Full wwPDB EM Validation Report

Mar 20, 2026 – 02:16 AM UTC

PDB ID	:	5O60 / pdb_00005o60
EMDB ID	:	EMD-3750
Title	:	Structure of the 50S large ribosomal subunit from Mycobacterium smegmatis
Authors	:	Hentschel, J.; Burnside, C.; Mignot, I.; Leibundgut, M.; Boehringer, D.; Ban, N.
Deposited on	:	2017-06-02
Resolution	:	3.18 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

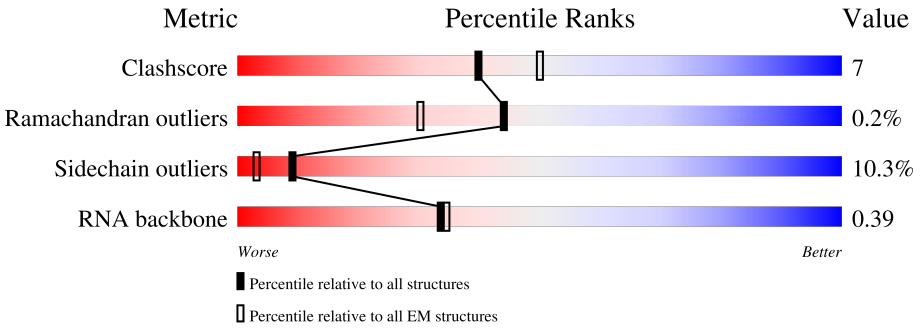
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

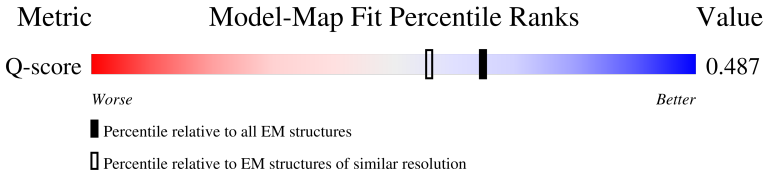
1 Overall quality at a glance

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

The reported resolution of this entry is 3.18 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14470 (2.68 - 3.68)

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	3	24	17% 54% 42% .
2	A	3120	10% 61% 31% 8%
3	B	118	. 63% 30% 8%

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Mol	Chain	Length	Quality of chain
4	C	278	13% 65% 30%
5	D	217	10% 66% 25% 7%
6	E	215	18% 73% 22%
7	F	187	33% 72% 22%
8	G	179	45% 69% 23% 6%
9	H	151	95% 83% 15%
10	I	175	71% 45% 24% 28%
11	J	142	94% 60% 27% 6% 6%
12	K	147	14% 76% 20%
13	L	122	26% 70% 25% 5%
14	M	147	15% 69% 24% 5%
15	N	138	17% 59% 33% 5%
16	O	199	41% 14% 41%
17	P	127	20% 76% 23%
18	Q	113	27% 65% 29% 5%
19	R	129	8% 71% 22%
20	S	103	17% 78% 17%
21	T	153	11% 54% 20% 25%
22	U	100	25% 75% 20%
23	V	105	29% 54% 34% 8%
24	W	215	44% 62% 24% 11%
25	X	88	9% 67% 19% 10%
26	Y	64	16% 67% 28%
27	Z	77	21% 64% 19% 17%
28	a	61	15% 77% 20%

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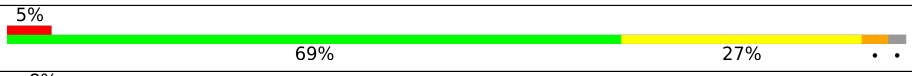
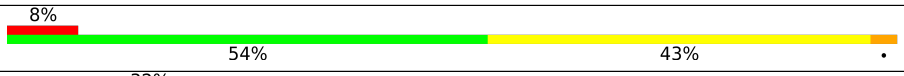
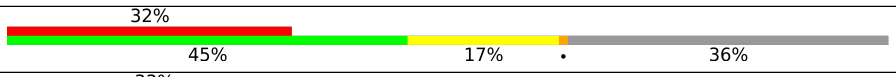
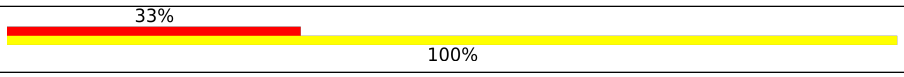
Mol	Chain	Length	Quality of chain
29	b	57	
30	c	55	
31	d	47	
32	e	64	
33	f	37	
34	g	75	
35	2	3	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 98153 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 50S ribosomal protein bL37.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	3	23	Total	C	N	O	0	0
			189	111	50	28		

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	3119	Total	C	N	O	P	0	0
			66981	29854	12313	21695	3119		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	118	Total	C	N	O	P	0	0
			2522	1126	468	810	118		

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	275	Total	C	N	O	S	0	0
			2110	1298	438	370	4		

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	214	Total	C	N	O	S	0	0
			1587	982	310	290	5		

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	209	Total	C	N	O	S	0	0
			1569	969	295	303	2		

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	182	Total	C	N	O	S	0	0
			1445	907	271	261	6		

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	176	Total	C	N	O	S	0	0
			1348	845	249	253	1		

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	151	Total	C	N	O	S	0	0
			1018	635	188	194	1		

- Molecule 10 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	126	Total	C	N	O	S	0	0
			918	580	156	180	2		

- Molecule 11 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	133	Total	C	N	O	S	0	0
			990	625	175	187	3		

- Molecule 12 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	146	Total	C	N	O	S	0	0
			1130	722	207	200	1		

- Molecule 13 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	122	Total	C	N	O	S	0	0
			938	586	179	170	3		

- Molecule 14 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	145	Total	C	N	O	S	0	0
			1078	676	205	194	3		

- Molecule 15 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	136	Total	C	N	O	S	0	0
			1092	690	213	187	2		

- Molecule 16 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	118	Total	C	N	O	S	0	0
			928	583	180	163	2		

- Molecule 17 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	P	126	Total	C	N	O	0	0
			956	586	199	171		

- Molecule 18 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	113	Total	C	N	O	S	0	0
			907	570	171	165	1		

- Molecule 19 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	R	124	Total	C	N	O	0	0
			988	613	203	172		

- Molecule 20 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	S	100	Total	C	N	O	0	0
			754	478	137	139		

- Molecule 21 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	T	114	Total 873	C 543	N 171	O 159	0	0

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	U	97	Total 756	C 479	N 138	O 139	0	0

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	97	Total 732	C 456	N 137	O 137	S 2	0	0

- Molecule 24 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	W	192	Total 1428	C 881	N 255	O 292	0	0

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	X	79	Total 586	C 361	N 123	O 102	0	0

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	63	Total 470	C 283	N 103	O 80	S 4	0	0

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	64	Total 531	C 324	N 103	O 103	S 1	0	0

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	a	59	Total 474	C 292	N 95	O 87	0	0

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	54	Total 423	C 260	N 93	O 69	S 1	0	0

- Molecule 30 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	49	Total 405	C 248	N 82	O 71	S 4	0	0

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	46	Total 377	C 225	N 97	O 54	S 1	0	0

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	e	63	Total 502	C 302	N 115	O 85	0	0

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	37	Total 299	C 181	N 66	O 47	S 5	0	0

- Molecule 34 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	48	Total 364	C 225	N 63	O 71	S 5	0	0

- Molecule 35 is a RNA chain called tRNA CCA-end acetylated (Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	2	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

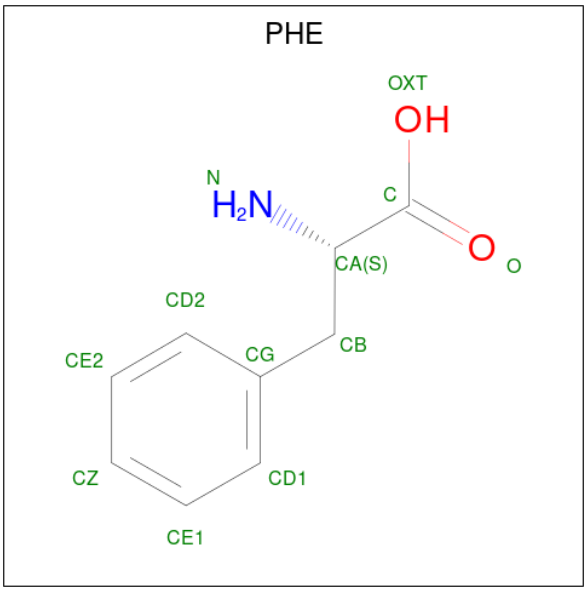
- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	A	388	Total	Mg	0
			388	388	
36	B	9	Total	Mg	0
			9	9	
36	C	4	Total	Mg	0
			4	4	
36	D	1	Total	Mg	0
			1	1	
36	F	1	Total	Mg	0
			1	1	
36	N	2	Total	Mg	0
			2	2	
36	T	1	Total	Mg	0
			1	1	
36	c	1	Total	Mg	0
			1	1	
36	2	1	Total	Mg	0
			1	1	

- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
37	Y	1	Total	Zn	0
			1	1	
37	c	1	Total	Zn	0
			1	1	
37	f	1	Total	Zn	0
			1	1	
37	g	1	Total	Zn	0
			1	1	

- Molecule 38 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



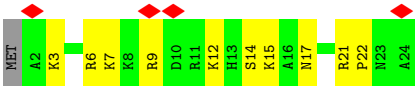
Mol	Chain	Residues	Atoms				AltConf
38	2	1	Total	C	N	O	0
			11	9	1	1	

3 Residue-property plots (i)

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

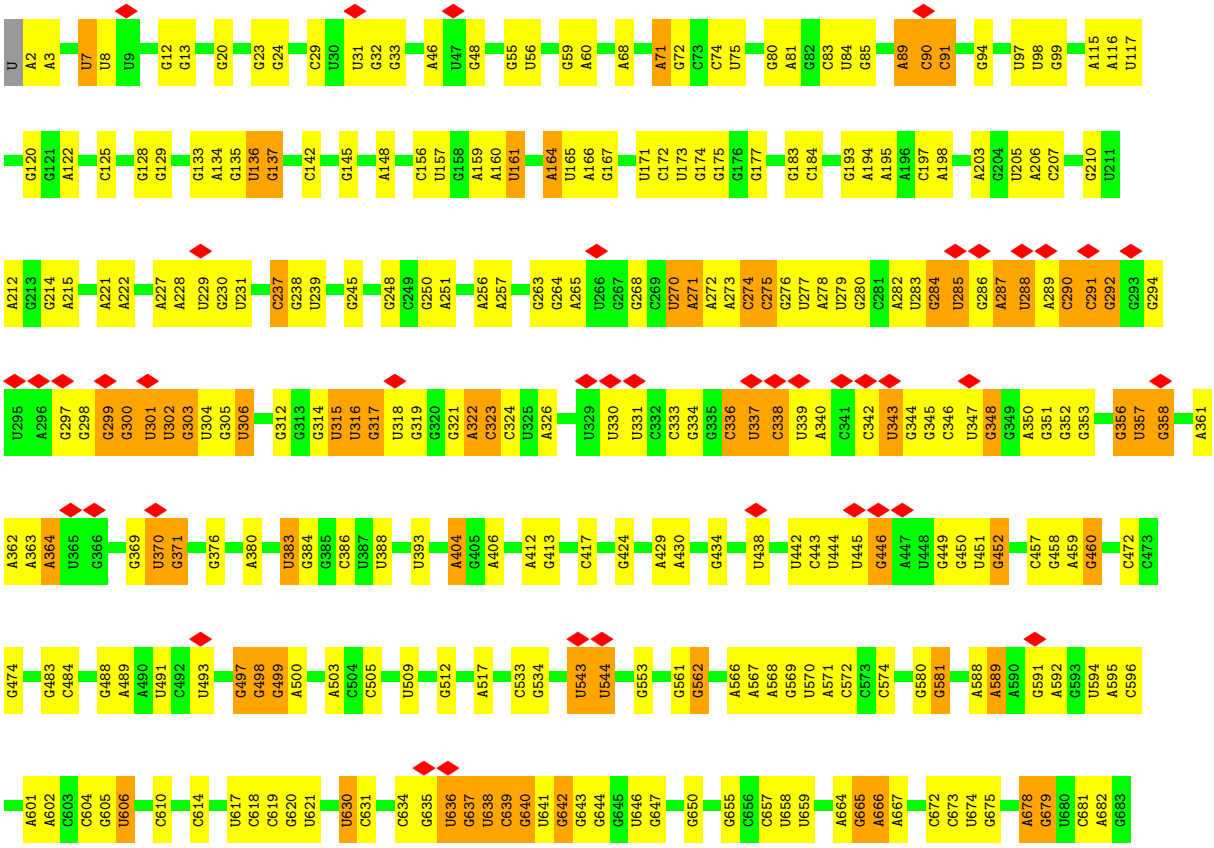
• Molecule 1: 50S ribosomal protein bL37

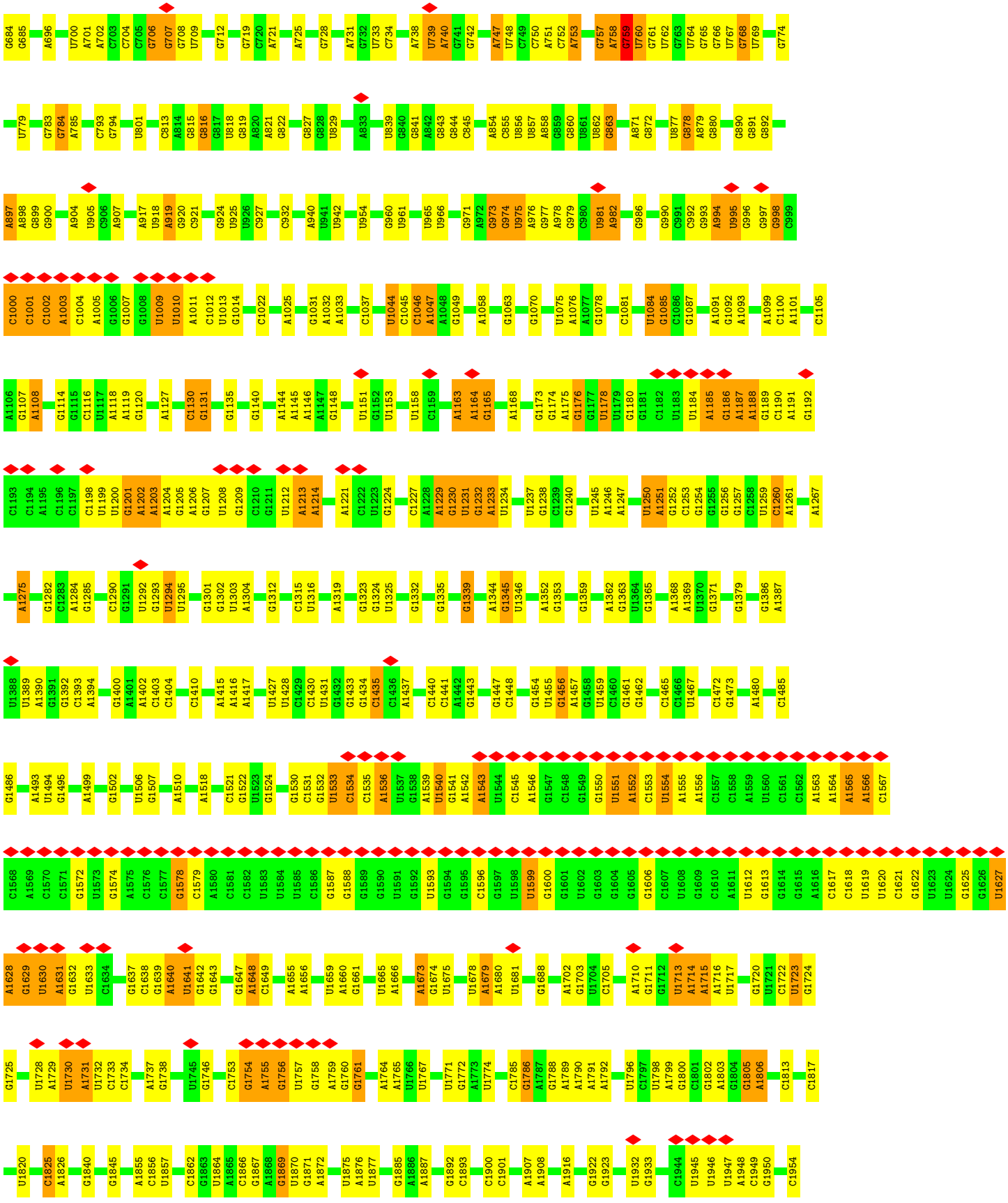
Chain 3:

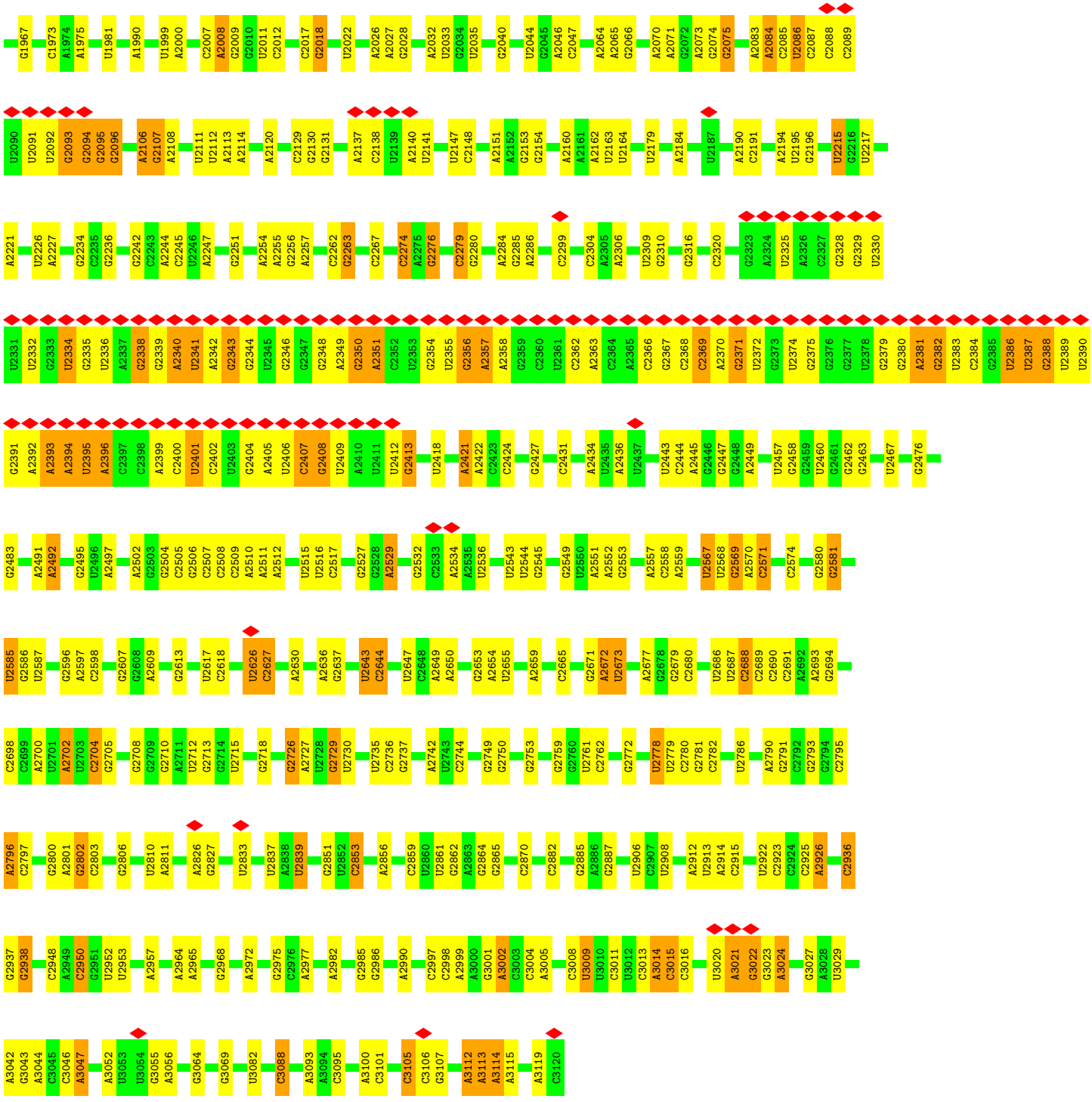


• Molecule 2: 23S rRNA

Chain A:

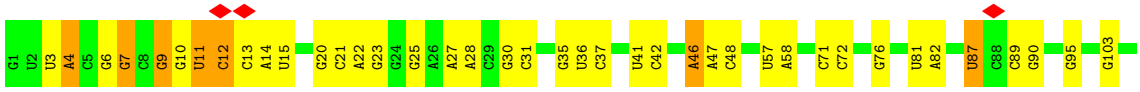


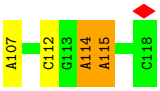




• Molecule 3: 5S rRNA

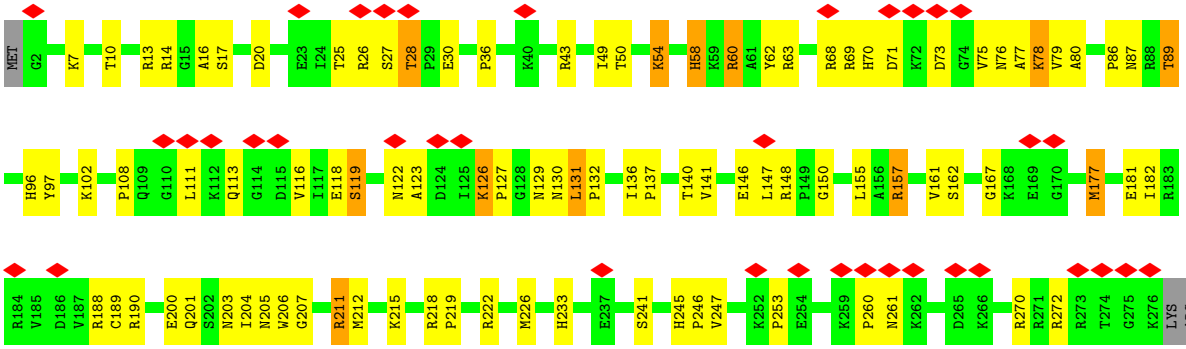
Chain B:





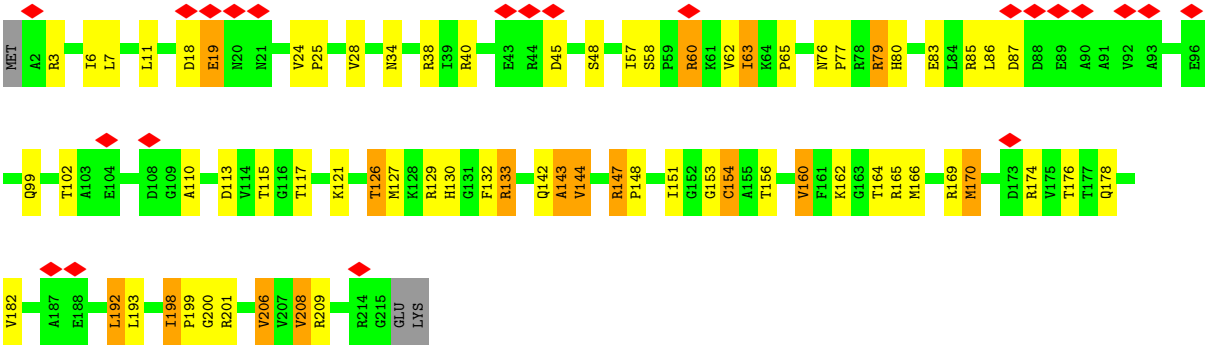
• Molecule 4: 50S ribosomal protein L2

Chain C:



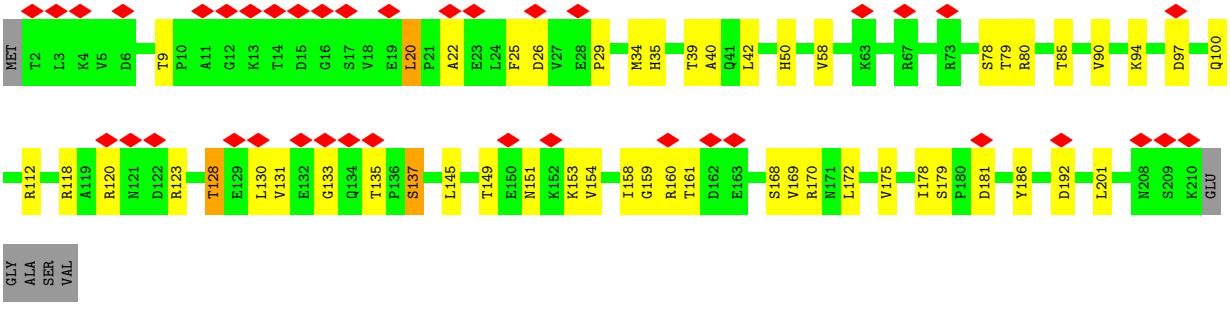
• Molecule 5: 50S ribosomal protein L3

Chain D:



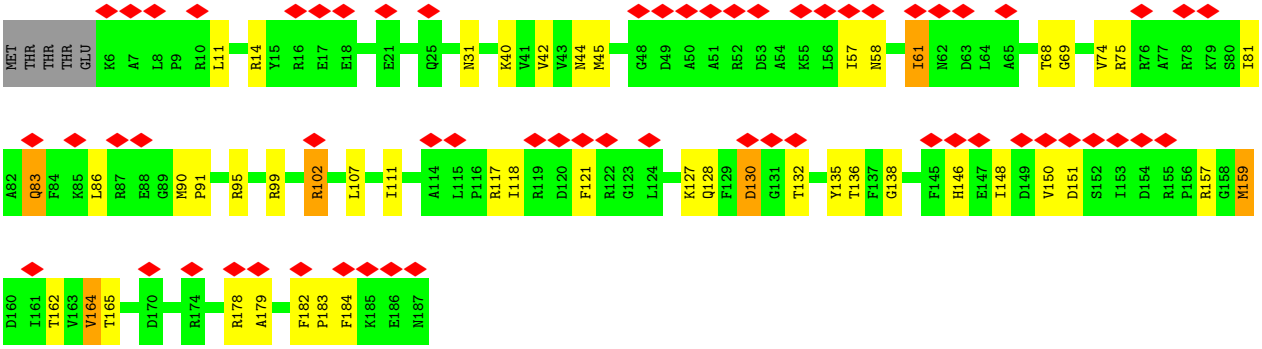
• Molecule 6: 50S ribosomal protein L4

Chain E:



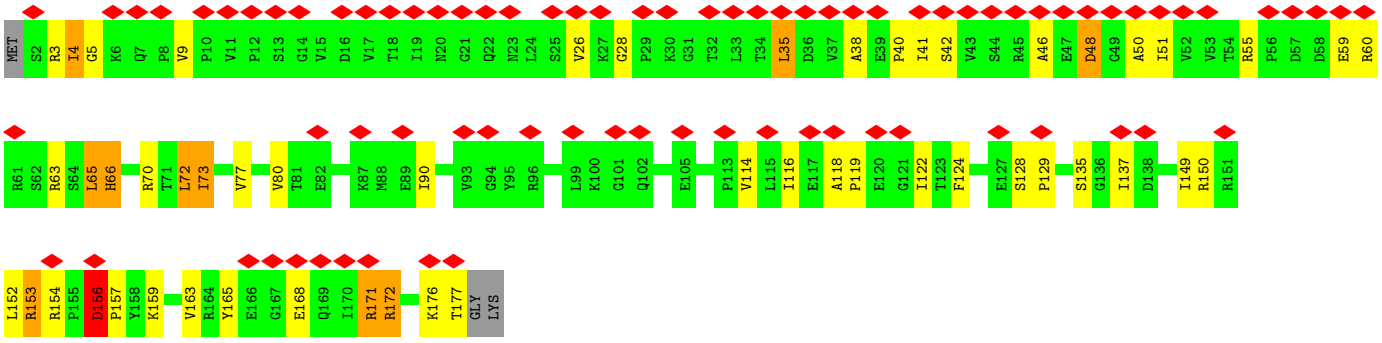
• Molecule 7: 50S ribosomal protein L5

Chain F:



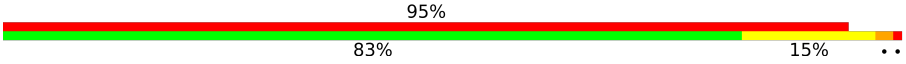
• Molecule 8: 50S ribosomal protein L6

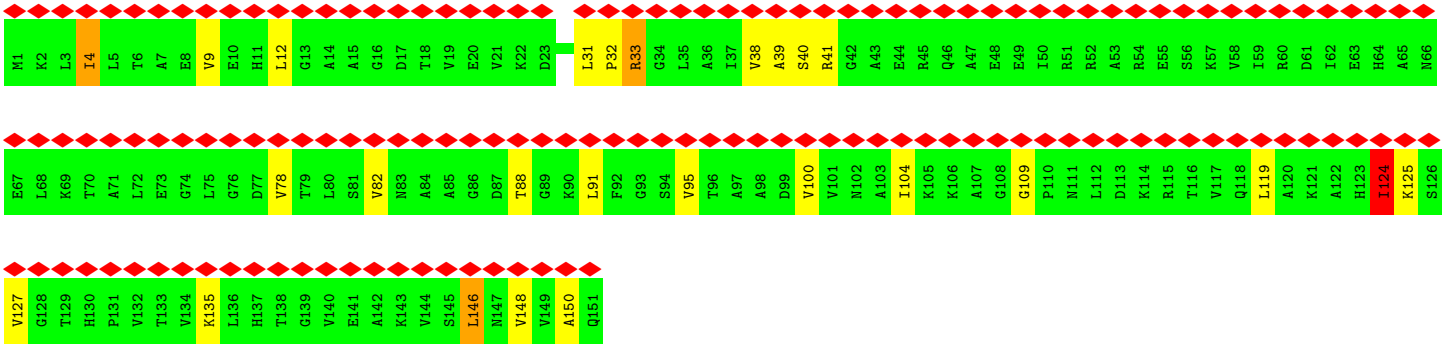
Chain G:



• Molecule 9: 50S ribosomal protein L9

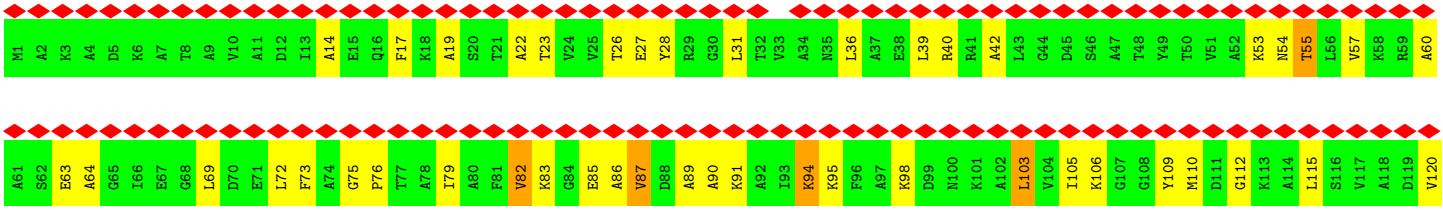
Chain H:

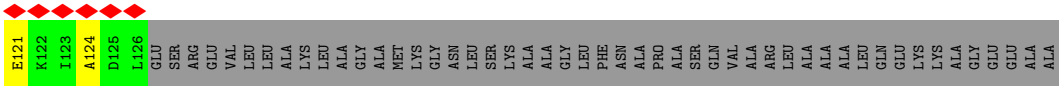




• Molecule 10: 50S ribosomal protein L10

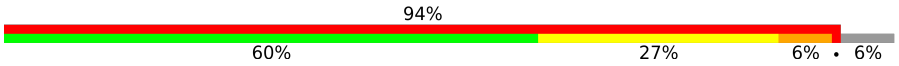
Chain I:

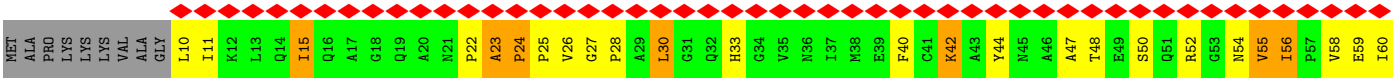


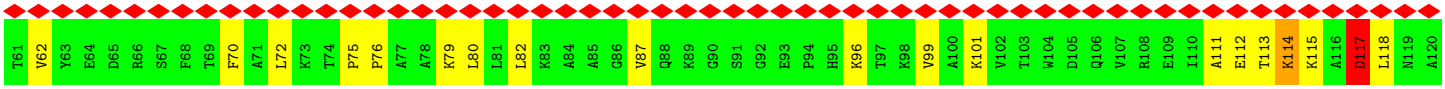


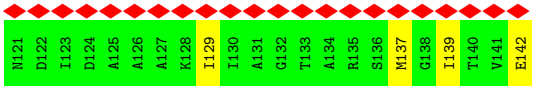
• Molecule 11: 50S ribosomal protein L11

Chain J:



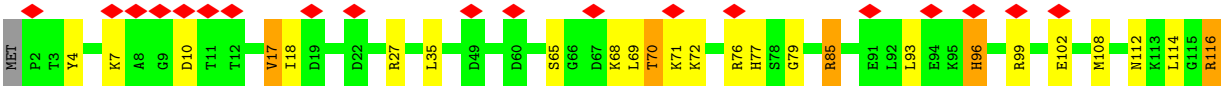


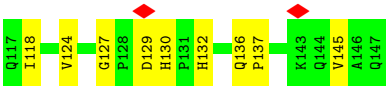




• Molecule 12: 50S ribosomal protein L13

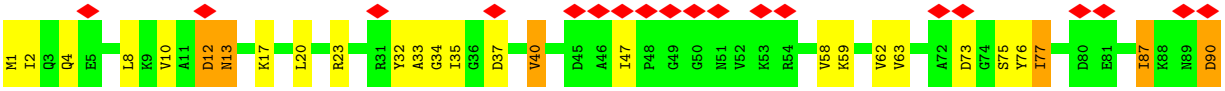
Chain K:





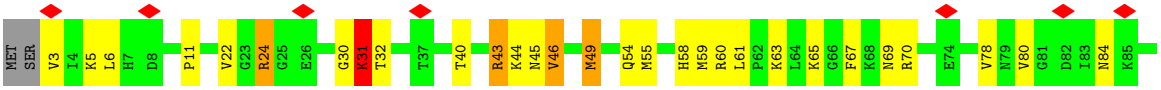
• Molecule 13: 50S ribosomal protein L14

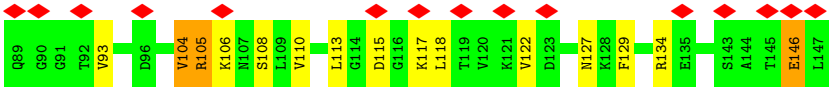
Chain L:



• Molecule 14: 50S ribosomal protein L15

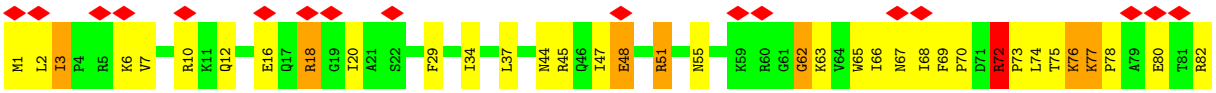
Chain M:

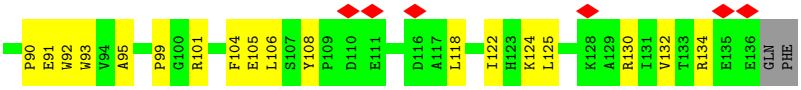




• Molecule 15: 50S ribosomal protein L16

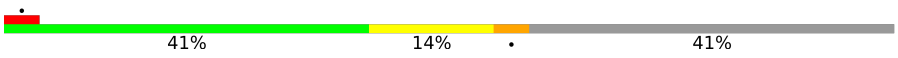
Chain N:

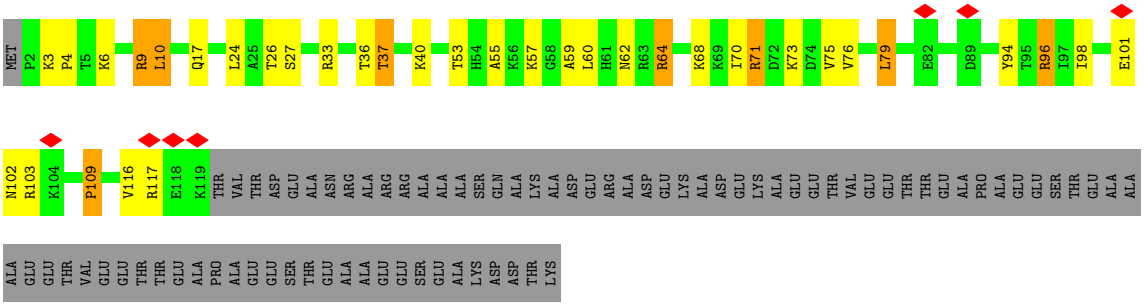




• Molecule 16: 50S ribosomal protein L17

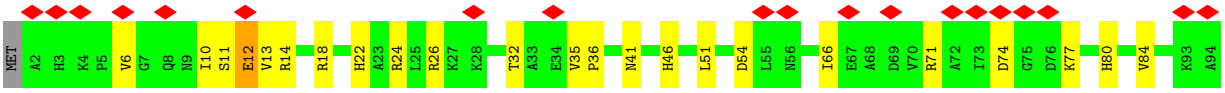
Chain O:





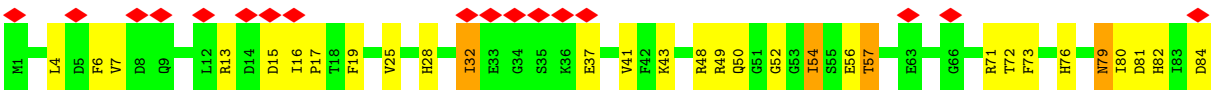
• Molecule 17: 50S ribosomal protein L18

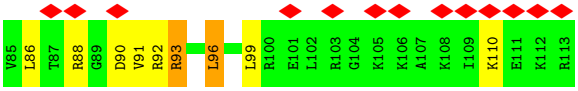
Chain P:



• Molecule 18: 50S ribosomal protein L19

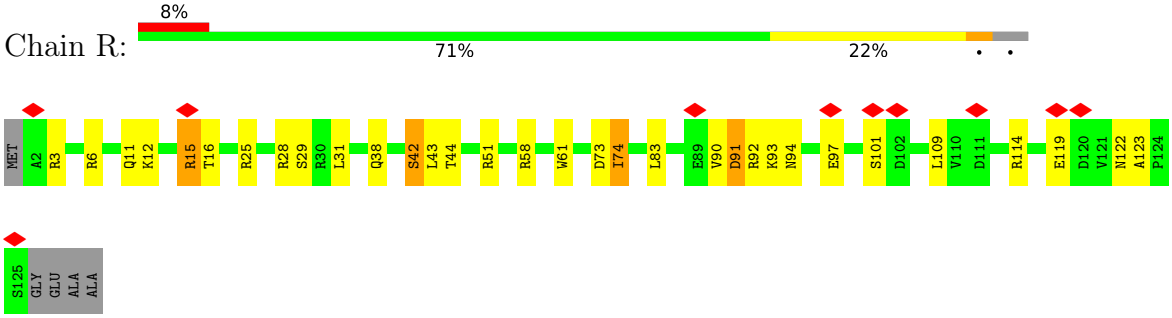
Chain Q:





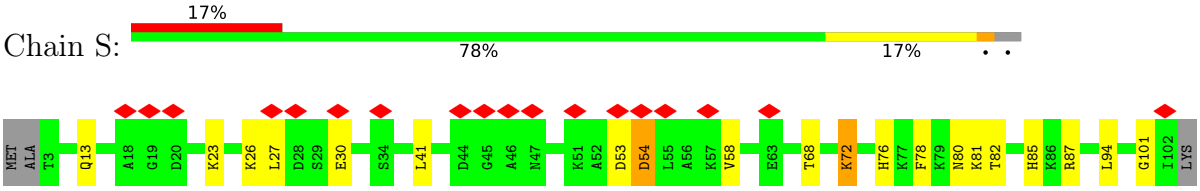
• Molecule 19: 50S ribosomal protein L20

Chain R:



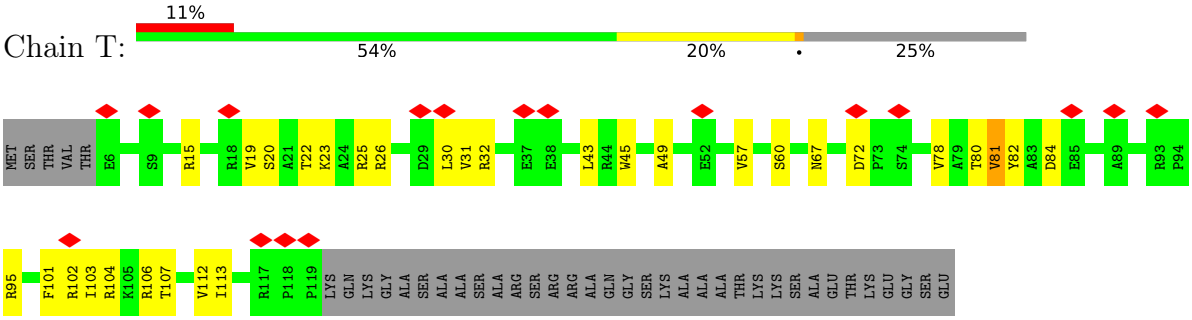
• Molecule 20: 50S ribosomal protein L21

Chain S:



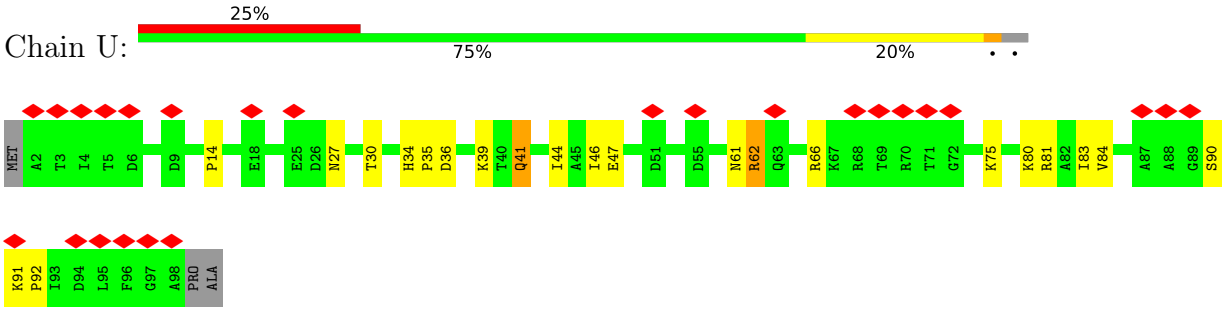
• Molecule 21: 50S ribosomal protein L22

Chain T:



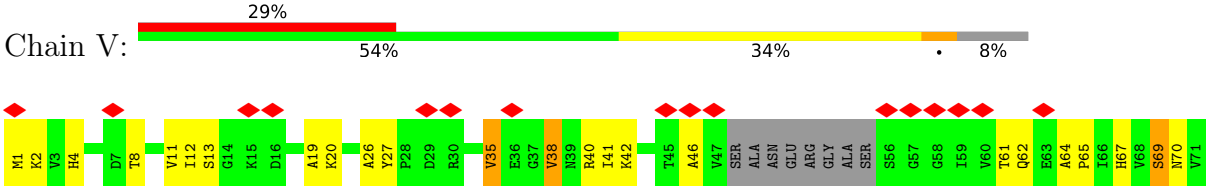
• Molecule 22: 50S ribosomal protein L23

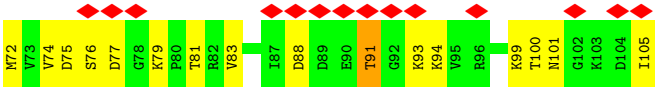
Chain U:



• Molecule 23: 50S ribosomal protein L24

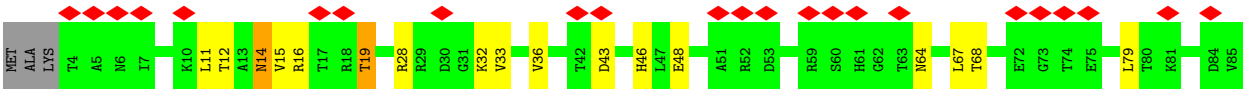
Chain V:

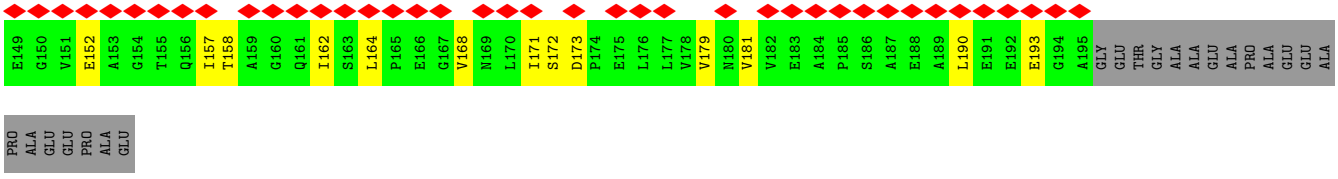




• Molecule 24: 50S ribosomal protein L25

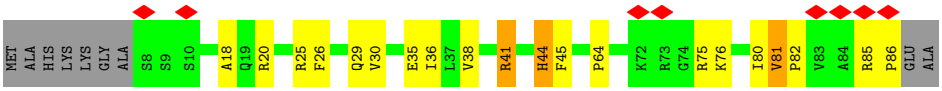
Chain W:





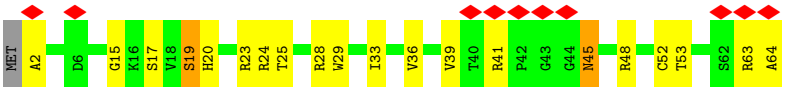
• Molecule 25: 50S ribosomal protein L27

Chain X:



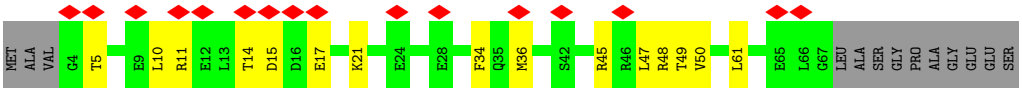
• Molecule 26: 50S ribosomal protein L28

Chain Y:



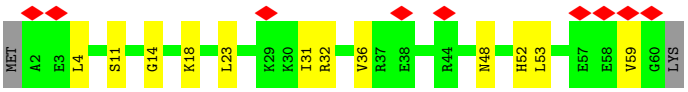
• Molecule 27: 50S ribosomal protein L29

Chain Z:



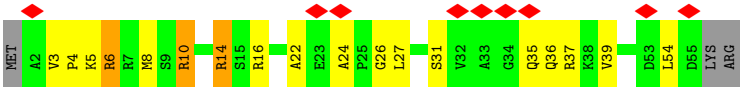
• Molecule 28: 50S ribosomal protein L30

Chain a:



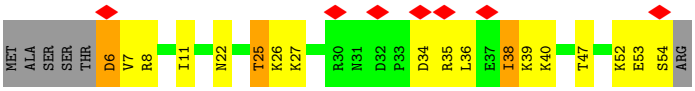
• Molecule 29: 50S ribosomal protein L32

Chain b:



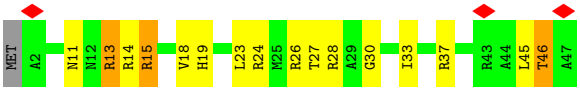
• Molecule 30: 50S ribosomal protein L33 1

Chain c:



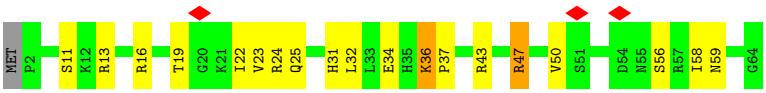
• Molecule 31: 50S ribosomal protein L34

Chain d:



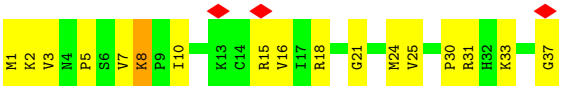
• Molecule 32: 50S ribosomal protein L35

Chain e:



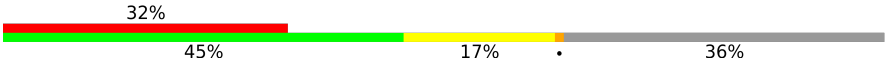
• Molecule 33: 50S ribosomal protein L36

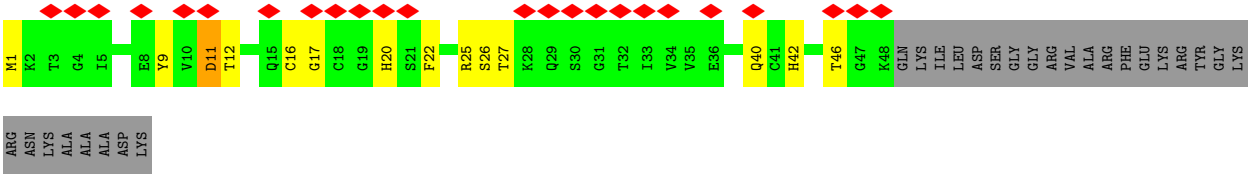
Chain f:



• Molecule 34: 50S ribosomal protein L31

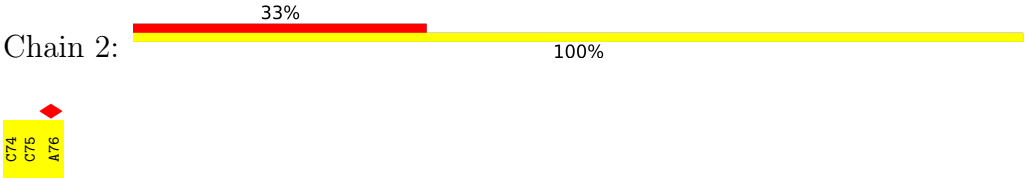
Chain g:





• Molecule 35: tRNA CCA-end acetylated (Phe)

Chain 2:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	224584	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF correction in Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	100719	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.570	Depositor
Minimum map value	-0.255	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	300.24, 300.24, 300.24	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	3	0.69	0/191	0.92	0/247
2	A	0.39	1/75001 (0.0%)	0.48	1/117027 (0.0%)
3	B	0.26	0/2821	0.41	0/4396
4	C	0.69	0/2153	1.07	10/2895 (0.3%)
5	D	0.73	0/1609	1.08	3/2165 (0.1%)
6	E	0.58	0/1592	1.04	7/2153 (0.3%)
7	F	0.44	0/1467	0.92	0/1973
8	G	0.45	0/1369	0.92	4/1848 (0.2%)
9	H	0.47	0/1027	0.87	3/1398 (0.2%)
10	I	0.60	0/925	0.91	1/1246 (0.1%)
11	J	0.67	1/1006 (0.1%)	0.98	6/1364 (0.4%)
12	K	0.64	0/1157	1.00	6/1567 (0.4%)
13	L	0.64	0/946	1.01	1/1268 (0.1%)
14	M	0.65	0/1091	1.12	5/1457 (0.3%)
15	N	0.69	0/1118	1.10	9/1506 (0.6%)
16	O	0.67	0/945	1.10	4/1267 (0.3%)
17	P	0.51	0/966	0.92	3/1298 (0.2%)
18	Q	0.60	0/921	0.98	0/1236
19	R	0.79	0/1000	0.96	2/1341 (0.1%)
20	S	0.63	0/764	1.02	1/1030 (0.1%)
21	T	0.78	0/887	1.07	4/1204 (0.3%)
22	U	0.61	0/766	0.99	1/1030 (0.1%)
23	V	0.62	0/738	0.96	2/987 (0.2%)
24	W	0.56	0/1443	0.95	5/1970 (0.3%)
25	X	0.72	0/595	1.00	3/798 (0.4%)
26	Y	0.76	0/478	1.10	0/641
27	Z	0.52	0/534	0.81	0/713
28	a	0.68	1/477 (0.2%)	0.96	0/640
29	b	0.64	0/427	0.91	0/572
30	c	0.59	0/413	0.86	0/553
31	d	0.69	0/380	1.07	0/500
32	e	0.64	0/507	1.01	2/672 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
33	f	0.75	0/303	1.13	3/401 (0.7%)
34	g	0.43	0/372	0.90	2/503 (0.4%)
35	2	0.32	0/68	0.58	0/103
All	All	0.46	3/106457 (0.0%)	0.64	88/159969 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1630	U	C1'-N1	6.79	1.58	1.48
28	a	59	VAL	N-CA	5.23	1.52	1.46
11	J	24	PRO	CA-C	5.03	1.56	1.52

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	N	125	LEU	CA-C-N	10.34	129.95	119.82
15	N	125	LEU	C-N-CA	10.34	129.95	119.82
16	O	70	ILE	N-CA-C	8.45	121.19	112.83
12	K	130	HIS	CA-C-N	8.31	128.52	119.87
12	K	130	HIS	C-N-CA	8.31	128.52	119.87
6	E	20	LEU	CA-C-N	8.31	128.38	119.90
6	E	20	LEU	C-N-CA	8.31	128.38	119.90
6	E	94	LYS	CA-C-N	-7.74	111.78	119.90
6	E	94	LYS	C-N-CA	-7.74	111.78	119.90
19	R	123	ALA	CA-C-N	7.57	127.24	119.82
19	R	123	ALA	C-N-CA	7.57	127.24	119.82
15	N	72	ARG	CA-C-N	7.57	128.16	120.14
15	N	72	ARG	C-N-CA	7.57	128.16	120.14
5	D	160	VAL	N-CA-C	7.47	120.23	112.83
8	G	156	ASP	CA-C-N	6.97	126.58	119.19
8	G	156	ASP	C-N-CA	6.97	126.58	119.19
6	E	133	GLY	N-CA-C	6.96	119.94	111.93
11	J	27	GLY	CA-C-N	6.84	126.64	119.05
11	J	27	GLY	C-N-CA	6.84	126.64	119.05
4	C	126	LYS	CA-C-N	6.71	126.74	119.90
4	C	126	LYS	C-N-CA	6.71	126.74	119.90
21	T	31	VAL	N-CA-C	6.61	119.38	112.83
11	J	117	ASP	N-CA-C	6.48	121.34	113.17
13	L	12	ASP	N-CA-C	6.37	118.87	109.69
21	T	72	ASP	CA-C-N	6.37	126.58	119.32
21	T	72	ASP	C-N-CA	6.37	126.58	119.32
25	X	81	VAL	CA-C-N	6.30	127.71	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	X	81	VAL	C-N-CA	6.30	127.71	119.84
16	O	60	LEU	N-CA-C	-6.29	104.43	111.28
10	I	85	GLU	CB-CA-C	-6.21	108.40	115.79
9	H	109	GLY	N-CA-C	6.11	124.80	112.34
11	J	24	PRO	N-CA-C	6.04	118.07	110.70
23	V	27	TYR	CA-C-N	6.03	126.47	119.47
23	V	27	TYR	C-N-CA	6.03	126.47	119.47
4	C	14	ARG	N-CA-C	6.02	117.53	110.97
14	M	46	VAL	CA-C-N	5.98	126.33	119.93
14	M	46	VAL	C-N-CA	5.98	126.33	119.93
24	W	116	GLY	N-CA-C	5.97	120.47	110.56
15	N	62	GLY	N-CA-C	-5.95	102.46	110.56
12	K	96	HIS	CA-C-N	5.89	125.36	119.24
12	K	96	HIS	C-N-CA	5.89	125.36	119.24
17	P	46	HIS	N-CA-C	5.85	117.11	108.86
8	G	28	GLY	CA-C-N	5.84	125.98	119.32
8	G	28	GLY	C-N-CA	5.84	125.98	119.32
4	C	245	HIS	CA-C-N	5.82	125.76	119.76
4	C	245	HIS	C-N-CA	5.82	125.76	119.76
24	W	173	ASP	CA-C-N	5.76	125.86	119.87
24	W	173	ASP	C-N-CA	5.76	125.86	119.87
14	M	106	LYS	N-CA-C	5.71	117.58	111.36
11	J	23	ALA	CA-C-N	-5.59	114.62	120.38
11	J	23	ALA	C-N-CA	-5.59	114.62	120.38
22	U	90	SER	N-CA-C	5.59	117.45	110.91
4	C	7	LYS	CA-C-N	5.58	126.81	119.84
4	C	7	LYS	C-N-CA	5.58	126.81	119.84
34	g	42	HIS	CA-C-N	5.58	125.25	119.56
34	g	42	HIS	C-N-CA	5.58	125.25	119.56
15	N	77	LYS	CA-C-N	5.57	125.58	119.90
15	N	77	LYS	C-N-CA	5.57	125.58	119.90
33	f	8	LYS	CA-C-N	5.53	126.75	119.84
33	f	8	LYS	C-N-CA	5.53	126.75	119.84
14	M	115	ASP	N-CA-C	5.50	116.97	110.97
32	e	36	LYS	CA-C-N	5.46	125.39	119.76
32	e	36	LYS	C-N-CA	5.46	125.39	119.76
5	D	133	ARG	N-CA-C	-5.46	102.80	110.50
4	C	20	ASP	CA-C-N	-5.40	114.47	122.41
4	C	20	ASP	C-N-CA	-5.40	114.47	122.41
5	D	200	GLY	N-CA-C	5.40	117.29	110.38
12	K	127	GLY	CA-C-N	5.40	125.02	119.56
12	K	127	GLY	C-N-CA	5.40	125.02	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	N	108	TYR	CA-C-N	5.40	124.86	119.24
15	N	108	TYR	C-N-CA	5.40	124.86	119.24
9	H	109	GLY	CA-C-N	-5.37	114.71	120.03
9	H	109	GLY	C-N-CA	-5.37	114.71	120.03
20	S	101	GLY	N-CA-C	5.35	118.91	111.10
21	T	82	TYR	N-CA-C	5.22	116.78	108.79
4	C	167	GLY	N-CA-C	5.16	118.11	110.42
14	M	108	SER	N-CA-C	5.14	117.44	110.35
17	P	35	VAL	CA-C-N	5.12	125.10	120.03
17	P	35	VAL	C-N-CA	5.12	125.10	120.03
25	X	44	HIS	N-CA-C	-5.11	105.40	111.69
33	f	10	ILE	N-CA-C	5.10	118.21	111.17
6	E	172	LEU	CA-C-N	5.09	124.27	118.97
6	E	172	LEU	C-N-CA	5.09	124.27	118.97
24	W	152	GLU	N-CA-C	5.09	117.41	109.52
24	W	122	THR	N-CA-C	5.07	117.76	109.59
16	O	109	PRO	CA-C-N	-5.01	114.39	122.81
16	O	109	PRO	C-N-CA	-5.01	114.39	122.81
2	A	759	G	C4'-C3'-O3'	5.01	116.91	109.40

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	3	189	0	205	6	0
2	A	66981	0	33699	543	0
3	B	2522	0	1285	21	0
4	C	2110	0	2165	71	0
5	D	1587	0	1630	46	0
6	E	1569	0	1607	26	0
7	F	1445	0	1476	37	0
8	G	1348	0	1399	35	0
9	H	1018	0	988	14	0
10	I	918	0	959	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	J	990	0	1021	29	0
12	K	1130	0	1167	31	0
13	L	938	0	1000	24	0
14	M	1078	0	1151	43	0
15	N	1092	0	1128	44	0
16	O	928	0	972	25	0
17	P	956	0	991	16	0
18	Q	907	0	938	30	0
19	R	988	0	1038	26	0
20	S	754	0	802	13	0
21	T	873	0	909	20	0
22	U	756	0	802	14	0
23	V	732	0	782	25	0
24	W	1428	0	1443	31	0
25	X	586	0	601	14	0
26	Y	470	0	480	14	0
27	Z	531	0	541	16	0
28	a	474	0	500	8	0
29	b	423	0	463	22	0
30	c	405	0	407	13	0
31	d	377	0	411	14	0
32	e	502	0	541	9	0
33	f	299	0	321	11	0
34	g	364	0	348	5	0
35	2	62	0	33	1	0
36	2	1	0	0	0	0
36	A	388	0	0	0	0
36	B	9	0	0	0	0
36	C	4	0	0	0	0
36	D	1	0	0	0	0
36	F	1	0	0	0	0
36	N	2	0	0	0	0
36	T	1	0	0	0	0
36	c	1	0	0	0	0
37	Y	1	0	0	0	0
37	c	1	0	0	0	0
37	f	1	0	0	0	0
37	g	1	0	0	0	0
38	2	11	0	8	0	0
All	All	98153	0	64211	1141	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 (1141) 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)
2:A:2422:A:O2'	26:Y:63:ARG:NH1	1.74	1.20
2:A:2509:C:OP2	30:c:8:ARG:NH1	1.91	1.03
2:A:142:C:H5"	22:U:41:GLN:HE21	1.27	0.99
2:A:301:U:H5'	2:A:302:U:H5"	1.47	0.96
2:A:2772:G:H1'	13:L:23:ARG:HH12	1.31	0.95
2:A:164:A:H4'	26:Y:41:ARG:HH12	1.31	0.95
2:A:1722:C:OP1	4:C:78:LYS:NZ	1.99	0.94
2:A:2245:C:OP1	19:R:25:ARG:NH1	2.00	0.94
7:F:75:ARG:HH21	7:F:95:ARG:NH1	1.66	0.94
2:A:1786:G:OP1	4:C:211:ARG:NH1	2.01	0.93
4:C:68:ARG:HH12	4:C:150:GLY:C	1.75	0.93
20:S:87:ARG:HG3	20:S:87:ARG:HH11	1.34	0.93
24:W:105:LYS:NZ	24:W:136:GLU:OE2	2.02	0.91
4:C:68:ARG:NH1	4:C:150:GLY:O	2.05	0.90
10:I:94:LYS:NZ	10:I:120:VAL:O	2.06	0.88
2:A:2343:G:O6	2:A:2399:A:N6	2.06	0.88
29:b:37:ARG:HH11	29:b:54:LEU:HB3	1.41	0.85
6:E:192:ASP:OD1	14:M:5:LYS:NZ	2.10	0.85
10:I:40:ARG:HG3	10:I:40:ARG:HH11	1.44	0.83
14:M:43:ARG:HG3	14:M:43:ARG:HH11	1.44	0.83
2:A:2276:G:H4'	5:D:153:GLY:O	1.80	0.82
4:C:132:PRO:HD3	4:C:190:ARG:HH11	1.44	0.82
2:A:2587:U:OP2	32:e:43:ARG:NH2	2.13	0.81
4:C:126:LYS:HD3	4:C:127:PRO:HD2	1.60	0.81
19:R:11:GLN:HB3	19:R:15:ARG:HH21	1.45	0.81
20:S:76:HIS:HE1	20:S:85:HIS:HB3	1.46	0.81
4:C:182:ILE:HD12	4:C:270:ARG:HH12	1.43	0.81
2:A:1186:G:N2	2:A:1213:A:O2'	2.15	0.80
2:A:2406:U:H5'	2:A:2407:C:OP2	1.81	0.80
2:A:1730:U:H5"	2:A:1731:A:C8	2.17	0.79
2:A:2279:C:OP1	29:b:5:LYS:NZ	2.14	0.79
23:V:88:ASP:HB2	23:V:93:LYS:HB2	1.64	0.79
2:A:2357:A:H1'	2:A:2382:G:H21	1.48	0.79
4:C:80:ALA:O	4:C:113:GLN:NE2	2.16	0.78
2:A:1365:G:OP2	14:M:24:ARG:NH1	2.15	0.78
2:A:2529:A:H5"	7:F:138:GLY:HA3	1.63	0.78
2:A:2363:A:H61	2:A:2374:U:H3	1.32	0.77
4:C:26:ARG:NH1	4:C:30:GLU:OE1	2.15	0.77
29:b:6:ARG:CG	29:b:6:ARG:HH11	1.96	0.77
2:A:1578:G:H22	2:A:1593:U:H3	1.29	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:85:ARG:HG3	12:K:85:ARG:HH11	1.49	0.77
19:R:73:ASP:O	19:R:114:ARG:NH2	2.17	0.77
14:M:84:ASN:HD21	14:M:118:LEU:HA	1.48	0.77
2:A:2862:G:O2'	2:A:3002:A:N6	2.18	0.77
10:I:17:PHE:CE2	10:I:64:ALA:HB3	2.20	0.76
12:K:4:TYR:OH	12:K:10:ASP:OD2	2.03	0.76
31:d:27:THR:HG23	31:d:30:GLY:H	1.50	0.76
2:A:2571:C:OP1	30:c:40:LYS:NZ	2.19	0.75
2:A:2977:A:O2'	33:f:15:ARG:NH1	2.19	0.75
2:A:2358:A:N6	2:A:2379:G:O2'	2.20	0.75
12:K:76:ARG:HB3	12:K:85:ARG:HH12	1.52	0.75
29:b:10:ARG:HG2	29:b:14:ARG:HH12	1.52	0.75
2:A:2032:A:OP2	4:C:54:LYS:NZ	2.19	0.75
2:A:1493:A:OP1	31:d:13:ARG:NH2	2.20	0.74
2:A:1730:U:H5"	2:A:1731:A:H8	1.49	0.74
7:F:117:ARG:HH11	7:F:146:HIS:CE1	2.05	0.74
2:A:1530:G:H22	2:A:1805:G:H1	1.36	0.74
12:K:76:ARG:HB3	12:K:85:ARG:NH1	2.02	0.73
13:L:2:ILE:HB	13:L:33:ALA:HB3	1.70	0.73
2:A:2386:U:OP1	2:A:2393:A:O2'	2.04	0.73
29:b:6:ARG:HH11	29:b:6:ARG:HG3	1.54	0.73
2:A:1260:C:H6	12:K:27:ARG:HH12	1.36	0.73
15:N:51:ARG:NH2	24:W:193:GLU:O	2.21	0.73
2:A:164:A:C4'	26:Y:41:ARG:HH12	2.02	0.73
2:A:659:U:OP2	14:M:31:LYS:NZ	2.21	0.73
2:A:2476:G:N2	35:2:74:C:O2	2.20	0.73
5:D:121:LYS:HG3	5:D:170:MET:HE3	1.70	0.73
7:F:136:THR:HG23	7:F:162:THR:HB	1.69	0.73
32:e:47:ARG:HB2	32:e:47:ARG:HH11	1.54	0.73
2:A:2009:G:H5'	4:C:205:ASN:ND2	2.04	0.72
2:A:81:A:OP1	23:V:4:HIS:NE2	2.22	0.72
2:A:679:G:OP2	14:M:24:ARG:NH2	2.23	0.72
4:C:247:VAL:HG12	4:C:253:PRO:HA	1.72	0.72
20:S:87:ARG:HG3	20:S:87:ARG:NH1	2.02	0.72
2:A:2691:C:OP1	33:f:8:LYS:NZ	2.23	0.71
2:A:543:U:H3'	2:A:544:U:H5"	1.70	0.71
2:A:1403:C:H5	2:A:1441:C:N3	1.87	0.71
9:H:32:PRO:HB3	26:Y:64:ALA:HA	1.73	0.71
2:A:2274:C:H1'	5:D:166:MET:HE3	1.70	0.71
2:A:753:A:H61	2:A:762:U:H3	1.38	0.71
2:A:2343:G:N2	2:A:2401:U:O2	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:31:C:H5'	17:P:11:SER:HB3	1.71	0.70
2:A:75:U:H5'	27:Z:11:ARG:HH22	1.57	0.70
2:A:1224:G:O2'	10:I:28:TYR:OH	2.09	0.70
2:A:2803:C:H4'	5:D:144:VAL:HG21	1.73	0.70
14:M:134:ARG:HH22	14:M:146:GLU:HG2	1.57	0.70
2:A:1554:U:H3	2:A:1617:C:H42	1.40	0.69
18:Q:48:ARG:HD2	18:Q:50:GLN:HE21	1.56	0.69
2:A:2348:G:O2'	2:A:2396:A:N6	2.22	0.69
13:L:76:TYR:HB2	18:Q:72:THR:HB	1.74	0.69
29:b:10:ARG:HG2	29:b:14:ARG:NH1	2.08	0.69
29:b:14:ARG:HG2	29:b:14:ARG:HH11	1.58	0.68
2:A:2332:U:H1'	2:A:2404:G:H21	1.57	0.68
2:A:2795:C:O2'	5:D:156:THR:O	2.10	0.68
2:A:2424:C:OP1	26:Y:48:ARG:NH2	2.21	0.68
13:L:63:VAL:HG12	13:L:106:LEU:HD11	1.75	0.68
2:A:290:C:H42	2:A:298:G:H22	1.41	0.68
2:A:1339:G:OP1	20:S:72:LYS:NZ	2.27	0.68
25:X:41:ARG:NE	25:X:41:ARG:HA	2.09	0.68
4:C:206:TRP:CH2	4:C:215:LYS:HE3	2.29	0.68
14:M:43:ARG:HH11	14:M:43:ARG:CG	2.07	0.68
2:A:160:A:H3'	2:A:161:U:H5"	1.75	0.68
2:A:164:A:O2'	26:Y:41:ARG:NH1	2.26	0.68
2:A:1673:A:O2'	2:A:2926:A:OP2	2.12	0.68
19:R:28:ARG:NH1	19:R:38:GLN:OE1	2.27	0.68
24:W:14:ASN:OD1	24:W:14:ASN:N	2.27	0.67
10:I:17:PHE:HE2	10:I:64:ALA:HB3	1.60	0.67
3:B:41:U:O4	34:g:1:MET:N	2.27	0.67
2:A:1410:C:H5"	16:O:71:ARG:NH1	2.10	0.67
2:A:2975:G:H4'	8:G:4:ILE:HD11	1.75	0.67
2:A:2350:G:O2'	2:A:2351:A:O4'	2.13	0.67
2:A:1260:C:O2'	12:K:27:ARG:NH2	2.28	0.67
2:A:287:A:N6	2:A:299:G:O2'	2.28	0.66
2:A:1260:C:H6	12:K:27:ARG:NH1	1.93	0.66
6:E:112:ARG:HG2	6:E:112:ARG:HH11	1.60	0.66
11:J:101:LYS:HE3	11:J:142:GLU:HB2	1.75	0.66
14:M:30:GLY:O	14:M:32:THR:N	2.27	0.66
7:F:75:ARG:HH21	7:F:95:ARG:HH11	1.43	0.66
12:K:77:HIS:CD2	12:K:79:GLY:H	2.14	0.66
11:J:30:LEU:HA	11:J:33:HIS:HD2	1.61	0.66
14:M:78:VAL:HG23	14:M:104:VAL:HG13	1.78	0.66
2:A:2936:C:OP1	2:A:2938:G:H4'	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:10:VAL:HG12	13:L:12:ASP:H	1.59	0.66
2:A:2557:A:OP1	25:X:75:ARG:NH2	2.29	0.66
2:A:380:A:P	23:V:99:LYS:HZ1	2.18	0.66
2:A:2626:U:H4'	2:A:2627:C:OP2	1.94	0.66
2:A:2569:G:H4'	2:A:2570:A:H5"	1.78	0.65
2:A:303:G:N2	2:A:304:U:O2	2.29	0.65
2:A:567:A:H4'	2:A:568:A:H5'	1.78	0.65
2:A:1552:A:H1'	2:A:1618:C:H42	1.59	0.65
2:A:1875:U:H4'	5:D:143:ALA:HB1	1.77	0.65
2:A:2862:G:HO2'	2:A:3002:A:N6	1.95	0.65
15:N:29:PHE:O	15:N:134:ARG:NH2	2.29	0.65
2:A:3113:A:H4'	2:A:3114:A:OP2	1.95	0.65
18:Q:90:ASP:HB2	18:Q:110:LYS:HB2	1.79	0.65
13:L:77:ILE:HD11	18:Q:71:ARG:HD2	1.78	0.65
2:A:2412:U:H2'	2:A:2413:G:C8	2.31	0.65
13:L:17:LYS:HE3	13:L:47:ILE:HG22	1.79	0.65
21:T:30:LEU:HD22	29:b:24:ALA:HB2	1.79	0.65
29:b:37:ARG:NH1	29:b:54:LEU:HB3	2.10	0.65
4:C:17:SER:O	4:C:211:ARG:NH2	2.29	0.65
2:A:1282:G:OP1	20:S:26:LYS:NZ	2.30	0.64
2:A:1002:C:H2'	2:A:1003:A:H5"	1.78	0.64
2:A:1037:C:O2'	25:X:29:GLN:NE2	2.29	0.64
20:S:76:HIS:CE1	20:S:85:HIS:HB3	2.31	0.64
2:A:998:G:H22	2:A:1009:U:H3	1.44	0.64
2:A:571:A:H4'	23:V:46:ALA:HB2	1.79	0.64
2:A:3013:C:H5'	2:A:3014:A:OP1	1.98	0.64
2:A:1456:G:OP1	2:A:1820:U:O2'	2.11	0.64
2:A:2422:A:HO2'	26:Y:63:ARG:NH1	1.91	0.64
2:A:2735:U:O2'	5:D:148:PRO:O	2.15	0.64
2:A:1224:G:HO2'	10:I:28:TYR:HH	1.39	0.63
8:G:118:ALA:HB2	8:G:124:PHE:CE2	2.33	0.63
16:O:59:ALA:HB3	16:O:62:ASN:H	1.62	0.63
10:I:23:THR:HG23	10:I:109:TYR:HB3	1.79	0.63
15:N:37:LEU:O	15:N:99:PRO:HB3	1.99	0.63
2:A:1233:A:H4'	2:A:1233:A:OP1	1.97	0.63
2:A:2803:C:C4'	5:D:144:VAL:HG21	2.29	0.63
13:L:93:PRO:HD2	13:L:113:LYS:HG2	1.79	0.63
18:Q:71:ARG:HG2	18:Q:73:PHE:CZ	2.34	0.62
2:A:290:C:N4	2:A:298:G:H22	1.96	0.62
16:O:57:LYS:O	16:O:62:ASN:ND2	2.32	0.62
18:Q:32:ILE:HG22	18:Q:37:GLU:HG2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1163:A:OP1	2:A:1164:A:O2'	2.18	0.62
30:c:35:ARG:NH2	30:c:53:GLU:O	2.32	0.62
2:A:706:G:O2'	6:E:160:ARG:NH2	2.32	0.62
2:A:1533:U:H3'	2:A:1534:C:H5"	1.81	0.62
10:I:36:LEU:O	10:I:40:ARG:HG2	1.99	0.62
14:M:84:ASN:ND2	14:M:117:LYS:O	2.33	0.62
17:P:26:ARG:NH1	17:P:54:ASP:OD2	2.31	0.62
2:A:291:C:O2'	2:A:337:U:O2'	2.16	0.62
2:A:333:C:H2'	2:A:334:G:H8	1.64	0.62
7:F:128:GLN:HB2	7:F:135:TYR:CE1	2.35	0.62
23:V:77:ASP:OD2	23:V:101:ASN:ND2	2.32	0.62
2:A:1410:C:H5"	16:O:71:ARG:HH11	1.64	0.61
4:C:26:ARG:HG2	4:C:28:THR:H	1.65	0.61
2:A:316:U:O2'	2:A:317:G:OP1	2.15	0.61
2:A:997:G:H1	2:A:1010:U:H3	1.45	0.61
29:b:14:ARG:NH1	29:b:14:ARG:HG2	2.14	0.61
2:A:2234:G:H5"	21:T:49:ALA:HB2	1.83	0.61
2:A:1551:U:H3'	2:A:1552:A:H8	1.64	0.61
2:A:1825:C:N4	2:A:1840:G:OP2	2.27	0.61
15:N:63:LYS:HD3	15:N:65:TRP:CH2	2.36	0.61
27:Z:45:ARG:NH1	27:Z:48:ARG:HE	1.99	0.61
2:A:2404:G:H2'	2:A:2405:A:C8	2.36	0.61
5:D:147:ARG:HB2	5:D:148:PRO:HD2	1.81	0.60
2:A:1201:G:N2	2:A:1203:A:H3'	2.16	0.60
2:A:1551:U:H3	2:A:1619:U:H3	1.48	0.60
2:A:1875:U:H5"	5:D:143:ALA:O	2.02	0.60
2:A:292:G:H1	2:A:343:U:H3	1.50	0.60
4:C:146:GLU:HB2	4:C:189:CYS:HB2	1.83	0.60
6:E:29:PRO:HD3	6:E:120:ARG:NH1	2.17	0.60
2:A:2093:G:O2'	2:A:2094:G:C8	2.54	0.60
2:A:2304:C:H4'	26:Y:25:THR:HG21	1.83	0.59
15:N:34:ILE:HD12	15:N:104:PHE:HB2	1.82	0.59
24:W:100:VAL:HG11	24:W:137:ALA:HB2	1.84	0.59
21:T:81:VAL:HG13	21:T:112:VAL:HG22	1.85	0.59
24:W:43:ASP:OD1	24:W:43:ASP:N	2.35	0.59
15:N:91:GLU:HB3	15:N:92:TRP:CE3	2.37	0.59
26:Y:19:SER:OG	26:Y:20:HIS:N	2.35	0.59
2:A:1187:A:H5"	2:A:1188:A:C8	2.37	0.59
5:D:7:LEU:H	5:D:34:ASN:ND2	2.01	0.59
22:U:61:ASN:HD21	22:U:80:LYS:HE2	1.68	0.59
5:D:154:CYS:C	5:D:156:THR:H	2.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2340:A:H61	2:A:2389:U:H3	1.49	0.59
26:Y:2:ALA:HA	26:Y:33:ILE:HD11	1.84	0.59
2:A:13:G:H5"	29:b:14:ARG:HB3	1.84	0.59
2:A:164:A:H2'	2:A:165:U:C6	2.38	0.59
5:D:7:LEU:HB2	5:D:34:ASN:HD21	1.68	0.59
7:F:81:ILE:HG22	7:F:86:LEU:HD23	1.84	0.59
11:J:40:PHE:HE1	11:J:58:VAL:HG21	1.67	0.59
23:V:91:THR:HB	23:V:93:LYS:HG3	1.83	0.59
27:Z:14:THR:HG23	27:Z:17:GLU:H	1.68	0.59
13:L:90:ASP:OD1	13:L:90:ASP:N	2.36	0.59
22:U:34:HIS:ND1	22:U:36:ASP:OD1	2.35	0.59
5:D:130:HIS:CD2	5:D:165:ARG:HB3	2.38	0.58
2:A:1679:A:H4'	2:A:1679:A:OP1	2.04	0.58
4:C:155:LEU:HB3	4:C:177:MET:HE1	1.86	0.58
23:V:67:HIS:HD2	23:V:69:SER:H	1.52	0.58
29:b:10:ARG:CG	29:b:14:ARG:HH12	2.16	0.58
29:b:31:SER:HB3	29:b:36:GLN:HE22	1.67	0.58
2:A:858:A:O2'	2:A:1877:U:OP1	2.19	0.58
2:A:918:U:H2'	2:A:919:A:H5"	1.86	0.58
2:A:2407:C:H2'	2:A:2408:G:C8	2.39	0.58
2:A:574:C:O2'	21:T:67:ASN:ND2	2.25	0.58
2:A:1116:C:O2	28:a:32:ARG:NH2	2.37	0.58
2:A:1551:U:H3'	2:A:1552:A:C8	2.39	0.58
12:K:85:ARG:HG3	12:K:85:ARG:NH1	2.17	0.58
2:A:1257:G:H5"	12:K:72:LYS:NZ	2.19	0.58
7:F:178:ARG:NH1	7:F:184:PHE:HB2	2.18	0.58
8:G:5:GLY:HA3	8:G:66:HIS:CD2	2.39	0.58
2:A:137:G:H21	2:A:1524:G:H1'	1.69	0.58
2:A:1044:U:H5'	2:A:1045:C:OP2	2.04	0.58
10:I:87:VAL:HG13	10:I:124:ALA:HA	1.84	0.58
14:M:49:MET:HE3	14:M:49:MET:H	1.69	0.58
2:A:314:G:H5'	2:A:315:U:OP2	2.04	0.57
2:A:1552:A:H2	2:A:1617:C:H5	1.52	0.57
2:A:2702:A:OP1	33:f:31:ARG:NH1	2.37	0.57
8:G:48:ASP:OD1	8:G:48:ASP:N	2.37	0.57
3:B:81:U:OP1	15:N:18:ARG:NH2	2.32	0.57
11:J:114:LYS:O	11:J:118:LEU:N	2.38	0.57
2:A:639:C:HO2'	2:A:640:G:H8	1.52	0.57
2:A:1153:U:H4'	8:G:60:ARG:CZ	2.34	0.57
2:A:1250:U:H3'	2:A:1251:A:H5"	1.85	0.57
2:A:2044:U:OP2	4:C:222:ARG:NH1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2708:G:OP1	15:N:45:ARG:NH1	2.37	0.57
10:I:69:LEU:HD22	10:I:72:LEU:HD12	1.86	0.57
14:M:134:ARG:NH2	14:M:146:GLU:HG2	2.19	0.57
2:A:752:C:H2'	2:A:753:A:C8	2.39	0.57
4:C:147:LEU:HD21	4:C:155:LEU:HD11	1.86	0.57
9:H:124:ILE:HG22	9:H:125:LYS:H	1.70	0.57
24:W:11:LEU:HD12	24:W:67:LEU:HD13	1.86	0.57
2:A:1530:G:N2	2:A:1805:G:H1	2.03	0.57
2:A:1612:U:H2'	2:A:1613:G:C8	2.39	0.57
2:A:543:U:H3'	2:A:544:U:C5'	2.35	0.57
2:A:2750:G:P	8:G:154:ARG:HH22	2.27	0.57
16:O:10:LEU:HB2	16:O:17:GLN:HE21	1.69	0.57
30:c:35:ARG:HE	30:c:52:LYS:HE2	1.69	0.57
2:A:2882:C:H5"	8:G:159:LYS:HD2	1.87	0.57
14:M:110:VAL:H	14:M:127:ASN:HD22	1.53	0.57
2:A:2394:A:O2'	2:A:2396:A:OP1	2.23	0.57
2:A:451:U:H2'	2:A:452:G:C8	2.40	0.56
2:A:860:G:HO2'	2:A:863:G:HO2'	1.49	0.56
2:A:1084:U:O2'	2:A:1085:G:OP1	2.17	0.56
2:A:2022:U:O2	4:C:50:THR:HB	2.06	0.56
2:A:2236:G:N7	21:T:23:LYS:NZ	2.51	0.56
6:E:137:SER:O	6:E:168:SER:OG	2.23	0.56
1:3:21:ARG:HG2	1:3:22:PRO:HD2	1.88	0.56
2:A:444:U:H5'	2:A:446:G:H4'	1.86	0.56
2:A:863:G:OP1	21:T:95:ARG:NH1	2.38	0.56
27:Z:10:LEU:HD21	27:Z:21:LYS:NZ	2.20	0.56
2:A:1454:G:OP2	22:U:62:ARG:NH2	2.39	0.56
30:c:6:ASP:OD1	30:c:6:ASP:N	2.38	0.56
2:A:2369:C:H5"	2:A:2370:A:C8	2.40	0.56
3:B:48:C:OP2	17:P:14:ARG:NH1	2.38	0.56
10:I:94:LYS:HZ3	10:I:120:VAL:C	2.10	0.56
14:M:110:VAL:H	14:M:127:ASN:ND2	2.04	0.56
23:V:40:ARG:HA	23:V:62:GLN:O	2.06	0.56
4:C:212:MET:HA	4:C:212:MET:HE2	1.88	0.56
18:Q:28:HIS:ND1	18:Q:41:VAL:HG12	2.20	0.56
8:G:171:ARG:HH21	33:f:30:PRO:HD3	1.71	0.56
2:A:273:A:H3'	2:A:274:C:H5"	1.86	0.55
2:A:1260:C:C6	12:K:27:ARG:NH1	2.74	0.55
2:A:2381:A:H4'	2:A:2382:G:O5'	2.04	0.55
4:C:206:TRP:CG	4:C:212:MET:HE3	2.41	0.55
2:A:380:A:P	23:V:99:LYS:NZ	2.78	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1640:A:H3'	2:A:1641:U:H5"	1.88	0.55
2:A:1755:A:H2	2:A:1759:A:N6	2.04	0.55
2:A:2147:U:H2'	2:A:2148:C:C6	2.41	0.55
2:A:2997:C:H2'	2:A:2998:C:H6	1.71	0.55
2:A:337:U:H5'	2:A:338:C:O5'	2.07	0.55
2:A:561:G:H2'	2:A:562:G:H5'	1.89	0.55
8:G:116:ILE:HD13	8:G:149:ILE:HG12	1.87	0.55
11:J:114:LYS:HB3	11:J:118:LEU:HG	1.88	0.55
2:A:1552:A:H2	2:A:1617:C:C5	2.25	0.55
2:A:2580:G:H2'	2:A:2581:G:O4'	2.05	0.55
2:A:1165:G:OP1	10:I:53:LYS:NZ	2.30	0.55
2:A:80:G:OP1	23:V:94:LYS:NZ	2.40	0.55
2:A:1713:U:H4'	2:A:1714:A:OP2	2.05	0.55
4:C:108:PRO:HG2	4:C:111:LEU:HB2	1.88	0.55
31:d:24:ARG:HG3	31:d:46:THR:HG21	1.88	0.55
5:D:6:ILE:HG22	5:D:208:VAL:HG22	1.89	0.55
10:I:40:ARG:HG3	10:I:40:ARG:NH1	2.14	0.55
2:A:2404:G:H2'	2:A:2405:A:H8	1.72	0.54
7:F:130:ASP:O	7:F:132:THR:N	2.33	0.54
2:A:1640:A:H3'	2:A:1641:U:C5'	2.37	0.54
4:C:96:HIS:CD2	4:C:102:LYS:HG2	2.42	0.54
8:G:35:LEU:HD11	8:G:72:LEU:HB3	1.89	0.54
2:A:1303:U:O2'	2:A:1304:A:H5'	2.08	0.54
2:A:1875:U:H2'	2:A:1876:A:H8	1.71	0.54
2:A:3023:G:H2'	2:A:3024:A:O4'	2.07	0.54
5:D:7:LEU:H	5:D:34:ASN:HD21	1.56	0.54
23:V:81:THR:HG23	23:V:100:THR:HG23	1.89	0.54
25:X:44:HIS:HD2	25:X:45:PHE:CE1	2.25	0.54
2:A:333:C:H2'	2:A:334:G:C8	2.42	0.54
2:A:630:U:H3	2:A:642:G:H1	1.55	0.54
6:E:40:ALA:HA	6:E:100:GLN:HE21	1.73	0.54
19:R:94:ASN:HD21	20:S:13:GLN:HB2	1.72	0.54
25:X:41:ARG:HA	25:X:41:ARG:HE	1.71	0.54
2:A:665:G:O2'	2:A:666:A:H3'	2.07	0.54
2:A:1158:U:H3	2:A:1233:A:H61	1.55	0.54
3:B:9:G:OP1	17:P:22:HIS:HE1	1.91	0.54
15:N:75:THR:HG22	15:N:90:PRO:HA	1.90	0.54
24:W:131:ILE:HD11	24:W:162:ILE:HD12	1.87	0.54
27:Z:10:LEU:HD21	27:Z:21:LYS:HZ3	1.73	0.54
28:a:11:SER:N	28:a:31:ILE:HD11	2.23	0.54
2:A:844:G:H4'	2:A:878:G:H5'	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:4:ILE:HG13	9:H:39:ALA:HB2	1.90	0.54
15:N:3:ILE:HG22	15:N:93:TRP:CD1	2.43	0.54
4:C:119:SER:HB3	4:C:130:ASN:HB3	1.89	0.54
14:M:44:LYS:HG3	14:M:45:ASN:H	1.73	0.54
15:N:76:LYS:HB3	15:N:91:GLU:HG3	1.90	0.54
2:A:974:G:O2'	2:A:975:U:O5'	2.25	0.54
6:E:118:ARG:NH1	14:M:3:VAL:HG13	2.23	0.54
10:I:91:LYS:HG2	10:I:95:LYS:HE3	1.90	0.54
14:M:43:ARG:CG	14:M:43:ARG:NH1	2.67	0.54
2:A:159:A:C6	2:A:160:A:C6	2.96	0.54
2:A:292:G:N2	2:A:343:U:O2	2.38	0.54
10:I:82:VAL:HG13	10:I:89:ALA:HB2	1.90	0.54
15:N:1:MET:HG2	15:N:48:GLU:HG3	1.89	0.54
29:b:10:ARG:HD3	29:b:14:ARG:HH12	1.73	0.54
2:A:287:A:C6	2:A:300:G:C6	2.96	0.53
2:A:604:C:O2'	21:T:25:ARG:NH2	2.41	0.53
4:C:212:MET:HE1	4:C:215:LYS:HD2	1.90	0.53
4:C:218:ARG:HB3	4:C:219:PRO:HD2	1.89	0.53
13:L:13:ASN:OD1	13:L:13:ASN:N	2.40	0.53
2:A:3021:A:H4'	2:A:3022:G:C8	2.43	0.53
6:E:29:PRO:CD	6:E:120:ARG:HH12	2.22	0.53
13:L:13:ASN:HD21	13:L:97:ARG:N	2.05	0.53
15:N:72:ARG:HB3	15:N:72:ARG:NH1	2.23	0.53
31:d:11:ASN:ND2	31:d:14:ARG:HB2	2.23	0.53
2:A:347:U:H2'	2:A:348:G:C8	2.43	0.53
2:A:383:U:O4	23:V:79:LYS:NZ	2.41	0.53
2:A:1756:G:H1'	2:A:1758:G:N1	2.23	0.53
4:C:141:VAL:HG13	4:C:162:SER:HB2	1.91	0.53
1:3:15:LYS:HA	3:B:87:U:O2	2.08	0.53
2:A:1756:G:H2'	2:A:1756:G:N3	2.22	0.53
11:J:114:LYS:HE3	11:J:117:ASP:HB3	1.90	0.53
2:A:897:A:C6	4:C:226:MET:HE2	2.43	0.53
2:A:2374:U:H2'	2:A:2375:G:C8	2.43	0.53
31:d:37:ARG:NH1	31:d:45:LEU:O	2.41	0.53
2:A:250:G:H2'	2:A:251:A:C8	2.44	0.53
6:E:192:ASP:HA	14:M:5:LYS:HZ3	1.73	0.53
2:A:1675:U:O2	16:O:64:ARG:NH1	2.42	0.53
6:E:29:PRO:HD3	6:E:120:ARG:HH12	1.73	0.53
15:N:132:VAL:HG13	24:W:90:ARG:HH22	1.73	0.53
16:O:26:THR:HG23	16:O:75:VAL:HG21	1.91	0.53
2:A:1427:U:H4'	2:A:1428:U:O5'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:198:ILE:HD12	5:D:206:VAL:HG11	1.91	0.53
10:I:69:LEU:HD21	10:I:109:TYR:HB2	1.90	0.53
15:N:62:GLY:HA2	24:W:123:LEU:HD11	1.90	0.53
31:d:27:THR:OG1	31:d:28:ARG:N	2.41	0.53
2:A:2106:A:H3'	2:A:2107:G:H5"	1.91	0.53
3:B:15:U:OP2	3:B:71:C:O2'	2.27	0.53
10:I:54:ASN:ND2	10:I:73:PHE:O	2.42	0.53
2:A:1875:U:H2'	2:A:1876:A:C8	2.44	0.52
2:A:2618:C:H5"	14:M:63:LYS:HD2	1.91	0.52
4:C:260:PRO:O	4:C:261:ASN:HB2	2.09	0.52
6:E:123:ARG:NH1	6:E:151:ASN:OD1	2.41	0.52
7:F:40:LYS:HG3	7:F:164:VAL:HG13	1.89	0.52
2:A:1146:A:N3	2:A:2710:G:O2'	2.33	0.52
2:A:1188:A:N7	2:A:1214:A:O2'	2.40	0.52
8:G:46:ALA:HB3	8:G:50:ALA:HB3	1.90	0.52
8:G:116:ILE:HD11	8:G:152:LEU:HD11	1.91	0.52
14:M:65:LYS:HG2	32:e:25:GLN:HE22	1.75	0.52
29:b:10:ARG:CD	29:b:14:ARG:HH12	2.22	0.52
2:A:206:A:H2'	2:A:207:C:O4'	2.10	0.52
2:A:1566:A:H2'	2:A:1567:C:C5	2.45	0.52
5:D:110:ALA:O	5:D:182:VAL:HG12	2.10	0.52
5:D:154:CYS:O	5:D:156:THR:N	2.41	0.52
24:W:16:ARG:HG2	24:W:48:GLU:HG3	1.91	0.52
2:A:270:U:H2'	2:A:271:A:H5'	1.90	0.52
2:A:2517:C:H5"	17:P:104:ARG:HH12	1.75	0.52
2:A:2543:U:H4'	2:A:2544:U:H5'	1.91	0.52
5:D:142:GLN:O	5:D:143:ALA:HB3	2.10	0.52
2:A:1722:C:H2'	2:A:1723:U:O4'	2.10	0.52
14:M:80:VAL:HG23	14:M:113:LEU:O	2.10	0.52
2:A:739:U:O3'	2:A:740:A:H2'	2.09	0.52
2:A:1312:G:O2'	19:R:12:LYS:NZ	2.43	0.52
2:A:1621:C:H2'	2:A:1622:G:C8	2.44	0.52
2:A:2914:A:OP1	16:O:9:ARG:NH1	2.43	0.52
15:N:63:LYS:HD3	15:N:65:TRP:CZ2	2.43	0.52
22:U:14:PRO:HD3	27:Z:34:PHE:CD1	2.45	0.52
4:C:16:ALA:HB2	4:C:207:GLY:HA3	1.92	0.52
4:C:182:ILE:HD12	4:C:270:ARG:NH1	2.18	0.52
11:J:56:ILE:HD11	11:J:72:LEU:HB3	1.92	0.52
12:K:116:ARG:HG3	12:K:116:ARG:HH11	1.74	0.52
1:3:6:ARG:NH2	2:A:2713:G:OP1	2.44	0.51
3:B:76:G:H5"	24:W:19:THR:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:118:GLU:H	4:C:129:ASN:ND2	2.09	0.51
10:I:57:VAL:HA	10:I:60:ALA:HB3	1.93	0.51
17:P:18:ARG:HD2	17:P:107:TYR:CZ	2.45	0.51
2:A:925:U:C4	14:M:31:LYS:O	2.63	0.51
33:f:16:VAL:HG22	33:f:25:VAL:HG22	1.92	0.51
2:A:210:G:P	31:d:28:ARG:HH21	2.33	0.51
2:A:1187:A:H5"	2:A:1188:A:H8	1.75	0.51
2:A:1430:C:H2'	2:A:1431:U:C6	2.45	0.51
8:G:118:ALA:HB2	8:G:124:PHE:HE2	1.74	0.51
11:J:96:LYS:HE2	24:W:120:PRO:HB2	1.92	0.51
2:A:84:U:H5"	2:A:85:G:H5"	1.91	0.51
2:A:356:G:H21	2:A:362:A:H62	1.56	0.51
2:A:733:U:H2'	2:A:734:C:C6	2.45	0.51
2:A:1665:U:H2'	2:A:1666:A:H8	1.75	0.51
2:A:877:U:H4'	2:A:878:G:O5'	2.11	0.51
6:E:112:ARG:HG2	6:E:112:ARG:NH1	2.25	0.51
21:T:15:ARG:HG3	21:T:15:ARG:HH11	1.74	0.51
2:A:758:A:H4'	2:A:758:A:OP2	2.11	0.51
2:A:759:G:H1	25:X:64:PRO:HB3	1.75	0.51
10:I:53:LYS:O	10:I:57:VAL:HG23	2.11	0.51
30:c:11:ILE:HG12	30:c:25:THR:O	2.10	0.51
2:A:326:A:H61	2:A:449:G:H1	1.59	0.51
2:A:672:C:H4'	19:R:31:LEU:HD13	1.93	0.51
9:H:82:VAL:HG11	9:H:91:LEU:HD22	1.93	0.51
9:H:100:VAL:HG22	9:H:146:LEU:HD21	1.92	0.51
30:c:35:ARG:HH22	30:c:54:SER:HA	1.76	0.51
2:A:752:C:H2'	2:A:753:A:H8	1.76	0.51
12:K:70:THR:OG1	12:K:71:LYS:HG2	2.10	0.51
19:R:119:GLU:CD	19:R:119:GLU:H	2.19	0.51
2:A:2018:G:H22	2:A:2028:G:P	2.34	0.50
15:N:51:ARG:HG2	15:N:66:ILE:HD11	1.92	0.50
2:A:74:C:O2'	27:Z:11:ARG:NH2	2.44	0.50
2:A:1817:C:OP2	22:U:39:LYS:HD2	2.11	0.50
2:A:2690:C:OP1	33:f:5:PRO:HD2	2.12	0.50
21:T:80:THR:OG1	21:T:113:ILE:HB	2.12	0.50
2:A:90:C:H2'	2:A:91:C:O4'	2.11	0.50
2:A:747:A:H2'	2:A:748:U:O4'	2.12	0.50
2:A:357:U:H4'	2:A:358:G:O5'	2.12	0.50
2:A:2351:A:N3	2:A:2396:A:O2'	2.41	0.50
4:C:137:PRO:O	4:C:140:THR:HG23	2.11	0.50
12:K:17:VAL:HG12	12:K:137:PRO:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:77:LYS:HB3	17:P:112:ARG:HD3	1.93	0.50
20:S:54:ASP:OD1	20:S:54:ASP:N	2.43	0.50
32:e:50:VAL:HG11	32:e:58:ILE:HD12	1.94	0.50
5:D:126:THR:HB	5:D:132:PHE:CD2	2.46	0.50
13:L:63:VAL:HB	13:L:102:VAL:HG12	1.93	0.50
2:A:380:A:N1	2:A:404:A:O2'	2.34	0.50
2:A:1164:A:H4'	10:I:55:THR:HB	1.93	0.50
2:A:2412:U:H2'	2:A:2413:G:H8	1.76	0.50
23:V:41:ILE:O	23:V:61:THR:HA	2.10	0.50
2:A:750:C:H2'	2:A:751:A:C8	2.46	0.50
2:A:2306:A:H61	2:A:2460:U:H3	1.60	0.50
13:L:77:ILE:CD1	18:Q:71:ARG:HD2	2.42	0.50
2:A:639:C:O2'	2:A:640:G:O5'	2.30	0.50
2:A:1678:U:H5'	2:A:1679:A:OP2	2.10	0.50
2:A:1754:G:C6	2:A:1755:A:C2	2.99	0.50
2:A:2691:C:O2	15:N:124:LYS:NZ	2.42	0.50
9:H:124:ILE:O	9:H:125:LYS:HB2	2.11	0.50
19:R:11:GLN:HB3	19:R:15:ARG:NH2	2.22	0.50
1:3:21:ARG:NH2	2:A:1100:C:N3	2.60	0.50
5:D:160:VAL:HG12	5:D:160:VAL:O	2.12	0.50
7:F:130:ASP:OD1	7:F:130:ASP:N	2.44	0.50
2:A:1627:U:H2'	2:A:1628:A:H8	1.76	0.49
2:A:2074:G:C6	2:A:2075:G:N1	2.80	0.49
3:B:4:A:N1	3:B:23:G:O2'	2.37	0.49
15:N:65:TRP:HB2	15:N:105:GLU:HB2	1.93	0.49
17:P:66:ILE:HG23	17:P:71:ARG:HH21	1.78	0.49
2:A:288:U:H4'	2:A:289:A:O5'	2.12	0.49
2:A:588:A:H2'	2:A:589:A:C8	2.47	0.49
11:J:23:ALA:HB3	11:J:24:PRO:HD3	1.93	0.49
14:M:84:ASN:ND2	14:M:118:LEU:HA	2.20	0.49
2:A:460:G:O2'	2:A:488:G:O6	2.28	0.49
2:A:2367:G:N2	2:A:2371:G:O6	2.45	0.49
8:G:41:ILE:HD11	8:G:65:LEU:HB3	1.94	0.49
11:J:137:MET:HE2	11:J:139:ILE:HD11	1.94	0.49
17:P:12:GLU:HG3	17:P:13:VAL:N	2.26	0.49
2:A:336:C:N4	2:A:337:U:O4	2.46	0.49
2:A:974:G:O2'	2:A:975:U:P	2.69	0.49
2:A:986:G:OP1	15:N:6:LYS:HE3	2.12	0.49
2:A:2086:U:H3	2:A:2096:G:H1	1.59	0.49
5:D:7:LEU:HB2	5:D:34:ASN:ND2	2.27	0.49
11:J:11:ILE:HG21	11:J:33:HIS:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:101:GLU:HG3	16:O:102:ASN:N	2.28	0.49
33:f:1:MET:HE2	33:f:33:LYS:HE2	1.92	0.49
2:A:1000:C:H3’	2:A:1001:C:H5”	1.94	0.49
2:A:1284:A:H2’	2:A:1285:G:C8	2.48	0.49
2:A:1572:G:N2	2:A:1599:U:H5	2.10	0.49
8:G:119:PRO:O	8:G:122:ILE:HG22	2.11	0.49
11:J:111:ALA:O	11:J:115:LYS:HB2	2.12	0.49
2:A:639:C:O2’	2:A:640:G:H8	1.96	0.49
2:A:2445:A:H4’	4:C:188:ARG:HH12	1.76	0.49
4:C:132:PRO:HD3	4:C:190:ARG:NH1	2.20	0.49
7:F:58:ASN:HA	7:F:61:ILE:HD12	1.93	0.49
9:H:82:VAL:HG21	9:H:148:VAL:HG13	1.95	0.49
25:X:25:ARG:NH2	25:X:35:GLU:OE2	2.46	0.49
2:A:1455:U:OP2	22:U:62:ARG:NH1	2.45	0.49
2:A:1642:G:C2	2:A:1643:G:C8	3.00	0.49
10:I:39:LEU:HD12	10:I:42:ALA:HB3	1.93	0.49
15:N:34:ILE:HG13	15:N:118:LEU:HD13	1.95	0.49
22:U:44:ILE:O	22:U:47:GLU:HG2	2.12	0.49
2:A:1530:G:N2	2:A:1805:G:H22	2.11	0.49
8:G:9:VAL:O	8:G:51:ILE:HG13	2.12	0.49
20:S:80:ASN:C	20:S:82:THR:H	2.20	0.49
2:A:2:A:H2’	2:A:3:A:C8	2.48	0.49
2:A:1619:U:H2’	2:A:1620:U:O4’	2.12	0.49
2:A:2009:G:H5’	4:C:205:ASN:HD21	1.76	0.49
2:A:2394:A:O2’	2:A:2395:U:H3’	2.12	0.49
2:A:1885:G:O2’	2:A:2215:U:O4	2.30	0.49
4:C:26:ARG:HD3	4:C:28:THR:O	2.12	0.49
8:G:171:ARG:NH2	33:f:30:PRO:HD3	2.27	0.49
14:M:55:MET:O	14:M:60:ARG:NH1	2.46	0.49
2:A:606:U:H5”	21:T:32:ARG:NH2	2.27	0.48
2:A:976:A:H2’	2:A:977:G:O4’	2.13	0.48
2:A:1715:A:H2’	2:A:1716:A:C8	2.48	0.48
2:A:2356:G:H2’	2:A:2380:G:H22	1.78	0.48
2:A:2636:A:H2’	2:A:2637:G:O4’	2.12	0.48
4:C:200:GLU:OE1	4:C:200:GLU:N	2.41	0.48
18:Q:43:LYS:HZ3	18:Q:86:LEU:HD13	1.78	0.48
2:A:300:G:N2	2:A:303:G:H5”	2.27	0.48
2:A:2350:G:O2’	2:A:2351:A:O5’	2.30	0.48
9:H:127:VAL:HG21	9:H:150:ALA:HB2	1.94	0.48
21:T:102:ARG:O	21:T:103:ILE:HD13	2.12	0.48
2:A:183:G:H2’	2:A:184:C:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2035:U:OP2	4:C:157:ARG:NH1	2.46	0.48
2:A:2491:A:H5"	2:A:2492:A:H5'	1.94	0.48
2:A:2552:A:H2'	2:A:2553:G:C8	2.48	0.48
4:C:233:HIS:NE2	4:C:246:PRO:HA	2.28	0.48
7:F:57:ILE:HD13	7:F:91:PRO:HB2	1.93	0.48
18:Q:32:ILE:O	18:Q:32:ILE:HG13	2.12	0.48
24:W:14:ASN:HD21	24:W:32:LYS:NZ	2.10	0.48
2:A:1294:U:H2'	2:A:1295:U:C6	2.49	0.48
2:A:1869:G:OP1	16:O:40:LYS:NZ	2.46	0.48
32:e:16:ARG:HG2	32:e:22:ILE:HD13	1.95	0.48
4:C:206:TRP:CD1	4:C:212:MET:HE3	2.49	0.48
2:A:1493:A:O2'	2:A:1495:G:N7	2.40	0.48
2:A:2997:C:H2'	2:A:2998:C:C6	2.48	0.48
3:B:76:G:O2'	24:W:94:HIS:HE1	1.97	0.48
2:A:1145:A:N1	2:A:1245:U:H5	2.12	0.48
12:K:102:GLU:HG3	12:K:124:VAL:HG11	1.95	0.48
24:W:157:ILE:HB	24:W:179:VAL:HB	1.96	0.48
2:A:2761:U:H2'	2:A:2762:C:C6	2.48	0.48
2:A:3014:A:N6	2:A:3112:A:H2'	2.28	0.48
34:g:26:SER:OG	34:g:27:THR:N	2.46	0.48
2:A:277:U:H2'	2:A:278:A:C8	2.49	0.48
2:A:1131:G:H21	19:R:122:ASN:HD22	1.62	0.48
2:A:2864:G:H5'	12:K:99:ARG:HH22	1.79	0.48
8:G:38:ALA:HB1	8:G:40:PRO:HD2	1.96	0.48
8:G:176:LYS:HG3	8:G:177:THR:H	1.78	0.48
15:N:70:PRO:HA	15:N:95:ALA:HB2	1.95	0.48
19:R:90:VAL:HG21	20:S:41:LEU:HD22	1.96	0.48
24:W:122:THR:HG23	24:W:181:VAL:HG13	1.96	0.48
2:A:383:U:H5"	23:V:72:MET:HE3	1.94	0.48
2:A:733:U:H2'	2:A:734:C:H6	1.76	0.48
4:C:68:ARG:NH1	4:C:150:GLY:C	2.57	0.48
4:C:108:PRO:HD2	4:C:111:LEU:HD22	1.95	0.48
6:E:154:VAL:HG12	6:E:175:VAL:HG22	1.95	0.48
8:G:26:VAL:HG12	8:G:80:VAL:HG21	1.96	0.48
10:I:75:GLY:HA3	10:I:106:LYS:HZ3	1.79	0.48
22:U:30:THR:HG23	22:U:83:ILE:HG12	1.96	0.48
23:V:13:SER:HB2	23:V:70:ASN:ND2	2.29	0.48
33:f:18:ARG:HE	33:f:21:GLY:HA2	1.79	0.48
2:A:2925:C:H3'	2:A:2926:A:C5'	2.44	0.47
4:C:77:ALA:HB2	4:C:97:TYR:CD1	2.48	0.47
8:G:9:VAL:HB	8:G:51:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:303:G:C2	2:A:304:U:C2	3.02	0.47
2:A:2859:C:O2'	5:D:83:GLU:OE1	2.28	0.47
4:C:79:VAL:HG21	4:C:111:LEU:HD21	1.95	0.47
5:D:18:ASP:HB3	5:D:19:GLU:OE2	2.14	0.47
5:D:28:VAL:HG22	5:D:193:LEU:HD22	1.96	0.47
8:G:159:LYS:C	8:G:172:ARG:HH22	2.22	0.47
23:V:1:MET:O	23:V:2:LYS:HB2	2.14	0.47
2:A:1259:U:OP2	12:K:65:SER:OG	2.30	0.47
2:A:2515:U:H2'	2:A:2516:U:C6	2.49	0.47
8:G:70:ARG:O	8:G:73:ILE:HG12	2.14	0.47
8:G:149:ILE:HG22	8:G:163:VAL:HG11	1.95	0.47
15:N:34:ILE:HD11	15:N:118:LEU:HD22	1.96	0.47
16:O:55:ALA:HB2	16:O:79:LEU:HD22	1.96	0.47
2:A:23:G:H1'	2:A:601:A:N6	2.29	0.47
13:L:113:LYS:HE3	13:L:117:LEU:HD11	1.96	0.47
2:A:137:G:H8	2:A:137:G:OP1	1.98	0.47
2:A:306:U:H5"	9:H:41:ARG:HG2	1.95	0.47
2:A:760:U:H2'	2:A:761:G:H8	1.79	0.47
2:A:2334:U:H4'	2:A:2341:U:O2'	2.13	0.47
7:F:117:ARG:HD2	7:F:146:HIS:CE1	2.50	0.47
9:H:78:VAL:HG21	9:H:104:ILE:HG12	1.94	0.47
10:I:94:LYS:HZ1	10:I:124:ALA:CB	2.28	0.47
10:I:94:LYS:HZ1	10:I:124:ALA:HB2	1.79	0.47
18:Q:52:GLY:H	18:Q:56:GLU:HB2	1.80	0.47
2:A:363:A:H2'	2:A:364:A:O4'	2.13	0.47
2:A:759:G:H5"	2:A:760:U:O4'	2.14	0.47
2:A:2950:C:H4'	13:L:1:MET:HE1	1.95	0.47
11:J:60:ILE:HD13	11:J:70:PHE:HB3	1.96	0.47
24:W:134:GLU:HB2	24:W:171:ILE:HD11	1.97	0.47
2:A:136:U:H4'	2:A:136:U:OP1	2.14	0.47
2:A:580:G:H2'	2:A:581:G:O4'	2.14	0.47
2:A:760:U:H2'	2:A:761:G:C8	2.50	0.47
2:A:1081:C:O2'	2:A:2497:A:N3	2.42	0.47
2:A:1702:A:H61	2:A:1732:U:H3	1.61	0.47
2:A:2421:A:O5'	9:H:33:ARG:NH2	2.42	0.47
4:C:43:ARG:NH2	4:C:49:ILE:HD11	2.30	0.47
16:O:102:ASN:OD1	16:O:109:PRO:HA	2.15	0.47
21:T:32:ARG:HH11	21:T:32:ARG:HG3	1.80	0.47
23:V:20:LYS:HZ3	23:V:74:VAL:HG23	1.80	0.47
25:X:18:ALA:HB3	25:X:20:ARG:NH1	2.29	0.47
2:A:159:A:N3	2:A:2431:C:O2'	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:256:A:H2'	2:A:257:A:C8	2.50	0.47
2:A:981:U:O2'	2:A:982:A:O5'	2.32	0.47
16:O:96:ARG:HD3	16:O:98:ILE:HD11	1.96	0.47
2:A:2964:A:H2'	2:A:2965:A:C8	2.50	0.47
8:G:150:ARG:HG2	8:G:150:ARG:HH11	1.80	0.47
16:O:24:LEU:HD23	16:O:24:LEU:HA	1.56	0.47
2:A:303:G:H2'	2:A:304:U:O4'	2.14	0.47
2:A:637:G:HO2'	2:A:638:U:H6	1.63	0.47
2:A:1105:C:O2'	2:A:1118:A:N3	2.46	0.47
2:A:2074:G:O6	2:A:2075:G:N1	2.48	0.47
8:G:55:ARG:HH11	8:G:63:ARG:HA	1.80	0.47
10:I:109:TYR:OH	10:I:112:GLY:HA2	2.14	0.47
2:A:2851:G:N2	2:A:3001:G:OP2	2.46	0.46
4:C:89:THR:HG22	4:C:201:GLN:HG2	1.97	0.46
5:D:40:ARG:O	5:D:48:SER:HA	2.15	0.46
14:M:24:ARG:HA	14:M:24:ARG:HD3	1.47	0.46
2:A:302:U:O2'	2:A:303:G:H3'	2.15	0.46
2:A:302:U:H1'	2:A:303:G:C8	2.50	0.46
9:H:9:VAL:HB	9:H:12:LEU:HD12	1.97	0.46
15:N:63:LYS:O	15:N:106:LEU:HD12	2.15	0.46
2:A:275:C:H6	2:A:275:C:H5"	1.81	0.46
2:A:973:G:OP1	25:X:76:LYS:HE3	2.15	0.46
2:A:2340:A:N6	2:A:2389:U:H3	2.14	0.46
3:B:46:A:O4'	7:F:99:ARG:NH1	2.48	0.46
15:N:12:GLN:OE1	15:N:72:ARG:NH1	2.48	0.46
15:N:69:PHE:HA	15:N:70:PRO:HD3	1.70	0.46
2:A:2778:U:H2'	2:A:2779:U:C6	2.50	0.46
5:D:40:ARG:HD2	5:D:45:ASP:CG	2.41	0.46
13:L:4:GLN:NE2	13:L:23:ARG:NH1	2.64	0.46
16:O:3:LYS:HA	16:O:4:PRO:HD3	1.79	0.46
21:T:106:ARG:HH11	21:T:106:ARG:HG2	1.80	0.46
24:W:164:LEU:HD13	24:W:168:VAL:HG12	1.96	0.46
2:A:636:U:H5"	2:A:637:G:C4	2.50	0.46
2:A:1256:G:N3	12:K:108:MET:HE2	2.30	0.46
2:A:2617:U:H2'	2:A:2618:C:O4'	2.15	0.46
16:O:10:LEU:HB2	16:O:17:GLN:NE2	2.29	0.46
17:P:120:ALA:O	17:P:125:LEU:HB2	2.14	0.46
2:A:135:G:H3'	2:A:136:U:H5"	1.97	0.46
2:A:498:G:H8	2:A:498:G:H5"	1.81	0.46
2:A:678:A:N1	2:A:924:G:O2'	2.46	0.46
2:A:2990:A:N3	2:A:2990:A:H2'	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3055:G:H5'	5:D:60:ARG:HH12	1.79	0.46
8:G:41:ILE:HD11	8:G:65:LEU:C	2.41	0.46
15:N:2:LEU:O	15:N:44:ASN:ND2	2.46	0.46
15:N:118:LEU:O	15:N:122:ILE:HG13	2.15	0.46
2:A:380:A:OP1	23:V:99:LYS:NZ	2.40	0.46
2:A:610:C:O2	2:A:646:U:O2'	2.34	0.46
2:A:2000:A:N1	2:A:2811:A:H2'	2.31	0.46
2:A:3052:A:O2'	2:A:3105:C:OP1	2.28	0.46
4:C:123:ALA:HB3	4:C:131:LEU:HD22	1.97	0.46
10:I:94:LYS:NZ	10:I:121:GLU:HA	2.30	0.46
23:V:67:HIS:CD2	23:V:69:SER:H	2.31	0.46
31:d:33:ILE:O	31:d:37:ARG:HG3	2.15	0.46
2:A:483:G:H2'	2:A:484:C:C6	2.51	0.46
2:A:2095:G:O2'	2:A:2096:G:O5'	2.31	0.46
11:J:75:PRO:HG2	11:J:80:LEU:HD21	1.97	0.46
18:Q:91:VAL:HG11	18:Q:96:LEU:HD11	1.97	0.46
2:A:1323:G:O2'	2:A:1352:A:N1	2.48	0.46
2:A:1760:G:H2'	2:A:1761:G:H8	1.81	0.46
2:A:1922:G:H2'	2:A:1923:G:C8	2.51	0.46
2:A:2262:C:H2'	2:A:2263:G:O4'	2.16	0.46
2:A:2839:U:C2	29:b:4:PRO:HA	2.51	0.46
7:F:118:ILE:HB	7:F:121:PHE:HB2	1.98	0.46
15:N:63:LYS:HB2	24:W:123:LEU:HD21	1.98	0.46
24:W:112:VAL:HG23	24:W:126:GLN:HE21	1.80	0.46
26:Y:39:VAL:HG21	26:Y:64:ALA:HB3	1.98	0.46
2:A:2366:C:H2'	2:A:2367:G:O4'	2.16	0.46
4:C:60:ARG:HH11	4:C:86:PRO:HB3	1.80	0.46
24:W:105:LYS:HA	24:W:105:LYS:HD3	1.80	0.46
2:A:2736:C:H2'	2:A:2737:G:O4'	2.16	0.45
4:C:62:TYR:HA	4:C:87:ASN:HD21	1.80	0.45
6:E:22:ALA:O	6:E:26:ASP:HB2	2.16	0.45
25:X:81:VAL:HA	25:X:82:PRO:HD3	1.60	0.45
33:f:3:VAL:HG12	33:f:37:GLY:HA3	1.98	0.45
2:A:1093:A:H1'	2:A:1108:A:C2	2.51	0.45
2:A:2387:U:H3'	2:A:2388:G:H8	1.80	0.45
2:A:2718:G:H4'	15:N:80:GLU:HG2	1.98	0.45
11:J:15:ILE:HD11	11:J:58:VAL:HG11	1.98	0.45
19:R:91:ASP:OD1	19:R:93:LYS:N	2.49	0.45
19:R:97:GLU:O	19:R:101:SER:OG	2.32	0.45
20:S:26:LYS:HE2	20:S:26:LYS:HB3	1.61	0.45
2:A:965:U:H2'	2:A:966:U:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2926:A:OP1	16:O:73:LYS:NZ	2.46	0.45
25:X:25:ARG:HD2	25:X:29:GLN:OE1	2.17	0.45
2:A:976:A:C2	2:A:1032:A:C4	3.05	0.45
2:A:1130:C:H6	2:A:1130:C:H5'	1.81	0.45
2:A:1760:G:H2'	2:A:1761:G:C8	2.50	0.45
5:D:113:ASP:OD1	5:D:178:GLN:HA	2.15	0.45
10:I:14:ALA:HB1	10:I:63:GLU:HG3	1.98	0.45
11:J:79:LYS:HD3	11:J:82:LEU:HD12	1.97	0.45
13:L:2:ILE:HG13	13:L:8:LEU:HD21	1.97	0.45
19:R:74:ILE:HB	19:R:114:ARG:HH21	1.81	0.45
19:R:83:LEU:HD23	19:R:83:LEU:HA	1.70	0.45
22:U:46:ILE:HD12	22:U:84:VAL:HG21	1.99	0.45
2:A:1457:A:O2'	2:A:1459:U:OP2	2.30	0.45
2:A:2534:A:C2	7:F:83:GLN:HG3	2.51	0.45
3:B:114:A:H3'	3:B:115:A:C8	2.52	0.45
5:D:79:ARG:HG2	5:D:80:HIS:CE1	2.52	0.45
7:F:40:LYS:HD3	7:F:99:ARG:NH2	2.32	0.45
7:F:130:ASP:C	7:F:132:THR:H	2.21	0.45
15:N:2:LEU:O	15:N:3:ILE:HG23	2.15	0.45
2:A:719:G:O6	14:M:105:ARG:HD3	2.16	0.45
2:A:2309:U:H2'	2:A:2310:G:C8	2.52	0.45
18:Q:28:HIS:CD2	18:Q:82:HIS:HB2	2.51	0.45
21:T:30:LEU:HD21	29:b:22:ALA:O	2.17	0.45
29:b:6:ARG:HH11	29:b:6:ARG:HG2	1.79	0.45
2:A:166:A:H2'	2:A:167:G:O4'	2.16	0.45
2:A:821:A:H2'	2:A:822:G:O4'	2.17	0.45
2:A:1168:A:C2	2:A:2975:G:C4	3.05	0.45
2:A:2729:G:N2	2:A:2730:U:O4	2.46	0.45
7:F:83:GLN:H	7:F:83:GLN:HG2	1.40	0.45
9:H:95:VAL:O	9:H:119:LEU:HD21	2.16	0.45
10:I:40:ARG:NH1	10:I:40:ARG:CG	2.79	0.45
10:I:82:VAL:HG21	10:I:86:ALA:O	2.17	0.45
28:a:52:HIS:CD2	28:a:53:LEU:HG	2.51	0.45
2:A:270:U:C2'	2:A:271:A:H5'	2.46	0.45
2:A:356:G:H5"	2:A:357:U:OP1	2.17	0.45
2:A:2527:G:O4'	7:F:130:ASP:HB3	2.17	0.45
7:F:14:ARG:NH2	7:F:179:ALA:O	2.50	0.45
18:Q:79:ASN:HD22	18:Q:79:ASN:HA	1.51	0.45
23:V:1:MET:HE3	23:V:26:ALA:HB1	1.98	0.45
2:A:289:A:N7	2:A:290:C:H5	2.15	0.45
2:A:657:C:H41	20:S:81:LYS:NZ	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1001:C:H4'	2:A:1001:C:OP1	2.17	0.45
2:A:1655:A:H2'	2:A:1656:A:O4'	2.16	0.45
2:A:1799:A:H2'	2:A:1800:G:O4'	2.17	0.45
2:A:2712:U:H2'	2:A:2713:G:O4'	2.17	0.45
14:M:31:LYS:HG3	14:M:32:THR:N	2.31	0.45
24:W:124:VAL:HG12	24:W:181:VAL:HG22	1.99	0.45
2:A:89:A:O2'	2:A:90:C:OP1	2.34	0.45
2:A:284:G:H5"	2:A:285:U:OP2	2.17	0.45
2:A:2585:U:H2'	2:A:2586:G:H5'	1.98	0.45
2:A:2643:U:H2'	2:A:2644:C:H6	1.82	0.45
21:T:95:ARG:HG3	21:T:101:PHE:CD2	2.51	0.45
26:Y:15:GLY:HA3	26:Y:29:TRP:HZ3	1.83	0.45
2:A:940:A:O2'	14:M:54:GLN:HB2	2.17	0.44
2:A:2581:G:OP2	2:A:2581:G:H8	2.00	0.44
11:J:23:ALA:O	11:J:28:PRO:HD2	2.17	0.44
30:c:27:LYS:NZ	30:c:34:ASP:O	2.50	0.44
1:3:3:LYS:HE2	2:A:1252:G:OP2	2.18	0.44
2:A:1002:C:H6	2:A:1003:A:H5"	1.82	0.44
2:A:1260:C:HO2'	12:K:27:ARG:NH2	2.13	0.44
6:E:130:LEU:HD23	6:E:130:LEU:HA	1.74	0.44
8:G:165:TYR:HB2	8:G:168:GLU:HB2	2.00	0.44
19:R:91:ASP:OD1	19:R:91:ASP:C	2.60	0.44
29:b:6:ARG:CG	29:b:6:ARG:NH1	2.63	0.44
4:C:70:HIS:CG	4:C:71:ASP:N	2.86	0.44
10:I:31:LEU:HD11	10:I:103:LEU:HD12	1.99	0.44
13:L:75:SER:CB	18:Q:71:ARG:HH21	2.30	0.44
27:Z:61:LEU:HD23	27:Z:61:LEU:HA	1.72	0.44
31:d:26:ARG:HE	31:d:26:ARG:HB2	1.59	0.44
2:A:534:G:OP1	19:R:3:ARG:NH2	2.50	0.44
2:A:1119:A:H2'	2:A:1120:G:O4'	2.17	0.44
3:B:47:A:H5"	17:P:14:ARG:HH12	1.82	0.44
4:C:69:ARG:H	4:C:69:ARG:HG3	1.62	0.44
7:F:45:MET:HG2	7:F:159:MET:HB2	1.99	0.44
10:I:90:ALA:O	10:I:94:LYS:HE3	2.17	0.44
13:L:34:GLY:H	13:L:37:ASP:HB2	1.81	0.44
19:R:114:ARG:HG3	19:R:114:ARG:HH11	1.82	0.44
23:V:75:ASP:OD1	23:V:76:SER:N	2.51	0.44
24:W:16:ARG:HD3	24:W:46:HIS:HB3	1.99	0.44
2:A:635:G:H4'	2:A:637:G:N2	2.33	0.44
2:A:673:C:H2'	2:A:674:U:C6	2.53	0.44
2:A:2083:A:C2'	2:A:2084:A:H5'	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2406:U:H2'	2:A:2407:C:C6	2.52	0.44
2:A:2922:U:H2'	2:A:2923:C:C6	2.53	0.44
4:C:155:LEU:HD13	4:C:177:MET:HE1	2.00	0.44
7:F:107:LEU:HD23	7:F:107:LEU:HA	1.81	0.44
10:I:19:ALA:HB1	10:I:83:LYS:HE3	1.99	0.44
21:T:57:VAL:O	21:T:60:SER:HB3	2.18	0.44
1:3:14:SER:HB3	1:3:17:ASN:HD22	1.82	0.44
2:A:7:U:H5	2:A:2853:C:N3	2.15	0.44
2:A:1178:U:C2	2:A:1180:G:H5'	2.52	0.44
2:A:1315:C:H2'	2:A:1316:U:O4'	2.17	0.44
2:A:1403:C:C5	2:A:1441:C:N3	2.77	0.44
11:J:75:PRO:HA	11:J:76:PRO:HD3	1.87	0.44
15:N:55:ASN:ND2	24:W:190:LEU:O	2.51	0.44
16:O:101:GLU:OE1	21:T:45:TRP:HZ3	2.00	0.44
30:c:36:LEU:HD23	30:c:38:ILE:HD11	1.99	0.44
2:A:498:G:H5'	2:A:499:G:O5'	2.18	0.44
2:A:974:G:H2'	2:A:1031:G:O6	2.17	0.44
2:A:978:A:C2	2:A:979:G:C4	3.06	0.44
2:A:1037:C:H1'	25:X:26:PHE:CD2	2.53	0.44
5:D:142:GLN:O	5:D:143:ALA:CB	2.65	0.44
7:F:42:VAL:HB	7:F:162:THR:HG23	1.99	0.44
12:K:145:VAL:HG12	19:R:73:ASP:OD1	2.18	0.44
14:M:67:PHE:HD2	14:M:69:ASN:H	1.64	0.44
30:c:26:LYS:HG3	32:e:34:GLU:OE2	2.18	0.44
2:A:621:U:H5'	19:R:42:SER:OG	2.18	0.44
2:A:919:A:H8	2:A:919:A:C5'	2.31	0.44
2:A:1165:G:H21	2:A:1229:A:H2	1.66	0.44
2:A:1400:G:H21	2:A:1443:G:H5"	1.83	0.44
2:A:1753:C:N4	2:A:1754:G:O6	2.51	0.44
6:E:9:THR:HG22	6:E:128:THR:HG21	2.00	0.44
8:G:152:LEU:HD23	8:G:152:LEU:HA	1.72	0.44
15:N:68:ILE:HD11	15:N:101:ARG:NE	2.32	0.44
2:A:672:C:H2'	2:A:673:C:C6	2.52	0.44
2:A:1379:G:OP1	29:b:16:ARG:NH2	2.36	0.44
2:A:2027:A:H2'	2:A:2028:G:O4'	2.17	0.44
2:A:2672:A:H4'	2:A:2673:U:OP2	2.17	0.44
2:A:2704:C:H5"	2:A:2704:C:H6	1.82	0.44
5:D:57:ILE:HG21	5:D:62:VAL:HG13	2.00	0.44
5:D:76:ASN:HA	5:D:77:PRO:HD3	1.86	0.44
7:F:102:ARG:H	7:F:102:ARG:HG2	1.52	0.44
11:J:54:ASN:HB3	11:J:75:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:72:ARG:H	15:N:72:ARG:HG2	1.31	0.44
23:V:8:THR:O	23:V:74:VAL:HG12	2.17	0.44
27:Z:14:THR:OG1	27:Z:15:ASP:N	2.51	0.44
30:c:35:ARG:NH2	30:c:54:SER:HA	2.32	0.44
34:g:11:ASP:OD1	34:g:25:ARG:NH1	2.51	0.44
2:A:497:G:H8	2:A:497:G:H5"	1.83	0.43
6:E:145:LEU:HD23	6:E:145:LEU:HA	1.84	0.43
23:V:35:VAL:HB	23:V:38:VAL:HG13	1.99	0.43
5:D:63:ILE:CG2	5:D:65:PRO:HD2	2.48	0.43
12:K:35:LEU:HD23	12:K:35:LEU:HA	1.73	0.43
15:N:1:MET:SD	15:N:45:ARG:HG2	2.58	0.43
18:Q:13:ARG:HH22	18:Q:81:ASP:HA	1.84	0.43
21:T:32:ARG:HG3	21:T:32:ARG:NH1	2.33	0.43
2:A:457:C:H5"	2:A:458:G:H5'	2.00	0.43
2:A:601:A:H2'	2:A:602:A:O4'	2.17	0.43
2:A:725:A:OP1	14:M:65:LYS:HE3	2.18	0.43
2:A:992:C:H2'	2:A:993:G:O4'	2.18	0.43
2:A:1764:A:H2'	2:A:1765:A:C8	2.53	0.43
2:A:1790:A:H2'	2:A:1791:A:C8	2.53	0.43
2:A:1922:G:H2'	2:A:1923:G:H8	1.82	0.43
10:I:75:GLY:CA	10:I:106:LYS:HZ3	2.31	0.43
21:T:43:LEU:HD23	21:T:43:LEU:HA	1.66	0.43
2:A:1660:A:H2'	2:A:1661:G:O4'	2.18	0.43
2:A:1788:G:H5'	4:C:60:ARG:HA	2.00	0.43
2:A:1907:A:H2'	2:A:1908:A:C8	2.53	0.43
2:A:2505:C:O2'	2:A:2506:G:H5'	2.17	0.43
4:C:26:ARG:HG2	4:C:27:SER:N	2.32	0.43
7:F:117:ARG:HD2	7:F:146:HIS:HE1	1.83	0.43
12:K:114:LEU:HD12	12:K:114:LEU:HA	1.71	0.43
17:P:22:HIS:CD2	17:P:105:GLY:HA2	2.53	0.43
31:d:18:VAL:HG12	31:d:19:HIS:CE1	2.53	0.43
2:A:273:A:N1	2:A:321:G:O2'	2.45	0.43
2:A:784:G:N3	2:A:784:G:H2'	2.33	0.43
2:A:1345:G:H2'	2:A:1346:U:O4'	2.19	0.43
2:A:1640:A:C3'	2:A:1641:U:H5"	2.48	0.43
2:A:2274:C:H1'	5:D:166:MET:CE	2.44	0.43
2:A:2534:A:N3	7:F:81:ILE:HD11	2.33	0.43
18:Q:17:PRO:O	18:Q:19:PHE:HD1	2.02	0.43
26:Y:33:ILE:HA	26:Y:52:CYS:HA	2.00	0.43
2:A:442:U:H2'	2:A:443:C:C6	2.54	0.43
2:A:1033:A:H5"	3:B:95:G:O2'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3014:A:O2'	2:A:3015:C:H5"	2.17	0.43
4:C:25:THR:HG21	4:C:113:GLN:NE2	2.34	0.43
8:G:55:ARG:HG2	8:G:66:HIS:CE1	2.54	0.43
12:K:7:LYS:HD3	12:K:7:LYS:HA	1.75	0.43
32:e:31:HIS:CD2	32:e:32:LEU:HG	2.53	0.43
2:A:857:U:H2'	2:A:858:A:C8	2.54	0.43
2:A:1627:U:C2	2:A:1628:A:H2'	2.53	0.43
11:J:42:LYS:N	11:J:42:LYS:HD2	2.34	0.43
31:d:24:ARG:O	31:d:30:GLY:HA3	2.19	0.43
34:g:16:CYS:SG	34:g:17:GLY:N	2.92	0.43
8:G:156:ASP:HA	8:G:157:PRO:HD3	1.60	0.43
13:L:1:MET:HE3	13:L:32:TYR:CZ	2.54	0.43
18:Q:4:LEU:HD23	18:Q:4:LEU:HA	1.66	0.43
18:Q:93:ARG:H	18:Q:93:ARG:HG2	1.65	0.43
2:A:757:G:H4'	2:A:758:A:O5'	2.19	0.43
2:A:1301:G:H2'	2:A:1302:G:O4'	2.18	0.43
2:A:2113:A:H2'	2:A:2114:A:C8	2.53	0.43
2:A:2686:U:H2'	2:A:2687:U:C6	2.54	0.43
2:A:2726:G:H5"	2:A:2727:A:H5"	2.01	0.43
2:A:2952:U:O2'	5:D:25:PRO:HG2	2.19	0.43
6:E:35:HIS:NE2	14:M:11:PRO:HD3	2.33	0.43
24:W:133:ILE:HD11	24:W:144:LEU:HD11	2.00	0.43
31:d:18:VAL:O	31:d:23:LEU:HD22	2.19	0.43
2:A:210:G:OP2	31:d:28:ARG:NH2	2.52	0.43
2:A:291:C:H42	2:A:338:C:H41	1.67	0.43
2:A:707:G:N3	2:A:707:G:H2'	2.34	0.43
2:A:1640:A:H2'	2:A:1642:G:N7	2.33	0.43
5:D:198:ILE:HA	5:D:199:PRO:HD3	1.83	0.43
16:O:94:TYR:O	16:O:116:VAL:HG22	2.19	0.43
2:A:2597:A:H2'	2:A:2598:C:C6	2.54	0.42
3:B:7:G:O2'	17:P:41:ASN:ND2	2.51	0.42
4:C:73:ASP:C	4:C:75:VAL:H	2.26	0.42
8:G:128:SER:HB3	8:G:129:PRO:HD2	2.00	0.42
10:I:22:ALA:HB2	10:I:110:MET:HE3	2.01	0.42
2:A:1185:A:O2'	2:A:1186:G:O4'	2.31	0.42
2:A:2338:G:H4'	2:A:2388:G:H22	1.84	0.42
2:A:2343:G:H2'	2:A:2344:G:C8	2.54	0.42
2:A:2457:U:H2'	2:A:2458:G:C8	2.54	0.42
2:A:3008:C:H2'	2:A:3009:U:O4'	2.19	0.42
6:E:158:ILE:HG22	6:E:159:GLY:O	2.19	0.42
10:I:98:LYS:HB2	10:I:98:LYS:HE2	1.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:19:PHE:HA	18:Q:88:ARG:NH1	2.34	0.42
18:Q:49:ARG:NE	18:Q:56:GLU:OE2	2.49	0.42
2:A:1855:A:H2'	2:A:1856:C:C6	2.54	0.42
2:A:3069:G:H3'	18:Q:92:ARG:O	2.19	0.42
4:C:60:ARG:HH11	4:C:86:PRO:CB	2.32	0.42
5:D:147:ARG:HB2	5:D:148:PRO:CD	2.49	0.42
16:O:73:LYS:HA	16:O:76:VAL:HG22	2.00	0.42
18:Q:13:ARG:NH1	18:Q:80:ILE:O	2.32	0.42
22:U:66:ARG:HG2	22:U:75:LYS:HG3	2.00	0.42
29:b:10:ARG:NH1	29:b:10:ARG:HG3	2.32	0.42
30:c:39:LYS:O	30:c:40:LYS:HG2	2.19	0.42
2:A:1174:G:O2'	2:A:1221:A:N6	2.51	0.42
2:A:2040:G:OP1	4:C:54:LYS:HE3	2.20	0.42
4:C:25:THR:HG21	4:C:113:GLN:HE22	1.83	0.42
5:D:192:LEU:HA	5:D:192:LEU:HD12	1.79	0.42
7:F:182:PHE:HA	7:F:183:PRO:HD3	1.64	0.42
12:K:65:SER:O	12:K:68:LYS:HE3	2.19	0.42
12:K:76:ARG:CB	12:K:85:ARG:HH12	2.26	0.42
16:O:117:ARG:HA	16:O:117:ARG:HD3	1.74	0.42
24:W:86:HIS:HA	24:W:87:PRO:HD3	1.87	0.42
24:W:104:GLU:O	24:W:136:GLU:HA	2.19	0.42
2:A:339:U:N3	2:A:340:A:N7	2.68	0.42
2:A:3046:C:H2'	2:A:3047:A:O4'	2.19	0.42
6:E:20:LEU:HB3	6:E:25:PHE:CD1	2.54	0.42
24:W:146:VAL:HG21	24:W:157:ILE:HG21	2.01	0.42
27:Z:36:MET:HE2	27:Z:36:MET:HB3	1.97	0.42
2:A:275:C:H6	2:A:275:C:C5'	2.31	0.42
2:A:561:G:C2'	2:A:562:G:H5'	2.50	0.42
2:A:1402:A:H5'	16:O:103:ARG:HD2	2.02	0.42
2:A:2443:U:H2'	2:A:2444:C:C6	2.55	0.42
2:A:3052:A:OP1	5:D:60:ARG:NH2	2.50	0.42
3:B:11:U:O2'	3:B:12:C:H5'	2.20	0.42
5:D:115:THR:HG21	5:D:174:ARG:HE	1.84	0.42
6:E:118:ARG:HH12	14:M:3:VAL:CG1	2.32	0.42
15:N:77:LYS:HB2	15:N:78:PRO:HD2	2.00	0.42
2:A:1202:A:O2'	2:A:1203:A:O4'	2.26	0.42
9:H:82:VAL:HG11	9:H:91:LEU:HD13	2.01	0.42
11:J:47:ALA:O	11:J:50:SER:HB2	2.20	0.42
22:U:34:HIS:HA	22:U:35:PRO:HD3	1.75	0.42
30:c:22:ASN:HD22	30:c:22:ASN:HA	1.57	0.42
2:A:263:G:O2'	2:A:517:A:N3	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1199:U:H2'	2:A:1200:U:C6	2.55	0.42
2:A:1900:C:H2'	2:A:1901:C:H6	1.85	0.42
2:A:2070:A:H2'	2:A:2071:A:C8	2.55	0.42
2:A:2780:C:H2'	2:A:2781:G:O4'	2.19	0.42
6:E:118:ARG:HH12	14:M:3:VAL:HG13	1.82	0.42
7:F:90:MET:HE2	7:F:90:MET:HB3	1.82	0.42
22:U:91:LYS:HA	22:U:92:PRO:HD2	1.92	0.42
2:A:7:U:H3'	2:A:8:U:H6	1.85	0.42
2:A:75:U:H5'	27:Z:11:ARG:NH2	2.31	0.42
2:A:194:A:H61	2:A:197:C:H3'	1.85	0.42
2:A:370:U:H4'	2:A:371:G:O5'	2.19	0.42
2:A:966:U:OP1	28:a:18:LYS:HD3	2.20	0.42
2:A:2495:G:OP1	25:X:18:ALA:HB1	2.20	0.42
5:D:127:MET:HE2	5:D:127:MET:HB3	1.81	0.42
10:I:27:GLU:HG3	10:I:76:PRO:HG2	2.01	0.42
11:J:22:PRO:HB2	11:J:25:PRO:HD2	2.02	0.42
15:N:72:ARG:HB3	15:N:72:ARG:HH11	1.84	0.42
20:S:78:PHE:HD1	20:S:85:HIS:HD2	1.68	0.42
28:a:23:LEU:HA	28:a:23:LEU:HD23	1.84	0.42
2:A:134:A:H2'	2:A:135:G:O4'	2.20	0.42
2:A:768:G:H2'	2:A:769:U:C6	2.55	0.42
2:A:1541:G:OP2	2:A:1629:G:N2	2.49	0.42
2:A:2007:C:H2'	2:A:2008:A:C5	2.54	0.42
2:A:2796:A:OP2	5:D:154:CYS:O	2.38	0.42
4:C:68:ARG:HH12	4:C:150:GLY:CA	2.31	0.42
4:C:131:LEU:HD12	4:C:136:ILE:HG12	2.01	0.42
8:G:153:ARG:HA	8:G:153:ARG:HD3	1.76	0.42
34:g:20:HIS:ND1	34:g:40:GLN:HG3	2.35	0.42
2:A:193:G:H2'	2:A:194:A:O4'	2.20	0.41
2:A:1084:U:H3'	2:A:1084:U:H6	1.84	0.41
2:A:1087:G:O3'	28:a:14:GLY:HA2	2.20	0.41
2:A:1131:G:H21	19:R:122:ASN:ND2	2.16	0.41
2:A:1539:A:H5"	2:A:1540:U:OP2	2.19	0.41
2:A:1756:G:H1'	2:A:1758:G:C2	2.55	0.41
3:B:27:A:C2	3:B:28:A:H1'	2.55	0.41
3:B:76:G:H1'	24:W:36:VAL:HG21	2.02	0.41
3:B:81:U:H2'	3:B:82:A:C8	2.54	0.41
6:E:58:VAL:HG21	6:E:80:ARG:HB3	2.02	0.41
7:F:74:VAL:CG1	7:F:91:PRO:HB3	2.49	0.41
11:J:30:LEU:HA	11:J:33:HIS:CD2	2.47	0.41
15:N:132:VAL:HG22	24:W:90:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:37:THR:HG23	16:O:40:LYS:HD2	2.02	0.41
2:A:159:A:C5	2:A:166:A:C2	3.08	0.41
2:A:719:G:N7	14:M:105:ARG:NH1	2.67	0.41
2:A:1392:G:H2'	2:A:1393:C:C6	2.55	0.41
2:A:1393:C:H2'	2:A:1394:A:C8	2.55	0.41
4:C:137:PRO:HG2	4:C:140:THR:CG2	2.50	0.41
4:C:147:LEU:HD23	4:C:147:LEU:HA	1.62	0.41
8:G:65:LEU:HD12	8:G:65:LEU:HA	1.74	0.41
15:N:37:LEU:HD23	15:N:37:LEU:HA	1.88	0.41
18:Q:19:PHE:HA	18:Q:88:ARG:HH12	1.84	0.41
2:A:994:A:C6	2:A:995:U:H1'	2.56	0.41
2:A:2567:U:H2'	2:A:2568:U:C6	2.55	0.41
4:C:132:PRO:HA	4:C:190:ARG:HA	2.02	0.41
7:F:11:LEU:HD23	7:F:11:LEU:HA	1.71	0.41
12:K:93:LEU:HA	12:K:93:LEU:HD23	1.73	0.41
19:R:109:LEU:HD23	19:R:109:LEU:HA	1.78	0.41
27:Z:49:THR:OG1	27:Z:50:VAL:N	2.53	0.41
2:A:1046:C:H4'	2:A:1047:A:OP2	2.21	0.41
2:A:1231:U:O2'	2:A:1232:G:OP1	2.33	0.41
2:A:1790:A:H5'	4:C:36:PRO:HB3	2.03	0.41
2:A:2011:U:H2'	2:A:2012:C:C6	2.55	0.41
11:J:59:GLU:O	11:J:70:PHE:HA	2.19	0.41
12:K:69:LEU:HA	12:K:69:LEU:HD12	1.78	0.41
14:M:31:LYS:HE3	14:M:32:THR:HG23	2.02	0.41
18:Q:16:ILE:HD13	18:Q:16:ILE:HA	1.91	0.41
21:T:106:ARG:HG2	21:T:106:ARG:NH1	2.35	0.41
22:U:14:PRO:HD3	27:Z:34:PHE:CE1	2.55	0.41
28:a:4:LEU:HD23	28:a:4:LEU:HA	1.85	0.41
32:e:36:LYS:HA	32:e:37:PRO:HD3	1.84	0.41
33:f:24:MET:HE2	33:f:24:MET:HB3	1.83	0.41
2:A:553:G:OP1	31:d:15:ARG:NH2	2.53	0.41
2:A:818:U:O4	2:A:819:G:N1	2.54	0.41
2:A:2861:U:H2'	2:A:2862:G:O4'	2.20	0.41
7:F:111:ILE:HD11	7:F:182:PHE:CD2	2.55	0.41
10:I:94:LYS:NZ	10:I:124:ALA:HB3	2.36	0.41
11:J:55:VAL:HG21	11:J:79:LYS:HE3	2.02	0.41
15:N:67:ASN:O	15:N:68:ILE:HD13	2.20	0.41
2:A:237:C:H5"	2:A:237:C:H6	1.85	0.41
2:A:854:A:H1'	2:A:855:C:H5	1.85	0.41
6:E:192:ASP:HA	14:M:5:LYS:NZ	2.35	0.41
11:J:44:TYR:HD1	11:J:72:LEU:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:23:ARG:HB3	13:L:40:VAL:HG13	2.02	0.41
15:N:74:LEU:HA	15:N:74:LEU:HD23	1.74	0.41
17:P:36:PRO:HG2	17:P:97:VAL:HG11	2.02	0.41
26:Y:45:ASN:HD22	26:Y:45:ASN:HA	1.55	0.41
2:A:322:A:H5'	2:A:323:C:OP2	2.20	0.41
2:A:664:A:H5"	2:A:665:G:OP2	2.21	0.41
2:A:932:C:O2'	2:A:954:U:H5"	2.20	0.41
2:A:1275:A:O4'	19:R:51:ARG:NH1	2.54	0.41
2:A:1472:C:H2'	2:A:1473:G:O4'	2.21	0.41
2:A:2358:A:O2'	2:A:2382:G:O2'	2.19	0.41
3:B:71:C:H2'	3:B:72:C:H6	1.86	0.41
7:F:127:LYS:HA	7:F:127:LYS:HD3	1.86	0.41
13:L:35:ILE:HA	13:L:62:VAL:O	2.21	0.41
14:M:6:LEU:HD23	14:M:6:LEU:HA	1.65	0.41
14:M:59:MET:HE2	14:M:59:MET:HB3	1.85	0.41
18:Q:82:HIS:HB3	18:Q:84:ASP:OD1	2.21	0.41
2:A:273:A:H61	2:A:314:G:H1'	1.86	0.41
2:A:856:U:H2'	2:A:857:U:O4'	2.20	0.41
2:A:1530:G:N2	2:A:1806:A:C6	2.89	0.41
2:A:1545:C:H2'	2:A:1546:A:H8	1.86	0.41
2:A:1755:A:C2	2:A:1758:G:O6	2.74	0.41
2:A:1771:U:H2'	2:A:1772:G:O4'	2.20	0.41
2:A:3119:A:H5'	12:K:136:GLN:HE21	1.86	0.41
8:G:55:ARG:NH1	8:G:63:ARG:HA	2.35	0.41
17:P:80:HIS:O	17:P:84:VAL:HG23	2.21	0.41
18:Q:6:PHE:CE1	18:Q:7:VAL:HG23	2.55	0.41
2:A:173:U:H2'	2:A:174:G:O4'	2.21	0.41
2:A:681:C:H2'	2:A:682:A:C8	2.55	0.41
2:A:758:A:O2'	2:A:759:G:OP2	2.35	0.41
2:A:1002:C:C2'	2:A:1003:A:H5"	2.50	0.41
2:A:1541:G:N2	2:A:1631:A:H61	2.19	0.41
2:A:2643:U:H2'	2:A:2644:C:C6	2.55	0.41
2:A:2801:A:H5"	2:A:2802:G:H5'	2.03	0.41
2:A:2908:U:OP1	18:Q:57:THR:HG21	2.21	0.41
6:E:42:LEU:HD21	6:E:186:TYR:CE2	2.56	0.41
7:F:159:MET:HE3	7:F:159:MET:HB3	1.82	0.41
11:J:10:LEU:N	11:J:62:VAL:HG22	2.36	0.41
11:J:112:GLU:O	11:J:115:LYS:HB3	2.21	0.41
13:L:59:LYS:HB3	13:L:87:ILE:HG22	2.02	0.41
14:M:110:VAL:N	14:M:127:ASN:HD22	2.18	0.41
18:Q:99:LEU:HA	18:Q:99:LEU:HD23	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:92:ARG:HG3	19:R:92:ARG:HH11	1.86	0.41
28:a:31:ILE:O	28:a:32:ARG:HB2	2.21	0.41
2:A:156:C:C4	2:A:157:U:C5	3.09	0.41
2:A:429:A:H2'	2:A:430:A:C8	2.56	0.41
2:A:815:G:H2'	2:A:816:G:O4'	2.21	0.41
2:A:965:U:H2'	2:A:966:U:C6	2.56	0.41
2:A:1733:C:H2'	2:A:1734:C:C6	2.56	0.41
2:A:2083:A:H2'	2:A:2084:A:H5'	2.01	0.41
2:A:2718:G:O2'	15:N:80:GLU:HA	2.21	0.41
2:A:3043:G:H2'	2:A:3044:A:H5"	2.03	0.41
3:B:114:A:H5'	3:B:115:A:OP2	2.21	0.41
4:C:58:HIS:ND1	4:C:58:HIS:C	2.78	0.41
7:F:68:THR:OG1	7:F:69:GLY:N	2.54	0.41
7:F:75:ARG:HH21	7:F:95:ARG:HH12	1.60	0.41
10:I:26:THR:HG22	10:I:105:ILE:HG23	2.02	0.41
14:M:49:MET:HB2	14:M:58:HIS:CE1	2.56	0.41
19:R:43:LEU:HA	19:R:43:LEU:HD23	1.75	0.41
2:A:56:U:O2'	2:A:71:A:OP2	2.36	0.40
2:A:2781:G:H2'	2:A:2782:C:C6	2.56	0.40
4:C:215:LYS:HB2	4:C:215:LYS:HE2	1.81	0.40
5:D:24:VAL:HA	5:D:25:PRO:HD3	1.85	0.40
16:O:68:LYS:HB3	16:O:68:LYS:HE2	1.96	0.40
18:Q:54:ILE:HA	18:Q:76:HIS:HD2	1.85	0.40
19:R:58:ARG:HA	19:R:61:TRP:CE3	2.56	0.40
2:A:23:G:C6	2:A:24:G:N1	2.89	0.40
2:A:357:U:OP2	2:A:357:U:H6	2.04	0.40
2:A:452:G:H8	2:A:452:G:OP2	2.04	0.40
2:A:1430:C:H2'	2:A:1431:U:H6	1.86	0.40
2:A:1555:A:H2'	2:A:1556:A:O4'	2.21	0.40
2:A:1647:G:C6	2:A:1648:A:C6	3.09	0.40
2:A:2407:C:H5"	2:A:2407:C:H6	1.85	0.40
15:N:72:ARG:HA	15:N:73:PRO:HD2	1.95	0.40
25:X:85:ARG:HA	25:X:86:PRO:HD3	1.91	0.40
27:Z:5:THR:HG21	27:Z:21:LYS:HZ1	1.86	0.40
2:A:3:A:O2'	12:K:132:HIS:HD2	2.03	0.40
2:A:287:A:H8	2:A:287:A:P	2.45	0.40
2:A:326:A:H2'	2:A:326:A:N3	2.36	0.40
2:A:1186:G:O2'	2:A:1187:A:H5'	2.22	0.40
2:A:1434:G:O2'	2:A:1435:C:H5'	2.21	0.40
2:A:1542:A:H2'	2:A:1543:A:C8	2.57	0.40
2:A:1565:A:N6	2:A:1606:G:H1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1759:A:O5’	2:A:1759:A:H8	2.04	0.40
2:A:2362:C:H2’	2:A:2363:A:C8	2.56	0.40
2:A:2444:C:H2’	2:A:2445:A:H8	1.87	0.40
4:C:206:TRP:CZ2	4:C:215:LYS:HE3	2.55	0.40
5:D:38:ARG:HD3	5:D:40:ARG:NH1	2.37	0.40
15:N:118:LEU:HA	15:N:118:LEU:HD23	1.65	0.40
16:O:36:THR:OG1	16:O:37:THR:N	2.54	0.40
17:P:66:ILE:HG23	17:P:71:ARG:NH2	2.37	0.40
24:W:28:ARG:HE	24:W:93:GLN:HA	1.86	0.40
27:Z:45:ARG:NH1	27:Z:48:ARG:NE	2.66	0.40
29:b:26:GLY:O	29:b:27:LEU:HD23	2.21	0.40
2:A:1229:A:H8	2:A:1230:G:H1’	1.85	0.40
2:A:1400:G:N2	2:A:1443:G:H5”	2.36	0.40
2:A:1485:C:H2’	2:A:1486:G:O4’	2.21	0.40
2:A:1540:U:H2’	2:A:1541:G:O4’	2.21	0.40
2:A:2998:C:H2’	2:A:2999:A:O4’	2.22	0.40
2:A:3088:C:H6	2:A:3088:C:H2’	1.76	0.40
4:C:76:ASN:ND2	4:C:118:GLU:HB3	2.35	0.40
13:L:109:LYS:O	13:L:110:LYS:HB2	2.21	0.40
14:M:61:LEU:HD13	32:e:24:ARG:HD2	2.03	0.40
27:Z:47:LEU:HA	27:Z:47:LEU:HD23	1.87	0.40
2:A:159:A:OP2	2:A:164:A:N6	2.53	0.40
2:A:238:G:H2’	2:A:239:U:O4’	2.22	0.40
2:A:650:G:OP1	12:K:112:ASN:HB2	2.21	0.40
2:A:1176:G:H21	11:J:129:ILE:HD13	1.87	0.40
2:A:1319:A:OP1	6:E:153:LYS:HD2	2.21	0.40
2:A:1535:C:H2’	2:A:1536:A:O4’	2.22	0.40
2:A:1665:U:H2’	2:A:1666:A:C8	2.57	0.40
2:A:2679:G:H2’	2:A:2680:C:C6	2.56	0.40
2:A:2687:U:H2’	2:A:2688:C:O4’	2.21	0.40
2:A:2729:G:O6	2:A:2800:G:H2’	2.22	0.40
12:K:77:HIS:HD2	12:K:79:GLY:H	1.64	0.40
14:M:129:PHE:CE1	14:M:146:GLU:HB3	2.57	0.40
23:V:11:VAL:HG23	23:V:19:ALA:O	2.22	0.40
23:V:64:ALA:HA	23:V:65:PRO:HD3	1.95	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	3	21/24 (88%)	21 (100%)	0	0	100	100
4	C	273/278 (98%)	259 (95%)	14 (5%)	0	100	100
5	D	212/217 (98%)	199 (94%)	12 (6%)	1 (0%)	24	57
6	E	207/215 (96%)	201 (97%)	5 (2%)	1 (0%)	24	57
7	F	180/187 (96%)	164 (91%)	15 (8%)	1 (1%)	21	53
8	G	174/179 (97%)	166 (95%)	7 (4%)	1 (1%)	21	53
9	H	149/151 (99%)	140 (94%)	8 (5%)	1 (1%)	18	50
10	I	124/175 (71%)	117 (94%)	7 (6%)	0	100	100
11	J	131/142 (92%)	124 (95%)	7 (5%)	0	100	100
12	K	144/147 (98%)	138 (96%)	6 (4%)	0	100	100
13	L	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
14	M	143/147 (97%)	135 (94%)	7 (5%)	1 (1%)	18	50
15	N	134/138 (97%)	124 (92%)	10 (8%)	0	100	100
16	O	116/199 (58%)	111 (96%)	5 (4%)	0	100	100
17	P	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
18	Q	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
19	R	122/129 (95%)	116 (95%)	6 (5%)	0	100	100
20	S	98/103 (95%)	96 (98%)	2 (2%)	0	100	100
21	T	112/153 (73%)	109 (97%)	3 (3%)	0	100	100
22	U	95/100 (95%)	91 (96%)	4 (4%)	0	100	100
23	V	93/105 (89%)	89 (96%)	4 (4%)	0	100	100
24	W	190/215 (88%)	186 (98%)	4 (2%)	0	100	100
25	X	77/88 (88%)	73 (95%)	4 (5%)	0	100	100
26	Y	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
27	Z	62/77 (80%)	61 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
28	a	57/61 (93%)	56 (98%)	1 (2%)	0	100 100
29	b	52/57 (91%)	51 (98%)	1 (2%)	0	100 100
30	c	47/55 (86%)	44 (94%)	2 (4%)	1 (2%)	5 27
31	d	44/47 (94%)	42 (96%)	2 (4%)	0	100 100
32	e	61/64 (95%)	61 (100%)	0	0	100 100
33	f	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
34	g	46/75 (61%)	46 (100%)	0	0	100 100
All	All	3615/3991 (91%)	3457 (96%)	151 (4%)	7 (0%)	44 72

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
30	c	7	VAL
5	D	143	ALA
14	M	31	LYS
8	G	66	HIS
6	E	90	VAL
9	H	124	ILE
7	F	61	ILE

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	3	18/19 (95%)	15 (83%)	3 (17%)	2 10
4	C	215/218 (99%)	192 (89%)	23 (11%)	6 25
5	D	160/163 (98%)	129 (81%)	31 (19%)	1 7
6	E	169/173 (98%)	150 (89%)	19 (11%)	6 23
7	F	151/156 (97%)	139 (92%)	12 (8%)	11 37
8	G	148/150 (99%)	130 (88%)	18 (12%)	5 20
9	H	90/116 (78%)	81 (90%)	9 (10%)	7 28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	I	89/120 (74%)	82 (92%)	7 (8%)	11 37
11	J	102/108 (94%)	89 (87%)	13 (13%)	4 19
12	K	119/120 (99%)	111 (93%)	8 (7%)	15 43
13	L	100/100 (100%)	91 (91%)	9 (9%)	9 31
14	M	112/114 (98%)	99 (88%)	13 (12%)	5 22
15	N	114/116 (98%)	101 (89%)	13 (11%)	5 22
16	O	97/158 (61%)	86 (89%)	11 (11%)	5 22
17	P	93/94 (99%)	86 (92%)	7 (8%)	12 39
18	Q	100/100 (100%)	92 (92%)	8 (8%)	11 37
19	R	97/99 (98%)	89 (92%)	8 (8%)	10 36
20	S	81/83 (98%)	72 (89%)	9 (11%)	6 23
21	T	90/117 (77%)	81 (90%)	9 (10%)	7 28
22	U	83/85 (98%)	79 (95%)	4 (5%)	23 53
23	V	81/86 (94%)	73 (90%)	8 (10%)	7 28
24	W	155/168 (92%)	136 (88%)	19 (12%)	4 20
25	X	58/63 (92%)	53 (91%)	5 (9%)	10 33
26	Y	50/51 (98%)	42 (84%)	8 (16%)	2 12
27	Z	58/66 (88%)	58 (100%)	0	100 100
28	a	52/54 (96%)	50 (96%)	2 (4%)	29 59
29	b	43/46 (94%)	36 (84%)	7 (16%)	2 11
30	c	47/52 (90%)	43 (92%)	4 (8%)	10 34
31	d	35/36 (97%)	32 (91%)	3 (9%)	10 33
32	e	53/54 (98%)	46 (87%)	7 (13%)	4 17
33	f	35/35 (100%)	33 (94%)	2 (6%)	18 48
34	g	43/63 (68%)	38 (88%)	5 (12%)	5 22
All	All	2938/3183 (92%)	2634 (90%)	304 (10%)	9 26

All (304) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	7	LYS
1	3	9	ARG
1	3	12	LYS

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Mol	Chain	Res	Type
4	C	10	THR
4	C	13	ARG
4	C	28	THR
4	C	54	LYS
4	C	58	HIS
4	C	60	ARG
4	C	63	ARG
4	C	78	LYS
4	C	89	THR
4	C	116	VAL
4	C	119	SER
4	C	122	ASN
4	C	131	LEU
4	C	148	ARG
4	C	157	ARG
4	C	161	VAL
4	C	177	MET
4	C	181	GLU
4	C	203	ASN
4	C	204	ILE
4	C	211	ARG
4	C	241	SER
4	C	272	ARG
5	D	3	ARG
5	D	11	LEU
5	D	19	GLU
5	D	58	SER
5	D	60	ARG
5	D	63	ILE
5	D	79	ARG
5	D	85	ARG
5	D	86	LEU
5	D	87	ASP
5	D	99	GLN
5	D	102	THR
5	D	117	THR
5	D	126	THR
5	D	129	ARG
5	D	133	ARG
5	D	144	VAL
5	D	147	ARG
5	D	151	ILE

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Mol	Chain	Res	Type
5	D	154	CYS
5	D	162	LYS
5	D	164	THR
5	D	169	ARG
5	D	170	MET
5	D	176	THR
5	D	192	LEU
5	D	198	ILE
5	D	201	ARG
5	D	206	VAL
5	D	208	VAL
5	D	209	ARG
6	E	34	MET
6	E	39	THR
6	E	50	HIS
6	E	78	SER
6	E	79	THR
6	E	85	THR
6	E	97	ASP
6	E	128	THR
6	E	131	VAL
6	E	135	THR
6	E	137	SER
6	E	149	THR
6	E	161	THR
6	E	169	VAL
6	E	170	ARG
6	E	178	ILE
6	E	179	SER
6	E	181	ASP
6	E	201	LEU
7	F	31	ASN
7	F	44	ASN
7	F	83	GLN
7	F	102	ARG
7	F	130	ASP
7	F	148	ILE
7	F	150	VAL
7	F	151	ASP
7	F	157	ARG
7	F	159	MET
7	F	164	VAL

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Mol	Chain	Res	Type
7	F	165	THR
8	G	3	ARG
8	G	4	ILE
8	G	35	LEU
8	G	42	SER
8	G	48	ASP
8	G	59	GLU
8	G	65	LEU
8	G	72	LEU
8	G	73	ILE
8	G	77	VAL
8	G	90	ILE
8	G	114	VAL
8	G	135	SER
8	G	137	ILE
8	G	153	ARG
8	G	156	ASP
8	G	171	ARG
8	G	172	ARG
9	H	4	ILE
9	H	31	LEU
9	H	33	ARG
9	H	38	VAL
9	H	40	SER
9	H	88	THR
9	H	124	ILE
9	H	135	LYS
9	H	146	LEU
10	I	55	THR
10	I	79	ILE
10	I	82	VAL
10	I	87	VAL
10	I	94	LYS
10	I	103	LEU
10	I	115	LEU
11	J	15	ILE
11	J	26	VAL
11	J	30	LEU
11	J	42	LYS
11	J	48	THR
11	J	52	ARG
11	J	55	VAL

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Mol	Chain	Res	Type
11	J	56	ILE
11	J	87	VAL
11	J	99	VAL
11	J	113	THR
11	J	114	LYS
11	J	117	ASP
12	K	17	VAL
12	K	18	ILE
12	K	70	THR
12	K	85	ARG
12	K	96	HIS
12	K	116	ARG
12	K	118	ILE
12	K	129	ASP
13	L	13	ASN
13	L	20	LEU
13	L	40	VAL
13	L	58	VAL
13	L	73	ASP
13	L	77	ILE
13	L	87	ILE
13	L	90	ASP
13	L	96	THR
14	M	22	VAL
14	M	24	ARG
14	M	31	LYS
14	M	40	THR
14	M	43	ARG
14	M	46	VAL
14	M	49	MET
14	M	70	ARG
14	M	93	VAL
14	M	104	VAL
14	M	105	ARG
14	M	122	VAL
14	M	146	GLU
15	N	3	ILE
15	N	7	VAL
15	N	10	ARG
15	N	16	GLU
15	N	18	ARG
15	N	20	ILE

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Mol	Chain	Res	Type
15	N	47	ILE
15	N	48	GLU
15	N	51	ARG
15	N	72	ARG
15	N	76	LYS
15	N	82	ARG
15	N	130	ARG
16	O	6	LYS
16	O	9	ARG
16	O	10	LEU
16	O	27	SER
16	O	33	ARG
16	O	37	THR
16	O	53	THR
16	O	64	ARG
16	O	71	ARG
16	O	79	LEU
16	O	96	ARG
17	P	6	VAL
17	P	10	ILE
17	P	12	GLU
17	P	24	ARG
17	P	32	THR
17	P	51	LEU
17	P	74	ASP
18	Q	15	ASP
18	Q	25	VAL
18	Q	32	ILE
18	Q	54	ILE
18	Q	57	THR
18	Q	79	ASN
18	Q	93	ARG
18	Q	96	LEU
19	R	6	ARG
19	R	15	ARG
19	R	16	THR
19	R	29	SER
19	R	42	SER
19	R	44	THR
19	R	74	ILE
19	R	91	ASP
20	S	23	LYS

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Mol	Chain	Res	Type
20	S	27	LEU
20	S	30	GLU
20	S	53	ASP
20	S	54	ASP
20	S	58	VAL
20	S	68	THR
20	S	72	LYS
20	S	94	LEU
21	T	19	VAL
21	T	20	SER
21	T	22	THR
21	T	26	ARG
21	T	78	VAL
21	T	81	VAL
21	T	84	ASP
21	T	104	ARG
21	T	107	THR
22	U	27	ASN
22	U	41	GLN
22	U	62	ARG
22	U	81	ARG
23	V	12	ILE
23	V	35	VAL
23	V	38	VAL
23	V	42	LYS
23	V	69	SER
23	V	83	VAL
23	V	91	THR
23	V	105	ILE
24	W	12	THR
24	W	14	ASN
24	W	15	VAL
24	W	19	THR
24	W	33	VAL
24	W	64	ASN
24	W	68	THR
24	W	79	LEU
24	W	91	ASN
24	W	92	ILE
24	W	99	VAL
24	W	112	VAL
24	W	114	VAL

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Mol	Chain	Res	Type
24	W	119	THR
24	W	131	ILE
24	W	139	SER
24	W	146	VAL
24	W	158	THR
24	W	172	SER
25	X	30	VAL
25	X	36	ILE
25	X	38	VAL
25	X	41	ARG
25	X	80	ILE
26	Y	17	SER
26	Y	19	SER
26	Y	23	ARG
26	Y	24	ARG
26	Y	28	ARG
26	Y	36	VAL
26	Y	45	ASN
26	Y	53	THR
28	a	36	VAL
28	a	48	ASN
29	b	3	VAL
29	b	6	ARG
29	b	8	MET
29	b	10	ARG
29	b	14	ARG
29	b	35	GLN
29	b	39	VAL
30	c	6	ASP
30	c	25	THR
30	c	38	ILE
30	c	47	THR
31	d	13	ARG
31	d	15	ARG
31	d	46	THR
32	e	11	SER
32	e	13	ARG
32	e	19	THR
32	e	23	VAL
32	e	47	ARG
32	e	56	SER
32	e	59	ASN

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Mol	Chain	Res	Type
33	f	2	LYS
33	f	7	VAL
34	g	9	TYR
34	g	11	ASP
34	g	12	THR
34	g	22	PHE
34	g	46	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	3	17	ASN
1	3	18	HIS
4	C	38	HIS
4	C	53	HIS
4	C	76	ASN
4	C	91	ASN
4	C	129	ASN
4	C	130	ASN
4	C	143	HIS
4	C	203	ASN
4	C	205	ASN
5	D	34	ASN
5	D	130	HIS
5	D	179	ASN
6	E	121	ASN
6	E	125	HIS
6	E	171	ASN
6	E	176	HIS
6	E	202	ASN
7	F	62	ASN
7	F	146	HIS
8	G	66	HIS
8	G	86	GLN
9	H	111	ASN
9	H	118	GLN
9	H	147	ASN
10	I	54	ASN
11	J	33	HIS
11	J	54	ASN
12	K	58	ASN
12	K	77	HIS

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Mol	Chain	Res	Type
12	K	103	ASN
12	K	132	HIS
13	L	13	ASN
13	L	51	ASN
14	M	58	HIS
14	M	76	GLN
14	M	107	ASN
14	M	127	ASN
15	N	123	HIS
16	O	17	GLN
17	P	22	HIS
17	P	41	ASN
17	P	53	ASN
18	Q	2	ASN
18	Q	26	ASN
18	Q	50	GLN
18	Q	79	ASN
19	R	41	HIS
19	R	72	ASN
19	R	94	ASN
19	R	122	ASN
20	S	76	HIS
20	S	85	HIS
21	T	67	ASN
22	U	41	GLN
22	U	58	ASN
22	U	61	ASN
23	V	31	ASN
23	V	67	HIS
23	V	101	ASN
24	W	46	HIS
24	W	61	HIS
24	W	76	GLN
24	W	94	HIS
24	W	126	GLN
24	W	161	GLN
25	X	29	GLN
25	X	44	HIS
26	Y	20	HIS
26	Y	22	HIS
26	Y	45	ASN
28	a	48	ASN

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Mol	Chain	Res	Type
28	a	51	HIS
29	b	36	GLN
30	c	22	ASN
30	c	48	HIS
31	d	36	ASN
32	e	25	GLN
32	e	28	ASN
32	e	31	HIS
32	e	63	ASN
33	f	20	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	3118/3120 (99%)	784 (25%)	30 (0%)
3	B	117/118 (99%)	28 (23%)	2 (1%)
35	2	2/3 (66%)	2 (100%)	0
All	All	3237/3241 (99%)	814 (25%)	32 (0%)

All (814) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	7	U
2	A	12	G
2	A	20	G
2	A	29	C
2	A	31	U
2	A	32	G
2	A	33	G
2	A	46	A
2	A	48	G
2	A	55	G
2	A	59	G
2	A	60	A
2	A	68	A
2	A	71	A
2	A	72	G
2	A	83	C
2	A	89	A
2	A	90	C
2	A	91	C

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Mol	Chain	Res	Type
2	A	94	G
2	A	98	U
2	A	99	G
2	A	115	A
2	A	116	A
2	A	117	U
2	A	120	G
2	A	122	A
2	A	125	C
2	A	128	G
2	A	129	G
2	A	133	G
2	A	136	U
2	A	137	G
2	A	145	G
2	A	148	A
2	A	161	U
2	A	164	A
2	A	171	U
2	A	172	C
2	A	175	G
2	A	177	G
2	A	195	A
2	A	198	A
2	A	203	A
2	A	205	U
2	A	212	A
2	A	214	G
2	A	215	A
2	A	221	A
2	A	222	A
2	A	227	A
2	A	228	A
2	A	229	U
2	A	230	G
2	A	231	U
2	A	237	C
2	A	245	G
2	A	248	G
2	A	264	G
2	A	265	A
2	A	268	G

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Mol	Chain	Res	Type
2	A	270	U
2	A	271	A
2	A	272	A
2	A	274	C
2	A	275	C
2	A	276	G
2	A	279	U
2	A	280	G
2	A	282	A
2	A	283	U
2	A	285	U
2	A	286	G
2	A	287	A
2	A	288	U
2	A	290	C
2	A	291	C
2	A	292	G
2	A	294	G
2	A	297	G
2	A	299	G
2	A	300	G
2	A	301	U
2	A	302	U
2	A	303	G
2	A	305	G
2	A	306	U
2	A	312	G
2	A	315	U
2	A	316	U
2	A	317	G
2	A	318	U
2	A	319	G
2	A	322	A
2	A	323	C
2	A	324	C
2	A	330	U
2	A	331	U
2	A	336	C
2	A	337	U
2	A	338	C
2	A	342	C
2	A	343	U

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Mol	Chain	Res	Type
2	A	344	G
2	A	345	G
2	A	346	C
2	A	348	G
2	A	350	A
2	A	351	G
2	A	352	G
2	A	353	G
2	A	356	G
2	A	357	U
2	A	358	G
2	A	361	A
2	A	364	A
2	A	369	G
2	A	370	U
2	A	371	G
2	A	376	G
2	A	383	U
2	A	384	G
2	A	386	C
2	A	388	U
2	A	393	U
2	A	404	A
2	A	406	A
2	A	412	A
2	A	413	G
2	A	417	C
2	A	424	G
2	A	434	G
2	A	438	U
2	A	445	U
2	A	446	G
2	A	450	G
2	A	452	G
2	A	459	A
2	A	460	G
2	A	472	C
2	A	474	G
2	A	489	A
2	A	491	U
2	A	493	U
2	A	497	G

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Mol	Chain	Res	Type
2	A	498	G
2	A	499	G
2	A	500	A
2	A	503	A
2	A	505	C
2	A	509	U
2	A	512	G
2	A	533	C
2	A	543	U
2	A	544	U
2	A	562	G
2	A	566	A
2	A	569	G
2	A	570	U
2	A	572	C
2	A	581	G
2	A	589	A
2	A	591	G
2	A	592	A
2	A	594	U
2	A	595	A
2	A	596	C
2	A	605	G
2	A	606	U
2	A	614	C
2	A	617	U
2	A	618	C
2	A	619	C
2	A	620	G
2	A	630	U
2	A	631	C
2	A	634	C
2	A	636	U
2	A	637	G
2	A	638	U
2	A	639	C
2	A	640	G
2	A	641	U
2	A	642	G
2	A	643	G
2	A	644	G
2	A	647	G

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Mol	Chain	Res	Type
2	A	655	G
2	A	658	U
2	A	665	G
2	A	666	A
2	A	667	A
2	A	675	G
2	A	678	A
2	A	679	G
2	A	684	G
2	A	685	G
2	A	696	A
2	A	700	U
2	A	701	A
2	A	702	A
2	A	704	C
2	A	706	G
2	A	707	G
2	A	708	G
2	A	709	U
2	A	712	G
2	A	721	A
2	A	728	G
2	A	731	A
2	A	738	A
2	A	739	U
2	A	740	A
2	A	742	G
2	A	747	A
2	A	753	A
2	A	757	G
2	A	758	A
2	A	760	U
2	A	764	U
2	A	765	G
2	A	766	G
2	A	767	U
2	A	768	G
2	A	774	G
2	A	779	U
2	A	783	G
2	A	784	G
2	A	785	A

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Mol	Chain	Res	Type
2	A	793	C
2	A	794	G
2	A	801	U
2	A	813	C
2	A	816	G
2	A	827	G
2	A	829	U
2	A	839	U
2	A	841	G
2	A	843	G
2	A	845	C
2	A	862	U
2	A	863	G
2	A	871	A
2	A	872	G
2	A	878	G
2	A	879	A
2	A	880	G
2	A	890	G
2	A	891	G
2	A	892	G
2	A	897	A
2	A	898	A
2	A	899	G
2	A	900	G
2	A	904	A
2	A	905	U
2	A	907	A
2	A	917	A
2	A	919	A
2	A	920	G
2	A	921	C
2	A	927	C
2	A	942	U
2	A	960	G
2	A	961	U
2	A	971	G
2	A	973	G
2	A	974	G
2	A	975	U
2	A	981	U
2	A	982	A

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Mol	Chain	Res	Type
2	A	990	G
2	A	994	A
2	A	995	U
2	A	996	G
2	A	998	G
2	A	1000	C
2	A	1001	C
2	A	1002	C
2	A	1003	A
2	A	1005	A
2	A	1007	G
2	A	1009	U
2	A	1011	A
2	A	1012	C
2	A	1013	U
2	A	1014	G
2	A	1022	C
2	A	1025	A
2	A	1044	U
2	A	1046	C
2	A	1047	A
2	A	1049	G
2	A	1058	A
2	A	1063	G
2	A	1070	G
2	A	1075	U
2	A	1076	A
2	A	1078	G
2	A	1084	U
2	A	1085	G
2	A	1091	A
2	A	1092	G
2	A	1099	A
2	A	1101	A
2	A	1107	G
2	A	1108	A
2	A	1114	G
2	A	1127	A
2	A	1130	C
2	A	1131	G
2	A	1135	G
2	A	1140	G

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Mol	Chain	Res	Type
2	A	1144	A
2	A	1148	G
2	A	1151	U
2	A	1163	A
2	A	1164	A
2	A	1165	G
2	A	1173	G
2	A	1175	A
2	A	1176	G
2	A	1178	U
2	A	1184	U
2	A	1185	A
2	A	1186	G
2	A	1187	A
2	A	1188	A
2	A	1189	G
2	A	1190	C
2	A	1191	A
2	A	1192	G
2	A	1198	C
2	A	1201	G
2	A	1202	A
2	A	1203	A
2	A	1204	A
2	A	1205	G
2	A	1206	A
2	A	1207	G
2	A	1208	U
2	A	1209	G
2	A	1212	U
2	A	1213	A
2	A	1214	A
2	A	1227	C
2	A	1229	A
2	A	1230	G
2	A	1232	G
2	A	1233	A
2	A	1234	U
2	A	1237	U
2	A	1238	G
2	A	1240	G
2	A	1246	A

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Mol	Chain	Res	Type
2	A	1247	A
2	A	1250	U
2	A	1251	A
2	A	1253	C
2	A	1254	G
2	A	1260	C
2	A	1261	A
2	A	1267	A
2	A	1275	A
2	A	1290	C
2	A	1292	U
2	A	1293	G
2	A	1294	U
2	A	1324	G
2	A	1325	U
2	A	1332	G
2	A	1335	G
2	A	1339	G
2	A	1344	A
2	A	1345	G
2	A	1353	G
2	A	1359	G
2	A	1362	A
2	A	1363	G
2	A	1368	A
2	A	1369	A
2	A	1371	G
2	A	1386	G
2	A	1387	A
2	A	1389	U
2	A	1390	A
2	A	1404	C
2	A	1415	A
2	A	1416	A
2	A	1417	A
2	A	1433	G
2	A	1435	C
2	A	1437	A
2	A	1440	C
2	A	1447	G
2	A	1448	C
2	A	1456	G

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Mol	Chain	Res	Type
2	A	1461	G
2	A	1462	G
2	A	1465	C
2	A	1467	U
2	A	1480	A
2	A	1494	U
2	A	1499	A
2	A	1502	G
2	A	1506	U
2	A	1507	G
2	A	1510	A
2	A	1518	A
2	A	1521	C
2	A	1522	G
2	A	1531	C
2	A	1532	G
2	A	1533	U
2	A	1534	C
2	A	1536	A
2	A	1540	U
2	A	1543	A
2	A	1550	G
2	A	1551	U
2	A	1552	A
2	A	1553	C
2	A	1554	U
2	A	1563	A
2	A	1564	A
2	A	1565	A
2	A	1566	A
2	A	1574	G
2	A	1578	G
2	A	1579	C
2	A	1587	G
2	A	1588	G
2	A	1596	C
2	A	1599	U
2	A	1600	G
2	A	1625	G
2	A	1627	U
2	A	1628	A
2	A	1629	G

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Mol	Chain	Res	Type
2	A	1630	U
2	A	1631	A
2	A	1632	G
2	A	1633	U
2	A	1637	G
2	A	1638	C
2	A	1639	G
2	A	1640	A
2	A	1641	U
2	A	1648	A
2	A	1649	C
2	A	1659	U
2	A	1673	A
2	A	1674	G
2	A	1679	A
2	A	1680	A
2	A	1681	U
2	A	1688	G
2	A	1703	G
2	A	1705	C
2	A	1710	A
2	A	1711	G
2	A	1714	A
2	A	1715	A
2	A	1717	U
2	A	1720	G
2	A	1723	U
2	A	1724	G
2	A	1725	G
2	A	1728	U
2	A	1729	A
2	A	1730	U
2	A	1731	A
2	A	1737	A
2	A	1738	G
2	A	1746	G
2	A	1754	G
2	A	1755	A
2	A	1756	G
2	A	1757	U
2	A	1761	G
2	A	1767	U

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Mol	Chain	Res	Type
2	A	1774	U
2	A	1785	C
2	A	1786	G
2	A	1789	A
2	A	1792	A
2	A	1796	U
2	A	1798	U
2	A	1802	G
2	A	1803	A
2	A	1805	G
2	A	1806	A
2	A	1813	C
2	A	1825	C
2	A	1826	A
2	A	1845	G
2	A	1857	U
2	A	1862	C
2	A	1864	U
2	A	1866	C
2	A	1867	G
2	A	1869	G
2	A	1870	U
2	A	1871	G
2	A	1872	A
2	A	1887	A
2	A	1892	G
2	A	1893	C
2	A	1916	A
2	A	1932	U
2	A	1933	G
2	A	1945	U
2	A	1946	U
2	A	1947	U
2	A	1948	A
2	A	1949	C
2	A	1950	G
2	A	1954	C
2	A	1967	G
2	A	1973	C
2	A	1975	A
2	A	1981	U
2	A	1990	A

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Mol	Chain	Res	Type
2	A	1999	U
2	A	2008	A
2	A	2017	C
2	A	2018	G
2	A	2026	A
2	A	2033	U
2	A	2046	A
2	A	2047	C
2	A	2064	A
2	A	2065	A
2	A	2066	G
2	A	2073	A
2	A	2075	G
2	A	2084	A
2	A	2085	C
2	A	2086	U
2	A	2087	C
2	A	2088	C
2	A	2089	C
2	A	2091	U
2	A	2092	U
2	A	2093	G
2	A	2094	G
2	A	2095	G
2	A	2096	G
2	A	2106	A
2	A	2107	G
2	A	2108	A
2	A	2111	U
2	A	2112	U
2	A	2120	A
2	A	2129	C
2	A	2130	G
2	A	2131	G
2	A	2137	A
2	A	2138	C
2	A	2140	A
2	A	2141	U
2	A	2151	A
2	A	2153	G
2	A	2154	G
2	A	2160	A

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Mol	Chain	Res	Type
2	A	2162	A
2	A	2163	U
2	A	2164	U
2	A	2179	U
2	A	2184	A
2	A	2190	A
2	A	2191	C
2	A	2194	A
2	A	2195	U
2	A	2196	G
2	A	2215	U
2	A	2217	U
2	A	2221	A
2	A	2226	U
2	A	2227	A
2	A	2242	G
2	A	2244	A
2	A	2247	A
2	A	2251	G
2	A	2254	A
2	A	2255	A
2	A	2256	G
2	A	2257	A
2	A	2263	G
2	A	2267	C
2	A	2274	C
2	A	2276	G
2	A	2279	C
2	A	2280	G
2	A	2284	A
2	A	2285	G
2	A	2286	A
2	A	2299	C
2	A	2316	G
2	A	2320	C
2	A	2325	U
2	A	2328	G
2	A	2329	G
2	A	2330	U
2	A	2334	U
2	A	2335	G
2	A	2336	U

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Mol	Chain	Res	Type
2	A	2338	G
2	A	2339	G
2	A	2340	A
2	A	2341	U
2	A	2342	A
2	A	2343	G
2	A	2346	G
2	A	2349	A
2	A	2351	A
2	A	2354	G
2	A	2355	U
2	A	2356	G
2	A	2357	A
2	A	2368	C
2	A	2369	C
2	A	2371	G
2	A	2372	U
2	A	2382	G
2	A	2383	U
2	A	2384	C
2	A	2386	U
2	A	2387	U
2	A	2388	G
2	A	2390	U
2	A	2391	G
2	A	2392	A
2	A	2393	A
2	A	2394	A
2	A	2395	U
2	A	2396	A
2	A	2400	C
2	A	2401	U
2	A	2402	C
2	A	2407	C
2	A	2408	G
2	A	2409	U
2	A	2413	G
2	A	2418	U
2	A	2421	A
2	A	2427	G
2	A	2434	A
2	A	2436	A

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Mol	Chain	Res	Type
2	A	2447	G
2	A	2449	A
2	A	2462	G
2	A	2463	G
2	A	2467	U
2	A	2483	G
2	A	2492	A
2	A	2502	A
2	A	2504	G
2	A	2507	C
2	A	2508	C
2	A	2510	A
2	A	2511	A
2	A	2512	A
2	A	2529	A
2	A	2532	G
2	A	2536	U
2	A	2545	G
2	A	2549	G
2	A	2551	A
2	A	2558	C
2	A	2559	A
2	A	2567	U
2	A	2569	G
2	A	2571	C
2	A	2574	C
2	A	2581	G
2	A	2585	U
2	A	2596	G
2	A	2607	G
2	A	2609	A
2	A	2613	G
2	A	2626	U
2	A	2627	C
2	A	2630	A
2	A	2643	U
2	A	2644	C
2	A	2647	U
2	A	2649	A
2	A	2650	A
2	A	2653	G
2	A	2654	A

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Mol	Chain	Res	Type
2	A	2655	U
2	A	2659	A
2	A	2665	C
2	A	2671	G
2	A	2672	A
2	A	2673	U
2	A	2677	A
2	A	2688	C
2	A	2689	C
2	A	2693	A
2	A	2694	G
2	A	2698	C
2	A	2700	A
2	A	2702	A
2	A	2704	C
2	A	2705	G
2	A	2715	U
2	A	2726	G
2	A	2729	G
2	A	2742	A
2	A	2744	C
2	A	2749	G
2	A	2753	G
2	A	2759	G
2	A	2778	U
2	A	2786	U
2	A	2790	A
2	A	2791	G
2	A	2793	G
2	A	2796	A
2	A	2797	C
2	A	2802	G
2	A	2806	G
2	A	2810	U
2	A	2826	A
2	A	2827	G
2	A	2833	U
2	A	2837	U
2	A	2839	U
2	A	2853	C
2	A	2856	A
2	A	2865	G

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Mol	Chain	Res	Type
2	A	2870	C
2	A	2885	G
2	A	2887	G
2	A	2906	U
2	A	2912	A
2	A	2913	U
2	A	2915	C
2	A	2926	A
2	A	2936	C
2	A	2937	G
2	A	2938	G
2	A	2948	C
2	A	2950	C
2	A	2953	U
2	A	2957	A
2	A	2968	G
2	A	2972	A
2	A	2982	A
2	A	2985	G
2	A	2986	G
2	A	3002	A
2	A	3004	C
2	A	3005	A
2	A	3009	U
2	A	3011	C
2	A	3014	A
2	A	3015	C
2	A	3016	C
2	A	3020	U
2	A	3021	A
2	A	3022	G
2	A	3024	A
2	A	3027	G
2	A	3029	U
2	A	3042	A
2	A	3047	A
2	A	3056	A
2	A	3064	G
2	A	3082	U
2	A	3088	C
2	A	3093	A
2	A	3095	C

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Mol	Chain	Res	Type
2	A	3100	A
2	A	3101	C
2	A	3105	C
2	A	3106	C
2	A	3107	G
2	A	3112	A
2	A	3113	A
2	A	3114	A
2	A	3115	A
3	B	4	A
3	B	6	G
3	B	7	G
3	B	9	G
3	B	11	U
3	B	12	C
3	B	13	C
3	B	14	A
3	B	20	G
3	B	21	C
3	B	22	A
3	B	25	G
3	B	30	G
3	B	35	G
3	B	36	U
3	B	37	C
3	B	42	C
3	B	46	A
3	B	57	U
3	B	58	A
3	B	87	U
3	B	89	C
3	B	90	G
3	B	103	G
3	B	107	A
3	B	112	C
3	B	114	A
3	B	115	A
35	2	75	C
35	2	76	A

All (32) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	89	A
2	A	97	U
2	A	284	G
2	A	287	A
2	A	316	U
2	A	357	U
2	A	445	U
2	A	759	G
2	A	919	A
2	A	974	G
2	A	981	U
2	A	1004	C
2	A	1010	U
2	A	1046	C
2	A	1084	U
2	A	1186	G
2	A	1231	U
2	A	1344	A
2	A	1368	A
2	A	1713	U
2	A	1730	U
2	A	1947	U
2	A	2085	C
2	A	2088	C
2	A	2094	G
2	A	2350	G
2	A	2381	A
2	A	2407	C
2	A	2626	U
2	A	3113	A
3	B	3	U
3	B	10	G

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 413 ligands modelled in this entry, 412 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
38	PHE	2	1002	35	10,11,12	0.73	0	8,13,15	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	PHE	2	1002	35	-	0/5/6/8	0/1/1/1

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.

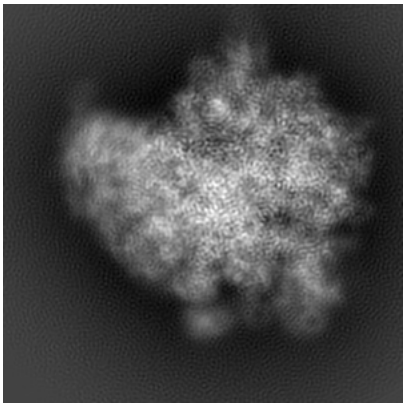
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3750. These allow visual inspection of the internal detail of the map and identification of artifacts.

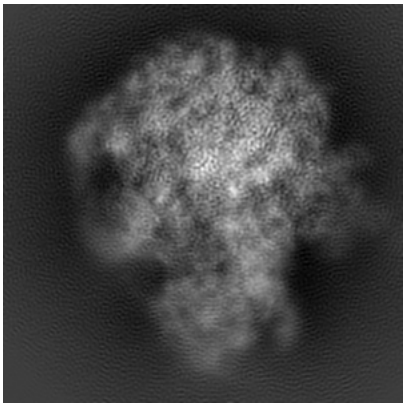
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

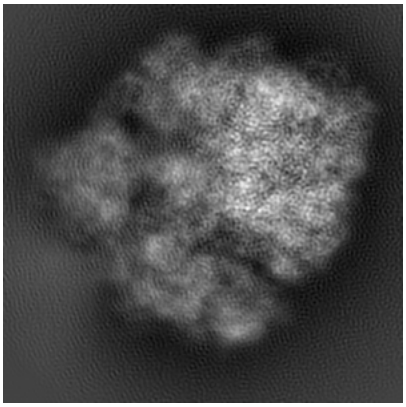
6.1.1 Primary map



X



Y

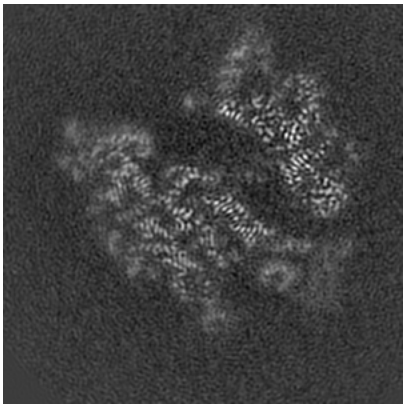


Z

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

6.2 Central slices

6.2.1 Primary map



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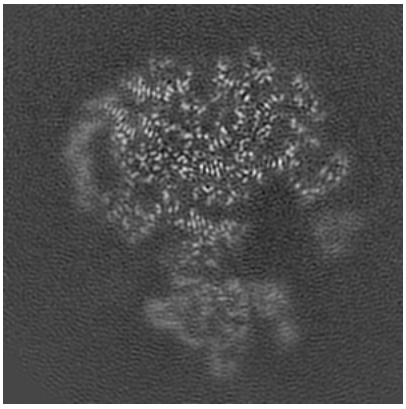
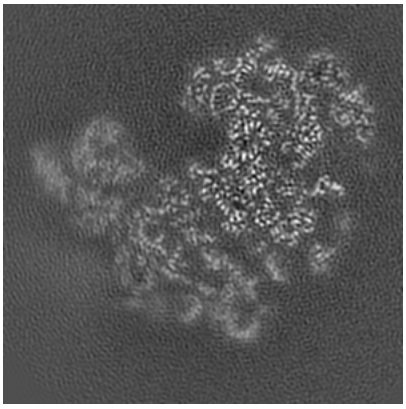


Y Index: 108

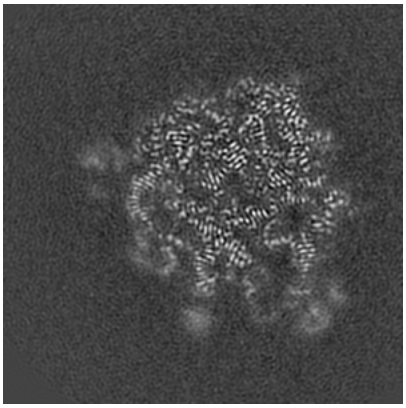


Z Index: 108

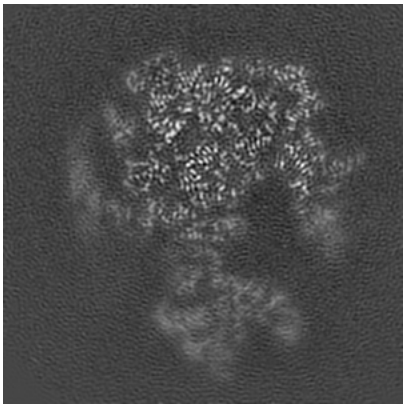
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

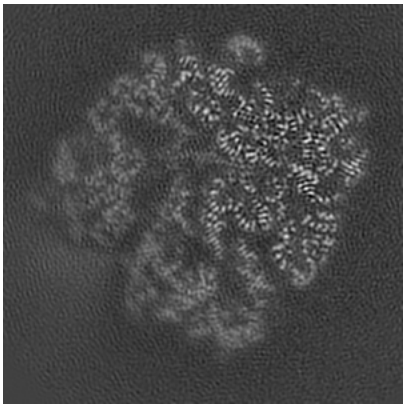
6.3.1 Primary map



X Index: 148



Y Index: 114

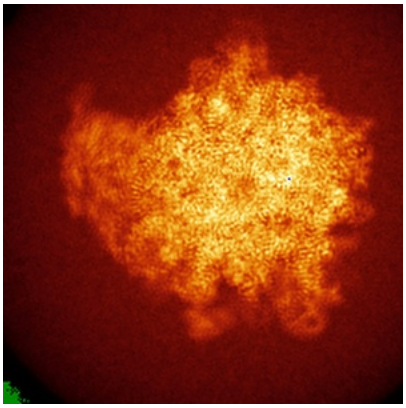


Z Index: 124

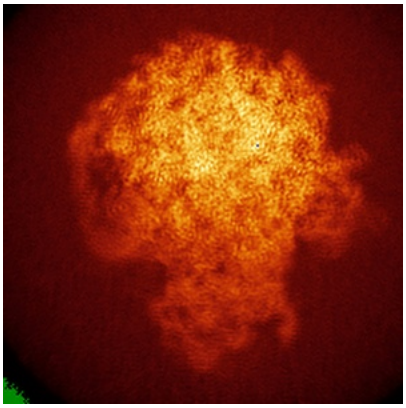
The images above show the largest variance slices of the map in three orthogonal directions.

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

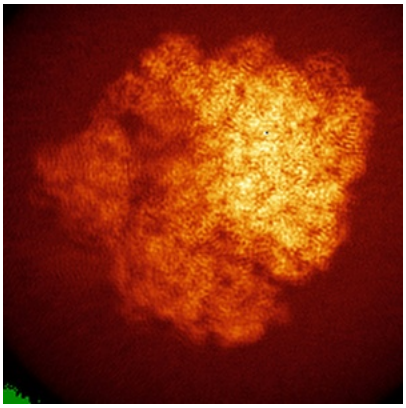
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

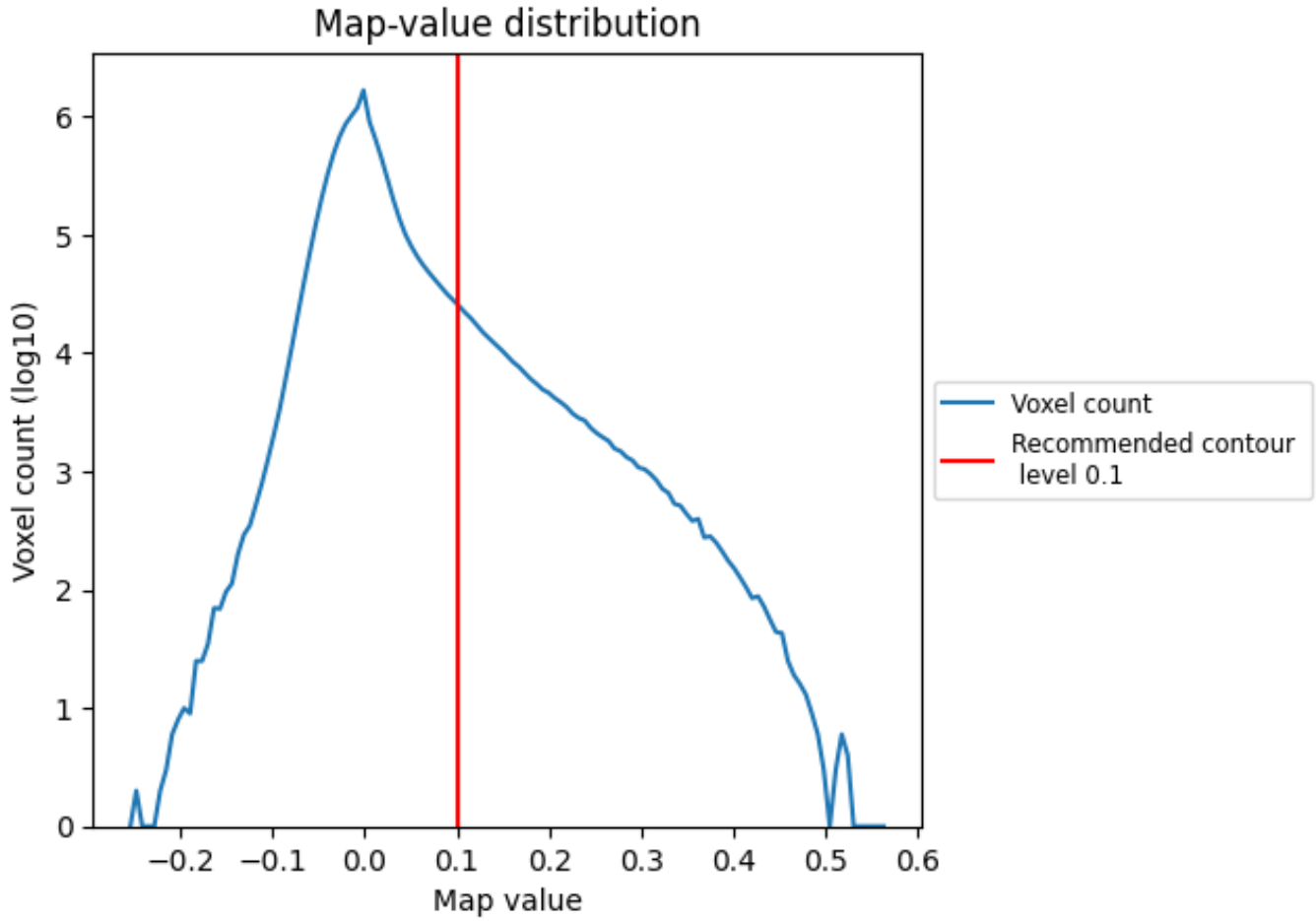
6.6 Mask visualisation (i)

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

7 Map analysis

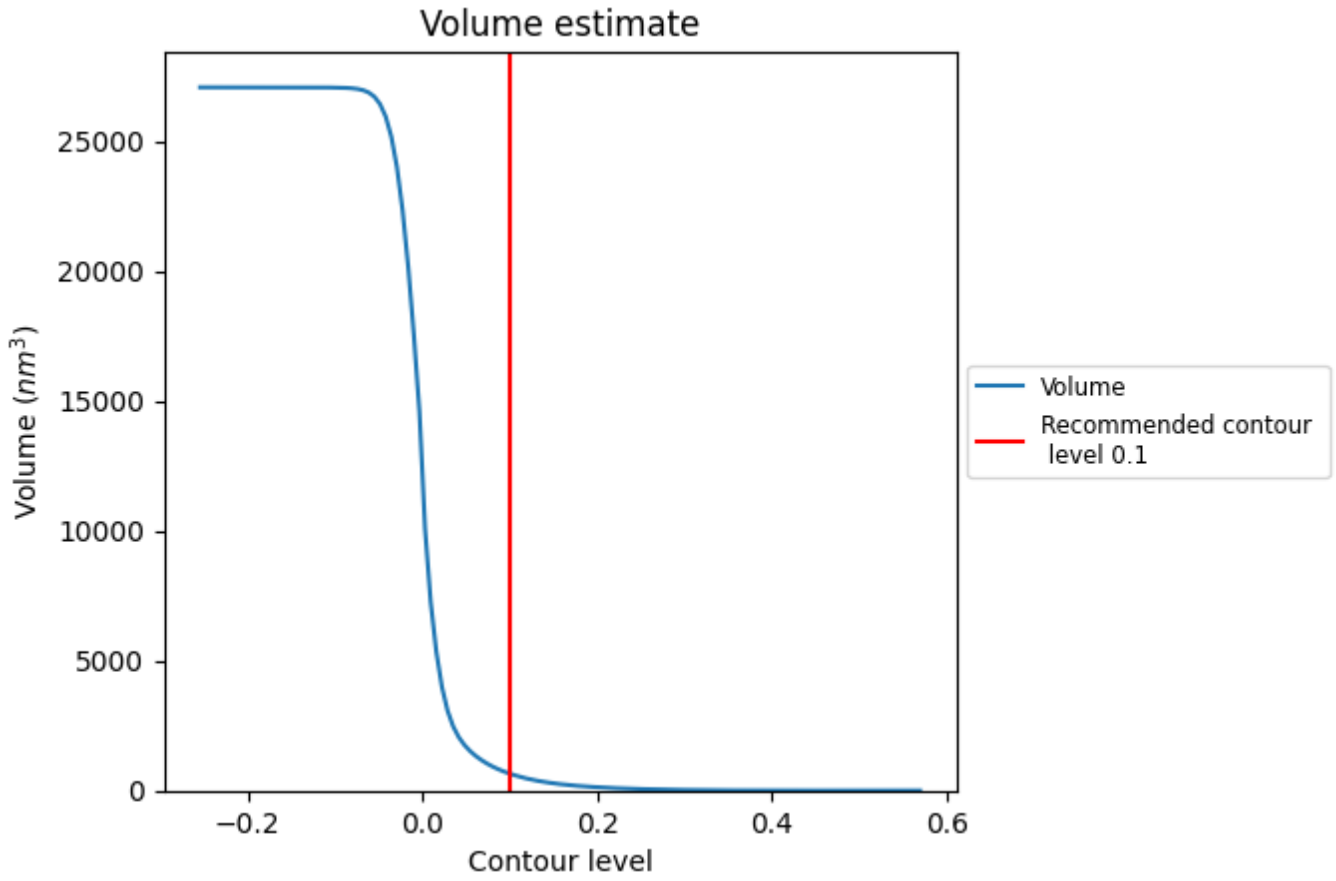
This section contains the results of statistical analysis of the map.

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.

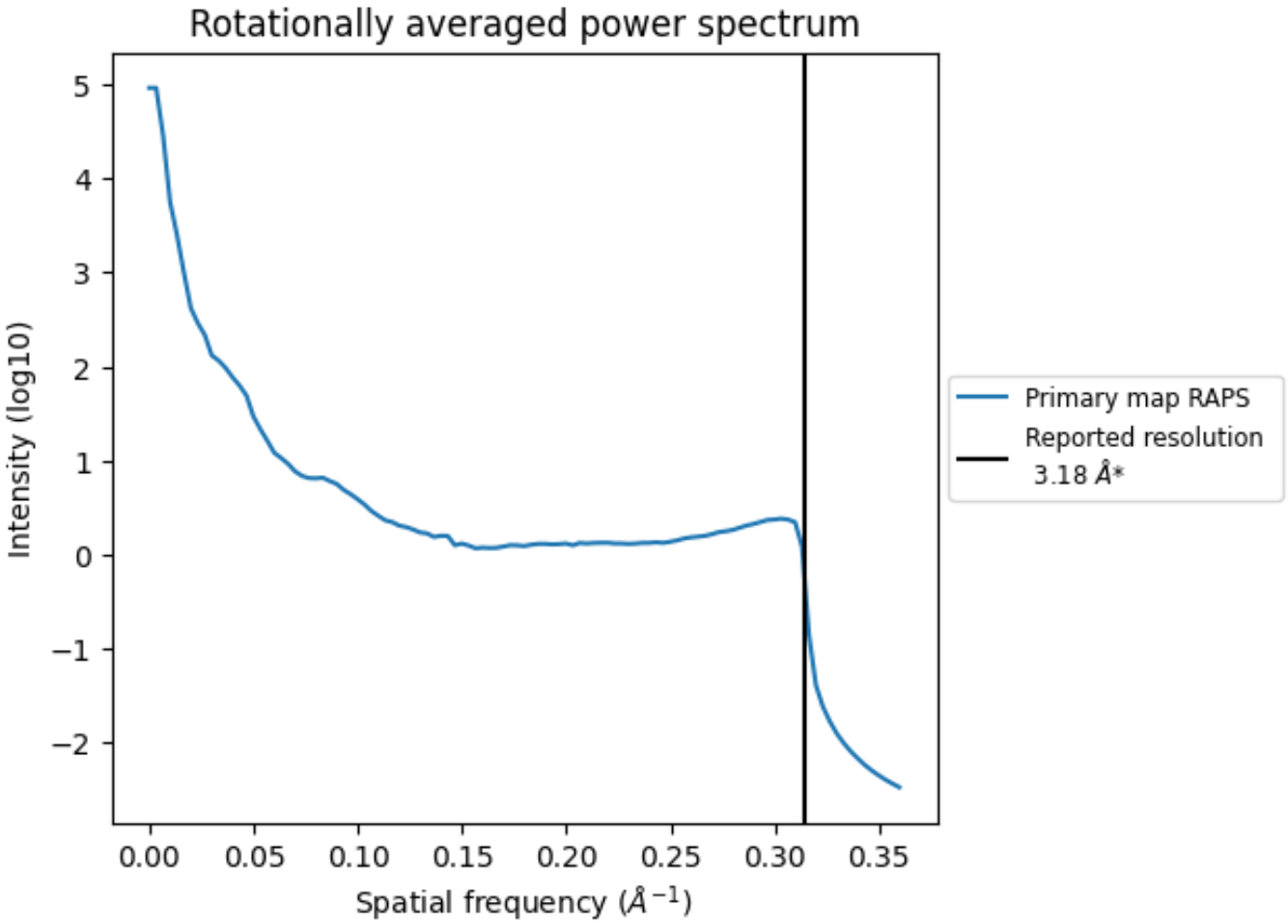
7.2 Volume estimate



The volume at the recommended contour level is 651 nm^3; this corresponds to an approximate mass of 588 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)

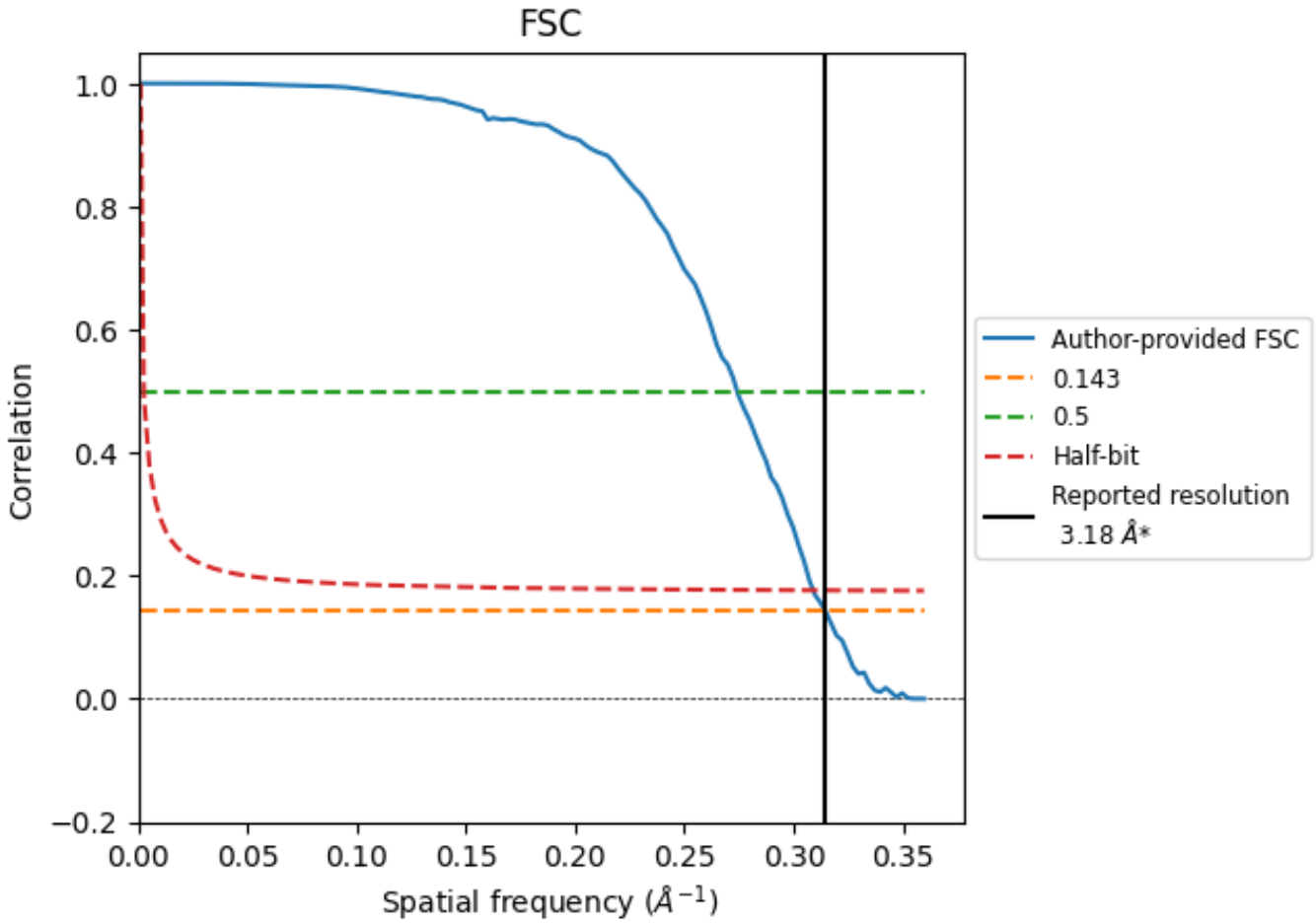


*Reported resolution corresponds to spatial frequency of 0.314 Å^{-1}

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 0.314 Å^{-1}

8.2 Resolution estimates (i)

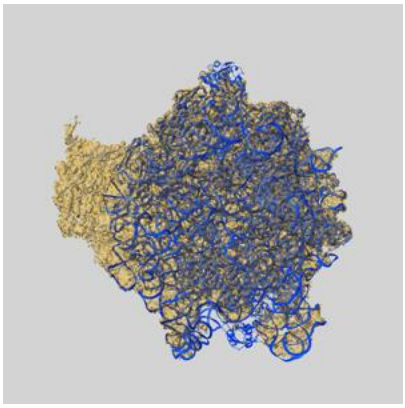
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	3.18	3.65	3.24
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

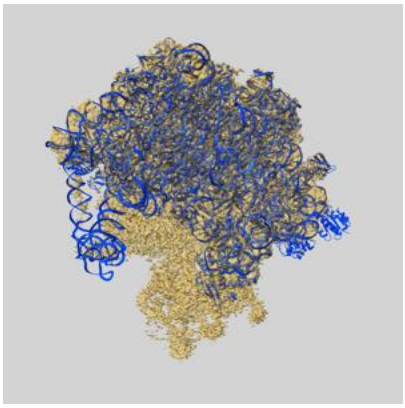
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3750 and PDB model 5O60. Per-residue inclusion information can be found in section 3 on page 12.

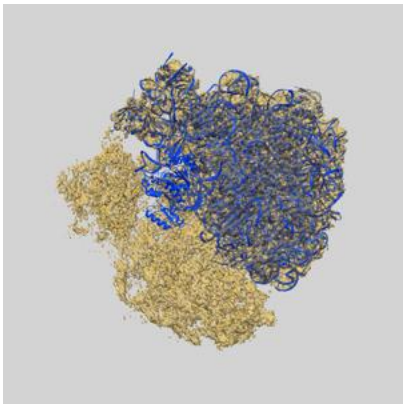
9.1 Map-model overlay



X



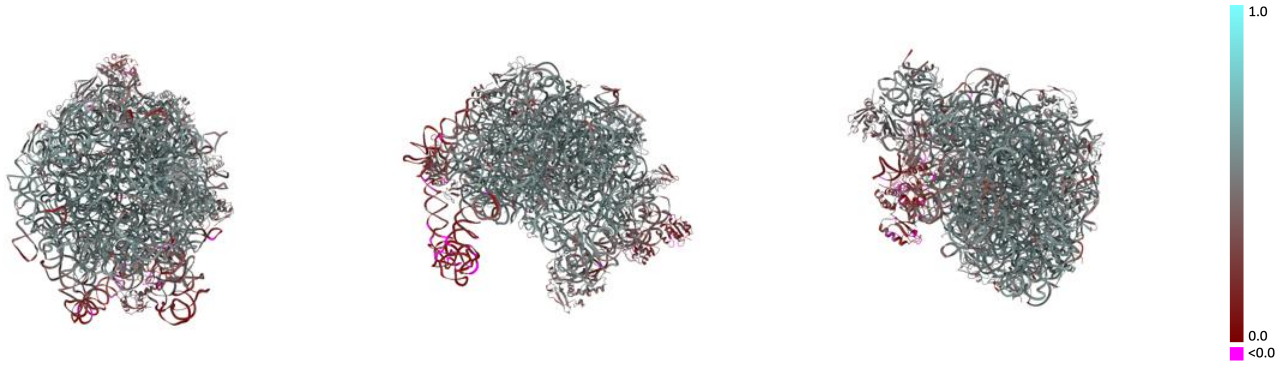
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

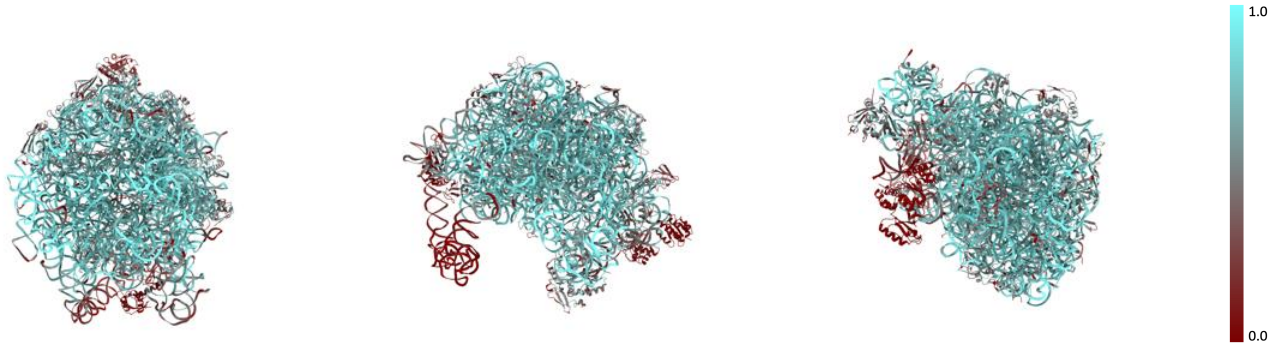
9.2 Q-score mapped to coordinate model (i)



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.

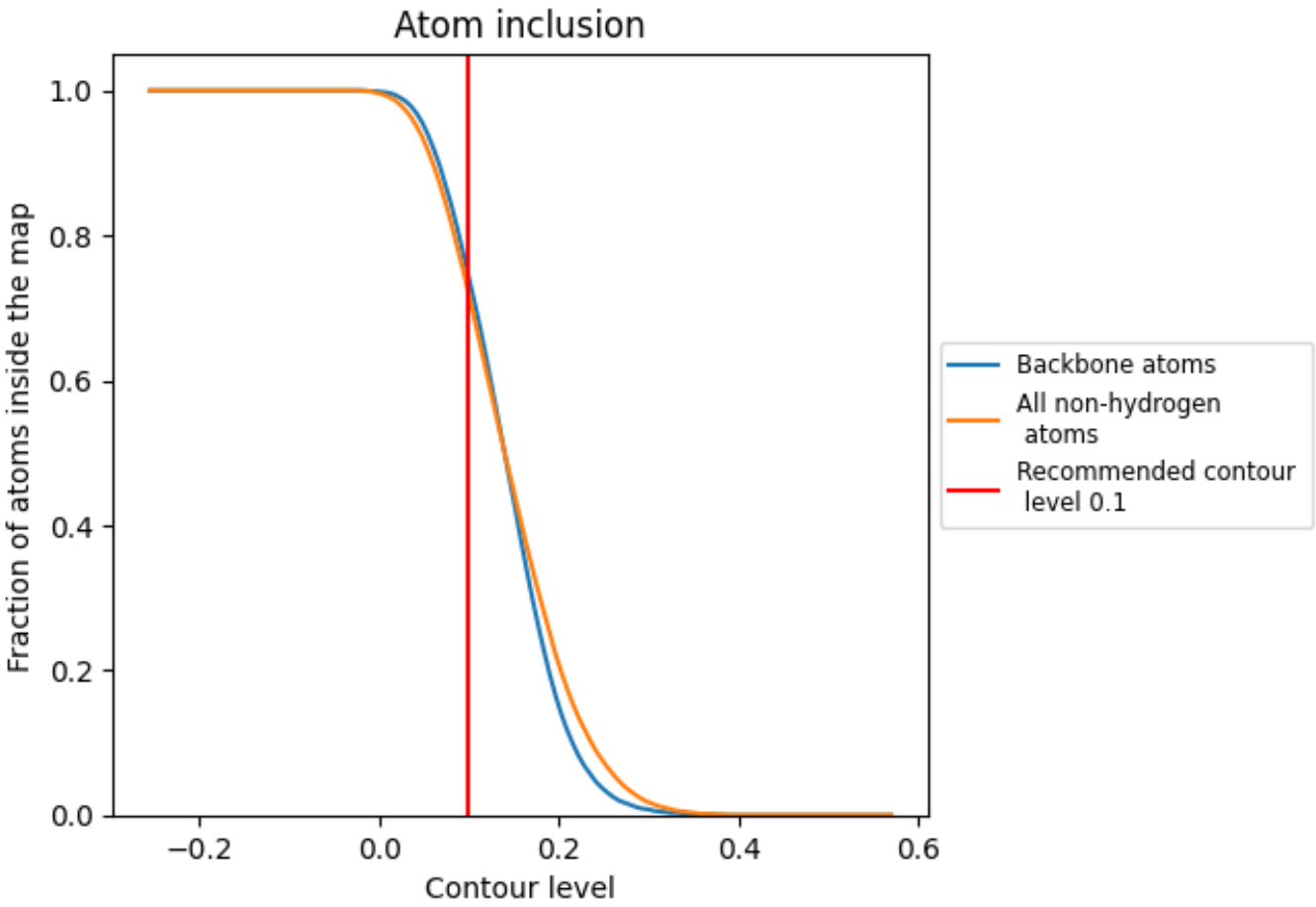
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 72% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7190	0.4870
2	0.3920	0.4480
3	0.6930	0.5360
A	0.7890	0.4960
B	0.8300	0.5010
C	0.6480	0.5250
D	0.6770	0.5280
E	0.6040	0.4950
F	0.4790	0.4130
G	0.4440	0.4210
H	0.1030	0.3400
I	0.0170	0.1790
J	0.0330	0.1890
K	0.6430	0.5110
L	0.5560	0.4970
M	0.6140	0.4920
N	0.6110	0.5130
O	0.7020	0.5290
P	0.6090	0.4780
Q	0.5620	0.4740
R	0.7060	0.5300
S	0.6040	0.5160
T	0.6270	0.5110
U	0.5460	0.4750
V	0.4850	0.4470
W	0.4050	0.4260
X	0.6960	0.5410
Y	0.6450	0.5160
Z	0.5780	0.4500
a	0.6600	0.5110
b	0.6140	0.5060
c	0.6360	0.4970
d	0.6930	0.5490
e	0.6750	0.5310
f	0.7050	0.5250
g	0.4320	0.4090