS8

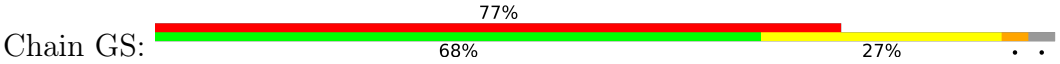


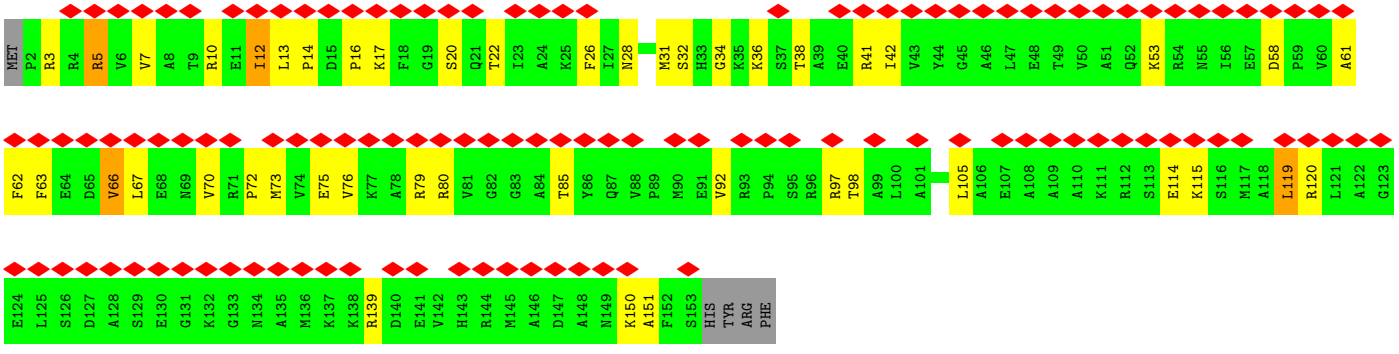


• Molecule 30: Large ribosomal subunit protein uL6



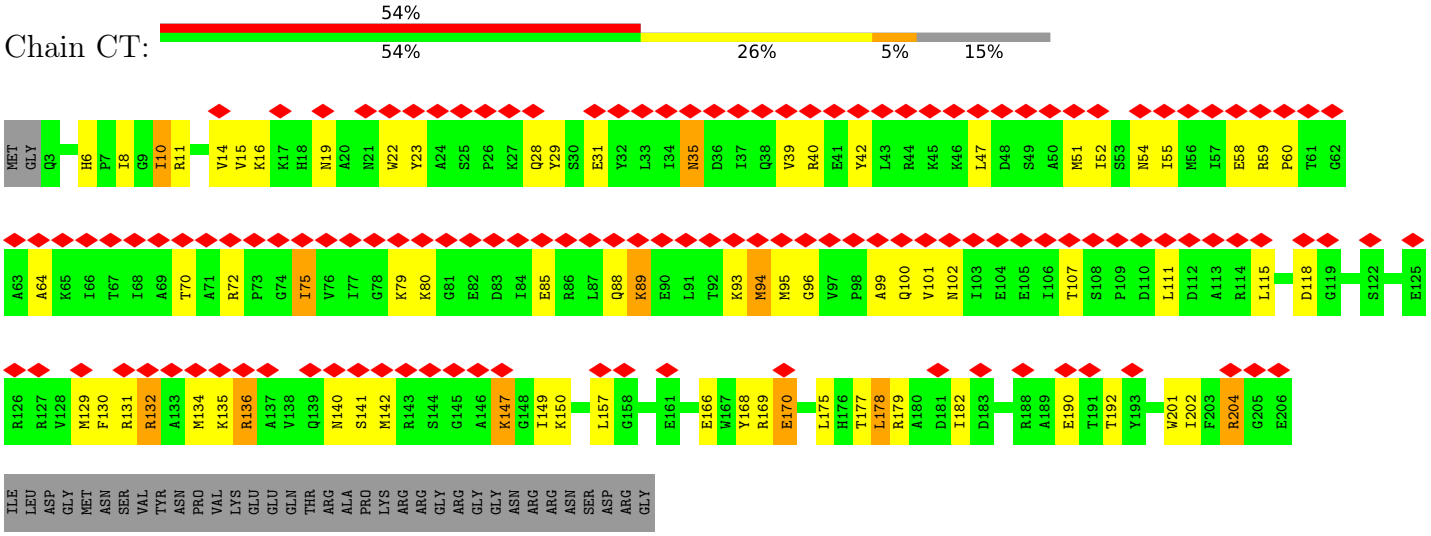
• Molecule 31: Small ribosomal subunit protein uS7





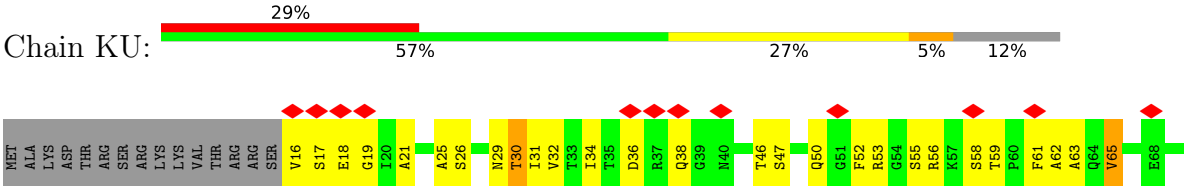
• Molecule 32: Small ribosomal subunit protein uS3

Chain CT:



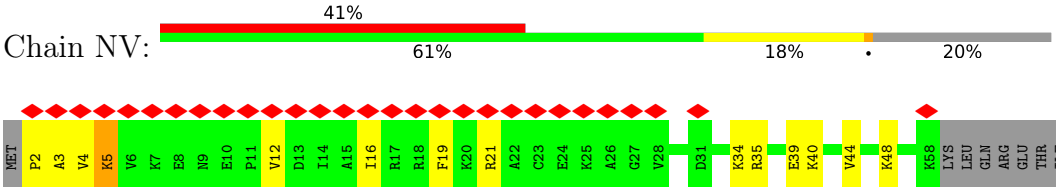
• Molecule 33: Small ribosomal subunit protein uS11

Chain KU:



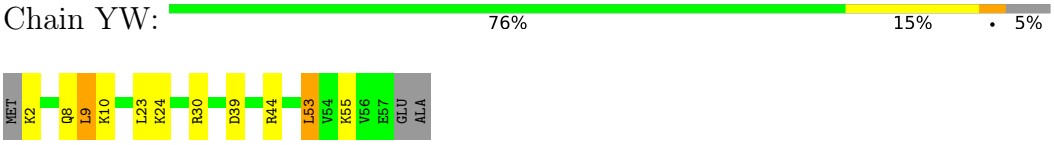
• Molecule 34: Small ribosomal subunit protein bS21

Chain NV:



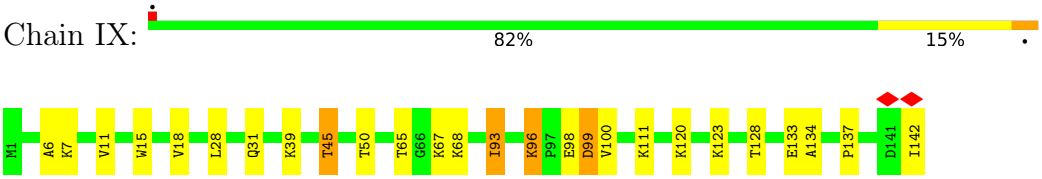
• Molecule 35: Large ribosomal subunit protein uL30

Chain YW:



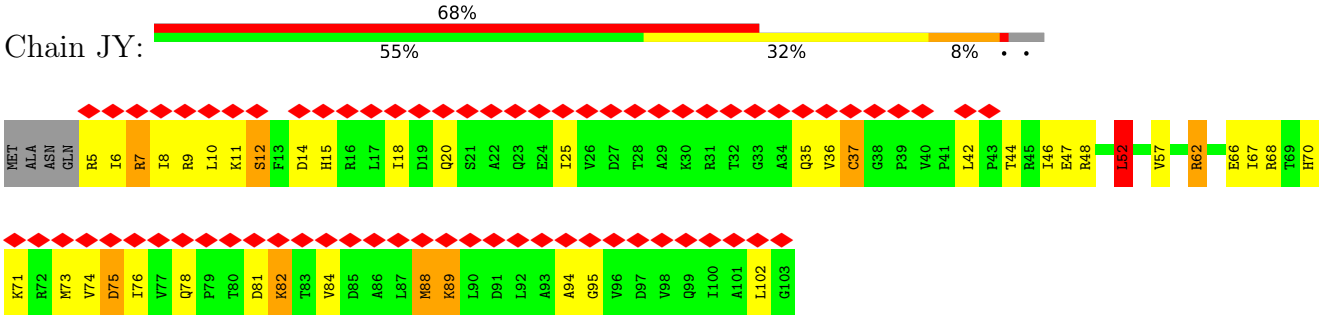
• Molecule 36: Large ribosomal subunit protein uL13

Chain IX:



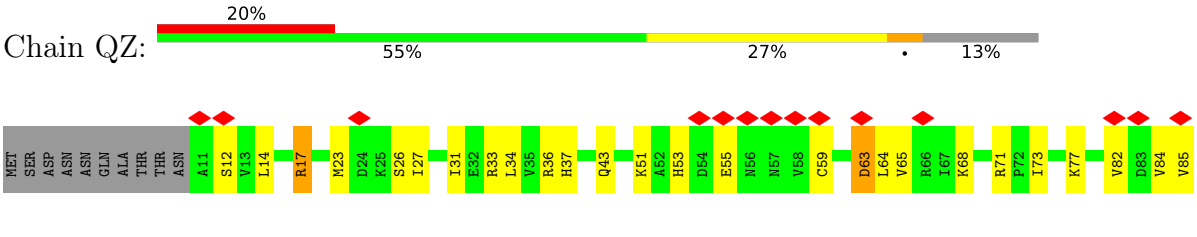
• Molecule 37: Small ribosomal subunit protein uS10

Chain JY:



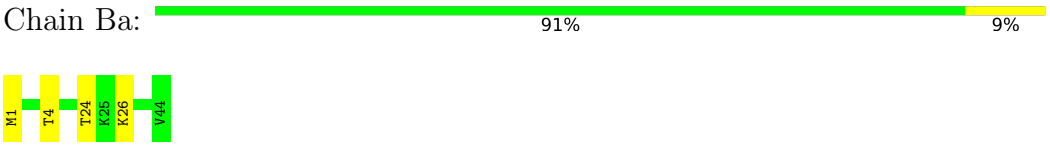
• Molecule 38: Small ribosomal subunit protein uS17

Chain QZ:



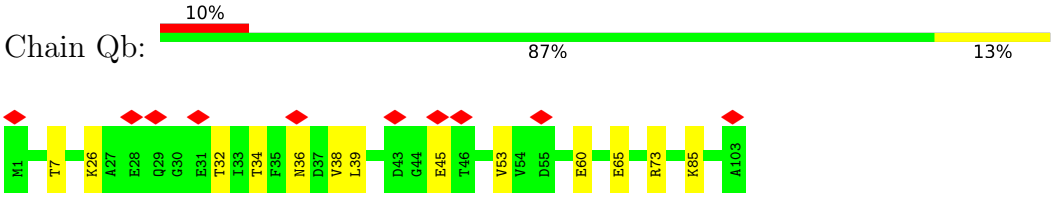
• Molecule 39: Large ribosomal subunit protein bL34

Chain Ba:



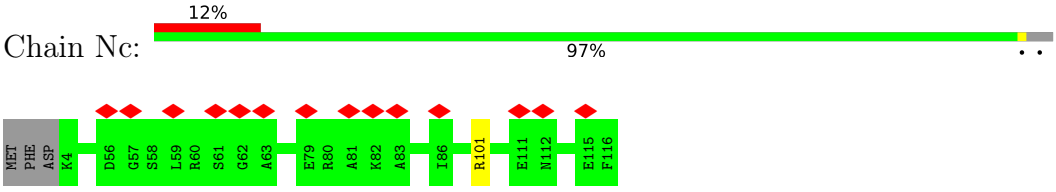
• Molecule 40: Large ribosomal subunit protein bL21

Chain Qb:



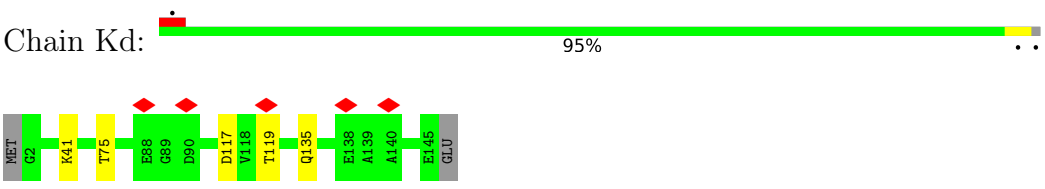
• Molecule 41: Large ribosomal subunit protein uL18

Chain Nc:



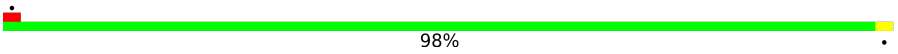
• Molecule 42: Large ribosomal subunit protein uL15

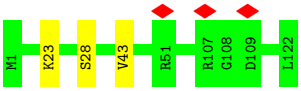
Chain Kd:



• Molecule 43: Large ribosomal subunit protein uL14

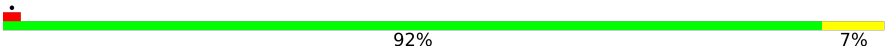
Chain Je:

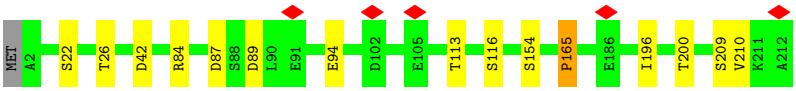




• Molecule 44: Large ribosomal subunit protein uL3

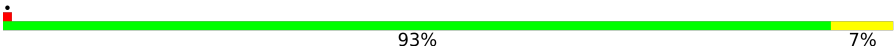
Chain Af:





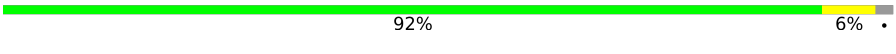
• Molecule 45: Large ribosomal subunit protein uL16

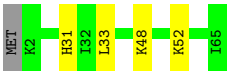
Chain Lg:



• Molecule 46: Large ribosomal subunit protein bL35

Chain dh:



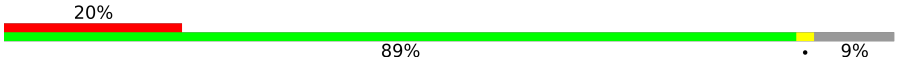


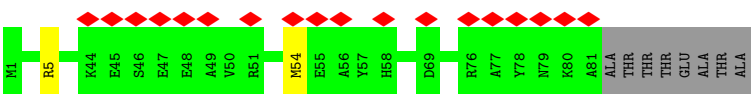
• Molecule 47: Large ribosomal subunit protein bL19

Chain Oi:

• Molecule 48: Small ribosomal subunit protein bS16

Chain Pj:



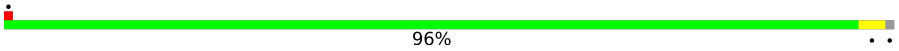


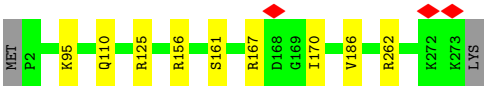
• Molecule 49: Large ribosomal subunit protein bL33

Chain bk:

• Molecule 50: Large ribosomal subunit protein uL2

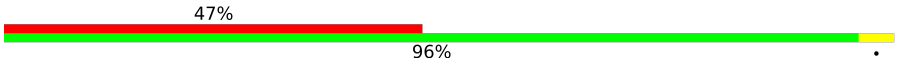
Chain Cl:

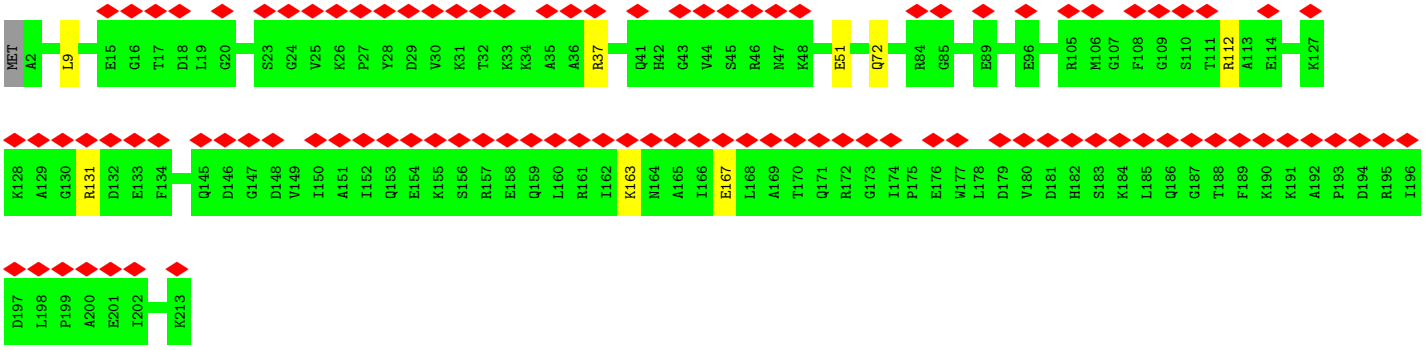




• Molecule 51: Small ribosomal subunit protein uS4

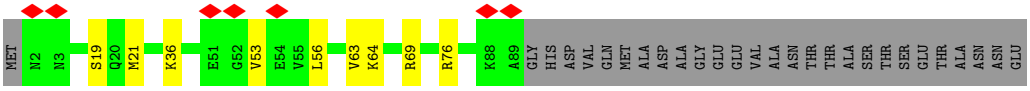
Chain Dm:





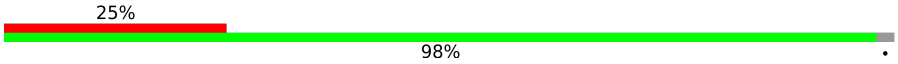
• Molecule 52: Large ribosomal subunit protein uL23

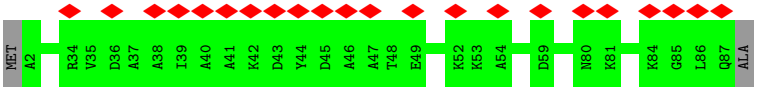
Chain Sn:



• Molecule 53: Small ribosomal subunit protein bS20

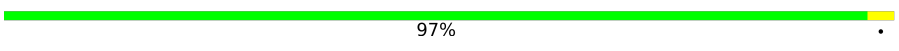
Chain To:





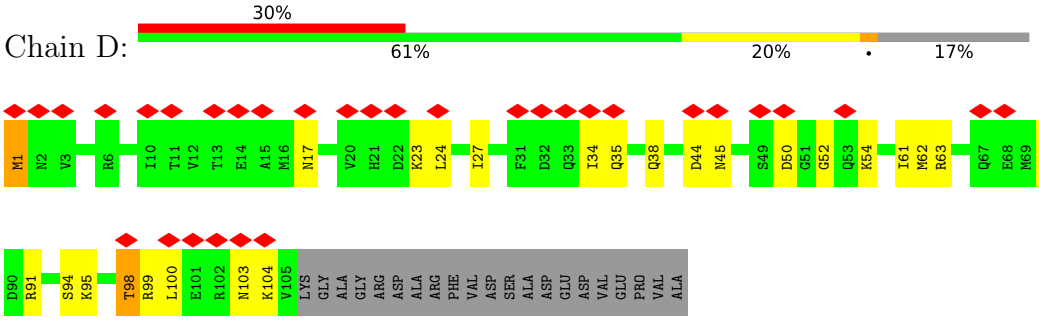
• Molecule 54: Large ribosomal subunit protein bL36

Chain ep:



• Molecule 55: 30S ribosomal protein S30

Chain D:


30%
61%
20%
17%
M1 N2 V3 R6 I10 T11 V12 T13 E14 A15 M16 N17 V20 H21 D22 K23 L24 I27 F31 D32 Q33 I34 Q35 Q38 D44 N45 S49 D50 Q51 G52 Q53 K54 I61 M62 R63 Q67 E68 M69 F70 E75 D76 D77 M78 Y79 K80 D87 K88 L89
D90 R91 S94 K95 T98 R99 L100 E101 R102 N103 K104 V105 LYS GLY ALA GLY ARG ASP ALA ARG PHE VAL ASP SER ALA ASP GLU ASP VAL GLU PRO VAL ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53372	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.211	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0198	Depositor
Map size (Å)	390.41998, 390.41998, 390.41998	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.723, 0.723, 0.723	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	B	0.34	0/2853	0.62	4/3869 (0.1%)
2	F	0.29	0/987	0.62	0/1322
3	H	0.29	0/1424	0.58	0/1918
4	C1	0.31	0/379	0.53	0/511
5	Z2	1.00	4/65009 (0.0%)	0.92	28/101385 (0.0%)
6	R3	0.32	0/465	0.50	0/629
7	A4	0.28	0/1848	0.50	0/2494
8	E5	0.35	0/1163	0.56	0/1564
9	L6	0.37	0/959	0.60	0/1282
10	F7	0.32	0/1383	0.55	0/1858
11	D8	0.71	0/2733	0.82	0/4256
12	E9	0.38	0/1559	0.57	0/2103
13	aA	0.41	0/450	0.65	0/596
14	MB	0.41	0/961	0.63	0/1282
15	UC	0.36	0/774	0.52	0/1043
16	WD	0.38	0/628	0.63	0/841
17	XE	0.27	0/503	0.56	0/670
18	RF	0.39	0/840	0.59	0/1125
19	FG	0.29	0/864	0.53	0/1169
20	VH	0.46	0/635	0.63	0/847
21	TI	0.34	0/790	0.52	0/1057
22	fJ	0.30	0/508	0.50	0/690
23	HK	0.28	0/821	0.56	0/1091
24	OL	0.32	0/702	0.54	0/941
25	MM	0.26	0/866	0.55	0/1166
26	iN	0.62	0/36108	0.80	2/56315 (0.0%)
27	PO	0.46	0/947	0.64	0/1261
28	SP	0.28	0/652	0.53	0/879
29	BQ	0.33	0/982	0.53	0/1318
30	GR	0.34	0/1377	0.54	0/1861
31	GS	0.28	0/1208	0.56	0/1619
32	CT	0.29	0/1633	0.57	0/2195

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	KU	0.30	0/851	0.55	0/1150
34	NV	0.32	0/478	0.52	0/632
35	YW	0.38	0/442	0.65	1/590 (0.2%)
36	IX	0.43	0/1134	0.52	0/1529
37	JY	0.32	0/794	0.65	1/1072 (0.1%)
38	QZ	0.32	0/638	0.58	0/858
39	Ba	0.44	0/373	0.75	0/489
40	Qb	0.40	0/839	0.58	0/1127
41	Nc	0.36	0/863	0.63	0/1158
42	Kd	0.41	0/1073	0.62	0/1429
43	Je	0.43	0/946	0.65	0/1271
44	Af	0.46	0/1566	0.67	2/2103 (0.1%)
45	Lg	0.44	0/1112	0.59	0/1483
46	dh	0.45	0/524	0.64	0/686
47	Oi	0.40	0/927	0.63	0/1239
48	Pj	0.36	0/660	0.59	0/887
49	bk	0.43	0/401	0.57	0/534
50	Cl	0.43	0/2147	0.65	0/2883
51	Dm	0.32	0/1712	0.58	0/2296
52	Sn	0.42	0/705	0.62	1/939 (0.1%)
53	To	0.30	0/679	0.58	0/904
54	ep	0.42	0/300	0.63	0/395
55	D	0.29	0/838	0.54	0/1121
All	All	0.75	4/153013 (0.0%)	0.80	39/227932 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Z2	2571	G	C8-N7	-5.22	1.27	1.30
5	Z2	555	G	C8-N7	-5.16	1.27	1.30
5	Z2	2428	G	C8-N7	-5.09	1.27	1.30
5	Z2	448	G	C8-N7	-5.07	1.27	1.30

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	99	PRO	CA-N-CD	-10.58	96.69	111.50
5	Z2	495	G	O4'-C1'-N9	8.27	114.82	108.20
44	Af	165	PRO	N-CD-CG	-8.00	91.21	103.20
5	Z2	1297	U	C2-N1-C1'	7.09	126.21	117.70
5	Z2	775	U	C2-N1-C1'	6.79	125.85	117.70
5	Z2	34	G	O4'-C1'-N9	6.64	113.51	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	Af	165	PRO	CA-CB-CG	-6.47	91.70	104.00
5	Z2	733	G	O4'-C1'-N9	6.43	113.34	108.20
5	Z2	1113	A	O4'-C1'-N9	6.42	113.34	108.20
1	B	96	LEU	CA-CB-CG	6.15	129.46	115.30
5	Z2	1765	U	O4'-C1'-N1	6.12	113.10	108.20
52	Sn	56	LEU	CA-CB-CG	5.93	128.95	115.30
5	Z2	1413	G	N9-C4-C5	-5.91	103.04	105.40
5	Z2	2814	G	O4'-C1'-N9	5.90	112.92	108.20
5	Z2	689	G	O4'-C1'-N9	5.89	112.91	108.20
1	B	98	THR	C-N-CD	5.66	140.29	128.40
5	Z2	189	G	C8-N9-C1'	-5.49	119.86	127.00
37	JY	52	LEU	CA-CB-CG	5.47	127.89	115.30
5	Z2	945	C	O5'-P-OP2	-5.45	100.80	105.70
5	Z2	702	C	N3-C2-O2	-5.40	118.12	121.90
35	YW	53	LEU	CA-CB-CG	5.38	127.67	115.30
5	Z2	1934	A	N1-C2-N3	-5.37	126.61	129.30
5	Z2	1833	A	O4'-C1'-N9	5.30	112.44	108.20
5	Z2	2672	U	N3-C2-O2	-5.29	118.50	122.20
5	Z2	775	U	N1-C2-O2	5.28	126.50	122.80
26	iN	1203	C	C2-N1-C1'	5.24	124.56	118.80
5	Z2	702	C	C2-N1-C1'	5.24	124.56	118.80
5	Z2	702	C	N1-C2-O2	5.23	122.04	118.90
5	Z2	1308	G	O4'-C1'-N9	5.20	112.36	108.20
5	Z2	331	G	N3-C4-N9	-5.18	122.89	126.00
1	B	99	PRO	N-CD-CG	-5.14	95.49	103.20
26	iN	1023	C	C2-N1-C1'	5.14	124.45	118.80
5	Z2	658	C	C2-N1-C1'	-5.12	113.16	118.80
5	Z2	218	A	O4'-C1'-N9	5.09	112.27	108.20
5	Z2	189	G	C4-N9-C1'	5.08	133.11	126.50
5	Z2	189	G	O4'-C1'-N9	5.06	112.25	108.20
5	Z2	1922	A	N9-C4-C5	-5.03	103.79	105.80
5	Z2	775	U	N3-C2-O2	-5.01	118.69	122.20
5	Z2	2021	G	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2812	0	2754	65	0
2	F	974	0	1022	24	0
3	H	1404	0	1411	33	0
4	C1	374	0	406	10	0
5	Z2	58043	0	29179	463	0
6	R3	457	0	466	6	0
7	A4	1816	0	1843	41	0
8	E5	1151	0	1205	16	0
9	L6	946	0	1008	6	0
10	F7	1362	0	1402	33	0
11	D8	2446	0	1241	11	0
12	E9	1537	0	1590	27	0
13	aA	442	0	432	0	0
14	MB	947	0	988	8	0
15	UC	760	0	774	12	0
16	WD	618	0	637	10	0
17	XE	502	0	527	11	0
18	RF	834	0	898	21	0
19	FG	849	0	838	15	0
20	VH	626	0	629	10	0
21	TI	784	0	820	9	0
22	fJ	493	0	441	0	0
23	HK	811	0	845	17	0
24	OL	694	0	710	6	0
25	MM	858	0	897	27	0
26	iN	32246	0	16224	0	0
27	PO	935	0	999	11	0
28	SP	637	0	665	12	0
29	BQ	974	0	1009	18	0
30	GR	1357	0	1397	29	0
31	GS	1190	0	1224	22	0
32	CT	1609	0	1674	41	0
33	KU	836	0	845	28	0
34	NV	472	0	520	9	0
35	YW	438	0	476	7	0
36	IX	1108	0	1145	18	0
37	JY	784	0	813	31	0
38	QZ	632	0	676	20	0
39	Ba	369	0	418	0	0
40	Qb	827	0	862	0	0
41	Nc	852	0	880	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	Kd	1062	0	1123	0	0
43	Je	937	0	1003	0	0
44	Af	1548	0	1574	0	0
45	Lg	1093	0	1188	0	0
46	dh	519	0	581	0	0
47	Oi	917	0	969	0	0
48	Pj	648	0	661	0	0
49	bk	394	0	412	0	0
50	Cl	2107	0	2195	0	0
51	Dm	1688	0	1745	0	0
52	Sn	698	0	750	0	0
53	To	675	0	716	0	0
54	ep	298	0	334	0	0
55	D	830	0	838	11	0
56	Z2	2	0	0	0	0
All	All	141222	0	96879	1073	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 7.

All (1073) 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)
5:Z2:1020:G:H1	5:Z2:1103:U:H3	1.25	0.85
5:Z2:219:C:H5	5:Z2:229:G:H21	1.25	0.83
5:Z2:271:A:H61	5:Z2:343:U:H3	1.29	0.81
5:Z2:2194:U:H3	5:Z2:2199:A:H61	1.30	0.80
17:XE:24:ASP:OD1	17:XE:27:ARG:NH1	2.16	0.78
1:B:174:ASP:OD1	1:B:174:ASP:N	2.16	0.78
5:Z2:2328:A:H4'	5:Z2:2329:A:H5"	1.65	0.76
5:Z2:68:A:OP2	17:XE:47:ARG:NH2	2.19	0.75
5:Z2:345:A:HO2'	5:Z2:346:A:H8	1.34	0.73
1:B:169:LEU:HD22	1:B:175:GLY:H	1.53	0.73
5:Z2:2053:G:H1	5:Z2:2426:U:H3	1.36	0.72
17:XE:16:GLN:NE2	17:XE:20:GLU:OE2	2.20	0.72
7:A4:189:ILE:HB	7:A4:203:TYR:HB2	1.70	0.72
8:E5:46:ASP:HB2	8:E5:50:ARG:HB2	1.70	0.72
10:F7:113:ASP:OD1	25:MM:71:ARG:NH1	2.22	0.72
25:MM:85:CYS:SG	25:MM:86:TYR:N	2.62	0.72
1:B:212:ILE:HB	1:B:235:THR:HG22	1.71	0.71
5:Z2:194:A:N6	5:Z2:2413:A:O2'	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:SP:4:SER:HB2	28:SP:7:LYS:HG3	1.72	0.71
5:Z2:1049:U:H3	5:Z2:1053:A:HO2'	1.37	0.71
7:A4:78:LYS:HG2	7:A4:80:ALA:H	1.54	0.71
28:SP:55:ARG:HG2	28:SP:56:THR:HG23	1.71	0.71
1:B:200:GLN:HG3	1:B:228:ARG:HE	1.55	0.71
5:Z2:477:G:H4'	18:RF:6:LYS:HB2	1.73	0.70
30:GR:42:GLU:HG3	30:GR:55:THR:HG22	1.73	0.70
1:B:99:PRO:HD2	1:B:99:PRO:O	1.90	0.70
5:Z2:2303:A:O2'	5:Z2:2305:A:N7	2.24	0.70
5:Z2:2288:U:H5"	10:F7:131:GLY:HA3	1.74	0.70
1:B:239:LEU:HD21	1:B:250:ILE:HA	1.73	0.69
5:Z2:2083:U:H3	5:Z2:2178:G:H1	1.40	0.69
37:JY:44:THR:HG22	37:JY:70:HIS:HA	1.74	0.69
18:RF:12:ILE:HD12	18:RF:42:LYS:HE2	1.75	0.69
36:IX:6:ALA:H	36:IX:45:THR:HG21	1.58	0.69
37:JY:12:SER:HB3	37:JY:18:ILE:HD13	1.75	0.68
24:OL:35:ILE:O	24:OL:39:GLN:NE2	2.26	0.68
5:Z2:1417:A:H2'	5:Z2:1418:A:C8	2.28	0.68
5:Z2:2226:U:H2'	5:Z2:2227:U:C6	2.29	0.68
29:BQ:11:LEU:HD22	29:BQ:77:ILE:HD11	1.75	0.68
5:Z2:2009:C:H5'	5:Z2:2600:U:H4'	1.75	0.67
10:F7:17:LYS:NZ	10:F7:22:LEU:O	2.26	0.67
10:F7:8:TYR:HA	10:F7:12:LEU:HB2	1.77	0.67
25:MM:23:PHE:HB3	25:MM:66:GLU:HB3	1.75	0.67
5:Z2:1788:A:H2'	5:Z2:1789:A:C8	2.29	0.67
15:UC:42:GLU:O	15:UC:99:ARG:NH2	2.27	0.67
5:Z2:2311:A:H2'	5:Z2:2312:A:C8	2.31	0.66
5:Z2:1348:G:H5"	16:WD:3:ARG:HH12	1.59	0.66
33:KU:112:ASP:HB3	34:NV:2:PRO:HB2	1.77	0.66
23:HK:64:CYS:HB2	23:HK:80:SER:HB3	1.77	0.66
37:JY:52:LEU:HB3	37:JY:62:ARG:HD2	1.78	0.66
32:CT:131:ARG:HA	32:CT:134:MET:HG3	1.78	0.66
7:A4:72:VAL:H	7:A4:94:MET:HE3	1.61	0.66
38:QZ:23:MET:HB2	38:QZ:26:SER:HB2	1.77	0.66
1:B:98:THR:OG1	1:B:101:ARG:NH2	2.29	0.65
5:Z2:593:A:H2'	5:Z2:594:A:C8	2.31	0.65
5:Z2:2274:U:H2'	5:Z2:2275:G:C8	2.30	0.65
29:BQ:81:SER:HB2	29:BQ:87:GLN:H	1.60	0.65
10:F7:34:ILE:HD11	10:F7:100:LEU:HD12	1.78	0.65
25:MM:48:LEU:HG	25:MM:52:GLN:HG3	1.78	0.65
33:KU:30:THR:HG21	33:KU:63:ALA:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ASP:HB2	1:B:95:PRO:O	1.97	0.65
7:A4:168:VAL:HG21	7:A4:178:ILE:HD11	1.79	0.65
5:Z2:1453:A:H2'	5:Z2:1454:A:C8	2.30	0.65
1:B:211:VAL:HG22	1:B:234:ALA:HB3	1.78	0.64
6:R3:63:ARG:HD3	6:R3:70:TYR:HA	1.78	0.64
18:RF:73:THR:HG23	18:RF:106:LYS:HB2	1.80	0.64
29:BQ:104:ALA:HB3	29:BQ:115:ASP:HB3	1.78	0.64
21:TI:12:VAL:HG22	21:TI:18:LYS:HA	1.79	0.64
5:Z2:1885:A:H8	5:Z2:1888:C:H41	1.45	0.64
12:E9:17:ALA:HA	12:E9:105:GLN:HG2	1.80	0.64
18:RF:13:SER:HB3	18:RF:16:LYS:HD2	1.79	0.64
33:KU:36:ASP:OD2	33:KU:38:GLN:NE2	2.31	0.64
10:F7:69:LYS:HD2	10:F7:82:GLU:HG3	1.80	0.64
5:Z2:977:G:OP1	27:PO:50:ARG:NH1	2.29	0.64
37:JY:88:MET:SD	37:JY:88:MET:N	2.70	0.64
37:JY:10:LEU:HD21	37:JY:25:ILE:HD12	1.80	0.64
5:Z2:197:U:H4'	16:WD:22:ASN:HB3	1.80	0.63
23:HK:76:LYS:HE2	37:JY:67:ILE:HD13	1.81	0.63
5:Z2:1089:U:H2'	5:Z2:1090:A:H8	1.63	0.63
18:RF:2:GLU:HG2	18:RF:106:LYS:HB3	1.80	0.63
2:F:49:PRO:HD3	2:F:78:ARG:HG3	1.81	0.62
10:F7:145:LYS:H	10:F7:145:LYS:HD3	1.64	0.62
24:OL:11:ILE:O	24:OL:15:GLN:HG2	1.99	0.62
2:F:125:PHE:HD2	2:F:127:LYS:HE2	1.64	0.62
5:Z2:732:U:H4'	18:RF:92:ARG:HH22	1.62	0.62
5:Z2:2574:C:H2'	5:Z2:2575:G:C8	2.34	0.62
27:PO:83:MET:HE1	27:PO:109:LEU:HB3	1.81	0.62
1:B:70:GLU:N	1:B:70:GLU:OE2	2.32	0.62
1:B:134:ARG:NH2	1:B:245:GLY:O	2.30	0.62
12:E9:144:ARG:HG2	12:E9:165:HIS:HB2	1.80	0.62
37:JY:6:ILE:HG22	37:JY:102:LEU:HA	1.81	0.62
37:JY:36:VAL:HG22	37:JY:76:ILE:HG22	1.80	0.62
17:XE:18:LEU:O	17:XE:22:GLN:HG2	1.98	0.62
5:Z2:818:A:H2'	5:Z2:819:G:C8	2.34	0.62
5:Z2:2310:A:H2'	5:Z2:2311:A:C8	2.34	0.62
10:F7:16:ILE:HD11	10:F7:172:ALA:HB2	1.81	0.62
3:H:249:GLY:O	3:H:251:ARG:N	2.33	0.62
38:QZ:87:LYS:HD2	38:QZ:88:VAL:N	2.14	0.62
5:Z2:932:C:H2'	5:Z2:933:G:C8	2.35	0.62
37:JY:37:CYS:SG	37:JY:75:ASP:HB2	2.40	0.61
5:Z2:578:U:H2'	5:Z2:579:U:C6	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z2:2216:U:H2'	5:Z2:2217:G:C8	2.36	0.61
5:Z2:798:U:H2'	5:Z2:799:C:C6	2.36	0.61
8:E5:39:THR:HG22	8:E5:57:LYS:HG2	1.80	0.61
5:Z2:2513:A:N7	30:GR:172:LYS:HE3	2.15	0.61
18:RF:33:LEU:O	18:RF:37:THR:HG22	2.00	0.61
12:E9:170:ASP:OD2	12:E9:172:SER:OG	2.18	0.61
25:MM:34:LEU:HD23	25:MM:41:PRO:HA	1.81	0.61
31:GS:80:ARG:NH1	31:GS:85:THR:OG1	2.26	0.61
1:B:282:LEU:HD11	1:B:364:ALA:HB1	1.83	0.61
5:Z2:2444:A:H2'	5:Z2:2445:C:C6	2.35	0.61
32:CT:85:GLU:HA	32:CT:88:GLN:HB2	1.83	0.61
37:JY:48:ARG:HD3	37:JY:66:GLU:HB3	1.83	0.61
55:D:95:LYS:O	55:D:99:ARG:HG3	2.00	0.61
5:Z2:984:A:H2'	5:Z2:985:A:C8	2.36	0.60
19:FG:94:ASP:OD1	19:FG:94:ASP:N	2.33	0.60
32:CT:47:LEU:HD23	32:CT:52:ILE:HG21	1.83	0.60
1:B:169:LEU:HD13	1:B:175:GLY:HA2	1.84	0.60
5:Z2:1370:U:H2'	5:Z2:1371:U:C6	2.37	0.60
5:Z2:1843:G:H1'	5:Z2:1871:A:H61	1.67	0.60
3:H:246:GLU:HB3	3:H:255:LYS:HD3	1.83	0.60
14:MB:33:LEU:HD13	14:MB:114:GLU:HG3	1.83	0.60
5:Z2:1378:U:H2'	5:Z2:1379:A:O4'	2.00	0.60
5:Z2:2671:G:N1	5:Z2:2703:U:OP2	2.23	0.60
25:MM:11:ASP:HA	25:MM:45:VAL:HB	1.83	0.60
1:B:160:ILE:HD11	20:VH:3:HIS:HB3	1.83	0.60
18:RF:88:ARG:HB2	18:RF:92:ARG:HE	1.65	0.60
5:Z2:564:G:O2'	5:Z2:2005:A:OP1	2.20	0.60
5:Z2:727:G:H2'	5:Z2:728:U:C6	2.36	0.60
1:B:61:LEU:HD13	1:B:64:ILE:HD11	1.83	0.59
25:MM:97:VAL:HG13	25:MM:98:ARG:HG2	1.84	0.59
37:JY:47:GLU:HG3	37:JY:67:ILE:HG23	1.84	0.59
5:Z2:645:C:H5"	12:E9:93:GLN:HG2	1.83	0.59
21:TI:70:ILE:HD13	21:TI:81:ILE:HD11	1.84	0.59
30:GR:61:ALA:O	30:GR:65:THR:HG22	2.03	0.59
35:YW:10:LYS:HB2	35:YW:53:LEU:HB2	1.84	0.59
2:F:15:ALA:HB2	2:F:65:VAL:HG13	1.82	0.59
10:F7:33:LYS:HG2	10:F7:157:THR:HB	1.84	0.59
31:GS:12:ILE:HD11	31:GS:28:ASN:HD21	1.67	0.59
7:A4:7:THR:HG23	7:A4:63:ASN:HD22	1.66	0.59
5:Z2:272:U:H3	5:Z2:342:G:H1	1.49	0.59
19:FG:26:ILE:HD11	19:FG:39:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:GS:92:VAL:HB	31:GS:97:ARG:HD3	1.85	0.59
31:GS:13:LEU:HD12	31:GS:14:PRO:HD2	1.85	0.59
32:CT:58:GLU:OE1	37:JY:94:ALA:HB1	2.02	0.59
12:E9:190:GLU:OE2	12:E9:190:GLU:N	2.28	0.59
7:A4:119:LEU:O	7:A4:123:GLU:HG2	2.02	0.58
1:B:23:THR:CG2	1:B:76:ASN:HB3	2.33	0.58
1:B:280:ASN:HD21	3:H:321:ARG:HA	1.68	0.58
5:Z2:1795:A:H2'	5:Z2:1796:A:C8	2.38	0.58
32:CT:72:ARG:HB3	32:CT:75:ILE:HG23	1.85	0.58
29:BQ:18:GLN:NE2	29:BQ:72:ALA:HB1	2.18	0.58
55:D:44:ASP:OD2	55:D:45:ASN:ND2	2.36	0.58
1:B:304:ARG:NH1	1:B:357:MET:O	2.36	0.58
7:A4:138:GLU:O	7:A4:141:GLU:HG3	2.03	0.58
4:C1:9:ILE:HD11	4:C1:12:LEU:HD23	1.84	0.58
5:Z2:52:G:H5"	5:Z2:53:G:H5'	1.83	0.58
5:Z2:1782:U:H2'	5:Z2:1783:C:H6	1.69	0.58
37:JY:9:ARG:HG2	37:JY:73:MET:HB2	1.86	0.58
5:Z2:2073:U:H2'	5:Z2:2074:A:H8	1.69	0.58
37:JY:35:GLN:H	37:JY:78:GLN:HE22	1.51	0.58
5:Z2:1708:A:N6	5:Z2:1724:G:O2'	2.37	0.58
5:Z2:688:U:H2'	5:Z2:689:G:O4'	2.04	0.57
5:Z2:2057:A:H2'	5:Z2:2058:C:C6	2.39	0.57
5:Z2:2295:U:H5'	10:F7:85:ILE:HD11	1.86	0.57
5:Z2:1012:A:N6	5:Z2:1109:G:H2'	2.19	0.57
5:Z2:1012:A:H2'	5:Z2:1013:A:C8	2.40	0.57
31:GS:38:THR:O	31:GS:42:ILE:HD12	2.04	0.57
5:Z2:37:G:H2'	5:Z2:38:C:C6	2.39	0.57
32:CT:95:MET:HG2	32:CT:96:GLY:H	1.69	0.57
36:IX:96:LYS:HD2	36:IX:99:ASP:OD2	2.04	0.57
5:Z2:886:A:O2'	5:Z2:887:C:OP1	2.22	0.57
5:Z2:2771:C:H2'	5:Z2:2772:C:C6	2.39	0.57
10:F7:14:GLN:O	10:F7:18:GLU:HG2	2.04	0.57
20:VH:53:MET:SD	20:VH:57:HIS:HA	2.44	0.57
55:D:75:GLU:HG2	55:D:80:LYS:HB2	1.87	0.57
5:Z2:2683:A:H2'	5:Z2:2684:C:C6	2.40	0.57
32:CT:19:ASN:O	32:CT:40:ARG:NH2	2.37	0.57
8:E5:86:LEU:HB2	8:E5:103:PRO:HG3	1.87	0.57
5:Z2:565:U:H2'	5:Z2:566:C:C6	2.39	0.57
5:Z2:2073:U:H2'	5:Z2:2074:A:C8	2.39	0.57
30:GR:105:LEU:HB2	30:GR:113:VAL:HG23	1.86	0.57
17:XE:24:ASP:O	17:XE:28:ILE:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z2:47:U:H2'	5:Z2:48:C:C6	2.40	0.57
5:Z2:397:C:H2'	5:Z2:398:A:C8	2.40	0.57
5:Z2:1581:A:H2'	5:Z2:1582:A:C8	2.40	0.57
21:TI:48:GLN:OE1	21:TI:48:GLN:N	2.34	0.57
29:BQ:81:SER:OG	29:BQ:126:GLU:OE2	2.20	0.57
1:B:22:LYS:H	1:B:100:GLU:HG3	1.70	0.56
5:Z2:1764:U:H2'	5:Z2:1770:A:N6	2.19	0.56
24:OL:25:GLU:HG3	24:OL:80:LEU:HD13	1.87	0.56
5:Z2:916:A:N6	5:Z2:1167:A:N3	2.53	0.56
5:Z2:1780:A:H2'	5:Z2:1781:C:C6	2.41	0.56
9:L6:67:ILE:HG12	9:L6:74:LEU:HD12	1.87	0.56
28:SP:11:ILE:HD12	28:SP:38:SER:HB3	1.87	0.56
38:QZ:87:LYS:HD2	38:QZ:88:VAL:H	1.68	0.56
32:CT:11:ARG:NH2	32:CT:177:THR:O	2.34	0.56
3:H:305:THR:OG1	3:H:364:GLU:OE2	2.23	0.56
5:Z2:517:U:H2'	5:Z2:518:A:C8	2.41	0.56
10:F7:162:THR:HB	10:F7:165:GLU:HG3	1.88	0.56
33:KU:59:THR:HG22	33:KU:61:PHE:H	1.71	0.56
5:Z2:1089:U:H2'	5:Z2:1090:A:C8	2.40	0.56
5:Z2:402:U:H2'	5:Z2:403:C:C6	2.40	0.56
5:Z2:836:C:H2'	5:Z2:837:A:C8	2.41	0.56
5:Z2:1782:U:H2'	5:Z2:1783:C:C6	2.40	0.56
17:XE:31:ALA:HA	17:XE:34:THR:HG22	1.87	0.56
1:B:17:VAL:HG11	1:B:44:VAL:HG21	1.86	0.56
5:Z2:2011:C:H2'	5:Z2:2012:A:C8	2.41	0.56
18:RF:86:LEU:HD22	18:RF:96:ILE:HD11	1.87	0.56
31:GS:12:ILE:HD12	31:GS:13:LEU:H	1.71	0.56
38:QZ:36:ARG:HG3	38:QZ:36:ARG:HH11	1.71	0.56
5:Z2:343:U:H2'	5:Z2:344:U:C6	2.41	0.56
25:MM:88:GLY:O	25:MM:92:ARG:HG2	2.05	0.56
30:GR:88:GLN:NE2	30:GR:130:GLU:OE1	2.39	0.56
5:Z2:2050:C:H2'	5:Z2:2051:C:C6	2.41	0.56
17:XE:34:THR:HG23	17:XE:36:GLN:HG2	1.88	0.56
32:CT:14:VAL:HG22	32:CT:15:VAL:HG13	1.87	0.56
20:VH:11:ARG:HG2	20:VH:11:ARG:HH11	1.71	0.55
25:MM:86:TYR:O	25:MM:90:ARG:HG2	2.06	0.55
37:JY:66:GLU:OE1	37:JY:68:ARG:NH1	2.38	0.55
2:F:116:LEU:HD22	2:F:122:ARG:HG2	1.88	0.55
5:Z2:1160:G:H4'	5:Z2:1161:U:H5'	1.89	0.55
5:Z2:841:G:H2'	5:Z2:842:G:C8	2.41	0.55
5:Z2:157:C:H2'	5:Z2:158:U:H6	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:GR:18:THR:O	30:GR:18:THR:OG1	2.24	0.55
33:KU:111:SER:HA	34:NV:3:ALA:HA	1.89	0.55
5:Z2:2360:A:H2'	5:Z2:2361:A:C8	2.42	0.55
15:UC:10:ALA:HB3	15:UC:71:VAL:HG22	1.89	0.55
5:Z2:2413:A:H2'	5:Z2:2413:A:N3	2.21	0.55
5:Z2:2632:C:H2'	5:Z2:2633:U:H6	1.71	0.55
5:Z2:247:G:H2'	5:Z2:248:A:C8	2.42	0.55
5:Z2:1154:A:H2'	5:Z2:1155:A:C8	2.41	0.55
5:Z2:1681:U:H5"	5:Z2:1682:C:H5	1.72	0.55
5:Z2:2328:A:N3	5:Z2:2364:A:H2'	2.22	0.55
10:F7:31:ILE:HG13	10:F7:169:LEU:HD21	1.87	0.55
3:H:263:MET:HE2	3:H:264:PHE:H	1.72	0.55
5:Z2:380:U:H5"	16:WD:32:ASN:HB2	1.89	0.55
28:SP:18:LYS:HE2	28:SP:31:ILE:HG23	1.89	0.55
5:Z2:307:G:N7	12:E9:131:LYS:NZ	2.54	0.55
5:Z2:1276:G:H2'	5:Z2:1277:C:C6	2.42	0.55
25:MM:11:ASP:O	25:MM:46:SER:OG	2.24	0.54
5:Z2:836:C:H2'	5:Z2:837:A:H8	1.70	0.54
5:Z2:1154:A:H2'	5:Z2:1155:A:H8	1.72	0.54
31:GS:62:PHE:O	31:GS:66:VAL:HG12	2.07	0.54
38:QZ:51:LYS:HB3	38:QZ:77:LYS:HG3	1.89	0.54
1:B:81:ALA:HB3	1:B:92:ILE:HG12	1.88	0.54
5:Z2:2256:A:H2'	5:Z2:2257:A:C8	2.43	0.54
5:Z2:1580:A:O2'	5:Z2:1581:A:OP1	2.23	0.54
19:FG:7:VAL:HG22	19:FG:61:LEU:HD12	1.89	0.54
28:SP:15:LEU:HD13	28:SP:33:THR:HG21	1.87	0.54
32:CT:202:ILE:HG22	32:CT:204:ARG:HD3	1.90	0.54
5:Z2:1426:U:H2'	5:Z2:1427:C:C6	2.42	0.54
5:Z2:695:G:H2'	5:Z2:696:C:C6	2.43	0.54
5:Z2:1918:A:H2'	5:Z2:1919:G:O4'	2.07	0.54
8:E5:43:VAL:HG11	8:E5:119:VAL:HA	1.90	0.54
30:GR:135:SER:HB3	30:GR:141:LEU:HB2	1.89	0.54
32:CT:85:GLU:O	32:CT:89:LYS:HE2	2.08	0.54
5:Z2:1006:G:OP2	36:IX:67:LYS:HE3	2.07	0.54
5:Z2:1850:U:OP1	5:Z2:2393:G:O2'	2.18	0.54
8:E5:84:ALA:HB1	8:E5:126:LYS:HB2	1.90	0.54
12:E9:147:ILE:HB	12:E9:168:VAL:HG22	1.90	0.54
31:GS:114:GLU:HB2	31:GS:120:ARG:HG2	1.90	0.54
12:E9:123:LEU:HG	12:E9:136:LYS:HE3	1.89	0.53
5:Z2:343:U:H2'	5:Z2:344:U:H6	1.73	0.53
5:Z2:1341:C:H2'	5:Z2:1342:G:O4'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F7:108:ILE:HG21	10:F7:176:PRO:HG2	1.90	0.53
11:D8:77:G:O6	15:UC:20:LYS:NZ	2.41	0.53
16:WD:31:PRO:HB2	16:WD:33:LEU:HG	1.90	0.53
16:WD:59:ILE:HD13	16:WD:67:VAL:HG21	1.89	0.53
38:QZ:53:HIS:HE2	38:QZ:55:GLU:HG2	1.73	0.53
1:B:304:ARG:NH2	1:B:354:GLN:HB3	2.23	0.53
1:B:305:ARG:O	1:B:354:GLN:NE2	2.41	0.53
10:F7:106:VAL:O	10:F7:110:ARG:HG3	2.08	0.53
5:Z2:1369:A:H62	5:Z2:1386:U:H3	1.57	0.53
34:NV:39:GLU:OE2	34:NV:44:VAL:HG22	2.09	0.53
1:B:154:GLN:HA	1:B:157:MET:HG3	1.91	0.53
5:Z2:1639:G:OP1	14:MB:37:THR:HG21	2.08	0.53
5:Z2:1996:G:H5"	18:RF:42:LYS:HB2	1.89	0.53
7:A4:122:LEU:O	7:A4:125:GLN:HG3	2.09	0.53
8:E5:45:GLY:HA3	8:E5:122:VAL:HG13	1.90	0.53
11:D8:11:A:N1	11:D8:67:G:O2'	2.30	0.53
1:B:23:THR:HG22	1:B:77:LEU:O	2.07	0.53
5:Z2:379:G:H1'	16:WD:29:PHE:HB3	1.90	0.53
5:Z2:1460:U:H2'	5:Z2:1461:A:H8	1.72	0.53
17:XE:2:LYS:HA	17:XE:5:GLU:HG3	1.91	0.53
5:Z2:653:A:H2'	5:Z2:655:A:H62	1.74	0.53
16:WD:52:SER:O	16:WD:56:MET:HG3	2.08	0.53
19:FG:28:LEU:HD23	19:FG:74:LEU:HD13	1.91	0.53
5:Z2:1585:A:H5"	5:Z2:1586:A:H5'	1.90	0.53
10:F7:38:MET:HG3	10:F7:152:MET:HG3	1.91	0.53
25:MM:4:ILE:HG23	25:MM:57:ARG:HG3	1.90	0.53
5:Z2:781:U:H2'	5:Z2:782:C:C6	2.44	0.53
5:Z2:1839:A:H2'	5:Z2:1840:A:C8	2.43	0.53
7:A4:122:LEU:HD23	7:A4:146:MET:HB2	1.90	0.53
33:KU:88:GLY:H	33:KU:114:THR:HB	1.73	0.53
36:IX:93:ILE:HD12	36:IX:100:VAL:HG21	1.91	0.53
55:D:61:ILE:HG13	55:D:70:PHE:HD2	1.74	0.53
1:B:132:LYS:HD2	1:B:133:ALA:N	2.24	0.52
7:A4:79:ARG:HD2	7:A4:79:ARG:N	2.24	0.52
33:KU:61:PHE:O	33:KU:65:VAL:HG13	2.09	0.52
23:HK:94:PRO:O	32:CT:29:TYR:OH	2.27	0.52
25:MM:4:ILE:HG13	25:MM:9:ILE:HD13	1.90	0.52
8:E5:43:VAL:HG12	8:E5:122:VAL:HG11	1.91	0.52
11:D8:46:U:H2'	11:D8:47:C:C6	2.44	0.52
37:JY:46:ILE:HG12	37:JY:68:ARG:HG2	1.90	0.52
55:D:94:SER:O	55:D:98:THR:OG1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z2:2497:U:H2'	5:Z2:2498:C:C6	2.44	0.52
7:A4:98:ASP:OD1	7:A4:98:ASP:N	2.41	0.52
32:CT:142:MET:HG2	32:CT:149:ILE:HG22	1.91	0.52
33:KU:47:SER:HB3	33:KU:62:ALA:HB1	1.91	0.52
5:Z2:566:C:H2'	5:Z2:567:A:C8	2.45	0.52
5:Z2:521:A:H5"	36:IX:7:LYS:HZ2	1.74	0.52
1:B:219:ILE:HD13	1:B:235:THR:HB	1.91	0.52
32:CT:132:ARG:HH12	32:CT:135:LYS:HB2	1.75	0.52
38:QZ:36:ARG:NH1	38:QZ:43:GLN:HG3	2.25	0.52
3:H:306:LYS:HG2	3:H:364:GLU:HG2	1.91	0.52
5:Z2:1843:G:H1'	5:Z2:1871:A:N6	2.24	0.52
7:A4:10:GLU:OE1	7:A4:11:MET:N	2.42	0.52
7:A4:230:LYS:O	7:A4:234:GLN:HG2	2.10	0.52
38:QZ:36:ARG:HG3	38:QZ:36:ARG:NH1	2.25	0.52
55:D:38:GLN:OE1	55:D:63:ARG:NH1	2.43	0.52
1:B:182:ASN:ND2	1:B:182:ASN:O	2.41	0.52
1:B:291:ARG:HG2	1:B:318:GLN:HG2	1.92	0.52
5:Z2:856:U:H2'	5:Z2:857:U:C6	2.45	0.52
5:Z2:2368:C:H2'	5:Z2:2369:U:C6	2.45	0.52
8:E5:162:ARG:O	29:BQ:66:LYS:NZ	2.43	0.52
29:BQ:81:SER:OG	29:BQ:81:SER:O	2.28	0.52
5:Z2:205:C:H2'	5:Z2:206:C:H6	1.75	0.51
5:Z2:244:G:H4'	5:Z2:369:G:C5	2.44	0.51
5:Z2:1273:C:H2'	5:Z2:1274:U:C6	2.45	0.51
23:HK:2:ALA:N	23:HK:67:THR:O	2.43	0.51
31:GS:151:ALA:HB1	33:KU:59:THR:HG21	1.92	0.51
32:CT:51:MET:HB3	32:CT:115:LEU:HD22	1.92	0.51
5:Z2:2696:U:O2'	5:Z2:2698:C:OP2	2.26	0.51
5:Z2:2823:G:N2	5:Z2:2826:A:OP2	2.31	0.51
15:UC:61:ALA:HB1	15:UC:65:HIS:ND1	2.25	0.51
4:C1:41:ALA:HA	4:C1:44:ILE:HG12	1.92	0.51
5:Z2:204:A:H2'	5:Z2:205:C:O4'	2.10	0.51
5:Z2:633:G:H4'	5:Z2:2334:G:H5'	1.92	0.51
5:Z2:1513:A:H2'	5:Z2:1514:A:H8	1.74	0.51
7:A4:25:THR:HG23	7:A4:44:HIS:CE1	2.46	0.51
37:JY:7:ARG:NH1	37:JY:75:ASP:OD2	2.42	0.51
1:B:213:VAL:HG11	1:B:239:LEU:HD23	1.92	0.51
12:E9:14:SER:N	12:E9:196:GLU:OE2	2.40	0.51
1:B:287:GLN:HG3	1:B:320:LEU:H	1.76	0.51
30:GR:37:LEU:HD12	30:GR:68:ILE:HD12	1.92	0.51
32:CT:6:HIS:HE1	32:CT:8:ILE:HD12	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:229:VAL:HG22	3:H:280:LEU:HG	1.91	0.51
5:Z2:1833:A:H1'	5:Z2:1834:A:N7	2.25	0.51
5:Z2:2051:C:H2'	5:Z2:2052:C:C6	2.46	0.51
38:QZ:14:LEU:HD13	38:QZ:31:ILE:HG21	1.93	0.51
2:F:5:TYR:HE1	2:F:16:ARG:HB3	1.74	0.51
2:F:45:VAL:HG13	2:F:78:ARG:HD3	1.93	0.51
5:Z2:178:A:H1'	5:Z2:418:C:O4'	2.11	0.51
20:VH:47:ALA:HB1	20:VH:51:VAL:HG23	1.93	0.51
32:CT:39:VAL:HG22	32:CT:94:MET:SD	2.51	0.51
32:CT:60:PRO:HD2	32:CT:64:ALA:HA	1.93	0.51
36:IX:65:THR:O	36:IX:68:LYS:HD3	2.11	0.51
5:Z2:1053:A:H5"	5:Z2:1054:A:C8	2.46	0.51
20:VH:3:HIS:O	20:VH:4:LYS:HB2	2.10	0.51
5:Z2:2196:A:H2'	5:Z2:2197:C:C6	2.46	0.50
5:Z2:2853:C:H2'	5:Z2:2854:U:C6	2.46	0.50
25:MM:65:THR:OG1	25:MM:66:GLU:OE1	2.23	0.50
30:GR:155:GLU:OE1	30:GR:160:LYS:N	2.43	0.50
5:Z2:824:U:H2'	5:Z2:825:C:C6	2.46	0.50
5:Z2:2650:C:H1'	30:GR:109:TYR:CD1	2.46	0.50
17:XE:39:ASN:OD1	17:XE:39:ASN:N	2.27	0.50
32:CT:102:ASN:OD1	32:CT:102:ASN:N	2.45	0.50
5:Z2:2311:A:H2'	5:Z2:2312:A:H8	1.76	0.50
5:Z2:2723:A:H2'	5:Z2:2724:A:C8	2.46	0.50
19:FG:39:LEU:HD13	19:FG:62:PHE:HB3	1.92	0.50
28:SP:35:SER:OG	28:SP:38:SER:OG	2.27	0.50
28:SP:43:GLN:N	28:SP:43:GLN:OE1	2.44	0.50
5:Z2:625:C:H2'	5:Z2:626:U:C6	2.46	0.50
5:Z2:1188:A:H4'	5:Z2:1189:A:H5"	1.93	0.50
5:Z2:1668:U:H2'	5:Z2:1669:G:O4'	2.11	0.50
5:Z2:2024:G:H2'	5:Z2:2025:U:O4'	2.12	0.50
19:FG:19:VAL:O	19:FG:23:GLU:HG2	2.12	0.50
5:Z2:2195:A:H2'	5:Z2:2196:A:H8	1.77	0.50
18:RF:37:THR:HB	18:RF:48:LYS:NZ	2.26	0.50
32:CT:142:MET:HG3	32:CT:170:GLU:HB3	1.93	0.50
5:Z2:624:U:H2'	5:Z2:625:C:C6	2.46	0.50
5:Z2:1285:A:O2'	5:Z2:1286:A:H3'	2.12	0.50
6:R3:73:ASN:O	6:R3:73:ASN:ND2	2.38	0.50
7:A4:10:GLU:HG3	7:A4:12:ARG:H	1.77	0.50
30:GR:47:ASP:O	30:GR:49:VAL:HG12	2.11	0.50
1:B:137:GLU:HG2	1:B:144:VAL:HB	1.93	0.50
3:H:297:LYS:HG3	3:H:298:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:PO:83:MET:CE	27:PO:109:LEU:HB3	2.42	0.50
32:CT:157:LEU:HD12	32:CT:166:GLU:HG3	1.93	0.50
35:YW:2:LYS:HG3	35:YW:39:ASP:HB3	1.94	0.50
5:Z2:157:C:H2'	5:Z2:158:U:C6	2.46	0.50
5:Z2:833:U:H2'	5:Z2:834:A:C8	2.47	0.50
32:CT:150:LYS:HB2	32:CT:169:ARG:HG3	1.94	0.50
33:KU:52:PHE:O	33:KU:53:ARG:HD2	2.12	0.50
2:F:31:LYS:HE2	2:F:36:TYR:HD2	1.77	0.50
5:Z2:2195:A:O2'	5:Z2:2196:A:OP1	2.26	0.50
5:Z2:2283:A:H2'	5:Z2:2284:A:C8	2.46	0.50
25:MM:50:ASP:HA	25:MM:53:LEU:HB2	1.94	0.50
36:IX:11:VAL:HG21	36:IX:50:THR:HG22	1.94	0.50
3:H:321:ARG:HG3	3:H:386:VAL:HG12	1.94	0.49
7:A4:48:LEU:HA	7:A4:51:THR:HG22	1.94	0.49
23:HK:28:LYS:HD3	23:HK:31:ILE:HD11	1.94	0.49
23:HK:64:CYS:HB3	23:HK:69:ARG:H	1.77	0.49
5:Z2:1006:G:O6	36:IX:68:LYS:NZ	2.39	0.49
5:Z2:2303:A:N3	5:Z2:2303:A:H2'	2.26	0.49
12:E9:149:THR:O	12:E9:170:ASP:HA	2.12	0.49
19:FG:11:HIS:ND1	19:FG:12:PRO:HD2	2.27	0.49
31:GS:75:GLU:HB2	31:GS:92:VAL:HG22	1.94	0.49
5:Z2:1629:A:H2'	5:Z2:1630:G:O4'	2.12	0.49
5:Z2:2530:A:H2'	5:Z2:2531:U:C6	2.47	0.49
5:Z2:1348:G:H5"	16:WD:3:ARG:NH1	2.27	0.49
5:Z2:1182:U:H2'	5:Z2:1183:U:C6	2.47	0.49
5:Z2:1776:C:H2'	5:Z2:1777:A:C5	2.47	0.49
24:OL:20:ASP:OD1	24:OL:21:THR:N	2.43	0.49
1:B:15:PRO:HB3	1:B:52:PHE:CZ	2.47	0.49
5:Z2:916:A:H4'	5:Z2:917:U:OP2	2.11	0.49
5:Z2:1923:A:O2'	5:Z2:1925:U:OP2	2.20	0.49
2:F:40:GLU:HG3	31:GS:16:PRO:HB2	1.95	0.49
5:Z2:71:G:H2'	5:Z2:72:C:C6	2.47	0.49
5:Z2:188:A:H2'	5:Z2:189:G:N3	2.28	0.49
5:Z2:732:U:O2	5:Z2:2000:A:H1'	2.13	0.49
5:Z2:2863:U:H2'	5:Z2:2864:U:C6	2.48	0.49
5:Z2:397:C:H2'	5:Z2:398:A:H8	1.78	0.49
5:Z2:1670:G:H2'	5:Z2:1671:U:C6	2.48	0.49
5:Z2:2865:G:H2'	5:Z2:2866:A:C8	2.48	0.49
3:H:314:LEU:HD22	3:H:318:GLU:HB2	1.95	0.49
5:Z2:579:U:H2'	5:Z2:580:C:C6	2.47	0.49
5:Z2:1166:A:H2'	5:Z2:1167:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z2:2632:C:H2'	5:Z2:2633:U:C6	2.47	0.49
1:B:60:ILE:O	1:B:64:ILE:HG23	2.13	0.49
5:Z2:533:U:H2'	5:Z2:534:U:C6	2.48	0.49
5:Z2:1592:C:O2'	5:Z2:1598:A:N1	2.35	0.49
5:Z2:2754:C:H2'	5:Z2:2755:C:C6	2.47	0.49
19:FG:74:LEU:HG	19:FG:78:PHE:CZ	2.46	0.49
30:GR:22:ARG:HH11	30:GR:39:ASP:HA	1.77	0.49
2:F:5:TYR:OH	2:F:7:THR:OG1	2.31	0.48
5:Z2:471:U:O2'	5:Z2:474:G:O6	2.29	0.48
5:Z2:2540:G:H2'	5:Z2:2541:C:C6	2.48	0.48
6:R3:36:ASN:HD21	6:R3:38:LYS:HD2	1.78	0.48
10:F7:29:PRO:HB3	10:F7:160:ALA:HB2	1.94	0.48
35:YW:23:LEU:HD21	35:YW:53:LEU:HD11	1.94	0.48
5:Z2:459:G:H4'	5:Z2:485:A:N1	2.27	0.48
5:Z2:932:C:H2'	5:Z2:933:G:H8	1.74	0.48
5:Z2:993:A:N3	5:Z2:1138:C:O2'	2.41	0.48
10:F7:22:LEU:HD22	10:F7:27:GLN:HB3	1.95	0.48
18:RF:11:ALA:HA	18:RF:100:THR:HG22	1.94	0.48
19:FG:42:TRP:HB2	19:FG:59:TYR:HB2	1.94	0.48
33:KU:19:GLY:O	33:KU:82:ILE:HA	2.13	0.48
2:F:5:TYR:HH	2:F:7:THR:HG1	1.61	0.48
5:Z2:1771:A:H2'	5:Z2:1773:A:N7	2.28	0.48
10:F7:103:LEU:HA	10:F7:107:ALA:HB3	1.95	0.48
5:Z2:386:G:H5"	5:Z2:387:A:OP1	2.13	0.48
5:Z2:642:U:H2'	5:Z2:643:U:C6	2.49	0.48
5:Z2:842:G:H2'	5:Z2:843:G:O4'	2.12	0.48
5:Z2:2356:A:H2'	5:Z2:2357:C:C6	2.48	0.48
5:Z2:2072:U:H2'	5:Z2:2073:U:C6	2.48	0.48
7:A4:48:LEU:HA	7:A4:51:THR:CG2	2.44	0.48
2:F:83:ARG:O	2:F:86:ILE:HG13	2.14	0.48
5:Z2:802:C:O2'	5:Z2:824:U:H5"	2.13	0.48
5:Z2:931:A:H2'	5:Z2:932:C:C6	2.48	0.48
5:Z2:2229:G:H2'	5:Z2:2230:A:C8	2.48	0.48
32:CT:88:GLN:NE2	32:CT:99:ALA:O	2.47	0.48
38:QZ:53:HIS:NE2	38:QZ:55:GLU:HG2	2.28	0.48
4:C1:12:LEU:HG	4:C1:19:VAL:HG21	1.95	0.48
5:Z2:575:A:H2'	5:Z2:576:U:C6	2.49	0.48
5:Z2:856:U:H2'	5:Z2:857:U:H6	1.79	0.48
10:F7:2:ALA:HB1	10:F7:5:LYS:HB3	1.96	0.48
55:D:77:ASP:HB3	55:D:80:LYS:HG3	1.95	0.48
5:Z2:833:U:H2'	5:Z2:834:A:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z2:2573:A:H2'	5:Z2:2574:C:C6	2.49	0.48
2:F:4:ASN:N	2:F:4:ASN:OD1	2.46	0.48
5:Z2:1078:U:H1'	5:Z2:1081:U:H5	1.78	0.48
5:Z2:1421:U:H2'	5:Z2:1422:U:C6	2.49	0.48
5:Z2:1780:A:H2'	5:Z2:1781:C:H6	1.76	0.48
5:Z2:2550:G:H2'	5:Z2:2551:A:C8	2.49	0.48
7:A4:76:GLY:O	7:A4:98:ASP:HA	2.14	0.48
9:L6:49:MET:O	9:L6:51:LYS:NZ	2.31	0.48
27:PO:76:TYR:CZ	27:PO:80:ILE:HG13	2.49	0.48
29:BQ:28:PRO:O	29:BQ:33:ARG:NH1	2.40	0.48
29:BQ:43:GLU:OE1	29:BQ:116:ARG:NH2	2.37	0.48
35:YW:23:LEU:HD11	35:YW:53:LEU:HD11	1.96	0.48
38:QZ:65:VAL:HG12	38:QZ:84:VAL:HG22	1.96	0.48
5:Z2:993:A:OP2	36:IX:39:LYS:NZ	2.41	0.48
5:Z2:2438:G:H2'	5:Z2:2439:C:C6	2.49	0.48
5:Z2:2670:U:H2'	5:Z2:2671:G:O4'	2.14	0.48
5:Z2:573:U:H2'	5:Z2:574:U:C6	2.49	0.47
5:Z2:2000:A:H2'	5:Z2:2001:A:C8	2.49	0.47
5:Z2:2233:G:OP1	5:Z2:2258:C:O2'	2.30	0.47
10:F7:17:LYS:HD2	10:F7:25:VAL:HA	1.95	0.47
12:E9:47:THR:H	12:E9:50:GLU:HG3	1.78	0.47
33:KU:52:PHE:HB3	33:KU:56:ARG:HB3	1.95	0.47
3:H:230:VAL:HG11	3:H:289:VAL:HG21	1.96	0.47
5:Z2:779:A:H2'	5:Z2:780:C:C6	2.49	0.47
5:Z2:1558:A:H2'	5:Z2:1559:A:C8	2.49	0.47
5:Z2:1660:A:C2	5:Z2:2565:G:H5'	2.48	0.47
10:F7:36:LEU:HD22	10:F7:61:ALA:HB2	1.96	0.47
10:F7:133:LYS:HB2	10:F7:133:LYS:HE2	1.62	0.47
7:A4:178:ILE:HD13	7:A4:188:VAL:HG21	1.95	0.47
10:F7:178:LYS:HD2	10:F7:178:LYS:C	2.35	0.47
33:KU:93:ARG:NH2	33:KU:112:ASP:OD2	2.47	0.47
5:Z2:644:G:O2'	12:E9:94:LYS:O	2.26	0.47
5:Z2:1843:G:HO2'	5:Z2:1844:A:H8	1.60	0.47
5:Z2:2058:C:H2'	5:Z2:2059:C:H6	1.78	0.47
7:A4:7:THR:HG23	7:A4:63:ASN:ND2	2.29	0.47
5:Z2:2051:C:H2'	5:Z2:2052:C:H6	1.80	0.47
20:VH:75:PHE:HB2	20:VH:77:ARG:HG2	1.95	0.47
1:B:172:THR:OG1	1:B:174:ASP:OD1	2.33	0.47
2:F:10:ARG:O	2:F:12:THR:N	2.48	0.47
5:Z2:205:C:H2'	5:Z2:206:C:C6	2.49	0.47
5:Z2:342:G:H2'	5:Z2:343:U:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z2:1401:C:O2'	5:Z2:1575:G:O2'	2.25	0.47
5:Z2:1719:U:H2'	5:Z2:1720:C:H6	1.80	0.47
11:D8:58:C:H2'	11:D8:59:A:C8	2.50	0.47
14:MB:114:GLU:HG2	14:MB:119:ASP:CB	2.44	0.47
27:PO:100:MET:HG2	27:PO:101:HIS:CD2	2.50	0.47
32:CT:130:PHE:O	32:CT:134:MET:HG3	2.15	0.47
3:H:291:ARG:HH11	3:H:291:ARG:HG3	1.79	0.47
5:Z2:179:A:H2'	5:Z2:180:C:C6	2.49	0.47
5:Z2:185:G:H5'	16:WD:14:VAL:HG11	1.97	0.47
5:Z2:334:A:H2'	5:Z2:335:C:C6	2.50	0.47
5:Z2:1223:G:H2'	5:Z2:1224:U:O4'	2.14	0.47
5:Z2:1253:A:H2'	5:Z2:1254:C:C6	2.50	0.47
5:Z2:2629:C:H2'	5:Z2:2630:U:O4'	2.14	0.47
33:KU:16:VAL:O	33:KU:18:GLU:N	2.46	0.47
34:NV:12:VAL:HG12	34:NV:16:ILE:HD12	1.96	0.47
38:QZ:34:LEU:HD13	38:QZ:43:GLN:NE2	2.29	0.47
18:RF:73:THR:CG2	18:RF:106:LYS:HB2	2.44	0.47
23:HK:63:ARG:NH2	23:HK:70:PRO:HG3	2.30	0.47
37:JY:15:HIS:HB3	37:JY:70:HIS:CE1	2.50	0.47
5:Z2:9:G:O2'	5:Z2:10:U:OP1	2.27	0.47
5:Z2:424:U:O2'	12:E9:40:GLN:OE1	2.25	0.47
5:Z2:727:G:H2'	5:Z2:728:U:H6	1.80	0.47
5:Z2:798:U:H2'	5:Z2:799:C:H6	1.79	0.47
33:KU:97:VAL:HG11	33:KU:110:ILE:HD13	1.96	0.47
34:NV:48:LYS:HE2	34:NV:48:LYS:HB2	1.67	0.47
36:IX:15:TRP:HB3	36:IX:137:PRO:HB3	1.97	0.47
5:Z2:849:G:H2'	5:Z2:850:C:C6	2.50	0.47
5:Z2:1012:A:N3	5:Z2:2469:C:O2'	2.41	0.47
5:Z2:1392:U:H2'	5:Z2:1393:U:C6	2.49	0.47
32:CT:88:GLN:NE2	32:CT:100:GLN:HA	2.30	0.47
33:KU:46:THR:O	33:KU:50:GLN:HG2	2.15	0.47
18:RF:80:ILE:O	18:RF:100:THR:OG1	2.29	0.46
33:KU:34:ILE:HG23	33:KU:82:ILE:HD11	1.97	0.46
5:Z2:273:G:H2'	5:Z2:274:C:H6	1.80	0.46
5:Z2:1209:A:H2'	5:Z2:1210:A:C8	2.51	0.46
5:Z2:2740:A:N1	30:GR:67:THR:HG21	2.30	0.46
28:SP:71:LEU:HD23	28:SP:71:LEU:HA	1.82	0.46
55:D:52:GLY:C	55:D:54:LYS:H	2.18	0.46
1:B:312:LYS:HD2	1:B:312:LYS:HA	1.63	0.46
5:Z2:117:A:H4'	17:XE:62:ARG:NH2	2.31	0.46
5:Z2:834:A:H2'	5:Z2:835:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BQ:43:GLU:HG3	29:BQ:103:VAL:HG21	1.97	0.46
32:CT:175:LEU:HD23	32:CT:182:ILE:HD13	1.96	0.46
5:Z2:26:A:H2'	5:Z2:27:C:C6	2.50	0.46
5:Z2:1472:U:H2'	5:Z2:1473:U:C6	2.50	0.46
5:Z2:2037:U:O2	5:Z2:2038:A:N6	2.45	0.46
5:Z2:2574:C:H2'	5:Z2:2575:G:H8	1.79	0.46
12:E9:72:ILE:HG13	12:E9:73:ARG:HD3	1.95	0.46
36:IX:133:GLU:CD	36:IX:133:GLU:H	2.18	0.46
37:JY:12:SER:HB2	37:JY:95:GLY:O	2.15	0.46
1:B:74:LYS:HD3	1:B:74:LYS:HA	1.69	0.46
1:B:213:VAL:HG22	1:B:236:VAL:HB	1.98	0.46
5:Z2:245:G:O5'	5:Z2:246:C:H5"	2.16	0.46
5:Z2:769:G:H5'	5:Z2:770:G:OP1	2.15	0.46
5:Z2:2683:A:H2'	5:Z2:2684:C:H6	1.81	0.46
30:GR:11:LEU:HD11	30:GR:50:VAL:HG23	1.98	0.46
32:CT:52:ILE:HG22	32:CT:70:THR:HB	1.97	0.46
33:KU:119:ASN:HA	34:NV:35:ARG:HH12	1.81	0.46
37:JY:81:ASP:HA	37:JY:84:VAL:HG12	1.96	0.46
2:F:125:PHE:CD2	2:F:127:LYS:HE2	2.50	0.46
3:H:262:GLU:HA	3:H:268:LEU:HG	1.98	0.46
5:Z2:2195:A:HO2'	5:Z2:2196:A:P	2.37	0.46
7:A4:159:MET:HG2	7:A4:161:GLY:O	2.16	0.46
12:E9:47:THR:N	12:E9:50:GLU:HG3	2.30	0.46
12:E9:127:ALA:O	12:E9:129:LYS:N	2.49	0.46
16:WD:55:GLY:O	16:WD:59:ILE:HG12	2.14	0.46
1:B:239:LEU:HD12	1:B:240:THR:H	1.80	0.46
4:C1:4:ILE:HD12	4:C1:4:ILE:N	2.30	0.46
4:C1:40:THR:OG1	4:C1:43:ASN:OD1	2.34	0.46
5:Z2:19:G:N7	5:Z2:2610:G:H5"	2.31	0.46
5:Z2:1183:U:H1'	27:PO:4:VAL:HG22	1.98	0.46
7:A4:72:VAL:HA	7:A4:165:ALA:O	2.16	0.46
25:MM:102:THR:O	25:MM:102:THR:OG1	2.33	0.46
5:Z2:565:U:H2'	5:Z2:566:C:H6	1.81	0.46
5:Z2:932:C:H1'	5:Z2:968:A:C8	2.51	0.46
5:Z2:1048:C:H2'	5:Z2:1049:U:O4'	2.16	0.46
5:Z2:2016:A:C2	5:Z2:2482:C:H5"	2.51	0.46
8:E5:31:LYS:HE3	8:E5:31:LYS:HB3	1.59	0.46
14:MB:37:THR:HG23	14:MB:39:PRO:HD2	1.98	0.46
5:Z2:724:A:H1'	5:Z2:725:C:H5	1.81	0.46
5:Z2:1338:A:H2'	5:Z2:1339:G:O4'	2.16	0.46
5:Z2:2314:G:O2'	5:Z2:2319:A:N1	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z2:2628:U:H4'	5:Z2:2715:G:O2'	2.16	0.46
5:Z2:2807:A:H2'	5:Z2:2808:G:C8	2.51	0.46
9:L6:56:ARG:HG3	9:L6:62:GLU:HG2	1.98	0.46
21:TI:85:PHE:HD1	21:TI:85:PHE:HA	1.66	0.46
25:MM:16:VAL:HB	25:MM:41:PRO:HB3	1.98	0.46
37:JY:82:LYS:HE2	37:JY:82:LYS:HB2	1.60	0.46
1:B:212:ILE:O	1:B:235:THR:HA	2.16	0.46
1:B:234:ALA:HB1	1:B:257:ALA:HB1	1.98	0.46
5:Z2:273:G:H2'	5:Z2:274:C:C6	2.51	0.46
5:Z2:629:A:H2'	5:Z2:631:A:C8	2.51	0.46
5:Z2:818:A:H2'	5:Z2:819:G:H8	1.80	0.46
5:Z2:977:G:OP2	27:PO:51:ARG:NH2	2.46	0.46
5:Z2:1215:U:H2'	5:Z2:1216:G:H8	1.81	0.46
5:Z2:1356:U:O2'	5:Z2:2196:A:N3	2.39	0.46
5:Z2:2216:U:H2'	5:Z2:2217:G:H8	1.81	0.46
5:Z2:2754:C:H2'	5:Z2:2755:C:H6	1.82	0.46
12:E9:150:LYS:HE2	12:E9:150:LYS:HB2	1.70	0.46
18:RF:17:VAL:HG11	18:RF:103:ILE:HD11	1.97	0.46
25:MM:33:ILE:HD13	25:MM:60:VAL:HG22	1.98	0.46
2:F:114:LEU:HD21	37:JY:62:ARG:HE	1.81	0.45
25:MM:48:LEU:HB3	25:MM:53:LEU:CD2	2.46	0.45
30:GR:127:THR:OG1	30:GR:128:GLN:N	2.49	0.45
30:GR:164:TYR:HB2	30:GR:167:GLU:HB3	1.99	0.45
5:Z2:85:U:H2'	5:Z2:86:C:C6	2.51	0.45
5:Z2:1418:A:H2'	5:Z2:1419:G:O4'	2.16	0.45
5:Z2:2786:A:O2'	5:Z2:2787:A:OP1	2.34	0.45
11:D8:46:U:H2'	11:D8:47:C:H6	1.80	0.45
23:HK:27:LEU:HD22	23:HK:48:LEU:HB2	1.97	0.45
34:NV:4:VAL:HG21	34:NV:19:PHE:HA	1.99	0.45
5:Z2:894:A:H2'	5:Z2:897:C:C5	2.52	0.45
5:Z2:1010:G:H2'	5:Z2:1011:A:C8	2.51	0.45
5:Z2:2298:U:H2'	5:Z2:2299:U:C6	2.51	0.45
6:R3:26:VAL:O	6:R3:30:LYS:HG2	2.16	0.45
9:L6:14:THR:O	9:L6:14:THR:OG1	2.30	0.45
36:IX:18:VAL:HG11	36:IX:28:LEU:HD11	1.97	0.45
3:H:263:MET:CE	3:H:264:PHE:H	2.29	0.45
5:Z2:627:U:O2'	5:Z2:629:A:N7	2.27	0.45
5:Z2:2521:C:H2'	5:Z2:2522:C:H6	1.82	0.45
5:Z2:2779:G:H2'	5:Z2:2780:C:H6	1.79	0.45
7:A4:14:LEU:HD23	7:A4:217:LEU:HD13	1.98	0.45
7:A4:118:ARG:O	7:A4:121:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:SP:63:SER:OG	28:SP:64:GLU:N	2.49	0.45
32:CT:28:GLN:O	32:CT:31:GLU:HG2	2.16	0.45
1:B:162:PHE:HZ	1:B:199:VAL:HG23	1.82	0.45
3:H:251:ARG:HH11	3:H:288:ASP:HA	1.81	0.45
5:Z2:59:A:H2'	5:Z2:60:A:C8	2.52	0.45
5:Z2:2546:U:H1'	5:Z2:2549:A:N6	2.32	0.45
21:TI:31:ARG:HB3	21:TI:62:PHE:HB3	1.99	0.45
23:HK:27:LEU:CD2	23:HK:48:LEU:HB2	2.45	0.45
37:JY:89:LYS:H	37:JY:89:LYS:HG2	1.63	0.45
55:D:1:MET:HA	55:D:35:GLN:O	2.16	0.45
1:B:247:ALA:O	1:B:251:ILE:HG12	2.17	0.45
8:E5:98:LYS:HB2	8:E5:98:LYS:HE2	1.56	0.45
20:VH:11:ARG:HG2	20:VH:11:ARG:NH1	2.31	0.45
3:H:335:PHE:HD2	3:H:375:LEU:HD21	1.81	0.45
5:Z2:887:C:H2'	5:Z2:888:C:C6	2.51	0.45
7:A4:88:GLN:HB3	7:A4:223:ALA:HB2	1.98	0.45
19:FG:9:LEU:O	19:FG:85:ILE:N	2.46	0.45
3:H:325:PHE:HB2	3:H:353:VAL:HB	1.99	0.45
4:C1:5:LEU:HD12	4:C1:7:GLN:O	2.17	0.45
5:Z2:656:C:H2'	5:Z2:657:C:C6	2.52	0.45
31:GS:70:VAL:HG21	31:GS:105:LEU:HD21	1.98	0.45
38:QZ:53:HIS:HB2	38:QZ:73:ILE:HD13	1.98	0.45
1:B:43:ILE:O	1:B:46:GLU:HG3	2.17	0.45
2:F:21:LYS:HE2	2:F:21:LYS:HB2	1.59	0.45
5:Z2:511:A:H2'	5:Z2:2028:A:N1	2.32	0.45
5:Z2:1072:A:N3	5:Z2:1072:A:H2'	2.32	0.45
5:Z2:1266:U:H2'	5:Z2:1267:G:O4'	2.16	0.45
5:Z2:1391:G:H2'	5:Z2:1392:U:C6	2.52	0.45
5:Z2:2207:G:H4'	5:Z2:2209:C:C2	2.52	0.45
5:Z2:2864:U:O2'	36:IX:134:ALA:O	2.21	0.45
28:SP:27:SER:OG	28:SP:29:LYS:HG2	2.16	0.45
5:Z2:1875:A:H2'	5:Z2:1876:A:C8	2.52	0.45
9:L6:8:ILE:HG12	38:QZ:37:HIS:CD2	2.52	0.45
12:E9:150:LYS:HE2	12:E9:194:GLN:OE1	2.17	0.45
5:Z2:199:U:H2'	5:Z2:200:C:O4'	2.17	0.44
5:Z2:216:A:N3	5:Z2:231:U:O2'	2.37	0.44
5:Z2:761:G:O2'	5:Z2:2224:A:OP1	2.35	0.44
5:Z2:847:G:H2'	5:Z2:848:A:O4'	2.17	0.44
5:Z2:1116:U:OP2	5:Z2:1117:A:H2'	2.17	0.44
5:Z2:1681:U:H5"	5:Z2:1682:C:C5	2.51	0.44
5:Z2:2240:U:O2'	5:Z2:2241:C:H5'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E9:144:ARG:HD3	12:E9:183:ASP:OD2	2.17	0.44
18:RF:37:THR:HG23	18:RF:38:TYR:CD2	2.51	0.44
23:HK:13:ARG:HG2	23:HK:60:LEU:HD23	1.99	0.44
36:IX:67:LYS:HE2	36:IX:67:LYS:HB2	1.80	0.44
1:B:279:ALA:CB	30:GR:177:LYS:HB3	2.47	0.44
3:H:218:GLU:HA	3:H:291:ARG:HH11	1.81	0.44
5:Z2:421:G:H2'	5:Z2:422:A:C8	2.52	0.44
5:Z2:1479:A:H2'	5:Z2:1480:A:C8	2.52	0.44
5:Z2:2060:U:H2'	5:Z2:2061:U:C6	2.52	0.44
5:Z2:2298:U:OP1	10:F7:33:LYS:NZ	2.47	0.44
10:F7:61:ALA:HB1	10:F7:91:LEU:HD11	2.00	0.44
3:H:334:TYR:CE1	3:H:380:ARG:HD2	2.52	0.44
5:Z2:178:A:H2'	5:Z2:179:A:C8	2.52	0.44
5:Z2:275:U:H2'	5:Z2:276:A:H8	1.83	0.44
5:Z2:1706:U:H2'	5:Z2:1707:G:O4'	2.18	0.44
11:D8:47:C:H2'	11:D8:48:A:C8	2.52	0.44
14:MB:28:LEU:HD21	14:MB:95:LEU:HD22	2.00	0.44
5:Z2:91:A:C2	5:Z2:109:A:C5	3.06	0.44
5:Z2:233:C:H2'	5:Z2:234:C:H6	1.82	0.44
5:Z2:1914:A:H2'	5:Z2:1915:G:O4'	2.16	0.44
11:D8:76:A:H2'	11:D8:77:G:O4'	2.18	0.44
11:D8:109:G:H2'	11:D8:110:U:C6	2.53	0.44
12:E9:122:GLU:HG2	12:E9:124:THR:HG23	2.00	0.44
29:BQ:55:GLU:OE1	29:BQ:55:GLU:N	2.47	0.44
31:GS:58:ASP:HB3	31:GS:61:ALA:HB3	2.00	0.44
5:Z2:732:U:H4'	18:RF:92:ARG:NH2	2.29	0.44
5:Z2:2023:U:H2'	5:Z2:2024:G:C8	2.53	0.44
5:Z2:2495:C:H2'	5:Z2:2496:A:O4'	2.18	0.44
32:CT:23:TYR:OH	37:JY:11:LYS:HE2	2.18	0.44
33:KU:29:ASN:OD1	33:KU:30:THR:N	2.50	0.44
33:KU:83:ASP:OD1	33:KU:83:ASP:N	2.45	0.44
35:YW:39:ASP:OD1	35:YW:44:ARG:NE	2.44	0.44
1:B:296:GLY:O	1:B:368:ARG:NH1	2.43	0.44
2:F:61:LEU:HD23	2:F:63:ILE:HD11	2.00	0.44
3:H:233:ARG:HE	3:H:233:ARG:HB3	1.44	0.44
25:MM:49:ASP:OD1	25:MM:50:ASP:N	2.51	0.44
30:GR:83:PHE:HB3	30:GR:141:LEU:HD22	1.99	0.44
32:CT:132:ARG:HA	32:CT:132:ARG:CZ	2.48	0.44
1:B:220:SER:HB2	5:Z2:2540:G:O3'	2.17	0.44
2:F:127:LYS:HD3	2:F:127:LYS:HA	1.82	0.44
5:Z2:1480:A:H2'	5:Z2:1482:C:C5	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z2:1890:G:O2'	5:Z2:1914:A:N1	2.36	0.44
5:Z2:2586:G:H2'	5:Z2:2587:U:O4'	2.18	0.44
7:A4:20:HIS:HB3	7:A4:48:LEU:HD11	1.99	0.44
7:A4:91:ARG:HH21	7:A4:227:ILE:HD12	1.83	0.44
10:F7:2:ALA:HB2	10:F7:94:GLU:HG2	1.99	0.44
33:KU:17:SER:OG	33:KU:18:GLU:N	2.51	0.44
37:JY:75:ASP:N	37:JY:75:ASP:OD1	2.49	0.44
38:QZ:63:ASP:N	38:QZ:63:ASP:OD2	2.51	0.44
5:Z2:156:U:H2'	5:Z2:157:C:C6	2.52	0.44
5:Z2:624:U:H2'	5:Z2:625:C:H6	1.81	0.44
5:Z2:2488:G:O2'	5:Z2:2489:U:H5"	2.18	0.44
11:D8:58:C:H2'	11:D8:59:A:H8	1.82	0.44
15:UC:81:LYS:HD2	15:UC:81:LYS:HA	1.81	0.44
32:CT:35:ASN:HD21	32:CT:59:ARG:HH22	1.65	0.44
1:B:20:PHE:HB3	1:B:98:THR:HG21	2.00	0.44
5:Z2:1579:U:H2'	5:Z2:1580:A:O4'	2.18	0.44
5:Z2:1842:U:H2'	5:Z2:1843:G:O4'	2.18	0.44
7:A4:204:ILE:O	7:A4:204:ILE:HG13	2.12	0.44
15:UC:68:THR:OG1	15:UC:77:GLN:OE1	2.31	0.44
55:D:23:LYS:O	55:D:27:ILE:HG13	2.18	0.44
2:F:117:ARG:HE	2:F:123:PRO:HG3	1.83	0.43
5:Z2:583:U:H2'	5:Z2:584:A:C8	2.53	0.43
5:Z2:708:C:H2'	5:Z2:709:C:O4'	2.18	0.43
5:Z2:1003:U:OP1	5:Z2:1019:U:O2'	2.20	0.43
5:Z2:1211:G:H5"	27:PO:12:ARG:NH1	2.33	0.43
5:Z2:2573:A:H2'	5:Z2:2574:C:H6	1.82	0.43
1:B:214:GLY:O	1:B:237:SER:HA	2.18	0.43
5:Z2:843:G:N3	5:Z2:2251:A:H2'	2.33	0.43
5:Z2:848:A:O2'	5:Z2:849:G:H5'	2.17	0.43
5:Z2:1460:U:H2'	5:Z2:1461:A:C8	2.52	0.43
5:Z2:2681:U:H2'	5:Z2:2682:C:C6	2.53	0.43
5:Z2:2759:A:H4'	5:Z2:2761:A:OP1	2.17	0.43
25:MM:79:ARG:O	25:MM:83:LEU:HB2	2.18	0.43
29:BQ:35:SER:OG	29:BQ:112:ILE:HD13	2.18	0.43
31:GS:12:ILE:HD11	31:GS:28:ASN:ND2	2.33	0.43
5:Z2:913:G:H2'	5:Z2:914:U:C6	2.52	0.43
5:Z2:953:G:H2'	5:Z2:954:U:C6	2.54	0.43
5:Z2:1633:G:H5"	5:Z2:1634:C:H5'	2.00	0.43
5:Z2:1816:U:H2'	5:Z2:1817:G:H8	1.82	0.43
5:Z2:2242:U:H2'	5:Z2:2243:C:H6	1.83	0.43
12:E9:193:LYS:O	12:E9:197:GLU:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z2:1250:G:O2'	5:Z2:1998:G:O6	2.25	0.43
5:Z2:2298:U:H2'	5:Z2:2299:U:H6	1.83	0.43
19:FG:45:ARG:HB2	19:FG:59:TYR:CD1	2.53	0.43
29:BQ:98:LYS:HE2	29:BQ:98:LYS:HB2	1.78	0.43
4:C1:29:PHE:CE1	4:C1:33:LEU:HD12	2.53	0.43
5:Z2:9:G:HO2'	5:Z2:10:U:P	2.39	0.43
5:Z2:140:U:H2'	5:Z2:141:A:C8	2.54	0.43
5:Z2:293:U:H2'	5:Z2:294:G:O4'	2.18	0.43
5:Z2:344:U:O2'	5:Z2:345:A:H5'	2.19	0.43
5:Z2:2056:A:H2'	5:Z2:2057:A:O4'	2.18	0.43
5:Z2:2068:A:H2'	5:Z2:2069:G:O4'	2.19	0.43
5:Z2:2274:U:OP1	5:Z2:2363:U:O2'	2.33	0.43
5:Z2:2374:G:O6	5:Z2:2408:A:H8	2.01	0.43
5:Z2:2654:G:H2'	5:Z2:2655:U:C6	2.53	0.43
28:SP:49:LEU:HD12	28:SP:71:LEU:HD21	2.00	0.43
30:GR:64:HIS:O	30:GR:67:THR:HG23	2.18	0.43
31:GS:119:LEU:HD12	31:GS:119:LEU:HA	1.83	0.43
32:CT:35:ASN:ND2	32:CT:59:ARG:HH22	2.17	0.43
3:H:333:PHE:O	3:H:339:ASP:HA	2.18	0.43
5:Z2:126:U:H5"	5:Z2:128:G:OP2	2.19	0.43
5:Z2:2290:G:H4'	5:Z2:2291:G:O5'	2.17	0.43
5:Z2:2372:G:H5"	5:Z2:2373:U:O4'	2.18	0.43
5:Z2:2567:U:H2'	5:Z2:2568:U:H2'	2.00	0.43
5:Z2:2797:G:H1'	5:Z2:2849:A:H2'	2.00	0.43
7:A4:75:VAL:HG22	7:A4:97:VAL:HG13	2.00	0.43
10:F7:145:LYS:H	10:F7:145:LYS:CD	2.31	0.43
30:GR:55:THR:OG1	30:GR:56:VAL:N	2.51	0.43
31:GS:63:PHE:CZ	31:GS:67:LEU:HD22	2.54	0.43
1:B:59:THR:O	1:B:63:LYS:HG2	2.19	0.43
5:Z2:12:A:H2'	5:Z2:13:A:C8	2.53	0.43
5:Z2:228:A:H2'	5:Z2:229:G:O4'	2.18	0.43
5:Z2:289:A:H2'	5:Z2:290:G:H8	1.83	0.43
5:Z2:375:U:H2'	5:Z2:376:C:H6	1.83	0.43
5:Z2:1504:U:H2'	5:Z2:1505:C:C6	2.53	0.43
15:UC:26:LEU:HG	15:UC:31:LEU:HB2	2.01	0.43
15:UC:82:ALA:HB3	15:UC:96:ASP:HB2	2.01	0.43
19:FG:54:ILE:HD12	19:FG:56:LYS:O	2.19	0.43
30:GR:22:ARG:NH1	30:GR:39:ASP:HA	2.33	0.43
3:H:317:GLU:OE1	3:H:317:GLU:N	2.52	0.43
5:Z2:582:G:H2'	5:Z2:583:U:C6	2.54	0.43
5:Z2:987:G:O2'	5:Z2:994:A:N1	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z2:2194:U:H3'	5:Z2:2195:A:H5"	2.00	0.43
8:E5:53:PHE:CZ	8:E5:143:ARG:HG3	2.53	0.43
17:XE:18:LEU:HA	17:XE:53:LEU:HD13	2.00	0.43
2:F:82:THR:HG23	2:F:96:LEU:HD21	2.01	0.43
5:Z2:709:C:H2'	5:Z2:710:G:C8	2.54	0.43
5:Z2:1593:C:H2'	5:Z2:1594:C:O4'	2.19	0.43
5:Z2:1940:G:O2'	5:Z2:1942:U:O4	2.23	0.43
5:Z2:2711:U:H2'	5:Z2:2712:U:C6	2.54	0.43
27:PO:58:ARG:HA	27:PO:61:TRP:CE3	2.54	0.43
5:Z2:739:C:H2'	5:Z2:740:C:C6	2.54	0.43
5:Z2:1369:A:H4'	5:Z2:1370:U:OP1	2.18	0.43
5:Z2:1514:A:H3'	5:Z2:1515:G:H5"	1.99	0.43
5:Z2:1864:G:H2'	5:Z2:1865:C:O4'	2.18	0.43
5:Z2:2058:C:H2'	5:Z2:2059:C:C6	2.52	0.43
7:A4:186:ILE:H	7:A4:186:ILE:HG12	1.65	0.43
9:L6:109:ASP:OD1	9:L6:109:ASP:N	2.33	0.43
18:RF:3:VAL:O	18:RF:106:LYS:HA	2.18	0.43
20:VH:51:VAL:HG12	20:VH:82:VAL:HG23	2.01	0.43
25:MM:56:ILE:O	25:MM:60:VAL:HG23	2.19	0.43
31:GS:42:ILE:HD12	31:GS:42:ILE:H	1.84	0.43
38:QZ:68:LYS:HB3	38:QZ:82:VAL:HG11	2.01	0.43
5:Z2:134:C:H2'	5:Z2:135:C:C6	2.54	0.42
5:Z2:462:A:N3	5:Z2:464:G:H5"	2.34	0.42
5:Z2:463:A:O2'	21:TI:41:THR:O	2.37	0.42
5:Z2:1401:C:HO2'	5:Z2:1575:G:HO2'	1.55	0.42
5:Z2:1501:A:H3'	5:Z2:1502:G:H8	1.84	0.42
5:Z2:2081:A:H2'	5:Z2:2082:C:C6	2.53	0.42
25:MM:37:VAL:HG11	25:MM:55:ALA:HB1	2.01	0.42
33:KU:53:ARG:HD2	33:KU:53:ARG:HA	1.80	0.42
5:Z2:289:A:H2'	5:Z2:290:G:C8	2.54	0.42
5:Z2:454:A:H2'	5:Z2:455:A:O4'	2.19	0.42
5:Z2:1065:U:H2'	5:Z2:1066:U:C6	2.54	0.42
5:Z2:1625:A:H5'	5:Z2:1746:C:O2'	2.19	0.42
5:Z2:2472:U:HO2'	5:Z2:2474:U:H5	1.65	0.42
5:Z2:2853:C:H2'	5:Z2:2854:U:H6	1.84	0.42
7:A4:73:LEU:HD11	7:A4:97:VAL:HG12	2.01	0.42
23:HK:28:LYS:HA	23:HK:31:ILE:HG12	2.00	0.42
30:GR:12:PRO:HD2	30:GR:15:VAL:HG21	2.00	0.42
38:QZ:17:ARG:HD2	38:QZ:64:LEU:HB2	2.01	0.42
5:Z2:124:A:OP2	5:Z2:125:A:H2'	2.20	0.42
5:Z2:745:G:H2'	5:Z2:746:A:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z2:1273:C:H2'	5:Z2:1274:U:H6	1.83	0.42
5:Z2:2717:U:H4'	5:Z2:2718:G:H5"	2.01	0.42
8:E5:159:ALA:HA	8:E5:169:ILE:HD12	2.01	0.42
1:B:98:THR:HG1	1:B:101:ARG:NH2	2.15	0.42
3:H:348:ASP:N	3:H:348:ASP:OD1	2.50	0.42
5:Z2:137:A:H2'	5:Z2:138:C:C6	2.54	0.42
5:Z2:1062:U:H5"	5:Z2:1063:C:H5'	2.02	0.42
5:Z2:1427:C:H2'	5:Z2:1428:A:O4'	2.19	0.42
5:Z2:2588:U:H2'	5:Z2:2589:C:C6	2.54	0.42
5:Z2:2735:C:H2'	5:Z2:2736:A:O4'	2.19	0.42
5:Z2:2767:U:H2'	5:Z2:2768:U:C6	2.54	0.42
8:E5:97:SER:OG	8:E5:135:SER:O	2.24	0.42
33:KU:25:ALA:O	33:KU:88:GLY:HA3	2.19	0.42
36:IX:120:LYS:O	36:IX:123:LYS:NZ	2.51	0.42
1:B:337:LEU:HD23	1:B:337:LEU:HA	1.91	0.42
5:Z2:2369:U:H2'	5:Z2:2370:U:C6	2.55	0.42
12:E9:4:LYS:HD2	12:E9:10:ALA:HA	2.02	0.42
23:HK:45:MET:O	23:HK:49:GLN:HG3	2.19	0.42
29:BQ:82:ARG:H	29:BQ:82:ARG:HG2	1.64	0.42
30:GR:96:ALA:HB2	30:GR:105:LEU:HD23	2.01	0.42
32:CT:132:ARG:HA	32:CT:132:ARG:NH1	2.35	0.42
1:B:99:PRO:HD3	1:B:101:ARG:HH21	1.84	0.42
3:H:256:THR:HG21	3:H:281:LEU:HD22	2.02	0.42
4:C1:12:LEU:HD12	4:C1:12:LEU:HA	1.85	0.42
5:Z2:295:G:H2'	5:Z2:296:G:C8	2.54	0.42
5:Z2:695:G:H2'	5:Z2:696:C:H6	1.84	0.42
10:F7:2:ALA:CB	10:F7:94:GLU:HG2	2.50	0.42
29:BQ:18:GLN:HE21	29:BQ:74:ILE:HB	1.85	0.42
38:QZ:27:ILE:HG21	38:QZ:59:CYS:SG	2.59	0.42
38:QZ:87:LYS:HD2	38:QZ:88:VAL:HG23	2.01	0.42
5:Z2:133:A:H5"	5:Z2:134:C:C6	2.54	0.42
5:Z2:315:U:H4'	21:TI:64:HIS:CD2	2.55	0.42
5:Z2:846:A:H2'	5:Z2:847:G:O4'	2.20	0.42
5:Z2:2549:A:H4'	5:Z2:2550:G:H5"	2.02	0.42
8:E5:74:ARG:HE	8:E5:74:ARG:HB2	1.56	0.42
30:GR:33:LEU:HD22	30:GR:137:ASP:HB3	2.02	0.42
32:CT:35:ASN:O	32:CT:39:VAL:HG23	2.19	0.42
33:KU:21:ALA:HB2	33:KU:82:ILE:HD13	2.01	0.42
33:KU:31:ILE:HG23	33:KU:46:THR:HG22	2.02	0.42
5:Z2:71:G:H2'	5:Z2:72:C:H6	1.85	0.42
5:Z2:482:U:H2'	5:Z2:483:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z2:617:A:H2'	5:Z2:618:A:C8	2.55	0.42
5:Z2:619:C:H2'	5:Z2:620:C:C6	2.55	0.42
5:Z2:985:A:H2'	5:Z2:986:G:O4'	2.20	0.42
5:Z2:2812:G:H2'	5:Z2:2813:U:C6	2.54	0.42
3:H:218:GLU:HA	3:H:291:ARG:NH1	2.34	0.42
5:Z2:1351:A:C5	5:Z2:1352:G:H1'	2.55	0.42
5:Z2:1459:G:O2'	5:Z2:1500:G:O6	2.31	0.42
5:Z2:2435:C:H2'	5:Z2:2436:A:C8	2.55	0.42
5:Z2:2528:G:H2'	5:Z2:2529:U:O4'	2.20	0.42
7:A4:20:HIS:HA	7:A4:46:ILE:HB	2.02	0.42
8:E5:90:ILE:HD11	8:E5:152:MET:SD	2.60	0.42
14:MB:117:ASP:O	14:MB:118:ARG:HB3	2.19	0.42
24:OL:53:ARG:HG2	24:OL:53:ARG:HH11	1.85	0.42
32:CT:147:LYS:HE3	32:CT:147:LYS:HB2	1.90	0.42
1:B:45:GLU:OE1	1:B:61:LEU:HG	2.20	0.42
2:F:41:THR:HA	31:GS:16:PRO:HG3	2.02	0.42
2:F:93:LYS:O	2:F:97:LYS:HB2	2.20	0.42
2:F:110:GLU:OE2	2:F:113:LYS:HE2	2.20	0.42
3:H:238:ILE:HD12	3:H:238:ILE:HA	1.88	0.42
14:MB:78:LYS:O	14:MB:82:THR:HG22	2.20	0.42
18:RF:20:VAL:HG11	18:RF:44:ALA:HA	2.01	0.42
5:Z2:1215:U:H2'	5:Z2:1216:G:C8	2.55	0.41
12:E9:3:LEU:HD12	12:E9:13:LEU:HD12	2.02	0.41
21:TI:63:LEU:HD23	21:TI:63:LEU:H	1.85	0.41
30:GR:40:LEU:C	30:GR:55:THR:HG23	2.41	0.41
1:B:332:ASP:OD1	1:B:332:ASP:N	2.30	0.41
3:H:213:PHE:HA	3:H:237:GLY:HA3	2.02	0.41
5:Z2:948:C:O2'	5:Z2:2256:A:N3	2.39	0.41
5:Z2:1205:U:H2'	5:Z2:1206:C:C6	2.55	0.41
5:Z2:1869:U:H2'	5:Z2:1870:G:O4'	2.21	0.41
5:Z2:1932:U:H2'	5:Z2:1933:C:C6	2.55	0.41
27:PO:83:MET:SD	27:PO:113:ALA:HB2	2.61	0.41
29:BQ:18:GLN:HE22	29:BQ:74:ILE:H	1.66	0.41
29:BQ:47:ALA:HB3	29:BQ:64:GLU:HB2	2.01	0.41
30:GR:158:LYS:HE3	30:GR:158:LYS:HB3	1.76	0.41
32:CT:10:ILE:HD13	32:CT:178:LEU:HD11	2.03	0.41
32:CT:136:ARG:NH2	32:CT:140:ASN:OD1	2.34	0.41
1:B:339:ILE:O	1:B:343:ILE:HG12	2.20	0.41
5:Z2:1384:A:H2'	5:Z2:1385:A:C8	2.56	0.41
5:Z2:1414:G:H2'	5:Z2:1415:A:O4'	2.21	0.41
5:Z2:1707:G:C6	5:Z2:1724:G:C6	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z2:2230:A:H2'	5:Z2:2231:C:H6	1.85	0.41
5:Z2:2312:A:H2'	5:Z2:2313:G:C8	2.54	0.41
5:Z2:2724:A:H2'	5:Z2:2725:C:O4'	2.20	0.41
8:E5:165:SER:OG	8:E5:168:GLU:HG3	2.20	0.41
23:HK:96:VAL:HG22	37:JY:67:ILE:HB	2.02	0.41
31:GS:53:LYS:HE3	31:GS:53:LYS:HB2	1.94	0.41
35:YW:9:LEU:HD21	35:YW:55:LYS:HB3	2.01	0.41
35:YW:24:LYS:HE2	35:YW:24:LYS:HB3	1.86	0.41
5:Z2:221:U:O4	5:Z2:403:C:H5'	2.20	0.41
5:Z2:814:A:N7	5:Z2:2231:C:H5'	2.35	0.41
5:Z2:1468:C:H2'	5:Z2:1469:A:H8	1.85	0.41
7:A4:59:LEU:HA	7:A4:62:VAL:HG22	2.01	0.41
25:MM:3:ARG:NH1	25:MM:6:GLY:HA2	2.35	0.41
32:CT:35:ASN:HD21	32:CT:59:ARG:HH12	1.68	0.41
1:B:280:ASN:HD22	3:H:316:LYS:NZ	2.18	0.41
3:H:295:LEU:HD23	3:H:295:LEU:HA	1.80	0.41
3:H:314:LEU:HD23	3:H:314:LEU:HA	1.94	0.41
4:C1:4:ILE:CD1	4:C1:39:ALA:HA	2.51	0.41
5:Z2:721:C:H2'	5:Z2:722:C:C6	2.56	0.41
5:Z2:982:C:H2'	5:Z2:983:U:O4'	2.20	0.41
5:Z2:1044:U:C2	5:Z2:1046:G:H5'	2.56	0.41
5:Z2:1852:A:H2'	5:Z2:1853:G:O4'	2.21	0.41
5:Z2:2520:U:H2'	5:Z2:2521:C:C6	2.55	0.41
7:A4:124:LYS:HE3	7:A4:124:LYS:HB2	1.71	0.41
10:F7:170:LEU:HD23	10:F7:170:LEU:HA	1.85	0.41
12:E9:33:ALA:HA	12:E9:93:GLN:OE1	2.21	0.41
31:GS:31:MET:HE3	31:GS:34:GLY:HA2	2.02	0.41
5:Z2:726:U:H2'	5:Z2:727:G:C8	2.55	0.41
5:Z2:1664:A:H2'	5:Z2:1665:A:O4'	2.21	0.41
5:Z2:2662:A:H2'	5:Z2:2663:C:O4'	2.21	0.41
7:A4:51:THR:O	7:A4:55:PHE:HB2	2.20	0.41
10:F7:4:LEU:HD13	10:F7:101:ASP:HB2	2.02	0.41
23:HK:99:ALA:HB2	37:JY:66:GLU:HG2	2.02	0.41
27:PO:52:ASN:HA	27:PO:55:ARG:HD2	2.02	0.41
28:SP:36:ARG:HD2	28:SP:52:HIS:O	2.20	0.41
29:BQ:76:THR:HG22	29:BQ:132:ALA:HB3	2.02	0.41
30:GR:107:VAL:HG23	30:GR:108:GLY:H	1.85	0.41
33:KU:34:ILE:H	33:KU:34:ILE:HD12	1.85	0.41
1:B:73:HIS:HA	1:B:76:ASN:ND2	2.36	0.41
5:Z2:993:A:P	36:IX:39:LYS:HZ1	2.42	0.41
5:Z2:1064:C:H2'	5:Z2:1065:U:H6	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z2:1671:U:H2'	5:Z2:1672:A:C8	2.56	0.41
5:Z2:1727:C:H2'	5:Z2:1728:U:O4'	2.21	0.41
5:Z2:2426:U:OP1	12:E9:62:LYS:HD3	2.20	0.41
15:UC:13:ARG:HB3	15:UC:45:SER:HB3	2.02	0.41
19:FG:11:HIS:CE1	19:FG:54:ILE:HG21	2.55	0.41
24:OL:15:GLN:HE22	24:OL:19:ASN:HA	1.84	0.41
33:KU:106:LYS:HE3	33:KU:106:LYS:HB3	1.79	0.41
1:B:69:LYS:HB2	1:B:69:LYS:HE3	1.87	0.41
5:Z2:179:A:H2'	5:Z2:180:C:H6	1.86	0.41
5:Z2:458:C:H2'	5:Z2:459:G:O4'	2.21	0.41
5:Z2:616:A:H2'	5:Z2:617:A:O4'	2.21	0.41
5:Z2:1854:C:H2'	5:Z2:1855:G:O4'	2.21	0.41
5:Z2:2229:G:H2'	5:Z2:2230:A:H8	1.85	0.41
11:D8:113:G:H2'	11:D8:114:C:C6	2.56	0.41
23:HK:20:TYR:HD2	23:HK:55:SER:HB3	1.86	0.41
23:HK:63:ARG:HH21	23:HK:70:PRO:HG3	1.86	0.41
31:GS:5:ARG:H	31:GS:5:ARG:HE	1.68	0.41
37:JY:52:LEU:HA	37:JY:62:ARG:HA	2.03	0.41
3:H:315:SER:OG	3:H:318:GLU:OE1	2.28	0.41
5:Z2:85:U:H2'	5:Z2:86:C:H6	1.86	0.41
5:Z2:448:G:H2'	5:Z2:449:A:C8	2.55	0.41
5:Z2:1084:C:H2'	5:Z2:1085:U:O4'	2.21	0.41
5:Z2:1226:U:H2'	5:Z2:1227:C:C6	2.56	0.41
5:Z2:1262:C:H2'	5:Z2:1263:G:H8	1.85	0.41
5:Z2:1425:G:H2'	5:Z2:1426:U:C6	2.56	0.41
5:Z2:1891:C:H2'	5:Z2:1916:G:C8	2.56	0.41
5:Z2:2049:C:O2	5:Z2:2433:A:N1	2.54	0.41
5:Z2:2297:G:H1'	10:F7:155:THR:HG21	2.02	0.41
5:Z2:2663:C:O2'	5:Z2:2664:C:H5'	2.20	0.41
7:A4:14:LEU:HD23	7:A4:14:LEU:HA	1.91	0.41
7:A4:167:PHE:HA	7:A4:189:ILE:O	2.20	0.41
11:D8:27:A:H2'	11:D8:28:C:O4'	2.21	0.41
15:UC:84:GLN:HB2	15:UC:94:HIS:HB3	2.03	0.41
15:UC:86:HIS:HB3	15:UC:90:GLY:H	1.86	0.41
19:FG:2:ARG:HE	19:FG:91:ARG:CZ	2.34	0.41
25:MM:64:MET:HG3	25:MM:68:ASP:HB3	2.02	0.41
25:MM:66:GLU:OE1	25:MM:66:GLU:N	2.53	0.41
34:NV:40:LYS:O	34:NV:44:VAL:HG23	2.21	0.41
1:B:37:LEU:O	1:B:41:LEU:HG	2.20	0.41
5:Z2:244:G:H4'	5:Z2:369:G:C4	2.56	0.41
5:Z2:335:C:H2'	5:Z2:336:A:N3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z2:554:U:H2'	5:Z2:555:G:O4'	2.21	0.41
5:Z2:1006:G:N7	36:IX:68:LYS:HD2	2.36	0.41
5:Z2:2197:C:H2'	5:Z2:2198:A:O4'	2.20	0.41
5:Z2:2269:G:N3	5:Z2:2269:G:H2'	2.36	0.41
7:A4:215:VAL:O	7:A4:219:VAL:HG23	2.21	0.41
23:HK:22:ASP:OD1	23:HK:23:LYS:N	2.54	0.41
32:CT:150:LYS:HG2	32:CT:201:TRP:CE3	2.56	0.41
55:D:24:LEU:HD23	55:D:24:LEU:HA	1.92	0.41
1:B:130:ARG:NH1	5:Z2:1928:C:OP1	2.54	0.40
5:Z2:707:A:H2'	5:Z2:708:C:O4'	2.21	0.40
5:Z2:1431:C:H2'	5:Z2:1432:U:C6	2.56	0.40
5:Z2:1453:A:H2'	5:Z2:1454:A:H8	1.82	0.40
5:Z2:1785:G:H5'	5:Z2:1805:A:N6	2.36	0.40
5:Z2:2825:G:H2'	5:Z2:2826:A:C8	2.56	0.40
7:A4:51:THR:HB	7:A4:206:PRO:O	2.21	0.40
12:E9:74:SER:O	12:E9:80:GLY:HA3	2.21	0.40
14:MB:55:ALA:HA	14:MB:80:PHE:CE2	2.56	0.40
15:UC:53:LEU:O	15:UC:57:LEU:HG	2.21	0.40
30:GR:46:GLU:HB2	30:GR:49:VAL:HG13	2.01	0.40
33:KU:72:LYS:HE2	33:KU:72:LYS:HB3	1.62	0.40
1:B:99:PRO:HD2	1:B:101:ARG:HE	1.86	0.40
1:B:160:ILE:HG12	20:VH:4:LYS:HG2	2.02	0.40
3:H:340:VAL:HG13	3:H:365:LEU:HD22	2.03	0.40
5:Z2:124:A:H5'	5:Z2:125:A:H8	1.87	0.40
5:Z2:2289:C:OP2	5:Z2:2290:G:O2'	2.28	0.40
7:A4:112:LEU:HD23	7:A4:112:LEU:HA	1.78	0.40
10:F7:8:TYR:OH	10:F7:29:PRO:O	2.37	0.40
20:VH:37:ILE:HG21	20:VH:80:VAL:HG11	2.02	0.40
21:TI:47:ASN:HD22	21:TI:50:THR:HG23	1.85	0.40
25:MM:49:ASP:O	25:MM:53:LEU:HD23	2.20	0.40
32:CT:22:TRP:HB3	32:CT:59:ARG:HG2	2.03	0.40
32:CT:136:ARG:HD2	32:CT:136:ARG:HA	1.85	0.40
36:IX:31:GLN:HB3	36:IX:142:ILE:HG13	2.03	0.40
37:JY:8:ILE:HB	37:JY:74:VAL:HG23	2.02	0.40
38:QZ:23:MET:HB2	38:QZ:26:SER:CB	2.50	0.40
1:B:177:SER:HB3	5:Z2:2435:C:OP1	2.21	0.40
5:Z2:37:G:H2'	5:Z2:38:C:H6	1.86	0.40
5:Z2:672:C:H2'	5:Z2:673:U:O4'	2.21	0.40
5:Z2:1447:A:H2'	5:Z2:1448:G:C8	2.57	0.40
5:Z2:1580:A:HO2'	5:Z2:1581:A:P	2.42	0.40
5:Z2:1602:A:P	5:Z2:1602:A:H8	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E9:155:ASN:OD1	12:E9:155:ASN:C	2.60	0.40
31:GS:72:PRO:O	31:GS:97:ARG:NE	2.54	0.40
37:JY:6:ILE:HG13	37:JY:76:ILE:HG12	2.03	0.40
1:B:127:VAL:HB	1:B:134:ARG:HB2	2.04	0.40
2:F:65:VAL:HG21	2:F:77:ILE:HD11	2.04	0.40
3:H:246:GLU:CD	3:H:298:PRO:HA	2.42	0.40
4:C1:9:ILE:HD11	4:C1:12:LEU:CD2	2.51	0.40
5:Z2:173:A:O2'	5:Z2:174:A:H5'	2.21	0.40
5:Z2:674:A:H2'	5:Z2:675:U:C6	2.57	0.40
5:Z2:943:A:H2'	5:Z2:944:A:C8	2.57	0.40
5:Z2:1402:G:N2	5:Z2:1567:A:N7	2.69	0.40
5:Z2:1513:A:H2'	5:Z2:1514:A:C8	2.55	0.40
5:Z2:1707:G:H8	5:Z2:1707:G:OP2	2.05	0.40
5:Z2:1999:A:H4'	18:RF:96:ILE:HD13	2.04	0.40
7:A4:78:LYS:HE2	7:A4:78:LYS:HB2	1.81	0.40
25:MM:65:THR:OG1	25:MM:66:GLU:N	2.54	0.40
37:JY:42:LEU:HD12	37:JY:71:LYS:HD3	2.02	0.40
5:Z2:281:A:H62	5:Z2:331:G:N2	2.19	0.40
5:Z2:560:A:H2'	5:Z2:561:U:H6	1.86	0.40
5:Z2:1750:G:H2'	5:Z2:1751:C:O4'	2.22	0.40
5:Z2:1866:U:H2'	5:Z2:1867:C:C6	2.57	0.40
5:Z2:2306:G:H2'	5:Z2:2307:U:O4'	2.21	0.40
5:Z2:2421:U:O2'	5:Z2:2423:C:OP1	2.28	0.40
5:Z2:2644:G:OP2	5:Z2:2644:G:H8	2.04	0.40
5:Z2:2852:G:H2'	5:Z2:2853:C:C6	2.56	0.40
6:R3:25:ASP:CG	19:FG:101:GLN:HE21	2.25	0.40
6:R3:36:ASN:HA	6:R3:72:ASP:HB3	2.03	0.40
18:RF:81:THR:HG21	18:RF:97:SER:HB3	2.02	0.40
30:GR:27:LYS:HB3	30:GR:27:LYS:HE2	1.86	0.40
34:NV:5:LYS:NZ	34:NV:5:LYS:HB2	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	356/369 (96%)	330 (93%)	24 (7%)	2 (1%)	25	45
2	F	123/128 (96%)	117 (95%)	5 (4%)	1 (1%)	19	36
3	H	182/396 (46%)	173 (95%)	7 (4%)	2 (1%)	14	27
4	C1	47/166 (28%)	46 (98%)	1 (2%)	0	100	100
6	R3	54/76 (71%)	54 (100%)	0	0	100	100
7	A4	231/269 (86%)	221 (96%)	10 (4%)	0	100	100
8	E5	154/171 (90%)	145 (94%)	9 (6%)	0	100	100
9	L6	120/124 (97%)	113 (94%)	7 (6%)	0	100	100
10	F7	175/178 (98%)	165 (94%)	10 (6%)	0	100	100
12	E9	197/200 (98%)	192 (98%)	5 (2%)	0	100	100
13	aA	51/60 (85%)	50 (98%)	1 (2%)	0	100	100
14	MB	117/119 (98%)	112 (96%)	4 (3%)	1 (1%)	17	33
15	UC	95/219 (43%)	91 (96%)	4 (4%)	0	100	100
16	WD	74/78 (95%)	72 (97%)	2 (3%)	0	100	100
17	XE	60/65 (92%)	60 (100%)	0	0	100	100
18	RF	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
19	FG	100/134 (75%)	98 (98%)	2 (2%)	0	100	100
20	VH	82/85 (96%)	75 (92%)	7 (8%)	0	100	100
21	TI	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
22	fJ	57/93 (61%)	55 (96%)	2 (4%)	0	100	100
23	HK	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
24	OL	84/88 (96%)	81 (96%)	3 (4%)	0	100	100
25	MM	108/118 (92%)	98 (91%)	9 (8%)	1 (1%)	17	33
27	PO	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
28	SP	78/91 (86%)	76 (97%)	2 (3%)	0	100	100
29	BQ	129/132 (98%)	128 (99%)	1 (1%)	0	100	100
30	GR	173/177 (98%)	162 (94%)	11 (6%)	0	100	100
31	GS	150/157 (96%)	140 (93%)	8 (5%)	2 (1%)	12	23
32	CT	202/241 (84%)	187 (93%)	15 (7%)	0	100	100
33	KU	112/129 (87%)	108 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	NV	55/71 (78%)	54 (98%)	1 (2%)	0	100	100
35	YW	54/59 (92%)	54 (100%)	0	0	100	100
36	IX	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
37	JY	97/103 (94%)	88 (91%)	9 (9%)	0	100	100
38	QZ	77/91 (85%)	72 (94%)	5 (6%)	0	100	100
39	Ba	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
40	Qb	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
41	Nc	111/116 (96%)	110 (99%)	1 (1%)	0	100	100
42	Kd	143/146 (98%)	135 (94%)	8 (6%)	0	100	100
43	Je	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
44	Af	209/212 (99%)	196 (94%)	12 (6%)	1 (0%)	29	50
45	Lg	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
46	dh	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
47	Oi	113/130 (87%)	107 (95%)	6 (5%)	0	100	100
48	Pj	79/89 (89%)	78 (99%)	1 (1%)	0	100	100
49	bk	47/51 (92%)	47 (100%)	0	0	100	100
50	Cl	270/274 (98%)	260 (96%)	10 (4%)	0	100	100
51	Dm	210/213 (99%)	200 (95%)	10 (5%)	0	100	100
52	Sn	86/116 (74%)	86 (100%)	0	0	100	100
53	To	84/88 (96%)	83 (99%)	1 (1%)	0	100	100
54	ep	36/38 (95%)	36 (100%)	0	0	100	100
55	D	103/126 (82%)	100 (97%)	3 (3%)	0	100	100
All	All	6104/7032 (87%)	5848 (96%)	246 (4%)	10 (0%)	50	69

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	96	LEU
3	H	250	ILE
31	GS	17	LYS
2	F	11	LYS
3	H	301	ILE
25	MM	109	ARG
1	B	95	PRO

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Mol	Chain	Res	Type
14	MB	118	ARG
44	Af	196	ILE
31	GS	150	LYS

5.3.2 Protein sidechains (i)

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	B	302/310 (97%)	262 (87%)	40 (13%)	4 6
2	F	102/105 (97%)	86 (84%)	16 (16%)	2 3
3	H	151/327 (46%)	129 (85%)	22 (15%)	3 4
4	C1	39/135 (29%)	39 (100%)	0	100 100
6	R3	51/67 (76%)	50 (98%)	1 (2%)	55 77
7	A4	188/211 (89%)	160 (85%)	28 (15%)	3 4
8	E5	118/131 (90%)	106 (90%)	12 (10%)	7 13
9	L6	102/103 (99%)	94 (92%)	8 (8%)	12 24
10	F7	139/146 (95%)	129 (93%)	10 (7%)	14 27
12	E9	159/159 (100%)	146 (92%)	13 (8%)	11 21
13	aA	46/53 (87%)	43 (94%)	3 (6%)	17 33
14	MB	101/102 (99%)	97 (96%)	4 (4%)	31 55
15	UC	79/184 (43%)	75 (95%)	4 (5%)	24 45
16	WD	67/71 (94%)	64 (96%)	3 (4%)	27 50
17	XE	54/57 (95%)	46 (85%)	8 (15%)	3 4
18	RF	88/88 (100%)	81 (92%)	7 (8%)	12 23
19	FG	92/121 (76%)	77 (84%)	15 (16%)	2 3
20	VH	60/62 (97%)	58 (97%)	2 (3%)	38 62
21	TI	83/85 (98%)	67 (81%)	16 (19%)	1 2
22	fJ	52/81 (64%)	41 (79%)	11 (21%)	1 1
23	HK	87/88 (99%)	85 (98%)	2 (2%)	50 73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	OL	75/77 (97%)	70 (93%)	5 (7%)	16 31
25	MM	91/99 (92%)	79 (87%)	12 (13%)	4 6
27	PO	88/90 (98%)	85 (97%)	3 (3%)	37 61
28	SP	71/79 (90%)	62 (87%)	9 (13%)	4 7
29	BQ	103/104 (99%)	96 (93%)	7 (7%)	16 30
30	GR	149/151 (99%)	133 (89%)	16 (11%)	6 11
31	GS	123/128 (96%)	104 (85%)	19 (15%)	2 4
32	CT	168/198 (85%)	140 (83%)	28 (17%)	2 3
33	KU	84/98 (86%)	72 (86%)	12 (14%)	3 5
34	NV	49/63 (78%)	46 (94%)	3 (6%)	18 36
35	YW	50/52 (96%)	47 (94%)	3 (6%)	19 37
36	IX	116/117 (99%)	109 (94%)	7 (6%)	19 37
37	JY	87/90 (97%)	74 (85%)	13 (15%)	3 4
38	QZ	73/84 (87%)	64 (88%)	9 (12%)	4 8
39	Ba	37/37 (100%)	33 (89%)	4 (11%)	6 11
40	Qb	89/89 (100%)	76 (85%)	13 (15%)	3 4
41	Nc	81/85 (95%)	80 (99%)	1 (1%)	71 86
42	Kd	108/110 (98%)	103 (95%)	5 (5%)	27 50
43	Je	102/102 (100%)	99 (97%)	3 (3%)	42 67
44	Af	161/162 (99%)	147 (91%)	14 (9%)	10 19
45	Lg	114/114 (100%)	105 (92%)	9 (8%)	12 23
46	dh	55/56 (98%)	51 (93%)	4 (7%)	14 27
47	Oi	97/108 (90%)	91 (94%)	6 (6%)	18 35
48	Pj	63/68 (93%)	61 (97%)	2 (3%)	39 63
49	bk	42/46 (91%)	37 (88%)	5 (12%)	5 8
50	Cl	219/221 (99%)	210 (96%)	9 (4%)	30 55
51	Dm	177/181 (98%)	169 (96%)	8 (4%)	27 50
52	Sn	76/97 (78%)	68 (90%)	8 (10%)	7 12
53	To	66/69 (96%)	66 (100%)	0	100 100
54	ep	33/33 (100%)	32 (97%)	1 (3%)	41 66
55	D	91/106 (86%)	80 (88%)	11 (12%)	5 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5098/5800 (88%)	4624 (91%)	474 (9%)	12 16

All (474) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	SER
1	B	10	GLU
1	B	14	ASN
1	B	46	GLU
1	B	69	LYS
1	B	86	VAL
1	B	87	ASP
1	B	91	LEU
1	B	92	ILE
1	B	94	MET
1	B	110	THR
1	B	112	ASP
1	B	117	MET
1	B	132	LYS
1	B	142	ARG
1	B	143	VAL
1	B	148	ASP
1	B	165	ASP
1	B	174	ASP
1	B	180	SER
1	B	189	LYS
1	B	200	GLN
1	B	201	GLU
1	B	210	LEU
1	B	215	ASP
1	B	220	SER
1	B	225	VAL
1	B	237	SER
1	B	244	ASP
1	B	288	ASP
1	B	300	THR
1	B	318	GLN
1	B	330	VAL
1	B	332	ASP
1	B	333	ASP
1	B	337	LEU
1	B	354	GLN

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Mol	Chain	Res	Type
1	B	356	MET
1	B	357	MET
1	B	369	TYR
2	F	3	ARG
2	F	4	ASN
2	F	5	TYR
2	F	14	THR
2	F	16	ARG
2	F	21	LYS
2	F	34	ASP
2	F	39	ARG
2	F	41	THR
2	F	44	MET
2	F	65	VAL
2	F	66	LYS
2	F	87	GLU
2	F	103	THR
2	F	104	ARG
2	F	126	SER
3	H	222	SER
3	H	230	VAL
3	H	233	ARG
3	H	257	THR
3	H	266	LYS
3	H	267	LEU
3	H	269	ASP
3	H	272	ARG
3	H	277	CYS
3	H	280	LEU
3	H	300	SER
3	H	305	THR
3	H	308	ASP
3	H	316	LYS
3	H	323	THR
3	H	336	ARG
3	H	339	ASP
3	H	352	MET
3	H	354	MET
3	H	364	GLU
3	H	375	LEU
3	H	376	ARG
6	R3	73	ASN

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Mol	Chain	Res	Type
7	A4	7	THR
7	A4	28	TRP
7	A4	43	ILE
7	A4	53	LYS
7	A4	55	PHE
7	A4	65	LEU
7	A4	67	SER
7	A4	72	VAL
7	A4	82	SER
7	A4	97	VAL
7	A4	112	LEU
7	A4	121	GLU
7	A4	124	LYS
7	A4	135	THR
7	A4	140	LEU
7	A4	141	GLU
7	A4	153	LEU
7	A4	158	ASP
7	A4	179	LYS
7	A4	186	ILE
7	A4	188	VAL
7	A4	189	ILE
7	A4	192	VAL
7	A4	194	THR
7	A4	196	SER
7	A4	204	ILE
7	A4	216	SER
7	A4	218	TYR
8	E5	16	LEU
8	E5	22	THR
8	E5	24	ASP
8	E5	37	SER
8	E5	70	GLU
8	E5	78	THR
8	E5	80	GLU
8	E5	91	LYS
8	E5	97	SER
8	E5	119	VAL
8	E5	164	LYS
8	E5	167	ASP
9	L6	13	LYS
9	L6	17	GLU

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Mol	Chain	Res	Type
9	L6	30	ARG
9	L6	41	THR
9	L6	62	GLU
9	L6	78	SER
9	L6	86	ARG
9	L6	108	LYS
10	F7	3	ARG
10	F7	7	LEU
10	F7	48	LYS
10	F7	71	ARG
10	F7	112	ARG
10	F7	120	LYS
10	F7	125	ARG
10	F7	144	ASP
10	F7	145	LYS
10	F7	178	LYS
12	E9	4	LYS
12	E9	12	GLU
12	E9	50	GLU
12	E9	74	SER
12	E9	94	LYS
12	E9	95	VAL
12	E9	110	GLU
12	E9	126	SER
12	E9	138	SER
12	E9	170	ASP
12	E9	171	THR
12	E9	172	SER
12	E9	178	SER
13	aA	12	ARG
13	aA	36	LYS
13	aA	39	ARG
14	MB	6	SER
14	MB	27	SER
14	MB	75	MET
14	MB	118	ARG
15	UC	5	HIS
15	UC	20	LYS
15	UC	47	SER
15	UC	55	LYS
16	WD	7	VAL
16	WD	24	LYS

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Mol	Chain	Res	Type
16	WD	25	THR
17	XE	2	LYS
17	XE	21	LYS
17	XE	23	LEU
17	XE	37	LEU
17	XE	39	ASN
17	XE	43	VAL
17	XE	45	VAL
17	XE	60	LYS
18	RF	1	MET
18	RF	2	GLU
18	RF	29	ILE
18	RF	45	VAL
18	RF	49	LYS
18	RF	70	LYS
18	RF	73	THR
19	FG	6	VAL
19	FG	9	LEU
19	FG	11	HIS
19	FG	18	VAL
19	FG	19	VAL
19	FG	56	LYS
19	FG	61	LEU
19	FG	63	ASN
19	FG	77	LEU
19	FG	81	ASN
19	FG	93	ASP
19	FG	94	ASP
19	FG	96	ILE
19	FG	97	THR
19	FG	100	SER
20	VH	4	LYS
20	VH	74	LYS
21	TI	2	SER
21	TI	6	LYS
21	TI	12	VAL
21	TI	21	GLN
21	TI	23	THR
21	TI	29	ASN
21	TI	33	LYS
21	TI	41	THR
21	TI	45	LYS

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Mol	Chain	Res	Type
21	TI	50	THR
21	TI	59	GLN
21	TI	75	THR
21	TI	85	PHE
21	TI	87	GLU
21	TI	98	ASN
21	TI	102	VAL
22	fJ	8	ASP
22	fJ	10	HIS
22	fJ	12	VAL
22	fJ	21	VAL
22	fJ	25	THR
22	fJ	35	ARG
22	fJ	36	GLU
22	fJ	37	TYR
22	fJ	42	TYR
22	fJ	47	LEU
22	fJ	74	ASN
23	HK	12	LYS
23	HK	34	MET
24	OL	1	MET
24	OL	9	GLN
24	OL	39	GLN
24	OL	53	ARG
24	OL	67	ASP
25	MM	4	ILE
25	MM	7	VAL
25	MM	9	ILE
25	MM	13	LYS
25	MM	27	ARG
25	MM	28	THR
25	MM	68	ASP
25	MM	85	CYS
25	MM	92	ARG
25	MM	98	ARG
25	MM	102	THR
25	MM	107	ARG
27	PO	31	VAL
27	PO	51	ARG
27	PO	83	MET
28	SP	3	ARG
28	SP	12	ASP

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Mol	Chain	Res	Type
28	SP	28	ARG
28	SP	29	LYS
28	SP	36	ARG
28	SP	50	SER
28	SP	58	VAL
28	SP	63	SER
28	SP	81	ARG
29	BQ	2	SER
29	BQ	12	THR
29	BQ	18	GLN
29	BQ	30	SER
29	BQ	35	SER
29	BQ	81	SER
29	BQ	107	SER
30	GR	17	VAL
30	GR	18	THR
30	GR	29	LYS
30	GR	30	ASN
30	GR	44	LYS
30	GR	56	VAL
30	GR	67	THR
30	GR	77	ILE
30	GR	95	ARG
30	GR	104	THR
30	GR	107	VAL
30	GR	152	ARG
30	GR	155	GLU
30	GR	167	GLU
30	GR	176	LYS
30	GR	177	LYS
31	GS	3	ARG
31	GS	5	ARG
31	GS	7	VAL
31	GS	10	ARG
31	GS	12	ILE
31	GS	20	SER
31	GS	22	THR
31	GS	26	PHE
31	GS	32	SER
31	GS	36	LYS
31	GS	41	ARG
31	GS	66	VAL

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Mol	Chain	Res	Type
31	GS	73	MET
31	GS	76	VAL
31	GS	79	ARG
31	GS	98	THR
31	GS	115	LYS
31	GS	119	LEU
31	GS	139	ARG
32	CT	10	ILE
32	CT	16	LYS
32	CT	35	ASN
32	CT	42	TYR
32	CT	54	ASN
32	CT	55	ILE
32	CT	75	ILE
32	CT	79	LYS
32	CT	80	LYS
32	CT	89	LYS
32	CT	93	LYS
32	CT	94	MET
32	CT	101	VAL
32	CT	107	THR
32	CT	111	LEU
32	CT	118	ASP
32	CT	129	MET
32	CT	132	ARG
32	CT	136	ARG
32	CT	141	SER
32	CT	147	LYS
32	CT	168	TYR
32	CT	170	GLU
32	CT	178	LEU
32	CT	179	ARG
32	CT	190	GLU
32	CT	192	THR
32	CT	204	ARG
33	KU	26	SER
33	KU	30	THR
33	KU	32	VAL
33	KU	55	SER
33	KU	58	SER
33	KU	65	VAL
33	KU	72	LYS

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Mol	Chain	Res	Type
33	KU	84	VAL
33	KU	106	LYS
33	KU	114	THR
33	KU	119	ASN
33	KU	128	ARG
34	NV	5	LYS
34	NV	21	ARG
34	NV	34	LYS
35	YW	8	GLN
35	YW	9	LEU
35	YW	30	ARG
36	IX	45	THR
36	IX	93	ILE
36	IX	96	LYS
36	IX	98	GLU
36	IX	99	ASP
36	IX	111	LYS
36	IX	128	THR
37	JY	5	ARG
37	JY	7	ARG
37	JY	12	SER
37	JY	14	ASP
37	JY	20	GLN
37	JY	37	CYS
37	JY	52	LEU
37	JY	57	VAL
37	JY	62	ARG
37	JY	75	ASP
37	JY	82	LYS
37	JY	88	MET
37	JY	89	LYS
38	QZ	12	SER
38	QZ	17	ARG
38	QZ	33	ARG
38	QZ	63	ASP
38	QZ	71	ARG
38	QZ	85	VAL
38	QZ	86	GLU
38	QZ	87	LYS
38	QZ	88	VAL
39	Ba	1	MET
39	Ba	4	THR

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Mol	Chain	Res	Type
39	Ba	24	THR
39	Ba	26	LYS
40	Qb	7	THR
40	Qb	26	LYS
40	Qb	32	THR
40	Qb	34	THR
40	Qb	36	ASN
40	Qb	38	VAL
40	Qb	39	LEU
40	Qb	45	GLU
40	Qb	53	VAL
40	Qb	60	GLU
40	Qb	65	GLU
40	Qb	73	ARG
40	Qb	85	LYS
41	Nc	101	ARG
42	Kd	41	LYS
42	Kd	75	THR
42	Kd	117	ASP
42	Kd	119	THR
42	Kd	135	GLN
43	Je	23	LYS
43	Je	28	SER
43	Je	43	VAL
44	Af	22	SER
44	Af	26	THR
44	Af	42	ASP
44	Af	84	ARG
44	Af	87	ASP
44	Af	89	ASP
44	Af	94	GLU
44	Af	113	THR
44	Af	116	SER
44	Af	154	SER
44	Af	165	PRO
44	Af	200	THR
44	Af	209	SER
44	Af	210	VAL
45	Lg	7	THR
45	Lg	16	ARG
45	Lg	26	THR
45	Lg	32	PHE

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Mol	Chain	Res	Type
45	Lg	60	ARG
45	Lg	85	LYS
45	Lg	90	VAL
45	Lg	102	MET
45	Lg	118	LEU
46	dh	31	HIS
46	dh	33	LEU
46	dh	48	LYS
46	dh	52	LYS
47	Oi	19	ARG
47	Oi	62	THR
47	Oi	70	VAL
47	Oi	84	GLU
47	Oi	108	LYS
47	Oi	116	LEU
48	Pj	5	ARG
48	Pj	54	MET
49	bk	18	THR
49	bk	31	GLU
49	bk	38	LYS
49	bk	46	LYS
49	bk	49	LYS
50	Cl	95	LYS
50	Cl	110	GLN
50	Cl	125	ARG
50	Cl	156	ARG
50	Cl	161	SER
50	Cl	167	ARG
50	Cl	170	ILE
50	Cl	186	VAL
50	Cl	262	ARG
51	Dm	9	LEU
51	Dm	37	ARG
51	Dm	51	GLU
51	Dm	72	GLN
51	Dm	112	ARG
51	Dm	131	ARG
51	Dm	163	LYS
51	Dm	167	GLU
52	Sn	19	SER
52	Sn	21	MET
52	Sn	36	LYS

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Mol	Chain	Res	Type
52	Sn	53	VAL
52	Sn	63	VAL
52	Sn	64	LYS
52	Sn	69	ARG
52	Sn	76	ARG
54	ep	19	ARG
55	D	1	MET
55	D	17	ASN
55	D	34	ILE
55	D	50	ASP
55	D	62	MET
55	D	77	ASP
55	D	91	ARG
55	D	98	THR
55	D	100	LEU
55	D	103	ASN
55	D	104	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	280	ASN
17	XE	16	GLN
18	RF	40	ASN
24	OL	39	GLN
29	BQ	18	GLN
32	CT	35	ASN
37	JY	78	GLN
38	QZ	43	GLN
44	Af	128	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	D8	114/115 (99%)	12 (10%)	1 (0%)
26	iN	1498/1590 (94%)	265 (17%)	0
5	Z2	2698/2882 (93%)	390 (14%)	14 (0%)
All	All	4310/4587 (93%)	667 (15%)	15 (0%)

All (667) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	Z2	10	U
5	Z2	16	A
5	Z2	19	G
5	Z2	21	A
5	Z2	22	G
5	Z2	30	G
5	Z2	41	U
5	Z2	49	A
5	Z2	53	G
5	Z2	58	G
5	Z2	62	G
5	Z2	70	A
5	Z2	78	A
5	Z2	81	A
5	Z2	82	G
5	Z2	99	A
5	Z2	124	A
5	Z2	125	A
5	Z2	126	U
5	Z2	137	A
5	Z2	146	A
5	Z2	148	G
5	Z2	193	A
5	Z2	196	A
5	Z2	202	G
5	Z2	213	A
5	Z2	219	C
5	Z2	221	U
5	Z2	222	C
5	Z2	226	U
5	Z2	227	G
5	Z2	245	G
5	Z2	271	A
5	Z2	274	C
5	Z2	298	A
5	Z2	311	U
5	Z2	314	G
5	Z2	317	A
5	Z2	325	G
5	Z2	332	A
5	Z2	333	A
5	Z2	339	A
5	Z2	345	A

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Mol	Chain	Res	Type
5	Z2	346	A
5	Z2	354	A
5	Z2	355	G
5	Z2	366	C
5	Z2	369	G
5	Z2	379	G
5	Z2	387	A
5	Z2	394	G
5	Z2	419	C
5	Z2	425	G
5	Z2	431	U
5	Z2	434	U
5	Z2	439	C
5	Z2	461	A
5	Z2	462	A
5	Z2	464	G
5	Z2	472	G
5	Z2	488	A
5	Z2	491	A
5	Z2	512	A
5	Z2	513	G
5	Z2	514	C
5	Z2	515	A
5	Z2	519	G
5	Z2	528	A
5	Z2	529	U
5	Z2	530	U
5	Z2	531	U
5	Z2	532	A
5	Z2	533	U
5	Z2	534	U
5	Z2	535	G
5	Z2	548	A
5	Z2	558	U
5	Z2	559	A
5	Z2	560	A
5	Z2	588	A
5	Z2	589	G
5	Z2	592	U
5	Z2	598	U
5	Z2	599	U
5	Z2	600	U

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Mol	Chain	Res	Type
5	Z2	612	A
5	Z2	622	A
5	Z2	630	U
5	Z2	654	G
5	Z2	671	U
5	Z2	702	C
5	Z2	715	A
5	Z2	732	U
5	Z2	749	A
5	Z2	760	G
5	Z2	761	G
5	Z2	767	A
5	Z2	769	G
5	Z2	770	G
5	Z2	776	C
5	Z2	790	G
5	Z2	797	C
5	Z2	812	U
5	Z2	813	U
5	Z2	815	G
5	Z2	844	G
5	Z2	849	G
5	Z2	851	A
5	Z2	854	G
5	Z2	887	C
5	Z2	892	G
5	Z2	895	A
5	Z2	899	C
5	Z2	912	A
5	Z2	916	A
5	Z2	917	U
5	Z2	929	A
5	Z2	930	C
5	Z2	937	G
5	Z2	945	C
5	Z2	958	G
5	Z2	967	A
5	Z2	980	A
5	Z2	983	U
5	Z2	987	G
5	Z2	995	U
5	Z2	996	U

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Mol	Chain	Res	Type
5	Z2	997	C
5	Z2	1001	G
5	Z2	1006	G
5	Z2	1010	G
5	Z2	1024	A
5	Z2	1030	A
5	Z2	1044	U
5	Z2	1053	A
5	Z2	1054	A
5	Z2	1063	C
5	Z2	1071	G
5	Z2	1072	A
5	Z2	1074	A
5	Z2	1081	U
5	Z2	1085	U
5	Z2	1094	G
5	Z2	1095	A
5	Z2	1096	G
5	Z2	1113	A
5	Z2	1114	U
5	Z2	1116	U
5	Z2	1119	C
5	Z2	1120	G
5	Z2	1133	G
5	Z2	1155	A
5	Z2	1156	A
5	Z2	1157	C
5	Z2	1158	U
5	Z2	1159	U
5	Z2	1160	G
5	Z2	1161	U
5	Z2	1163	U
5	Z2	1164	U
5	Z2	1168	G
5	Z2	1179	G
5	Z2	1189	A
5	Z2	1190	G
5	Z2	1211	G
5	Z2	1234	G
5	Z2	1237	A
5	Z2	1240	G
5	Z2	1255	G

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Mol	Chain	Res	Type
5	Z2	1256	A
5	Z2	1257	U
5	Z2	1260	U
5	Z2	1264	A
5	Z2	1284	G
5	Z2	1285	A
5	Z2	1287	G
5	Z2	1290	C
5	Z2	1305	A
5	Z2	1313	U
5	Z2	1329	C
5	Z2	1336	U
5	Z2	1343	A
5	Z2	1349	A
5	Z2	1354	C
5	Z2	1363	U
5	Z2	1364	G
5	Z2	1367	A
5	Z2	1369	A
5	Z2	1370	U
5	Z2	1379	A
5	Z2	1380	U
5	Z2	1400	G
5	Z2	1401	C
5	Z2	1404	U
5	Z2	1405	G
5	Z2	1408	G
5	Z2	1411	A
5	Z2	1412	C
5	Z2	1419	G
5	Z2	1420	G
5	Z2	1435	C
5	Z2	1436	G
5	Z2	1443	G
5	Z2	1444	U
5	Z2	1466	U
5	Z2	1474	A
5	Z2	1477	C
5	Z2	1478	A
5	Z2	1481	U
5	Z2	1483	C
5	Z2	1497	G

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Mol	Chain	Res	Type
5	Z2	1501	A
5	Z2	1515	G
5	Z2	1542	U
5	Z2	1548	G
5	Z2	1551	U
5	Z2	1554	A
5	Z2	1557	A
5	Z2	1566	U
5	Z2	1580	A
5	Z2	1581	A
5	Z2	1584	G
5	Z2	1596	A
5	Z2	1598	A
5	Z2	1603	C
5	Z2	1606	A
5	Z2	1622	A
5	Z2	1635	U
5	Z2	1636	U
5	Z2	1642	A
5	Z2	1662	G
5	Z2	1681	U
5	Z2	1710	A
5	Z2	1724	G
5	Z2	1731	C
5	Z2	1732	G
5	Z2	1750	G
5	Z2	1759	A
5	Z2	1762	G
5	Z2	1768	U
5	Z2	1770	A
5	Z2	1777	A
5	Z2	1785	G
5	Z2	1786	C
5	Z2	1787	A
5	Z2	1796	A
5	Z2	1802	C
5	Z2	1806	U
5	Z2	1815	A
5	Z2	1824	C
5	Z2	1848	G
5	Z2	1851	U
5	Z2	1855	G

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Mol	Chain	Res	Type
5	Z2	1856	U
5	Z2	1857	A
5	Z2	1880	C
5	Z2	1892	G
5	Z2	1899	A
5	Z2	1915	G
5	Z2	1916	G
5	Z2	1917	U
5	Z2	1923	A
5	Z2	1924	A
5	Z2	1925	U
5	Z2	1941	U
5	Z2	1948	C
5	Z2	1949	U
5	Z2	1951	C
5	Z2	1953	C
5	Z2	1956	A
5	Z2	1957	U
5	Z2	1958	G
5	Z2	1968	U
5	Z2	1977	U
5	Z2	1979	U
5	Z2	1983	C
5	Z2	2009	C
5	Z2	2016	A
5	Z2	2017	A
5	Z2	2019	A
5	Z2	2029	C
5	Z2	2041	C
5	Z2	2042	G
5	Z2	2046	A
5	Z2	2047	G
5	Z2	2048	A
5	Z2	2055	G
5	Z2	2079	G
5	Z2	2178	G
5	Z2	2184	A
5	Z2	2189	A
5	Z2	2190	G
5	Z2	2195	A
5	Z2	2196	A
5	Z2	2206	G

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Mol	Chain	Res	Type
5	Z2	2208	A
5	Z2	2221	G
5	Z2	2222	G
5	Z2	2225	G
5	Z2	2242	U
5	Z2	2251	A
5	Z2	2261	A
5	Z2	2266	U
5	Z2	2270	A
5	Z2	2271	A
5	Z2	2288	U
5	Z2	2291	G
5	Z2	2294	A
5	Z2	2302	U
5	Z2	2303	A
5	Z2	2305	A
5	Z2	2306	G
5	Z2	2308	A
5	Z2	2310	A
5	Z2	2319	A
5	Z2	2328	A
5	Z2	2329	A
5	Z2	2330	C
5	Z2	2333	C
5	Z2	2337	A
5	Z2	2360	A
5	Z2	2365	G
5	Z2	2366	G
5	Z2	2368	C
5	Z2	2374	G
5	Z2	2385	U
5	Z2	2389	U
5	Z2	2408	A
5	Z2	2412	G
5	Z2	2413	A
5	Z2	2414	U
5	Z2	2417	A
5	Z2	2422	A
5	Z2	2424	U
5	Z2	2431	A
5	Z2	2452	A
5	Z2	2453	G

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Mol	Chain	Res	Type
5	Z2	2459	A
5	Z2	2461	A
5	Z2	2474	U
5	Z2	2485	G
5	Z2	2486	A
5	Z2	2488	G
5	Z2	2489	U
5	Z2	2501	A
5	Z2	2503	C
5	Z2	2512	G
5	Z2	2530	A
5	Z2	2537	U
5	Z2	2539	C
5	Z2	2545	U
5	Z2	2549	A
5	Z2	2550	G
5	Z2	2556	C
5	Z2	2565	G
5	Z2	2585	A
5	Z2	2592	U
5	Z2	2596	U
5	Z2	2598	U
5	Z2	2604	G
5	Z2	2612	U
5	Z2	2619	U
5	Z2	2623	G
5	Z2	2646	G
5	Z2	2668	G
5	Z2	2672	U
5	Z2	2673	U
5	Z2	2697	G
5	Z2	2709	C
5	Z2	2716	A
5	Z2	2731	A
5	Z2	2740	A
5	Z2	2744	G
5	Z2	2761	A
5	Z2	2762	U
5	Z2	2763	U
5	Z2	2769	U
5	Z2	2770	C
5	Z2	2772	C

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Mol	Chain	Res	Type
5	Z2	2773	U
5	Z2	2774	A
5	Z2	2775	A
5	Z2	2784	U
5	Z2	2786	A
5	Z2	2787	A
5	Z2	2815	G
5	Z2	2827	U
5	Z2	2838	A
5	Z2	2839	A
5	Z2	2850	U
11	D8	13	A
11	D8	22	G
11	D8	28	C
11	D8	33	U
11	D8	38	U
11	D8	39	C
11	D8	50	A
11	D8	54	G
11	D8	88	A
11	D8	96	A
11	D8	105	C
11	D8	106	A
26	iN	51	C
26	iN	52	U
26	iN	54	A
26	iN	56	G
26	iN	69	G
26	iN	79	A
26	iN	80	A
26	iN	86	G
26	iN	94	C
26	iN	95	U
26	iN	97	A
26	iN	98	A
26	iN	116	G
26	iN	118	A
26	iN	122	G
26	iN	125	G
26	iN	127	A
26	iN	128	G
26	iN	130	U

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Mol	Chain	Res	Type
26	iN	131	U
26	iN	132	G
26	iN	135	U
26	iN	136	C
26	iN	137	U
26	iN	139	G
26	iN	143	A
26	iN	161	A
26	iN	164	A
26	iN	166	U
26	iN	167	A
26	iN	172	G
26	iN	174	A
26	iN	175	A
26	iN	176	U
26	iN	187	G
26	iN	197	G
26	iN	200	C
26	iN	206	A
26	iN	208	C
26	iN	210	C
26	iN	218	U
26	iN	225	U
26	iN	233	A
26	iN	234	C
26	iN	238	A
26	iN	240	A
26	iN	242	A
26	iN	247	G
26	iN	259	U
26	iN	263	G
26	iN	288	U
26	iN	289	A
26	iN	290	G
26	iN	294	G
26	iN	309	G
26	iN	310	C
26	iN	332	G
26	iN	351	C
26	iN	364	A
26	iN	371	C
26	iN	372	A

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Mol	Chain	Res	Type
26	iN	373	C
26	iN	375	G
26	iN	395	C
26	iN	397	G
26	iN	406	A
26	iN	410	U
26	iN	415	C
26	iN	416	A
26	iN	427	C
26	iN	435	C
26	iN	441	U
26	iN	449	G
26	iN	450	U
26	iN	452	U
26	iN	454	A
26	iN	456	G
26	iN	457	A
26	iN	464	U
26	iN	465	U
26	iN	466	U
26	iN	467	G
26	iN	472	U
26	iN	477	C
26	iN	479	C
26	iN	488	G
26	iN	496	G
26	iN	497	A
26	iN	502	G
26	iN	508	A
26	iN	510	U
26	iN	511	A
26	iN	521	G
26	iN	522	A
26	iN	525	A
26	iN	527	A
26	iN	529	U
26	iN	540	U
26	iN	552	A
26	iN	554	C
26	iN	556	C
26	iN	561	C
26	iN	564	G

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Mol	Chain	Res	Type
26	iN	567	G
26	iN	570	G
26	iN	574	U
26	iN	575	A
26	iN	578	A
26	iN	582	A
26	iN	583	G
26	iN	590	A
26	iN	607	C
26	iN	615	A
26	iN	616	A
26	iN	617	A
26	iN	619	G
26	iN	620	G
26	iN	622	G
26	iN	631	G
26	iN	639	A
26	iN	675	U
26	iN	686	A
26	iN	697	A
26	iN	709	A
26	iN	719	A
26	iN	730	U
26	iN	739	A
26	iN	747	G
26	iN	761	U
26	iN	765	G
26	iN	767	U
26	iN	768	G
26	iN	789	U
26	iN	798	C
26	iN	799	A
26	iN	821	A
26	iN	825	A
26	iN	837	U
26	iN	838	A
26	iN	843	G
26	iN	854	C
26	iN	859	A
26	iN	861	C
26	iN	872	A
26	iN	880	G

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Mol	Chain	Res	Type
26	iN	891	G
26	iN	897	G
26	iN	911	G
26	iN	914	A
26	iN	916	A
26	iN	928	U
26	iN	958	A
26	iN	970	G
26	iN	971	G
26	iN	978	C
26	iN	979	A
26	iN	1002	A
26	iN	1004	U
26	iN	1010	G
26	iN	1011	C
26	iN	1013	A
26	iN	1019	A
26	iN	1020	G
26	iN	1021	A
26	iN	1033	U
26	iN	1036	U
26	iN	1043	U
26	iN	1044	C
26	iN	1046	A
26	iN	1048	A
26	iN	1050	U
26	iN	1053	U
26	iN	1056	A
26	iN	1070	G
26	iN	1072	C
26	iN	1074	U
26	iN	1075	C
26	iN	1077	G
26	iN	1078	G
26	iN	1080	A
26	iN	1081	U
26	iN	1084	G
26	iN	1085	A
26	iN	1089	C
26	iN	1108	G
26	iN	1109	U
26	iN	1114	U

Continued on next page...

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Mol	Chain	Res	Type
26	iN	1129	U
26	iN	1133	G
26	iN	1138	G
26	iN	1139	U
26	iN	1145	A
26	iN	1168	G
26	iN	1197	A
26	iN	1202	A
26	iN	1204	U
26	iN	1209	G
26	iN	1213	C
26	iN	1214	A
26	iN	1216	A
26	iN	1241	A
26	iN	1242	A
26	iN	1247	U
26	iN	1257	U
26	iN	1258	A
26	iN	1259	C
26	iN	1260	G
26	iN	1271	C
26	iN	1272	A
26	iN	1278	G
26	iN	1281	A
26	iN	1283	A
26	iN	1284	A
26	iN	1291	G
26	iN	1302	A
26	iN	1303	G
26	iN	1305	U
26	iN	1323	G
26	iN	1331	A
26	iN	1332	A
26	iN	1333	A
26	iN	1345	G
26	iN	1347	C
26	iN	1348	C
26	iN	1350	G
26	iN	1360	U
26	iN	1362	C
26	iN	1363	A
26	iN	1365	C

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Mol	Chain	Res	Type
26	iN	1367	C
26	iN	1377	A
26	iN	1383	G
26	iN	1391	A
26	iN	1398	G
26	iN	1408	A
26	iN	1415	G
26	iN	1424	G
26	iN	1426	U
26	iN	1427	C
26	iN	1428	C
26	iN	1439	A
26	iN	1443	A
26	iN	1448	C
26	iN	1474	C
26	iN	1477	G
26	iN	1486	A
26	iN	1490	U
26	iN	1491	A
26	iN	1496	U
26	iN	1497	C
26	iN	1520	G
26	iN	1532	G
26	iN	1538	A
26	iN	1542	G
26	iN	1548	A
26	iN	1549	G
26	iN	1551	U
26	iN	1562	G
26	iN	1564	A
26	iN	1565	C
26	iN	1574	G
26	iN	1575	G
26	iN	1576	A
26	iN	1577	U
26	iN	1578	C

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	Z2	9	G
5	Z2	532	A

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Mol	Chain	Res	Type
5	Z2	749	A
5	Z2	769	G
5	Z2	812	U
5	Z2	886	A
5	Z2	916	A
5	Z2	968	A
5	Z2	1053	A
5	Z2	1379	A
5	Z2	1580	A
5	Z2	2195	A
5	Z2	2413	A
5	Z2	2739	U
11	D8	13	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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.

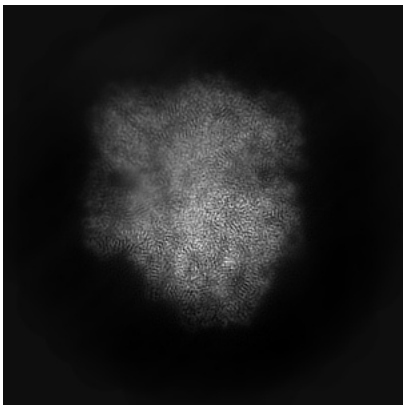
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19067. These allow visual inspection of the internal detail of the map and identification of artifacts.

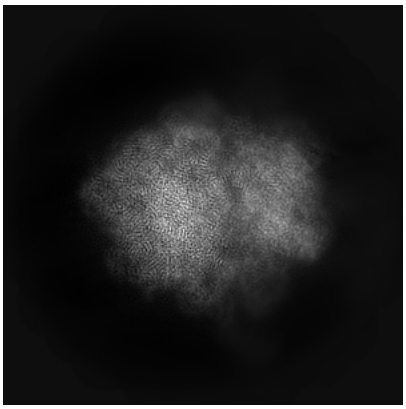
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

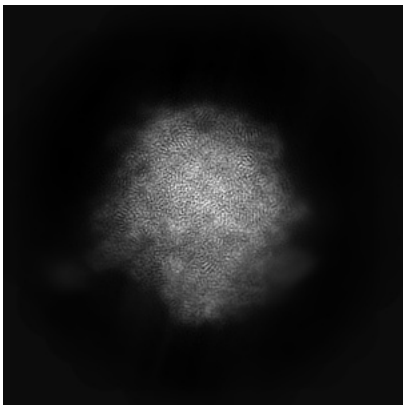
6.1.1 Primary map



X

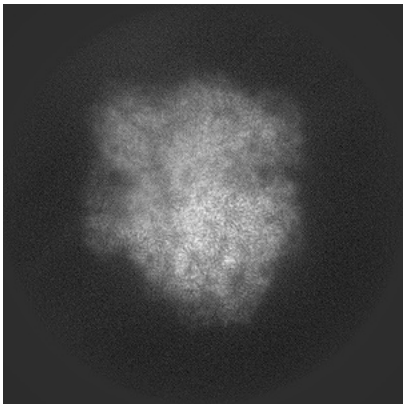


Y

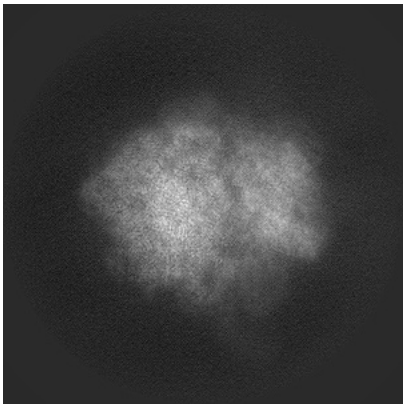


Z

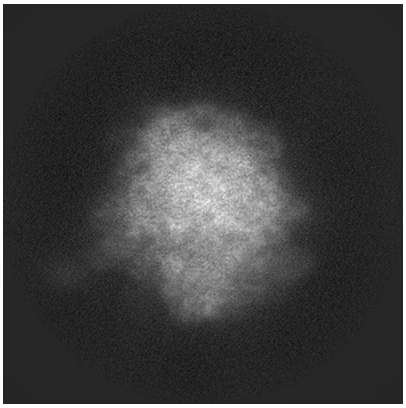
6.1.2 Raw map



X



Y

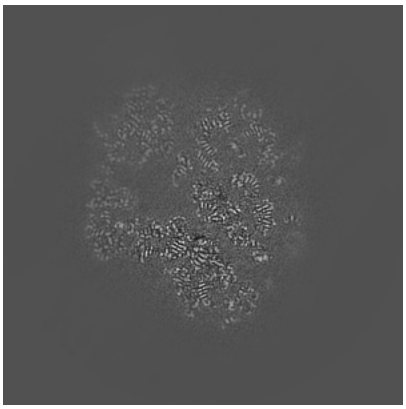


Z

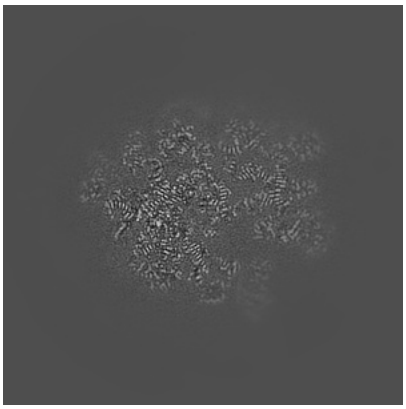
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

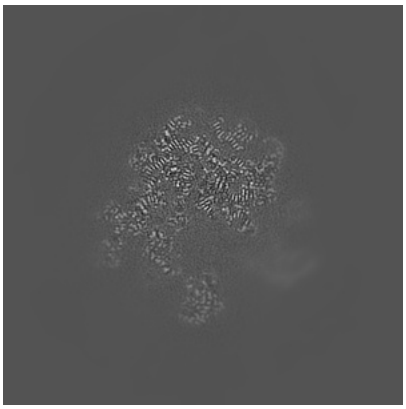
6.2.1 Primary map



X Index: 270

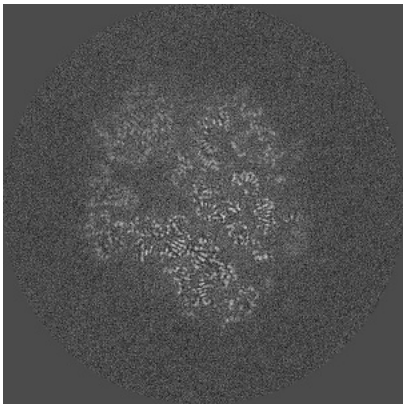


Y Index: 270

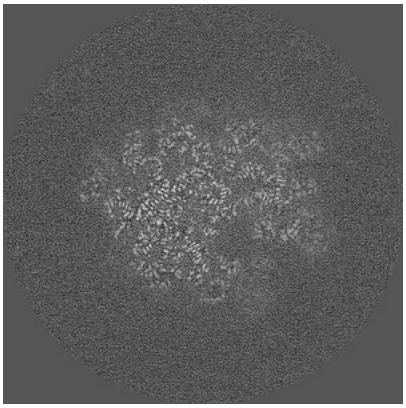


Z Index: 270

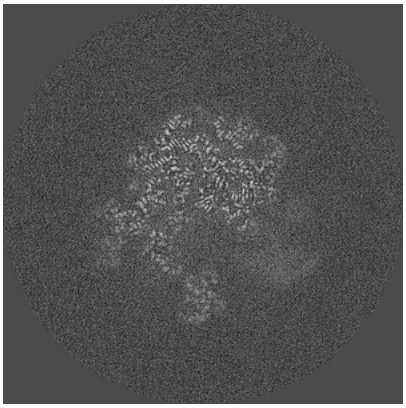
6.2.2 Raw map



X Index: 270



Y Index: 270

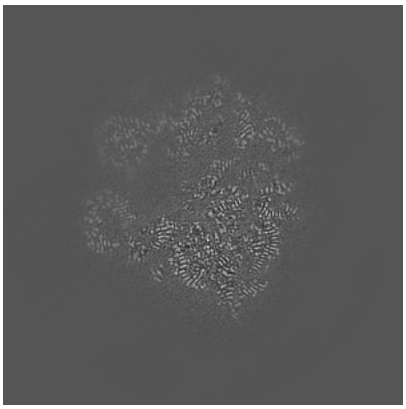


Z Index: 270

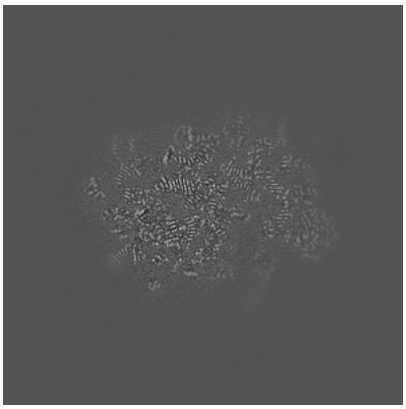
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

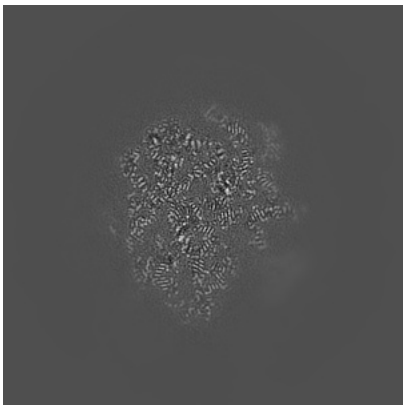
6.3.1 Primary map



X Index: 250

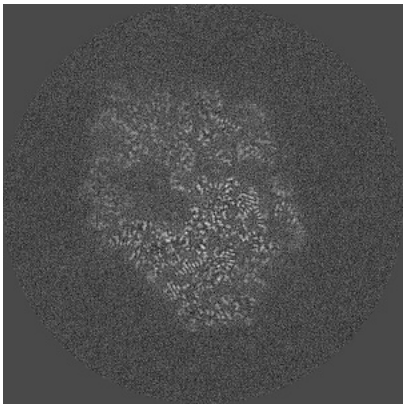


Y Index: 290

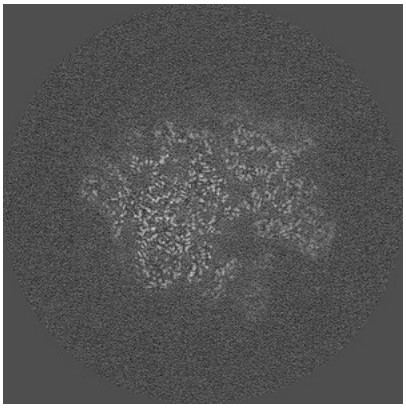


Z Index: 234

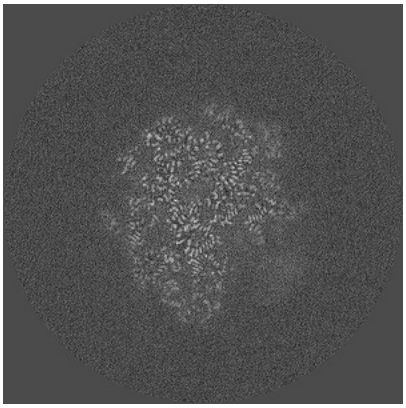
6.3.2 Raw map



X Index: 286



Y Index: 276

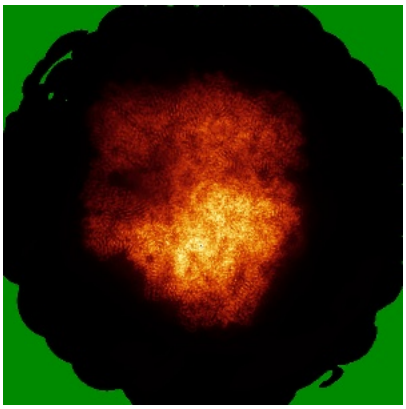


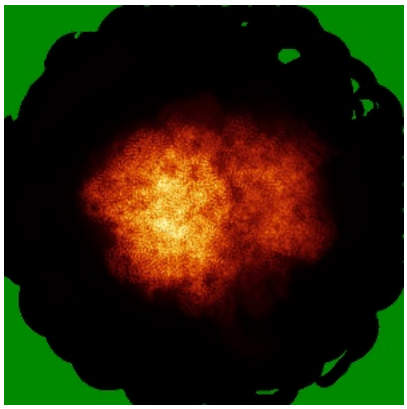
Z Index: 237

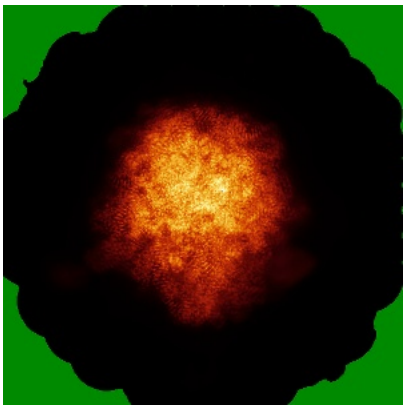
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

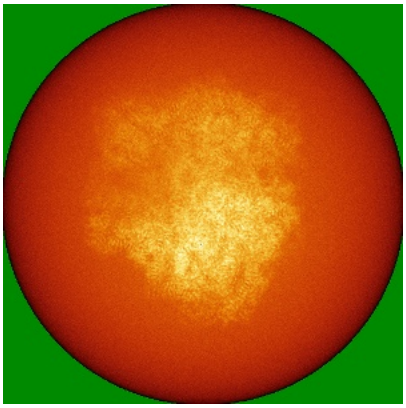
6.4.1 Primary map

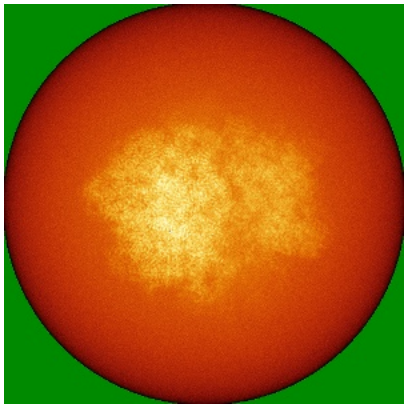

X

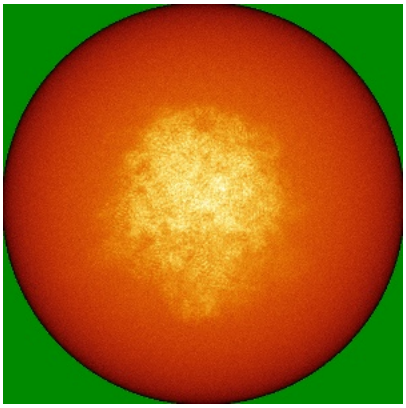

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0198. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

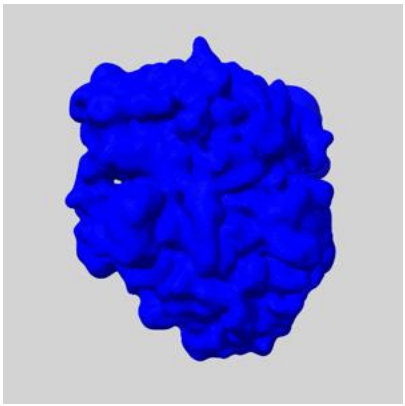
6.6 Mask visualisation

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

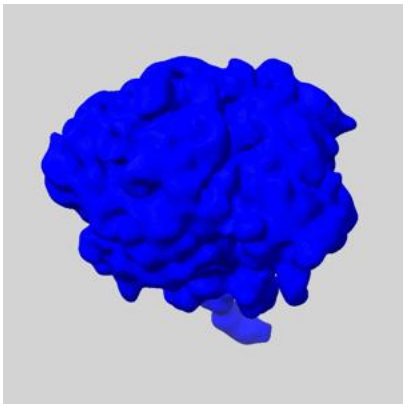
A mask typically either:

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

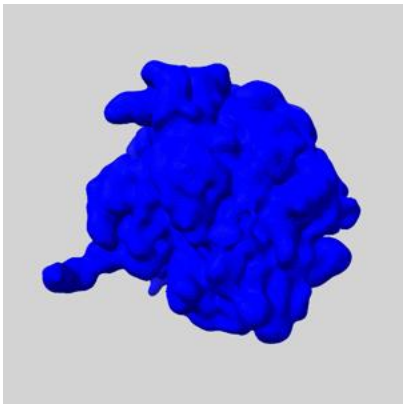
6.6.1 emd_19067_msk_1.map



X



Y

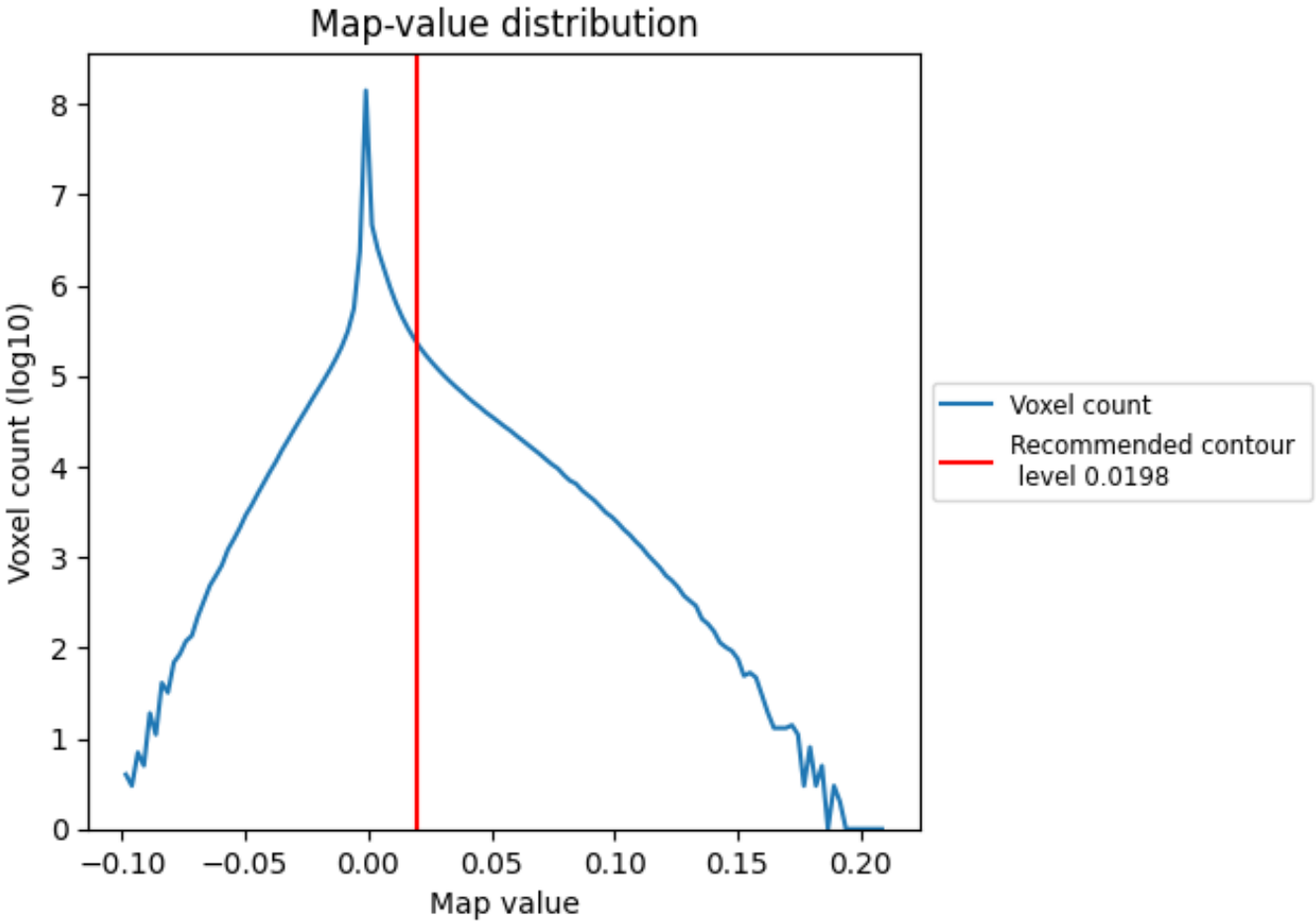


Z

7 Map analysis

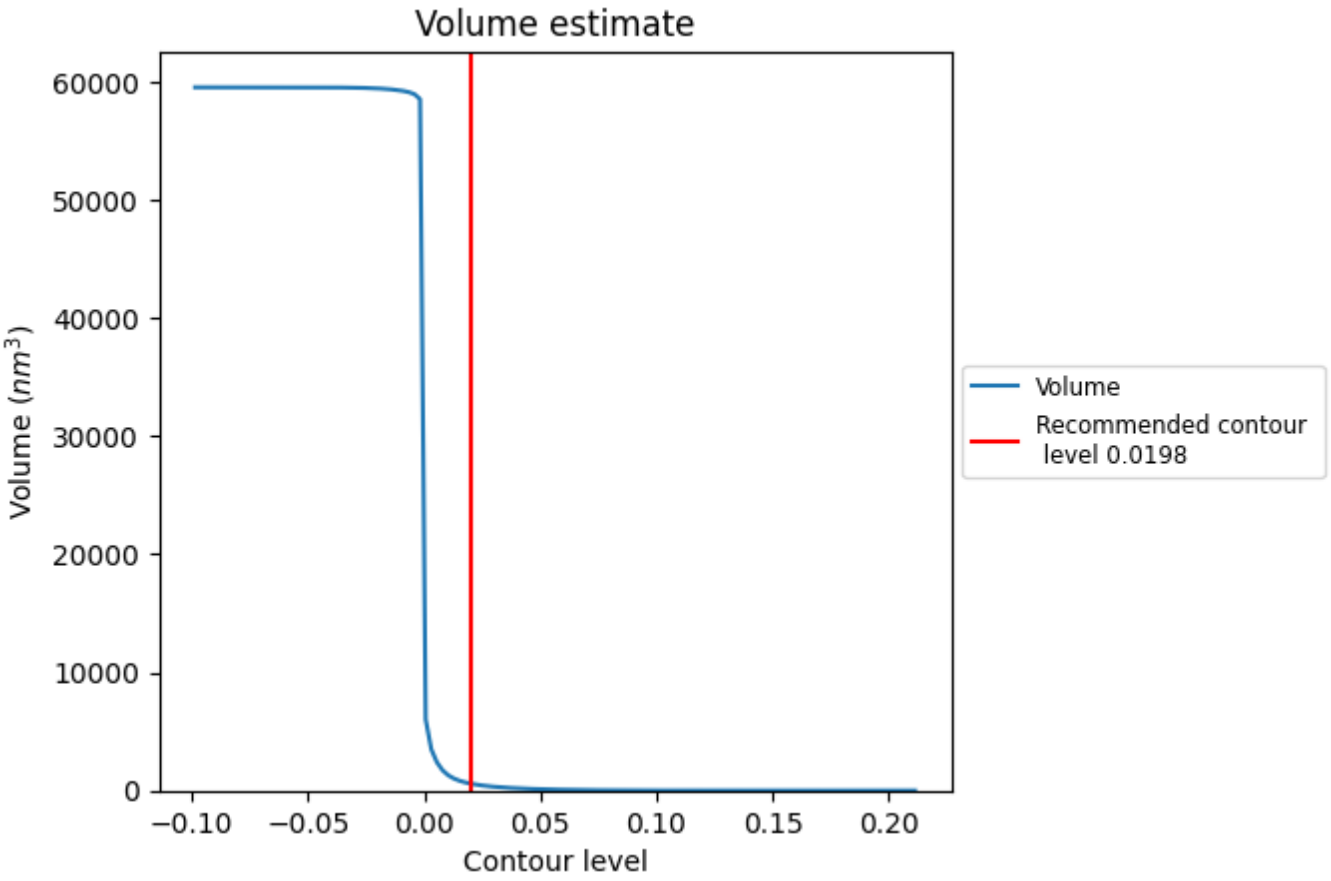
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

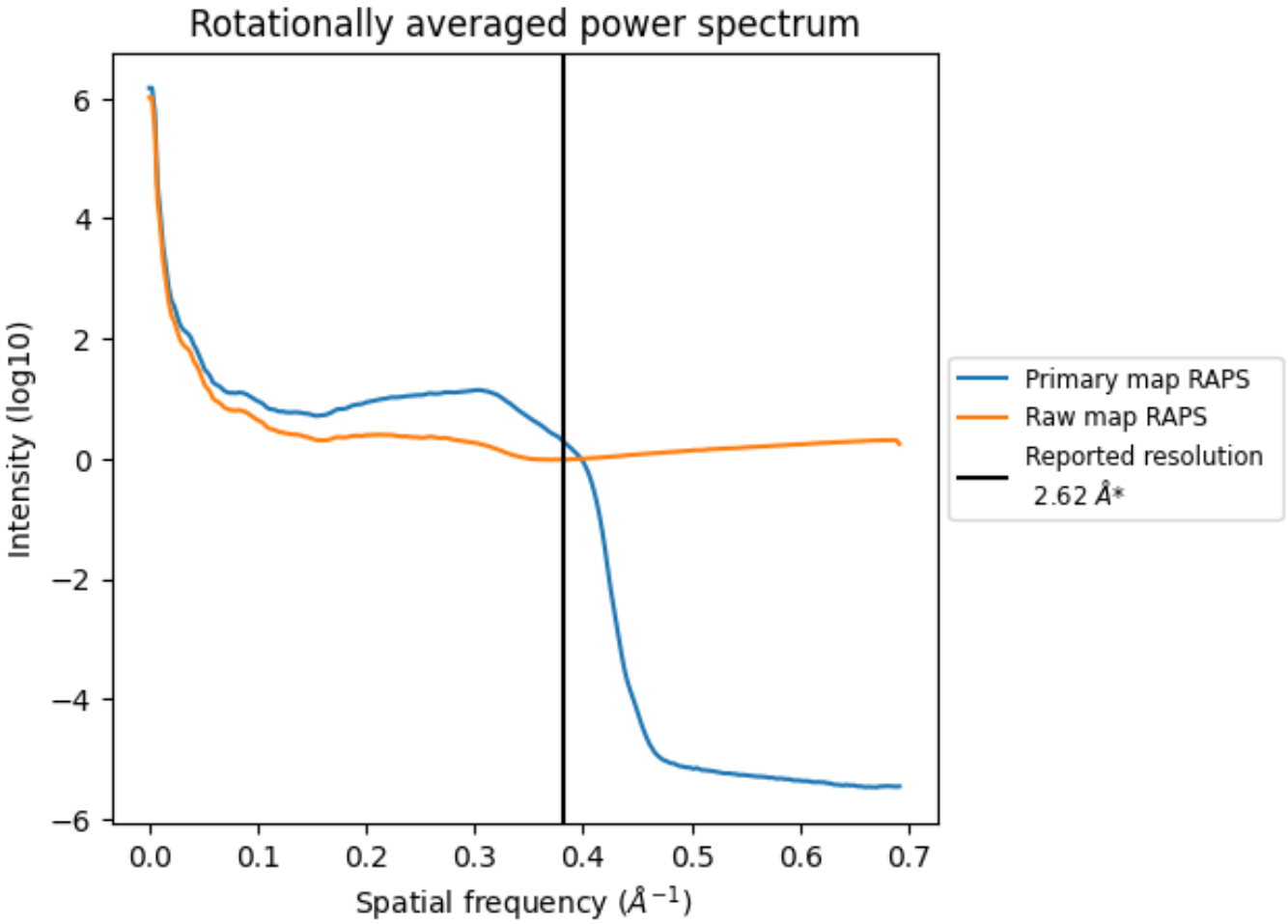
7.2 Volume estimate



The volume at the recommended contour level is 598 nm^3; this corresponds to an approximate mass of 540 kDa.

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

7.3 Rotationally averaged power spectrum (i)

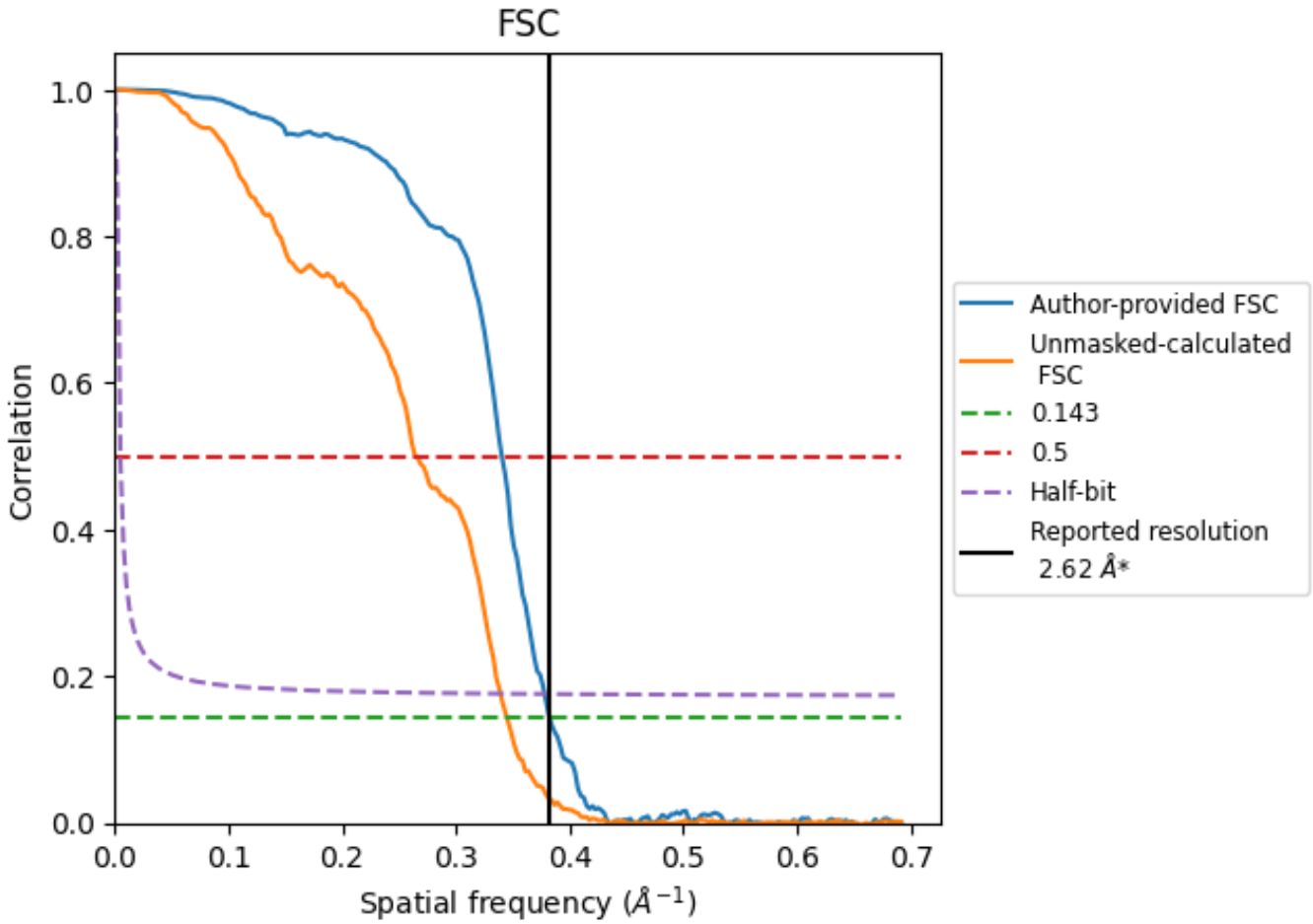


*Reported resolution corresponds to spatial frequency of 0.382 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.382 $Å^{-1}$

8.2 Resolution estimates (i)

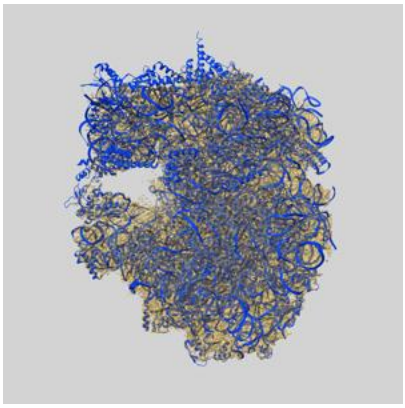
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.62	-	-
Author-provided FSC curve	2.62	2.94	2.65
Unmasked-calculated*	2.90	3.77	2.95

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.90 differs from the reported value 2.62 by more than 10 %

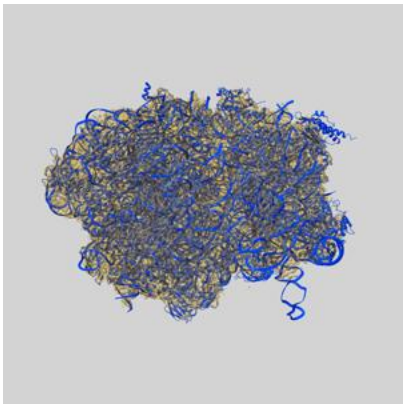
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19067 and PDB model 8RD8. Per-residue inclusion information can be found in section 3 on page 14.

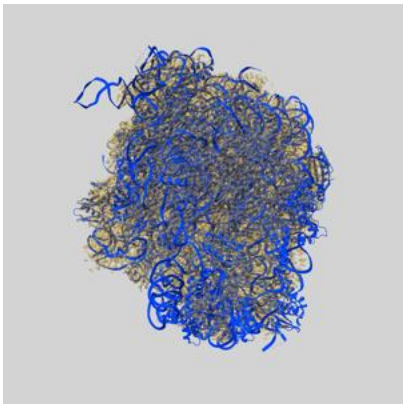
9.1 Map-model overlay



X



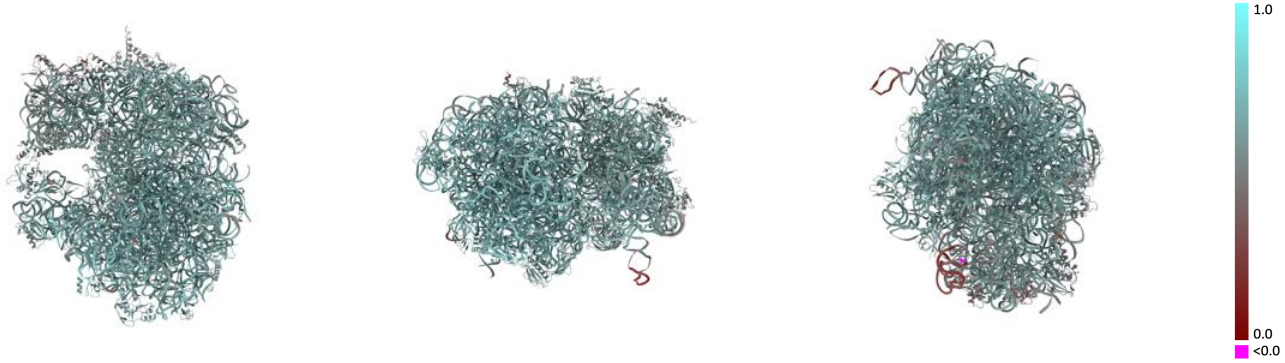
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0198 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.

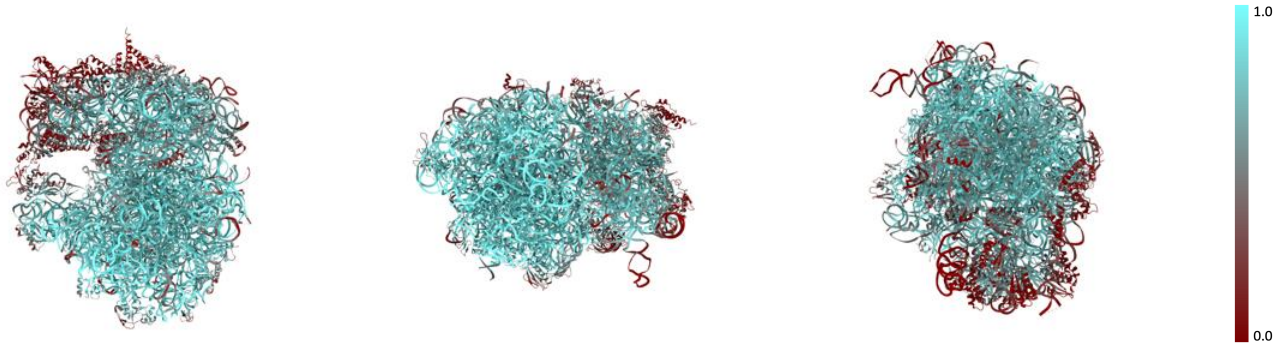
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

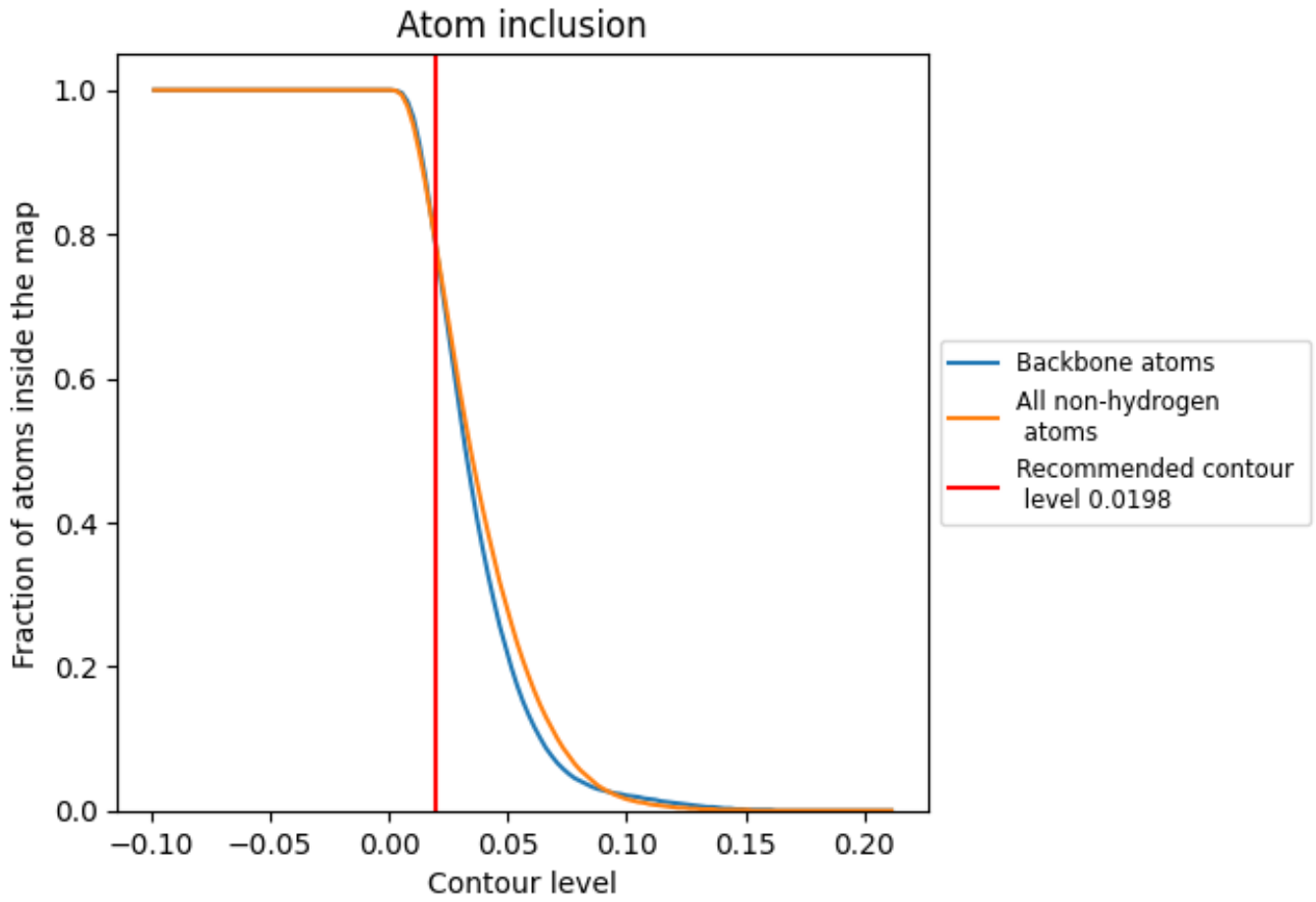
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0198).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0198) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7860	0.6370
A4	0.2270	0.5450
Af	0.9160	0.6860
B	0.6660	0.6290
BQ	0.6980	0.6390
Ba	0.9910	0.7030
C1	0.5090	0.5390
CT	0.3250	0.5580
Cl	0.9370	0.6830
D	0.5200	0.5840
D8	0.8440	0.6350
Dm	0.4010	0.5550
E5	0.6950	0.6290
E9	0.8040	0.6660
F	0.2910	0.5540
F7	0.4130	0.5640
FG	0.3870	0.5870
GR	0.5680	0.6090
GS	0.2190	0.5320
H	0.1270	0.5690
HK	0.3230	0.5310
IX	0.9310	0.6870
JY	0.2520	0.5170
Je	0.8910	0.6630
KU	0.5210	0.5990
Kd	0.8800	0.6700
L6	0.8260	0.6340
Lg	0.9070	0.6700
MB	0.9640	0.6930
MM	0.1820	0.5460
NV	0.4050	0.5820
Nc	0.7480	0.6260
OL	0.7000	0.6270
Oi	0.9000	0.6740
PO	0.9430	0.6980

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Chain	Atom inclusion	Q-score
Pj	0.6470	0.6000
QZ	0.6490	0.6250
Qb	0.8000	0.6630
R3	0.6050	0.5890
RF	0.9110	0.6780
SP	0.1300	0.5300
Sn	0.8010	0.6430
TI	0.6480	0.6160
To	0.6770	0.6230
UC	0.7700	0.6480
VH	0.8950	0.6690
WD	0.8610	0.6540
XE	0.5760	0.6160
YW	0.9300	0.6810
Z2	0.9320	0.6670
aA	0.9030	0.6820
bk	0.8910	0.6650
dh	0.9720	0.7020
ep	0.9510	0.6730
fJ	0.1600	0.5480
iN	0.7450	0.6060