



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 02:48 am BST

PDB ID : 9TVU / pdb_00009tvu
EMDB ID : EMD-56352
Title : Structure of the Chlamydomonas reinhardtii chlororibosome
Authors : Waltz, F.; Kater, L.; Engel, B.D.
Deposited on : 2026-01-13
Resolution : 2.52 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

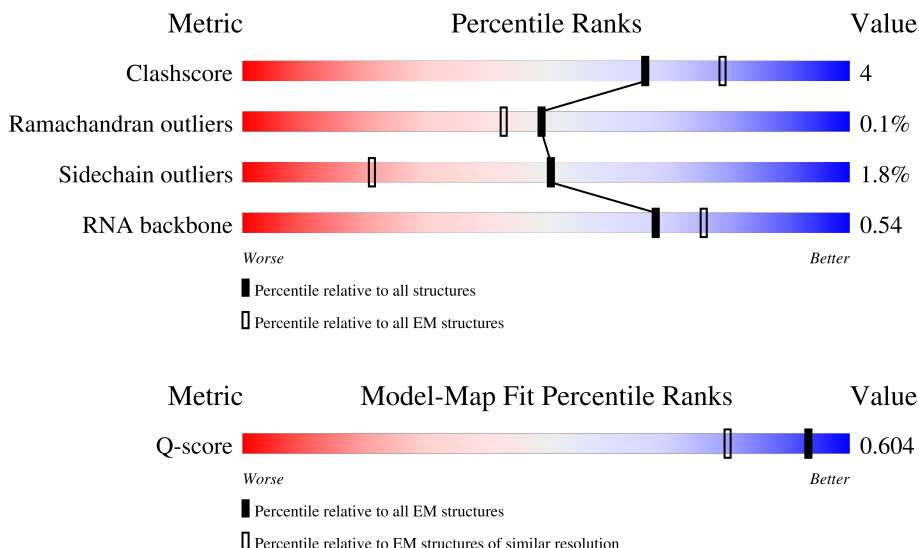
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

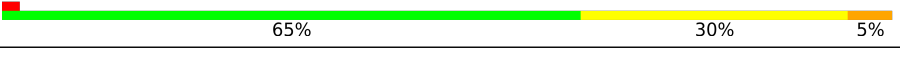
The reported resolution of this entry is 2.52 Å.

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.



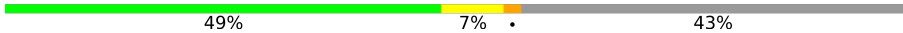
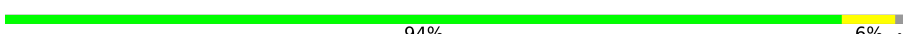
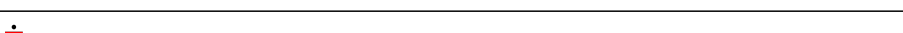
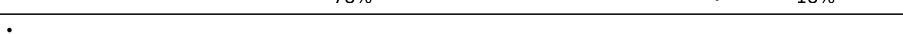
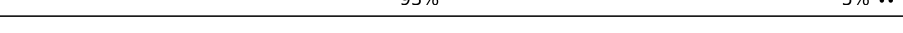
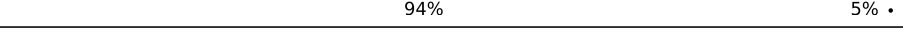
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7226 (2.02 - 3.02)

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

Mol	Chain	Length	Quality of chain
1	0	66	
2	3	121	
3	5	47	

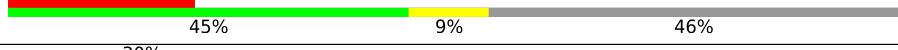
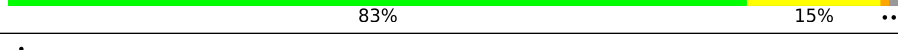
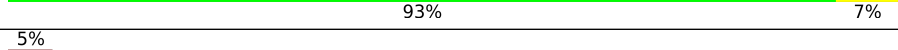
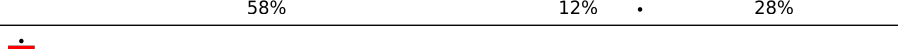
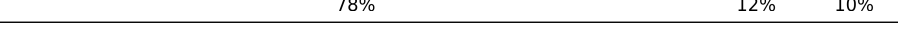
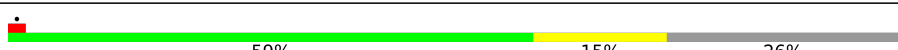
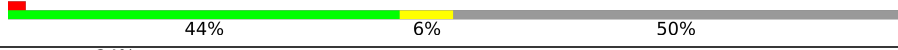
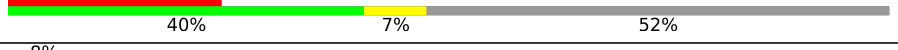
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Mol	Chain	Length	Quality of chain
4	6	101	
5	7	124	
6	8	114	
7	9	37	
8	B	278	
9	C	259	
10	D	243	
11	E	179	
12	F	207	
13	G	200	
14	H	235	
15	I	176	
16	J	225	
17	K	122	
18	L	241	
19	M	136	
20	N	173	
21	O	145	
22	P	153	
23	Q	112	
24	R	179	
25	S	175	
26	T	111	
27	U	170	
28	V	161	

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Mol	Chain	Length	Quality of chain
29	W	195	
30	X	134	
31	Z	98	
32	a	436	
33	d	257	
34	f	171	
35	g	168	
36	h	141	
37	j	169	
38	k	130	
39	l	133	
40	m	164	
41	n	100	
42	o	141	
43	p	128	
44	q	105	
45	r	137	
46	s	92	
47	t	166	
48	u	184	
49	v	298	
50	x	120	
51	Y	136	
52	w	560	
53	1	2375	

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Mol	Chain	Length	Quality of chain
54	4	272	81%17%
55	2	1470	76%22%
56	b	910	8% 63%12%25%
57	c	712	10% 72%13%15%
58	e	673	16% 68%12%20%
59	i	191	20% 68%11%20%

2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 158406 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 cL38/PSRP6.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	47	Total	C	N	O	0	0
			369	233	76	60		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	121	Total	C	N	O	P	0	0
			2571	1148	449	853	121		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	47	Total	C	N	O	P	0	0
			1006	450	185	324	47		

- Molecule 4 is a protein called bL33c.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	58	Total	C	N	O	S	0	0
			473	293	91	86	3		

- Molecule 5 is a protein called bL34c.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	60	Total	C	N	O	S	0	0
			455	271	104	77	3		

- Molecule 6 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	68	Total	C	N	O	S	0	0
			520	322	104	91	3		

- Molecule 7 is a protein called Large ribosomal subunit protein bL36c.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	37	Total	C	N	O	S	0	0
			292	177	63	46	6		

- Molecule 8 is a protein called Large ribosomal subunit protein uL2c.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	276	Total	C	N	O	S	0	0
			2159	1347	431	377	4		

- Molecule 9 is a protein called Large ribosomal subunit protein uL3c.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	223	Total	C	N	O	S	0	0
			1681	1057	310	305	9		

- Molecule 10 is a protein called Large ribosomal subunit protein uL4c.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	216	Total	C	N	O	S	0	0
			1599	997	290	306	6		

- Molecule 11 is a protein called Large ribosomal subunit protein uL5c.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	178	Total	C	N	O	S	0	0
			1413	900	247	260	6		

- Molecule 12 is a protein called Plastid ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	177	Total	C	N	O	S	0	0
			1338	845	245	244	4		

- Molecule 13 is a protein called Large ribosomal subunit protein bL9c.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	54	Total	C	N	O	S	0	0
			418	272	72	73	1		

- Molecule 14 is a protein called uL10c.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	141	Total	C	N	O	S	0	0
			1114	711	189	209	5		

- Molecule 15 is a protein called Large ribosomal subunit protein uL11c.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	132	Total	C	N	O	S	0	0
			980	623	171	181	5		

- Molecule 16 is a protein called uL13c.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	173	Total	C	N	O	S	0	0
			1346	857	243	243	3		

- Molecule 17 is a protein called Large ribosomal subunit protein uL14c.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	122	Total	C	N	O	S	0	0
			942	588	180	169	5		

- Molecule 18 is a protein called uL15c.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	198	Total	C	N	O	S	0	0
			1484	921	282	276	5		

- Molecule 19 is a protein called Large ribosomal subunit protein uL16c.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	135	Total	C	N	O	S	0	0
			1080	689	211	173	7		

- Molecule 20 is a protein called Large ribosomal subunit protein bL17c.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	117	Total	C	N	O	S	0	0
			937	585	185	162	5		

- Molecule 21 is a protein called Large ribosomal subunit protein uL18c.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	118	Total	C	N	O	S	0	0
			902	557	173	168	4		

- Molecule 22 is a protein called bL19c.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	130	Total	C	N	O	S	0	0
			995	620	199	174	2		

- Molecule 23 is a protein called Large ribosomal subunit protein bL20c.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	111	Total	C	N	O	S	0	0
			943	592	193	152	6		

- Molecule 24 is a protein called bL21c.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	115	Total	C	N	O	S	0	0
			907	585	161	157	4		

- Molecule 25 is a protein called Large ribosomal subunit protein uL22c.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	115	Total	C	N	O	S	0	0
			903	564	174	157	8		

- Molecule 26 is a protein called Large ribosomal subunit protein uL23c.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	107	Total	C	N	O	S	0	0
			837	542	148	146	1		

- Molecule 27 is a protein called KOW domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	132	Total	C	N	O	S	0	0
			1020	650	189	178	3		

- Molecule 28 is a protein called bL27c.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	114	Total	C	N	O	S	0	0
			869	535	172	159	3		

- Molecule 29 is a protein called Large ribosomal subunit protein bL28c.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	138	Total	C	N	O	S	0	0
			1104	700	205	193	6		

- Molecule 30 is a protein called uL29c.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	106	Total	C	N	O	S	0	0
			843	518	169	153	3		

- Molecule 31 is a protein called bL32c.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Z	41	Total	C	N	O	0	0
			323	213	57	53		

- Molecule 32 is a protein called Ribosomal protein S1 homologue.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	236	Total	C	N	O	S	0	0
			1868	1175	285	395	13		

- Molecule 33 is a protein called Small ribosomal subunit protein uS4c.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	256	Total	C	N	O	S	0	0
			2107	1356	403	341	7		

- Molecule 34 is a protein called bS6c.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	103	Total	C	N	O	S	0	0
			850	543	148	156	3		

- Molecule 35 is a protein called Small ribosomal subunit protein uS7c.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	167	Total	C	N	O	S	0	0
			1334	846	253	229	6		

- Molecule 36 is a protein called Small ribosomal subunit protein uS8c.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	141	Total	C	N	O	S	0	0
			1113	698	206	203	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	122	Total	C	N	O	S	0	0
			957	597	173	178	9		

- Molecule 38 is a protein called Small ribosomal subunit protein uS11c.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	117	Total	C	N	O	S	0	0
			894	560	179	151	4		

- Molecule 39 is a protein called Small ribosomal subunit protein uS12c.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	l	121	Total	C	N	O	S	0	0
			941	591	190	157	3		

- Molecule 40 is a protein called uS13c.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	m	114	Total	C	N	O	S	0	0
			924	569	181	172	2		

- Molecule 41 is a protein called Small ribosomal subunit protein uS14c.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	n	99	Total	C	N	O	S	0	0
			814	513	163	132	6		

- Molecule 42 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o	101	Total	C	N	O	S	0	0
			813	502	156	151	4		

- Molecule 43 is a protein called 30S ribosomal protein S16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	p	80	Total	C	N	O	S	0	0
			666	433	120	112	1		

- Molecule 44 is a protein called Small ribosomal subunit protein uS17c.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	78	Total	C	N	O	S	0	0
			621	386	117	116	2		

- Molecule 45 is a protein called Small ribosomal subunit protein bS18c.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	81	Total	C	N	O	S	0	0
			664	434	123	106	1		

- Molecule 46 is a protein called Small ribosomal subunit protein uS19c.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	81	Total	C	N	O	S	0	0
			645	414	122	106	3		

- Molecule 47 is a protein called bS20c.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	t	119	Total	C	N	O	S	0	0
			935	592	172	167	4		

- Molecule 48 is a protein called bS21c.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	u	92	Total	C	N	O	S	0	0
			789	494	144	147	4		

- Molecule 49 is a protein called 30S ribosomal protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	v	181	Total	C	N	O	S	0	0
			1430	907	245	276	2		

- Molecule 50 is a protein called cS26/PSRP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	x	60	Total	C	N	O	S	0	0
			462	299	80	81	2		

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Y	65	Total	C	N	O	S	0	0
			521	331	90	98	2		

- Molecule 52 is a protein called Plastid-specific ribosomal protein-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	w	365	Total	C	N	O	S	0	0
			2786	1749	429	598	10		

- Molecule 53 is a RNA chain called 23S.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1	2375	Total	C	N	O	P	0	0
			50934	22751	9345	16463	2375		

- Molecule 54 is a RNA chain called 7S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	272	Total	C	N	O	P	0	0
			5856	2616	1106	1862	272		

- Molecule 55 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	2	1470	Total	C	N	O	P	0	0
			31537	14077	5779	10211	1470		

- Molecule 56 is a protein called Small ribosomal subunit protein uS2c.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	b	685	Total	C	N	O	S	0	0
			5545	3581	1010	934	20		

- Molecule 57 is a protein called Small ribosomal subunit protein uS3c.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	c	607	Total	C	N	O	S	0	0
			4939	3179	905	844	11		

- Molecule 58 is a protein called uS5c.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	e	536	Total	C	N	O	S	0	0
			3988	2477	658	838	15		

- Molecule 59 is a protein called Small ribosomal subunit protein uS9c.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	i	153	Total	C	N	O	S	0	0
			1189	750	219	217	3		

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	3	5	Total	Mg	0
			5	5	
60	5	4	Total	Mg	0
			4	4	
60	7	1	Total	Mg	0
			1	1	
60	L	1	Total	Mg	0
			1	1	
60	1	206	Total	Mg	0
			206	206	
60	4	7	Total	Mg	0
			7	7	
60	2	99	Total	Mg	0
			99	99	

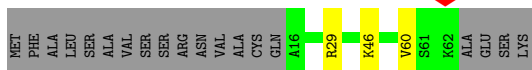
- Molecule 61 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
61	U	1	Total 1	K 1	0
61	1	86	Total 86	K 86	0
61	4	4	Total 4	K 4	0
61	2	47	Total 47	K 47	0

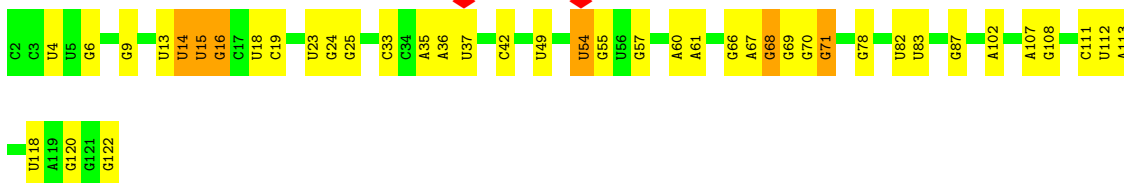
3 Residue-property plots [i](#)

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

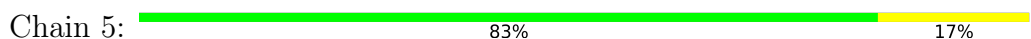
- Molecule 1: cL38/PSRP6



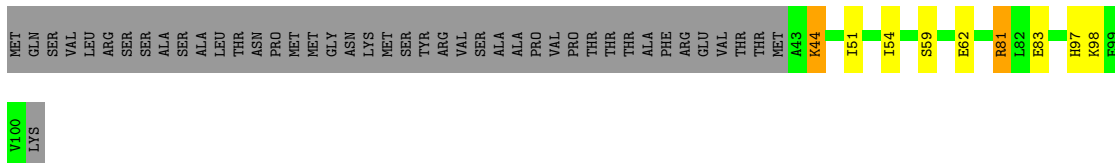
- Molecule 2: 5S rRNA



- Molecule 3: 3S rRNA

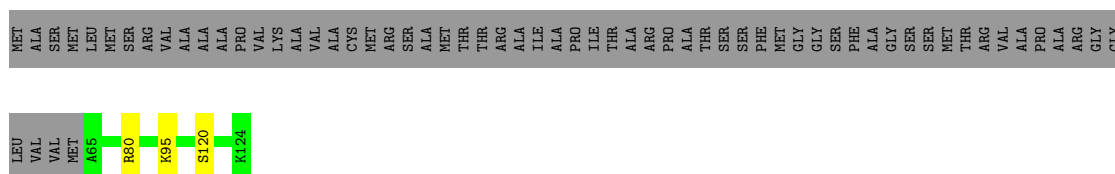


- Molecule 4: bL33c

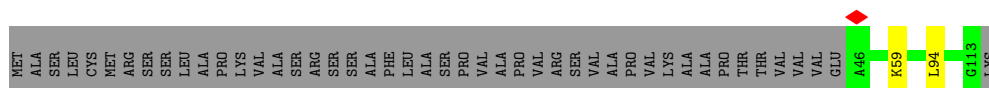


- Molecule 5: bL34c

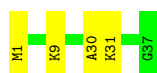
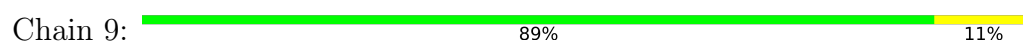




- Molecule 6: 50S ribosomal protein L35



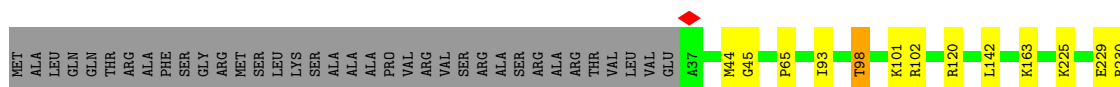
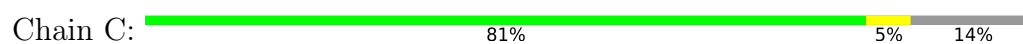
- Molecule 7: Large ribosomal subunit protein bL36c



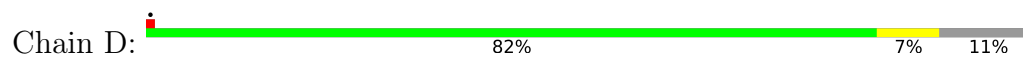
- Molecule 8: Large ribosomal subunit protein uL2c



- Molecule 9: Large ribosomal subunit protein uL3c

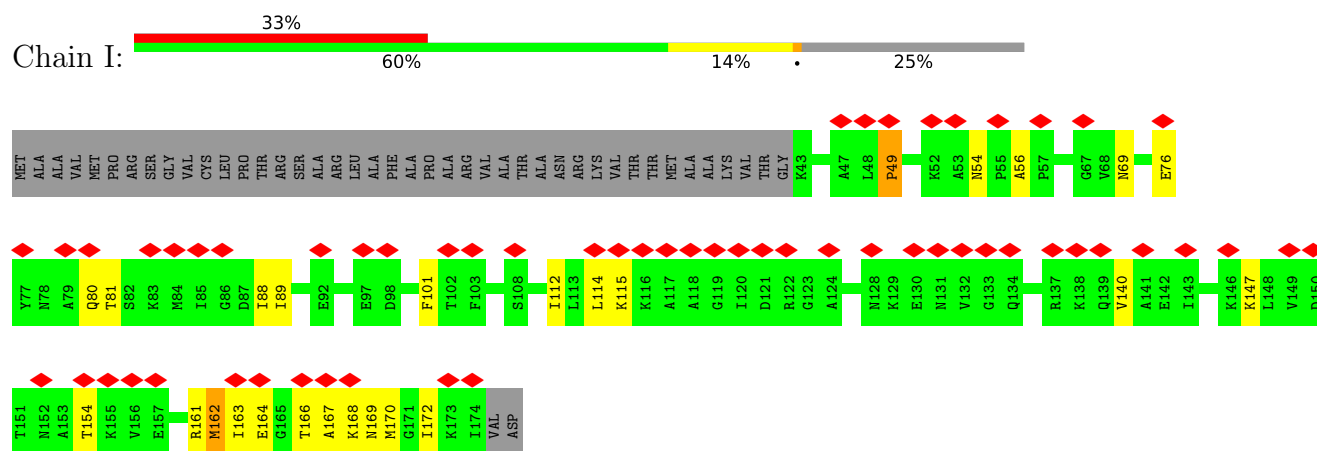


- Molecule 10: Large ribosomal subunit protein uL4c

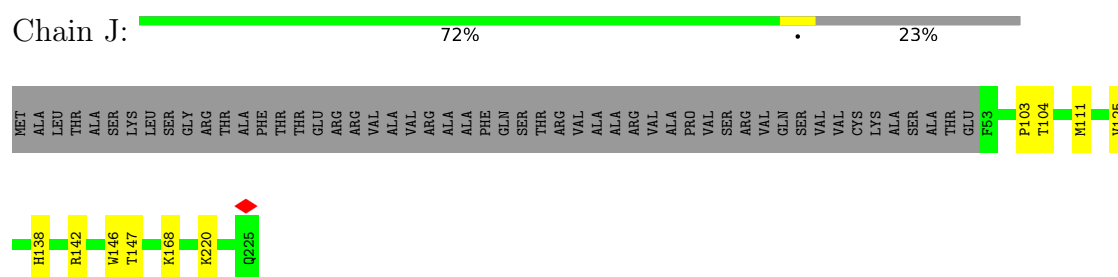


- Molecule 11: Large ribosomal subunit protein uL5c

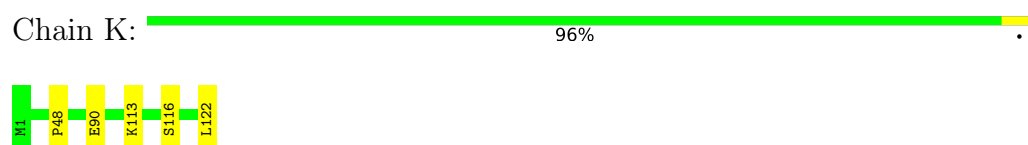
• Molecule 15: Large ribosomal subunit protein uL11c



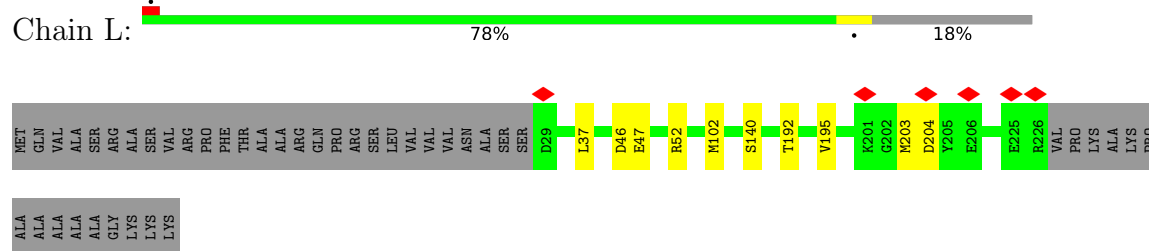
• Molecule 16: uL13c



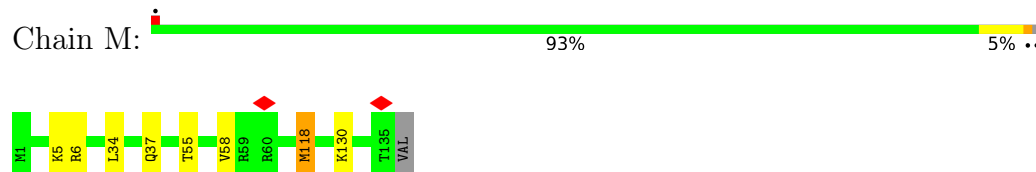
• Molecule 17: Large ribosomal subunit protein uL14c

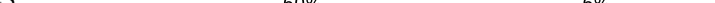


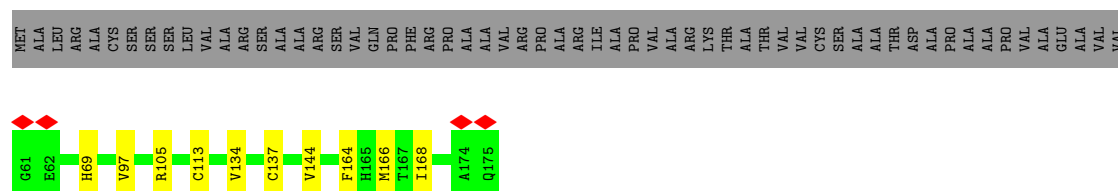
• Molecule 18: uL15c



• Molecule 19: Large ribosomal subunit protein uL16c



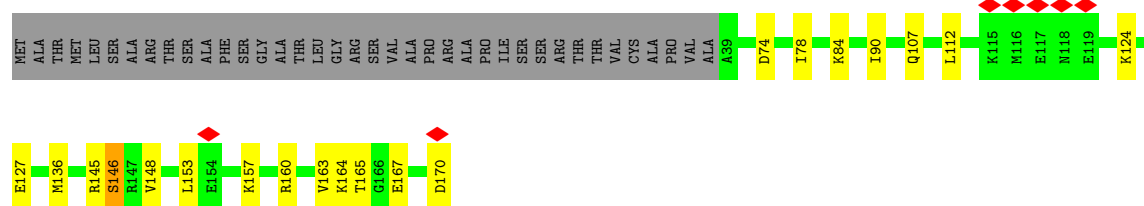
- Chain S: 



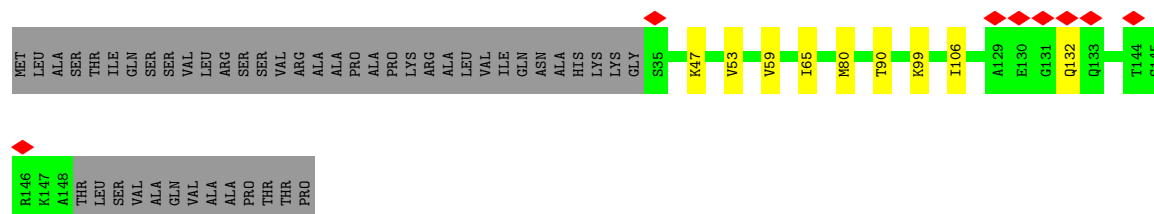
- Molecule 26: Large ribosomal subunit protein uL23c



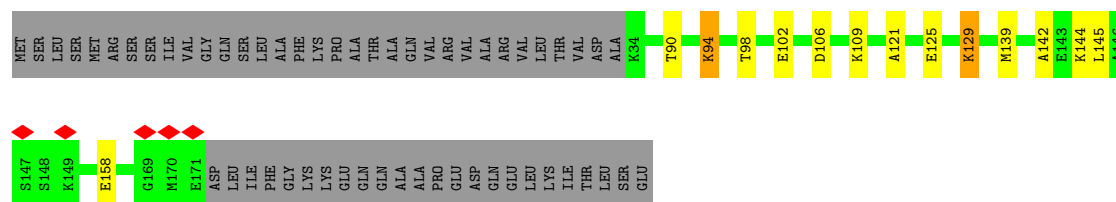
- Molecule 27: KOW domain-containing protein



- Molecule 28: bL27c



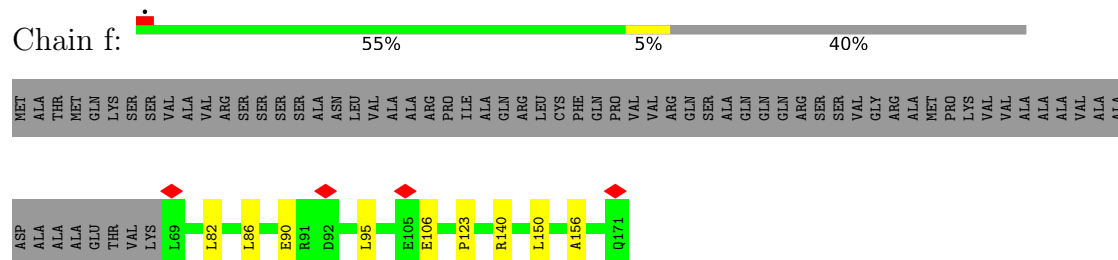
- Molecule 29: Large ribosomal subunit protein bL28c



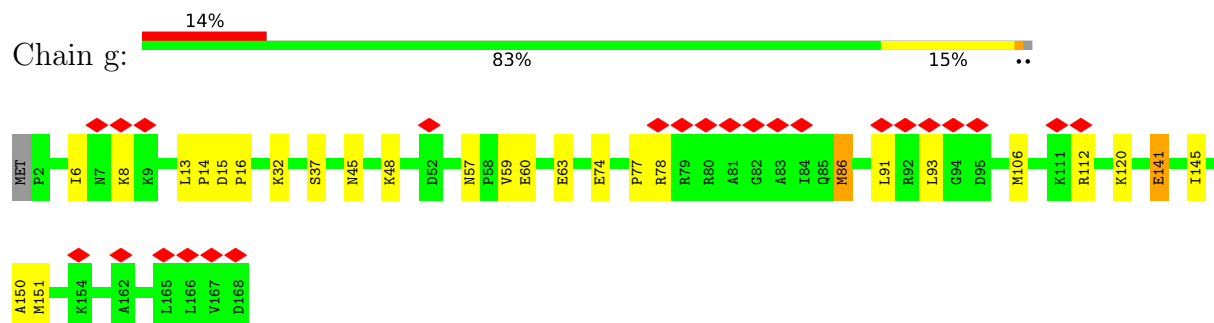
- Molecule 30: uL29c



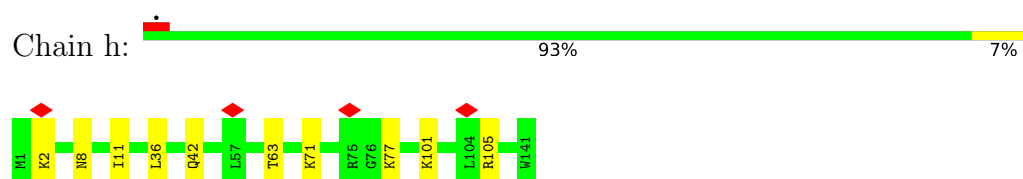
- Molecule 34: bS6c



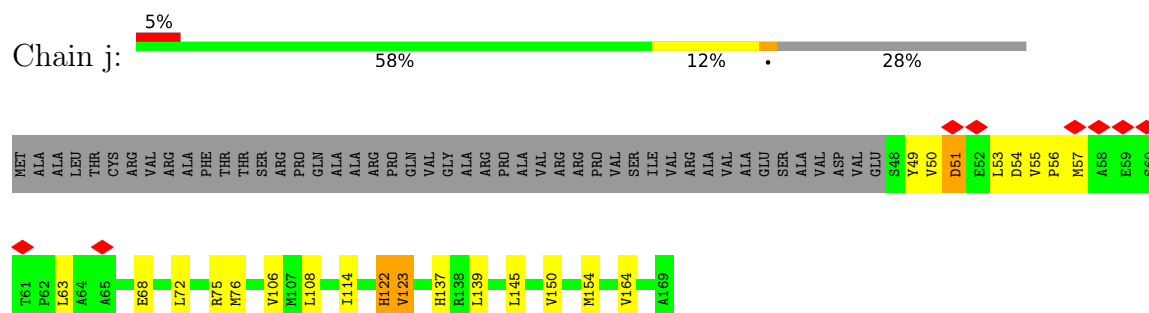
- Molecule 35: Small ribosomal subunit protein uS7c



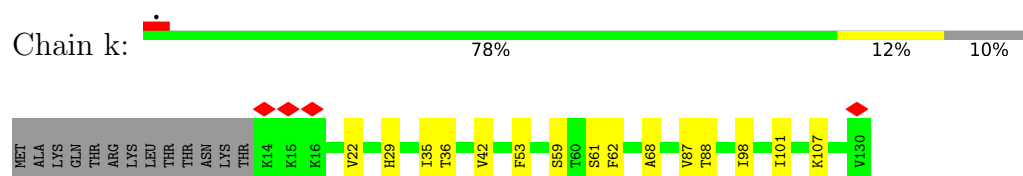
- Molecule 36: Small ribosomal subunit protein uS8c



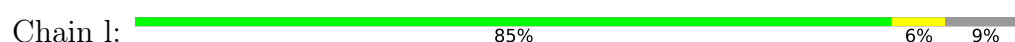
- Molecule 37: Small ribosomal subunit protein uS10 domain-containing protein



- Molecule 38: Small ribosomal subunit protein uS11c

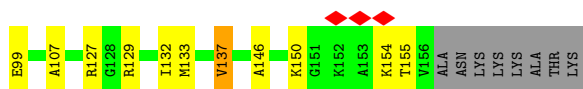
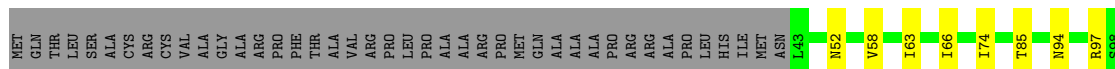


- Molecule 39: Small ribosomal subunit protein uS12c

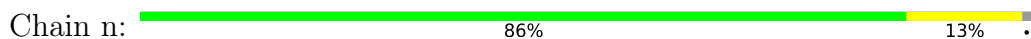




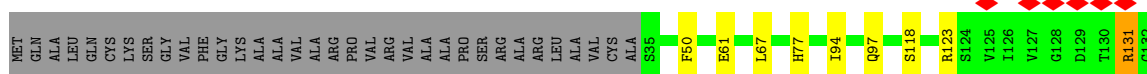
- Molecule 40: uS13c



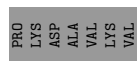
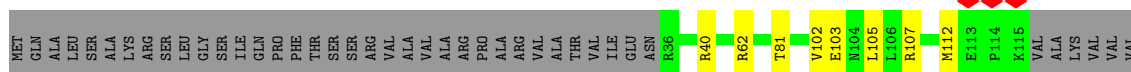
- Molecule 41: Small ribosomal subunit protein uS14c



- Molecule 42: 30S ribosomal protein S15



- Molecule 43: 30S ribosomal protein S16, chloroplastic

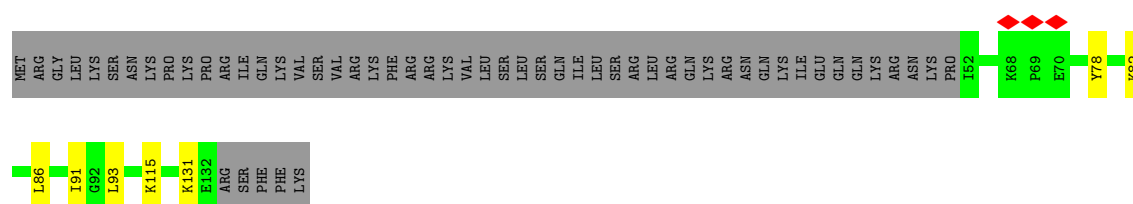


- Molecule 44: Small ribosomal subunit protein uS17c



- Molecule 45: Small ribosomal subunit protein bS18c

Chain r: 



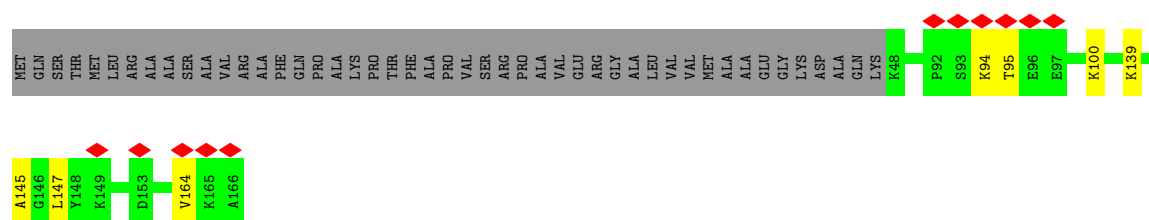
- Molecule 46: Small ribosomal subunit protein uS19c

Chain s: 



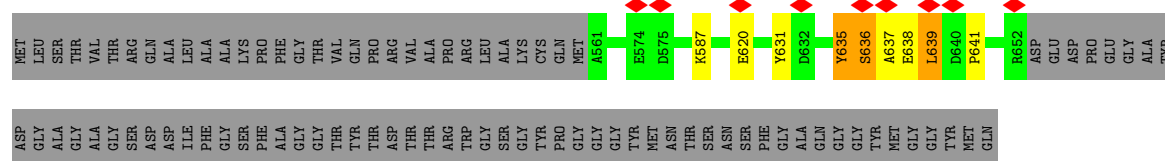
- Molecule 47: bS20c

Chain t: 

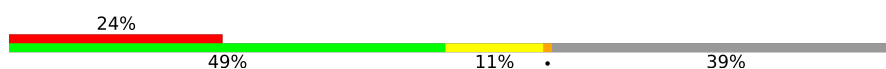


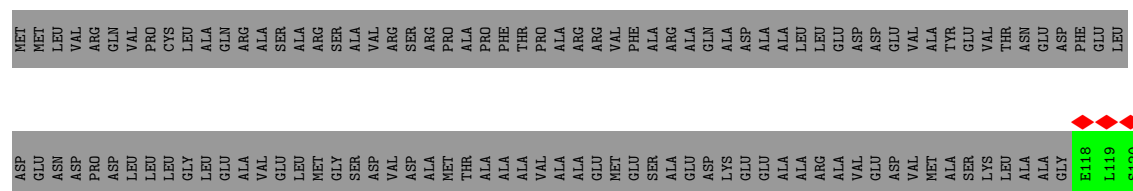
- Molecule 48: bS21c

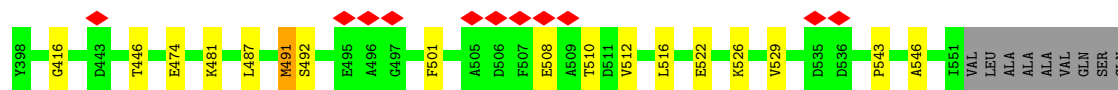
Chain u: 



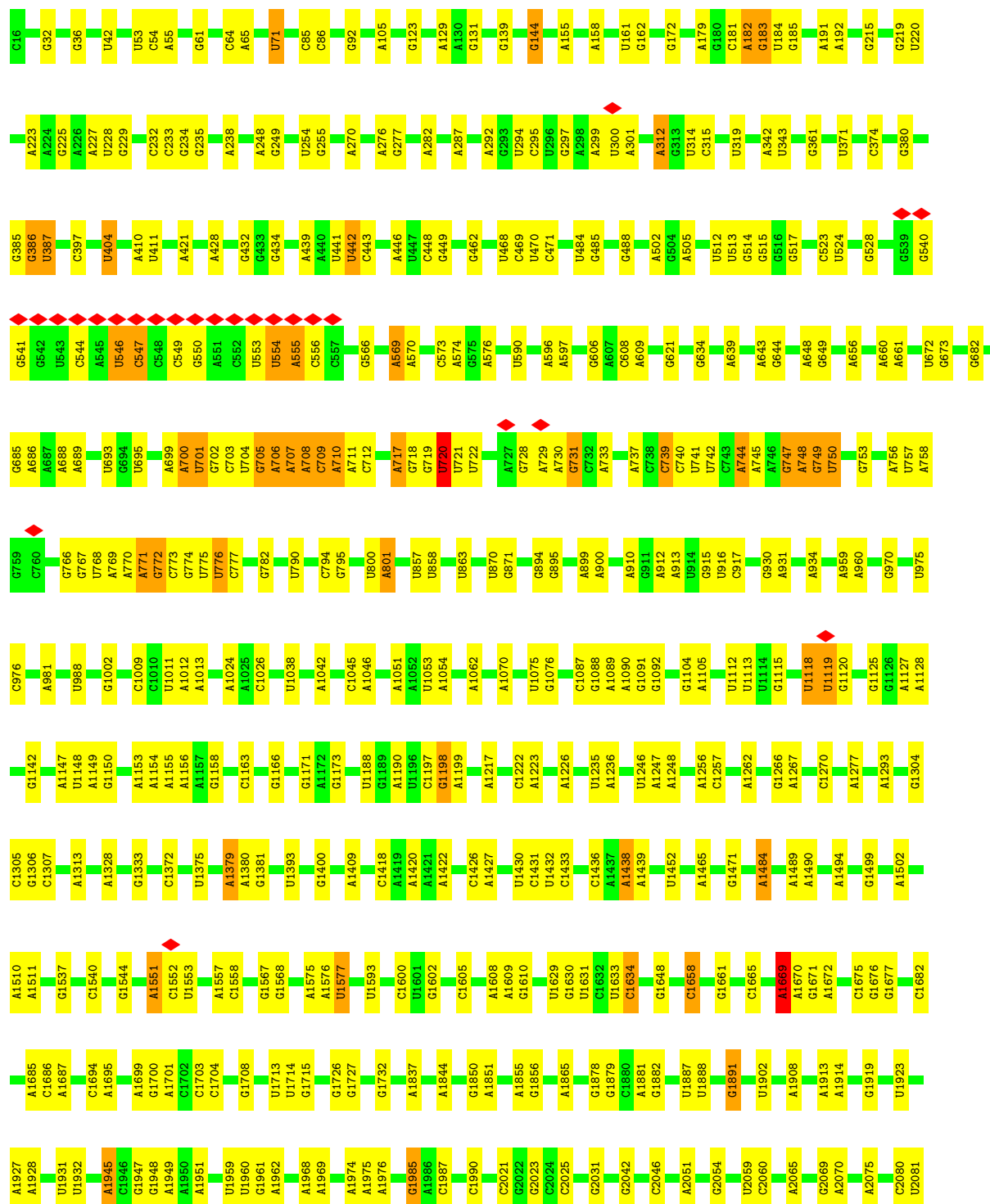
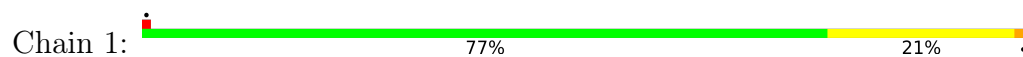
- Molecule 49: 30S ribosomal protein 3, chloroplastic

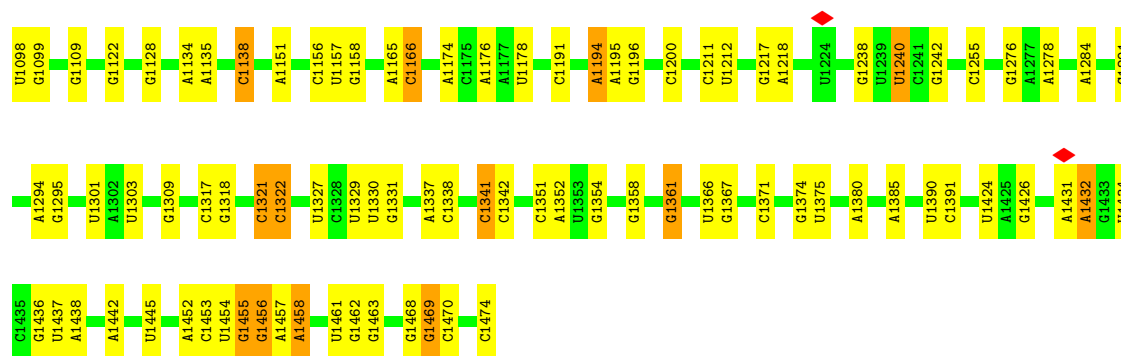
Chain v: 



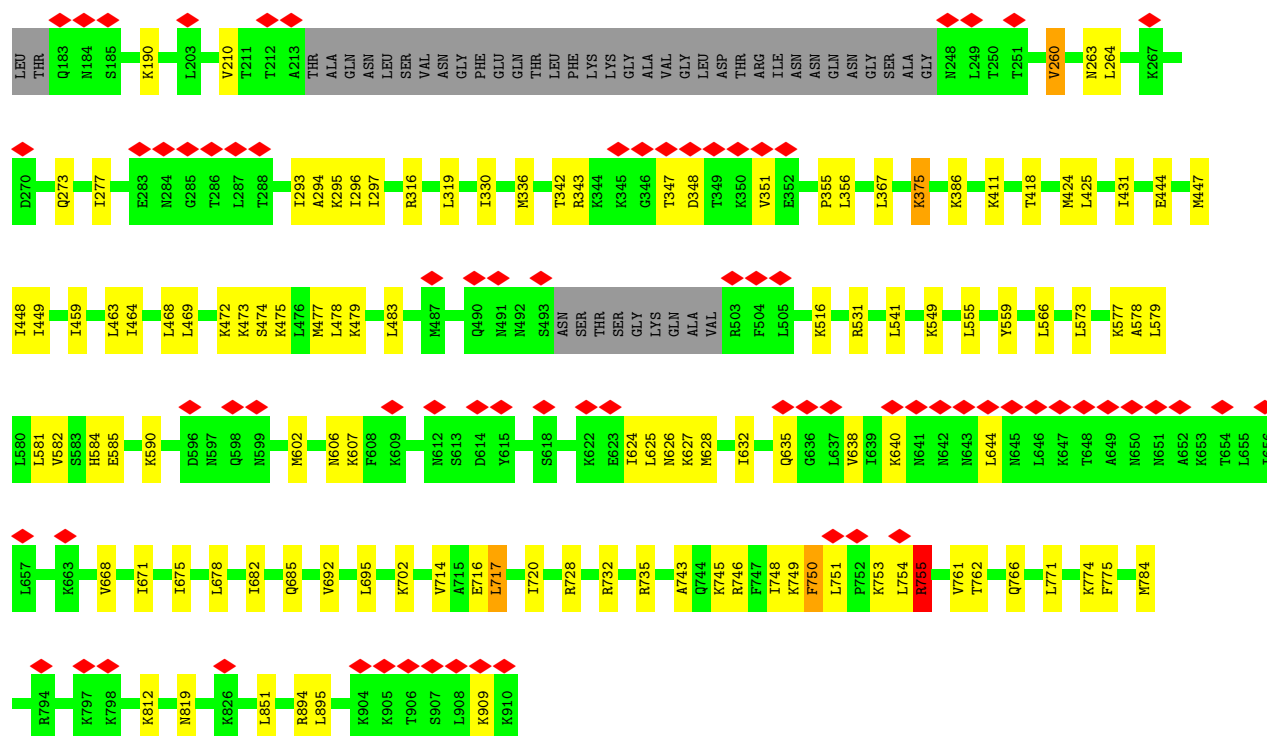
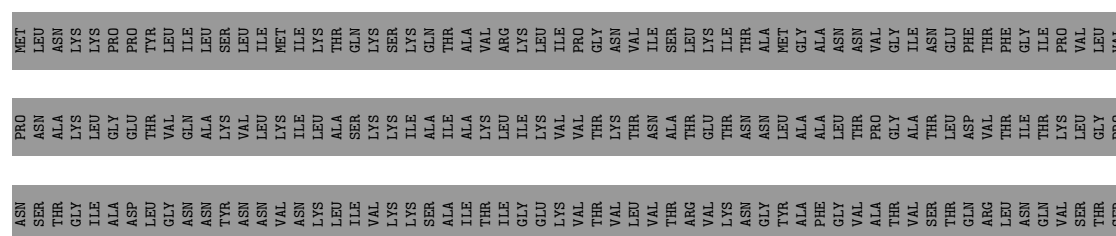


• Molecule 53: 23S



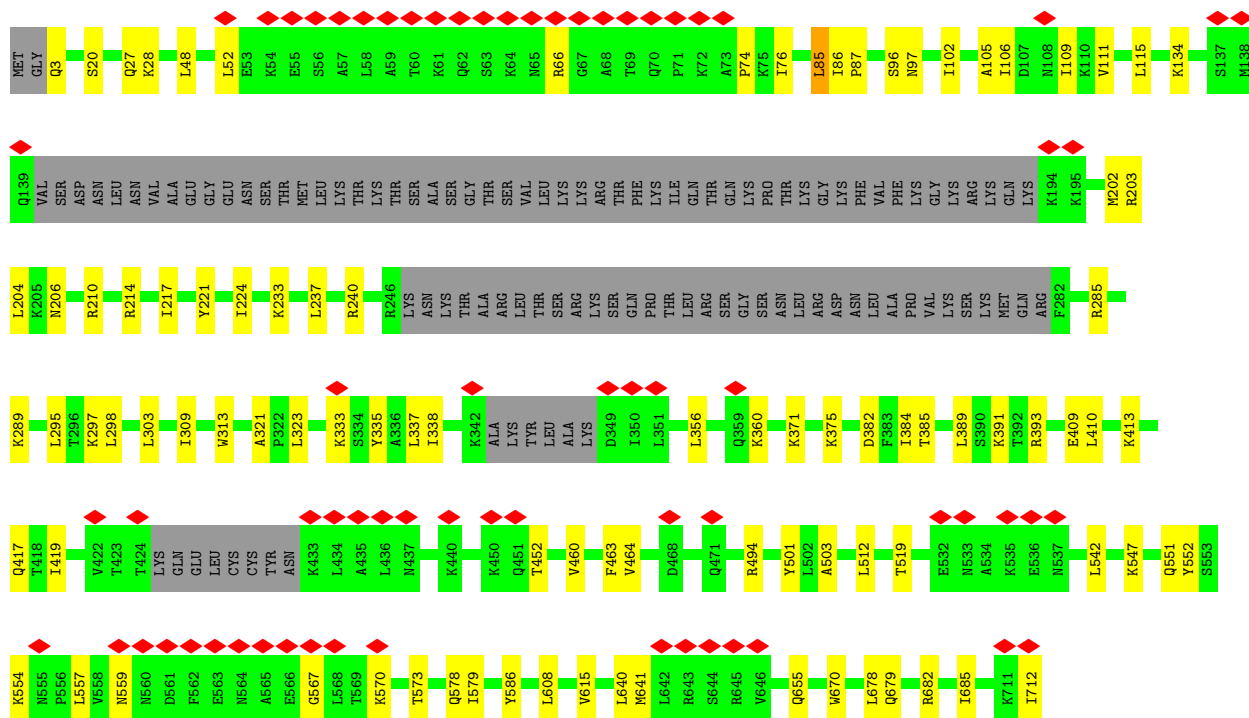


• Molecule 56: Small ribosomal subunit protein uS2c

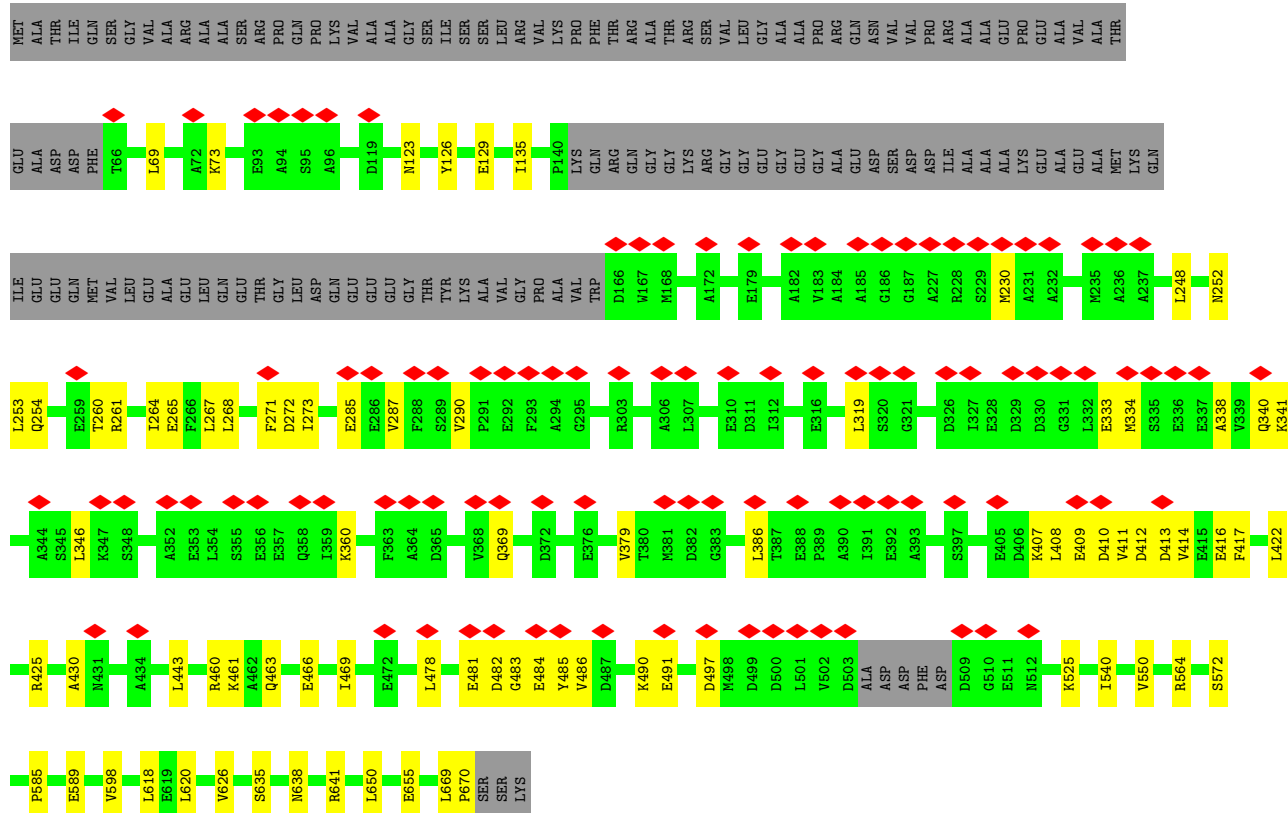


• Molecule 57: Small ribosomal subunit protein uS3c

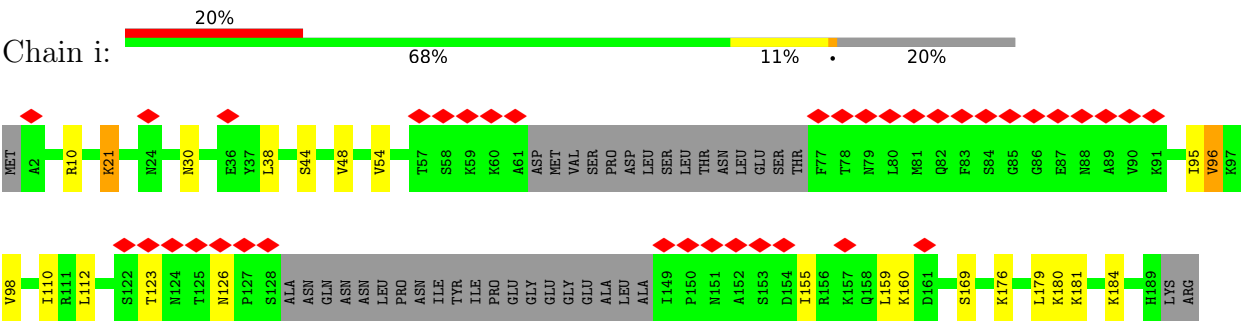




• Molecule 58: uS5c



• Molecule 59: Small ribosomal subunit protein uS9c



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	225199	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	75000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.555	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.102	Depositor
Map size (Å)	544.3072, 544.3072, 544.3072	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0631, 1.0631, 1.0631	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 6MZ, UR3, 2MA, 2MG, OMC, 5MU, 4OC, H2U, K, MG, G7M, 5MC, OMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.27	0/382	0.36	0/518
2	3	0.23	0/2871	0.38	0/4471
3	5	0.33	0/1126	0.41	0/1753
4	6	0.28	0/479	0.43	0/640
5	7	0.34	0/457	0.45	0/595
6	8	0.31	0/528	0.43	0/702
7	9	0.30	0/292	0.40	0/379
8	B	0.32	0/2200	0.48	0/2965
9	C	0.31	0/1711	0.46	0/2304
10	D	0.29	0/1619	0.45	0/2183
11	E	0.21	0/1433	0.52	1/1920 (0.1%)
12	F	0.20	0/1354	0.40	0/1821
13	G	0.28	0/424	0.57	0/570
14	H	0.22	0/1131	0.54	1/1520 (0.1%)
15	I	1.81	2/992 (0.2%)	1.25	7/1336 (0.5%)
16	J	0.29	0/1375	0.47	0/1855
17	K	0.29	0/952	0.45	0/1280
18	L	0.29	0/1505	0.50	0/2009
19	M	0.30	0/1105	0.41	0/1482
20	N	0.29	0/951	0.47	0/1275
21	O	0.22	0/913	0.51	0/1222
22	P	0.27	0/1005	0.44	0/1351
23	Q	0.35	0/958	0.51	0/1272
24	R	0.31	0/927	0.44	0/1247
25	S	0.28	0/915	0.47	0/1221
26	T	0.30	0/772	0.48	0/1043
27	U	0.26	0/1036	0.40	0/1381
28	V	0.27	0/884	0.47	0/1187
29	W	0.30	0/1126	0.42	0/1507
30	X	0.26	0/853	0.43	0/1141
31	Z	0.29	0/328	0.43	0/436
32	a	0.20	0/1899	0.52	0/2570

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.19	0/2144	0.43	0/2867
34	f	0.16	0/868	0.35	0/1172
35	g	0.29	0/1354	0.53	1/1820 (0.1%)
36	h	0.17	0/1125	0.36	0/1505
37	j	0.40	0/974	0.58	0/1316
38	k	0.17	0/908	0.40	0/1210
39	l	0.17	0/955	0.36	0/1282
40	m	0.36	0/931	0.48	0/1246
41	n	0.41	0/827	0.47	0/1097
42	o	0.21	0/822	0.45	0/1098
43	p	0.18	0/682	0.42	0/917
44	q	0.18	0/626	0.37	0/836
45	r	0.20	0/676	0.41	0/907
46	s	0.40	0/661	0.47	0/887
47	t	0.20	0/948	0.42	0/1269
48	u	0.45	1/801 (0.1%)	0.60	1/1070 (0.1%)
49	v	0.28	1/1463 (0.1%)	0.65	3/1994 (0.2%)
50	x	0.17	0/472	0.37	0/637
51	Y	0.24	0/532	0.59	0/715
52	w	0.24	0/2835	0.47	0/3845
53	1	0.59	6/56765 (0.0%)	0.43	5/88499 (0.0%)
54	4	0.36	0/6566	0.41	0/10240
55	2	0.31	1/35103 (0.0%)	0.37	0/54745
56	b	0.23	0/5616	0.57	4/7512 (0.1%)
57	c	0.31	0/5008	0.46	0/6698
58	e	0.22	0/4029	0.53	1/5461 (0.0%)
59	i	0.34	0/1202	0.52	0/1605
All	All	0.44	11/169396 (0.0%)	0.44	24/249606 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
18	L	0	1
37	j	0	1
49	v	0	1
53	1	2	1
56	b	0	1
57	c	0	1
58	e	0	1
All	All	2	7

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	I	162	MET	CA-C	55.46	2.30	1.52
53	1	720	U	N3-C4	50.30	2.39	1.38
53	1	720	U	C2-N3	46.90	2.31	1.37
53	1	720	U	N1-C2	46.14	2.30	1.38
53	1	720	U	N1-C6	44.06	2.26	1.38
53	1	720	U	C4-C5	39.98	2.23	1.43
53	1	720	U	C5-C6	38.77	2.11	1.34
48	u	635	TYR	CA-C	-8.07	1.46	1.52
15	I	162	MET	C-N	7.04	1.42	1.33
49	v	188	ASP	CA-CB	5.38	1.60	1.52
55	2	480	G7M	O3'-P	5.10	1.61	1.56

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	I	162	MET	O-C-N	-23.45	93.02	122.34
15	I	162	MET	N-CA-CB	-19.95	80.97	110.49
15	I	162	MET	CB-CA-C	16.51	137.67	110.09
15	I	162	MET	CA-C-O	10.92	132.13	119.35
15	I	162	MET	N-CA-C	10.51	126.41	113.17
15	I	49	PRO	CA-N-CD	-7.68	101.25	112.00
48	u	639	LEU	N-CA-C	-6.92	101.36	110.43
53	1	720	U	N1-C1'-C2'	6.88	122.32	112.00
35	g	86	MET	CB-CG-SD	6.16	131.19	112.70
53	1	312	A	O4'-C1'-N9	6.06	117.59	108.50
15	I	162	MET	CG-SD-CE	-5.91	87.89	100.90
14	H	163	MET	CB-CG-SD	5.70	129.81	112.70
49	v	141	ASP	CA-C-N	5.69	132.40	121.54
49	v	141	ASP	C-N-CA	5.69	132.40	121.54
53	1	1379	A	N9-C1'-C2'	5.63	120.44	112.00
49	v	193	LYS	CB-CG-CD	5.61	124.19	111.30
56	b	748	ILE	N-CA-C	-5.56	106.97	111.91
53	1	1379	A	O4'-C1'-N9	5.55	116.82	108.50
53	1	162	G	O4'-C1'-N9	5.49	116.43	108.20
56	b	477	MET	CA-CB-CG	5.33	124.76	114.10
56	b	755	ARG	CA-CB-CG	5.30	124.70	114.10
56	b	602	MET	CB-CG-SD	5.29	128.56	112.70
58	e	271	PHE	CB-CA-C	5.18	119.70	111.51
11	E	79	LYS	CB-CG-CD	5.01	122.81	111.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	1	312	A	C1'
53	1	1379	A	C1'

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
53	1	720	U	Sidechain
18	L	204	ASP	Peptide
56	b	755	ARG	Peptide
57	c	85	LEU	Peptide
58	e	333	GLU	Peptide
37	j	122	HIS	Peptide
49	v	141	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	369	0	381	2	0
2	3	2571	0	1300	19	0
3	5	1006	0	507	3	0
4	6	473	0	498	14	0
5	7	455	0	500	4	0
6	8	520	0	543	0	0
7	9	292	0	332	4	0
8	B	2159	0	2239	22	0
9	C	1681	0	1736	15	0
10	D	1599	0	1659	8	0
11	E	1413	0	1479	16	0
12	F	1338	0	1434	15	0
13	G	418	0	456	6	0
14	H	1114	0	1149	24	0
15	I	980	0	1056	44	0
16	J	1346	0	1389	5	0
17	K	942	0	998	2	0
18	L	1484	0	1530	8	0
19	M	1080	0	1143	7	0
20	N	937	0	978	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	O	902	0	920	7	0
22	P	995	0	1057	7	0
23	Q	943	0	992	5	0
24	R	907	0	951	10	0
25	S	903	0	948	7	0
26	T	837	0	823	7	0
27	U	1020	0	1097	11	0
28	V	869	0	882	5	0
29	W	1104	0	1151	8	0
30	X	843	0	884	4	0
31	Z	323	0	367	1	0
32	a	1868	0	1762	26	0
33	d	2107	0	2303	42	0
34	f	850	0	852	8	0
35	g	1334	0	1441	27	0
36	h	1113	0	1184	8	0
37	j	957	0	968	33	0
38	k	894	0	956	17	0
39	l	941	0	1029	5	0
40	m	924	0	970	22	0
41	n	814	0	877	11	0
42	o	813	0	828	6	0
43	p	666	0	697	5	0
44	q	621	0	658	13	0
45	r	664	0	743	8	0
46	s	645	0	677	7	0
47	t	935	0	1008	4	0
48	u	789	0	794	7	0
49	v	1430	0	1333	18	0
50	x	462	0	480	5	0
51	Y	521	0	500	9	0
52	w	2786	0	2612	56	0
53	1	50934	0	25632	234	0
54	4	5856	0	2947	21	0
55	2	31537	0	15884	137	0
56	b	5545	0	6140	112	0
57	c	4939	0	5338	99	0
58	e	3988	0	3837	81	0
59	i	1189	0	1243	15	0
60	1	206	0	0	0	0
60	2	99	0	0	0	0
60	3	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	4	7	0	0	0	0
60	5	4	0	0	0	0
60	7	1	0	0	0	0
60	L	1	0	0	0	0
61	1	86	0	0	0	0
61	2	47	0	0	0	0
61	4	4	0	0	0	0
61	U	1	0	0	0	0
All	All	158406	0	115072	1067	0

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

All (1067) 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)
35:g:151:MET:HE1	38:k:53:PHE:CE1	1.05	1.54
35:g:151:MET:CE	38:k:53:PHE:CE1	1.98	1.46
35:g:151:MET:CE	38:k:53:PHE:HE1	1.28	1.41
53:1:720:U:C6	53:1:720:U:C5	2.11	1.38
37:j:49:TYR:OH	56:b:606:ASN:HB3	1.17	1.31
56:b:753:LYS:HE3	58:e:265:GLU:OE2	1.13	1.30
53:1:720:U:C5	53:1:720:U:C4	2.23	1.26
15:I:162:MET:HA	53:1:720:U:C2	1.76	1.21
33:d:12:ILE:HD11	33:d:22:THR:CG2	1.71	1.20
33:d:34:PHE:CD1	57:c:66:ARG:HD3	1.74	1.20
37:j:49:TYR:OH	56:b:606:ASN:CB	1.91	1.19
5:7:95:LYS:NZ	54:4:191:G:OP1	1.78	1.16
56:b:625:LEU:HD12	56:b:628:MET:CE	1.75	1.15
56:b:753:LYS:CE	58:e:265:GLU:OE2	1.94	1.15
33:d:34:PHE:CD1	57:c:66:ARG:CD	2.30	1.14
56:b:625:LEU:HD12	56:b:628:MET:HE1	1.20	1.13
33:d:34:PHE:CE1	57:c:66:ARG:HB2	1.84	1.13
35:g:151:MET:HE1	38:k:53:PHE:CZ	1.84	1.12
33:d:34:PHE:CE1	57:c:66:ARG:HD3	1.84	1.12
57:c:335:TYR:CE2	58:e:410:ASP:OD2	2.03	1.11
53:1:1551:A:C2	55:2:1432:A:C4	2.39	1.10
52:w:178:ARG:NH1	56:b:909:LYS:HE2	1.68	1.09
35:g:151:MET:HE2	38:k:62:PHE:HD2	1.11	1.09
22:P:66:ARG:NH2	55:2:322:G:OP1	1.86	1.07
8:B:55:HIS:CE1	8:B:221:THR:HG22	1.89	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:162:MET:C	15:I:162:MET:CA	2.30	1.05
57:c:86:ILE:HG22	57:c:87:PRO:HD3	1.39	1.04
53:1:720:U:C6	53:1:720:U:N1	2.26	1.04
35:g:151:MET:HE2	38:k:62:PHE:CD2	1.92	1.04
37:j:49:TYR:CZ	56:b:606:ASN:HB3	1.93	1.03
15:I:162:MET:C	53:1:720:U:C2	2.36	1.02
33:d:34:PHE:HE1	57:c:66:ARG:HB2	1.18	1.02
56:b:625:LEU:CD1	56:b:628:MET:HE1	1.90	1.02
33:d:12:ILE:HD11	33:d:22:THR:HG22	1.38	1.00
35:g:150:ALA:O	35:g:151:MET:HG2	1.61	1.00
53:1:720:U:C2	53:1:720:U:N1	2.30	0.99
4:6:83:GLU:OE2	4:6:98:LYS:HE2	1.62	0.98
58:e:460:ARG:NH1	58:e:481:GLU:OE2	1.96	0.98
33:d:34:PHE:HD1	57:c:66:ARG:CD	1.69	0.98
53:1:720:U:C2	53:1:720:U:N3	2.31	0.97
52:w:178:ARG:HH11	56:b:909:LYS:HE2	1.21	0.97
55:2:47:G:N1	55:2:371:A:C2	2.33	0.95
37:j:53:LEU:HB3	56:b:626:ASN:HD21	1.29	0.95
15:I:162:MET:HA	53:1:720:U:N1	1.82	0.94
33:d:34:PHE:CE1	57:c:66:ARG:CG	2.50	0.94
33:d:34:PHE:CE1	57:c:66:ARG:CB	2.51	0.94
57:c:335:TYR:HE2	58:e:410:ASP:OD2	1.48	0.94
33:d:11:VAL:HG13	33:d:15:ILE:HD12	1.48	0.93
33:d:12:ILE:HD11	33:d:22:THR:HG21	1.52	0.92
33:d:34:PHE:CE1	57:c:66:ARG:CD	2.51	0.92
33:d:12:ILE:CD1	33:d:22:THR:CG2	2.47	0.92
53:1:540:G:H2'	53:1:541:G:H8	1.33	0.92
55:2:1352:A:C2	55:2:1426:G:N1	2.38	0.92
15:I:162:MET:C	53:1:720:U:C4	2.48	0.91
4:6:83:GLU:OE2	4:6:98:LYS:CE	2.19	0.91
55:2:47:G:N1	55:2:371:A:H2	1.65	0.91
15:I:162:MET:C	53:1:720:U:N3	2.29	0.90
53:1:720:U:C4	53:1:720:U:N3	2.39	0.90
55:2:1352:A:H2	55:2:1426:G:H1	0.96	0.89
8:B:82:ARG:HD2	8:B:84:GLU:OE2	1.72	0.89
20:N:152:ARG:HD3	20:N:154:LYS:HE3	1.54	0.89
33:d:12:ILE:CD1	33:d:22:THR:HG21	2.04	0.88
15:I:162:MET:CA	53:1:720:U:C2	2.58	0.86
8:B:55:HIS:ND1	8:B:221:THR:HG22	1.88	0.86
54:4:252:A:H62	54:4:273:G:N2	1.73	0.86
33:d:34:PHE:HE1	57:c:66:ARG:CB	1.88	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:2:47:G:H1	55:2:371:A:H2	0.89	0.85
15:I:162:MET:C	53:1:720:U:C5	2.54	0.85
35:g:151:MET:HB3	38:k:62:PHE:HB3	1.57	0.85
41:n:55:SER:OG	41:n:57:VAL:HG12	1.75	0.85
33:d:11:VAL:CG1	33:d:15:ILE:HD12	2.06	0.84
55:2:791:C:H42	55:2:795:A:H61	1.26	0.84
15:I:163:ILE:N	53:1:720:U:C4	2.46	0.84
52:w:334:LYS:HE3	57:c:375:LYS:HE2	1.61	0.83
15:I:162:MET:C	53:1:720:U:C6	2.57	0.83
59:i:44:SER:O	59:i:48:VAL:HG23	1.79	0.82
40:m:129:ARG:HH12	53:1:546:U:H5'	1.43	0.82
57:c:409:GLU:OE2	58:e:413:ASP:HB2	1.81	0.81
53:1:540:G:H2'	53:1:541:G:C8	2.16	0.81
54:4:252:A:H62	54:4:273:G:H21	1.29	0.81
53:1:540:G:H1	53:1:554:U:H3	1.26	0.81
55:2:1352:A:H2	55:2:1426:G:N1	1.74	0.81
37:j:122:HIS:O	37:j:123:VAL:HG12	1.81	0.80
10:D:193:THR:HA	10:D:204:MET:HE1	1.62	0.80
56:b:753:LYS:HE3	58:e:265:GLU:CD	2.07	0.80
8:B:55:HIS:CG	8:B:221:THR:HG22	2.17	0.79
25:S:134:VAL:CG1	25:S:137:CYS:SG	2.71	0.79
52:w:491:MET:HE2	52:w:501:PHE:CZ	2.17	0.79
56:b:761:VAL:HG21	58:e:483:GLY:HA2	1.62	0.79
9:C:98:THR:HG21	9:C:120:ARG:NH2	1.99	0.78
55:2:220:U:O2	55:2:259:G:N1	2.14	0.78
57:c:285:ARG:NH1	58:e:482:ASP:OD2	2.16	0.78
33:d:34:PHE:CD1	57:c:66:ARG:CG	2.65	0.78
19:M:37:GLN:NE2	19:M:130:LYS:HB3	1.99	0.78
57:c:335:TYR:CE1	58:e:407:LYS:O	2.36	0.77
15:I:162:MET:C	53:1:720:U:N1	2.42	0.77
55:2:1021:U:OP2	58:e:564:ARG:NH1	2.16	0.77
53:1:773:C:H2'	53:1:774:G:H8	1.48	0.77
15:I:162:MET:CA	53:1:720:U:C4	2.68	0.77
35:g:151:MET:HB3	38:k:62:PHE:CB	2.15	0.76
53:1:1551:A:H2	55:2:1432:A:C4	2.03	0.75
53:1:254:U:H3	53:1:312:A:H61	1.34	0.75
33:d:34:PHE:HD1	57:c:66:ARG:HD2	1.52	0.75
56:b:464:ILE:HD11	58:e:486:VAL:HG11	1.68	0.75
15:I:169:ASN:ND2	53:1:748:A:N7	2.35	0.74
8:B:26:ASP:OD1	8:B:82:ARG:NH1	2.20	0.74
15:I:162:MET:HA	15:I:162:MET:C	2.09	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:c:335:TYR:OH	58:e:409:GLU:N	2.20	0.74
15:I:162:MET:CA	53:1:720:U:N3	2.50	0.74
37:j:53:LEU:HB3	56:b:626:ASN:ND2	2.02	0.74
53:1:219:G:H21	53:1:223:A:H8	1.34	0.74
27:U:165:THR:OG1	27:U:167:GLU:HG2	1.89	0.73
51:Y:56:VAL:HG23	51:Y:57:MET:HG2	1.71	0.73
53:1:1551:A:C2	55:2:1432:A:C5	2.78	0.72
52:w:283:ASP:OD2	57:c:333:LYS:HE3	1.90	0.72
15:I:163:ILE:N	53:1:720:U:N3	2.37	0.72
35:g:141:GLU:O	35:g:145:ILE:HG13	1.89	0.72
52:w:334:LYS:CE	57:c:375:LYS:HE2	2.21	0.71
37:j:122:HIS:C	37:j:123:VAL:HG12	2.16	0.71
29:W:98:THR:O	29:W:102:GLU:HG3	1.90	0.71
57:c:335:TYR:HE1	58:e:407:LYS:O	1.74	0.71
44:q:67:MET:HE2	44:q:92:THR:OG1	1.91	0.70
53:1:708:A:H5'	53:1:709:C:H5	1.54	0.70
53:1:1551:A:H2	55:2:1432:A:H2'	1.55	0.70
33:d:34:PHE:CD1	57:c:66:ARG:HG3	2.27	0.70
32:a:178:LEU:HA	49:v:224:ARG:HH22	1.56	0.70
53:1:220:U:H1'	53:1:1669:6MZ:H9C1	1.74	0.70
18:L:192:THR:OG1	18:L:195:VAL:HG13	1.92	0.70
37:j:53:LEU:HD21	56:b:625:LEU:HD23	1.73	0.70
58:e:252:ASN:ND2	58:e:254:GLN:HE21	1.90	0.70
15:I:162:MET:O	53:1:720:U:N1	2.24	0.69
53:1:719:G:H2'	53:1:720:U:H3'	1.73	0.69
56:b:463:LEU:O	58:e:267:LEU:HD22	1.92	0.69
58:e:252:ASN:CG	58:e:254:GLN:HE21	2.01	0.69
58:e:460:ARG:HH12	58:e:481:GLU:CD	1.98	0.69
27:U:146:SER:HB3	27:U:164:LYS:HB2	1.73	0.69
55:2:618:G:H22	55:2:695:G:H1	1.41	0.69
57:c:86:ILE:HG22	57:c:87:PRO:CD	2.21	0.69
55:2:875:G:H1	55:2:1327:U:H3	1.41	0.69
41:n:3:LYS:HG2	55:2:996:G:H5''	1.74	0.68
52:w:202:GLU:HB2	58:e:461:LYS:HD2	1.75	0.68
52:w:178:ARG:NH1	56:b:909:LYS:CE	2.52	0.68
55:2:347:G:H1	55:2:366:G:H1	1.42	0.68
33:d:34:PHE:HD1	57:c:66:ARG:HD3	1.33	0.68
55:2:1352:A:N1	55:2:1426:G:O6	2.27	0.68
12:F:112:MET:HE3	12:F:189:TYR:CE1	2.29	0.68
56:b:625:LEU:CD1	56:b:628:MET:CE	2.58	0.68
56:b:464:ILE:HD11	58:e:486:VAL:CG1	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:4:258:G:H1	54:4:267:U:H3	1.42	0.68
12:F:48:LEU:HG	12:F:61:THR:HG22	1.76	0.67
5:7:95:LYS:HZ1	54:4:191:G:P	2.12	0.67
30:X:130:ALA:HB2	54:4:123:A:H62	1.58	0.67
56:b:717:LEU:HD21	58:e:411:VAL:HG11	1.77	0.67
14:H:61:LEU:HB3	14:H:115:ALA:HB3	1.75	0.67
15:I:162:MET:CA	53:1:720:U:N1	2.57	0.67
35:g:15:ASP:OD1	35:g:16:PRO:HD2	1.95	0.67
37:j:57:MET:HE2	57:c:547:LYS:NZ	2.10	0.67
44:q:31:LYS:NZ	44:q:82:ARG:HH12	1.93	0.67
15:I:161:ARG:NH1	15:I:161:ARG:O	2.28	0.67
56:b:625:LEU:HD12	56:b:628:MET:HE3	1.74	0.67
4:6:81:ARG:HH12	4:6:98:LYS:CG	2.08	0.67
37:j:54:ASP:HB2	56:b:626:ASN:OD1	1.94	0.67
11:E:79:LYS:HZ3	11:E:81:ARG:HH22	1.40	0.66
53:1:1551:A:N1	55:2:1432:A:C5	2.64	0.66
25:S:134:VAL:HG12	25:S:137:CYS:SG	2.35	0.66
59:i:98:VAL:HG11	59:i:110:ILE:HD11	1.76	0.66
14:H:62:ARG:HD2	14:H:113:GLU:HB2	1.78	0.66
53:1:32:G:H22	53:1:42:U:H3	1.44	0.66
48:u:635:TYR:O	48:u:636:SER:C	2.39	0.66
4:6:83:GLU:CD	4:6:98:LYS:HE3	2.21	0.66
2:3:15:U:H4'	2:3:16:G:H5'	1.78	0.65
18:L:102:MET:HE2	53:1:287:A:O4'	1.96	0.65
14:H:84:VAL:HG22	14:H:117:VAL:HG13	1.77	0.65
33:d:34:PHE:HE1	57:c:66:ARG:HD3	1.55	0.65
36:h:71:LYS:NZ	58:e:655:GLU:OE1	2.30	0.65
52:w:202:GLU:CB	58:e:461:LYS:HD2	2.27	0.65
56:b:468:LEU:HD22	58:e:483:GLY:O	1.95	0.65
55:2:791:C:N4	55:2:795:A:H61	1.92	0.65
56:b:746:ARG:HH21	58:e:272:ASP:HB2	1.62	0.65
8:B:55:HIS:CD2	8:B:221:THR:HG22	2.31	0.65
40:m:97:ARG:NH1	51:Y:52:ASN:OD1	2.30	0.65
21:O:28:ALA:HB3	21:O:32:ALA:H	1.62	0.65
57:c:86:ILE:CG2	57:c:87:PRO:HD3	2.21	0.65
12:F:180:GLU:OE2	12:F:185:LYS:HD3	1.97	0.64
15:I:147:LYS:NZ	53:1:720:U:OP1	2.28	0.64
55:2:1330:U:H2'	55:2:1331:G:C8	2.33	0.64
53:1:1902:U:H4'	53:1:1968:A:H2	1.61	0.64
53:1:238:A:H62	53:1:910:A:H2	1.46	0.64
53:1:701:U:H2'	53:1:702:G:H8	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:48:PRO:HB3	55:2:1361:G:O5'	1.99	0.63
53:1:1551:A:C2	55:2:1432:A:N3	2.66	0.63
53:1:1558:C:OP1	55:2:1456:G:C8	2.51	0.63
25:S:134:VAL:HG11	25:S:137:CYS:SG	2.37	0.63
58:e:248:LEU:O	58:e:268:LEU:HD21	1.98	0.63
4:6:83:GLU:OE2	4:6:98:LYS:HE3	1.97	0.63
35:g:151:MET:HE3	38:k:53:PHE:HE1	1.49	0.63
12:F:112:MET:HE3	12:F:189:TYR:CD1	2.33	0.63
8:B:55:HIS:CE1	8:B:221:THR:CG2	2.75	0.62
8:B:55:HIS:NE2	8:B:221:THR:HG22	2.14	0.62
24:R:122:LYS:HE3	24:R:124:THR:HG22	1.80	0.62
53:1:773:C:H2'	53:1:774:G:C8	2.33	0.62
12:F:180:GLU:OE2	12:F:185:LYS:HB2	1.97	0.62
56:b:573:LEU:HD13	56:b:678:LEU:HD11	1.80	0.62
55:2:346:C:H42	55:2:367:A:H61	1.46	0.62
33:d:34:PHE:CE1	57:c:66:ARG:HG3	2.32	0.62
38:k:29:HIS:HA	38:k:59:SER:HB3	1.80	0.62
12:F:48:LEU:CG	12:F:61:THR:HG22	2.29	0.62
15:I:162:MET:N	53:1:720:U:C4	2.67	0.62
35:g:57:ASN:HB3	35:g:60:GLU:HG3	1.81	0.62
15:I:81:THR:HG23	15:I:89:ILE:HD12	1.82	0.62
57:c:221:TYR:HA	57:c:224:ILE:HD12	1.82	0.62
11:E:132:GLY:HA3	53:1:1945:A:H5''	1.82	0.61
15:I:49:PRO:HA	15:I:88:ILE:HA	1.82	0.61
37:j:49:TYR:OH	56:b:606:ASN:HB2	1.97	0.61
55:2:1294:A:H2'	55:2:1295:G:C8	2.34	0.61
11:E:8:LEU:O	11:E:12:THR:HB	2.00	0.61
57:c:202:MET:O	57:c:206:ASN:ND2	2.33	0.61
35:g:151:MET:CB	38:k:62:PHE:HB3	2.30	0.61
9:C:98:THR:CG2	9:C:120:ARG:HH21	2.13	0.61
32:a:149:ILE:HG22	32:a:150:GLU:HG2	1.83	0.61
52:w:491:MET:HE2	52:w:501:PHE:HZ	1.65	0.61
27:U:136:MET:HG2	27:U:145:ARG:HB2	1.82	0.61
56:b:474:SER:HB3	56:b:755:ARG:HH11	1.64	0.61
57:c:106:ILE:HA	57:c:109:ILE:HD13	1.83	0.61
9:C:163:LYS:CD	20:N:57:MET:SD	2.89	0.61
32:a:93:LYS:HB2	49:v:156:VAL:HG23	1.83	0.61
55:2:47:G:O6	55:2:371:A:N1	2.33	0.61
57:c:52:LEU:HD13	57:c:105:ALA:HB1	1.81	0.61
2:3:111:C:H2'	2:3:112:U:C6	2.36	0.60
35:g:6:ILE:HG22	35:g:8:LYS:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:1931:U:H2'	53:1:1932:U:C6	2.37	0.60
55:2:38:U:H3	55:2:373:G:H1	1.49	0.60
56:b:190:LYS:HB2	56:b:273:GLN:HE21	1.66	0.60
4:6:83:GLU:CD	4:6:98:LYS:CE	2.75	0.60
54:4:252:A:N6	54:4:273:G:H21	1.98	0.60
56:b:762:THR:O	56:b:766:GLN:HG2	2.01	0.60
15:I:162:MET:CA	53:1:720:U:C5	2.84	0.60
53:1:775:U:H2'	53:1:776:U:C6	2.36	0.60
35:g:151:MET:SD	38:k:53:PHE:CE1	2.95	0.60
53:1:514:G:H2'	53:1:515:G:C8	2.37	0.60
55:2:365:G:H3'	55:2:366:G:C8	2.37	0.60
15:I:162:MET:CA	53:1:720:U:C6	2.85	0.59
16:J:104:THR:HB	16:J:111:MET:HE2	1.83	0.59
52:w:375:GLU:HG3	57:c:337:LEU:HD22	1.83	0.59
57:c:554:LYS:HB3	57:c:559:ASN:HD22	1.68	0.59
54:4:59:G:H1	54:4:66:C:H5	1.50	0.59
9:C:163:LYS:HD3	20:N:57:MET:SD	2.43	0.59
40:m:129:ARG:HH12	53:1:546:U:C5'	2.15	0.59
56:b:468:LEU:CD2	58:e:483:GLY:O	2.50	0.59
52:w:212:LEU:O	57:c:297:LYS:NZ	2.35	0.59
53:1:747:G:O2'	53:1:749:G:OP2	2.19	0.59
29:W:139:MET:HE1	29:W:144:LYS:HB3	1.85	0.59
15:I:162:MET:HB3	53:1:720:U:C6	2.37	0.58
40:m:127:ARG:HG2	40:m:137:VAL:HG13	1.85	0.58
55:2:352:G:H1	55:2:363:A:H2	1.49	0.58
9:C:98:THR:CG2	9:C:120:ARG:NH2	2.66	0.58
15:I:162:MET:O	53:1:720:U:C6	2.56	0.58
59:i:38:LEU:HD13	59:i:44:SER:HB3	1.83	0.58
55:2:1352:A:N1	55:2:1426:G:C6	2.71	0.58
49:v:230:LEU:HD23	49:v:231:THR:HG23	1.85	0.58
52:w:170:LEU:HD11	52:w:176:GLU:HB2	1.86	0.58
53:1:702:G:C6	53:1:774:G:C6	2.92	0.58
56:b:751:LEU:HD22	58:e:443:LEU:HD21	1.86	0.58
56:b:894:ARG:HH22	58:e:491:GLU:HG2	1.69	0.58
8:B:82:ARG:CD	8:B:84:GLU:HG2	2.33	0.58
53:1:771:A:H8	53:1:772:G:H1'	1.67	0.58
40:m:129:ARG:NH1	53:1:546:U:H5'	2.16	0.58
40:m:129:ARG:HH22	53:1:546:U:P	2.26	0.58
49:v:155:ALA:HB1	56:b:264:LEU:HD11	1.86	0.58
12:F:52:LYS:HE2	12:F:57:THR:HG23	1.85	0.57
57:c:356:LEU:O	57:c:360:LYS:NZ	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:c:678:LEU:HD23	57:c:685:ILE:HD13	1.86	0.57
20:N:66:LEU:HD21	20:N:99:VAL:HG21	1.86	0.57
37:j:57:MET:HG2	57:c:551:GLN:OE1	2.04	0.57
57:c:382:ASP:OD2	57:c:393:ARG:NH1	2.37	0.57
2:3:6:G:H1	2:3:118:U:H3	1.51	0.57
55:2:350:A:N6	55:2:366:G:H21	2.02	0.57
52:w:334:LYS:HZ3	52:w:368:GLU:HG2	1.69	0.57
59:i:96:VAL:HG11	59:i:110:ILE:HG12	1.84	0.57
4:6:81:ARG:HH12	4:6:98:LYS:HG2	1.69	0.57
11:E:33:GLU:HG2	11:E:34:LYS:HG2	1.85	0.57
53:1:729:A:H61	53:1:733:A:H62	1.51	0.57
44:q:41:LYS:HD2	55:2:231:U:H5'	1.86	0.57
59:i:54:VAL:HG11	59:i:155:ILE:HG23	1.86	0.57
14:H:62:ARG:NH1	14:H:113:GLU:OE2	2.38	0.57
37:j:154:MET:HE3	57:c:578:GLN:CD	2.30	0.57
52:w:347:LEU:HG	57:c:204:LEU:HD11	1.86	0.57
59:i:30:ASN:HD21	59:i:98:VAL:CG2	2.18	0.57
14:H:88:LYS:HG2	53:1:766:G:H5''	1.87	0.56
8:B:134:LEU:HD23	8:B:137:ILE:HD12	1.85	0.56
9:C:98:THR:HG21	9:C:120:ARG:CZ	2.35	0.56
15:I:162:MET:HE1	53:1:719:G:N3	2.21	0.56
49:v:160:ASP:HA	49:v:163:LEU:HD12	1.86	0.56
52:w:260:ASP:O	57:c:210:ARG:NH2	2.38	0.56
56:b:424:MET:HA	56:b:431:ILE:HD12	1.87	0.56
29:W:121:ALA:O	29:W:125:GLU:HG2	2.06	0.56
37:j:106:VAL:HB	37:j:139:LEU:HB3	1.86	0.56
24:R:141:GLU:HB3	24:R:171:LYS:HB3	1.88	0.56
40:m:94:ASN:HD22	51:Y:52:ASN:HD22	1.54	0.56
35:g:74:GLU:HB2	35:g:91:LEU:HD13	1.87	0.56
11:E:107:LEU:HD23	11:E:140:PRO:HG2	1.87	0.56
57:c:519:THR:HG22	57:c:579:ILE:HD13	1.88	0.56
7:9:31:LYS:HE2	53:1:2118:A:H5'	1.88	0.56
52:w:209:GLU:OE1	56:b:472:LYS:HB3	2.05	0.56
55:2:668:G:H2'	55:2:669:A:C8	2.41	0.56
55:2:791:C:H42	55:2:795:A:N6	2.00	0.56
14:H:175:ARG:O	14:H:175:ARG:NE	2.31	0.56
25:S:164:PHE:HE2	25:S:166:MET:HE2	1.71	0.56
52:w:202:GLU:HG2	58:e:461:LYS:HD3	1.88	0.56
58:e:484:GLU:O	58:e:485:TYR:C	2.48	0.56
14:H:134:PHE:HA	14:H:137:ASP:HB2	1.89	0.55
53:1:699:A:H2'	53:1:700:A:C8	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:710:A:C2	53:1:711:A:H1'	2.41	0.55
9:C:225:LYS:NZ	9:C:230:ARG:HH21	2.04	0.55
10:D:66:VAL:HG22	53:1:270:A:H4'	1.87	0.55
49:v:137:ALA:HB3	56:b:210:VAL:HA	1.87	0.55
52:w:296:ASP:HA	52:w:299:LEU:HB3	1.88	0.55
5:7:95:LYS:NZ	54:4:191:G:P	2.75	0.55
53:1:731:G:N2	53:1:749:G:O2'	2.40	0.55
18:L:140:SER:HB2	53:1:277:G:H5''	1.88	0.55
54:4:269:U:H2'	54:4:270:A:H8	1.71	0.55
53:1:737:A:H2	53:1:748:A:H8	1.55	0.55
58:e:123:ASN:H	58:e:126:TYR:HB2	1.72	0.55
52:w:329:THR:OG1	57:c:214:ARG:NH2	2.38	0.55
52:w:334:LYS:NZ	52:w:368:GLU:HG2	2.21	0.55
53:1:710:A:C4	53:1:2391:G:C2	2.95	0.55
55:2:345:U:H3	55:2:368:G:H1	1.53	0.55
57:c:298:LEU:HD21	57:c:384:ILE:HA	1.89	0.55
55:2:350:A:H61	55:2:366:G:H21	1.54	0.55
56:b:728:ARG:HH22	58:e:416:GLU:HG3	1.71	0.55
56:b:753:LYS:NZ	58:e:265:GLU:OE2	2.40	0.55
57:c:413:LYS:HD3	58:e:412:ASP:OD2	2.07	0.55
12:F:48:LEU:CD1	12:F:61:THR:HG22	2.37	0.55
14:H:169:SER:OG	14:H:172:GLU:OE1	2.25	0.55
19:M:55:THR:O	19:M:58:VAL:HG22	2.07	0.55
44:q:75:LEU:HD11	44:q:97:VAL:HG11	1.89	0.55
4:6:81:ARG:NH1	4:6:98:LYS:HG3	2.21	0.54
37:j:122:HIS:O	37:j:123:VAL:CG1	2.55	0.54
56:b:418:THR:HG21	56:b:812:LYS:HD3	1.89	0.54
50:x:99:LYS:HZ1	58:e:129:GLU:HG2	1.71	0.54
52:w:329:THR:CB	57:c:214:ARG:HH22	2.20	0.54
30:X:125:LYS:HG2	30:X:134:MET:HE1	1.90	0.54
52:w:341:VAL:HG21	52:w:371:ALA:H	1.73	0.54
18:L:192:THR:O	18:L:195:VAL:HG22	2.07	0.54
42:o:123:ARG:NE	53:1:371:U:OP2	2.41	0.54
56:b:342:THR:HA	56:b:355:PRO:HA	1.89	0.54
22:P:54:VAL:HG21	22:P:101:MET:HE1	1.90	0.54
8:B:43:LYS:HD3	8:B:57:GLY:HA2	1.89	0.54
37:j:56:PRO:HA	57:c:551:GLN:HE22	1.72	0.54
41:n:52:ARG:HH12	55:2:1158:G:P	2.30	0.54
12:F:48:LEU:HD12	12:F:61:THR:HG22	1.90	0.54
37:j:53:LEU:HD21	56:b:625:LEU:CD2	2.38	0.54
53:1:1188:U:H3	53:1:1198:G:H1	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:2:1200:C:H42	55:2:1211:C:H42	1.56	0.54
59:i:54:VAL:HG21	59:i:159:LEU:HG	1.90	0.54
15:I:161:ARG:HH21	53:1:740:C:H1'	1.72	0.54
40:m:132:ILE:HD13	53:1:547:C:C5	2.43	0.54
40:m:132:ILE:HG23	53:1:547:C:O4'	2.08	0.54
56:b:750:PHE:HB2	56:b:754:LEU:HB3	1.90	0.53
2:3:4:U:H3	2:3:120:G:H1	1.54	0.53
2:3:23:U:H2'	2:3:24:G:C8	2.43	0.53
14:H:62:ARG:HH11	14:H:113:GLU:H	1.55	0.53
15:I:167:ALA:HB1	15:I:172:ILE:HB	1.88	0.53
8:B:136:ASN:C	34:f:156:ALA:CB	2.81	0.53
53:1:1537:G:H21	53:1:1540:C:N4	2.06	0.53
20:N:79:SER:O	20:N:83:GLU:HG2	2.07	0.53
53:1:1902:U:H4'	53:1:1968:A:C2	2.41	0.53
2:3:111:C:H2'	2:3:112:U:H6	1.74	0.53
8:B:136:ASN:O	34:f:156:ALA:HB2	2.08	0.53
12:F:58:LEU:HB3	12:F:100:LEU:HD22	1.90	0.53
53:1:701:U:O2	53:1:774:G:N2	2.40	0.53
14:H:88:LYS:NZ	53:1:767:G:OP2	2.38	0.53
33:d:201:LEU:HD22	33:d:240:LEU:HD23	1.89	0.53
40:m:97:ARG:NE	51:Y:69:ASP:OD2	2.42	0.53
57:c:240:ARG:NH2	57:c:385:THR:O	2.38	0.53
44:q:47:ALA:HB3	44:q:66:TYR:HE1	1.73	0.53
55:2:47:G:C6	55:2:371:A:N1	2.77	0.53
59:i:10:ARG:H	59:i:112:LEU:HD23	1.74	0.53
7:9:1:MET:SD	53:1:2382:C:OP1	2.66	0.53
24:R:135:VAL:HG13	24:R:177:ILE:HG12	1.90	0.53
56:b:745:LYS:HD2	58:e:430:ALA:CB	2.39	0.53
57:c:210:ARG:O	57:c:214:ARG:HG2	2.08	0.53
55:2:1056:G:H5'	57:c:679:GLN:HG3	1.91	0.53
19:M:55:THR:HA	19:M:58:VAL:HG22	1.91	0.53
29:W:142:ALA:HA	29:W:145:LEU:HD12	1.91	0.53
53:1:1676:G:H2'	53:1:1677:G:C8	2.44	0.53
58:e:260:THR:O	58:e:264:ILE:HG13	2.08	0.53
53:1:749:G:N2	53:1:750:U:O4	2.40	0.52
53:1:1304:G:H5''	53:1:1305:C:H5'	1.91	0.52
58:e:252:ASN:OD1	58:e:254:GLN:NE2	2.42	0.52
58:e:466:GLU:HA	58:e:469:ILE:HG12	1.91	0.52
52:w:334:LYS:CE	57:c:375:LYS:CE	2.88	0.52
53:1:608:C:H2'	53:1:609:A:H8	1.75	0.52
23:Q:6:ARG:NH2	53:1:910:A:H2'	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:w:181:LEU:HD13	52:w:182:PRO:HD2	1.91	0.52
33:d:7:PRO:HB2	33:d:10:ARG:HG2	1.91	0.52
40:m:129:ARG:HG3	40:m:133:MET:CE	2.39	0.52
58:e:422:LEU:HA	58:e:425:ARG:HE	1.74	0.52
2:3:13:U:C4	28:V:99:LYS:HD3	2.44	0.52
9:C:163:LYS:HD2	20:N:57:MET:SD	2.49	0.52
36:h:11:ILE:HD11	36:h:36:LEU:HD23	1.91	0.52
53:1:710:A:H1'	53:1:2391:G:N2	2.25	0.52
58:e:252:ASN:OD1	58:e:254:GLN:HG3	2.10	0.52
10:D:48:LEU:HD22	10:D:235:TYR:HB2	1.92	0.52
11:E:131:LEU:HD11	11:E:155:ILE:HD12	1.91	0.52
33:d:184:LYS:HD3	33:d:187:LEU:HD12	1.92	0.52
38:k:22:VAL:HG22	38:k:35:ILE:HG12	1.92	0.52
55:2:723:G:H4'	55:2:1452:A:H4'	1.92	0.52
16:J:138:HIS:CD2	16:J:146:TRP:HB3	2.45	0.52
44:q:31:LYS:NZ	44:q:82:ARG:NH1	2.56	0.52
55:2:921:A:H4'	55:2:922:G:H5''	1.91	0.52
53:1:705:G:C2	53:1:771:A:C2	2.98	0.52
53:1:753:G:H21	53:1:758:A:H62	1.56	0.52
53:1:1557:A:N1	55:2:1434:U:O2'	2.38	0.52
56:b:559:TYR:HB2	56:b:692:VAL:HG11	1.91	0.52
2:3:68:G:H2'	2:3:69:G:O4'	2.10	0.52
2:3:70:G:H3'	2:3:71:G:H5''	1.92	0.52
11:E:114:ASP:OD1	40:m:107:ALA:HB1	2.10	0.52
53:1:1118:U:H4'	53:1:1119:U:H5'	1.92	0.52
59:i:30:ASN:HD21	59:i:98:VAL:HG22	1.74	0.52
15:I:76:GLU:OE1	15:I:80:GLN:NE2	2.43	0.51
55:2:627:G:H2'	55:2:628:G:C8	2.45	0.51
59:i:30:ASN:ND2	59:i:98:VAL:HG22	2.25	0.51
41:n:4:LYS:HD3	55:2:995:G:H5''	1.93	0.51
33:d:11:VAL:HG13	33:d:15:ILE:CD1	2.30	0.51
43:p:62:ARG:HG2	55:2:97:G:H5''	1.93	0.51
46:s:11:VAL:HG11	46:s:16:LEU:HD13	1.92	0.51
56:b:469:LEU:HG	56:b:473:LYS:HE3	1.91	0.51
25:S:113:CYS:HB3	25:S:168:ILE:HD12	1.91	0.51
55:2:351:U:H3	55:2:365:G:H1	1.58	0.51
53:1:294:U:H2'	53:1:295:C:C6	2.46	0.51
53:1:553:U:H2'	53:1:554:U:O4'	2.11	0.51
53:1:772:G:C6	53:1:773:C:C4	2.98	0.51
54:4:171:A:H2'	54:4:172:C:C6	2.46	0.51
55:2:131:G:H1	55:2:163:C:H5	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:e:585:PRO:HD2	58:e:650:LEU:HD22	1.93	0.51
14:H:90:SER:HB3	53:1:706:A:H4'	1.92	0.51
35:g:77:PRO:O	35:g:78:ARG:HG3	2.10	0.51
37:j:57:MET:HE2	57:c:547:LYS:HZ2	1.75	0.51
52:w:187:ILE:HD11	57:c:295:LEU:HD11	1.92	0.51
11:E:57:GLU:HG2	11:E:142:ILE:HD13	1.93	0.51
27:U:112:LEU:HD21	27:U:124:LYS:HE3	1.91	0.51
52:w:269:LEU:HD21	52:w:294:LEU:HD11	1.93	0.51
37:j:154:MET:HE3	57:c:578:GLN:NE2	2.26	0.51
56:b:348:ASP:HB3	56:b:351:VAL:HG12	1.93	0.51
40:m:146:ALA:HB3	40:m:150:LYS:HE2	1.92	0.50
53:1:53:U:H4'	53:1:54:C:H5'	1.92	0.50
20:N:152:ARG:CD	20:N:154:LYS:HE3	2.34	0.50
27:U:107:GLN:HG2	27:U:127:GLU:HG3	1.93	0.50
31:Z:42:LYS:HG3	53:1:1658:C:H5	1.76	0.50
55:2:628:G:H2'	55:2:629:A:C8	2.46	0.50
56:b:682:ILE:HA	56:b:685:GLN:HG3	1.94	0.50
58:e:422:LEU:HD23	58:e:425:ARG:HE	1.75	0.50
2:3:54:U:H2'	2:3:55:G:H8	1.76	0.50
4:6:81:ARG:HH12	4:6:98:LYS:HG3	1.75	0.50
37:j:49:TYR:CE2	56:b:606:ASN:HB3	2.46	0.50
51:Y:69:ASP:OD1	51:Y:69:ASP:O	2.28	0.50
53:1:1537:G:H21	53:1:1540:C:H41	1.59	0.50
32:a:127:VAL:HG21	56:b:367:LEU:HD11	1.94	0.50
54:4:76:A:H62	54:4:93:G:H8	1.57	0.50
56:b:627:LYS:HD2	58:e:334:MET:HE1	1.93	0.50
53:1:546:U:H4'	53:1:547:C:H5	1.76	0.50
53:1:1713:U:H2'	53:1:1714:U:C6	2.47	0.50
55:2:365:G:H3'	55:2:366:G:H8	1.76	0.50
55:2:667:G:H2'	55:2:668:G:C8	2.47	0.50
8:B:82:ARG:HD2	8:B:84:GLU:CD	2.36	0.50
17:K:122:LEU:HD13	22:P:97:VAL:HG11	1.94	0.50
52:w:416:GLY:HA2	52:w:474:GLU:HG2	1.93	0.50
52:w:543:PRO:HG2	52:w:546:ALA:HB2	1.94	0.50
53:1:708:A:H5'	53:1:709:C:C5	2.40	0.50
55:2:1341:4OC:H2'	55:2:1342:C:O4'	2.11	0.50
14:H:172:GLU:OE1	14:H:172:GLU:N	2.45	0.50
55:2:347:G:H21	55:2:349:A:N6	2.09	0.50
55:2:347:G:H22	55:2:366:G:N2	2.09	0.50
32:a:88:GLN:HG2	56:b:895:LEU:HD11	1.94	0.50
33:d:12:ILE:HD12	33:d:22:THR:HG21	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:m:74:ILE:HG23	40:m:99:GLU:HG2	1.92	0.50
23:Q:6:ARG:HH22	53:1:910:A:H2'	1.77	0.50
52:w:344:TYR:HD1	52:w:355:LEU:HD12	1.76	0.50
44:q:91:LYS:HB2	55:2:242:G:H3'	1.94	0.49
53:1:540:G:N2	53:1:554:U:O2	2.38	0.49
53:1:1489:A:H2'	53:1:1490:A:C8	2.47	0.49
56:b:644:LEU:HB3	58:e:369:GLN:HB3	1.94	0.49
3:5:40:C:H5''	27:U:136:MET:HE1	1.94	0.49
21:O:52:PRO:HG2	21:O:118:VAL:HG12	1.94	0.49
52:w:289:PRO:HA	57:c:321:ALA:HB3	1.92	0.49
53:1:707:A:C2	53:1:770:A:H1'	2.48	0.49
58:e:252:ASN:HD21	58:e:254:GLN:HE21	1.58	0.49
15:I:162:MET:N	53:1:720:U:N3	2.60	0.49
23:Q:31:LEU:HD13	53:1:232:C:H4'	1.94	0.49
39:l:50:ARG:HB3	39:l:66:TYR:HE1	1.76	0.49
53:1:184:U:H2'	53:1:185:G:C8	2.46	0.49
53:1:702:G:C4	53:1:774:G:C2	3.00	0.49
2:3:18:U:H3	2:3:67:A:H2	1.60	0.49
55:2:1351:C:H2'	55:2:1352:A:C8	2.47	0.49
58:e:589:GLU:HG2	58:e:598:VAL:HG22	1.94	0.49
41:n:17:VAL:HG11	41:n:59:LEU:HD11	1.95	0.49
50:x:74:PRO:HD2	50:x:77:LEU:HD12	1.93	0.49
55:2:133:G:H2'	55:2:134:G:C8	2.48	0.49
20:N:152:ARG:HD3	20:N:154:LYS:CE	2.36	0.49
55:2:60:A:H5''	55:2:363:A:H5''	1.95	0.49
55:2:1010:U:H2'	55:2:1011:C:C6	2.48	0.49
15:I:169:ASN:HB3	53:1:748:A:H62	1.77	0.49
53:1:1968:A:H2'	53:1:1969:A:C8	2.47	0.49
57:c:76:ILE:HD13	57:c:96:SER:HB3	1.95	0.49
14:H:88:LYS:HB2	14:H:91:LEU:HG	1.94	0.49
53:1:386:G:H5''	53:1:387:U:H5''	1.94	0.49
53:1:1127:A:H2'	53:1:1128:A:C8	2.48	0.49
55:2:47:G:C2	55:2:371:A:H2	2.29	0.49
55:2:311:C:H2'	55:2:312:A:H8	1.77	0.49
4:6:83:GLU:OE1	4:6:98:LYS:HE3	2.12	0.49
43:p:107:ARG:NH1	43:p:112:MET:HE2	2.27	0.49
53:1:688:A:H2'	53:1:689:A:C8	2.48	0.49
56:b:743:ALA:HA	56:b:746:ARG:HG2	1.95	0.49
56:b:771:LEU:HD21	58:e:264:ILE:HG23	1.94	0.49
37:j:51:ASP:HA	57:c:547:LYS:HD3	1.95	0.49
49:v:190:PHE:HB3	56:b:784:MET:HE3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:72:PRO:HB3	54:4:50:G:H5'	1.94	0.48
53:1:1432:U:H2'	53:1:1433:C:C6	2.48	0.48
22:P:133:LYS:HB2	55:2:1371:C:OP1	2.13	0.48
52:w:244:LEU:HD13	52:w:313:ALA:HB2	1.94	0.48
53:1:1855:A:H2'	53:1:1856:G:C8	2.48	0.48
55:2:1455:2MG:HM21	55:2:1458:MA6:N7	2.28	0.48
56:b:516:LYS:HG2	58:e:290:VAL:HG11	1.95	0.48
4:6:81:ARG:NH1	4:6:98:LYS:CG	2.76	0.48
14:H:133:LYS:O	14:H:137:ASP:N	2.44	0.48
37:j:53:LEU:CB	56:b:626:ASN:HD21	2.14	0.48
40:m:52:ASN:HA	40:m:85:THR:HB	1.94	0.48
55:2:1461:U:H2'	55:2:1462:G:H8	1.78	0.48
8:B:260:LEU:HD23	53:1:1433:C:H5''	1.96	0.48
23:Q:44:ARG:HD2	24:R:153:MET:HB3	1.95	0.48
55:2:669:A:H2'	55:2:670:A:C8	2.48	0.48
24:R:173:MET:HE2	24:R:173:MET:HB2	1.78	0.48
53:1:701:U:H2'	53:1:702:G:C8	2.44	0.48
56:b:277:ILE:HD11	56:b:295:LYS:HG2	1.94	0.48
57:c:682:ARG:HD2	57:c:712:ILE:HD11	1.95	0.48
55:2:392:G:H2'	55:2:393:G:H8	1.78	0.48
55:2:628:G:H2'	55:2:629:A:H8	1.78	0.48
58:e:460:ARG:HA	58:e:463:GLN:HG2	1.95	0.48
44:q:31:LYS:HZ3	44:q:82:ARG:HH12	1.60	0.48
58:e:253:LEU:HD12	58:e:261:ARG:HG2	1.96	0.48
11:E:62:ALA:HB1	11:E:92:LEU:HD21	1.95	0.48
32:a:131:LEU:HD23	56:b:319:LEU:HD21	1.96	0.48
32:a:174:SER:HB3	32:a:178:LEU:HD21	1.96	0.48
47:t:94:LYS:HD2	47:t:145:ALA:HB2	1.95	0.48
50:x:81:LYS:HB2	50:x:84:VAL:HB	1.94	0.48
53:1:233:C:H2'	53:1:234:G:C8	2.49	0.48
53:1:1686:C:H2'	53:1:1687:A:C8	2.49	0.48
9:C:225:LYS:HZ1	9:C:230:ARG:HH21	1.61	0.48
32:a:281:LEU:HD11	32:a:293:SER:HB2	1.96	0.48
40:m:129:ARG:HG3	40:m:133:MET:HE2	1.96	0.48
49:v:268:THR:HA	49:v:271:ILE:HG12	1.95	0.48
9:C:44:MET:HE3	9:C:45:GLY:O	2.14	0.48
42:o:67:LEU:HD11	42:o:97:GLN:HG2	1.95	0.48
52:w:306:GLN:N	52:w:306:GLN:OE1	2.47	0.48
53:1:705:G:H4'	53:1:706:A:H5''	1.96	0.48
55:2:1329:U:H2'	55:2:1330:U:C6	2.49	0.48
57:c:338:ILE:HG12	57:c:410:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:82:LEU:HD11	34:f:95:LEU:HD21	1.95	0.47
53:1:1247:A:H2'	53:1:1248:A:C8	2.49	0.47
53:1:1913:A:H2'	53:1:1914:A:C8	2.49	0.47
56:b:343:ARG:HD3	56:b:356:LEU:HD13	1.96	0.47
56:b:475:LYS:HD2	56:b:478:LEU:HD21	1.96	0.47
58:e:618:LEU:HD13	58:e:626:VAL:HG11	1.95	0.47
39:l:110:ARG:HB3	39:l:119:VAL:HG21	1.97	0.47
57:c:552:TYR:HB3	57:c:573:THR:HB	1.96	0.47
58:e:490:LYS:HD2	58:e:490:LYS:HA	1.69	0.47
15:l:164:GLU:OE1	15:l:164:GLU:N	2.42	0.47
29:W:90:THR:HG22	29:W:94:LYS:HG3	1.96	0.47
52:w:178:ARG:NH1	56:b:909:LYS:HG2	2.29	0.47
53:1:64:C:H2'	53:1:65:A:C8	2.49	0.47
53:1:699:A:H2'	53:1:700:A:H8	1.78	0.47
53:1:1551:A:C2	55:2:1432:A:H2'	2.40	0.47
58:e:253:LEU:N	58:e:253:LEU:HD23	2.30	0.47
13:G:42:ILE:HD11	13:G:73:LYS:HG3	1.96	0.47
21:O:55:ALA:HA	21:O:121:ASP:HB3	1.96	0.47
53:1:71:U:H5'	54:4:202:A:H3'	1.96	0.47
53:1:1247:A:H2'	53:1:1248:A:H8	1.78	0.47
35:g:77:PRO:HG3	35:g:86:MET:HE1	1.96	0.47
53:1:1575:A:H1'	53:1:1577:5MU:H72	1.95	0.47
33:d:34:PHE:CZ	57:c:66:ARG:HB2	2.45	0.47
53:1:1484:A:H1'	55:2:656:A:O4'	2.14	0.47
55:2:1030:G:OP1	58:e:525:LYS:HE2	2.14	0.47
56:b:579:LEU:HD11	56:b:628:MET:HB2	1.97	0.47
56:b:632:ILE:HA	56:b:635:GLN:HE21	1.79	0.47
57:c:641:MET:HB3	57:c:641:MET:HE3	1.84	0.47
26:T:28:VAL:HB	26:T:32:LEU:HD12	1.97	0.47
33:d:147:PRO:HD2	55:2:379:C:H5''	1.97	0.47
53:1:297:G:H22	53:1:300:U:H5'	1.79	0.47
53:1:1088:G:H2'	53:1:1089:A:C8	2.49	0.47
55:2:320:A:H5''	55:2:321:C:H5	1.80	0.47
55:2:1366:U:H2'	55:2:1367:G:C8	2.50	0.47
57:c:52:LEU:HD11	57:c:109:ILE:HD11	1.96	0.47
57:c:460:VAL:HG23	57:c:557:LEU:HD22	1.97	0.47
16:J:103:PRO:HB3	23:Q:68:ALA:HB2	1.97	0.47
19:M:34:LEU:HB2	19:M:118:MET:HG2	1.97	0.47
43:p:103:GLU:HG3	43:p:112:MET:HE1	1.97	0.47
53:1:1091:G:H2'	53:1:1092:G:C8	2.50	0.47
56:b:625:LEU:HA	56:b:628:MET:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:55:HIS:ND1	8:B:221:THR:CG2	2.69	0.47
19:M:55:THR:HA	19:M:58:VAL:CG2	2.45	0.47
37:j:122:HIS:C	37:j:123:VAL:CG1	2.86	0.47
55:2:347:G:H21	55:2:349:A:H62	1.61	0.47
55:2:1366:U:H2'	55:2:1367:G:H8	1.79	0.47
42:o:67:LEU:HD22	42:o:94:ILE:HG23	1.96	0.46
55:2:1174:A:H4'	55:2:1242:G:H4'	1.96	0.46
56:b:578:ALA:O	56:b:582:VAL:HG23	2.15	0.46
19:M:6:ARG:NH1	53:1:528:G:O3'	2.48	0.46
52:w:487:LEU:HD12	52:w:512:VAL:HG11	1.97	0.46
53:1:1045:C:H2'	53:1:1046:A:C8	2.51	0.46
54:4:66:C:H5''	54:4:67:G:O4'	2.16	0.46
55:2:1354:G:H1	55:2:1424:U:H3	1.63	0.46
56:b:566:LEU:HD12	56:b:685:GLN:HE22	1.80	0.46
10:D:213:PHE:O	10:D:217:ASN:HB2	2.16	0.46
53:1:2322:A:H61	53:1:2369:C:H1'	1.80	0.46
58:e:69:LEU:O	58:e:73:LYS:HG3	2.15	0.46
9:C:98:THR:HG22	9:C:120:ARG:HH21	1.81	0.46
40:m:97:ARG:HD3	51:Y:52:ASN:HD21	1.80	0.46
55:2:438:G:H1'	55:2:439:U:H5	1.80	0.46
56:b:555:LEU:HD22	56:b:695:LEU:HD13	1.96	0.46
58:e:338:ALA:HA	58:e:341:LYS:HD3	1.96	0.46
27:U:78:ILE:HG22	27:U:84:LYS:HA	1.96	0.46
46:s:4:SER:HB2	46:s:7:LYS:HG3	1.97	0.46
48:u:587:LYS:HD2	48:u:587:LYS:O	2.16	0.46
53:1:700:A:H3'	53:1:701:U:C6	2.51	0.46
53:1:774:G:C6	53:1:775:U:C4	3.03	0.46
56:b:459:ILE:O	56:b:463:LEU:HG	2.15	0.46
47:t:100:LYS:HB2	47:t:100:LYS:HE2	1.73	0.46
12:F:48:LEU:HA	12:F:61:THR:HA	1.96	0.46
33:d:122:ALA:HB2	33:d:131:LEU:HD22	1.97	0.46
41:n:57:VAL:HG11	55:2:1255:C:H5	1.81	0.46
53:1:540:G:N2	53:1:555:A:C2	2.78	0.46
56:b:668:VAL:HA	56:b:671:ILE:HG12	1.98	0.46
56:b:702:LYS:HE2	56:b:702:LYS:HB2	1.65	0.46
56:b:819:ASN:HD21	58:e:497:ASP:HA	1.80	0.46
57:c:97:ASN:HB3	57:c:608:LEU:HD13	1.98	0.46
13:G:53:GLU:HG3	13:G:55:LYS:HD3	1.97	0.46
14:H:140:VAL:HG23	14:H:143:LYS:HE3	1.98	0.46
34:f:123:PRO:HD2	45:r:131:LYS:HD2	1.97	0.46
45:r:93:LEU:O	48:u:635:TYR:OH	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:w:329:THR:OG1	52:w:330:HIS:N	2.48	0.46
53:1:123:G:H21	54:4:26:A:N6	2.14	0.46
53:1:703:C:C4	53:1:704:U:C4	3.03	0.46
3:5:14:A:H2'	3:5:35:A:H2	1.81	0.45
15:I:114:LEU:HD22	15:I:163:ILE:HB	1.98	0.45
44:q:37:THR:HG22	44:q:43:VAL:HG12	1.98	0.45
52:w:334:LYS:HE2	57:c:375:LYS:NZ	2.31	0.45
53:1:1246:U:H2'	53:1:1247:A:C8	2.51	0.45
56:b:263:ASN:H	56:b:296:ILE:HD12	1.81	0.45
40:m:154:LYS:HB2	40:m:154:LYS:HE2	1.68	0.45
52:w:491:MET:HE2	52:w:501:PHE:CE2	2.52	0.45
54:4:257:U:H3	54:4:268:G:H1	1.63	0.45
2:3:82:U:H2'	2:3:83:U:C6	2.50	0.45
37:j:123:VAL:O	37:j:123:VAL:HG22	2.17	0.45
53:1:161:U:H4'	53:1:894:G:H4'	1.99	0.45
55:2:347:G:N2	55:2:366:G:H22	2.15	0.45
55:2:492:A:H2'	55:2:493:G:C8	2.51	0.45
32:a:88:GLN:HE21	49:v:174:LEU:HD11	1.82	0.45
42:o:131:ARG:HA	42:o:131:ARG:HD3	1.84	0.45
53:1:1438:A:H2'	53:1:1439:A:C8	2.52	0.45
57:c:567:GLY:HA2	57:c:570:LYS:HB2	1.98	0.45
47:t:95:THR:HG23	47:t:147:LEU:HD11	1.99	0.45
55:2:892:A:H2'	55:2:893:U:C6	2.52	0.45
56:b:775:PHE:HZ	58:e:252:ASN:O	1.98	0.45
14:H:51:LYS:HA	14:H:54:LYS:HZ3	1.81	0.45
36:h:101:LYS:HB2	36:h:101:LYS:HE2	1.74	0.45
53:1:470:U:H2'	53:1:471:C:C6	2.51	0.45
53:1:772:G:C5	53:1:773:C:C5	3.03	0.45
57:c:615:VAL:HG21	57:c:640:LEU:HD11	1.99	0.45
9:C:93:ILE:HG21	9:C:142:LEU:HD11	1.97	0.45
39:l:17:LYS:H	39:l:17:LYS:HG2	1.60	0.45
45:r:91:ILE:HG13	48:u:631:TYR:HB2	1.98	0.45
53:1:254:U:H3	53:1:312:A:N6	2.10	0.45
53:1:660:A:H2'	53:1:661:A:C8	2.52	0.45
53:1:857:U:H2'	53:1:858:U:C6	2.51	0.45
55:2:57:U:H2'	55:2:58:G:C8	2.52	0.45
56:b:531:ARG:HB2	56:b:720:ILE:HG21	1.97	0.45
38:k:87:VAL:HG21	38:k:98:ILE:HD11	1.98	0.45
52:w:337:SER:HB2	52:w:369:VAL:HA	1.99	0.45
52:w:366:GLU:HB2	52:w:370:LEU:HD12	1.99	0.45
55:2:311:C:H2'	55:2:312:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:58:LEU:HD13	12:F:104:VAL:HG12	1.98	0.45
33:d:11:VAL:O	33:d:15:ILE:HB	2.17	0.45
52:w:508:GLU:HB3	52:w:510:THR:HG23	1.98	0.45
53:1:1432:U:H2'	53:1:1433:C:H6	1.81	0.45
53:1:2377:G:H2'	53:1:2378:A:C8	2.52	0.45
55:2:444:G:H2'	55:2:445:A:H8	1.82	0.45
56:b:695:LEU:HD21	58:e:319:LEU:HD21	1.98	0.45
15:I:154:THR:HG23	53:1:742:U:H4'	1.99	0.45
24:R:119:HIS:CD2	24:R:120:GLU:OE2	2.70	0.45
28:V:53:VAL:HG21	28:V:59:VAL:HG23	1.99	0.45
49:v:243:GLU:O	49:v:247:ILE:HG12	2.16	0.45
55:2:896:U:H2'	55:2:897:G:C8	2.51	0.45
58:e:635:SER:HB3	58:e:638:ASN:HB2	1.99	0.45
32:a:143:LYS:HB2	32:a:143:LYS:HE2	1.76	0.44
53:1:771:A:C8	53:1:772:G:H1'	2.50	0.44
53:1:2287:C:H2'	53:1:2288:U:C6	2.52	0.44
55:2:1454:U:H2'	55:2:1455:2MG:C8	2.52	0.44
58:e:360:LYS:HE3	58:e:360:LYS:HB3	1.79	0.44
8:B:97:ARG:HG3	8:B:103:LYS:HD3	1.98	0.44
14:H:62:ARG:HB3	14:H:157:GLU:HB2	2.00	0.44
15:I:69:ASN:H	15:I:101:PHE:HE2	1.66	0.44
15:I:166:THR:HA	53:1:748:A:H61	1.82	0.44
16:J:111:MET:HE3	16:J:111:MET:HB3	1.89	0.44
40:m:155:THR:HA	55:2:1166:C:H4'	1.98	0.44
53:1:314:U:H2'	53:1:315:C:C6	2.52	0.44
53:1:711:A:H2'	53:1:712:C:C6	2.52	0.44
53:1:2287:C:H2'	53:1:2288:U:H6	1.81	0.44
55:2:1156:C:H2'	55:2:1157:U:C6	2.52	0.44
56:b:425:LEU:HB3	56:b:851:LEU:HD12	1.98	0.44
58:e:669:LEU:HD23	58:e:670:PRO:HD2	1.99	0.44
15:I:54:ASN:ND2	15:I:56:ALA:HB2	2.31	0.44
24:R:141:GLU:HG2	24:R:143:LEU:HD22	1.98	0.44
26:T:38:LYS:O	26:T:42:GLU:HG3	2.17	0.44
33:d:101:GLY:HA3	50:x:108:GLU:HG3	1.98	0.44
33:d:177:TYR:O	33:d:180:MET:HG2	2.17	0.44
35:g:106:MET:HE3	35:g:106:MET:HA	1.98	0.44
55:2:988:G:H2'	55:2:989:A:H8	1.82	0.44
2:3:68:G:H3'	2:3:69:G:H8	1.83	0.44
32:a:71:VAL:HG23	56:b:316:ARG:HD2	2.00	0.44
44:q:44:VAL:HG22	44:q:67:MET:HG2	1.98	0.44
50:x:106:GLN:HB3	50:x:108:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:e:414:VAL:HA	58:e:417:PHE:HD2	1.81	0.44
2:3:14:U:O4'	2:3:71:G:O2'	2.36	0.44
24:R:92:PRO:HD3	24:R:177:ILE:HD12	1.99	0.44
52:w:522:GLU:HG2	52:w:526:LYS:HE2	1.98	0.44
53:1:2369:C:H2'	53:1:2370:A:C8	2.52	0.44
56:b:295:LYS:HE2	56:b:297:ILE:HD11	1.99	0.44
9:C:101:LYS:HG3	9:C:102:ARG:HD2	2.00	0.44
24:R:119:HIS:NE2	24:R:120:GLU:OE2	2.51	0.44
46:s:22:LEU:HD12	46:s:31:ILE:HD11	1.99	0.44
49:v:210:THR:HG22	49:v:212:LYS:H	1.83	0.44
52:w:192:GLU:HB2	52:w:195:ASP:HB2	1.99	0.44
53:1:608:C:H2'	53:1:609:A:C8	2.53	0.44
55:2:1008:U:H2'	55:2:1009:G:H8	1.83	0.44
57:c:417:GLN:OE1	58:e:409:GLU:OE2	2.36	0.44
14:H:128:VAL:HG11	14:H:176:CYS:HB2	2.00	0.44
21:O:118:VAL:HG23	21:O:145:PHE:HB3	2.00	0.44
55:2:454:C:H2'	55:2:455:A:C8	2.52	0.44
56:b:746:ARG:HA	56:b:749:LYS:HG2	1.98	0.44
57:c:85:LEU:H	57:c:85:LEU:HG	1.48	0.44
57:c:86:ILE:CG2	57:c:87:PRO:CD	2.90	0.44
59:i:21:LYS:HD3	59:i:95:ILE:HD13	2.00	0.44
20:N:126:LEU:HD12	20:N:132:VAL:HG22	2.00	0.44
29:W:106:ASP:OD2	29:W:109:LYS:HG2	2.17	0.44
53:1:442:U:H2'	53:1:443:C:C6	2.52	0.44
53:1:569:A:H2'	53:1:570:A:C8	2.52	0.44
53:1:608:C:H1'	53:1:644:G:C8	2.53	0.44
53:1:705:G:C6	53:1:771:A:C4	3.06	0.44
55:2:1374:G:H2'	55:2:1375:U:C6	2.53	0.44
56:b:468:LEU:O	56:b:472:LYS:HG2	2.18	0.44
7:9:30:ALA:HB1	53:1:2167:C:H5''	2.00	0.43
48:u:637:ALA:HB3	48:u:639:LEU:HG	2.00	0.43
53:1:768:U:H3'	53:1:769:A:C8	2.53	0.43
53:1:2476:U:H2'	53:1:2477:A:C8	2.53	0.43
55:2:1321:C:H2'	55:2:1322:C:H6	1.83	0.43
4:6:54:ILE:HB	4:6:97:HIS:HB3	1.99	0.43
14:H:50:GLY:O	14:H:54:LYS:NZ	2.50	0.43
33:d:84:ARG:NH1	55:2:377:C:OP2	2.51	0.43
55:2:1001:G:N7	55:2:1138:C:H5''	2.31	0.43
11:E:106:HIS:HB3	51:Y:57:MET:HE1	2.00	0.43
11:E:110:PRO:HG3	51:Y:78:TYR:HE2	1.82	0.43
26:T:20:LYS:HB3	26:T:20:LYS:HE2	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:32:LYS:HA	35:g:32:LYS:HD3	1.79	0.43
40:m:63:ILE:HB	40:m:66:ILE:HD12	2.00	0.43
41:n:49:GLN:NE2	46:s:13:ASP:OD2	2.37	0.43
53:1:2231:C:H2'	53:1:2232:G:C8	2.53	0.43
55:2:947:A:H2'	55:2:948:A:C8	2.54	0.43
58:e:248:LEU:C	58:e:268:LEU:HD21	2.43	0.43
11:E:114:ASP:OD1	40:m:107:ALA:CB	2.66	0.43
32:a:130:MET:HB3	56:b:319:LEU:HD11	2.00	0.43
36:h:8:ASN:HB2	55:2:540:G:H4'	1.99	0.43
38:k:68:ALA:HB1	38:k:101:ILE:CD1	2.48	0.43
49:v:221:VAL:HG23	49:v:225:GLY:HA2	2.00	0.43
52:w:316:LEU:HG	57:c:217:ILE:HD13	2.01	0.43
54:4:206:A:H5'	54:4:237:C:H4'	1.99	0.43
55:2:1019:C:H2'	55:2:1020:G:H8	1.84	0.43
8:B:82:ARG:HG2	8:B:84:GLU:HG2	2.00	0.43
35:g:45:ASN:HA	35:g:48:LYS:HE3	2.00	0.43
41:n:49:GLN:HE22	46:s:13:ASP:CG	2.21	0.43
46:s:22:LEU:HD22	46:s:27:LYS:HB3	2.00	0.43
52:w:178:ARG:HH12	56:b:909:LYS:HG2	1.83	0.43
53:1:707:A:C8	53:1:770:A:C2	3.06	0.43
53:1:1089:A:H2'	53:1:1090:A:C8	2.53	0.43
53:1:1426:C:H2'	53:1:1427:A:C5	2.53	0.43
56:b:447:MET:HG3	58:e:230:MET:HE3	2.01	0.43
56:b:638:VAL:HG13	56:b:640:LYS:HG3	2.00	0.43
57:c:413:LYS:HD3	58:e:412:ASP:CG	2.43	0.43
58:e:252:ASN:HD21	58:e:254:GLN:NE2	2.17	0.43
33:d:45:GLY:HA3	55:2:495:G:H5'	2.01	0.43
36:h:105:ARG:HD3	58:e:669:LEU:HG	2.00	0.43
39:l:89:ASP:HB2	55:2:476:A:H61	1.84	0.43
48:u:638:GLU:N	48:u:638:GLU:CD	2.76	0.43
52:w:516:LEU:HD13	57:c:463:PHE:CE2	2.54	0.43
54:4:139:A:H2'	54:4:140:A:C8	2.54	0.43
55:2:477:G:H2'	55:2:478:C:C6	2.54	0.43
8:B:136:ASN:O	34:f:156:ALA:CB	2.66	0.43
10:D:119:LYS:HA	10:D:119:LYS:HD3	1.89	0.43
32:a:243:MET:HE2	32:a:254:ILE:HB	2.01	0.43
49:v:250:GLU:HG2	49:v:260:ARG:HH22	1.84	0.43
52:w:287:GLU:HG2	52:w:288:MET:HG3	2.00	0.43
53:1:728:G:N2	53:1:756:A:O4'	2.52	0.43
53:1:744:A:H2'	53:1:745:A:C8	2.54	0.43
58:e:620:LEU:HD23	58:e:620:LEU:HA	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:62:GLU:H	4:6:62:GLU:HG2	1.68	0.43
13:G:73:LYS:HE3	13:G:79:ILE:HD13	2.00	0.43
28:V:47:LYS:HA	28:V:47:LYS:HD3	1.80	0.43
55:2:313:G:H2'	55:2:314:A:C8	2.53	0.43
55:2:951:A:C5	55:2:952:C:H1'	2.54	0.43
56:b:584:HIS:HA	58:e:379:VAL:HG21	2.01	0.43
58:e:540:ILE:HG12	58:e:550:VAL:HG22	2.00	0.43
4:6:44:LYS:HB3	4:6:51:ILE:HG12	2.01	0.43
21:O:104:LYS:O	21:O:108:GLU:HG3	2.19	0.43
32:a:191:ARG:HE	32:a:209:LEU:HD11	1.82	0.43
32:a:197:GLU:HB2	32:a:206:ILE:HB	2.01	0.43
36:h:2:LYS:HD3	36:h:2:LYS:HA	1.66	0.43
37:j:72:LEU:HB2	37:j:145:LEU:HD11	2.00	0.43
57:c:48:LEU:HD11	57:c:109:ILE:HG12	2.01	0.43
16:J:168:LYS:HB3	16:J:168:LYS:HE2	1.67	0.43
36:h:36:LEU:HD12	36:h:36:LEU:HA	1.92	0.43
45:r:78:TYR:O	45:r:86:LEU:CD2	2.67	0.43
51:Y:90:GLY:HA3	51:Y:93:ASN:HB2	2.01	0.43
53:1:1985:G:N3	53:1:2021:C:H2'	2.34	0.43
55:2:347:G:H22	55:2:366:G:H22	1.65	0.43
57:c:313:TRP:NE1	57:c:391:LYS:O	2.38	0.43
59:i:181:LYS:HB2	59:i:184:LYS:HB3	2.00	0.43
8:B:169:LYS:HG2	8:B:174:VAL:HG22	2.00	0.42
13:G:41:LEU:HD13	13:G:45:ILE:HD12	2.01	0.42
15:I:168:LYS:NZ	53:1:739:C:O4'	2.52	0.42
29:W:129:LYS:HE3	29:W:129:LYS:HB2	1.81	0.42
53:1:975:U:H2'	53:1:976:C:C6	2.53	0.42
55:2:513:A:H4'	55:2:514:U:H5''	2.00	0.42
55:2:885:G:H2'	55:2:886:C:C6	2.53	0.42
56:b:336:MET:HE3	56:b:336:MET:HB3	1.88	0.42
57:c:134:LYS:HB3	57:c:464:VAL:HG13	2.01	0.42
33:d:17:LYS:HB3	33:d:17:LYS:HE2	1.72	0.42
42:o:50:PHE:HB3	42:o:61:GLU:HB3	2.01	0.42
53:1:916:U:H2'	53:1:917:C:C6	2.54	0.42
53:1:2154:U:H2'	53:1:2155:C:C6	2.54	0.42
53:1:2155:C:H2'	53:1:2156:A:H8	1.84	0.42
55:2:553:U:H2'	55:2:554:A:C8	2.54	0.42
57:c:233:LYS:HB3	57:c:233:LYS:HE3	1.84	0.42
2:3:67:A:C3'	2:3:68:G:H5''	2.49	0.42
7:9:9:LYS:HB3	7:9:9:LYS:HE2	1.81	0.42
9:C:65:PRO:HB3	53:1:2322:A:C6	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:99:ALA:HB1	21:O:134:VAL:HG23	2.02	0.42
32:a:115:PHE:CZ	56:b:375:LYS:HD2	2.54	0.42
49:v:265:ASN:HA	49:v:268:THR:HG22	2.01	0.42
53:1:512:U:H2'	53:1:513:U:C6	2.54	0.42
53:1:1633:U:H3'	53:1:1634:C:H2'	2.01	0.42
56:b:330:ILE:HD12	56:b:330:ILE:H	1.85	0.42
57:c:86:ILE:HD12	57:c:86:ILE:HA	1.90	0.42
58:e:285:GLU:H	58:e:285:GLU:HG2	1.71	0.42
33:d:237:THR:HG22	33:d:250:PHE:HA	2.01	0.42
52:w:178:ARG:HH11	56:b:909:LYS:CE	2.11	0.42
53:1:729:A:N6	53:1:733:A:H62	2.16	0.42
55:2:42:G:H2'	55:2:43:G:C8	2.55	0.42
56:b:607:LYS:HB3	56:b:607:LYS:HE3	1.78	0.42
59:i:176:LYS:HB2	59:i:179:LEU:HD12	2.01	0.42
14:H:161:ALA:O	14:H:168:LEU:N	2.37	0.42
24:R:95:TRP:HB3	24:R:173:MET:HE2	2.02	0.42
25:S:69:HIS:HB2	53:1:144:G:H4'	2.02	0.42
49:v:218:ILE:HD13	49:v:230:LEU:HD22	2.01	0.42
53:1:1887:U:H2'	53:1:1888:U:H6	1.84	0.42
55:2:1026:U:O2'	58:e:641:ARG:NH1	2.52	0.42
55:2:1068:U:H2'	55:2:1069:U:C6	2.55	0.42
57:c:393:ARG:HD2	57:c:393:ARG:HA	1.80	0.42
12:F:188:ARG:CZ	12:F:194:ILE:HD12	2.49	0.42
13:G:53:GLU:HG3	13:G:55:LYS:CD	2.49	0.42
38:k:107:LYS:HD3	38:k:107:LYS:HA	1.81	0.42
46:s:22:LEU:HD23	46:s:22:LEU:HA	1.89	0.42
49:v:208:LEU:H	49:v:215:ALA:HB3	1.83	0.42
52:w:283:ASP:OD1	52:w:283:ASP:N	2.51	0.42
53:1:700:A:H3'	53:1:701:U:H6	1.85	0.42
53:1:1430:U:H2'	53:1:1431:C:C6	2.54	0.42
53:1:1881:A:H2'	53:1:1882:G:C8	2.54	0.42
53:1:2288:U:H2'	53:1:2289:U:C6	2.54	0.42
55:2:1194:A:H2'	57:c:27:GLN:HG2	2.00	0.42
56:b:714:VAL:HG22	58:e:408:LEU:HD22	2.00	0.42
56:b:716:GLU:O	56:b:720:ILE:HG12	2.19	0.42
57:c:74:PRO:HB2	57:c:102:ILE:HD11	2.01	0.42
57:c:419:ILE:HD13	57:c:419:ILE:HA	1.90	0.42
14:H:163:MET:HE3	14:H:163:MET:O	2.20	0.42
32:a:109:MET:SD	36:h:77:LYS:HD3	2.60	0.42
37:j:150:VAL:O	37:j:154:MET:HG3	2.20	0.42
41:n:64:MET:HE3	41:n:64:MET:HB2	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:t:139:LYS:HE3	47:t:139:LYS:HB2	1.80	0.42
55:2:444:G:H2'	55:2:445:A:C8	2.55	0.42
55:2:454:C:H2'	55:2:455:A:H8	1.84	0.42
56:b:549:LYS:HE2	56:b:549:LYS:HB2	1.80	0.42
56:b:732:ARG:HA	56:b:735:ARG:HG2	2.01	0.42
49:v:258:ARG:O	49:v:262:ILE:HG13	2.19	0.42
53:1:228:U:H2'	53:1:229:G:C8	2.54	0.42
55:2:275:G:H2'	55:2:276:A:C8	2.55	0.42
55:2:553:U:H2'	55:2:554:A:H8	1.84	0.42
55:2:1019:C:H2'	55:2:1020:G:C8	2.54	0.42
56:b:590:LYS:HB2	56:b:590:LYS:HE3	1.86	0.42
14:H:138:LEU:HD23	14:H:138:LEU:HA	1.91	0.42
15:I:140:VAL:HG13	15:I:163:ILE:HD11	2.01	0.42
26:T:15:TYR:CZ	30:X:78:GLN:HG2	2.55	0.42
29:W:158:GLU:H	29:W:158:GLU:HG3	1.70	0.42
32:a:73:PRO:HA	32:a:76:VAL:HG22	2.01	0.42
32:a:295:LYS:HE2	32:a:295:LYS:HB3	1.89	0.42
53:1:1012:A:H2'	53:1:1013:A:C8	2.54	0.42
15:I:112:ILE:HA	15:I:115:LYS:HB2	2.01	0.42
18:L:47:GLU:HG3	53:1:319:U:H5''	2.01	0.42
28:V:80:MET:HE3	28:V:90:THR:HG21	2.01	0.42
52:w:332:THR:HG23	52:w:334:LYS:H	1.85	0.42
55:2:285:A:H2'	55:2:286:G:H8	1.84	0.42
55:2:392:G:H2'	55:2:393:G:C8	2.54	0.42
56:b:581:LEU:HD12	56:b:581:LEU:HA	1.84	0.42
57:c:111:VAL:HG22	57:c:115:LEU:HD12	2.01	0.42
33:d:37:PHE:HD1	33:d:40:LYS:HD2	1.84	0.41
33:d:96:ILE:HG22	33:d:98:GLU:H	1.85	0.41
41:n:64:MET:HE2	41:n:77:GLY:HA3	2.02	0.41
45:r:115:LYS:HB3	45:r:115:LYS:HE2	1.89	0.41
53:1:766:G:H2'	53:1:767:G:H8	1.85	0.41
53:1:863:U:H5	53:1:900:A:N1	2.16	0.41
9:C:163:LYS:HE3	53:1:2365:U:OP1	2.19	0.41
33:d:11:VAL:HG12	33:d:15:ILE:HD12	1.93	0.41
37:j:57:MET:HE2	57:c:547:LYS:HZ1	1.84	0.41
37:j:63:LEU:HD23	37:j:63:LEU:HA	1.86	0.41
45:r:78:TYR:O	45:r:86:LEU:HD22	2.21	0.41
53:1:248:A:H2'	53:1:249:G:C8	2.55	0.41
53:1:1891:OMG:HM23	53:1:1891:OMG:H1'	1.70	0.41
53:1:2372:G:H2'	53:1:2373:G:C8	2.55	0.41
59:i:180:LYS:HB2	59:i:184:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:7:95:LYS:HD3	53:1:1026:C:O2'	2.21	0.41
26:T:1:MET:HE2	30:X:133:THR:HG22	2.01	0.41
32:a:235:VAL:HA	32:a:245:VAL:HG12	2.02	0.41
35:g:15:ASP:OD1	35:g:16:PRO:CD	2.66	0.41
35:g:48:LYS:HE3	35:g:48:LYS:HB3	1.79	0.41
40:m:58:VAL:HG21	55:2:1240:U:C5	2.55	0.41
43:p:40:ARG:HA	43:p:102:VAL:HG21	2.02	0.41
53:1:485:G:H4'	53:1:488:G:N1	2.35	0.41
58:e:252:ASN:HD21	58:e:254:GLN:CG	2.34	0.41
28:V:65:ILE:HG21	28:V:106:ILE:HG21	2.02	0.41
32:a:106:LEU:HD11	56:b:386:LYS:HG3	2.02	0.41
34:f:86:LEU:HD22	34:f:90:GLU:HB3	2.02	0.41
35:g:112:ARG:HB2	35:g:120:LYS:HE2	2.01	0.41
37:j:49:TYR:CE2	56:b:606:ASN:CB	3.03	0.41
37:j:49:TYR:HE2	56:b:606:ASN:HA	1.85	0.41
52:w:317:GLU:HG2	52:w:321:VAL:HB	2.03	0.41
52:w:529:VAL:HG21	57:c:542:LEU:HA	2.02	0.41
53:1:1053:U:H2'	53:1:1054:A:O4'	2.21	0.41
53:1:1372:C:H5	53:1:1381:G:H1	1.68	0.41
54:4:162:A:H2'	54:4:163:C:H6	1.86	0.41
57:c:494:ARG:HG2	57:c:501:TYR:CZ	2.55	0.41
2:3:49:U:H4'	21:O:128:HIS:HD2	1.84	0.41
45:r:93:LEU:O	48:u:635:TYR:CE2	2.74	0.41
53:1:1551:A:H2	55:2:1432:A:C2'	2.28	0.41
55:2:1469:G:H2'	55:2:1470:C:C6	2.56	0.41
25:S:105:ARG:HB2	53:1:1648:G:H5''	2.01	0.41
34:f:106:GLU:HB2	34:f:140:ARG:HH12	1.86	0.41
41:n:26:ALA:O	41:n:30:GLN:HG3	2.21	0.41
43:p:81:THR:HG21	43:p:105:LEU:HD21	2.03	0.41
52:w:178:ARG:HG3	56:b:909:LYS:NZ	2.35	0.41
53:1:774:G:C5	53:1:775:U:C5	3.08	0.41
55:2:35:C:H2'	55:2:36:G:H8	1.85	0.41
55:2:505:U:H2'	55:2:506:G:H8	1.86	0.41
59:i:123:THR:HA	59:i:126:ASN:HB2	2.02	0.41
8:B:82:ARG:HD2	8:B:84:GLU:HG2	2.03	0.41
10:D:127:MET:HG2	10:D:132:ARG:HG3	2.03	0.41
12:F:84:ARG:HE	53:1:695:U:H5''	1.85	0.41
32:a:160:ILE:HG21	32:a:207:VAL:HG11	2.03	0.41
44:q:31:LYS:HZ3	44:q:82:ARG:NH1	2.17	0.41
52:w:354:GLU:HA	52:w:357:LYS:HD2	2.02	0.41
53:1:576:A:H5''	53:1:1908:A:H61	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:717:A:H2'	53:1:718:G:C8	2.55	0.41
53:1:2059:U:H2'	53:1:2060:C:C6	2.55	0.41
55:2:1452:A:H2'	55:2:1453:C:C6	2.56	0.41
56:b:479:LYS:HE2	56:b:479:LYS:HB2	1.86	0.41
56:b:573:LEU:O	56:b:577:LYS:HG3	2.21	0.41
13:G:55:LYS:HE2	13:G:55:LYS:HA	2.03	0.41
18:L:52:ARG:HA	53:1:468:U:H2'	2.03	0.41
44:q:45:VAL:HG21	44:q:83:LEU:HD21	2.03	0.41
53:1:702:G:C5	53:1:774:G:N1	2.89	0.41
53:1:1499:G:H4'	53:1:2051:A:H4'	2.02	0.41
53:1:2289:U:H2'	53:1:2290:U:C6	2.56	0.41
55:2:1352:A:H2	55:2:1426:G:C2	2.38	0.41
57:c:309:ILE:HD12	57:c:391:LYS:HA	2.03	0.41
57:c:512:LEU:HD13	57:c:586:TYR:HB2	2.03	0.41
10:D:25:VAL:HG21	10:D:237:ALA:HB2	2.03	0.41
26:T:2:LEU:HD23	26:T:2:LEU:HA	1.90	0.41
27:U:153:LEU:HD23	27:U:153:LEU:HA	1.86	0.41
35:g:13:LEU:HD13	35:g:14:PRO:HD2	2.01	0.41
44:q:36:SER:HB3	44:q:44:VAL:HB	2.01	0.41
53:1:410:A:H2'	53:1:411:U:C6	2.56	0.41
53:1:2184:G:H1'	53:1:2286:C:H5'	2.02	0.41
54:4:267:U:H2'	54:4:268:G:C8	2.56	0.41
55:2:682:A:H2'	55:2:683:A:C8	2.55	0.41
56:b:260:VAL:HB	56:b:294:ALA:HB3	2.02	0.41
56:b:444:GLU:O	56:b:448:ILE:HD12	2.21	0.41
56:b:761:VAL:HG11	58:e:483:GLY:HA3	2.02	0.41
57:c:413:LYS:HD2	57:c:413:LYS:HA	1.92	0.41
2:3:60:A:H2'	2:3:61:A:C8	2.56	0.41
2:3:82:U:H2'	2:3:83:U:H6	1.85	0.41
3:5:25:A:H4'	3:5:27:A:N7	2.36	0.41
18:L:102:MET:HE2	53:1:287:A:C4'	2.51	0.41
32:a:115:PHE:HZ	56:b:375:LYS:HD2	1.86	0.41
32:a:169:PRO:HD2	32:a:172:GLU:HB2	2.03	0.41
38:k:36:THR:HG22	38:k:42:VAL:HG22	2.03	0.41
55:2:42:G:H2'	55:2:43:G:H8	1.86	0.41
55:2:947:A:H2'	55:2:948:A:H8	1.86	0.41
56:b:469:LEU:HD12	56:b:469:LEU:HA	1.93	0.41
56:b:577:LYS:NZ	58:e:386:LEU:HA	2.35	0.41
57:c:28:LYS:HG2	57:c:503:ALA:HB1	2.02	0.41
57:c:202:MET:SD	57:c:203:ARG:N	2.94	0.41
10:D:60:HIS:HB2	18:L:37:LEU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:179:LYS:HE2	11:E:179:LYS:HB2	1.69	0.40
15:I:161:ARG:HG2	53:1:741:U:H5'	2.03	0.40
19:M:37:GLN:HE22	19:M:130:LYS:HB3	1.84	0.40
27:U:157:LYS:HB2	27:U:157:LYS:HE2	1.68	0.40
39:I:30:ARG:HA	39:I:30:ARG:HD2	1.87	0.40
49:v:214:LEU:HD11	49:v:270:LEU:HD21	2.03	0.40
53:1:710:A:H3'	53:1:711:A:H8	1.85	0.40
53:1:2338:U:H2'	53:1:2339:C:C6	2.56	0.40
57:c:371:LYS:HD3	57:c:371:LYS:HA	1.78	0.40
57:c:655:GLN:HG3	57:c:670:TRP:HB3	2.04	0.40
14:H:140:VAL:HA	14:H:143:LYS:HG2	2.03	0.40
27:U:160:ARG:H	27:U:170:ASP:HB2	1.86	0.40
32:a:141:GLY:HA2	32:a:194:MET:HE3	2.03	0.40
42:o:77:HIS:HB2	55:2:694:U:H5'	2.03	0.40
45:r:82:LYS:HB2	45:r:82:LYS:HE2	1.80	0.40
52:w:224:PRO:HG3	52:w:246:PHE:HZ	1.86	0.40
52:w:243:PHE:HD1	52:w:243:PHE:HA	1.77	0.40
53:1:1703:C:H2'	53:1:1704:C:C6	2.56	0.40
53:1:2194:U:H2'	53:1:2195:U:C6	2.56	0.40
2:3:55:G:H21	11:E:27:HIS:CE1	2.39	0.40
14:H:49:LYS:O	14:H:53:GLU:HG3	2.22	0.40
27:U:74:ASP:HB2	27:U:90:ILE:HD12	2.03	0.40
35:g:59:VAL:O	35:g:63:GLU:HG2	2.21	0.40
37:j:75:ARG:HD3	37:j:139:LEU:HD13	2.03	0.40
37:j:108:LEU:HB2	37:j:137:HIS:HB2	2.04	0.40
53:1:64:C:H2'	53:1:65:A:H8	1.86	0.40
53:1:1053:U:H4'	53:1:1262:A:H4'	2.03	0.40
53:1:1246:U:H2'	53:1:1247:A:H8	1.85	0.40
53:1:2187:U:H2'	53:1:2188:G:C8	2.56	0.40
1:0:29:ARG:HA	1:0:29:ARG:HD2	1.86	0.40
1:0:46:LYS:HB2	1:0:46:LYS:HE2	1.84	0.40
11:E:58:LEU:HD23	11:E:58:LEU:HA	1.93	0.40
11:E:105:ILE:HG22	11:E:106:HIS:ND1	2.36	0.40
22:P:58:VAL:HB	22:P:66:ARG:HG3	2.03	0.40
32:a:221:ILE:O	32:a:225:GLN:HG3	2.21	0.40
33:d:121:MET:HG2	33:d:169:VAL:HG13	2.03	0.40
53:1:182:A:H4'	53:1:183:G:C8	2.56	0.40
53:1:191:A:H2'	53:1:192:A:C8	2.56	0.40
53:1:512:U:H2'	53:1:513:U:H6	1.86	0.40
53:1:800:U:H4'	53:1:801:A:O4'	2.21	0.40
53:1:899:A:H2'	53:1:900:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:1002:G:H1'	53:1:1256:A:C5	2.57	0.40
55:2:1194:A:H62	55:2:1217:G:N2	2.20	0.40
56:b:774:LYS:HE2	56:b:774:LYS:HB3	1.78	0.40
57:c:557:LEU:HD23	57:c:557:LEU:HA	1.92	0.40
58:e:252:ASN:CG	58:e:254:GLN:HG3	2.46	0.40
8:B:136:ASN:C	34:f:156:ALA:HB1	2.46	0.40
12:F:148:VAL:HG13	12:F:158:ILE:HG13	2.02	0.40
15:I:161:ARG:HG3	15:I:162:MET:HG2	2.02	0.40
22:P:100:VAL:HG11	53:1:2324:U:H5''	2.03	0.40
22:P:116:ARG:HD2	22:P:143:VAL:HG21	2.02	0.40
37:j:76:MET:HG2	37:j:164:VAL:HG22	2.03	0.40
53:1:299:A:H2'	53:1:301:A:C8	2.57	0.40
55:2:22:G:H2'	55:2:23:G:C8	2.56	0.40
55:2:353:G:H1	55:2:362:G:H1	1.69	0.40
55:2:1462:G:H2'	55:2:1463:G:C8	2.57	0.40
56:b:411:LYS:HA	56:b:411:LYS:HD3	1.75	0.40
57:c:289:LYS:HE2	57:c:289:LYS:HB3	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	45/66 (68%)	45 (100%)	0	0	100	100
4	6	56/101 (55%)	54 (96%)	2 (4%)	0	100	100
5	7	58/124 (47%)	57 (98%)	1 (2%)	0	100	100
6	8	66/114 (58%)	65 (98%)	1 (2%)	0	100	100
7	9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
8	B	274/278 (99%)	271 (99%)	3 (1%)	0	100	100
9	C	221/259 (85%)	217 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	D	214/243 (88%)	210 (98%)	4 (2%)	0	100	100
11	E	176/179 (98%)	170 (97%)	6 (3%)	0	100	100
12	F	175/207 (84%)	169 (97%)	6 (3%)	0	100	100
13	G	52/200 (26%)	51 (98%)	1 (2%)	0	100	100
14	H	139/235 (59%)	136 (98%)	3 (2%)	0	100	100
15	I	130/176 (74%)	118 (91%)	12 (9%)	0	100	100
16	J	171/225 (76%)	165 (96%)	6 (4%)	0	100	100
17	K	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
18	L	196/241 (81%)	188 (96%)	8 (4%)	0	100	100
19	M	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
20	N	115/173 (66%)	111 (96%)	4 (4%)	0	100	100
21	O	116/145 (80%)	114 (98%)	2 (2%)	0	100	100
22	P	128/153 (84%)	123 (96%)	5 (4%)	0	100	100
23	Q	109/112 (97%)	109 (100%)	0	0	100	100
24	R	113/179 (63%)	113 (100%)	0	0	100	100
25	S	113/175 (65%)	111 (98%)	2 (2%)	0	100	100
26	T	90/111 (81%)	88 (98%)	2 (2%)	0	100	100
27	U	130/170 (76%)	128 (98%)	2 (2%)	0	100	100
28	V	112/161 (70%)	108 (96%)	3 (3%)	1 (1%)	14	26
29	W	136/195 (70%)	134 (98%)	2 (2%)	0	100	100
30	X	104/134 (78%)	103 (99%)	1 (1%)	0	100	100
31	Z	39/98 (40%)	37 (95%)	2 (5%)	0	100	100
32	a	234/436 (54%)	225 (96%)	8 (3%)	1 (0%)	30	47
33	d	254/257 (99%)	246 (97%)	8 (3%)	0	100	100
34	f	101/171 (59%)	99 (98%)	2 (2%)	0	100	100
35	g	165/168 (98%)	163 (99%)	2 (1%)	0	100	100
36	h	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
37	j	120/169 (71%)	112 (93%)	5 (4%)	3 (2%)	4	6
38	k	115/130 (88%)	113 (98%)	2 (2%)	0	100	100
39	l	119/133 (90%)	114 (96%)	5 (4%)	0	100	100
40	m	112/164 (68%)	108 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	n	97/100 (97%)	96 (99%)	1 (1%)	0	100	100
42	o	99/141 (70%)	96 (97%)	3 (3%)	0	100	100
43	p	78/128 (61%)	78 (100%)	0	0	100	100
44	q	76/105 (72%)	74 (97%)	2 (3%)	0	100	100
45	r	79/137 (58%)	76 (96%)	3 (4%)	0	100	100
46	s	79/92 (86%)	77 (98%)	2 (2%)	0	100	100
47	t	117/166 (70%)	116 (99%)	1 (1%)	0	100	100
48	u	90/184 (49%)	84 (93%)	5 (6%)	1 (1%)	11	21
49	v	179/298 (60%)	163 (91%)	12 (7%)	4 (2%)	5	8
50	x	58/120 (48%)	57 (98%)	1 (2%)	0	100	100
51	Y	61/136 (45%)	51 (84%)	10 (16%)	0	100	100
52	w	361/560 (64%)	354 (98%)	7 (2%)	0	100	100
56	b	679/910 (75%)	656 (97%)	22 (3%)	1 (0%)	48	67
57	c	597/712 (84%)	579 (97%)	18 (3%)	0	100	100
58	e	528/673 (78%)	497 (94%)	30 (6%)	1 (0%)	43	62
59	i	147/191 (77%)	137 (93%)	10 (7%)	0	100	100
All	All	8250/11171 (74%)	7984 (97%)	254 (3%)	12 (0%)	49	67

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
37	j	51	ASP
37	j	123	VAL
32	a	71	VAL
37	j	50	VAL
49	v	142	PHE
49	v	131	VAL
56	b	347	THR
49	v	146	LEU
28	V	132	GLN
48	u	641	PRO
49	v	141	ASP
58	e	273	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	39/54 (72%)	38 (97%)	1 (3%)	40	66
4	6	53/90 (59%)	50 (94%)	3 (6%)	18	36
5	7	45/90 (50%)	43 (96%)	2 (4%)	25	47
6	8	55/92 (60%)	53 (96%)	2 (4%)	31	55
7	9	33/33 (100%)	33 (100%)	0	100	100
8	B	228/230 (99%)	227 (100%)	1 (0%)	84	92
9	C	176/204 (86%)	174 (99%)	2 (1%)	65	83
10	D	167/187 (89%)	164 (98%)	3 (2%)	51	75
11	E	156/157 (99%)	155 (99%)	1 (1%)	78	90
12	F	145/168 (86%)	140 (97%)	5 (3%)	32	57
13	G	46/167 (28%)	45 (98%)	1 (2%)	45	71
14	H	122/197 (62%)	121 (99%)	1 (1%)	73	88
15	I	106/138 (77%)	105 (99%)	1 (1%)	70	86
16	J	140/180 (78%)	136 (97%)	4 (3%)	37	63
17	K	101/101 (100%)	98 (97%)	3 (3%)	36	62
18	L	149/180 (83%)	147 (99%)	2 (1%)	61	81
19	M	110/111 (99%)	108 (98%)	2 (2%)	51	75
20	N	97/140 (69%)	96 (99%)	1 (1%)	68	85
21	O	93/116 (80%)	90 (97%)	3 (3%)	34	60
22	P	104/122 (85%)	103 (99%)	1 (1%)	68	85
23	Q	100/101 (99%)	98 (98%)	2 (2%)	48	73
24	R	97/145 (67%)	96 (99%)	1 (1%)	68	85
25	S	94/136 (69%)	92 (98%)	2 (2%)	47	72
26	T	85/89 (96%)	85 (100%)	0	100	100
27	U	109/137 (80%)	106 (97%)	3 (3%)	38	64
28	V	90/127 (71%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	W	116/164 (71%)	114 (98%)	2 (2%)	53	77
30	X	89/109 (82%)	87 (98%)	2 (2%)	45	71
31	Z	33/81 (41%)	33 (100%)	0	100	100
32	a	206/368 (56%)	202 (98%)	4 (2%)	50	74
33	d	233/234 (100%)	231 (99%)	2 (1%)	70	86
34	f	89/140 (64%)	88 (99%)	1 (1%)	65	83
35	g	146/147 (99%)	143 (98%)	3 (2%)	47	72
36	h	125/125 (100%)	123 (98%)	2 (2%)	55	78
37	j	107/143 (75%)	104 (97%)	3 (3%)	38	64
38	k	93/105 (89%)	91 (98%)	2 (2%)	45	71
39	l	103/111 (93%)	102 (99%)	1 (1%)	68	85
40	m	101/138 (73%)	100 (99%)	1 (1%)	68	85
41	n	88/89 (99%)	87 (99%)	1 (1%)	65	83
42	o	86/115 (75%)	84 (98%)	2 (2%)	44	70
43	p	69/108 (64%)	69 (100%)	0	100	100
44	q	69/90 (77%)	69 (100%)	0	100	100
45	r	73/128 (57%)	73 (100%)	0	100	100
46	s	71/80 (89%)	66 (93%)	5 (7%)	14	27
47	t	99/133 (74%)	98 (99%)	1 (1%)	68	85
48	u	85/149 (57%)	83 (98%)	2 (2%)	43	69
49	v	143/246 (58%)	139 (97%)	4 (3%)	38	64
50	x	50/95 (53%)	50 (100%)	0	100	100
51	Y	55/106 (52%)	52 (94%)	3 (6%)	19	38
52	w	287/434 (66%)	279 (97%)	8 (3%)	38	64
56	b	620/807 (77%)	609 (98%)	11 (2%)	51	75
57	c	541/634 (85%)	534 (99%)	7 (1%)	61	81
58	e	411/527 (78%)	405 (98%)	6 (2%)	57	79
59	i	126/159 (79%)	122 (97%)	4 (3%)	34	60
All	All	7054/9257 (76%)	6930 (98%)	124 (2%)	51	75

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	60	VAL
4	6	44	LYS
4	6	59	SER
4	6	81	ARG
5	7	80	ARG
5	7	120	SER
6	8	59	LYS
6	8	94	LEU
8	B	203	TYR
9	C	98	THR
9	C	229	GLU
10	D	30	SER
10	D	106	SER
10	D	203	THR
11	E	130	SER
12	F	43	THR
12	F	59	GLU
12	F	87	MET
12	F	132	VAL
12	F	152	LYS
13	G	44	ASP
14	H	89	ASN
15	I	170	MET
16	J	125	VAL
16	J	142	ARG
16	J	147	THR
16	J	220	LYS
17	K	90	GLU
17	K	113	LYS
17	K	116	SER
18	L	46	ASP
18	L	203	MET
19	M	5	LYS
19	M	118	MET
20	N	156	GLU
21	O	61	GLU
21	O	89	SER
21	O	111	LYS
22	P	112	GLU
23	Q	74	LEU
23	Q	94	VAL
24	R	148	VAL
25	S	97	VAL

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Mol	Chain	Res	Type
25	S	144	VAL
27	U	146	SER
27	U	148	VAL
27	U	163	VAL
29	W	94	LYS
29	W	129	LYS
30	X	31	LYS
30	X	71	GLU
32	a	101	THR
32	a	170	VAL
32	a	217	PHE
32	a	292	PHE
33	d	196	LEU
33	d	218	VAL
34	f	150	LEU
35	g	37	SER
35	g	93	LEU
35	g	141	GLU
36	h	42	GLN
36	h	63	THR
37	j	55	VAL
37	j	68	GLU
37	j	114	ILE
38	k	61	SER
38	k	88	THR
39	l	113	SER
40	m	137	VAL
41	n	11	LEU
42	o	118	SER
42	o	131	ARG
46	s	27	LYS
46	s	32	LYS
46	s	39	MET
46	s	63	SER
46	s	79	THR
47	t	164	VAL
48	u	620	GLU
48	u	636	SER
49	v	170	SER
49	v	207	VAL
49	v	208	LEU
49	v	221	VAL

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Mol	Chain	Res	Type
51	Y	49	VAL
51	Y	68	VAL
51	Y	96	LYS
52	w	264	VAL
52	w	330	HIS
52	w	355	LEU
52	w	372	PHE
52	w	446	THR
52	w	481	LYS
52	w	491	MET
52	w	492	SER
56	b	260	VAL
56	b	293	ILE
56	b	375	LYS
56	b	449	ILE
56	b	483	LEU
56	b	541	LEU
56	b	585	GLU
56	b	624	ILE
56	b	675	ILE
56	b	717	LEU
56	b	750	PHE
57	c	3	GLN
57	c	20	SER
57	c	237	LEU
57	c	303	LEU
57	c	323	LEU
57	c	389	LEU
57	c	452	THR
58	e	135	ILE
58	e	287	VAL
58	e	340	GLN
58	e	346	LEU
58	e	478	LEU
58	e	572	SER
59	i	21	LYS
59	i	96	VAL
59	i	160	LYS
59	i	169	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	21	HIS
1	0	26	HIS
8	B	119	GLN
8	B	155	GLN
8	B	189	ASN
9	C	89	ASN
11	E	48	GLN
12	F	153	ASN
20	N	61	ASN
23	Q	81	ASN
23	Q	108	GLN
25	S	124	ASN
26	T	53	ASN
26	T	55	HIS
27	U	150	HIS
28	V	74	ASN
29	W	45	ASN
29	W	67	ASN
33	d	46	GLN
33	d	141	ASN
34	f	171	GLN
36	h	51	GLN
37	j	82	GLN
37	j	90	GLN
38	k	29	HIS
40	m	94	ASN
41	n	48	GLN
42	o	81	ASN
42	o	103	GLN
46	s	65	GLN
48	u	591	GLN
49	v	239	GLN
52	w	466	GLN
56	b	273	GLN
56	b	275	GLN
56	b	317	GLN
56	b	557	ASN
56	b	626	ASN
56	b	766	GLN
57	c	559	ASN
57	c	679	GLN
58	e	254	GLN
58	e	275	ASN

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Mol	Chain	Res	Type
58	e	283	ASN
59	i	30	ASN
59	i	31	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	3	120/121 (99%)	22 (18%)	1 (0%)
3	5	46/47 (97%)	3 (6%)	0
53	1	2362/2375 (99%)	333 (14%)	5 (0%)
54	4	270/272 (99%)	35 (12%)	1 (0%)
55	2	1468/1470 (99%)	209 (14%)	3 (0%)
All	All	4266/4285 (99%)	602 (14%)	10 (0%)

All (602) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	3	9	G
2	3	14	U
2	3	16	G
2	3	19	C
2	3	25	G
2	3	33	C
2	3	35	A
2	3	36	A
2	3	37	U
2	3	42	C
2	3	54	U
2	3	57	G
2	3	66	G
2	3	68	G
2	3	71	G
2	3	78	G
2	3	87	G
2	3	102	A
2	3	107	A
2	3	108	G
2	3	113	A
2	3	122	G
3	5	16	U
3	5	34	G

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Mol	Chain	Res	Type
3	5	36	A
53	1	36	G
53	1	55	A
53	1	61	G
53	1	71	U
53	1	85	C
53	1	86	C
53	1	92	G
53	1	105	A
53	1	129	A
53	1	131	G
53	1	139	G
53	1	144	G
53	1	155	A
53	1	158	A
53	1	172	G
53	1	179	A
53	1	181	C
53	1	182	A
53	1	183	G
53	1	215	G
53	1	225	G
53	1	227	A
53	1	235	G
53	1	255	G
53	1	276	A
53	1	282	A
53	1	292	A
53	1	342	A
53	1	343	U
53	1	361	G
53	1	374	C
53	1	380	G
53	1	385	G
53	1	386	G
53	1	387	U
53	1	397	C
53	1	404	5MU
53	1	421	A
53	1	428	A
53	1	432	G
53	1	434	G

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Mol	Chain	Res	Type
53	1	439	A
53	1	441	U
53	1	442	U
53	1	446	A
53	1	448	C
53	1	449	G
53	1	462	G
53	1	469	C
53	1	484	U
53	1	502	A
53	1	505	A
53	1	517	G
53	1	523	C
53	1	524	U
53	1	544	C
53	1	546	U
53	1	547	C
53	1	549	C
53	1	550	G
53	1	554	U
53	1	555	A
53	1	556	C
53	1	566	G
53	1	569	A
53	1	573	C
53	1	574	A
53	1	590	U
53	1	596	A
53	1	597	A
53	1	606	G
53	1	621	G
53	1	634	G
53	1	639	A
53	1	643	A
53	1	648	A
53	1	649	G
53	1	656	A
53	1	672	U
53	1	673	G
53	1	682	G
53	1	685	G
53	1	686	A

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Mol	Chain	Res	Type
53	1	693	U
53	1	700	A
53	1	701	U
53	1	705	G
53	1	706	A
53	1	707	A
53	1	708	A
53	1	709	C
53	1	710	A
53	1	717	A
53	1	720	U
53	1	721	U
53	1	722	U
53	1	730	A
53	1	731	G
53	1	739	C
53	1	744	A
53	1	747	G
53	1	748	A
53	1	749	G
53	1	750	U
53	1	757	U
53	1	771	A
53	1	772	G
53	1	776	U
53	1	777	C
53	1	782	G
53	1	790	U
53	1	794	C
53	1	795	G
53	1	801	A
53	1	870	U
53	1	871	G
53	1	895	G
53	1	912	A
53	1	913	A
53	1	915	G
53	1	930	G
53	1	931	A
53	1	934	A
53	1	959	A
53	1	960	A

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Mol	Chain	Res	Type
53	1	970	G
53	1	981	A
53	1	988	U
53	1	1009	C
53	1	1011	U
53	1	1024	A
53	1	1038	U
53	1	1042	A
53	1	1051	A
53	1	1062	A
53	1	1070	A
53	1	1075	U
53	1	1076	G
53	1	1087	C
53	1	1104	G
53	1	1105	A
53	1	1112	U
53	1	1113	U
53	1	1115	G
53	1	1118	U
53	1	1119	U
53	1	1120	G
53	1	1125	G
53	1	1142	G
53	1	1147	A
53	1	1148	U
53	1	1149	A
53	1	1150	G
53	1	1153	A
53	1	1154	A
53	1	1155	A
53	1	1156	A
53	1	1158	G
53	1	1163	C
53	1	1166	G
53	1	1171	G
53	1	1173	G
53	1	1190	A
53	1	1197	C
53	1	1198	G
53	1	1199	A
53	1	1217	A

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Mol	Chain	Res	Type
53	1	1222	C
53	1	1223	A
53	1	1226	A
53	1	1235	U
53	1	1236	A
53	1	1257	C
53	1	1266	G
53	1	1267	A
53	1	1270	C
53	1	1277	A
53	1	1293	A
53	1	1306	G
53	1	1307	C
53	1	1313	A
53	1	1328	A
53	1	1333	G
53	1	1375	U
53	1	1379	A
53	1	1380	A
53	1	1393	U
53	1	1400	G
53	1	1409	A
53	1	1418	C
53	1	1420	A
53	1	1422	A
53	1	1436	C
53	1	1438	A
53	1	1452	U
53	1	1465	A
53	1	1484	A
53	1	1494	A
53	1	1502	A
53	1	1510	A
53	1	1511	A
53	1	1544	G
53	1	1551	A
53	1	1552	C
53	1	1553	U
53	1	1567	G
53	1	1568	G
53	1	1576	A
53	1	1593	U

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Mol	Chain	Res	Type
53	1	1602	G
53	1	1605	C
53	1	1608	A
53	1	1609	A
53	1	1610	G
53	1	1629	U
53	1	1630	G
53	1	1631	U
53	1	1634	C
53	1	1658	C
53	1	1661	G
53	1	1665	C
53	1	1669	6MZ
53	1	1670	A
53	1	1671	G
53	1	1672	A
53	1	1675	C
53	1	1682	C
53	1	1685	A
53	1	1694	C
53	1	1695	A
53	1	1699	A
53	1	1700	G
53	1	1701	A
53	1	1708	G
53	1	1715	G
53	1	1726	G
53	1	1727	G
53	1	1732	G
53	1	1837	A
53	1	1844	A
53	1	1850	G
53	1	1851	A
53	1	1865	A
53	1	1878	G
53	1	1879	G
53	1	1919	G
53	1	1923	U
53	1	1927	A
53	1	1928	A
53	1	1945	A
53	1	1947	G

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Mol	Chain	Res	Type
53	1	1948	G
53	1	1949	A
53	1	1951	A
53	1	1959	U
53	1	1960	U
53	1	1961	G
53	1	1962	A
53	1	1974	A
53	1	1975	A
53	1	1976	A
53	1	1985	G
53	1	1987	C
53	1	1990	C
53	1	2023	G
53	1	2025	C
53	1	2031	G
53	1	2042	G
53	1	2046	C
53	1	2054	G
53	1	2065	A
53	1	2069	G
53	1	2070	A
53	1	2075	A
53	1	2080	C
53	1	2081	U
53	1	2088	A
53	1	2110	G
53	1	2118	A
53	1	2131	U
53	1	2134	G
53	1	2138	OMC
53	1	2142	G
53	1	2145	G
53	1	2158	A
53	1	2160	C
53	1	2169	G
53	1	2175	G
53	1	2204	A
53	1	2206	A
53	1	2207	G
53	1	2213	C
53	1	2218	G

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Mol	Chain	Res	Type
53	1	2222	G
53	1	2225	U
53	1	2242	A
53	1	2249	U
53	1	2253	U
53	1	2269	U
53	1	2270	A
53	1	2281	A
53	1	2286	C
53	1	2294	A
53	1	2303	G
53	1	2308	U
53	1	2325	U
53	1	2329	U
53	1	2352	A
53	1	2353	A
53	1	2354	C
53	1	2355	G
53	1	2366	A
53	1	2367	C
53	1	2384	G
53	1	2388	A
53	1	2406	G
53	1	2418	A
53	1	2420	G
53	1	2430	U
53	1	2460	U
53	1	2461	A
53	1	2463	A
53	1	2471	U
53	1	2473	A
53	1	2476	U
53	1	2501	U
53	1	2513	A
53	1	2519	A
53	1	2520	C
53	1	2523	A
53	1	2530	U
53	1	2531	U
53	1	2532	U
54	4	8	G
54	4	26	A

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Mol	Chain	Res	Type
54	4	27	G
54	4	35	G
54	4	38	A
54	4	43	G
54	4	47	G
54	4	63	A
54	4	66	C
54	4	67	G
54	4	92	U
54	4	93	G
54	4	101	G
54	4	109	A
54	4	110	A
54	4	111	U
54	4	123	A
54	4	124	U
54	4	139	A
54	4	142	U
54	4	155	A
54	4	176	A
54	4	179	A
54	4	195	G
54	4	196	A
54	4	202	A
54	4	203	A
54	4	206	A
54	4	208	A
54	4	213	A
54	4	228	G
54	4	275	U
54	4	277	G
54	4	278	U
54	4	279	G
55	2	6	U
55	2	10	G
55	2	20	C
55	2	23	G
55	2	33	A
55	2	40	G
55	2	48	C
55	2	49	U
55	2	52	A

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Mol	Chain	Res	Type
55	2	55	C
55	2	59	C
55	2	80	U
55	2	86	U
55	2	106	A
55	2	107	C
55	2	116	A
55	2	117	C
55	2	128	G
55	2	130	G
55	2	137	A
55	2	149	C
55	2	168	C
55	2	169	A
55	2	181	A
55	2	183	A
55	2	191	A
55	2	192	A
55	2	195	G
55	2	204	G
55	2	220	U
55	2	222	G
55	2	226	G
55	2	231	U
55	2	235	G
55	2	242	G
55	2	243	C
55	2	256	C
55	2	259	G
55	2	265	G
55	2	282	A
55	2	297	A
55	2	304	C
55	2	305	A
55	2	320	A
55	2	327	G
55	2	328	C
55	2	330	G
55	2	343	U
55	2	348	C
55	2	349	A
55	2	360	G

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Mol	Chain	Res	Type
55	2	374	U
55	2	382	G
55	2	388	A
55	2	389	G
55	2	391	A
55	2	397	G
55	2	398	U
55	2	399	G
55	2	400	G
55	2	405	U
55	2	414	U
55	2	415	U
55	2	429	G
55	2	430	U
55	2	431	U
55	2	434	G
55	2	437	G
55	2	438	G
55	2	439	U
55	2	448	A
55	2	449	A
55	2	462	A
55	2	464	C
55	2	471	C
55	2	474	G
55	2	477	G
55	2	480	G7M
55	2	484	U
55	2	485	A
55	2	500	A
55	2	512	A
55	2	515	G
55	2	517	U
55	2	525	A
55	2	526	A
55	2	527	A
55	2	529	C
55	2	530	G
55	2	571	C
55	2	595	U
55	2	596	A
55	2	606	U

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Mol	Chain	Res	Type
55	2	607	U
55	2	619	G
55	2	620	G
55	2	640	G
55	2	657	G
55	2	665	G
55	2	675	A
55	2	677	U
55	2	678	G
55	2	688	C
55	2	703	A
55	2	709	A
55	2	714	G
55	2	731	A
55	2	747	U
55	2	748	A
55	2	766	G
55	2	769	A
55	2	771	C
55	2	775	G
55	2	786	G
55	2	792	G
55	2	793	C
55	2	794	A
55	2	816	U
55	2	830	U
55	2	836	G
55	2	860	A
55	2	872	G
55	2	880	C
55	2	904	A
55	2	906	U
55	2	907	U
55	2	915	A
55	2	917	G
55	2	918	C
55	2	921	A
55	2	922	G
55	2	923	A
55	2	939	G
55	2	949	G
55	2	950	A

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Mol	Chain	Res	Type
55	2	971	U
55	2	972	G
55	2	978	A
55	2	980	G
55	2	981	G
55	2	982	A
55	2	986	U
55	2	1001	G
55	2	1013	U
55	2	1018	U
55	2	1034	A
55	2	1036	A
55	2	1042	G
55	2	1043	U
55	2	1049	A
55	2	1053	A
55	2	1072	G
55	2	1073	U
55	2	1074	U
55	2	1079	U
55	2	1080	U
55	2	1081	U
55	2	1082	G
55	2	1096	A
55	2	1098	U
55	2	1099	G
55	2	1109	G
55	2	1122	G
55	2	1128	G
55	2	1134	A
55	2	1135	A
55	2	1138	C
55	2	1151	A
55	2	1165	A
55	2	1166	C
55	2	1176	A
55	2	1178	U
55	2	1191	C
55	2	1194	A
55	2	1195	A
55	2	1196	G
55	2	1212	U

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Mol	Chain	Res	Type
55	2	1218	A
55	2	1238	G
55	2	1240	U
55	2	1276	G
55	2	1278	A
55	2	1284	A
55	2	1291	G
55	2	1301	U
55	2	1303	U
55	2	1309	G
55	2	1317	C
55	2	1318	G
55	2	1321	C
55	2	1322	C
55	2	1337	A
55	2	1338	C
55	2	1358	G
55	2	1361	G
55	2	1380	A
55	2	1385	A
55	2	1390	U
55	2	1391	C
55	2	1431	A
55	2	1432	A
55	2	1436	G
55	2	1438	A
55	2	1442	A
55	2	1445	U
55	2	1456	G
55	2	1468	G
55	2	1469	G
55	2	1474	C

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	3	15	U
53	1	484	U
53	1	1154	A
53	1	1379	A
53	1	1961	G
53	1	2352	A

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Mol	Chain	Res	Type
54	4	277	G
55	2	191	A
55	2	595	U
55	2	980	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
53	2MG	1	1471	53	23,26,27	2.73	8 (34%)	32,38,41	2.76	12 (37%)
55	UR3	2	1437	55	19,22,23	2.75	8 (42%)	26,32,35	1.33	2 (7%)
55	MA6	2	1457	55	23,26,27	1.65	5 (21%)	34,38,41	3.36	11 (32%)
53	2MG	1	2085	53	23,26,27	2.63	8 (34%)	32,38,41	2.48	13 (40%)
55	2MG	2	912	55	23,26,27	2.83	8 (34%)	32,38,41	2.89	10 (31%)
53	5MC	1	1600	61,53	18,22,23	3.40	7 (38%)	26,32,35	0.98	2 (7%)
53	OMG	1	1891	61,53	23,26,27	2.34	7 (30%)	33,38,41	2.25	10 (30%)
53	6MZ	1	1669	53	22,25,26	4.32	13 (59%)	30,36,39	3.02	14 (46%)
55	G7M	2	480	61,55	23,26,27	2.25	7 (30%)	35,39,42	2.94	10 (28%)
55	5MC	2	913	55	18,22,23	3.33	7 (38%)	26,32,35	1.09	2 (7%)
53	OMC	1	2138	60,53	19,22,23	2.74	7 (36%)	26,31,34	0.84	0
53	OMU	1	2192	61,53	19,22,23	2.93	7 (36%)	26,31,34	1.76	5 (19%)
55	MA6	2	1458	55	23,26,27	1.69	5 (21%)	34,38,41	3.49	12 (35%)
55	4OC	2	1341	55	20,23,24	3.36	8 (40%)	26,32,35	0.84	1 (3%)
53	5MU	1	404	53	19,22,23	1.43	6 (31%)	28,32,35	2.20	7 (25%)
55	2MG	2	1455	55	23,26,27	2.78	7 (30%)	32,38,41	2.92	13 (40%)
53	5MU	1	1577	61,53	19,22,23	1.47	5 (26%)	28,32,35	2.22	6 (21%)
53	2MA	1	2143	60,61,53	22,25,26	4.02	7 (31%)	33,37,40	2.45	10 (30%)
53	H2U	1	2089	53	18,21,22	0.61	0	21,30,33	0.91	1 (4%)

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
53	2MG	1	1471	53	-	0/9/27/28	0/3/3/3
55	UR3	2	1437	55	-	0/7/25/26	0/2/2/2
55	MA6	2	1457	55	-	0/11/29/30	0/3/3/3
53	2MG	1	2085	53	-	1/9/27/28	0/3/3/3
55	2MG	2	912	55	-	0/9/27/28	0/3/3/3
53	5MC	1	1600	61,53	-	0/7/25/26	0/2/2/2
53	OMG	1	1891	61,53	-	3/9/27/28	0/3/3/3
53	6MZ	1	1669	53	-	2/9/27/28	0/3/3/3
55	G7M	2	480	61,55	-	3/7/25/26	0/3/3/3
55	5MC	2	913	55	-	1/7/25/26	0/2/2/2
53	OMC	1	2138	60,53	-	0/9/27/28	0/2/2/2
53	OMU	1	2192	61,53	-	0/9/27/28	0/2/2/2
55	MA6	2	1458	55	-	1/11/29/30	0/3/3/3
55	4OC	2	1341	55	-	1/9/29/30	0/2/2/2
53	5MU	1	404	53	-	0/7/25/26	0/2/2/2
55	2MG	2	1455	55	-	0/9/27/28	0/3/3/3
53	5MU	1	1577	61,53	-	0/7/25/26	0/2/2/2
53	2MA	1	2143	60,61,53	-	2/7/25/26	0/3/3/3
53	H2U	1	2089	53	-	0/7/38/39	0/2/2/2

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	1	2143	2MA	C4-N3	13.33	1.51	1.34
53	1	1669	6MZ	C6-N6	13.28	1.48	1.34
53	1	1600	5MC	C6-C5	8.24	1.48	1.34
55	2	913	5MC	C6-C5	7.96	1.47	1.34
53	1	2143	2MA	C2-N3	7.46	1.47	1.34
55	2	1341	4OC	C4-N3	7.44	1.45	1.32
55	2	912	2MG	C2-N2	7.44	1.50	1.33
53	1	1669	6MZ	O4'-C1'	7.37	1.59	1.42
55	2	912	2MG	C2-N3	7.25	1.45	1.31
55	2	1455	2MG	C2-N2	7.23	1.49	1.33
55	2	1455	2MG	C2-N3	7.15	1.45	1.31
53	1	1471	2MG	C2-N2	7.13	1.49	1.33
55	2	1437	UR3	C2-N1	7.01	1.48	1.38
53	1	1471	2MG	C2-N3	6.98	1.45	1.31
53	1	2085	2MG	C2-N2	6.95	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	1	1600	5MC	C4-N3	6.69	1.45	1.34
53	1	2192	OMU	C2-N3	6.61	1.49	1.38
55	2	1341	4OC	C2-N3	6.53	1.49	1.36
55	2	1341	4OC	C6-C5	6.49	1.50	1.35
55	2	913	5MC	C4-N3	6.41	1.45	1.34
53	1	2192	OMU	C2-N1	6.38	1.48	1.38
53	1	1891	OMG	C4-N3	6.24	1.49	1.34
55	2	480	G7M	C4-N3	6.23	1.49	1.34
53	1	1669	6MZ	C2'-C1'	-6.19	1.33	1.53
53	1	2143	2MA	C6-N1	6.15	1.43	1.35
53	1	2085	2MG	C2-N3	6.07	1.43	1.31
55	2	1437	UR3	C6-C5	6.04	1.49	1.35
53	1	1669	6MZ	O4'-C4'	-6.01	1.31	1.45
55	2	1341	4OC	C4-N4	5.93	1.48	1.35
53	1	1600	5MC	C2-N3	5.86	1.48	1.36
55	2	913	5MC	C2-N3	5.68	1.47	1.36
55	2	912	2MG	C4-N3	5.60	1.47	1.34
53	1	2138	OMC	C2-N3	5.60	1.47	1.36
53	1	2138	OMC	C6-C5	5.48	1.47	1.35
53	1	1471	2MG	C4-N3	5.46	1.47	1.34
53	1	2192	OMU	C6-C5	5.24	1.47	1.35
55	2	1455	2MG	C4-N3	5.23	1.46	1.34
53	1	1891	OMG	C2-N3	5.22	1.45	1.33
55	2	1437	UR3	C2-N3	5.16	1.49	1.39
53	1	2143	2MA	C2-N1	5.10	1.43	1.34
53	1	2143	2MA	C5-C6	5.00	1.54	1.41
53	1	1600	5MC	C6-N1	4.95	1.46	1.38
53	1	2085	2MG	C4-N3	4.92	1.46	1.34
55	2	1457	MA6	C6-N6	4.80	1.51	1.36
55	2	1458	MA6	C6-N6	4.70	1.50	1.36
55	2	913	5MC	C6-N1	4.68	1.46	1.38
55	2	1455	2MG	C2-N1	4.54	1.44	1.36
53	1	2138	OMC	C4-N3	4.48	1.43	1.34
53	1	1669	6MZ	C5-C4	-4.25	1.31	1.39
53	1	2138	OMC	C4-N4	4.24	1.43	1.33
55	2	913	5MC	C4-N4	4.18	1.45	1.34
55	2	480	G7M	C2-N2	4.16	1.44	1.34
55	2	912	2MG	C2-N1	4.15	1.43	1.36
53	1	1891	OMG	C2-N2	4.07	1.43	1.34
53	1	2138	OMC	C2-N1	4.06	1.48	1.40
53	1	2085	2MG	C2-N1	4.01	1.43	1.36
55	2	1341	4OC	C5-C4	3.96	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	1	1471	2MG	C2-N1	3.96	1.43	1.36
53	1	1669	6MZ	C5-N7	-3.93	1.31	1.39
53	1	2192	OMU	C4-N3	3.91	1.45	1.38
53	1	1600	5MC	C4-N4	3.86	1.44	1.34
55	2	1341	4OC	C2-N1	3.86	1.48	1.40
55	2	480	G7M	C2-N3	3.76	1.42	1.33
53	1	1669	6MZ	C8-N9	-3.73	1.30	1.37
55	2	480	G7M	C5-N7	-3.73	1.34	1.39
53	1	2143	2MA	C6-N6	-3.71	1.24	1.34
53	1	1669	6MZ	O3'-C3'	-3.68	1.34	1.43
53	1	1891	OMG	C5-N7	-3.57	1.32	1.39
53	1	2192	OMU	O4-C4	-3.47	1.17	1.24
53	1	2138	OMC	O2-C2	-3.35	1.17	1.23
55	2	1341	4OC	C6-N1	3.27	1.45	1.38
55	2	1458	MA6	C5-N7	-3.19	1.33	1.39
55	2	913	5MC	O2-C2	-3.14	1.17	1.23
55	2	913	5MC	C2-N1	3.10	1.46	1.40
53	1	1600	5MC	C2-N1	3.09	1.46	1.40
53	1	2085	2MG	C4-N9	-3.08	1.30	1.38
53	1	2192	OMU	O2-C2	-3.05	1.17	1.23
53	1	2192	OMU	C6-N1	3.02	1.45	1.38
53	1	1669	6MZ	C4-N9	-3.02	1.31	1.37
53	1	2138	OMC	C6-N1	2.96	1.45	1.38
53	1	1891	OMG	O6-C6	-2.95	1.18	1.23
55	2	1437	UR3	C6-N1	2.92	1.45	1.38
55	2	480	G7M	C6-N1	2.92	1.44	1.38
53	1	1577	5MU	C4-N3	-2.91	1.33	1.38
53	1	1669	6MZ	C6-N1	-2.89	1.30	1.35
53	1	1600	5MC	O2-C2	-2.89	1.18	1.23
53	1	404	5MU	C4-N3	-2.85	1.33	1.38
55	2	1458	MA6	C5-C4	-2.80	1.33	1.39
53	1	1669	6MZ	C9-N6	2.78	1.49	1.45
53	1	2143	2MA	C5-N7	-2.76	1.33	1.39
55	2	480	G7M	C5-C6	2.74	1.50	1.43
55	2	1457	MA6	C5-C4	-2.73	1.33	1.39
55	2	1455	2MG	C5-C6	2.72	1.54	1.44
55	2	1458	MA6	C10-N6	2.66	1.51	1.45
53	1	1577	5MU	C6-C5	2.65	1.39	1.34
53	1	404	5MU	C6-C5	2.62	1.38	1.34
55	2	1457	MA6	C5-N7	-2.62	1.34	1.39
55	2	1341	4OC	O2-C2	-2.60	1.18	1.23
55	2	912	2MG	C5-N7	-2.58	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2	1457	MA6	C10-N6	2.46	1.51	1.45
55	2	480	G7M	C2-N1	2.44	1.43	1.37
55	2	1437	UR3	O2-C2	-2.44	1.18	1.22
55	2	1458	MA6	C8-N9	-2.44	1.33	1.37
53	1	1577	5MU	C6-N1	-2.44	1.33	1.38
53	1	1577	5MU	C2-N3	-2.43	1.33	1.38
55	2	1455	2MG	C6-N1	2.40	1.43	1.38
53	1	2085	2MG	C5-C6	2.38	1.53	1.44
55	2	1457	MA6	C8-N9	-2.37	1.33	1.37
53	1	1669	6MZ	O2'-C2'	2.36	1.48	1.43
55	2	1437	UR3	O4-C4	-2.35	1.18	1.23
53	1	1471	2MG	C5-N7	-2.35	1.34	1.39
53	1	404	5MU	C6-N1	-2.34	1.34	1.38
53	1	1471	2MG	C5-C6	2.34	1.53	1.44
55	2	912	2MG	C6-N1	2.32	1.43	1.38
55	2	1437	UR3	C5-C4	2.29	1.49	1.43
53	1	404	5MU	C4-C5	2.25	1.48	1.44
55	2	912	2MG	C5-C6	2.24	1.52	1.44
53	1	1891	OMG	C5-C6	2.23	1.52	1.44
53	1	1891	OMG	C2-N1	2.22	1.43	1.37
55	2	1437	UR3	C4-N3	2.20	1.45	1.40
53	1	404	5MU	C2-N3	-2.19	1.34	1.38
53	1	1471	2MG	C6-N1	2.18	1.42	1.38
53	1	2085	2MG	C6-N1	2.17	1.42	1.38
53	1	1577	5MU	C4-C5	2.13	1.48	1.44
53	1	1471	2MG	C4-N9	-2.12	1.32	1.38
53	1	2085	2MG	C5-N7	-2.12	1.35	1.39
55	2	1455	2MG	C5-N7	-2.08	1.35	1.39
55	2	912	2MG	C4-N9	-2.07	1.32	1.38
53	1	404	5MU	C2-N1	2.03	1.41	1.38
53	1	1669	6MZ	C8-N7	2.01	1.35	1.31

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2	1458	MA6	N1-C6-N6	-12.91	102.97	117.08
55	2	1457	MA6	N1-C6-N6	-12.85	103.04	117.08
55	2	480	G7M	CN7-N7-C5	9.09	138.07	126.77
53	1	2143	2MA	C5-C4-N3	-8.26	117.90	127.19
55	2	912	2MG	C1'-N9-C8	-8.10	103.64	126.70
53	1	1669	6MZ	N1-C2-N3	-7.85	116.32	128.60
55	2	912	2MG	C1'-N9-C4	7.81	149.69	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	1	1471	2MG	C1'-N9-C8	-7.55	105.20	126.70
53	1	1471	2MG	C1'-N9-C4	7.21	147.90	126.50
53	1	1669	6MZ	C1'-N9-C8	-7.18	110.92	127.14
55	2	1455	2MG	C1'-N9-C8	-7.16	106.33	126.70
55	2	1455	2MG	C1'-N9-C4	7.11	147.61	126.50
55	2	1458	MA6	C5-C6-N6	7.05	137.59	125.30
55	2	480	G7M	CN7-N7-C8	-7.04	113.98	124.84
55	2	1457	MA6	C5-C6-N6	7.03	137.55	125.30
53	1	2085	2MG	C1'-N9-C8	-6.46	108.30	126.70
55	2	912	2MG	C2-N3-C4	6.45	120.04	112.04
55	2	1455	2MG	C2-N3-C4	6.30	119.85	112.04
55	2	480	G7M	C1'-N9-C4	6.27	145.12	126.50
53	1	1471	2MG	C2-N3-C4	6.10	119.61	112.04
53	1	1669	6MZ	C4-N9-C1'	6.06	141.03	126.59
53	1	1891	OMG	C5-C4-N3	-5.94	118.83	128.46
53	1	2085	2MG	C1'-N9-C4	5.92	144.09	126.50
53	1	2143	2MA	N3-C4-N9	5.79	135.02	126.99
55	2	480	G7M	C1'-N9-C8	-5.72	107.41	126.74
53	1	2085	2MG	C2-N3-C4	5.69	119.09	112.04
55	2	1457	MA6	N1-C2-N3	-5.63	119.80	128.60
53	1	1577	5MU	C4-N3-C2	-5.57	120.14	127.35
55	2	1458	MA6	N9-C8-N7	-5.54	106.33	113.91
55	2	1458	MA6	C5-C4-N3	-5.53	119.53	126.75
53	1	404	5MU	C4-N3-C2	-5.38	120.38	127.35
55	2	1458	MA6	N1-C2-N3	-5.30	120.31	128.60
53	1	2192	OMU	C4-N3-C2	-5.25	119.65	126.58
53	1	404	5MU	N3-C2-N1	5.18	121.76	114.89
55	2	1455	2MG	C2-N1-C6	-5.16	118.54	124.48
55	2	1455	2MG	CM2-N2-C2	-5.15	112.49	123.86
53	1	1577	5MU	N3-C2-N1	5.09	121.65	114.89
53	1	1891	OMG	C1'-N9-C4	-5.07	111.44	126.50
55	2	1457	MA6	N9-C8-N7	-5.05	107.00	113.91
53	1	1577	5MU	C5-C4-N3	4.97	119.56	115.31
53	1	1669	6MZ	N9-C8-N7	-4.91	107.20	113.91
55	2	1457	MA6	C5-C4-N3	-4.89	120.37	126.75
55	2	1437	UR3	C4-N3-C2	-4.88	119.96	124.56
53	1	1891	OMG	C1'-N9-C8	4.77	140.28	126.70
55	2	912	2MG	C5-C4-N3	-4.68	120.87	128.46
53	1	404	5MU	C5-C4-N3	4.57	119.21	115.31
55	2	1455	2MG	C5-C4-N3	-4.57	121.05	128.46
55	2	480	G7M	C2-N3-C4	4.54	120.38	112.30
55	2	1458	MA6	C4-C5-C6	4.50	120.91	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	1	1577	5MU	C5-C6-N1	-4.44	118.77	123.34
55	2	912	2MG	C2-N1-C6	-4.42	119.40	124.48
53	1	1471	2MG	C2-N1-C6	-4.36	119.46	124.48
55	2	1458	MA6	C5-N7-C8	4.31	109.63	103.51
53	1	1891	OMG	C2-N3-C4	4.27	119.91	112.30
53	1	1471	2MG	C5-C4-N3	-4.22	121.61	128.46
53	1	1891	OMG	N9-C4-N3	4.07	134.12	125.94
53	1	2143	2MA	N9-C8-N7	-4.06	108.36	113.91
55	2	1458	MA6	N3-C4-N9	4.06	133.77	127.08
53	1	1669	6MZ	C2-N3-C4	4.03	121.27	111.75
53	1	1577	5MU	O4-C4-C5	-4.00	120.26	124.90
53	1	404	5MU	C5-C6-N1	-3.92	119.31	123.34
55	2	480	G7M	C5-C6-N1	3.87	119.88	111.79
53	1	404	5MU	O4-C4-C5	-3.84	120.45	124.90
53	1	2192	OMU	C5-C4-N3	3.75	120.45	114.84
55	2	480	G7M	C5-C4-N3	-3.74	120.98	128.15
55	2	1457	MA6	C2-N1-C6	3.72	120.54	111.75
55	2	1457	MA6	C4-C5-C6	3.72	120.04	115.88
53	1	1669	6MZ	C6-C5-N7	3.71	136.41	132.39
53	1	2192	OMU	N3-C2-N1	3.71	119.81	114.89
55	2	1457	MA6	C4-N9-C8	3.59	109.62	105.73
55	2	1458	MA6	C2-N1-C6	3.50	120.02	111.75
55	2	1458	MA6	C4-N9-C8	3.49	109.51	105.73
55	2	1457	MA6	N3-C4-N9	3.49	132.83	127.08
53	1	2192	OMU	O4-C4-C5	-3.47	119.06	125.16
55	2	1457	MA6	C2-N3-C4	3.42	119.84	111.75
53	1	2085	2MG	C2-N1-C6	-3.42	120.54	124.48
55	2	480	G7M	O6-C6-C5	-3.42	120.35	128.06
53	1	2143	2MA	C4-N9-C1'	-3.41	118.46	126.59
55	2	1458	MA6	C2-N3-C4	3.40	119.79	111.75
53	1	1669	6MZ	C5-C4-N9	3.39	109.72	105.78
53	1	2143	2MA	N3-C2-N1	-3.38	119.50	125.72
53	1	1891	OMG	C2-N1-C6	-3.37	118.96	125.10
53	1	2085	2MG	N9-C8-N7	-3.36	107.06	113.39
55	2	1457	MA6	C5-N7-C8	3.34	108.25	103.51
53	1	2143	2MA	C5-N7-C8	3.23	108.10	103.51
53	1	1471	2MG	CM2-N2-C2	-3.17	116.85	123.86
53	1	1600	5MC	C5-C6-N1	-3.15	120.10	123.34
55	2	913	5MC	CM5-C5-C6	-3.03	118.80	122.85
53	1	1669	6MZ	C5-N7-C8	3.00	107.78	103.51
55	2	912	2MG	CM2-N2-C2	-3.00	117.23	123.86
55	2	1455	2MG	C5-C4-N9	2.99	111.05	105.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	1	2085	2MG	C6-C5-N7	2.96	135.75	130.25
53	1	2143	2MA	C1'-N9-C8	2.92	133.74	127.14
53	1	1669	6MZ	C5-C4-N3	-2.90	122.97	126.75
53	1	2089	H2U	C5-C4-N3	-2.88	113.42	116.65
55	2	912	2MG	O6-C6-C5	-2.87	118.99	126.60
55	2	480	G7M	C2-N1-C6	-2.85	119.91	125.10
55	2	913	5MC	C5-C6-N1	-2.84	120.42	123.34
53	1	2085	2MG	C5-C4-N3	-2.82	123.89	128.46
53	1	2085	2MG	C5-C4-N9	2.79	110.69	105.63
53	1	1471	2MG	N9-C8-N7	-2.79	108.14	113.39
53	1	2085	2MG	N1-C2-N3	-2.78	119.65	123.95
53	1	1471	2MG	C5-C6-N1	2.76	120.20	113.19
53	1	1669	6MZ	C4-C5-N7	-2.76	107.26	110.62
55	2	912	2MG	C5-C6-N1	2.74	120.15	113.19
55	2	1455	2MG	C4-C5-N7	-2.71	106.42	110.72
53	1	1891	OMG	C5-C6-N1	2.69	120.03	113.19
55	2	1455	2MG	C5-C6-N1	2.69	120.01	113.19
53	1	1891	OMG	N9-C8-N7	-2.67	108.37	113.39
55	2	1455	2MG	N9-C8-N7	-2.65	108.39	113.39
53	1	1669	6MZ	C9-N6-C6	-2.65	120.59	122.87
53	1	1669	6MZ	C2-N1-C6	2.59	123.93	115.25
53	1	404	5MU	C3'-C2'-C1'	2.53	106.24	101.43
55	2	480	G7M	N2-C2-N1	2.52	122.09	116.71
55	2	912	2MG	N1-C2-N3	-2.52	120.05	123.95
53	1	2143	2MA	C6-C5-C4	2.52	120.57	117.18
53	1	1577	5MU	O2-C2-N1	-2.49	119.48	122.79
53	1	2085	2MG	C4-C5-N7	-2.48	106.80	110.72
53	1	2085	2MG	C5-C6-N1	2.44	119.39	113.19
53	1	1891	OMG	O6-C6-C5	-2.42	120.19	126.60
55	2	1455	2MG	O6-C6-C5	-2.37	120.31	126.60
55	2	912	2MG	N9-C8-N7	-2.36	108.94	113.39
53	1	1471	2MG	O6-C6-C5	-2.36	120.35	126.60
53	1	404	5MU	O2-C2-N1	-2.36	119.66	122.79
53	1	1471	2MG	N1-C2-N3	-2.32	120.36	123.95
53	1	1471	2MG	C5-C4-N9	2.31	109.81	105.63
55	2	1458	MA6	C4-C5-N7	-2.31	107.81	110.62
53	1	2192	OMU	O2-C2-N1	-2.26	119.78	122.79
55	2	1341	4OC	C6-C5-C4	2.20	119.65	116.96
53	1	2085	2MG	O6-C6-C5	-2.20	120.77	126.60
55	2	1437	UR3	C1'-N1-C2	2.18	120.66	116.99
53	1	2085	2MG	CM2-N2-C2	-2.16	119.09	123.86
53	1	2143	2MA	CM2-C2-N3	2.14	120.50	117.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	1	1669	6MZ	C4-N9-C8	2.14	108.04	105.73
53	1	1471	2MG	C4-C5-N7	-2.13	107.34	110.72
55	2	1455	2MG	C8-N7-C5	2.13	108.10	104.24
53	1	1891	OMG	C8-N7-C5	2.12	108.08	104.24
55	2	1455	2MG	C6-C5-N7	2.10	134.15	130.25
53	1	1600	5MC	CM5-C5-C6	-2.09	120.06	122.85
53	1	2143	2MA	C2-N3-C4	2.05	122.03	116.99
53	1	1669	6MZ	C5'-C4'-C3'	-2.03	107.56	115.18

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	1	1669	6MZ	C3'-C4'-C5'-O5'
53	1	1891	OMG	C1'-C2'-O2'-CM2
53	1	1669	6MZ	O4'-C4'-C5'-O5'
55	2	480	G7M	C3'-C4'-C5'-O5'
55	2	480	G7M	C4'-C5'-O5'-P
53	1	1891	OMG	O4'-C4'-C5'-O5'
55	2	480	G7M	O4'-C4'-C5'-O5'
53	1	2085	2MG	C3'-C4'-C5'-O5'
53	1	1891	OMG	C3'-C4'-C5'-O5'
55	2	913	5MC	O4'-C4'-C5'-O5'
53	1	2143	2MA	O4'-C4'-C5'-O5'
55	2	1341	4OC	O4'-C4'-C5'-O5'
53	1	2143	2MA	C4'-C5'-O5'-P
55	2	1458	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	1	1891	OMG	1	0
53	1	1669	6MZ	1	0
55	2	1458	MA6	1	0
55	2	1341	4OC	1	0
55	2	1455	2MG	2	0
53	1	1577	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 461 ligands modelled in this entry, 461 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
53	1	12
55	2	2
58	e	1
54	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	e	187:GLY	C	227:ALA	N	24.83
1	4	259:U	O3'	266:A	P	16.47
1	1	1190:A	O3'	1196:U	P	16.31
1	1	1506:C	O3'	1509:G	P	16.24
1	1	1738:G	O3'	1830:G	P	15.47
1	1	828:U	O3'	840:U	P	14.87
1	1	194:A	O3'	201:G	P	12.10
1	1	2430:U	O3'	2449:A	P	11.17
1	1	308:A	O3'	312:A	P	9.40

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	590:U	O3'	592:C	P	9.07
1	1	586:A	O3'	588:U	P	8.90
1	2	76:G	O3'	79:A	P	8.36
1	1	1242:U	O3'	1245:A	P	7.61
1	1	502:A	O3'	504:G	P	5.44
1	1	139:G	O3'	141:U	P	5.03
1	2	1472:C	O3'	1473:A	P	3.18

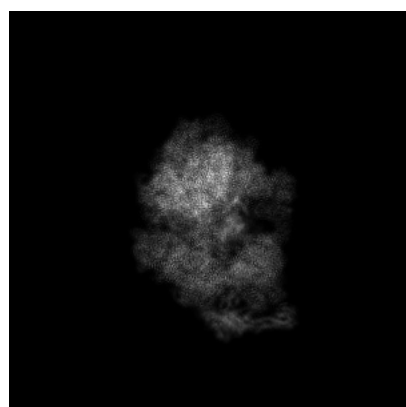
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56352. These allow visual inspection of the internal detail of the map and identification of artifacts.

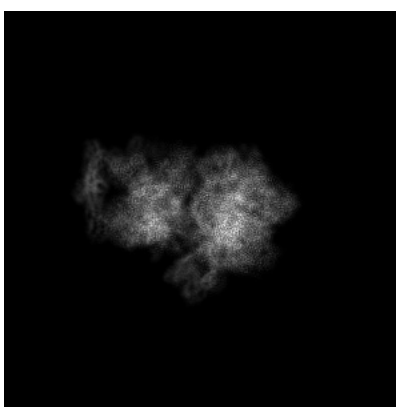
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

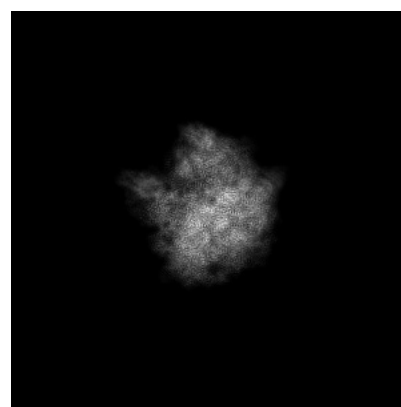
6.1.1 Primary map



X



Y



Z

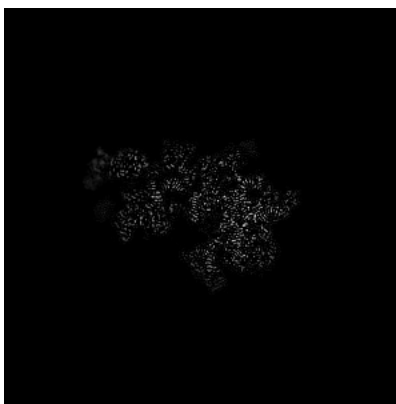
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

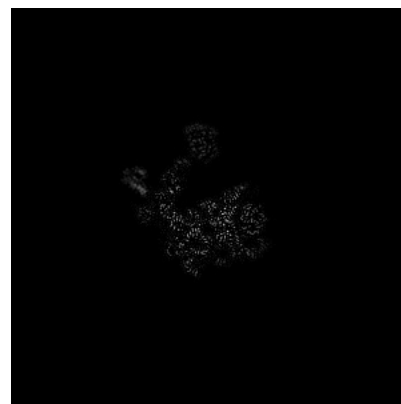
6.2.1 Primary map



X Index: 256



Y Index: 256

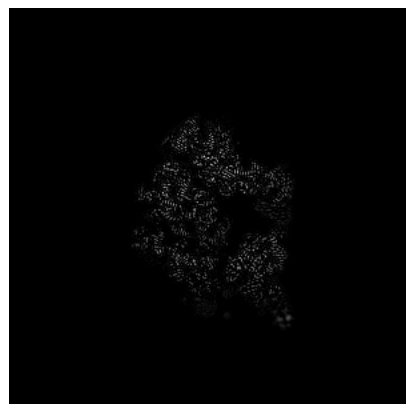


Z Index: 256

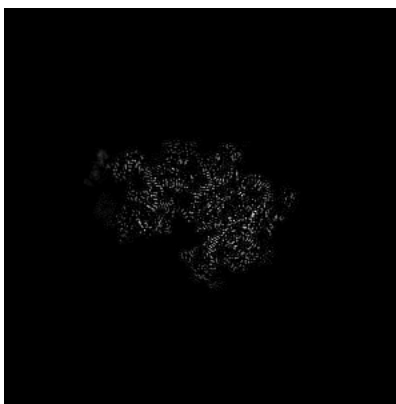
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

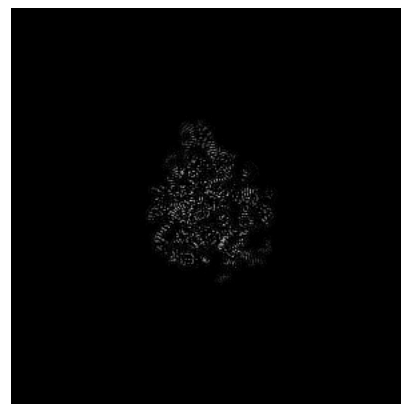
6.3.1 Primary map



X Index: 251



Y Index: 250

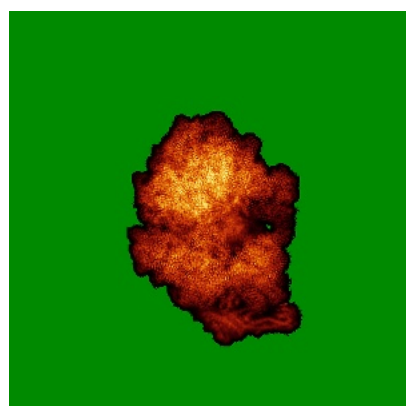


Z Index: 295

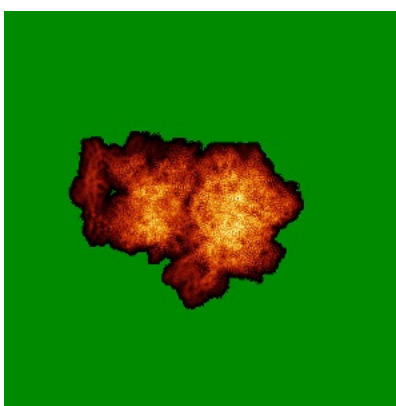
The images above show the largest variance slices of the map in three orthogonal directions.

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

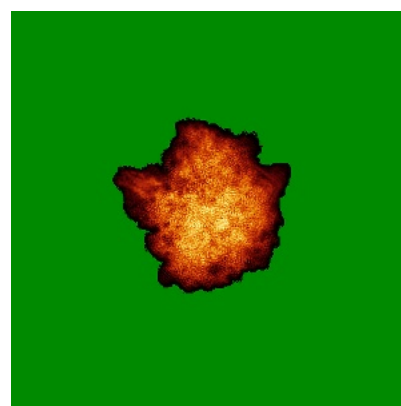
6.4.1 Primary map



X



Y

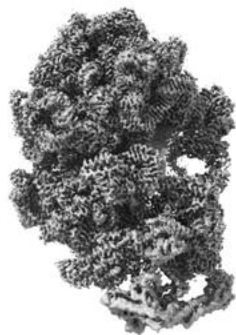


Z

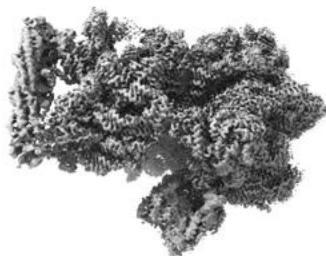
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.102. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

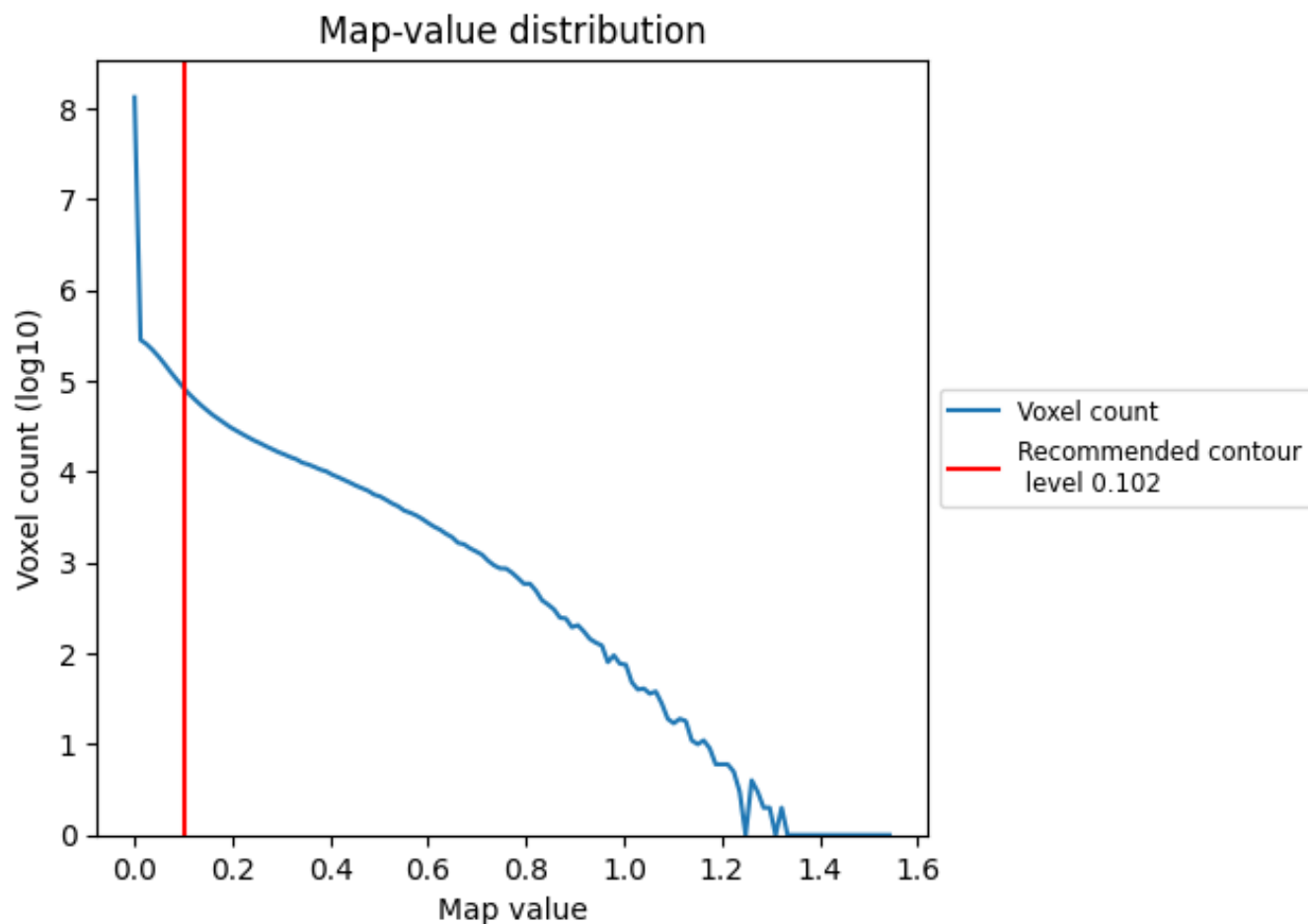
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

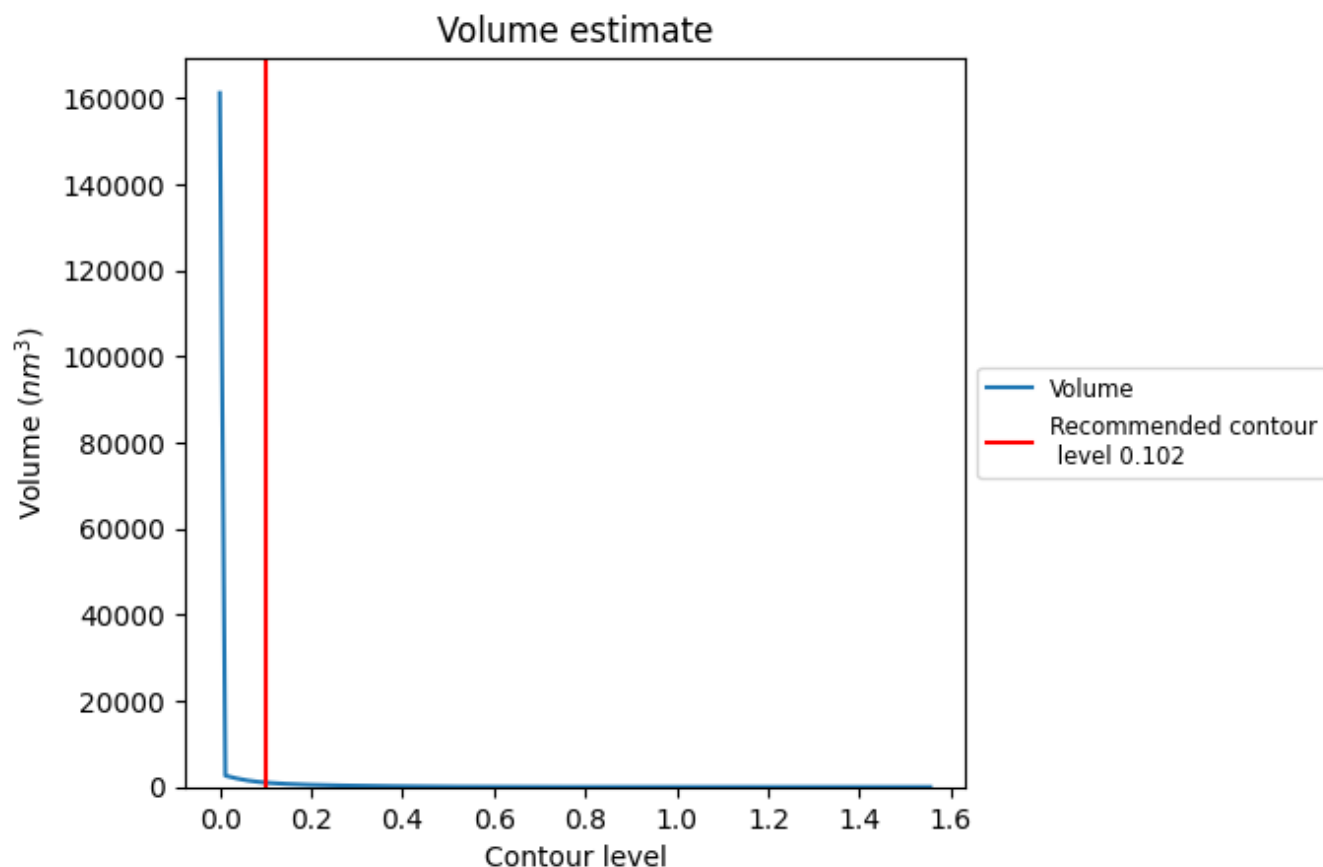
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

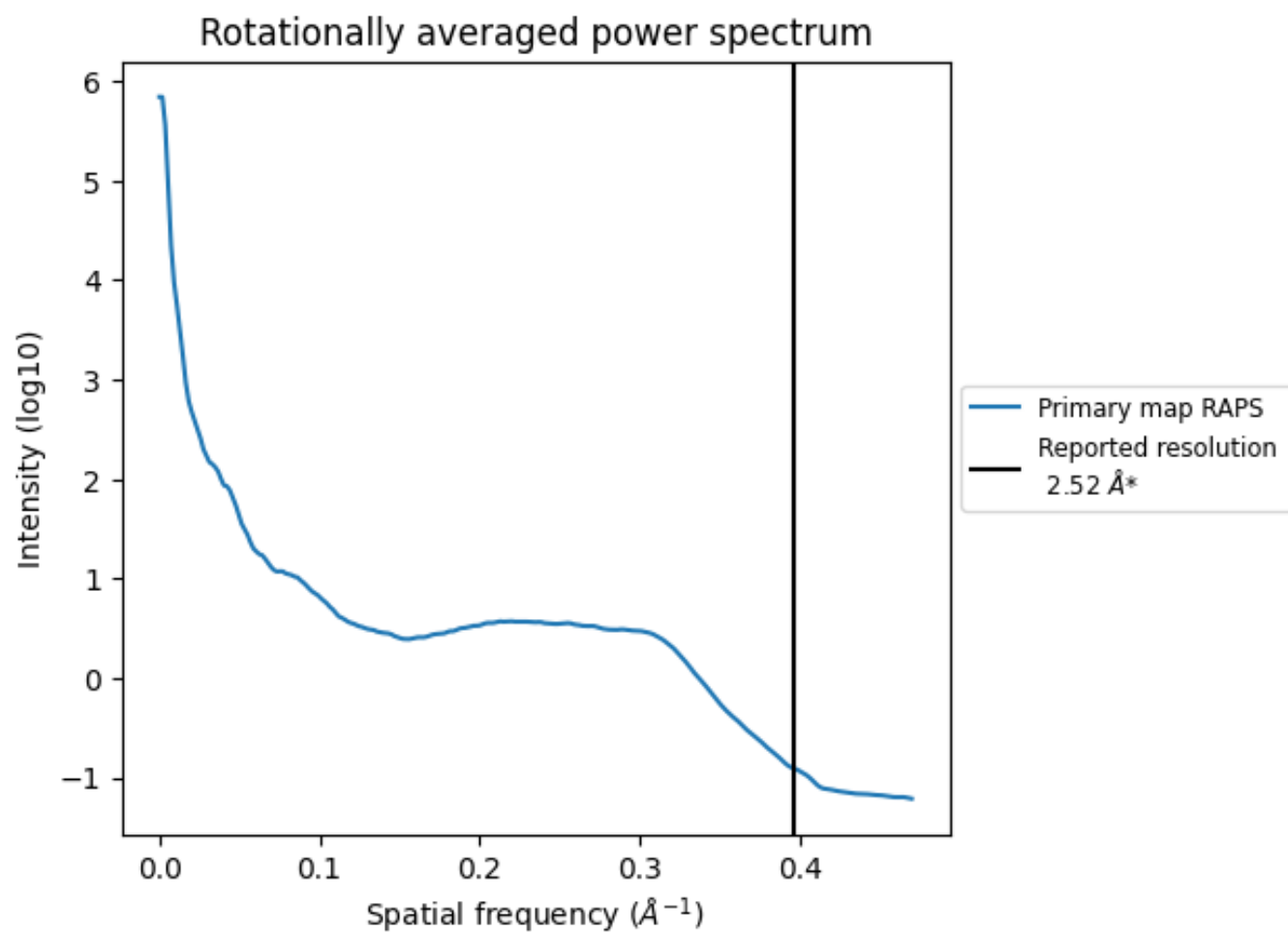
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1003 nm^3 ; this corresponds to an approximate mass of 906 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.397 Å⁻¹

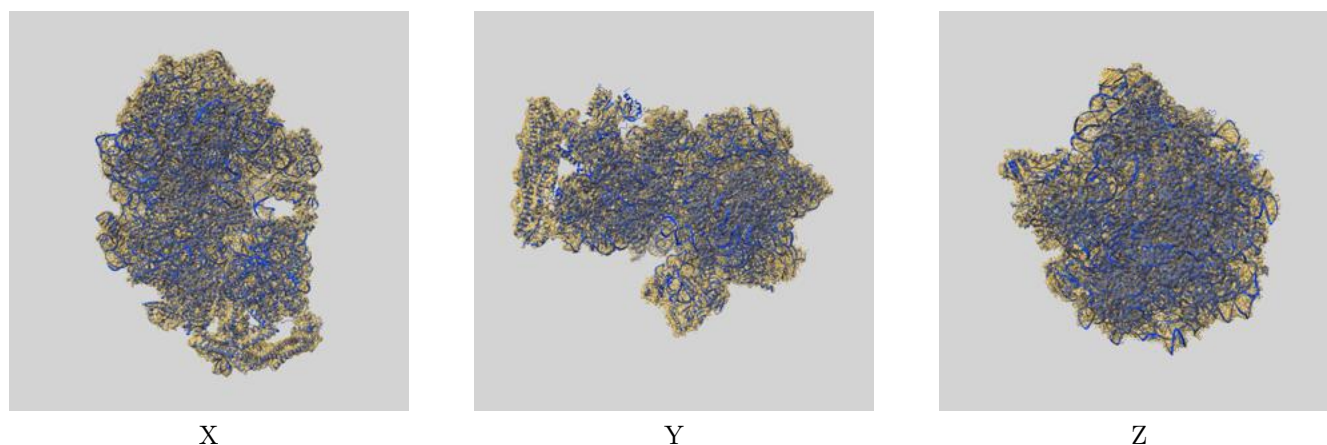
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

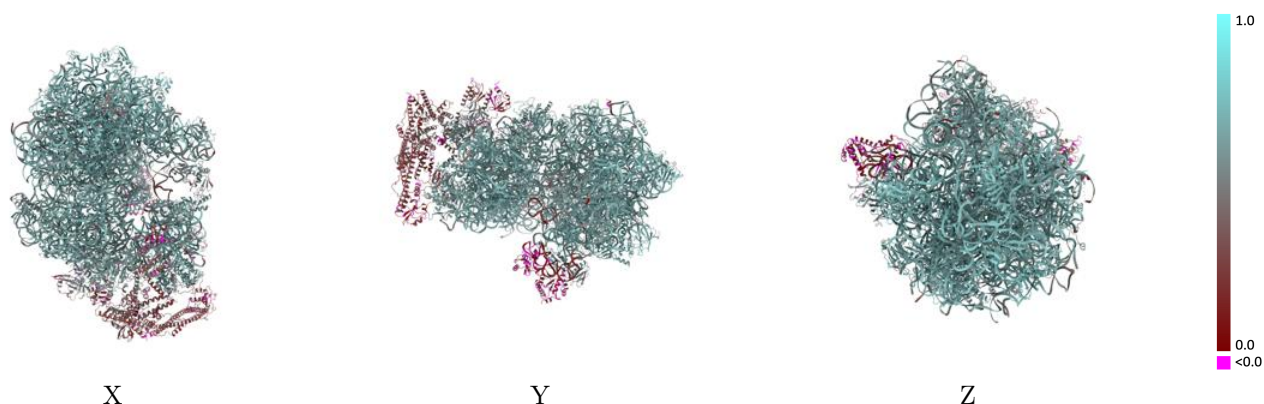
This section contains information regarding the fit between EMDB map EMD-56352 and PDB model 9TVU. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



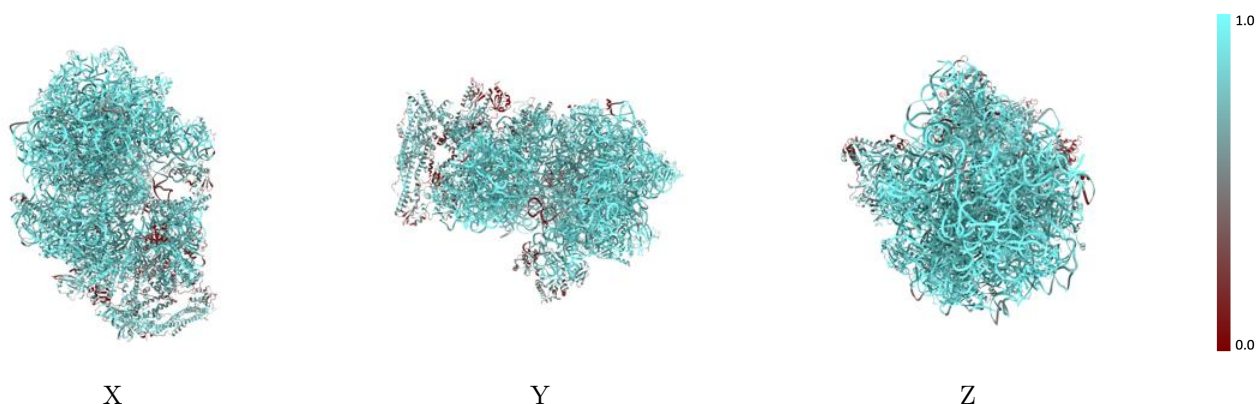
The images above show the 3D surface view of the map at the recommended contour level 0.102 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



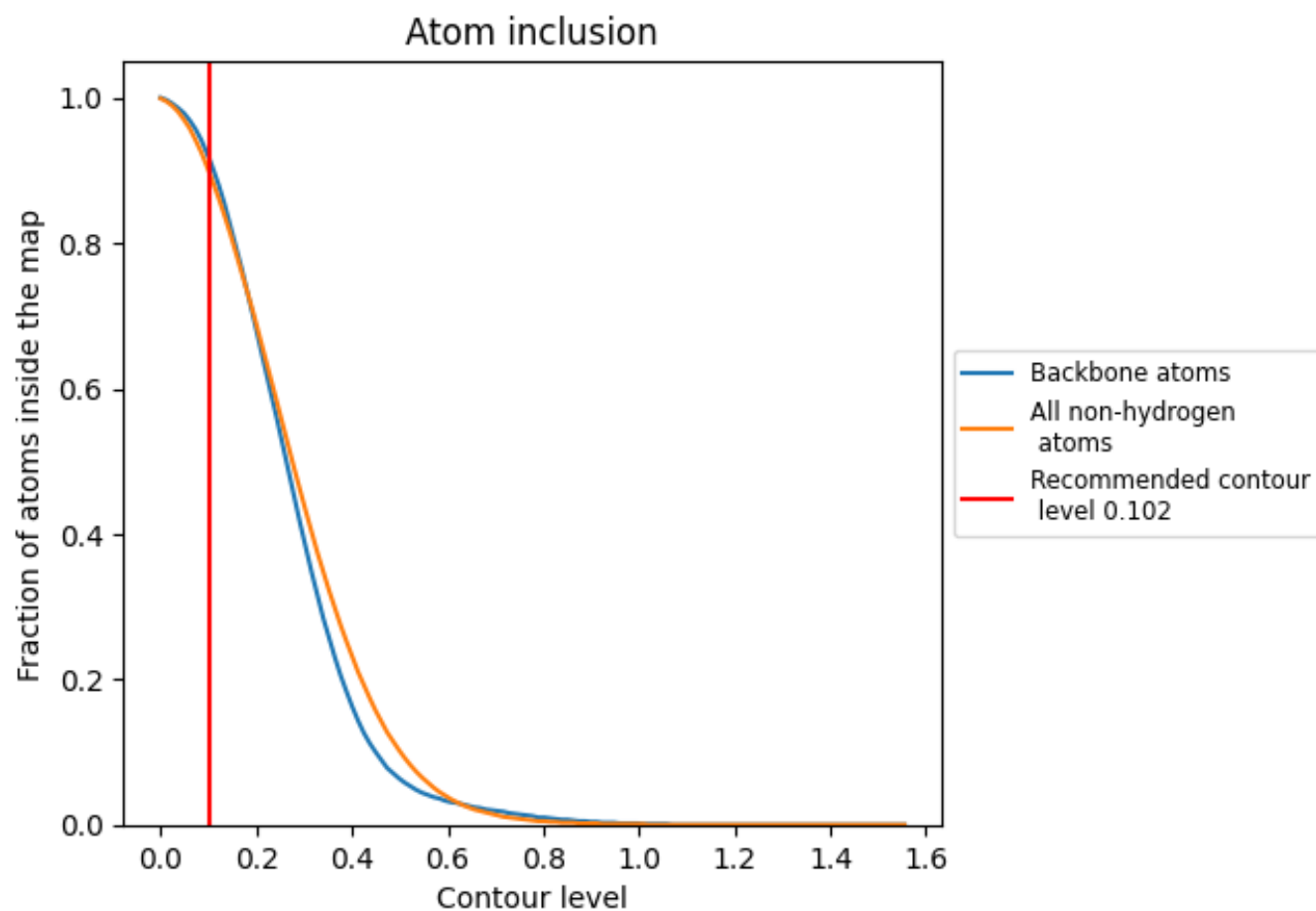
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.102).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.102) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8970	 0.6040
0	 0.9140	 0.6710
1	 0.9660	 0.6470
2	 0.9710	 0.6450
3	 0.9060	 0.5840
4	 0.9650	 0.6580
5	 0.9830	 0.6690
6	 0.9170	 0.6620
7	 0.9610	 0.6920
8	 0.9710	 0.6940
9	 0.9510	 0.6750
B	 0.9630	 0.6910
C	 0.9580	 0.6820
D	 0.9540	 0.6820
E	 0.6440	 0.5330
F	 0.7660	 0.5780
G	 0.7490	 0.5660
H	 0.5450	 0.0890
I	 0.4760	 0.0530
J	 0.9440	 0.6760
K	 0.9410	 0.6870
L	 0.9010	 0.6560
M	 0.9470	 0.6800
N	 0.9670	 0.6850
O	 0.8630	 0.6070
P	 0.8780	 0.6450
Q	 0.9860	 0.6970
R	 0.9470	 0.6830
S	 0.9330	 0.6720
T	 0.9520	 0.6690
U	 0.8880	 0.6500
V	 0.8690	 0.6140
W	 0.9170	 0.6600
X	 0.8940	 0.6540
Y	 0.4480	 0.4490



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Chain	Atom inclusion	Q-score
Z	 0.9280	 0.6680
a	 0.5110	 0.3570
b	 0.7340	 0.3830
c	 0.7670	 0.4910
d	 0.6570	 0.4990
e	 0.6830	 0.4120
f	 0.7870	 0.6200
g	 0.7200	 0.5590
h	 0.8980	 0.6370
i	 0.6650	 0.5200
j	 0.8510	 0.6160
k	 0.8470	 0.6310
l	 0.9310	 0.6620
m	 0.8390	 0.6170
n	 0.9390	 0.6610
o	 0.8470	 0.6200
p	 0.9180	 0.6520
q	 0.8610	 0.6250
r	 0.8680	 0.6390
s	 0.9220	 0.6540
t	 0.8080	 0.5960
u	 0.7330	 0.5940
v	 0.5190	 0.3490
w	 0.7130	 0.4060
x	 0.8810	 0.6410