



Full wwPDB EM Validation Report ⓘ

Jul 21, 2025 – 11:06 AM EDT

PDB ID : 9MKK / pdb_00009mkk
EMDB ID : EMD-48329
Title : Structure of arbekacin bound Escherichia coli 70S ribosome
Authors : Majumdar, S.; Parajuli, N.P.; Ge, X.; Emmerich, A.; Sanyal, S.
Deposited on : 2024-12-17
Resolution : 3.20 Å(reported)
Based on initial model : 7K00

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:

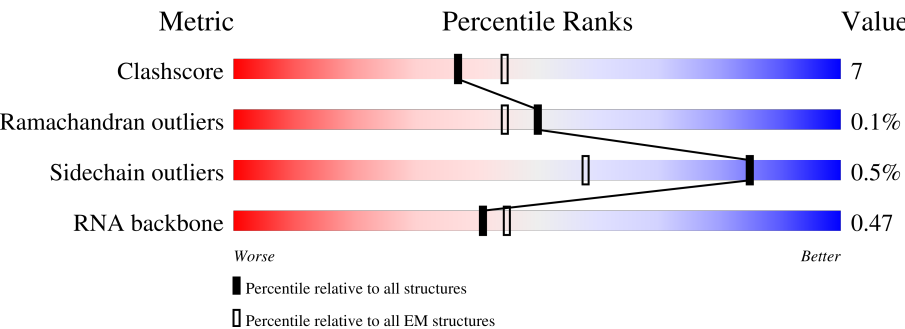
EMDB validation analysis : 0.0.1.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	0	55	<div> <div>69%</div> <div>24%</div> <div>7%</div> </div>
2	1	46	<div> <div>85%</div> <div>15%</div> </div>
3	2	65	<div> <div>74%</div> <div>25%</div> </div>
4	3	38	<div> <div>74%</div> <div>26%</div> </div>
5	4	70	<div> <div>14%</div> <div>56%</div> <div>30%</div> <div>14%</div> </div>
6	B	241	<div> <div>35%</div> <div>67%</div> <div>25%</div> <div>7%</div> </div>
7	C	233	<div> <div>5%</div> <div>70%</div> <div>18%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
8	D	206	
9	E	167	
10	F	135	
11	G	179	
12	H	130	
13	I	130	
14	J	103	
15	K	129	
16	L	124	
17	M	118	
18	N	101	
19	O	89	
20	P	82	
21	Q	84	
22	R	75	
23	S	92	
24	T	87	
25	U	71	
26	X	28	
27	Z	76	
28	b	120	
29	c	273	
30	d	209	
31	e	201	
32	f	179	

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Mol	Chain	Length	Quality of chain
33	g	177	
34	i	142	
35	j	123	
36	k	144	
37	l	136	
38	m	127	
39	n	117	
40	o	115	
41	p	118	
42	q	103	
43	s	100	
44	t	104	
45	u	94	
46	v	85	
47	w	78	
48	x	63	
49	y	59	
50	z	57	
51	A	1542	
52	a	2904	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 137440 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called 50S ribosomal protein L34.

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

- Molecule 3 is a protein called 50S ribosomal protein L35.

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

- Molecule 4 is a protein called 50S ribosomal protein L36.

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

- Molecule 5 is a protein called 50S ribosomal protein L31.

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

- Molecule 6 is a protein called 30S ribosomal protein S2.

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

- Molecule 7 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 8 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 10 is a protein called Small ribosomal subunit protein bS6.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	153	Total	C	N	O	S	0	0
			1197	747	228	218	4		

- Molecule 12 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	127	Total	C	N	O	S	0	0
			1019	632	206	179	2		

- Molecule 14 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 15 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	116	Total	C	N	O	S	0	0
			869	536	172	158	3		

- Molecule 16 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	122	Total	C	N	O	S	0	0
			944	583	195	162	4		

- Molecule 17 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 20 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 21 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 22 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 23 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 24 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 25 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 26 is a RNA chain called mRNA.

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

- Molecule 27 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 28 is a RNA chain called 5S rRNA.

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

- Molecule 29 is a protein called 50S ribosomal protein L2.

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

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	208	Total	C	N	O	S	0	0
			1556	974	286	292	4		

- Molecule 31 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 32 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 34 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	142	Total	C	N	O	S	0	0
			1123	711	209	199	4		

- Molecule 35 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	134	Total	C	N	O	S	0	0
			1055	675	200	175	5		

- Molecule 38 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 40 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	54	Total	C	N	O		0	0
			431	270	96	65			

- Molecule 42 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	92	Total	C	N	O	S	0	0
			730	461	138	130	1		

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 45 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 46 is a protein called Large ribosomal subunit protein bL27.

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

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	x	62	Total	C	N	O	S	0	0
			485	300	91	93	1		

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	y	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	z	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

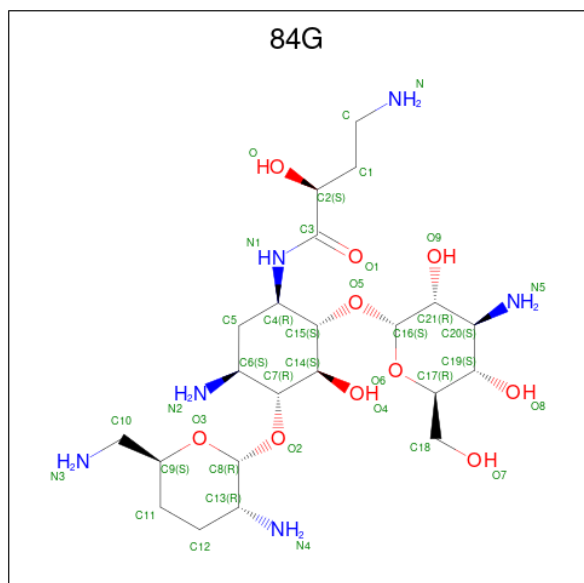
- Molecule 51 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	A	1512	Total	C	N	O	P	0	0
			32450	14473	5962	10503	1512		

- Molecule 52 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	a	2732	Total	C	N	O	P	0	0
			58675	26173	10829	18941	2732		

- Molecule 53 is Arbekacin (CCD ID: 84G) (formula: $C_{22}H_{44}N_6O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
53	A	1	Total	C	N	O	0
			38	22	6	10	

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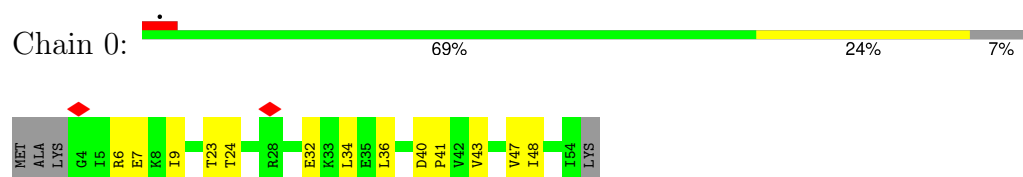
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
53	a	1	38	22	6	10	0

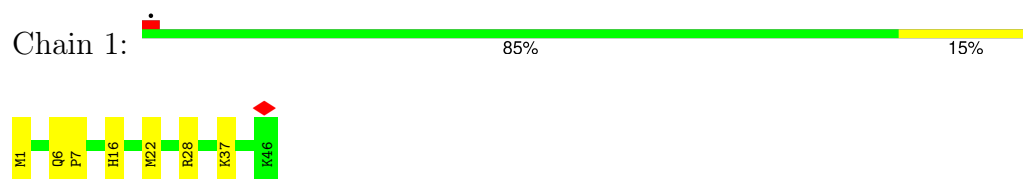
3 Residue-property plots [i](#)

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.

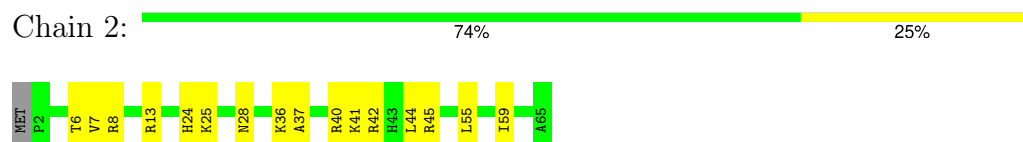
- Molecule 1: 50S ribosomal protein L33



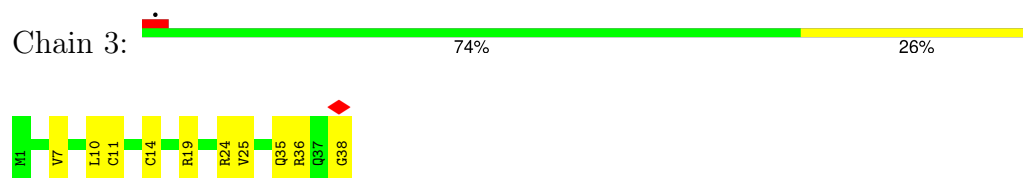
- Molecule 2: 50S ribosomal protein L34



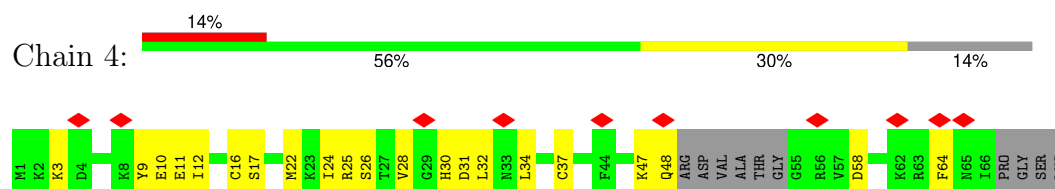
- Molecule 3: 50S ribosomal protein L35



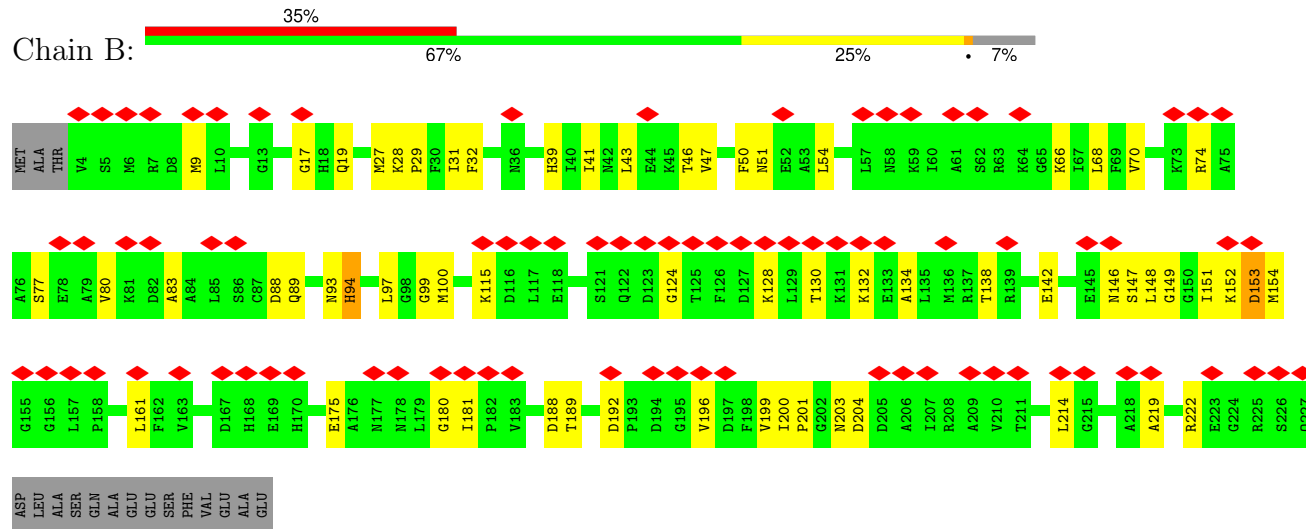
- Molecule 4: 50S ribosomal protein L36



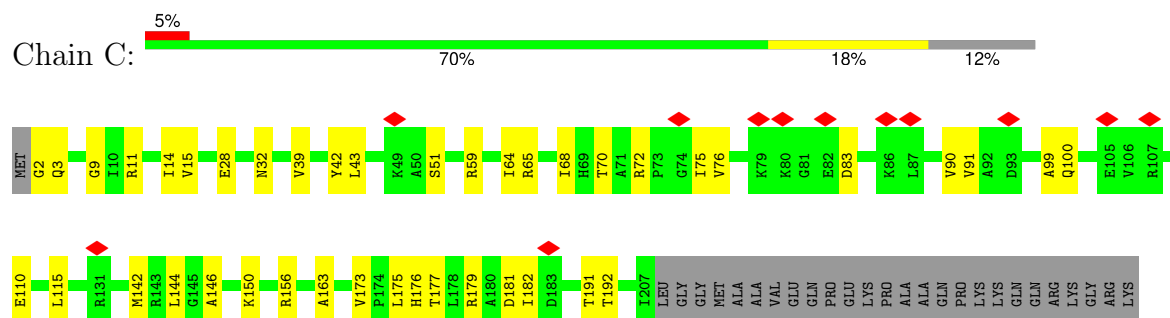
- Molecule 5: 50S ribosomal protein L31



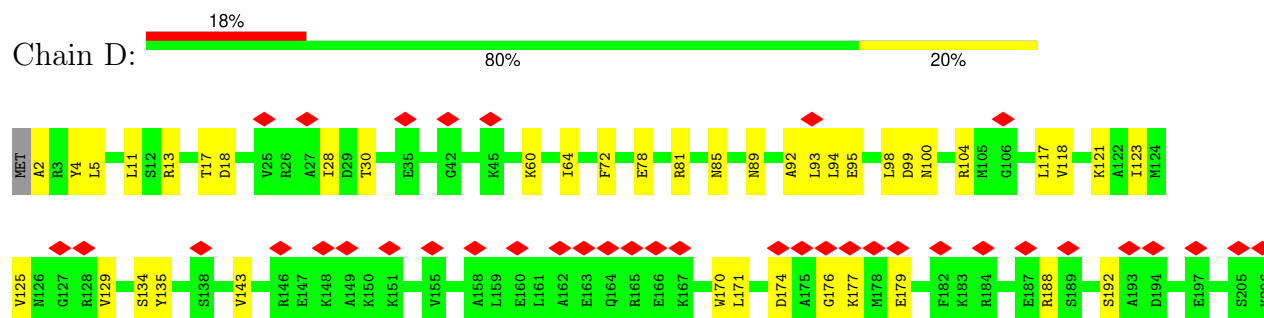
- Molecule 6: 30S ribosomal protein S2



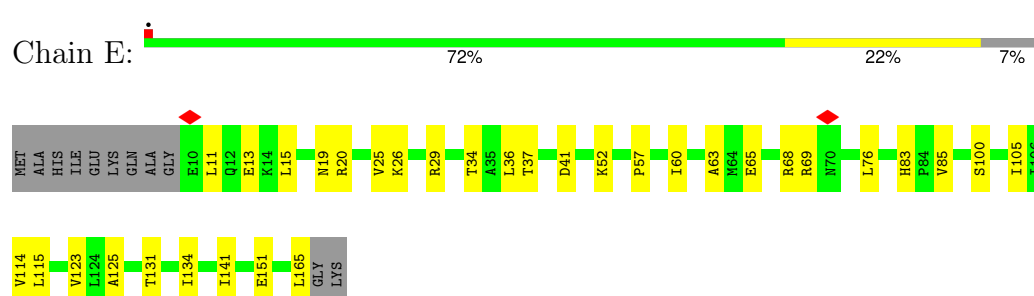
- Molecule 7: Small ribosomal subunit protein uS3



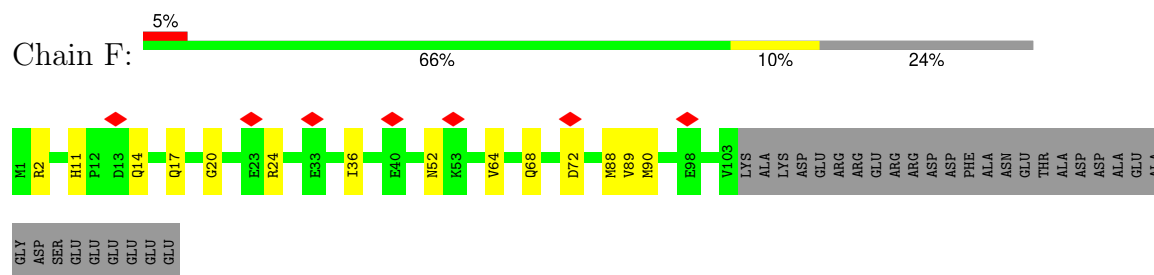
- Molecule 8: Small ribosomal subunit protein uS4



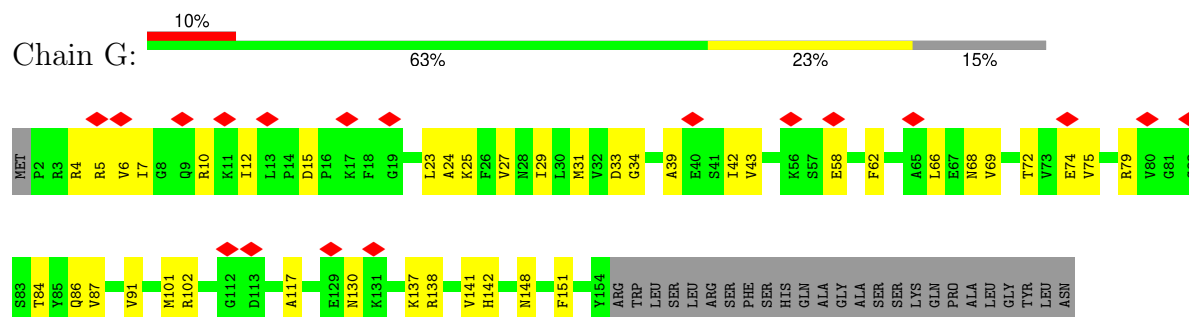
- Molecule 9: Small ribosomal subunit protein uS5



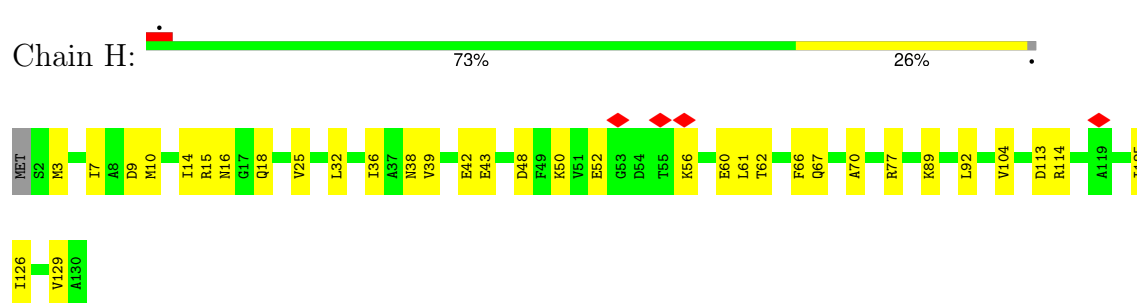
- Molecule 10: Small ribosomal subunit protein bS6



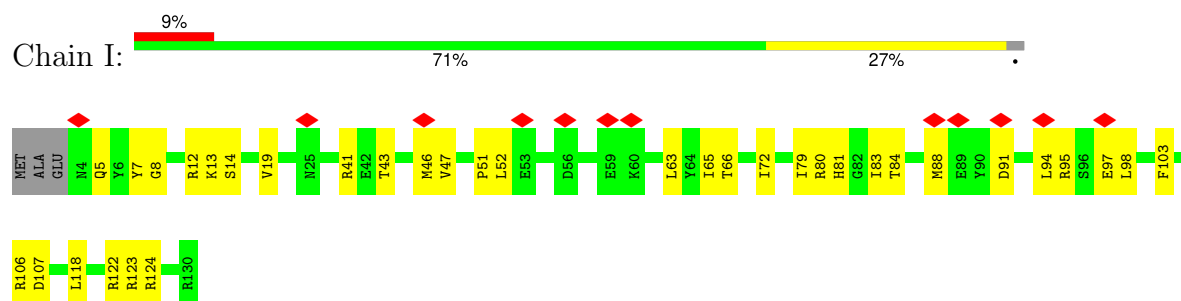
- Molecule 11: Small ribosomal subunit protein uS7



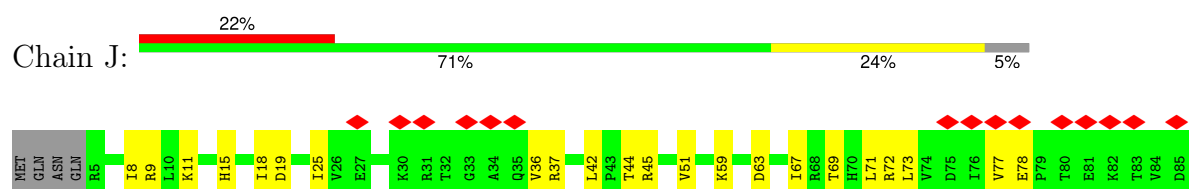
- Molecule 12: Small ribosomal subunit protein uS8

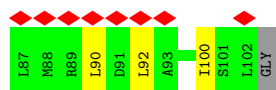


- Molecule 13: Small ribosomal subunit protein uS9

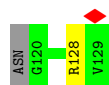
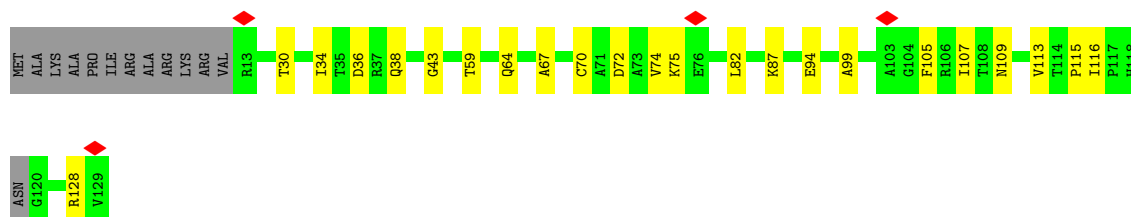


- Molecule 14: Small ribosomal subunit protein uS10

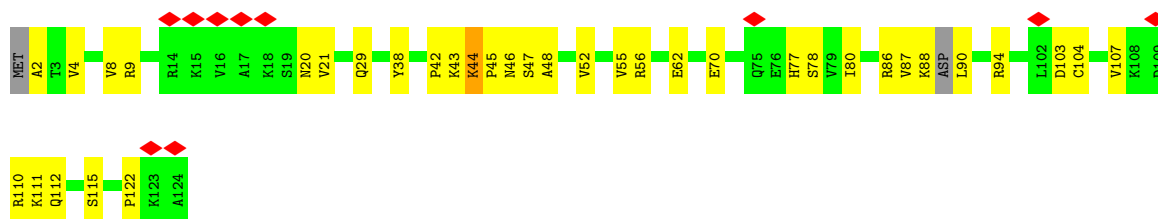




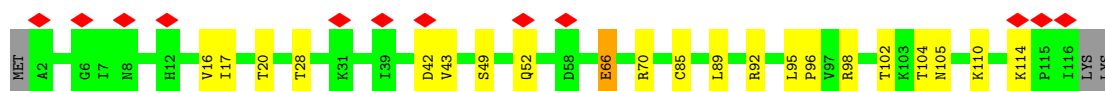
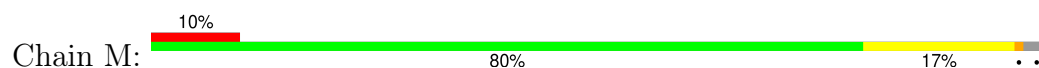
- Molecule 15: 30S ribosomal protein S11



- Molecule 16: 30S ribosomal protein S12



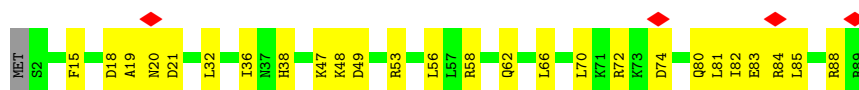
- Molecule 17: Small ribosomal subunit protein uS13



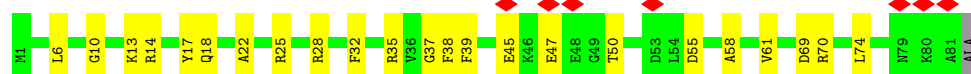
- Molecule 18: Small ribosomal subunit protein uS14



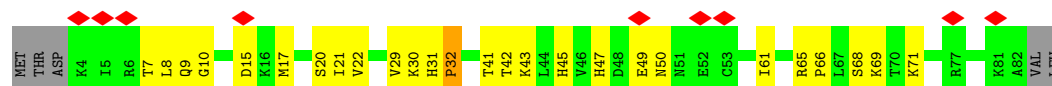
- Molecule 19: Small ribosomal subunit protein uS15



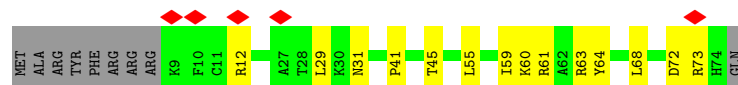
- Molecule 20: Small ribosomal subunit protein bS16



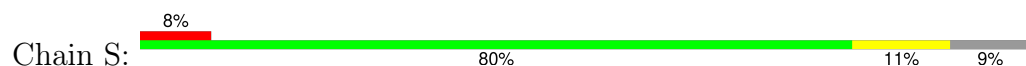
- Molecule 21: Small ribosomal subunit protein uS17



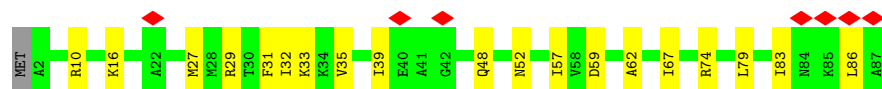
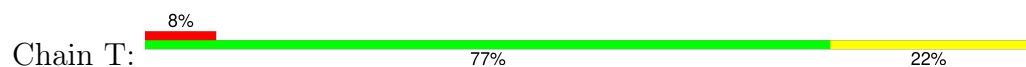
- Molecule 22: Small ribosomal subunit protein bS18



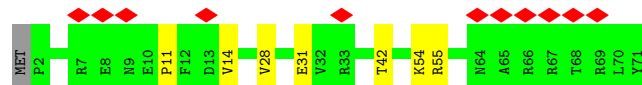
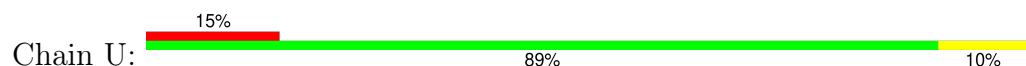
- Molecule 23: Small ribosomal subunit protein uS19



- Molecule 24: Small ribosomal subunit protein bS20



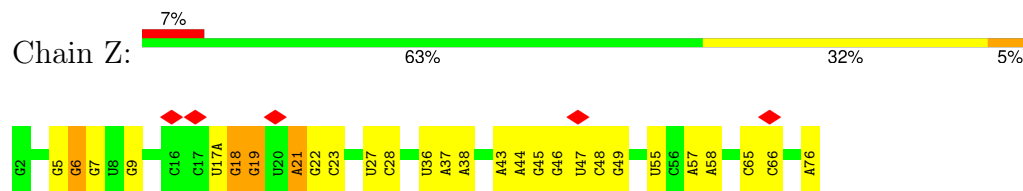
- Molecule 25: Small ribosomal subunit protein bS21



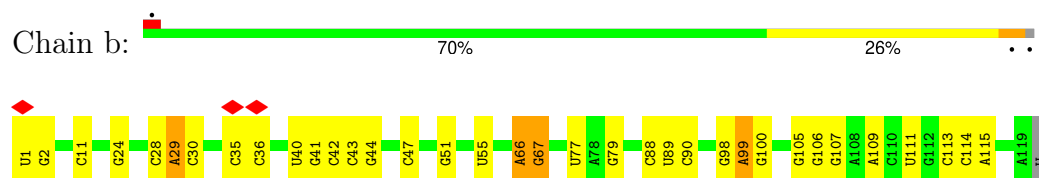
- Molecule 26: mRNA



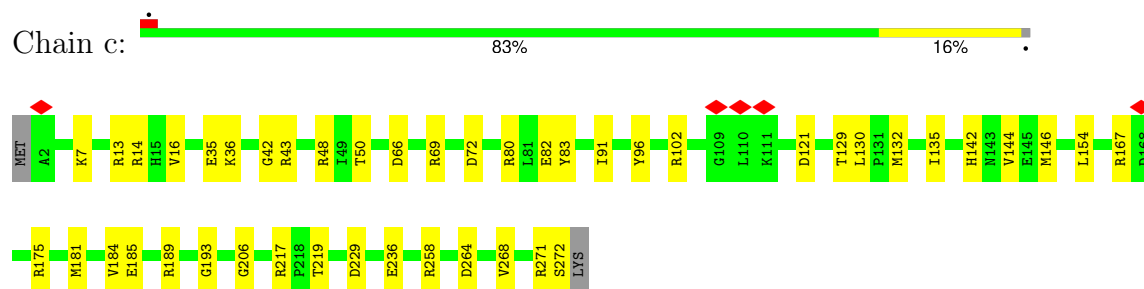
- Molecule 27: tRNA-fMet



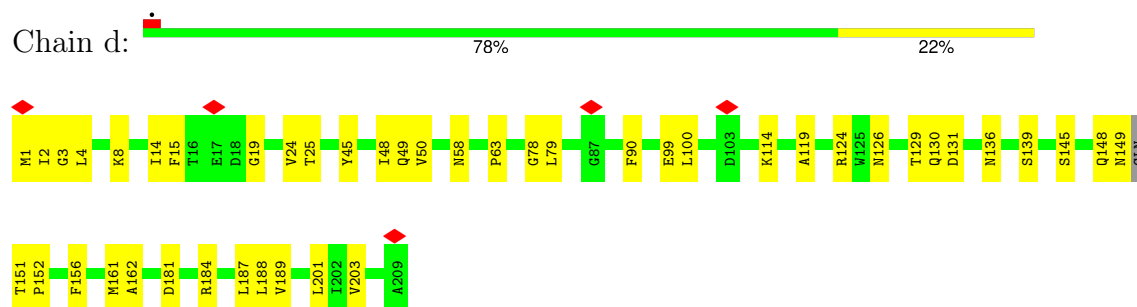
- Molecule 28: 5S rRNA



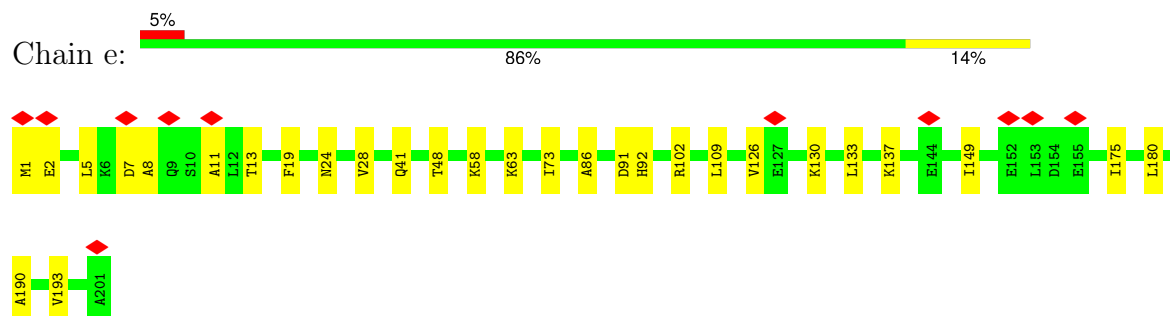
- Molecule 29: 50S ribosomal protein L2



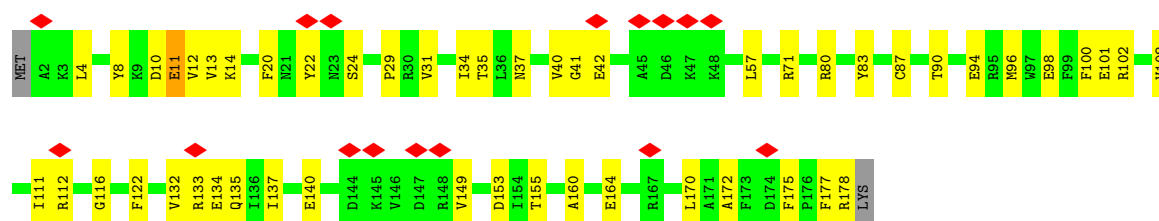
- Molecule 30: 50S ribosomal protein L3



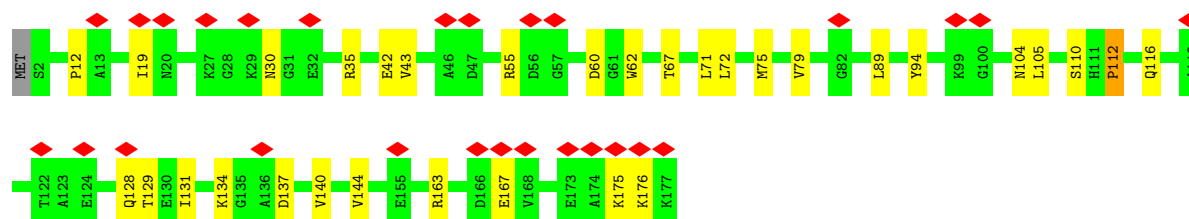
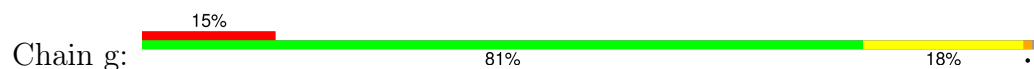
- Molecule 31: Large ribosomal subunit protein uL4



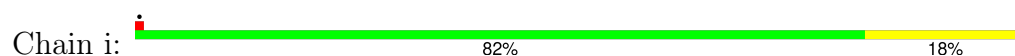
- Molecule 32: Large ribosomal subunit protein uL5



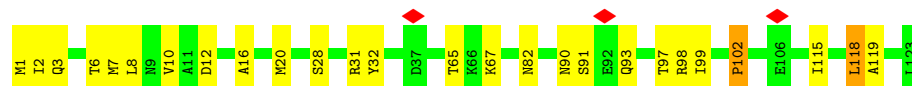
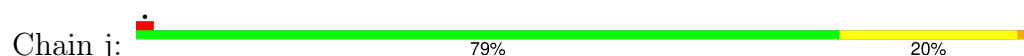
- Molecule 33: Large ribosomal subunit protein uL6



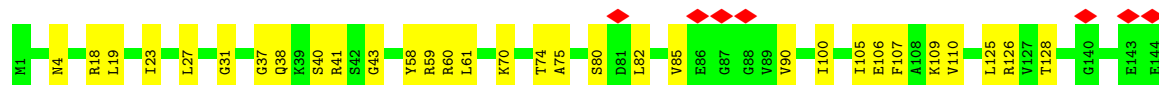
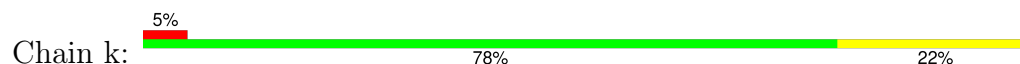
- Molecule 34: Large ribosomal subunit protein uL13



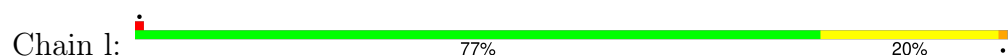
- Molecule 35: Large ribosomal subunit protein uL14




- Molecule 36: Large ribosomal subunit protein uL15



- Molecule 37: 50S ribosomal protein L16




- Molecule 38: Large ribosomal subunit protein bL17

Chain m:  76% 16% 7%




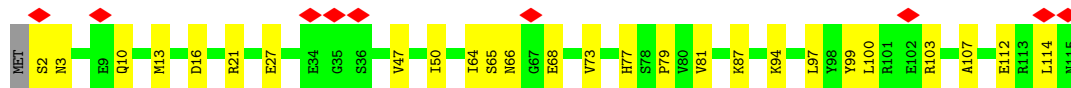
- Molecule 39: Large ribosomal subunit protein uL18

Chain n:  7% 79% 21%




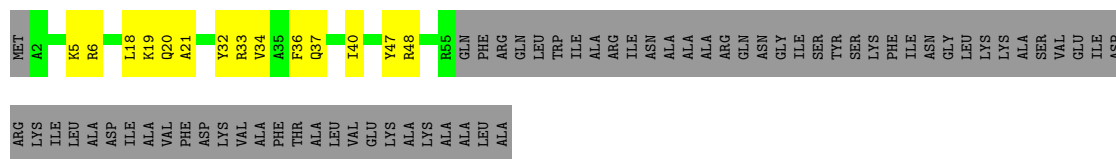
- Molecule 40: Large ribosomal subunit protein bL19

Chain o:  8% 77% 23%




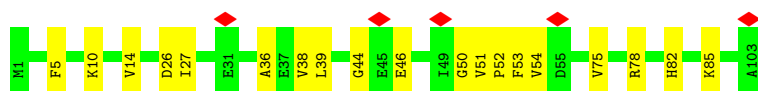
- Molecule 41: 50S ribosomal protein L20

Chain p:  34% 12% 54%



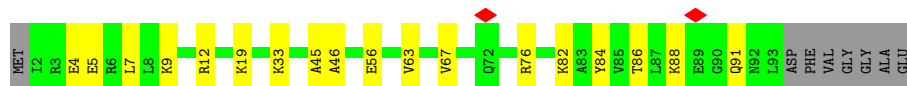
- Molecule 42: Large ribosomal subunit protein bL21

Chain q:  5% 82% 18%




- Molecule 43: 50S ribosomal protein L23

Chain s:  74% 18% 8%

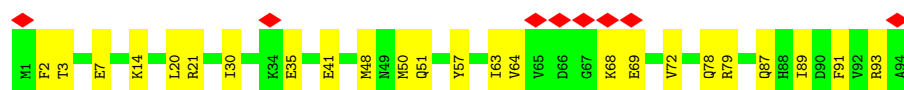
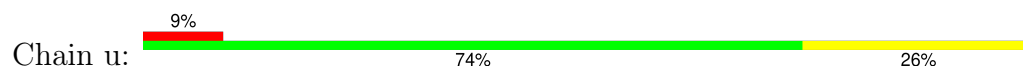


- Molecule 44: 50S ribosomal protein L24

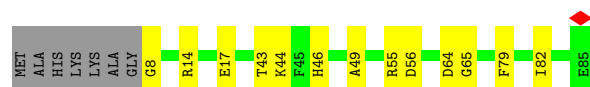
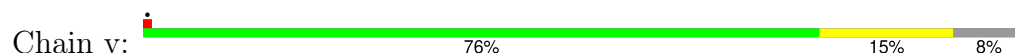
Chain t:  78% 20%



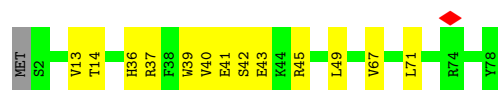
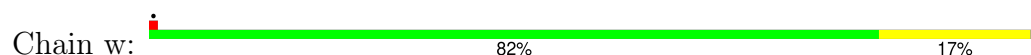
- Molecule 45: Large ribosomal subunit protein bL25



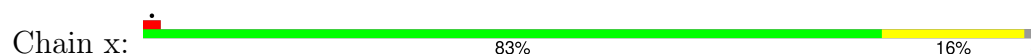
- Molecule 46: Large ribosomal subunit protein bL27



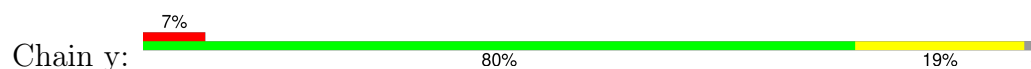
- Molecule 47: 50S ribosomal protein L28



- Molecule 48: Large ribosomal subunit protein uL29



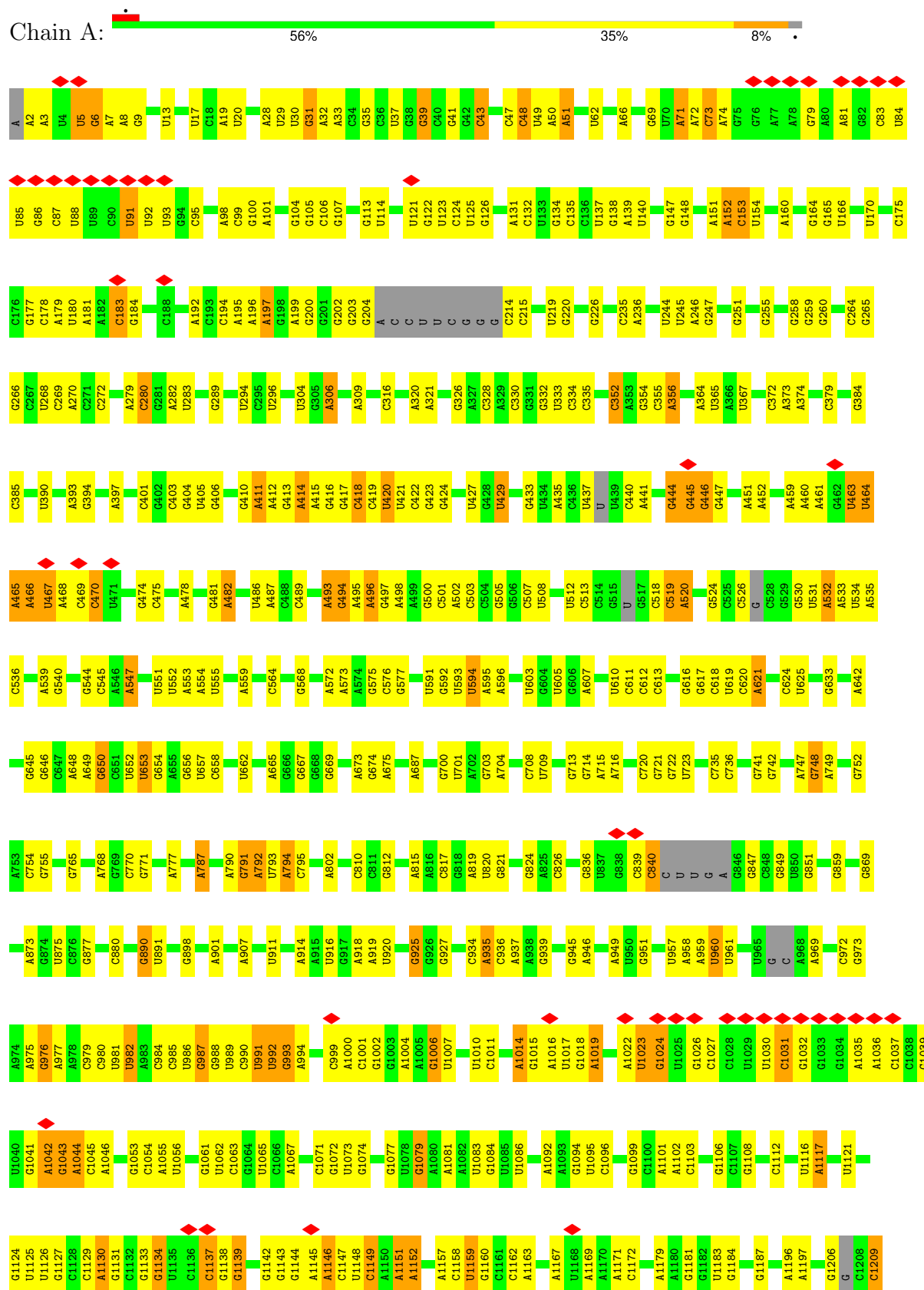
- Molecule 49: 50S ribosomal protein L30

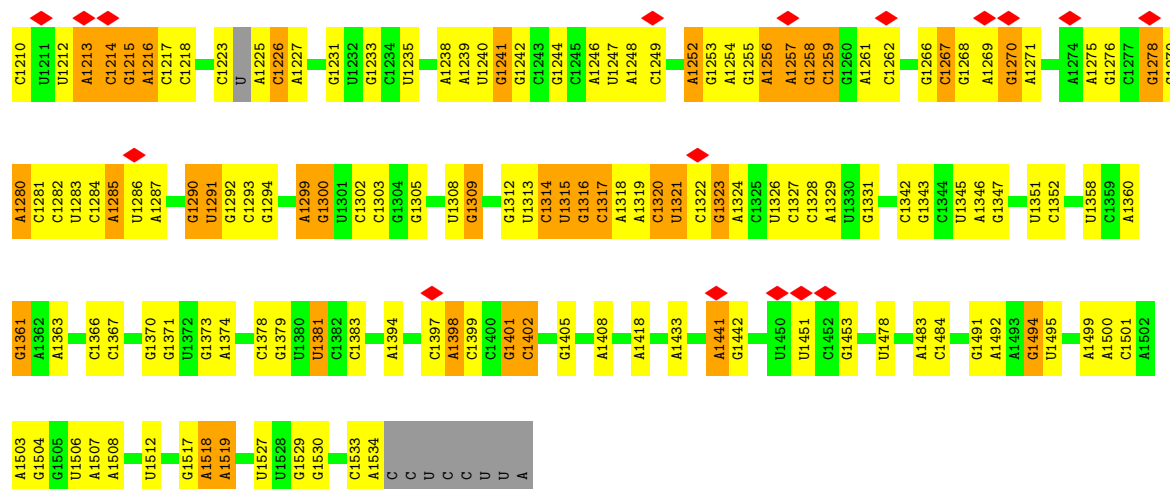


- Molecule 50: 50S ribosomal protein L32

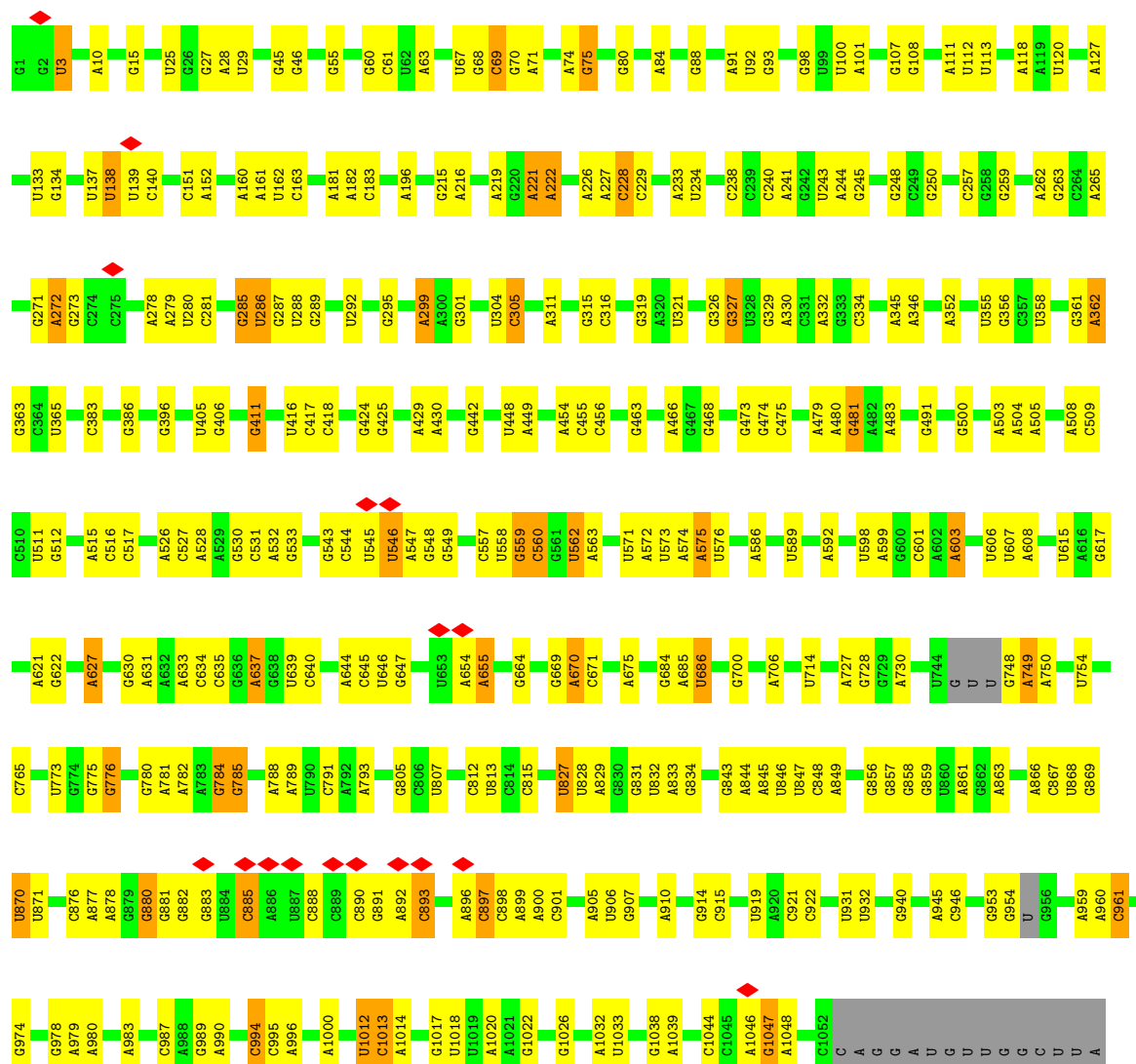


- Molecule 51: 16S rRNA

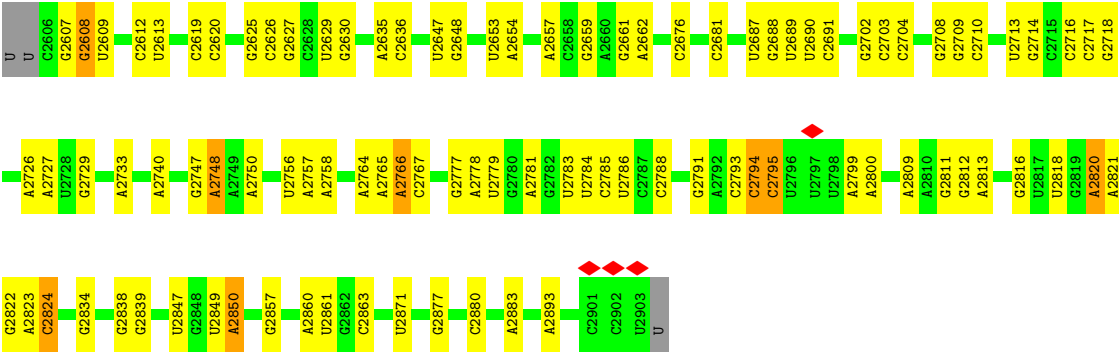




• Molecule 52: 23S rRNA







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	46282	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 ($e^-/\text{\AA}^2$)	1.37	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.105	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	425.0, 425.0, 425.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 84G

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	0.46	1/424 (0.2%)	0.81	2/565 (0.4%)
2	1	0.25	0/380	0.41	0/498
3	2	0.22	0/513	0.43	0/676
4	3	0.23	0/303	0.48	0/397
5	4	0.24	0/488	0.51	0/649
6	B	0.21	0/1784	0.46	0/2403
7	C	0.20	0/1651	0.40	0/2225
8	D	0.19	0/1665	0.40	0/2227
9	E	0.24	0/1165	0.46	0/1568
10	F	0.22	0/858	0.44	0/1160
11	G	0.22	0/1213	0.42	0/1628
12	H	0.22	0/989	0.43	0/1326
13	I	0.26	0/1031	0.55	0/1372
14	J	0.23	0/796	0.41	0/1077
15	K	0.22	0/884	0.46	0/1191
16	L	0.26	0/957	0.48	0/1282
17	M	0.20	0/900	0.41	0/1204
18	N	0.20	0/817	0.43	0/1088
19	O	0.24	0/722	0.43	0/964
20	P	0.21	0/653	0.45	0/877
21	Q	1.21	4/650 (0.6%)	1.31	5/871 (0.6%)
22	R	0.18	0/553	0.45	0/742
23	S	0.20	0/685	0.41	0/922
24	T	0.23	0/676	0.44	0/895
25	U	0.20	0/597	0.42	0/792
26	X	0.17	0/72	0.26	0/110
27	Z	0.17	0/1813	0.33	0/2825
28	b	0.18	0/2850	0.30	0/4444
29	c	0.24	0/2121	0.43	0/2852
30	d	0.27	0/1576	0.48	0/2119
31	e	0.23	0/1571	0.40	0/2113
32	f	0.21	0/1434	0.45	0/1926

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.47	3/1343 (0.2%)	0.82	6/1816 (0.3%)
34	i	0.30	0/1146	0.47	0/1544
35	j	0.26	0/955	0.57	1/1279 (0.1%)
36	k	0.25	0/1062	0.45	0/1413
37	l	0.32	0/1073	0.53	1/1433 (0.1%)
38	m	0.76	1/958 (0.1%)	1.22	7/1281 (0.5%)
39	n	0.21	0/902	0.42	0/1209
40	o	0.22	0/929	0.42	0/1242
41	p	0.27	0/436	0.55	1/578 (0.2%)
42	q	0.24	0/829	0.44	0/1107
43	s	0.22	0/736	0.40	0/984
44	t	0.21	0/787	0.42	0/1051
45	u	0.23	0/766	0.43	0/1025
46	v	0.22	0/593	0.43	0/785
47	w	0.34	0/635	0.43	0/848
48	x	0.21	0/486	0.44	0/648
49	y	0.22	0/453	0.39	0/605
50	z	0.22	0/450	0.44	0/599
51	A	0.19	1/36330 (0.0%)	0.32	0/56657
52	a	0.20	0/65703	0.31	0/102459
All	All	0.23	10/149363 (0.0%)	0.38	23/223551 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Q	32	PRO	CB-CG	22.09	2.60	1.49
38	m	50	PRO	CG-CD	-20.28	0.81	1.50
21	Q	32	PRO	CG-CD	-18.25	0.88	1.50
33	g	112	PRO	CG-CD	-8.93	1.20	1.50
1	0	41	PRO	CG-CD	-7.24	1.26	1.50
33	g	112	PRO	CB-CG	6.00	1.79	1.49
21	Q	32	PRO	CA-CB	-5.61	1.45	1.53
33	g	110	SER	C-N	5.50	1.40	1.32
51	A	1402	C	C1'-N1	5.21	1.56	1.48
21	Q	32	PRO	N-CD	5.19	1.55	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Q	32	PRO	CB-CG-CD	-29.43	11.92	106.10
38	m	50	PRO	CB-CG-CD	23.07	179.91	106.10
38	m	50	PRO	N-CD-CG	-19.44	74.03	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	g	112	PRO	CA-N-CD	-15.69	90.04	112.00
38	m	50	PRO	CA-CB-CG	-15.44	75.17	104.50
21	Q	32	PRO	N-CA-CB	-12.42	89.10	103.26
38	m	49	GLU	CA-C-N	-12.34	107.10	119.56
38	m	49	GLU	C-N-CA	-12.34	107.10	119.56
33	g	12	PRO	N-CD-CG	-11.75	85.58	103.20
21	Q	32	PRO	N-CD-CG	-10.24	87.84	103.20
1	0	41	PRO	N-CD-CG	-9.34	89.19	103.20
21	Q	32	PRO	CA-CB-CG	-9.20	87.03	104.50
1	0	41	PRO	CA-CB-CG	-8.77	87.84	104.50
35	j	102	PRO	CA-N-CD	-8.49	100.12	112.00
33	g	12	PRO	CA-N-CD	-8.09	100.67	112.00
38	m	50	PRO	CA-N-CD	-7.26	101.84	112.00
37	l	78	LEU	N-CA-C	6.63	118.16	111.07
33	g	112	PRO	CA-CB-CG	-6.38	92.38	104.50
21	Q	32	PRO	CA-N-CD	-6.30	103.18	112.00
33	g	12	PRO	N-CA-CB	-6.03	96.92	103.25
38	m	49	GLU	C-N-CD	5.88	149.09	125.00
33	g	112	PRO	N-CD-CG	-5.61	94.79	103.20
41	p	34	VAL	N-CA-C	-5.05	108.36	113.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	417	0	451	9	0
2	1	377	0	418	6	0
3	2	504	0	572	14	0
4	3	302	0	340	8	0
5	4	480	0	482	26	0
6	B	1753	0	1780	50	0
7	C	1624	0	1696	28	0
8	D	1643	0	1707	26	0
9	E	1152	0	1196	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	F	839	0	833	11	0
11	G	1197	0	1243	29	0
12	H	979	0	1031	25	0
13	I	1019	0	1063	30	0
14	J	786	0	828	37	0
15	K	869	0	880	18	0
16	L	944	0	1002	30	0
17	M	891	0	952	18	0
18	N	805	0	844	19	0
19	O	714	0	734	26	0
20	P	643	0	661	21	0
21	Q	641	0	682	34	0
22	R	544	0	565	12	0
23	S	668	0	693	10	0
24	T	670	0	719	13	0
25	U	589	0	629	7	0
26	X	65	0	33	1	0
27	Z	1623	0	825	16	0
28	b	2549	0	1291	18	0
29	c	2082	0	2154	37	0
30	d	1556	0	1607	35	0
31	e	1552	0	1619	21	0
32	f	1410	0	1444	44	0
33	g	1323	0	1371	21	0
34	i	1123	0	1151	24	0
35	j	946	0	1023	21	0
36	k	1053	0	1129	33	0
37	l	1055	0	1134	28	0
38	m	945	0	989	19	0
39	n	892	0	923	19	0
40	o	917	0	962	19	0
41	p	431	0	454	10	0
42	q	816	0	839	15	0
43	s	730	0	795	12	0
44	t	779	0	831	19	0
45	u	753	0	780	20	0
46	v	586	0	596	14	0
47	w	625	0	652	14	0
48	x	485	0	503	7	0
49	y	449	0	488	12	0
50	z	444	0	458	10	0
51	A	32450	0	16337	409	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	a	58675	0	29536	426	0
53	A	38	0	0	2	0
53	a	38	0	0	1	0
All	All	137440	0	91925	1659	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1659) 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)
21:Q:32:PRO:N	21:Q:32:PRO:CG	1.75	1.47
33:g:112:PRO:CB	33:g:112:PRO:CG	1.79	1.42
21:Q:32:PRO:CD	21:Q:32:PRO:HG3	1.65	1.06
21:Q:32:PRO:CG	21:Q:32:PRO:HD3	1.57	1.05
21:Q:32:PRO:CD	21:Q:32:PRO:HG2	1.65	1.04
21:Q:32:PRO:CG	21:Q:32:PRO:HD2	1.57	1.04
52:a:1779:U:OP2	52:a:1784:A:N6	1.91	1.02
24:T:16:LYS:NZ	51:A:104:G:OP1	1.97	0.98
28:b:66:A:O2'	28:b:67:G:OP2	1.83	0.95
31:e:58:LYS:NZ	52:a:675:A:OP1	2.01	0.94
6:B:115:LYS:NZ	6:B:153:ASP:OD1	2.02	0.93
16:L:2:ALA:N	51:A:568:G:O6	2.02	0.93
51:A:69:G:N2	51:A:100:G:O6	2.02	0.92
52:a:259:G:HO2'	52:a:621:A:HO2'	1.02	0.92
13:I:7:TYR:OH	51:A:1147:C:O2'	1.82	0.91
51:A:126:G:OP1	51:A:605:U:O2'	1.88	0.91
20:P:38:PHE:O	20:P:50:THR:OG1	1.89	0.91
38:m:106:ASP:OD2	52:a:1649:G:O2'	1.88	0.91
51:A:1235:U:O2'	51:A:1305:G:OP1	1.88	0.90
51:A:1209:C:O2'	51:A:1214:C:N4	2.04	0.90
28:b:40:U:O2'	28:b:43:C:OP2	1.89	0.90
52:a:748:G:O2'	52:a:749:A:OP1	1.89	0.89
21:Q:32:PRO:CG	21:Q:32:PRO:CD	0.88	0.88
52:a:299:A:N3	52:a:319:G:O2'	2.05	0.88
42:q:51:VAL:HG22	42:q:52:PRO:HD2	1.57	0.87
51:A:401:C:O2'	51:A:621:A:N3	2.07	0.87
51:A:1213:A:N7	51:A:1215:G:N2	2.22	0.86
46:v:17:GLU:N	46:v:17:GLU:OE2	2.09	0.86
5:4:3:LYS:HE3	5:4:3:LYS:HA	1.58	0.86
8:D:177:LYS:NZ	8:D:179:GLU:OE1	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:A:840:C:HO2'	51:A:849:G:H1	1.22	0.86
52:a:27:G:O2'	52:a:28:A:OP2	1.93	0.86
51:A:17:U:O2	51:A:1079:G:N2	2.09	0.85
14:J:36:VAL:O	14:J:37:ARG:NH1	2.09	0.85
29:c:69:ARG:NH1	29:c:129:THR:OG1	2.10	0.85
7:C:142:MET:HE1	7:C:146:ALA:O	1.77	0.85
27:Z:7:G:O2'	27:Z:49:G:OP2	1.93	0.84
16:L:78:SER:OG	16:L:103:ASP:OD2	1.94	0.84
33:g:42:GLU:OE1	33:g:55:ARG:NH2	2.10	0.84
52:a:219:A:N3	52:a:234:U:O2'	2.10	0.84
51:A:140:U:O2	51:A:183:C:N4	2.11	0.83
52:a:2469:A:N6	52:a:2481:G:O2'	2.10	0.83
38:m:69:ARG:O	38:m:70:THR:OG1	1.94	0.83
13:I:97:GLU:N	13:I:97:GLU:OE1	2.12	0.83
8:D:78:GLU:OE1	8:D:81:ARG:NH1	2.12	0.83
51:A:1290:G:O2'	51:A:1291:U:OP2	1.97	0.83
16:L:44:LYS:HE3	16:L:46:ASN:H	1.42	0.82
28:b:77:U:OP1	45:u:21:ARG:NH1	2.11	0.82
36:k:109:LYS:NZ	52:a:635:C:OP2	2.10	0.82
21:Q:31:HIS:HA	21:Q:32:PRO:HG2	1.62	0.82
51:A:1256:A:N6	51:A:1278:G:OP2	2.12	0.82
16:L:4:VAL:O	16:L:8:VAL:HG23	1.78	0.82
51:A:1031:C:O3'	51:A:1032:G:N2	2.12	0.82
51:A:1261:A:HO2'	51:A:1282:C:HO2'	1.24	0.82
34:i:129:GLU:OE1	34:i:129:GLU:N	2.12	0.82
52:a:2857:G:N2	52:a:2860:A:OP2	2.13	0.81
11:G:102:ARG:NH2	51:A:939:G:OP1	2.13	0.81
6:B:74:ARG:O	6:B:77:SER:OG	1.99	0.81
11:G:86:GLN:O	11:G:148:ASN:ND2	2.13	0.81
51:A:203:G:N2	51:A:204:G:O6	2.13	0.81
13:I:5:GLN:OE1	51:A:1130:A:O2'	1.99	0.81
51:A:28:A:O2'	51:A:296:U:OP1	1.99	0.81
45:u:51:GLN:OE1	45:u:57:TYR:OH	1.98	0.81
52:a:25:U:O2	52:a:515:A:N6	2.14	0.81
21:Q:71:LYS:NZ	51:A:255:G:OP1	2.14	0.80
52:a:240:C:O2	52:a:257:C:N4	2.15	0.80
7:C:179:ARG:NH1	51:A:1112:C:O2'	2.15	0.80
51:A:1041:G:O2'	51:A:1042:A:O5'	2.00	0.80
52:a:685:A:O2'	52:a:773:U:O4	1.98	0.80
30:d:130:GLN:OE1	30:d:139:SER:OG	1.99	0.79
32:f:37:ASN:ND2	52:a:2312:U:O2	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:a:1864:U:OP1	52:a:2410:G:O2'	1.99	0.79
21:Q:31:HIS:C	21:Q:32:PRO:CG	2.54	0.79
17:M:66:GLU:OE1	32:f:112:ARG:NH2	2.16	0.78
33:g:89:LEU:O	33:g:129:THR:OG1	2.00	0.78
46:v:55:ARG:NH1	52:a:2364:C:OP1	2.15	0.78
44:t:43:LYS:O	52:a:480:A:O2'	2.01	0.78
52:a:1814:G:OP2	52:a:1815:A:O2'	2.01	0.78
7:C:2:GLY:N	51:A:1062:U:O4	2.17	0.78
29:c:80:ARG:NH1	29:c:82:GLU:OE2	2.17	0.78
37:l:18:ARG:NH2	52:a:953:G:OP2	2.15	0.77
50:z:49:TYR:OH	52:a:2883:A:OP1	2.02	0.77
51:A:662:U:O2'	51:A:836:G:OP1	2.02	0.77
32:f:37:ASN:ND2	52:a:2313:C:O4'	2.17	0.77
30:d:181:ASP:OD2	30:d:184:ARG:NH1	2.18	0.77
17:M:49:SER:OG	17:M:52:GLN:OE1	2.01	0.77
30:d:145:SER:HG	52:a:2575:C:HO2'	1.29	0.77
20:P:13:LYS:NZ	51:A:43:C:OP1	2.18	0.77
24:T:10:ARG:NE	51:A:107:G:O6	2.18	0.76
36:k:23:ILE:HD13	42:q:82:HIS:CE1	2.19	0.76
29:c:271:ARG:NH2	52:a:1798:U:OP2	2.18	0.76
32:f:42:GLU:OE1	32:f:42:GLU:N	2.18	0.76
41:p:47:TYR:O	41:p:48:ARG:NE	2.19	0.76
52:a:304:U:O2'	52:a:305:C:OP1	2.04	0.75
12:H:7:ILE:HD11	12:H:32:LEU:HD23	1.67	0.75
29:c:132:MET:O	29:c:167:ARG:NH2	2.17	0.75
13:I:46:MET:O	13:I:46:MET:HE3	1.86	0.75
14:J:36:VAL:O	14:J:37:ARG:CZ	2.34	0.75
1:O:6:ARG:NH1	52:a:2285:C:OP2	2.19	0.75
8:D:125:VAL:HG12	8:D:143:VAL:HG22	1.69	0.75
51:A:958:A:N3	51:A:985:C:O2'	2.19	0.75
52:a:475:C:O2	52:a:479:A:N6	2.20	0.75
52:a:1509:A:O2'	52:a:1510:G:O5'	2.02	0.75
13:I:66:THR:HG22	13:I:66:THR:O	1.86	0.75
51:A:1494:G:N7	53:A:1601:84G:N2	2.35	0.75
23:S:70:LYS:NZ	51:A:1320:C:OP1	2.20	0.74
4:3:19:ARG:NE	52:a:2756:U:OP2	2.19	0.74
7:C:32:ASN:OD1	7:C:59:ARG:NH2	2.20	0.74
27:Z:38:A:O2'	51:A:790:A:OP1	2.05	0.74
40:o:21:ARG:NH1	52:a:2849:U:O4	2.20	0.74
9:E:151:GLU:OE1	9:E:151:GLU:N	2.21	0.74
52:a:2794:C:O2'	52:a:2795:C:OP1	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:A:1244:G:O6	51:A:1293:C:N4	2.21	0.74
11:G:10:ARG:NH2	51:A:1346:A:N7	2.35	0.73
9:E:13:GLU:OE1	9:E:68:ARG:NH2	2.22	0.73
30:d:8:LYS:HB2	30:d:201:LEU:HD11	1.70	0.73
48:x:16:THR:O	48:x:20:ASN:ND2	2.21	0.73
9:E:134:ILE:H	9:E:134:ILE:HD12	1.53	0.73
8:D:89:ASN:O	8:D:93:LEU:HD13	1.89	0.73
31:e:102:ARG:NH1	52:a:617:G:OP1	2.22	0.73
49:y:12:SER:OG	52:a:989:G:OP2	2.04	0.73
52:a:411:G:OP2	52:a:2406:A:O2'	2.07	0.73
52:a:161:A:OP2	52:a:162:U:O2'	2.02	0.73
52:a:877:A:O2'	52:a:900:A:N6	2.22	0.73
52:a:332:A:O2'	52:a:334:C:OP2	2.05	0.72
20:P:25:ARG:NH1	51:A:134:G:O6	2.23	0.72
15:K:64:GLN:HG2	15:K:99:ALA:HB2	1.71	0.72
30:d:124:ARG:NH1	30:d:161:MET:O	2.22	0.72
43:s:4:GLU:OE1	43:s:5:GLU:N	2.23	0.72
39:n:74:VAL:O	39:n:78:VAL:HG22	1.89	0.72
21:Q:49:GLU:O	21:Q:50:ASN:ND2	2.23	0.72
25:U:42:THR:HG23	51:A:1527:U:OP2	1.90	0.72
51:A:1484:C:HO2'	52:a:1960:A:HO2'	1.33	0.72
52:a:80:G:OP1	52:a:346:A:O2'	2.08	0.72
52:a:1721:G:O2'	52:a:1739:A:N6	2.23	0.71
29:c:217:ARG:NH2	52:a:781:A:OP1	2.24	0.71
52:a:603:A:N6	52:a:655:A:O4'	2.24	0.71
12:H:15:ARG:NH1	51:A:875:U:O2'	2.23	0.71
51:A:335:C:O2'	51:A:1433:A:N3	2.23	0.70
3:2:42:ARG:NH1	52:a:2349:G:OP2	2.24	0.70
11:G:15:ASP:OD2	11:G:23:LEU:HD23	1.90	0.70
51:A:1319:A:O2'	51:A:1323:G:N7	2.19	0.70
1:0:34:LEU:HD11	1:0:36:LEU:HD21	1.73	0.70
11:G:74:GLU:N	11:G:74:GLU:OE2	2.25	0.70
29:c:185:GLU:OE1	29:c:185:GLU:N	2.25	0.70
45:u:51:GLN:O	45:u:51:GLN:NE2	2.25	0.70
51:A:840:C:O2'	51:A:849:G:N1	2.23	0.70
1:0:7:GLU:N	1:0:7:GLU:OE2	2.25	0.70
6:B:134:ALA:O	6:B:138:THR:HG23	1.92	0.70
43:s:7:LEU:HD11	43:s:46:ALA:HB2	1.74	0.69
45:u:69:GLU:N	45:u:69:GLU:OE2	2.25	0.69
52:a:2816:G:N3	52:a:2883:A:O2'	2.23	0.69
51:A:5:U:O2'	51:A:6:G:O5'	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:84:ARG:HG3	19:O:85:LEU:HD12	1.75	0.69
5:4:9:TYR:OH	5:4:25:ARG:O	2.07	0.69
20:P:28:ARG:NH2	51:A:390:U:O2'	2.25	0.69
52:a:1352:U:O2'	52:a:1570:A:N3	2.25	0.69
8:D:117:LEU:HB3	8:D:123:ILE:HD11	1.75	0.69
33:g:35:ARG:NH1	33:g:71:LEU:HD21	2.07	0.69
51:A:1000:A:N6	51:A:1041:G:O6	2.26	0.69
21:Q:31:HIS:CG	21:Q:32:PRO:HG3	2.28	0.68
37:l:3:GLN:HE21	37:l:92:TRP:NE1	1.91	0.68
45:u:48:MET:HE3	45:u:48:MET:O	1.92	0.68
6:B:27:MET:HE2	6:B:188:ASP:O	1.93	0.68
21:Q:31:HIS:HA	21:Q:32:PRO:CG	2.24	0.68
32:f:135:GLN:OE1	32:f:135:GLN:N	2.24	0.68
50:z:38:HIS:ND1	50:z:39:LEU:O	2.27	0.68
51:A:1015:G:O2'	51:A:1016:A:O4'	2.10	0.68
32:f:140:GLU:N	32:f:140:GLU:OE2	2.25	0.68
51:A:1041:G:HO2'	51:A:1042:A:P	2.16	0.68
51:A:1043:G:O2'	51:A:1044:A:OP2	2.10	0.68
52:a:2532:G:O2'	52:a:2657:A:N1	2.26	0.68
28:b:29:A:OP2	39:n:31:THR:OG1	2.10	0.68
52:a:2834:G:H21	52:a:2883:A:H62	1.41	0.68
22:R:31:ASN:O	22:R:31:ASN:ND2	2.27	0.68
52:a:2092:U:OP1	52:a:2199:A:O2'	2.13	0.67
18:N:3:LYS:HB2	18:N:6:MET:HE2	1.75	0.67
51:A:701:U:O2	51:A:703:G:N1	2.28	0.67
38:m:54:LEU:O	38:m:62:ASN:ND2	2.28	0.67
42:q:51:VAL:HG22	42:q:52:PRO:CD	2.25	0.67
51:A:1279:G:O2'	51:A:1282:C:N4	2.27	0.67
52:a:630:G:N2	52:a:633:A:OP2	2.26	0.67
52:a:669:G:O2'	52:a:670:A:O5'	2.12	0.67
51:A:1484:C:O2'	52:a:1960:A:O2'	2.05	0.67
1:0:40:ASP:OD2	1:0:43:VAL:HG22	1.95	0.66
19:O:36:ILE:HG23	19:O:56:LEU:HD11	1.78	0.66
52:a:228:C:N4	52:a:417:C:O2'	2.25	0.66
21:Q:17:MET:HE3	21:Q:20:SER:OG	1.95	0.66
52:a:527:C:N4	52:a:2777:G:O2'	2.26	0.66
47:w:39:TRP:CZ3	47:w:41:GLU:HB3	2.30	0.66
49:y:51:VAL:HG12	49:y:51:VAL:O	1.95	0.66
51:A:976:G:OP2	51:A:1358:U:O2'	2.13	0.66
52:a:1769:U:O2'	52:a:1958:C:OP1	2.12	0.66
16:L:38:TYR:CD1	16:L:52:VAL:HG23	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:142:HIS:ND1	29:c:193:GLY:O	2.28	0.66
4:3:36:ARG:NH1	4:3:38:GLY:O	2.28	0.66
32:f:40:VAL:O	32:f:40:VAL:HG13	1.95	0.66
6:B:9:MET:HE1	6:B:47:VAL:HG22	1.76	0.66
21:Q:31:HIS:ND1	21:Q:32:PRO:HG3	2.10	0.66
34:i:37:ARG:HA	34:i:118:MET:HE2	1.76	0.66
16:L:110:ARG:NH2	16:L:112:GLN:O	2.29	0.66
52:a:700:G:O2'	52:a:1632:A:N3	2.29	0.65
12:H:113:ASP:OD1	12:H:114:ARG:N	2.29	0.65
51:A:62:U:O2	51:A:379:C:O2'	2.14	0.65
52:a:2659:G:N2	52:a:2662:A:OP2	2.27	0.65
21:Q:22:VAL:O	21:Q:22:VAL:HG13	1.97	0.65
51:A:2:A:O2'	51:A:3:A:O4'	2.08	0.65
13:I:19:VAL:HG12	13:I:65:ILE:HD12	1.77	0.65
13:I:91:ASP:O	13:I:91:ASP:OD2	2.14	0.65
30:d:14:ILE:HD12	30:d:24:VAL:HG11	1.78	0.65
37:l:17:ASN:O	37:l:38:ARG:NH1	2.29	0.65
8:D:99:ASP:OD1	8:D:100:ASN:N	2.30	0.65
21:Q:31:HIS:CA	21:Q:32:PRO:CG	2.75	0.64
37:l:53:MET:HE1	37:l:117:PHE:CE1	2.32	0.64
37:l:84:LYS:HA	52:a:2275:C:H1'	1.80	0.64
23:S:11:ILE:HD13	23:S:41:PHE:HE2	1.60	0.64
37:l:136:MET:O	45:u:79:ARG:NH2	2.30	0.64
46:v:8:GLY:O	52:a:2255:G:N2	2.25	0.64
46:v:49:ALA:O	46:v:82:ILE:HG22	1.96	0.64
51:A:1518:A:O2'	51:A:1519:A:O5'	2.06	0.64
16:L:44:LYS:HD2	16:L:45:PRO:CD	2.27	0.64
32:f:134:GLU:OE2	32:f:149:VAL:HG13	1.98	0.64
1:0:32:GLU:OE1	1:0:32:GLU:N	2.30	0.64
15:K:128:ARG:O	51:A:795:C:O2'	2.16	0.64
18:N:59:ARG:NH1	51:A:979:C:O2	2.30	0.64
28:b:47:C:OP1	39:n:3:LYS:NZ	2.31	0.64
47:w:39:TRP:CH2	47:w:41:GLU:CB	2.81	0.64
21:Q:9:GLN:OE1	21:Q:10:GLY:N	2.31	0.63
50:z:13:ARG:O	50:z:17:ARG:HG3	1.98	0.63
52:a:1129:A:N6	52:a:2491:U:OP1	2.31	0.63
51:A:1255:G:N3	51:A:1259:C:O2'	2.25	0.63
24:T:27:MET:SD	24:T:31:PHE:CE1	2.91	0.63
52:a:2627:G:O2'	52:a:2781:A:N1	2.30	0.63
11:G:33:ASP:OD1	11:G:33:ASP:O	2.16	0.63
52:a:1332:G:N7	52:a:1609:A:O2'	2.22	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:2:ARG:NH2	10:F:68:GLN:OE1	2.31	0.63
12:H:16:ASN:ND2	51:A:826:C:O2	2.31	0.63
24:T:27:MET:HE1	24:T:57:ILE:CG2	2.28	0.63
51:A:991:U:O2'	51:A:992:U:O5'	2.16	0.63
14:J:37:ARG:NH1	14:J:77:VAL:HG21	2.14	0.63
51:A:294:U:OP1	51:A:610:U:O2'	2.12	0.63
3:2:45:ARG:NH2	52:a:2349:G:OP1	2.32	0.63
34:i:43:GLU:OE1	34:i:43:GLU:N	2.31	0.63
52:a:1378:A:O2'	52:a:1379:U:OP2	2.11	0.63
37:l:66:ARG:NH2	52:a:906:U:O2'	2.31	0.62
9:E:65:GLU:OE2	9:E:69:ARG:NH1	2.31	0.62
37:l:47:GLU:OE1	37:l:50:ARG:NH2	2.32	0.62
3:2:24:HIS:ND1	3:2:25:LYS:O	2.30	0.62
32:f:153:ASP:OD2	52:a:2304:G:O2'	2.09	0.62
23:S:13:LEU:HD12	23:S:13:LEU:O	1.98	0.62
39:n:34:HIS:O	39:n:102:ARG:NH2	2.31	0.62
44:t:36:VAL:CG1	44:t:39:ILE:HD12	2.29	0.62
51:A:1067:A:N1	51:A:1108:G:O2'	2.25	0.62
10:F:17:GLN:OE1	10:F:17:GLN:N	2.32	0.62
34:i:128:ASN:C	34:i:129:GLU:OE1	2.42	0.62
46:v:43:THR:O	46:v:43:THR:HG23	1.99	0.62
22:R:12:ARG:NH2	22:R:31:ASN:OD1	2.33	0.62
51:A:1030:U:N3	51:A:1032:G:O6	2.33	0.62
51:A:1279:G:O2'	51:A:1281:C:OP2	2.16	0.62
11:G:66:LEU:CD2	11:G:101:MET:HE2	2.29	0.61
29:c:42:GLY:O	29:c:50:THR:OG1	2.14	0.61
51:A:417:G:O6	51:A:418:C:N4	2.33	0.61
19:O:81:LEU:O	19:O:85:LEU:HD13	1.99	0.61
29:c:264:ASP:OD2	29:c:264:ASP:N	2.33	0.61
46:v:65:GLY:CA	46:v:82:ILE:HD11	2.31	0.61
8:D:13:ARG:NH1	51:A:427:U:OP1	2.31	0.61
29:c:36:LYS:NZ	52:a:1354:A:OP1	2.33	0.61
52:a:1363:C:O2'	52:a:1809:A:N3	2.27	0.61
31:e:48:THR:HG23	31:e:86:ALA:HB3	1.81	0.61
37:l:84:LYS:HG2	52:a:2275:C:O2	2.00	0.61
43:s:7:LEU:CD1	43:s:46:ALA:HB2	2.31	0.61
7:C:14:ILE:HG22	7:C:15:VAL:HG13	1.82	0.61
18:N:33:ASP:O	18:N:41:ARG:NH2	2.33	0.61
46:v:56:ASP:OD1	46:v:56:ASP:N	2.33	0.61
47:w:39:TRP:CH2	47:w:41:GLU:HB3	2.36	0.61
51:A:1261:A:O2'	51:A:1282:C:O2'	2.03	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:A:507:C:OP2	51:A:508:U:O2'	2.10	0.60
37:l:53:MET:CE	37:l:117:PHE:CE1	2.84	0.60
52:a:262:A:N3	52:a:430:A:O2'	2.33	0.60
9:E:107:ALA:HB3	9:E:112:ARG:HG3	1.82	0.60
11:G:66:LEU:HD21	11:G:101:MET:HE2	1.83	0.60
13:I:106:ARG:NH1	13:I:107:ASP:O	2.34	0.60
12:H:66:PHE:O	12:H:67:GLN:OE1	2.20	0.60
17:M:17:ILE:O	17:M:20:THR:HG23	2.02	0.60
7:C:173:VAL:O	7:C:173:VAL:HG13	2.01	0.60
14:J:45:ARG:NH2	51:A:1255:G:OP2	2.33	0.60
8:D:134:SER:OG	51:A:403:C:OP1	2.12	0.60
51:A:1086:U:H3	51:A:1099:G:H22	1.50	0.60
14:J:9:ARG:CZ	51:A:1279:G:OP2	2.50	0.60
52:a:2653:U:OP2	52:a:2654:A:O2'	2.20	0.60
34:i:49:ASP:O	34:i:49:ASP:OD2	2.19	0.60
51:A:51:A:N7	51:A:114:U:O2'	2.35	0.59
12:H:77:ARG:NH1	12:H:126:ILE:O	2.35	0.59
15:K:115:PRO:O	15:K:116:ILE:HG23	2.02	0.59
18:N:24:ARG:NH1	18:N:56:SER:OG	2.35	0.59
51:A:309:A:O2'	51:A:607:A:N1	2.34	0.59
11:G:27:VAL:HG12	11:G:43:VAL:HG21	1.84	0.59
16:L:38:TYR:CE1	16:L:52:VAL:HG23	2.37	0.59
29:c:7:LYS:NZ	52:a:706:A:OP1	2.35	0.59
36:k:4:ASN:O	52:a:1243:C:O2'	2.06	0.59
51:A:195:A:O2'	51:A:196:A:O4'	2.18	0.59
52:a:1754:A:N1	52:a:2716:C:O2'	2.34	0.59
3:2:7:VAL:HG23	3:2:7:VAL:O	2.02	0.59
32:f:108:VAL:O	32:f:111:ILE:HG13	2.02	0.59
52:a:869:G:H2'	52:a:870:U:H5'	1.84	0.59
25:U:42:THR:HG21	51:A:1527:U:H5	1.66	0.59
40:o:27:GLU:OE2	40:o:87:LYS:NZ	2.33	0.59
47:w:39:TRP:CH2	47:w:41:GLU:CA	2.85	0.59
15:K:34:ILE:HD12	15:K:43:GLY:O	2.03	0.59
37:l:76:LYS:HB3	37:l:77:PRO:HD2	1.84	0.59
36:k:106:GLU:HB3	36:k:107:PHE:CE2	2.38	0.59
14:J:36:VAL:O	14:J:37:ARG:NH2	2.35	0.58
16:L:44:LYS:HD2	16:L:45:PRO:HD2	1.84	0.58
6:B:94:HIS:CE1	6:B:146:ASN:HD22	2.21	0.58
51:A:374:A:O2'	51:A:451:A:OP2	2.20	0.58
14:J:9:ARG:NH2	14:J:71:LEU:HD11	2.19	0.58
37:l:51:ARG:NH2	52:a:2483:C:O2'	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:w:36:HIS:ND1	47:w:37:ARG:O	2.37	0.58
3:2:8:ARG:NH1	52:a:245:G:N7	2.50	0.58
29:c:229:ASP:OD1	52:a:780:G:N1	2.35	0.58
51:A:1253:G:N2	51:A:1285:A:H61	2.02	0.58
3:2:40:ARG:O	3:2:44:LEU:HG	2.02	0.58
51:A:1405:G:N7	53:A:1601:84G:N5	2.51	0.58
52:a:788:A:OP1	52:a:791:C:N4	2.35	0.58
21:Q:66:PRO:O	51:A:264:C:O2'	2.22	0.58
42:q:10:LYS:NZ	52:a:994:C:O2	2.28	0.58
12:H:14:ILE:HD11	12:H:61:LEU:HD13	1.85	0.58
17:M:92:ARG:HD2	52:a:888:C:C4	2.39	0.58
44:t:36:VAL:HG11	44:t:39:ILE:HD12	1.86	0.58
48:x:46:VAL:O	48:x:50:VAL:HG23	2.04	0.58
48:x:47:ARG:NH2	52:a:61:C:OP2	2.29	0.58
51:A:1290:G:H1'	51:A:1291:U:H5'	1.86	0.58
52:a:2718:G:O2'	52:a:2847:U:OP1	2.22	0.58
19:O:58:ARG:NH2	51:A:742:G:OP1	2.36	0.57
32:f:10:ASP:HB2	32:f:11:GLU:OE1	2.03	0.57
36:k:70:LYS:HE2	36:k:107:PHE:HE1	1.69	0.57
51:A:768:A:N3	51:A:1512:U:O2'	2.38	0.57
31:e:5:LEU:HD23	31:e:7:ASP:N	2.18	0.57
3:2:8:ARG:NH2	52:a:244:A:OP2	2.37	0.57
21:Q:22:VAL:HG23	21:Q:45:HIS:CD2	2.39	0.57
37:l:53:MET:CE	37:l:117:PHE:CD1	2.88	0.57
6:B:124:GLY:O	6:B:128:LYS:NZ	2.26	0.57
11:G:62:PHE:CZ	11:G:66:LEU:HD13	2.39	0.57
33:g:112:PRO:O	33:g:112:PRO:HD2	1.96	0.57
34:i:114:LEU:O	34:i:118:MET:HG3	2.05	0.57
52:a:954:G:O2'	52:a:2274:A:N1	2.31	0.57
5:4:22:MET:HA	5:4:22:MET:HE3	1.86	0.57
47:w:39:TRP:CH2	47:w:41:GLU:HA	2.40	0.57
30:d:1:MET:O	30:d:2:ILE:HG23	2.05	0.57
52:a:793:A:OP2	52:a:2071:A:O2'	2.20	0.57
34:i:45:THR:HG22	34:i:46:PRO:HD2	1.86	0.57
34:i:82:GLY:N	52:a:1131:G:OP1	2.33	0.57
13:I:14:SER:O	13:I:14:SER:OG	2.22	0.57
19:O:32:LEU:O	19:O:36:ILE:HG13	2.05	0.57
22:R:29:LEU:HD23	22:R:29:LEU:C	2.29	0.57
12:H:43:GLU:OE1	12:H:43:GLU:HA	2.04	0.56
33:g:112:PRO:O	33:g:112:PRO:CD	2.50	0.56
36:k:23:ILE:CD1	42:q:82:HIS:CE1	2.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:k:59:ARG:NH1	52:a:250:G:O5'	2.38	0.56
42:q:44:GLY:O	42:q:46:GLU:N	2.38	0.56
15:K:82:LEU:HD21	15:K:107:ILE:HD13	1.87	0.56
36:k:19:LEU:HD11	36:k:31:GLY:O	2.05	0.56
48:x:18:LEU:HD12	48:x:18:LEU:O	2.06	0.56
30:d:25:THR:O	30:d:25:THR:HG23	2.05	0.56
32:f:31:VAL:HG11	32:f:96:MET:SD	2.45	0.56
37:l:83:GLY:O	37:l:84:LYS:HB2	2.05	0.56
52:a:664:G:O2'	52:a:940:G:OP1	2.21	0.56
52:a:1392:A:N7	52:a:1393:A:N6	2.53	0.56
52:a:2291:U:OP1	52:a:2380:C:O2'	2.23	0.56
5:4:30:HIS:ND1	5:4:31:ASP:O	2.38	0.56
28:b:40:U:N3	28:b:44:G:OP2	2.30	0.56
39:n:100:HIS:HA	39:n:104:GLN:OE1	2.06	0.56
52:a:1535:A:O2'	52:a:1537:G:N7	2.38	0.56
32:f:164:GLU:OE1	32:f:164:GLU:N	2.32	0.56
36:k:19:LEU:HD22	36:k:31:GLY:HA2	1.88	0.56
51:A:592:G:N2	51:A:648:A:N3	2.52	0.56
19:O:74:ASP:O	19:O:74:ASP:OD2	2.23	0.56
23:S:12:ASP:OD1	23:S:12:ASP:N	2.35	0.56
51:A:1247:U:N3	51:A:1290:G:O6	2.39	0.56
6:B:50:PHE:O	6:B:54:LEU:HD22	2.06	0.56
21:Q:22:VAL:O	21:Q:22:VAL:CG1	2.54	0.56
23:S:78:ARG:NH2	51:A:1321:U:O2'	2.30	0.56
52:a:2834:G:N2	52:a:2883:A:H62	2.04	0.56
25:U:54:LYS:NZ	51:A:1533:C:O2	2.35	0.56
30:d:149:ASN:C	30:d:151:THR:N	2.64	0.56
44:t:74:ASN:OD1	44:t:77:THR:N	2.38	0.56
51:A:791:G:O6	51:A:792:A:N6	2.39	0.56
14:J:9:ARG:HH22	14:J:71:LEU:HD11	1.71	0.56
51:A:1270:G:C2	51:A:1271:A:C8	2.94	0.56
52:a:1047:G:O2'	52:a:1110:G:N1	2.34	0.56
13:I:95:ARG:NH2	51:A:1179:A:OP2	2.39	0.56
22:R:41:PRO:O	22:R:45:THR:HG23	2.06	0.56
48:x:26:PHE:CE1	48:x:30:MET:HE2	2.41	0.56
51:A:898:G:N2	51:A:901:A:OP2	2.38	0.56
51:A:1083:U:O2'	51:A:1102:A:OP2	2.22	0.56
29:c:13:ARG:NH1	52:a:727:A:O2'	2.38	0.55
31:e:24:ASN:O	31:e:28:VAL:HG22	2.06	0.55
45:u:20:LEU:HD21	45:u:41:GLU:OE2	2.06	0.55
47:w:43:GLU:OE1	47:w:45:ARG:NE	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:A:13:U:N3	51:A:916:U:O4	2.39	0.55
52:a:2049:G:N2	52:a:2620:C:C2	2.74	0.55
19:O:49:ASP:OD1	51:A:667:G:O2'	2.21	0.55
36:k:70:LYS:NZ	52:a:634:C:OP1	2.35	0.55
51:A:673:A:H2'	51:A:674:G:C8	2.41	0.55
51:A:1151:A:HO2'	51:A:1152:A:H8	1.53	0.55
24:T:62:ALA:HA	24:T:67:ILE:HG13	1.88	0.55
32:f:35:THR:HB	32:f:155:THR:OG1	2.06	0.55
7:C:11:ARG:NH2	7:C:177:THR:O	2.40	0.55
13:I:84:THR:HG23	13:I:98:LEU:HD23	1.87	0.55
29:c:146:MET:HE1	29:c:154:LEU:HD21	1.87	0.55
40:o:47:VAL:HG11	40:o:50:ILE:HD11	1.88	0.55
43:s:7:LEU:HD21	43:s:45:ALA:C	2.32	0.55
51:A:1270:G:C2	51:A:1271:A:N7	2.75	0.55
52:a:1421:G:O2'	52:a:1493:C:N4	2.36	0.55
42:q:5:PHE:HE1	42:q:14:VAL:HG11	1.71	0.55
49:y:41:THR:HG22	49:y:43:ALA:H	1.70	0.55
51:A:1276:G:N2	51:A:1279:G:H21	2.05	0.55
7:C:76:VAL:O	7:C:83:ASP:OD1	2.23	0.55
13:I:80:ARG:HE	13:I:103:PHE:HD1	1.55	0.55
18:N:49:GLN:OE1	23:S:13:LEU:N	2.38	0.55
32:f:20:PHE:CB	32:f:22:TYR:CE1	2.89	0.55
51:A:1405:G:O2'	51:A:1518:A:O2'	2.19	0.55
7:C:156:ARG:NH1	51:A:1055:A:N3	2.54	0.55
19:O:47:LYS:O	19:O:53:ARG:NH2	2.39	0.55
25:U:55:ARG:NH2	51:A:723:U:OP1	2.39	0.55
51:A:859:G:OP2	51:A:869:G:N1	2.35	0.55
6:B:147:SER:OG	6:B:148:LEU:N	2.40	0.55
17:M:66:GLU:OE1	17:M:70:ARG:NH2	2.40	0.55
39:n:93:ASP:OD1	39:n:95:SER:N	2.40	0.55
36:k:82:LEU:HD22	36:k:90:VAL:HG21	1.89	0.55
51:A:446:G:N2	51:A:489:C:O2	2.40	0.55
13:I:51:PRO:HG3	13:I:80:ARG:HG3	1.89	0.55
24:T:35:VAL:HG11	24:T:79:LEU:HD13	1.89	0.55
35:j:10:VAL:HG21	35:j:16:ALA:HB3	1.89	0.55
51:A:447:G:H21	51:A:487:A:H62	1.53	0.55
51:A:1215:G:N7	51:A:1216:A:N6	2.55	0.55
23:S:66:MET:HE3	23:S:74:PHE:CE2	2.41	0.54
51:A:992:U:H4'	51:A:993:G:H5''	1.89	0.54
6:B:19:GLN:OE1	6:B:19:GLN:N	2.40	0.54
6:B:50:PHE:O	6:B:54:LEU:CD2	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:19:VAL:HG12	13:I:65:ILE:CD1	2.37	0.54
14:J:37:ARG:NH1	14:J:77:VAL:CG2	2.70	0.54
16:L:21:VAL:HG23	16:L:21:VAL:O	2.08	0.54
36:k:106:GLU:C	36:k:107:PHE:CD2	2.85	0.54
52:a:2625:G:H2'	52:a:2626:C:O4'	2.07	0.54
6:B:50:PHE:CD1	6:B:54:LEU:HD21	2.42	0.54
37:l:55:ARG:HD2	52:a:2469:A:H4'	1.88	0.54
40:o:97:LEU:HD13	40:o:100:LEU:HD11	1.88	0.54
51:A:1518:A:HO2'	51:A:1519:A:P	2.28	0.54
52:a:1914:C:H2'	52:a:1915:U:C6	2.42	0.54
21:Q:49:GLU:O	21:Q:50:ASN:CG	2.51	0.54
32:f:116:GLY:O	32:f:178:ARG:NH2	2.40	0.54
51:A:1305:G:H22	51:A:1331:G:H2'	1.72	0.54
52:a:1362:C:HO2'	52:a:1810:A:HO2'	1.53	0.54
32:f:8:TYR:HA	32:f:12:VAL:HG23	1.88	0.54
9:E:165:LEU:O	12:H:114:ARG:NH1	2.40	0.54
14:J:37:ARG:HG2	14:J:37:ARG:HH11	1.73	0.54
31:e:41:GLN:NE2	52:a:442:G:O4'	2.41	0.54
37:l:3:GLN:HE21	37:l:92:TRP:CD1	2.25	0.54
51:A:1316:G:N1	51:A:1319:A:OP2	2.37	0.54
14:J:11:LYS:NZ	51:A:1278:G:O2'	2.40	0.54
35:j:91:SER:O	35:j:93:GLN:NE2	2.40	0.54
11:G:25:LYS:O	11:G:29:ILE:HG13	2.08	0.54
24:T:10:ARG:NH2	51:A:107:G:N7	2.56	0.54
35:j:1:MET:CB	35:j:67:LYS:HD3	2.38	0.54
52:a:980:A:N3	52:a:2037:A:O2'	2.40	0.54
23:S:65:GLU:OE1	23:S:65:GLU:N	2.38	0.54
39:n:93:ASP:OD1	39:n:93:ASP:C	2.50	0.54
51:A:178:C:C2	51:A:179:A:C8	2.97	0.54
52:a:75:G:H22	52:a:111:A:H2	1.55	0.54
52:a:1607:C:H4'	52:a:1608:A:O5'	2.08	0.54
52:a:2564:A:OP1	52:a:2648:G:O2'	2.19	0.54
6:B:41:ILE:HD11	6:B:189:THR:HG22	1.90	0.53
9:E:111:MET:HA	9:E:114:VAL:HG12	1.90	0.53
22:R:29:LEU:HD21	22:R:59:ILE:HG12	1.91	0.53
34:i:37:ARG:HA	34:i:118:MET:CE	2.38	0.53
51:A:440:C:C2	51:A:441:A:C8	2.95	0.53
52:a:607:U:O2	52:a:608:A:C8	2.61	0.53
27:Z:21:A:N6	27:Z:46:G:H2'	2.24	0.53
32:f:101:GLU:OE2	32:f:102:ARG:N	2.41	0.53
52:a:2038:G:H2'	52:a:2039:U:O4'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:88:ARG:NH2	52:a:714:U:OP2	2.40	0.53
52:a:2794:C:HO2'	52:a:2795:C:P	2.30	0.53
4:3:11:CYS:N	4:3:14:CYS:SG	2.80	0.53
18:N:52:PRO:O	18:N:55:SER:OG	2.19	0.53
20:P:55:ASP:N	20:P:55:ASP:OD1	2.41	0.53
29:c:181:MET:HB2	29:c:268:VAL:HB	1.91	0.53
35:j:1:MET:CG	35:j:67:LYS:HD3	2.38	0.53
35:j:12:ASP:N	35:j:12:ASP:OD1	2.42	0.53
21:Q:41:THR:OG1	51:A:280:C:N3	2.37	0.53
52:a:84:A:N1	52:a:98:G:O2'	2.39	0.53
15:K:87:LYS:HE2	15:K:113:VAL:HG23	1.89	0.53
3:2:36:LYS:O	3:2:41:LYS:NZ	2.42	0.53
12:H:14:ILE:HD13	12:H:25:VAL:HG21	1.90	0.53
52:a:848:C:H2'	52:a:849:A:H8	1.74	0.53
52:a:885:C:N3	52:a:892:A:N6	2.57	0.53
5:4:24:ILE:HG21	32:f:102:ARG:HG3	1.91	0.53
27:Z:55:U:O2'	27:Z:57:A:N7	2.33	0.53
51:A:1142:G:O6	51:A:1143:G:N2	2.42	0.53
52:a:754:U:O2'	52:a:1272:A:N1	2.42	0.53
16:L:44:LYS:HB2	16:L:45:PRO:HD2	1.91	0.53
17:M:105:ASN:ND2	51:A:949:A:OP2	2.40	0.53
31:e:1:MET:O	31:e:13:THR:OG1	2.16	0.53
51:A:1290:G:C5	51:A:1291:U:C4	2.96	0.53
52:a:326:G:O2'	52:a:327:G:OP1	2.24	0.53
52:a:2691:C:HO2'	52:a:2871:U:HO2'	1.54	0.53
16:L:62:GLU:OE1	16:L:62:GLU:N	2.42	0.53
30:d:48:ILE:HD12	30:d:50:VAL:CG2	2.39	0.53
30:d:58:ASN:OD1	30:d:58:ASN:N	2.41	0.53
32:f:80:ARG:HB3	32:f:83:TYR:CZ	2.44	0.53
51:A:1071:C:H2'	51:A:1072:G:H8	1.74	0.53
13:I:66:THR:O	13:I:66:THR:CG2	2.56	0.52
28:b:55:U:HO2'	32:f:24:SER:HG	1.55	0.52
30:d:25:THR:CG2	30:d:189:VAL:HG22	2.38	0.52
38:m:69:ARG:C	38:m:70:THR:HG1	2.12	0.52
52:a:238:C:O2'	52:a:608:A:N3	2.41	0.52
32:f:20:PHE:HB2	32:f:22:TYR:CE1	2.44	0.52
51:A:98:A:H2'	51:A:99:C:O4'	2.08	0.52
6:B:204:ASP:C	6:B:204:ASP:OD1	2.51	0.52
20:P:69:ASP:OD1	20:P:70:ARG:N	2.43	0.52
49:y:37:GLU:OE2	49:y:37:GLU:N	2.42	0.52
51:A:1124:G:N2	51:A:1125:U:O4	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:1:MET:N	52:a:1620:G:O4'	2.41	0.52
32:f:20:PHE:HB3	32:f:22:TYR:CE1	2.45	0.52
33:g:60:ASP:O	33:g:62:TRP:N	2.42	0.52
52:a:987:C:O2'	52:a:1000:A:N3	2.40	0.52
13:I:43:THR:O	13:I:47:VAL:HG23	2.10	0.52
38:m:2:ARG:NH2	52:a:1653:G:OP1	2.36	0.52
39:n:79:ALA:CB	39:n:113:ALA:HB3	2.39	0.52
51:A:1223:C:OP2	51:A:1322:C:N4	2.41	0.52
52:a:1551:A:H2'	52:a:1552:A:O4'	2.09	0.52
52:a:2250:G:N2	52:a:2497:A:OP2	2.43	0.52
16:L:115:SER:OG	51:A:35:G:N3	2.42	0.52
17:M:42:ASP:C	17:M:42:ASP:OD2	2.52	0.52
24:T:48:GLN:O	24:T:52:ASN:ND2	2.43	0.52
51:A:1014:A:N7	51:A:1015:G:N2	2.58	0.52
51:A:1116:U:H2'	51:A:1117:A:H5'	1.91	0.52
51:A:1252:A:H61	51:A:1285:A:H2	1.57	0.52
52:a:827:U:O2'	52:a:2068:U:N3	2.41	0.52
49:y:44:ILE:O	49:y:48:ILE:HG22	2.10	0.52
52:a:463:G:N2	52:a:466:A:OP2	2.38	0.52
52:a:1858:A:H2'	52:a:1859:U:O4'	2.10	0.52
14:J:9:ARG:NH1	14:J:71:LEU:HD11	2.24	0.52
33:g:30:ASN:ND2	33:g:79:VAL:O	2.41	0.52
33:g:71:LEU:O	33:g:75:MET:HG3	2.09	0.52
47:w:40:VAL:HG22	47:w:42:SER:H	1.75	0.52
51:A:437:U:O2'	51:A:493:A:N6	2.42	0.52
31:e:2:GLU:OE2	31:e:11:ALA:HB1	2.10	0.52
51:A:1162:C:N3	51:A:1163:A:N7	2.58	0.52
9:E:29:ARG:NH2	51:A:1397:C:OP2	2.43	0.52
21:Q:17:MET:CE	21:Q:20:SER:OG	2.58	0.52
30:d:2:ILE:HD12	30:d:48:ILE:HD11	1.91	0.52
33:g:35:ARG:HH11	33:g:71:LEU:HD21	1.75	0.52
6:B:17:GLY:HA3	6:B:189:THR:HG21	1.90	0.51
28:b:1:U:H2'	28:b:2:G:H8	1.74	0.51
31:e:130:LYS:HB2	31:e:133:LEU:HD13	1.92	0.51
31:e:190:ALA:O	31:e:193:VAL:HG22	2.10	0.51
52:a:2197:U:O2'	52:a:2198:A:OP2	2.23	0.51
14:J:9:ARG:NH1	51:A:1279:G:OP2	2.43	0.51
34:i:4:PHE:CE2	34:i:5:THR:O	2.63	0.51
40:o:97:LEU:HD22	40:o:99:TYR:CE1	2.44	0.51
51:A:1035:A:C2	51:A:1036:A:C2	2.99	0.51
51:A:1408:A:N6	51:A:1494:G:O6	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:a:2794:C:O2'	52:a:2795:C:P	2.68	0.51
8:D:170:TRP:NE1	8:D:171:LEU:HD21	2.25	0.51
11:G:58:GLU:OE1	11:G:58:GLU:N	2.41	0.51
11:G:75:VAL:HB	11:G:86:GLN:HG2	1.92	0.51
19:O:62:GLN:O	19:O:66:LEU:HG	2.10	0.51
43:s:12:ARG:HB2	43:s:33:LYS:HG2	1.91	0.51
45:u:72:VAL:HG12	45:u:93:ARG:HA	1.92	0.51
49:y:51:VAL:HG13	49:y:54:MET:HE3	1.93	0.51
51:A:1267:C:O2	51:A:1268:G:N2	2.44	0.51
14:J:9:ARG:NH2	51:A:1279:G:OP2	2.43	0.51
25:U:11:PRO:O	25:U:14:VAL:HG22	2.10	0.51
46:v:64:ASP:C	46:v:64:ASP:OD1	2.53	0.51
20:P:39:PHE:CE1	20:P:74:LEU:HD13	2.46	0.51
38:m:48:VAL:O	38:m:49:GLU:C	2.52	0.51
52:a:2560:A:H2'	52:a:2561:U:O4'	2.11	0.51
7:C:39:VAL:HG21	7:C:91:VAL:HG23	1.93	0.51
14:J:9:ARG:NH2	51:A:1280:A:OP1	2.44	0.51
39:n:52:SER:OG	39:n:54:VAL:HG22	2.11	0.51
51:A:179:A:C5	51:A:180:U:C5	2.99	0.51
51:A:840:C:OP1	51:A:847:G:N1	2.40	0.51
1:O:47:VAL:HG12	1:O:48:ILE:N	2.25	0.51
6:B:50:PHE:CD1	6:B:54:LEU:CD2	2.93	0.51
24:T:59:ASP:OD1	24:T:59:ASP:C	2.53	0.51
35:j:118:LEU:O	35:j:118:LEU:HD23	2.10	0.51
37:l:79:ALA:O	37:l:80:VAL:HG13	2.11	0.51
37:l:90:GLU:HG3	37:l:91:TYR:HD2	1.74	0.51
49:y:48:ILE:HD11	49:y:57:VAL:CG2	2.40	0.51
52:a:1493:C:O2	52:a:1493:C:H2'	2.11	0.51
52:a:2031:A:N3	52:a:2455:G:O2'	2.40	0.51
12:H:36:ILE:O	12:H:39:VAL:HG12	2.11	0.51
16:L:9:ARG:NH1	51:A:880:C:OP1	2.40	0.51
42:q:5:PHE:HE1	42:q:14:VAL:CG1	2.23	0.51
8:D:118:VAL:HG12	8:D:123:ILE:HD12	1.92	0.51
44:t:42:VAL:HG11	44:t:63:ALA:HB2	1.93	0.51
13:I:91:ASP:OD2	13:I:94:LEU:HB2	2.11	0.50
29:c:121:ASP:OD1	29:c:121:ASP:N	2.36	0.50
51:A:1255:G:O3'	51:A:1258:G:O2'	2.24	0.50
52:a:2260:C:HO2'	52:a:2388:A:HO2'	1.58	0.50
52:a:2328:A:H2'	52:a:2329:U:C6	2.46	0.50
52:a:2619:C:H2'	52:a:2620:C:C6	2.47	0.50
52:a:2766:A:C2	52:a:2767:C:C6	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:10:LEU:HD11	4:3:35:GLN:HE21	1.76	0.50
5:4:48:GLN:N	5:4:48:GLN:OE1	2.44	0.50
14:J:63:ASP:C	14:J:63:ASP:OD2	2.54	0.50
28:b:51:G:OP1	39:n:63:LYS:NZ	2.45	0.50
38:m:100:CYS:SG	38:m:101:GLY:N	2.85	0.50
44:t:82:ARG:NH2	52:a:301:G:OP2	2.45	0.50
51:A:197:A:N1	51:A:220:G:O2'	2.31	0.50
51:A:393:A:C2	51:A:394:G:C8	2.99	0.50
51:A:1210:C:O2'	51:A:1213:A:O3'	2.28	0.50
16:L:87:VAL:O	16:L:88:LYS:C	2.52	0.50
36:k:19:LEU:HD21	36:k:27:LEU:HD22	1.92	0.50
52:a:631:A:N3	52:a:2415:G:O2'	2.34	0.50
52:a:1577:C:H2'	52:a:1578:U:C1'	2.42	0.50
5:4:32:LEU:HB3	5:4:34:LEU:HD21	1.93	0.50
18:N:66:GLN:HE21	18:N:79:LEU:HD21	1.77	0.50
30:d:78:GLY:C	30:d:79:LEU:HD12	2.37	0.50
30:d:131:ASP:O	30:d:136:ASN:ND2	2.44	0.50
51:A:1360:A:N3	51:A:1360:A:OP1	2.45	0.50
52:a:137:U:O2'	52:a:138:U:OP1	2.28	0.50
52:a:1802:A:H2'	52:a:1803:A:C8	2.46	0.50
16:L:70:GLU:OE2	16:L:107:VAL:HG21	2.10	0.50
38:m:44:LEU:O	38:m:48:VAL:HG23	2.11	0.50
51:A:333:U:N3	51:A:334:C:C5	2.79	0.50
9:E:19:ASN:OD1	9:E:20:ARG:N	2.42	0.50
13:I:12:ARG:NH2	51:A:1347:G:O6	2.44	0.50
19:O:85:LEU:HD12	19:O:85:LEU:N	2.26	0.50
51:A:79:G:N1	51:A:91:U:O4	2.45	0.50
51:A:765:G:N1	51:A:812:G:O2'	2.38	0.50
51:A:935:A:O2'	51:A:1383:C:N3	2.43	0.50
51:A:1124:G:O2'	51:A:1144:G:O6	2.29	0.50
17:M:98:ARG:NH2	51:A:1309:G:OP2	2.45	0.50
30:d:49:GLN:OE1	52:a:2635:A:O2'	2.29	0.50
2:l:6:GLN:O	52:a:686:U:O2	2.29	0.50
23:S:6:LYS:NZ	51:A:1313:U:OP2	2.44	0.50
25:U:42:THR:HG21	51:A:1527:U:C5	2.46	0.50
37:l:53:MET:CE	37:l:117:PHE:HE1	2.25	0.50
33:g:72:LEU:HD23	33:g:72:LEU:O	2.11	0.50
18:N:9:ARG:NH1	51:A:1217:C:OP1	2.44	0.49
19:O:70:LEU:HD12	19:O:70:LEU:O	2.12	0.49
47:w:49:LEU:N	47:w:49:LEU:HD23	2.27	0.49
52:a:2822:G:N2	52:a:2824:C:OP1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:11:GLU:OE2	5:4:24:ILE:N	2.45	0.49
41:p:5:LYS:NZ	52:a:29:U:OP1	2.30	0.49
51:A:445:G:H4'	51:A:446:G:OP2	2.12	0.49
51:A:1323:G:H2'	51:A:1324:A:C8	2.47	0.49
52:a:1641:A:H2'	52:a:1642:G:O4'	2.12	0.49
52:a:1918:A:O2'	52:a:1920:C:N4	2.45	0.49
3:2:13:ARG:NE	36:k:58:TYR:O	2.45	0.49
6:B:97:LEU:N	6:B:100:MET:HE3	2.27	0.49
15:K:82:LEU:HD22	15:K:105:PHE:HB3	1.94	0.49
28:b:79:G:O6	45:u:14:LYS:NZ	2.24	0.49
51:A:496:A:H61	51:A:498:A:H62	1.61	0.49
51:A:1483:A:O2'	52:a:1947:C:O2'	2.24	0.49
5:4:11:GLU:HA	5:4:25:ARG:HA	1.93	0.49
6:B:50:PHE:CE1	6:B:54:LEU:HD21	2.48	0.49
7:C:28:GLU:HG3	7:C:28:GLU:O	2.12	0.49
14:J:37:ARG:CZ	14:J:37:ARG:HA	2.43	0.49
29:c:66:ASP:OD2	29:c:102:ARG:NH1	2.45	0.49
36:k:70:LYS:HE2	36:k:107:PHE:CE1	2.48	0.49
38:m:82:GLU:OE1	38:m:82:GLU:N	2.45	0.49
39:n:24:THR:O	39:n:90:VAL:HG23	2.13	0.49
51:A:1171:A:H2'	51:A:1172:C:C6	2.48	0.49
52:a:562:U:O2	52:a:2035:G:O2'	2.29	0.49
52:a:2468:A:H2'	52:a:2476:A:C6	2.46	0.49
52:a:2784:U:O2'	52:a:2785:C:H5'	2.12	0.49
33:g:175:LYS:O	33:g:176:LYS:C	2.55	0.49
35:j:32:TYR:OH	52:a:1996:C:N4	2.32	0.49
39:n:111:ARG:NH2	39:n:117:PHE:O	2.45	0.49
49:y:48:ILE:HD11	49:y:57:VAL:HG22	1.95	0.49
51:A:264:C:H2'	51:A:265:G:O4'	2.12	0.49
51:A:364:A:H2'	51:A:365:U:O2	2.12	0.49
51:A:1062:U:H2'	51:A:1063:C:C6	2.48	0.49
52:a:2691:C:O2'	52:a:2871:U:O2'	2.29	0.49
1:0:34:LEU:CD1	1:0:36:LEU:HD21	2.40	0.49
8:D:18:ASP:CG	8:D:28:ILE:HG21	2.38	0.49
38:m:8:ARG:HD2	38:m:43:GLU:CG	2.42	0.49
45:u:35:GLU:OE1	45:u:35:GLU:HA	2.11	0.49
52:a:2687:U:H2'	52:a:2688:G:O4'	2.13	0.49
34:i:7:LYS:HD3	34:i:7:LYS:N	2.28	0.49
43:s:67:VAL:HG22	43:s:76:ARG:HG2	1.93	0.49
51:A:373:A:C2	51:A:374:A:C8	3.01	0.49
51:A:1315:U:H1'	51:A:1360:A:H2'	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:a:1419:A:O2'	52:a:1421:G:N7	2.30	0.49
45:u:7:GLU:OE1	45:u:7:GLU:N	2.46	0.49
52:a:2260:C:O2'	52:a:2388:A:O2'	2.28	0.49
52:a:2540:C:O2'	52:a:2740:A:N3	2.43	0.49
52:a:2788:C:O2'	52:a:2809:A:N3	2.45	0.49
6:B:46:THR:O	6:B:50:PHE:HB2	2.12	0.49
30:d:156:PHE:CD1	34:i:81:ILE:HD13	2.48	0.49
51:A:1256:A:H4'	51:A:1258:G:H1'	1.94	0.49
52:a:1141:U:H4'	52:a:1142:A:O4'	2.12	0.49
4:3:11:CYS:SG	4:3:14:CYS:N	2.86	0.48
21:Q:31:HIS:CE1	21:Q:32:PRO:HG3	2.48	0.48
35:j:102:PRO:HD2	35:j:102:PRO:O	2.13	0.48
11:G:72:THR:O	11:G:91:VAL:HG12	2.14	0.48
16:L:87:VAL:O	16:L:90:LEU:N	2.46	0.48
51:A:139:A:H2'	51:A:140:U:O4'	2.13	0.48
52:a:279:A:H2'	52:a:280:U:O4'	2.14	0.48
15:K:34:ILE:HD13	15:K:74:VAL:HG21	1.95	0.48
51:A:919:A:C2	51:A:920:U:C5	3.01	0.48
52:a:2703:C:C2	52:a:2704:C:C5	3.01	0.48
10:F:36:ILE:HG13	10:F:64:VAL:HG12	1.95	0.48
32:f:133:ARG:C	32:f:133:ARG:HD3	2.39	0.48
36:k:37:GLY:N	36:k:40:SER:OG	2.47	0.48
36:k:60:ARG:O	36:k:61:LEU:HD23	2.13	0.48
51:A:214:C:C2	51:A:215:C:C5	3.01	0.48
51:A:936:C:C2	51:A:937:A:C8	3.02	0.48
51:A:1183:U:H3'	51:A:1184:G:H5''	1.95	0.48
9:E:37:THR:HG22	9:E:63:ALA:HB1	1.96	0.48
11:G:5:ARG:CZ	11:G:7:ILE:HG22	2.42	0.48
14:J:9:ARG:CZ	14:J:71:LEU:HD11	2.44	0.48
37:l:3:GLN:HE21	37:l:92:TRP:HE1	1.56	0.48
52:a:880:G:C2	52:a:881:G:C8	3.00	0.48
52:a:2523:G:HO2'	52:a:2764:A:HO2'	1.62	0.48
2:1:37:LYS:NZ	52:a:468:G:OP2	2.45	0.48
40:o:112:GLU:OE2	51:A:1441:A:N6	2.34	0.48
52:a:1145:C:N3	52:a:1146:C:C5	2.81	0.48
52:a:2506:U:OP2	52:a:2576:G:N1	2.42	0.48
9:E:115:LEU:HD13	9:E:123:VAL:HG11	1.95	0.48
51:A:1255:G:H1'	51:A:1259:C:O2'	2.14	0.48
52:a:2756:U:H4'	52:a:2757:A:OP1	2.13	0.48
7:C:163:ALA:HB2	51:A:1056:U:H4'	1.96	0.48
35:j:115:ILE:O	35:j:119:ALA:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:m:32:GLU:N	38:m:32:GLU:OE2	2.46	0.48
43:s:82:LYS:NZ	52:a:1340:U:OP2	2.46	0.48
51:A:951:G:C6	51:A:1231:G:O6	2.66	0.48
51:A:1023:U:H2'	51:A:1024:G:C1'	2.43	0.48
20:P:18:GLN:OE1	20:P:35:ARG:HD2	2.14	0.48
32:f:34:ILE:HD11	32:f:100:PHE:HD1	1.78	0.48
51:A:37:U:O2	51:A:547:A:H2	1.97	0.48
51:A:945:G:C2	51:A:946:A:C8	3.02	0.48
51:A:1133:G:H3'	51:A:1134:G:C8	2.48	0.48
12:H:3:MET:HE3	12:H:9:ASP:OD2	2.14	0.48
14:J:9:ARG:HH12	14:J:71:LEU:HD11	1.78	0.48
22:R:29:LEU:HD22	22:R:68:LEU:HD11	1.96	0.48
36:k:19:LEU:HD13	36:k:31:GLY:HA3	1.96	0.48
40:o:81:VAL:HG23	40:o:81:VAL:O	2.14	0.48
51:A:988:G:O2'	51:A:1014:A:N6	2.47	0.48
51:A:1018:G:H3'	51:A:1019:A:O4'	2.13	0.48
51:A:1254:A:H2'	51:A:1255:G:O4'	2.14	0.48
50:z:48:TYR:CE1	50:z:53:LYS:HG2	2.49	0.47
51:A:179:A:C6	51:A:180:U:C5	3.02	0.47
51:A:417:G:C6	51:A:418:C:C5	3.02	0.47
51:A:552:U:N3	51:A:553:A:N7	2.62	0.47
52:a:544:C:H2'	52:a:545:U:H2'	1.94	0.47
17:M:28:THR:HG21	51:A:1328:C:OP1	2.15	0.47
20:P:47:GLU:OE1	51:A:617:G:H4'	2.14	0.47
29:c:175:ARG:HG3	29:c:181:MET:HE2	1.96	0.47
51:A:1257:A:O2'	51:A:1258:G:OP1	2.31	0.47
52:a:2607:G:H2'	52:a:2608:G:O4'	2.14	0.47
7:C:72:ARG:O	7:C:75:ILE:HG22	2.14	0.47
16:L:44:LYS:HE3	16:L:46:ASN:N	2.21	0.47
24:T:74:ARG:NH1	51:A:260:G:OP2	2.42	0.47
40:o:10:GLN:HA	40:o:13:MET:HG2	1.95	0.47
43:s:5:GLU:OE2	43:s:9:LYS:NZ	2.34	0.47
51:A:792:A:C4	51:A:794:A:N6	2.82	0.47
51:A:1381:U:O2	51:A:1381:U:H2'	2.14	0.47
52:a:1866:A:C6	52:a:1876:A:N7	2.82	0.47
5:4:12:ILE:CD1	5:4:32:LEU:HD12	2.44	0.47
8:D:72:PHE:HE2	8:D:94:LEU:HD21	1.78	0.47
11:G:31:MET:HE1	11:G:34:GLY:HA2	1.97	0.47
41:p:6:ARG:CG	41:p:6:ARG:O	2.62	0.47
47:w:39:TRP:CZ3	47:w:41:GLU:N	2.82	0.47
51:A:552:U:C2	51:A:553:A:C8	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:A:645:G:C2	51:A:646:G:C8	3.03	0.47
51:A:765:G:H1	51:A:812:G:HO2'	1.61	0.47
52:a:133:U:H2'	52:a:134:G:H8	1.78	0.47
52:a:870:U:H2'	52:a:871:U:O4'	2.14	0.47
52:a:1020:A:C2	52:a:1141:U:C2	3.02	0.47
5:4:47:LYS:O	5:4:48:GLN:C	2.57	0.47
35:j:2:ILE:HD11	35:j:82:ASN:HB3	1.95	0.47
51:A:259:G:C4	51:A:260:G:C8	3.03	0.47
51:A:714:G:H2'	51:A:715:A:C8	2.48	0.47
51:A:1014:A:N7	51:A:1015:G:C2	2.82	0.47
51:A:1269:A:N6	51:A:1312:G:H1'	2.29	0.47
52:a:151:C:H2'	52:a:152:A:H8	1.80	0.47
52:a:1433:A:H2'	52:a:1434:A:O4'	2.15	0.47
51:A:611:C:C4	51:A:612:C:C5	3.02	0.47
52:a:480:A:H2'	52:a:481:G:OP1	2.14	0.47
4:3:10:LEU:HD11	4:3:35:GLN:NE2	2.29	0.47
9:E:34:THR:HG22	9:E:52:LYS:HB3	1.96	0.47
12:H:18:GLN:CG	12:H:70:ALA:HB1	2.45	0.47
15:K:30:THR:HG23	15:K:30:THR:O	2.13	0.47
22:R:61:ARG:NH1	51:A:736:C:OP1	2.47	0.47
27:Z:19:G:C2	27:Z:57:A:C2	3.03	0.47
36:k:105:ILE:HD13	36:k:105:ILE:N	2.29	0.47
38:m:69:ARG:C	38:m:70:THR:OG1	2.56	0.47
46:v:65:GLY:HA3	46:v:82:ILE:HD11	1.97	0.47
51:A:19:A:H2'	51:A:20:U:O4'	2.15	0.47
51:A:500:G:H2'	51:A:501:C:C6	2.50	0.47
51:A:610:U:C2	51:A:611:C:C5	3.03	0.47
52:a:897:C:H2'	52:a:898:C:C6	2.49	0.47
52:a:1197:G:C2	52:a:1198:U:C5	3.03	0.47
52:a:1980:G:O2'	52:a:1982:U:OP2	2.32	0.47
9:E:100:SER:N	51:A:6:G:O6	2.42	0.47
27:Z:18:G:C4	27:Z:58:A:C2	3.02	0.47
28:b:28:C:OP1	39:n:31:THR:HG21	2.15	0.47
33:g:94:TYR:N	33:g:94:TYR:HD1	2.13	0.47
52:a:1858:A:C6	52:a:1885:A:C8	3.03	0.47
28:b:79:G:O2'	52:a:861:A:N3	2.48	0.47
34:i:113:PRO:HD2	52:a:558:U:OP1	2.14	0.47
41:p:37:GLN:HB3	42:q:75:VAL:HG21	1.97	0.47
51:A:31:G:C8	51:A:306:A:H1'	2.50	0.47
52:a:285:G:C8	52:a:286:U:C5	3.03	0.47
52:a:2250:G:O5'	52:a:2252:G:P	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:11:LEU:HD23	9:E:41:ASP:HA	1.96	0.46
28:b:106:G:H2'	28:b:107:G:O4'	2.15	0.46
52:a:326:G:O2'	52:a:327:G:P	2.72	0.46
12:H:50:LYS:HG3	12:H:52:GLU:OE1	2.14	0.46
14:J:25:ILE:HD12	14:J:90:LEU:HD13	1.97	0.46
43:s:19:LYS:NZ	43:s:84:TYR:OH	2.47	0.46
51:A:1256:A:O5'	51:A:1258:G:H1'	2.15	0.46
52:a:2534:A:C2	52:a:2535:G:H1'	2.50	0.46
11:G:24:ALA:HA	11:G:27:VAL:HG22	1.97	0.46
18:N:28:LYS:NZ	51:A:1317:C:OP2	2.38	0.46
20:P:39:PHE:HE1	20:P:74:LEU:HD13	1.80	0.46
29:c:132:MET:HE1	29:c:184:VAL:HG21	1.98	0.46
33:g:67:THR:HG21	52:a:2757:A:N1	2.30	0.46
36:k:125:LEU:HD12	36:k:125:LEU:N	2.29	0.46
51:A:592:G:H2'	51:A:593:U:O4'	2.14	0.46
52:a:285:G:O6	52:a:355:U:O2	2.33	0.46
52:a:866:A:O2'	52:a:867:C:H5'	2.16	0.46
52:a:2007:U:C2	52:a:2008:C:C5	3.03	0.46
19:O:48:LYS:NZ	51:A:669:G:OP1	2.45	0.46
20:P:45:GLU:O	20:P:47:GLU:HG3	2.16	0.46
30:d:187:LEU:HD21	30:d:203:VAL:HG11	1.97	0.46
31:e:175:ILE:HD11	31:e:180:LEU:HG	1.97	0.46
32:f:13:VAL:HG23	32:f:14:LYS:N	2.30	0.46
36:k:85:VAL:O	36:k:85:VAL:HG13	2.15	0.46
44:t:15:THR:HG22	44:t:69:ASN:HB3	1.97	0.46
51:A:123:U:C2	51:A:124:C:C5	3.04	0.46
52:a:289:G:C6	52:a:352:A:N6	2.84	0.46
52:a:1264:A:OP2	52:a:1265:A:O2'	2.22	0.46
32:f:8:TYR:HA	32:f:12:VAL:CG2	2.44	0.46
51:A:532:A:N1	51:A:1206:G:O2'	2.42	0.46
51:A:1315:U:C5'	51:A:1361:G:O5'	2.63	0.46
51:A:1323:G:H2'	51:A:1324:A:H8	1.80	0.46
51:A:1494:G:C2	51:A:1495:U:C6	3.04	0.46
52:a:1198:U:C2	52:a:1199:U:C5	3.04	0.46
52:a:1462:C:C4'	52:a:2702:G:H21	2.28	0.46
10:F:20:GLY:O	10:F:24:ARG:HG3	2.15	0.46
16:L:111:LYS:HE3	16:L:122:PRO:HB3	1.96	0.46
29:c:35:GLU:OE2	52:a:1816:C:N4	2.47	0.46
30:d:25:THR:HG22	30:d:189:VAL:HG22	1.98	0.46
36:k:18:ARG:NH2	52:a:1250:G:N7	2.55	0.46
52:a:221:A:N1	52:a:265:A:O2'	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:a:473:G:O2'	52:a:474:G:H5'	2.16	0.46
52:a:1607:C:N4	52:a:1622:G:OP2	2.48	0.46
5:4:24:ILE:HG12	32:f:101:GLU:OE1	2.15	0.46
12:H:7:ILE:CD1	12:H:32:LEU:HD23	2.42	0.46
20:P:70:ARG:NH1	51:A:374:A:O3'	2.49	0.46
32:f:96:MET:SD	32:f:96:MET:C	2.98	0.46
38:m:15:SER:OG	52:a:2710:C:OP1	2.30	0.46
44:t:27:ASN:N	44:t:27:ASN:OD1	2.45	0.46
51:A:554:A:H2'	51:A:555:U:H6	1.81	0.46
7:C:3:GLN:HG3	51:A:1061:G:OP2	2.16	0.46
12:H:48:ASP:C	12:H:48:ASP:OD2	2.58	0.46
15:K:36:ASP:C	15:K:36:ASP:OD1	2.59	0.46
31:e:19:PHE:HE2	31:e:109:LEU:HD13	1.80	0.46
35:j:28:SER:HB2	52:a:2563:U:O2'	2.16	0.46
45:u:2:PHE:HB3	45:u:50:MET:HE2	1.98	0.46
52:a:2533:U:H2'	52:a:2534:A:O4'	2.16	0.46
8:D:85:ASN:O	8:D:89:ASN:OD1	2.33	0.46
9:E:76:LEU:HD23	9:E:76:LEU:N	2.31	0.46
14:J:51:VAL:HB	18:N:81:ARG:HB2	1.97	0.46
15:K:74:VAL:O	15:K:74:VAL:HG12	2.15	0.46
29:c:236:GLU:OE2	52:a:2599:G:C8	2.69	0.46
35:j:90:ASN:OD1	35:j:91:SER:N	2.48	0.46
51:A:71:A:C2	51:A:72:A:C8	3.04	0.46
51:A:618:C:H5'	51:A:619:U:H5''	1.97	0.46
51:A:951:G:C6	51:A:1231:G:C6	3.03	0.46
52:a:2283:C:C2	52:a:2284:A:C8	3.04	0.46
13:I:41:ARG:NH2	13:I:72:ILE:HD11	2.31	0.46
14:J:90:LEU:HB2	14:J:92:LEU:HD13	1.98	0.46
18:N:93:ILE:HD12	18:N:96:LEU:HD23	1.98	0.46
20:P:35:ARG:NH1	20:P:38:PHE:HB3	2.31	0.46
51:A:153:C:C2	51:A:154:U:C5	3.04	0.46
51:A:787:A:N1	51:A:795:C:N4	2.58	0.46
52:a:1432:G:H2'	52:a:1433:A:C8	2.51	0.46
52:a:2590:A:C2	52:a:2591:C:C5	3.04	0.46
52:a:2838:G:C4	52:a:2839:G:C8	3.04	0.46
6:B:51:ASN:HA	6:B:54:LEU:HD23	1.97	0.45
6:B:196:VAL:HG11	6:B:199:VAL:HA	1.99	0.45
9:E:57:PRO:O	9:E:60:ILE:HG13	2.16	0.45
15:K:87:LYS:CE	15:K:113:VAL:HG23	2.46	0.45
34:i:76:HIS:ND1	34:i:76:HIS:O	2.48	0.45
44:t:13:VAL:HG21	44:t:39:ILE:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:A:656:G:H2'	51:A:657:U:H6	1.82	0.45
52:a:137:U:HO2'	52:a:138:U:P	2.40	0.45
52:a:669:G:H2'	52:a:670:A:C8	2.52	0.45
52:a:828:U:H2'	52:a:829:A:C8	2.51	0.45
6:B:132:LYS:NZ	51:A:1160:G:OP1	2.47	0.45
7:C:65:ARG:NH1	7:C:100:GLN:OE1	2.50	0.45
9:E:52:LYS:NZ	51:A:1081:A:N7	2.64	0.45
21:Q:8:LEU:HD22	21:Q:8:LEU:N	2.31	0.45
33:g:19:ILE:HG22	33:g:43:VAL:HG11	1.98	0.45
33:g:94:TYR:N	33:g:94:TYR:CD1	2.84	0.45
41:p:32:TYR:O	41:p:32:TYR:CG	2.69	0.45
45:u:48:MET:HE3	45:u:51:GLN:HB3	1.98	0.45
46:v:65:GLY:C	46:v:82:ILE:HD11	2.41	0.45
51:A:925:G:C2	51:A:927:G:C8	3.04	0.45
52:a:101:A:H2'	52:a:101:A:N3	2.31	0.45
3:2:28:ASN:O	3:2:36:LYS:NZ	2.49	0.45
12:H:89:LYS:O	12:H:92:LEU:HD12	2.17	0.45
17:M:42:ASP:OD2	17:M:43:VAL:N	2.49	0.45
29:c:13:ARG:O	29:c:14:ARG:C	2.59	0.45
30:d:2:ILE:HD11	30:d:90:PHE:CZ	2.51	0.45
30:d:24:VAL:HG21	30:d:188:LEU:HD23	1.98	0.45
51:A:31:G:C2'	51:A:48:C:H41	2.28	0.45
6:B:180:GLY:O	6:B:181:ILE:HG13	2.17	0.45
17:M:95:LEU:HB3	17:M:96:PRO:HD2	1.99	0.45
19:O:21:ASP:OD2	19:O:21:ASP:C	2.59	0.45
19:O:72:ARG:NH2	51:A:754:C:OP1	2.50	0.45
37:l:117:PHE:HD2	37:l:130:PHE:CD2	2.34	0.45
50:z:43:ILE:HD13	50:z:49:TYR:HB2	1.97	0.45
51:A:410:G:C2	51:A:429:U:O2	2.70	0.45
51:A:618:C:C5'	51:A:619:U:H5''	2.47	0.45
51:A:992:U:O4	51:A:1045:C:C5	2.70	0.45
52:a:1400:U:O2'	52:a:1401:G:H5'	2.16	0.45
52:a:1599:U:N3	52:a:1600:C:C5	2.84	0.45
2:1:7:PRO:HB2	52:a:1309:G:H4'	1.99	0.45
5:4:34:LEU:N	5:4:34:LEU:HD23	2.32	0.45
7:C:51:SER:HB3	7:C:115:LEU:HD11	1.98	0.45
14:J:37:ARG:HA	14:J:37:ARG:NE	2.31	0.45
21:Q:68:SER:OG	21:Q:69:LYS:N	2.50	0.45
22:R:59:ILE:O	22:R:63:ARG:HD2	2.16	0.45
28:b:113:C:H2'	28:b:114:C:O4'	2.15	0.45
39:n:31:THR:HG23	39:n:33:ARG:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:a:526:A:O2'	52:a:2043:C:O2	2.33	0.45
52:a:858:G:N3	52:a:2268:A:H2'	2.30	0.45
52:a:1118:C:H2'	52:a:1119:U:O4'	2.17	0.45
52:a:1395:A:HO2'	52:a:1397:U:H5	1.59	0.45
5:4:11:GLU:OE1	5:4:12:ILE:N	2.50	0.45
11:G:138:ARG:HH11	11:G:142:HIS:CE1	2.34	0.45
14:J:18:ILE:HG21	14:J:72:ARG:CD	2.47	0.45
28:b:36:C:O2	28:b:36:C:H2'	2.16	0.45
31:e:91:ASP:OD1	31:e:92:HIS:N	2.50	0.45
36:k:100:ILE:O	36:k:100:ILE:HG22	2.16	0.45
37:l:102:LEU:HD12	37:l:102:LEU:N	2.31	0.45
44:t:39:ILE:N	44:t:62:GLU:OE1	2.48	0.45
44:t:97:LYS:O	44:t:98:SER:OG	2.31	0.45
51:A:713:G:H2'	51:A:714:G:C8	2.50	0.45
51:A:1309:G:O6	51:A:1329:A:C6	2.70	0.45
52:a:45:G:H5'	52:a:46:G:O5'	2.17	0.45
52:a:362:A:C5	52:a:363:G:C8	3.05	0.45
9:E:114:VAL:HG13	9:E:115:LEU:N	2.30	0.45
24:T:86:LEU:HD12	24:T:86:LEU:O	2.16	0.45
31:e:5:LEU:HD22	31:e:8:ALA:H	1.81	0.45
49:y:16:ARG:HD3	49:y:54:MET:HE1	1.97	0.45
51:A:269:C:N4	51:A:270:A:H62	2.15	0.45
51:A:417:G:H2'	51:A:418:C:C5'	2.47	0.45
51:A:1313:U:H2'	51:A:1314:C:O5'	2.16	0.45
52:a:2071:A:H2'	52:a:2072:C:C6	2.52	0.45
52:a:2075:U:H1'	52:a:2597:G:N2	2.31	0.45
6:B:32:PHE:O	6:B:32:PHE:HD2	1.99	0.45
8:D:4:TYR:CE1	8:D:11:LEU:HD11	2.52	0.45
8:D:174:ASP:OD1	8:D:176:GLY:N	2.50	0.45
11:G:4:ARG:HG3	11:G:6:VAL:HG22	1.99	0.45
15:K:36:ASP:OD1	15:K:38:GLN:N	2.37	0.45
51:A:411:A:C5	51:A:413:G:C6	3.04	0.45
51:A:413:G:H4'	51:A:414:A:C5'	2.47	0.45
51:A:979:C:C4	51:A:980:C:C6	3.05	0.45
2:1:16:HIS:ND1	52:a:684:G:OP1	2.45	0.45
2:1:22:MET:O	2:1:28:ARG:NH1	2.50	0.45
5:4:58:ASP:OD2	5:4:58:ASP:C	2.59	0.45
15:K:67:ALA:HA	15:K:70:CYS:SG	2.57	0.45
16:L:43:LYS:O	16:L:44:LYS:HG3	2.17	0.45
17:M:102:THR:O	51:A:1226:C:O2'	2.24	0.45
17:M:110:LYS:O	17:M:114:LYS:NZ	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:70:LEU:HD23	19:O:81:LEU:CD2	2.47	0.45
19:O:70:LEU:HD23	19:O:81:LEU:HD22	1.98	0.45
19:O:81:LEU:HD12	19:O:85:LEU:HD13	1.99	0.45
27:Z:18:G:C6	27:Z:57:A:C6	3.05	0.45
27:Z:36:U:C2	27:Z:37:A:C8	3.05	0.45
33:g:140:VAL:O	33:g:144:VAL:HG22	2.16	0.45
34:i:58:ASN:ND2	34:i:128:ASN:OD1	2.50	0.45
36:k:19:LEU:HD23	36:k:27:LEU:HB3	1.99	0.45
49:y:5:ILE:N	49:y:5:ILE:HD12	2.32	0.45
51:A:152:A:C6	51:A:170:U:O2	2.70	0.45
52:a:1829:A:C8	52:a:1830:C:C5	3.05	0.45
52:a:2439:A:H8	52:a:2586:U:O3'	1.99	0.45
52:a:2812:G:H2'	52:a:2813:A:O4'	2.17	0.45
33:g:104:ASN:OD1	33:g:105:LEU:N	2.50	0.45
34:i:101:ILE:CG2	34:i:124:VAL:HG11	2.47	0.45
36:k:38:GLN:OE1	52:a:831:G:O2'	2.35	0.45
47:w:67:VAL:O	47:w:71:LEU:HD23	2.17	0.45
51:A:1290:G:HO2'	51:A:1291:U:P	2.29	0.45
52:a:2370:G:H2'	52:a:2371:G:O4'	2.17	0.45
9:E:25:VAL:HG22	9:E:26:LYS:N	2.32	0.44
12:H:38:ASN:O	12:H:42:GLU:HG2	2.16	0.44
27:Z:5:G:H2'	27:Z:6:G:O4'	2.17	0.44
32:f:35:THR:HG21	52:a:2313:C:O2'	2.16	0.44
51:A:649:A:C6	51:A:650:G:C8	3.05	0.44
51:A:949:A:C6	51:A:1233:G:N1	2.85	0.44
51:A:1073:U:C2	51:A:1074:G:C8	3.05	0.44
6:B:192:ASP:OD1	6:B:192:ASP:C	2.61	0.44
6:B:200:ILE:O	6:B:200:ILE:HG22	2.17	0.44
9:E:83:HIS:O	9:E:85:VAL:HG13	2.17	0.44
10:F:11:HIS:ND1	10:F:14:GLN:OE1	2.50	0.44
34:i:99:ARG:O	34:i:103:ILE:HG22	2.17	0.44
51:A:592:G:N2	51:A:648:A:C4	2.82	0.44
52:a:1038:G:H2'	52:a:1039:A:C8	2.52	0.44
52:a:1394:U:H4'	52:a:1603:A:H4'	1.98	0.44
52:a:2049:G:O2'	52:a:2050:C:H5'	2.17	0.44
52:a:2460:U:C2	52:a:2461:A:C8	3.05	0.44
6:B:130:THR:HG22	6:B:130:THR:O	2.16	0.44
9:E:100:SER:OG	51:A:6:G:O6	2.30	0.44
18:N:10:GLU:HA	18:N:10:GLU:OE2	2.17	0.44
30:d:151:THR:N	30:d:152:PRO:CD	2.80	0.44
49:y:51:VAL:O	49:y:51:VAL:CG1	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:A:180:U:N3	51:A:181:A:N7	2.65	0.44
51:A:949:A:N6	51:A:1233:G:C6	2.85	0.44
9:E:111:MET:SD	9:E:125:ALA:HB1	2.58	0.44
10:F:88:MET:HE3	22:R:64:TYR:CD2	2.53	0.44
14:J:9:ARG:HH22	14:J:71:LEU:CD1	2.29	0.44
16:L:45:PRO:O	16:L:46:ASN:C	2.60	0.44
32:f:71:ARG:N	52:a:2312:U:OP1	2.49	0.44
38:m:71:ARG:NH1	52:a:2708:G:O4'	2.50	0.44
51:A:104:G:C2	51:A:105:G:N7	2.86	0.44
51:A:413:G:H4'	51:A:414:A:H5''	2.00	0.44
51:A:701:U:O2	51:A:703:G:C2	2.71	0.44
51:A:1006:G:N1	51:A:1007:U:H1'	2.32	0.44
52:a:1530:G:C2'	52:a:1531:C:H5'	2.47	0.44
3:2:7:VAL:O	3:2:7:VAL:CG2	2.66	0.44
12:H:104:VAL:HG12	12:H:125:ILE:HD12	1.98	0.44
16:L:80:ILE:HG22	16:L:104:CYS:SG	2.57	0.44
19:O:20:ASN:OD1	51:A:749:A:O2'	2.36	0.44
32:f:94:GLU:O	32:f:98:GLU:HG2	2.17	0.44
38:m:8:ARG:HD2	38:m:43:GLU:HG2	2.00	0.44
51:A:181:A:O2'	51:A:194:C:N4	2.37	0.44
51:A:820:U:H4'	51:A:821:G:OP2	2.17	0.44
51:A:1158:C:H2'	51:A:1159:U:H5''	1.99	0.44
52:a:827:U:O2'	52:a:2068:U:C2	2.70	0.44
52:a:892:A:C2	52:a:893:C:H1'	2.53	0.44
52:a:1013:C:H2'	52:a:1014:A:H8	1.83	0.44
52:a:1142:A:C4	52:a:1144:A:N7	2.86	0.44
6:B:130:THR:O	6:B:132:LYS:N	2.50	0.44
18:N:4:GLN:OE1	18:N:7:LYS:NZ	2.39	0.44
19:O:38:HIS:C	19:O:38:HIS:HD1	2.25	0.44
27:Z:18:G:N2	27:Z:58:A:O4'	2.51	0.44
35:j:1:MET:HB2	35:j:67:LYS:HD3	1.98	0.44
38:m:107:ASN:O	38:m:107:ASN:ND2	2.49	0.44
40:o:10:GLN:HA	40:o:10:GLN:OE1	2.17	0.44
51:A:147:G:H2'	51:A:148:G:C8	2.52	0.44
51:A:520:A:N1	51:A:536:C:H1'	2.33	0.44
51:A:1084:G:OP1	51:A:1086:U:C6	2.70	0.44
51:A:1418:A:C2	51:A:1483:A:C2	3.06	0.44
52:a:898:C:C2	52:a:899:A:C8	3.06	0.44
52:a:1349:C:O2	52:a:1349:C:H2'	2.16	0.44
52:a:1720:U:H2'	52:a:1721:G:O4'	2.17	0.44
52:a:1733:G:C2	52:a:1734:G:C8	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:a:2521:C:C2	52:a:2522:U:C6	3.06	0.44
9:E:105:ILE:HG22	9:E:123:VAL:HG12	1.99	0.44
10:F:68:GLN:O	10:F:72:ASP:OD1	2.35	0.44
11:G:39:ALA:HA	11:G:42:ILE:HG22	2.00	0.44
13:I:8:GLY:O	13:I:19:VAL:HG22	2.18	0.44
34:i:27:ARG:NH1	52:a:1143:A:N7	2.66	0.44
44:t:74:ASN:O	44:t:96:PHE:HE1	1.99	0.44
51:A:466:A:O2'	51:A:467:U:OP1	2.27	0.44
52:a:2249:U:H3'	52:a:2252:G:OP1	2.17	0.44
19:O:84:ARG:HG3	19:O:85:LEU:CD1	2.46	0.44
22:R:55:LEU:O	22:R:59:ILE:HG13	2.18	0.44
24:T:29:ARG:O	24:T:33:LYS:HG2	2.17	0.44
27:Z:44:A:H2'	27:Z:45:G:O4'	2.18	0.44
28:b:100:G:N2	52:a:863:A:O3'	2.44	0.44
35:j:97:THR:O	35:j:98:ARG:HG2	2.18	0.44
36:k:109:LYS:HG3	36:k:126:ARG:HB2	2.00	0.44
40:o:2:SER:OG	40:o:3:ASN:N	2.44	0.44
40:o:16:ASP:OD1	40:o:16:ASP:N	2.51	0.44
44:t:96:PHE:CE2	44:t:103:ILE:HG21	2.53	0.44
51:A:352:C:H4'	51:A:354:G:OP1	2.17	0.44
51:A:411:A:C5	51:A:413:G:O6	2.71	0.44
51:A:890:G:N2	51:A:907:A:OP2	2.47	0.44
52:a:3:U:O2	52:a:3:U:H2'	2.17	0.44
52:a:271:G:O2'	52:a:272:A:O5'	2.32	0.44
52:a:527:C:HO2'	52:a:2779:U:HO2'	1.64	0.44
52:a:644:A:C2'	52:a:645:C:O5'	2.66	0.44
52:a:1197:G:H2'	52:a:1198:U:H6	1.82	0.44
6:B:9:MET:HE1	6:B:47:VAL:CG2	2.47	0.44
6:B:142:GLU:O	6:B:146:ASN:OD1	2.35	0.44
16:L:42:PRO:HD2	16:L:48:ALA:O	2.18	0.44
32:f:41:GLY:HA3	52:a:2311:A:C2	2.53	0.44
51:A:177:G:N3	51:A:177:G:O4'	2.51	0.44
52:a:259:G:O2'	52:a:621:A:O2'	1.99	0.44
52:a:961:C:O2	52:a:2031:A:N6	2.51	0.44
6:B:70:VAL:HG13	6:B:161:LEU:HD11	2.00	0.43
13:I:122:ARG:HH12	51:A:1346:A:H5''	1.82	0.43
26:X:18:G:OP2	51:A:1402:C:N4	2.50	0.43
28:b:42:C:N3	32:f:90:THR:HG22	2.33	0.43
30:d:114:LYS:NZ	52:a:2681:C:OP2	2.40	0.43
30:d:131:ASP:OD2	30:d:136:ASN:ND2	2.51	0.43
32:f:132:VAL:HG21	32:f:137:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:z:16:ARG:NH1	52:a:1266:G:OP2	2.51	0.43
50:z:23:THR:OG1	50:z:24:ALA:N	2.50	0.43
51:A:1127:G:H1	51:A:1145:A:H61	1.64	0.43
51:A:1366:C:H2'	51:A:1367:C:C6	2.53	0.43
52:a:278:A:N6	52:a:362:A:N7	2.67	0.43
52:a:1292:G:H2'	52:a:1293:C:C6	2.53	0.43
52:a:1689:A:C5	52:a:1700:A:C6	3.06	0.43
52:a:2092:U:H4'	52:a:2093:G:O5'	2.16	0.43
8:D:125:VAL:HG23	8:D:125:VAL:O	2.18	0.43
13:I:79:ILE:HG22	13:I:83:ILE:HG13	2.00	0.43
30:d:19:GLY:HA2	40:o:79:PRO:HG2	2.00	0.43
47:w:13:VAL:CG1	47:w:14:THR:N	2.81	0.43
51:A:544:G:C6	51:A:545:C:C4	3.06	0.43
52:a:454:A:H4'	52:a:455:C:OP2	2.18	0.43
52:a:869:G:C2'	52:a:870:U:H5'	2.48	0.43
52:a:960:A:H5''	52:a:961:C:OP1	2.18	0.43
52:a:1152:C:H2'	52:a:1153:C:C6	2.53	0.43
4:3:7:VAL:CG1	4:3:25:VAL:HG23	2.48	0.43
6:B:68:LEU:HD22	6:B:161:LEU:HD13	2.00	0.43
6:B:99:GLY:N	6:B:175:GLU:OE2	2.52	0.43
12:H:10:MET:HE3	12:H:61:LEU:CD1	2.49	0.43
13:I:81:HIS:O	13:I:84:THR:HB	2.18	0.43
17:M:104:THR:O	17:M:105:ASN:OD1	2.36	0.43
30:d:100:LEU:HD12	30:d:100:LEU:O	2.18	0.43
36:k:19:LEU:CD2	36:k:27:LEU:HB3	2.48	0.43
36:k:41:ARG:NH2	52:a:807:U:OP2	2.51	0.43
38:m:45:ARG:NH1	38:m:97:ILE:HD12	2.33	0.43
51:A:420:U:O2	51:A:424:G:O6	2.36	0.43
51:A:1000:A:C6	51:A:1041:G:O6	2.70	0.43
52:a:304:U:O2'	52:a:305:C:P	2.76	0.43
52:a:527:C:H4'	52:a:528:A:O5'	2.19	0.43
52:a:1204:A:O4'	52:a:1206:G:C8	2.71	0.43
52:a:1477:A:H2'	52:a:1478:G:O4'	2.19	0.43
6:B:46:THR:HG23	6:B:201:PRO:O	2.19	0.43
19:O:70:LEU:HD12	19:O:70:LEU:C	2.43	0.43
32:f:11:GLU:OE1	32:f:11:GLU:N	2.51	0.43
32:f:31:VAL:O	32:f:31:VAL:HG12	2.17	0.43
32:f:57:LEU:HD22	32:f:87:CYS:SG	2.58	0.43
35:j:2:ILE:HD13	35:j:8:LEU:HD21	2.00	0.43
35:j:12:ASP:HB3	35:j:99:ILE:HD13	2.00	0.43
51:A:612:C:C2	51:A:613:C:C5	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:A:674:G:H2'	51:A:675:A:H8	1.81	0.43
52:a:1185:G:H5''	52:a:1186:G:OP1	2.19	0.43
52:a:1498:C:N3	52:a:1499:C:C5	2.86	0.43
52:a:2066:C:O2'	52:a:2067:G:H5'	2.18	0.43
52:a:2350:C:H2'	52:a:2351:G:O4'	2.17	0.43
6:B:66:LYS:NZ	6:B:154:MET:O	2.45	0.43
8:D:104:ARG:HB2	8:D:171:LEU:CD1	2.49	0.43
16:L:20:ASN:O	16:L:94:ARG:HD2	2.18	0.43
29:c:13:ARG:HD2	52:a:728:G:H4'	2.00	0.43
42:q:36:ALA:O	42:q:38:VAL:HG23	2.18	0.43
49:y:5:ILE:HD12	49:y:5:ILE:H	1.83	0.43
51:A:463:U:H3'	51:A:464:U:H5''	1.99	0.43
51:A:1137:C:H1'	51:A:1138:G:H22	1.84	0.43
52:a:222:A:C2	52:a:233:A:H4'	2.54	0.43
52:a:1312:U:H4'	52:a:1313:U:O5'	2.17	0.43
52:a:2236:U:H2'	52:a:2237:G:O4'	2.19	0.43
11:G:69:VAL:O	11:G:69:VAL:HG12	2.18	0.43
14:J:44:THR:HG23	14:J:69:THR:O	2.18	0.43
35:j:65:THR:HG22	35:j:67:LYS:N	2.34	0.43
51:A:100:G:C6	51:A:101:A:N7	2.87	0.43
51:A:113:G:H1'	51:A:354:G:H5'	2.01	0.43
51:A:1043:G:HO2'	51:A:1044:A:P	2.36	0.43
51:A:1281:C:OP2	51:A:1282:C:N4	2.45	0.43
51:A:1282:C:H2'	51:A:1283:U:C6	2.54	0.43
51:A:1320:C:H2'	51:A:1321:U:O4'	2.19	0.43
52:a:900:A:C5	52:a:901:C:C5	3.07	0.43
52:a:1353:A:H2'	52:a:1354:A:C8	2.53	0.43
52:a:2308:G:H2'	52:a:2308:G:N3	2.33	0.43
10:F:52:ASN:CG	10:F:52:ASN:O	2.61	0.43
35:j:3:GLN:O	35:j:6:THR:OG1	2.28	0.43
51:A:957:U:O2	51:A:959:A:C8	2.72	0.43
51:A:1006:G:C2	51:A:1007:U:H1'	2.53	0.43
51:A:1046:A:N6	51:A:1213:A:H61	2.16	0.43
51:A:1501:C:OP2	51:A:1504:G:H2'	2.19	0.43
52:a:1407:G:H2'	52:a:1408:G:H8	1.83	0.43
52:a:1599:U:C2	52:a:1600:C:C5	3.07	0.43
52:a:2291:U:H2'	52:a:2292:U:C6	2.53	0.43
52:a:2602:A:H2'	52:a:2602:A:N3	2.34	0.43
6:B:180:GLY:C	6:B:181:ILE:HG13	2.44	0.43
14:J:25:ILE:HD12	14:J:90:LEU:CD1	2.49	0.43
16:L:38:TYR:HD1	16:L:52:VAL:HG23	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:99:TYR:CZ	39:n:104:GLN:HG3	2.53	0.43
42:q:39:LEU:N	42:q:39:LEU:HD22	2.34	0.43
51:A:469:C:H4'	51:A:470:C:OP1	2.19	0.43
51:A:981:U:H3'	51:A:982:U:H5''	2.00	0.43
51:A:1036:A:C5	51:A:1037:C:C6	3.07	0.43
51:A:1258:G:N2	51:A:1279:G:H22	2.17	0.43
52:a:28:A:C5	52:a:29:U:C5	3.06	0.43
52:a:511:U:C5	52:a:512:G:C5	3.07	0.43
52:a:776:G:H2'	52:a:776:G:N3	2.34	0.43
52:a:1499:C:C2	52:a:1500:G:C8	3.06	0.43
52:a:2661:G:H2'	52:a:2662:A:O4'	2.19	0.43
52:a:2784:U:C2	52:a:2785:C:C5	3.07	0.43
5:4:16:CYS:HG	5:4:37:CYS:HG	1.65	0.43
11:G:62:PHE:CE1	11:G:66:LEU:HD13	2.54	0.43
27:Z:27:U:C2	27:Z:28:C:C5	3.07	0.43
31:e:130:LYS:CB	31:e:133:LEU:HD13	2.49	0.43
51:A:505:G:C8	51:A:535:A:C8	3.06	0.43
51:A:1370:G:C2	51:A:1371:G:C8	3.07	0.43
52:a:1370:C:H2'	52:a:1371:G:O4'	2.19	0.43
52:a:2081:U:H2'	52:a:2082:A:H8	1.84	0.43
52:a:2436:G:OP1	53:a:3001:84G:N3	2.52	0.43
6:B:192:ASP:OD1	6:B:192:ASP:O	2.37	0.43
7:C:42:TYR:CE1	7:C:90:VAL:HG11	2.54	0.43
11:G:87:VAL:HG23	11:G:151:PHE:O	2.19	0.43
19:O:15:PHE:HE2	19:O:85:LEU:HD11	1.84	0.43
29:c:181:MET:CB	29:c:268:VAL:HB	2.48	0.43
40:o:73:VAL:O	40:o:73:VAL:HG23	2.19	0.43
40:o:103:ARG:NH1	40:o:107:ALA:O	2.51	0.43
42:q:78:ARG:NH2	52:a:990:A:N1	2.67	0.43
45:u:64:VAL:O	45:u:64:VAL:HG23	2.19	0.43
51:A:687:A:C2	51:A:704:A:C5	3.07	0.43
51:A:935:A:H2'	51:A:936:C:H6	1.84	0.43
51:A:1133:G:C3'	51:A:1134:G:C8	3.01	0.43
52:a:1349:C:C2	52:a:1350:C:C5	3.07	0.43
52:a:1843:C:N3	52:a:1844:C:C5	2.87	0.43
52:a:2043:C:C2	52:a:2044:C:C5	3.06	0.43
52:a:2303:G:H2'	52:a:2304:G:O4'	2.18	0.43
52:a:2783:U:C2	52:a:2784:U:C5	3.07	0.43
4:3:19:ARG:HH11	4:3:24:ARG:HD2	1.84	0.42
13:I:52:LEU:HD21	13:I:63:LEU:HD21	2.01	0.42
14:J:37:ARG:HH11	14:J:77:VAL:CG2	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:18:ASP:OD2	19:O:19:ALA:N	2.52	0.42
31:e:149:ILE:O	31:e:149:ILE:HG22	2.18	0.42
32:f:122:PHE:HZ	32:f:170:LEU:HD12	1.82	0.42
34:i:27:ARG:NH2	52:a:1143:A:OP1	2.50	0.42
51:A:39:G:N2	51:A:404:G:C4	2.86	0.42
51:A:575:G:O2'	51:A:821:G:OP2	2.27	0.42
51:A:1148:U:H3'	51:A:1149:C:H5''	2.01	0.42
51:A:1312:G:C2	51:A:1313:U:C6	3.07	0.42
51:A:1326:U:H2'	51:A:1327:C:C6	2.54	0.42
52:a:1348:C:C4	52:a:1349:C:C6	3.07	0.42
52:a:1989:G:H2'	52:a:1990:C:O4'	2.19	0.42
9:E:15:LEU:HD12	9:E:36:LEU:O	2.19	0.42
14:J:8:ILE:O	14:J:73:LEU:HD12	2.19	0.42
20:P:13:LYS:CE	51:A:43:C:OP1	2.67	0.42
29:c:132:MET:HE1	29:c:184:VAL:CG2	2.48	0.42
30:d:15:PHE:CE2	40:o:77:HIS:O	2.72	0.42
35:j:3:GLN:NE2	52:a:1995:U:O2	2.46	0.42
40:o:94:LYS:HZ2	52:a:2717:C:HO2'	1.60	0.42
42:q:50:GLY:HA3	42:q:54:VAL:CG2	2.49	0.42
51:A:594:U:H2'	51:A:595:A:O4'	2.19	0.42
52:a:598:U:H2'	52:a:599:A:H8	1.84	0.42
52:a:1987:A:C2	52:a:1988:G:C5	3.08	0.42
52:a:2202:U:O2'	52:a:2204:G:OP1	2.30	0.42
52:a:2783:U:H2'	52:a:2784:U:H6	1.83	0.42
14:J:77:VAL:O	14:J:78:GLU:C	2.62	0.42
15:K:34:ILE:HD13	15:K:74:VAL:CG2	2.49	0.42
20:P:6:LEU:HD22	20:P:17:TYR:HB3	2.01	0.42
20:P:22:ALA:HB2	20:P:32:PHE:HA	2.00	0.42
28:b:98:G:O2'	28:b:99:A:O4'	2.37	0.42
29:c:144:VAL:HG23	29:c:154:LEU:HD12	2.01	0.42
39:n:79:ALA:HB1	39:n:113:ALA:HB3	2.01	0.42
51:A:493:A:H2'	51:A:494:G:C8	2.54	0.42
51:A:652:U:O4	51:A:752:G:O2'	2.35	0.42
51:A:741:G:H2'	51:A:742:G:O4'	2.19	0.42
52:a:55:G:O2'	52:a:127:A:N1	2.44	0.42
52:a:921:C:C2	52:a:922:C:C5	3.06	0.42
52:a:2514:U:H2'	52:a:2515:C:C6	2.54	0.42
16:L:55:VAL:HG12	16:L:56:ARG:N	2.34	0.42
19:O:80:GLN:O	19:O:84:ARG:HG2	2.20	0.42
29:c:16:VAL:HG22	29:c:206:GLY:HA3	2.01	0.42
36:k:74:THR:HG22	36:k:75:ALA:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:79:ALA:C	37:l:80:VAL:HG22	2.45	0.42
43:s:56:GLU:HB3	43:s:86:THR:HG23	2.02	0.42
51:A:501:C:H2'	51:A:502:A:C8	2.54	0.42
51:A:539:A:H2'	51:A:540:G:C8	2.54	0.42
51:A:715:A:H2'	51:A:716:A:C8	2.54	0.42
51:A:1026:G:H2'	51:A:1026:G:N3	2.34	0.42
51:A:1151:A:O2'	51:A:1152:A:H8	2.00	0.42
52:a:315:G:H2'	52:a:316:C:H6	1.84	0.42
52:a:882:G:C2	52:a:883:G:C5	3.07	0.42
52:a:1246:A:H2'	52:a:1247:A:O5'	2.20	0.42
52:a:1773:A:C8	52:a:1829:A:C8	3.07	0.42
7:C:175:LEU:HD23	7:C:182:ILE:HD13	2.02	0.42
12:H:56:LYS:NZ	51:A:653:U:OP1	2.49	0.42
13:I:88:MET:HG2	13:I:95:ARG:HG3	2.01	0.42
22:R:60:LYS:HD2	51:A:735:C:H5'	2.01	0.42
37:l:53:MET:HE1	37:l:117:PHE:CD1	2.52	0.42
39:n:33:ARG:O	39:n:34:HIS:ND1	2.52	0.42
41:p:33:ARG:O	41:p:36:PHE:CE2	2.71	0.42
45:u:89:ILE:HG21	45:u:91:PHE:CZ	2.55	0.42
46:v:43:THR:HG22	52:a:2331:G:O2'	2.18	0.42
51:A:203:G:O2'	51:A:465:A:N6	2.52	0.42
51:A:444:G:N2	51:A:446:G:OP1	2.53	0.42
51:A:708:C:C2	51:A:709:U:C5	3.07	0.42
51:A:1145:A:H4'	51:A:1146:A:H5'	2.00	0.42
51:A:1398:A:OP1	51:A:1401:G:H4'	2.19	0.42
52:a:500:G:N1	52:a:503:A:OP2	2.44	0.42
52:a:516:C:O2'	52:a:517:C:H5'	2.19	0.42
52:a:1333:G:C2	52:a:1334:G:C8	3.07	0.42
52:a:2473:U:O2	52:a:2473:U:H2'	2.19	0.42
52:a:2811:G:H2'	52:a:2812:G:O4'	2.19	0.42
7:C:181:ASP:OD2	7:C:181:ASP:C	2.62	0.42
8:D:121:LYS:NZ	51:A:440:C:OP1	2.53	0.42
12:H:60:GLU:OE2	12:H:62:THR:OG1	2.25	0.42
36:k:19:LEU:CD2	36:k:27:LEU:HD22	2.50	0.42
51:A:1137:C:O3'	51:A:1138:G:N2	2.53	0.42
51:A:1321:U:OP2	51:A:1321:U:C6	2.72	0.42
52:a:91:A:N3	52:a:92:U:C4	2.88	0.42
52:a:417:C:H2'	52:a:418:C:C6	2.54	0.42
52:a:1854:A:H2	52:a:2088:A:O4'	2.02	0.42
52:a:2703:C:N3	52:a:2704:C:C5	2.87	0.42
6:B:149:GLY:O	6:B:152:LYS:NZ	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:151:ILE:HG13	6:B:154:MET:HE2	2.01	0.42
10:F:14:GLN:OE1	10:F:14:GLN:N	2.52	0.42
13:I:91:ASP:OD2	13:I:94:LEU:HD23	2.19	0.42
21:Q:15:ASP:O	21:Q:15:ASP:CG	2.61	0.42
51:A:451:A:H1'	51:A:452:A:C2	2.55	0.42
51:A:824:G:C6	51:A:877:G:C6	3.08	0.42
51:A:1223:C:OP2	51:A:1322:C:C5	2.73	0.42
51:A:1256:A:O4'	51:A:1258:G:C4	2.73	0.42
51:A:1267:C:O2'	51:A:1268:G:H5'	2.20	0.42
51:A:1270:G:N2	51:A:1271:A:C8	2.87	0.42
51:A:1346:A:N1	51:A:1374:A:H5''	2.34	0.42
52:a:813:U:O2'	52:a:1225:G:H1'	2.19	0.42
5:4:28:VAL:HG13	5:4:30:HIS:H	1.84	0.42
7:C:70:THR:HG21	7:C:76:VAL:HG11	2.02	0.42
16:L:20:ASN:OD1	16:L:86:ARG:NH2	2.52	0.42
18:N:100:SER:HB3	51:A:1187:G:O2'	2.19	0.42
29:c:43:ARG:HA	29:c:48:ARG:O	2.20	0.42
31:e:73:ILE:O	31:e:73:ILE:HG22	2.19	0.42
34:i:30:THR:OG1	52:a:1012:U:O4	2.36	0.42
36:k:110:VAL:O	36:k:128:THR:HG23	2.19	0.42
44:t:6:ARG:NH1	52:a:84:A:OP1	2.53	0.42
44:t:74:ASN:O	44:t:96:PHE:CE1	2.73	0.42
47:w:39:TRP:HH2	47:w:41:GLU:CB	2.32	0.42
51:A:519:C:H2'	51:A:520:A:O5'	2.20	0.42
51:A:591:U:H2'	51:A:592:G:C8	2.55	0.42
51:A:1129:C:O2'	51:A:1139:G:N7	2.39	0.42
51:A:1130:A:N7	51:A:1131:G:C5	2.88	0.42
52:a:559:G:H2'	52:a:560:C:C5'	2.50	0.42
52:a:784:G:H5'	52:a:785:G:OP1	2.20	0.42
52:a:1212:G:O2'	52:a:1213:A:OP2	2.30	0.42
5:4:24:ILE:HG22	5:4:25:ARG:N	2.35	0.42
7:C:150:LYS:CE	7:C:173:VAL:HG11	2.50	0.42
14:J:90:LEU:HD12	14:J:92:LEU:HD22	2.01	0.42
29:c:72:ASP:OD1	29:c:189:ARG:NH2	2.53	0.42
29:c:258:ARG:NH1	52:a:1799:G:OP1	2.53	0.42
32:f:175:PHE:HB3	32:f:177:PHE:CE2	2.54	0.42
44:t:36:VAL:HB	44:t:39:ILE:HD12	2.02	0.42
51:A:373:A:C2	51:A:482:A:C6	3.08	0.42
51:A:747:A:H5'	51:A:748:G:OP2	2.20	0.42
51:A:960:U:H4'	51:A:961:U:H5''	2.02	0.42
51:A:1242:G:N2	51:A:1302:C:O2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:A:1315:U:O2'	51:A:1360:A:H2'	2.20	0.42
52:a:263:G:O2'	52:a:429:A:N3	2.51	0.42
52:a:546:U:H2'	52:a:548:G:N2	2.34	0.42
52:a:1469:A:H2'	52:a:1470:A:C8	2.54	0.42
52:a:2708:G:H2'	52:a:2709:G:H8	1.84	0.42
5:4:9:TYR:CE2	5:4:25:ARG:HB3	2.55	0.42
5:4:31:ASP:OD1	5:4:31:ASP:N	2.52	0.42
14:J:59:LYS:NZ	51:A:973:G:OP1	2.52	0.42
18:N:6:MET:SD	18:N:9:ARG:NH2	2.93	0.42
20:P:35:ARG:NH1	20:P:37:GLY:C	2.78	0.42
30:d:45:TYR:OH	52:a:2636:C:O2'	2.25	0.42
50:z:33:THR:OG1	50:z:34:SER:N	2.53	0.42
51:A:1001:C:H2'	51:A:1002:G:C8	2.55	0.42
51:A:1046:A:H62	51:A:1213:A:H61	1.66	0.42
52:a:548:G:H2'	52:a:549:G:O4'	2.20	0.42
52:a:575:A:C2	52:a:576:U:C5	3.08	0.42
52:a:1242:U:H2'	52:a:1243:C:O4'	2.20	0.42
52:a:1392:A:C5	52:a:1393:A:C6	3.08	0.42
52:a:1527:G:N2	52:a:1544:A:N7	2.67	0.42
52:a:1731:G:C6	52:a:1733:G:C5	3.08	0.42
52:a:2783:U:H2'	52:a:2784:U:C6	2.55	0.42
1:0:9:ILE:HG12	1:0:23:THR:O	2.20	0.41
6:B:28:LYS:HA	6:B:31:ILE:HD12	2.01	0.41
9:E:111:MET:SD	9:E:125:ALA:CB	3.08	0.41
14:J:15:HIS:O	14:J:19:ASP:OD2	2.39	0.41
17:M:92:ARG:HG2	52:a:888:C:C6	2.55	0.41
27:Z:19:G:N2	27:Z:57:A:N3	2.68	0.41
29:c:219:THR:O	29:c:219:THR:HG23	2.20	0.41
44:t:7:ARG:HB3	44:t:8:ASP:OD1	2.19	0.41
51:A:657:U:N3	51:A:658:C:C5	2.88	0.41
51:A:1015:G:C4	51:A:1016:A:C6	3.08	0.41
51:A:1157:A:C2	51:A:1181:G:C4	3.08	0.41
51:A:1342:C:H2'	51:A:1343:G:H8	1.85	0.41
52:a:1432:G:N2	52:a:1562:U:O2	2.53	0.41
52:a:2218:G:O2'	52:a:2219:U:H5'	2.20	0.41
52:a:2820:A:N3	52:a:2820:A:H2'	2.34	0.41
5:4:10:GLU:O	5:4:26:SER:O	2.38	0.41
8:D:95:GLU:OE2	8:D:100:ASN:ND2	2.37	0.41
13:I:123:ARG:NH1	13:I:124:ARG:O	2.53	0.41
27:Z:65:C:H2'	27:Z:66:C:C6	2.55	0.41
29:c:82:GLU:O	29:c:91:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:m:70:THR:O	38:m:71:ARG:C	2.62	0.41
40:o:65:SER:O	40:o:66:ASN:C	2.62	0.41
41:p:47:TYR:CD1	41:p:47:TYR:C	2.98	0.41
45:u:78:GLN:O	45:u:87:GLN:N	2.52	0.41
50:z:38:HIS:HB3	50:z:44:THR:HG22	2.02	0.41
51:A:164:G:H2'	51:A:165:G:O4'	2.21	0.41
51:A:258:G:C2	51:A:259:G:C8	3.09	0.41
51:A:410:G:H1'	51:A:433:G:H22	1.85	0.41
51:A:418:C:H2'	51:A:419:C:C1'	2.50	0.41
52:a:876:C:H2'	52:a:877:A:O4'	2.20	0.41
52:a:2302:U:H2'	52:a:2303:G:H5'	2.02	0.41
52:a:2850:A:H2'	52:a:2850:A:N3	2.34	0.41
5:4:64:PHE:CZ	18:N:38:ASP:OD2	2.73	0.41
13:I:118:LEU:HG	13:I:124:ARG:HG2	2.02	0.41
15:K:109:ASN:OD1	15:K:109:ASN:C	2.61	0.41
21:Q:65:ARG:HG3	21:Q:65:ARG:HH11	1.85	0.41
22:R:72:ASP:HB3	22:R:73:ARG:HD2	2.02	0.41
23:S:11:ILE:HD13	23:S:41:PHE:CE2	2.49	0.41
29:c:146:MET:HE2	29:c:146:MET:HB2	1.97	0.41
30:d:148:GLN:O	30:d:149:ASN:C	2.63	0.41
32:f:4:LEU:CD1	32:f:101:GLU:HB2	2.51	0.41
36:k:106:GLU:O	36:k:107:PHE:HD2	2.02	0.41
51:A:134:G:C4	51:A:135:C:C6	3.08	0.41
51:A:134:G:C5	51:A:135:C:C5	3.08	0.41
51:A:417:G:H2'	51:A:418:C:H5''	2.02	0.41
51:A:648:A:N1	51:A:649:A:C5	2.89	0.41
51:A:1275:A:H2'	51:A:1276:G:O4'	2.20	0.41
52:a:100:U:O2	52:a:101:A:N6	2.53	0.41
52:a:639:U:H2'	52:a:640:C:C6	2.54	0.41
52:a:1184:U:C2'	52:a:1185:G:O5'	2.68	0.41
6:B:28:LYS:N	6:B:29:PRO:CD	2.83	0.41
7:C:110:GLU:HB2	7:C:144:LEU:HD12	2.02	0.41
7:C:181:ASP:O	7:C:182:ILE:HG13	2.20	0.41
8:D:60:LYS:O	8:D:64:ILE:HG13	2.20	0.41
11:G:68:ASN:OD1	11:G:130:ASN:ND2	2.53	0.41
12:H:129:VAL:O	12:H:129:VAL:HG12	2.20	0.41
15:K:72:ASP:HA	15:K:75:LYS:HE3	2.03	0.41
19:O:82:ILE:HG13	19:O:83:GLU:N	2.35	0.41
21:Q:42:THR:HG22	21:Q:43:LYS:N	2.35	0.41
36:k:43:GLY:N	52:a:671:C:OP1	2.53	0.41
42:q:26:ASP:O	42:q:27:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:v:46:HIS:HB2	46:v:79:PHE:CD1	2.55	0.41
46:v:82:ILE:HG23	46:v:82:ILE:O	2.20	0.41
51:A:259:G:C2	51:A:268:U:C2	3.09	0.41
51:A:418:C:H2'	51:A:419:C:O4'	2.21	0.41
51:A:986:U:H2'	51:A:987:G:O4'	2.21	0.41
51:A:1014:A:H62	51:A:1015:G:N2	2.18	0.41
51:A:1041:G:C2	51:A:1042:A:C5	3.08	0.41
51:A:1142:G:H2'	51:A:1143:G:H5'	2.02	0.41
51:A:1266:G:N1	51:A:1270:G:C6	2.89	0.41
52:a:1693:U:H4'	52:a:1694:C:OP2	2.20	0.41
52:a:2243:U:H2'	52:a:2244:U:C6	2.55	0.41
52:a:2364:C:H2'	52:a:2365:G:O4'	2.21	0.41
6:B:83:ALA:HB3	6:B:214:LEU:HD12	2.02	0.41
6:B:219:ALA:HA	6:B:222:ARG:HG2	2.01	0.41
13:I:46:MET:O	13:I:46:MET:CE	2.64	0.41
20:P:50:THR:HG21	20:P:74:LEU:HD11	2.02	0.41
20:P:58:ALA:HA	20:P:61:VAL:HG22	2.02	0.41
30:d:25:THR:O	30:d:25:THR:CG2	2.68	0.41
30:d:181:ASP:C	30:d:181:ASP:OD1	2.63	0.41
37:l:53:MET:CE	37:l:117:PHE:HD1	2.33	0.41
47:w:39:TRP:HZ3	47:w:41:GLU:HB3	1.84	0.41
50:z:16:ARG:NH2	52:a:1264:A:OP1	2.43	0.41
51:A:125:U:O2'	51:A:126:G:H5'	2.20	0.41
52:a:784:G:C5'	52:a:785:G:OP1	2.68	0.41
52:a:843:G:H2'	52:a:844:A:C8	2.55	0.41
52:a:2047:C:O2'	52:a:2823:A:N1	2.51	0.41
6:B:97:LEU:H	6:B:100:MET:CE	2.34	0.41
8:D:5:LEU:HD11	51:A:405:U:C2	2.56	0.41
8:D:188:ARG:NH1	8:D:192:SER:O	2.49	0.41
11:G:137:LYS:O	11:G:141:VAL:HG23	2.19	0.41
32:f:29:PRO:HB3	32:f:160:ALA:HB2	2.02	0.41
51:A:255:G:N1	51:A:272:C:N3	2.68	0.41
51:A:554:A:H2'	51:A:555:U:C6	2.54	0.41
52:a:776:G:H8	52:a:793:A:C2	2.38	0.41
52:a:1737:G:O3'	52:a:1738:G:O4'	2.38	0.41
52:a:2784:U:N3	52:a:2785:C:C5	2.88	0.41
3:2:55:LEU:O	3:2:59:ILE:HG13	2.21	0.41
6:B:31:ILE:HG21	6:B:39:HIS:ND1	2.35	0.41
6:B:88:ASP:O	6:B:89:GLN:NE2	2.45	0.41
8:D:2:ALA:N	51:A:404:G:N7	2.69	0.41
8:D:98:LEU:N	8:D:135:TYR:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:39:ALA:HA	11:G:42:ILE:CG2	2.50	0.41
14:J:8:ILE:HG22	14:J:100:ILE:HA	2.03	0.41
14:J:42:LEU:HD11	14:J:73:LEU:HB3	2.02	0.41
30:d:3:GLY:O	30:d:4:LEU:HD23	2.20	0.41
37:l:26:VAL:HG13	37:l:104:GLU:CD	2.45	0.41
37:l:35:ALA:HB2	37:l:102:LEU:HD11	2.03	0.41
51:A:220:G:N3	51:A:220:G:H2'	2.34	0.41
51:A:416:G:C6	51:A:417:G:C4	3.09	0.41
51:A:502:A:H2'	51:A:503:C:H6	1.83	0.41
51:A:951:G:N1	51:A:1231:G:C6	2.89	0.41
51:A:1405:G:HO2'	51:A:1518:A:HO2'	1.62	0.41
52:a:1533:C:H2'	52:a:1534:U:O4'	2.19	0.41
52:a:1774:C:O2	52:a:1774:C:H2'	2.20	0.41
52:a:1791:A:C8	52:a:1792:G:C8	3.09	0.41
52:a:2303:G:O6	52:a:2314:A:C6	2.74	0.41
10:F:88:MET:HG2	10:F:90:MET:HE2	2.02	0.41
14:J:72:ARG:NH1	51:A:1152:A:OP1	2.43	0.41
21:Q:31:HIS:CG	21:Q:32:PRO:CG	3.00	0.41
24:T:39:ILE:HD11	24:T:83:ILE:HG13	2.03	0.41
32:f:12:VAL:HG13	32:f:172:ALA:HB1	2.02	0.41
45:u:3:THR:O	45:u:50:MET:HE1	2.21	0.41
51:A:140:U:H1'	51:A:183:C:H42	1.86	0.41
51:A:332:G:C2	51:A:333:U:C5	3.09	0.41
51:A:502:A:H2'	51:A:503:C:C6	2.55	0.41
51:A:810:C:O2	51:A:810:C:H2'	2.20	0.41
51:A:989:U:H2'	51:A:990:C:H6	1.86	0.41
51:A:1116:U:C2'	51:A:1117:A:H5'	2.50	0.41
51:A:1216:A:N7	51:A:1217:C:H5	2.19	0.41
52:a:867:C:O2'	52:a:868:U:H5'	2.21	0.41
52:a:2018:G:O2'	52:a:2019:A:P	2.79	0.41
52:a:2564:A:C2	52:a:2647:U:H4'	2.55	0.41
1:O:23:THR:OG1	1:O:24:THR:N	2.53	0.41
5:4:3:LYS:HE3	5:4:3:LYS:CA	2.35	0.41
6:B:203:ASN:OD1	6:B:204:ASP:N	2.53	0.41
7:C:181:ASP:OD2	7:C:181:ASP:O	2.38	0.41
8:D:92:ALA:O	8:D:95:GLU:O	2.38	0.41
16:L:46:ASN:HD22	16:L:47:SER:N	2.18	0.41
17:M:95:LEU:HB3	17:M:96:PRO:CD	2.51	0.41
20:P:14:ARG:NH2	51:A:618:C:O2'	2.48	0.41
21:Q:29:VAL:HG22	21:Q:30:LYS:N	2.36	0.41
29:c:83:TYR:OH	52:a:1567:G:OP2	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:271:ARG:O	29:c:272:SER:C	2.64	0.41
33:g:137:ASP:OD1	33:g:137:ASP:N	2.54	0.41
34:i:54:ILE:HD12	34:i:54:ILE:N	2.36	0.41
39:n:114:GLY:O	39:n:116:GLN:NE2	2.53	0.41
41:p:18:LEU:HG	41:p:19:LYS:N	2.35	0.41
41:p:37:GLN:HA	41:p:40:ILE:HD12	2.03	0.41
42:q:85:LYS:NZ	52:a:815:C:OP2	2.45	0.41
46:v:14:ARG:HD2	52:a:2280:G:O6	2.20	0.41
51:A:72:A:C8	51:A:73:C:C5	3.09	0.41
51:A:355:C:C4	51:A:356:A:N7	2.88	0.41
51:A:474:G:H2'	51:A:475:C:O4'	2.21	0.41
51:A:494:G:N3	51:A:496:A:N7	2.68	0.41
51:A:551:U:N3	51:A:552:U:C5	2.89	0.41
51:A:1083:U:H2'	51:A:1084:G:O4'	2.20	0.41
51:A:1124:G:C6	51:A:1145:A:C2	3.09	0.41
52:a:10:A:C2	52:a:2800:A:C4	3.08	0.41
52:a:69:C:O2'	52:a:70:G:H5'	2.21	0.41
52:a:74:A:H5''	52:a:75:G:O4'	2.20	0.41
52:a:111:A:O5'	52:a:111:A:H8	2.04	0.41
52:a:627:A:O4'	52:a:637:A:N6	2.53	0.41
52:a:833:A:H2'	52:a:834:G:H8	1.86	0.41
52:a:856:G:H2'	52:a:857:G:C8	2.56	0.41
52:a:1017:G:C6	52:a:1018:U:C4	3.09	0.41
52:a:1131:G:O6	52:a:2024:G:O2'	2.22	0.41
52:a:1246:A:C2'	52:a:1247:A:O5'	2.68	0.41
52:a:1509:A:O2'	52:a:1510:G:P	2.78	0.41
52:a:2283:C:C5	52:a:2389:G:C4	3.09	0.41
3:2:6:THR:HG21	52:a:243:U:OP1	2.21	0.41
5:4:9:TYR:CZ	5:4:25:ARG:O	2.74	0.41
6:B:80:VAL:HB	6:B:93:ASN:OD1	2.21	0.41
7:C:43:LEU:HD21	7:C:68:ILE:HD11	2.01	0.41
7:C:191:THR:OG1	7:C:192:THR:N	2.53	0.41
9:E:105:ILE:O	9:E:112:ARG:NH1	2.53	0.41
11:G:42:ILE:HD11	11:G:117:ALA:HA	2.03	0.41
12:H:104:VAL:O	12:H:104:VAL:HG23	2.19	0.41
13:I:52:LEU:HD11	13:I:83:ILE:HD13	2.01	0.41
15:K:94:GLU:OE1	15:K:94:GLU:N	2.54	0.41
17:M:16:VAL:HG23	17:M:17:ILE:N	2.35	0.41
31:e:63:LYS:NZ	52:a:2061:G:OP1	2.37	0.41
31:e:190:ALA:O	31:e:193:VAL:CG2	2.69	0.41
43:s:88:LYS:O	43:s:91:GLN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:t:7:ARG:C	44:t:8:ASP:OD1	2.64	0.41
45:u:30:ILE:HD11	45:u:63:ILE:CD1	2.51	0.41
48:x:2:LYS:HA	48:x:5:GLU:OE2	2.20	0.41
51:A:384:G:H2'	51:A:385:C:C6	2.55	0.41
51:A:770:C:O2	51:A:771:G:C8	2.74	0.41
51:A:1006:G:C6	51:A:1007:U:C6	3.09	0.41
52:a:160:A:N3	52:a:2208:C:O2'	2.48	0.41
52:a:272:A:H2'	52:a:273:G:H8	1.85	0.41
52:a:606:U:O2	52:a:622:G:O6	2.39	0.41
52:a:978:G:O2'	52:a:979:A:H5'	2.20	0.41
52:a:1263:U:H2'	52:a:1264:A:C8	2.57	0.41
52:a:1590:A:C5	52:a:1591:A:N7	2.89	0.41
52:a:1779:U:O2	52:a:1779:U:C2'	2.68	0.41
10:F:88:MET:HG2	10:F:89:VAL:N	2.36	0.40
12:H:10:MET:HE3	12:H:61:LEU:HD11	2.02	0.40
21:Q:47:HIS:HB2	21:Q:71:LYS:HD2	2.03	0.40
25:U:28:VAL:HA	25:U:31:GLU:HG3	2.03	0.40
33:g:134:LYS:C	33:g:134:LYS:CD	2.94	0.40
34:i:102:GLU:HG3	34:i:124:VAL:HG21	2.03	0.40
35:j:7:MET:HE2	35:j:20:MET:SD	2.61	0.40
43:s:7:LEU:HD21	43:s:45:ALA:O	2.21	0.40
48:x:26:PHE:CZ	48:x:30:MET:HE2	2.56	0.40
51:A:1360:A:OP1	51:A:1360:A:H3'	2.20	0.40
52:a:67:U:C2	52:a:68:G:C8	3.09	0.40
52:a:832:U:H2'	52:a:833:A:H8	1.85	0.40
52:a:2415:G:C4	52:a:2416:C:C5	3.09	0.40
52:a:2747:G:N2	52:a:2748:A:N6	2.69	0.40
5:4:16:CYS:SG	5:4:17:SER:N	2.95	0.40
8:D:17:THR:HG22	8:D:18:ASP:N	2.36	0.40
16:L:29:GLN:OE1	16:L:29:GLN:HA	2.22	0.40
16:L:107:VAL:HG23	16:L:110:ARG:CG	2.51	0.40
27:Z:21:A:H62	27:Z:46:G:H2'	1.85	0.40
30:d:119:ALA:O	30:d:162:ALA:HB1	2.21	0.40
31:e:1:MET:HE2	31:e:1:MET:HB2	1.95	0.40
41:p:20:GLN:O	41:p:21:ALA:HB3	2.21	0.40
44:t:45:HIS:HB3	52:a:483:A:O4'	2.20	0.40
45:u:20:LEU:HD11	45:u:41:GLU:OE2	2.20	0.40
51:A:29:U:O2'	51:A:30:U:H5'	2.21	0.40
51:A:113:G:H1'	51:A:354:G:C5'	2.51	0.40
51:A:269:C:H2'	51:A:270:A:H8	1.86	0.40
51:A:1225:A:O2'	51:A:1226:C:O5'	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:A:1299:A:H2'	51:A:1300:G:O5'	2.20	0.40
52:a:285:G:N7	52:a:286:U:C4	2.90	0.40
52:a:1108:U:H2'	52:a:1109:C:C6	2.56	0.40
52:a:1527:G:N2	52:a:1544:A:C8	2.89	0.40
52:a:2272:U:H5''	52:a:2273:A:OP1	2.22	0.40
52:a:2393:U:C2	52:a:2394:C:C6	3.09	0.40
52:a:2396:G:N1	52:a:2421:G:C6	2.89	0.40
52:a:2532:G:H2'	52:a:2533:U:H5'	2.02	0.40
52:a:2756:U:H3	52:a:2758:A:H62	1.70	0.40
5:4:3:LYS:HA	5:4:3:LYS:CE	2.34	0.40
6:B:43:LEU:HA	6:B:46:THR:OG1	2.21	0.40
7:C:9:GLY:HA3	18:N:89:MET:SD	2.61	0.40
11:G:79:ARG:HG2	11:G:84:THR:HG22	2.02	0.40
17:M:85:CYS:O	17:M:89:LEU:HG	2.21	0.40
21:Q:15:ASP:HB2	21:Q:21:ILE:HA	2.04	0.40
27:Z:22:G:C2	27:Z:23:C:C5	3.08	0.40
29:c:130:LEU:HB2	29:c:135:ILE:HD11	2.02	0.40
30:d:99:GLU:O	30:d:100:LEU:C	2.65	0.40
32:f:34:ILE:HD11	32:f:100:PHE:CD1	2.56	0.40
35:j:31:ARG:NH2	52:a:2676:C:OP1	2.48	0.40
40:o:64:ILE:HA	40:o:68:GLU:O	2.22	0.40
45:u:64:VAL:HA	45:u:68:LYS:O	2.21	0.40
51:A:199:A:H2'	51:A:200:G:C8	2.57	0.40
51:A:235:C:H2'	51:A:236:A:H8	1.86	0.40
51:A:246:A:C2	51:A:282:A:C5	3.09	0.40
51:A:255:G:C2	51:A:272:C:C2	3.10	0.40
51:A:418:C:H2'	51:A:419:C:N1	2.36	0.40
51:A:918:A:H2'	51:A:919:A:O4'	2.20	0.40
51:A:1022:A:N7	51:A:1023:U:C4	2.89	0.40
51:A:1126:U:O2	51:A:1280:A:H2'	2.21	0.40
51:A:1351:U:O2'	51:A:1352:C:H5'	2.21	0.40
52:a:1348:C:O2	52:a:1348:C:H2'	2.20	0.40
3:2:37:ALA:O	3:2:40:ARG:HG2	2.21	0.40
6:B:43:LEU:HD23	6:B:46:THR:HB	2.02	0.40
11:G:66:LEU:HD21	11:G:101:MET:HG2	2.04	0.40
14:J:67:ILE:O	14:J:67:ILE:HG22	2.22	0.40
18:N:87:ALA:HB3	18:N:93:ILE:HD11	2.03	0.40
21:Q:7:THR:HB	21:Q:61:ILE:O	2.22	0.40
29:c:96:TYR:CE2	29:c:102:ARG:HD2	2.57	0.40
31:e:126:VAL:HG22	31:e:137:LYS:HE3	2.03	0.40
34:i:32:LEU:HD11	34:i:54:ILE:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:i:114:LEU:HD12	34:i:114:LEU:HA	1.96	0.40
37:l:134:THR:HG22	37:l:135:VAL:N	2.36	0.40
39:n:31:THR:OG1	39:n:32:PRO:CD	2.70	0.40
40:o:114:LEU:HD21	51:A:1442:G:C4'	2.52	0.40
51:A:1077:G:N2	51:A:1079:G:H3'	2.37	0.40
51:A:1500:A:O2'	51:A:1501:C:H5'	2.22	0.40
52:a:182:A:H2'	52:a:183:C:H6	1.86	0.40
52:a:833:A:H2'	52:a:834:G:C8	2.56	0.40
52:a:891:G:H2'	52:a:892:A:H8	1.87	0.40
52:a:1358:G:N2	52:a:1372:U:C5	2.90	0.40
52:a:1548:A:H2'	52:a:1549:A:C8	2.56	0.40
52:a:1570:A:H2'	52:a:1571:A:C8	2.56	0.40
52:a:2025:C:H2'	52:a:2026:U:C6	2.56	0.40
7:C:64:ILE:O	7:C:99:ALA:HA	2.22	0.40
18:N:27:LEU:HA	18:N:30:ILE:HG22	2.04	0.40
20:P:10:GLY:HA2	51:A:624:C:O3'	2.21	0.40
30:d:63:PRO:O	52:a:2786:U:O2'	2.38	0.40
33:g:163:ARG:HB2	33:g:167:GLU:OE1	2.22	0.40
38:m:45:ARG:HH11	38:m:97:ILE:HD12	1.85	0.40
51:A:512:U:H2'	51:A:513:C:C6	2.57	0.40
51:A:1225:A:H2'	51:A:1226:C:C5	2.56	0.40
51:A:1239:A:C2	51:A:1241:G:N1	2.90	0.40
51:A:1290:G:C6	51:A:1291:U:C4	3.10	0.40
51:A:1315:U:H5''	51:A:1361:G:O5'	2.21	0.40
52:a:362:A:C2	52:a:363:G:H1'	2.56	0.40
52:a:515:A:H2	52:a:1261:C:O4'	2.05	0.40
52:a:1360:G:C8	52:a:1361:G:C8	3.10	0.40
52:a:1890:A:C5	52:a:1891:G:C8	3.08	0.40
52:a:2321:U:H3'	52:a:2321:U:O2	2.21	0.40
52:a:2328:A:H2'	52:a:2329:U:H6	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	45 (92%)	4 (8%)	0	100	100
2	1	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
3	2	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
4	3	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
5	4	56/70 (80%)	48 (86%)	8 (14%)	0	100	100
6	B	222/241 (92%)	197 (89%)	25 (11%)	0	100	100
7	C	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
8	D	203/206 (98%)	188 (93%)	15 (7%)	0	100	100
9	E	154/167 (92%)	140 (91%)	14 (9%)	0	100	100
10	F	101/135 (75%)	99 (98%)	2 (2%)	0	100	100
11	G	151/179 (84%)	140 (93%)	11 (7%)	0	100	100
12	H	127/130 (98%)	111 (87%)	16 (13%)	0	100	100
13	I	125/130 (96%)	110 (88%)	14 (11%)	1 (1%)	16	51
14	J	96/103 (93%)	88 (92%)	8 (8%)	0	100	100
15	K	112/129 (87%)	105 (94%)	7 (6%)	0	100	100
16	L	118/124 (95%)	104 (88%)	13 (11%)	1 (1%)	16	51
17	M	113/118 (96%)	107 (95%)	6 (5%)	0	100	100
18	N	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
19	O	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
20	P	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
21	Q	77/84 (92%)	65 (84%)	12 (16%)	0	100	100
22	R	64/75 (85%)	57 (89%)	7 (11%)	0	100	100
23	S	82/92 (89%)	76 (93%)	6 (7%)	0	100	100
24	T	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
25	U	68/71 (96%)	68 (100%)	0	0	100	100
29	c	269/273 (98%)	249 (93%)	20 (7%)	0	100	100
30	d	204/209 (98%)	191 (94%)	13 (6%)	0	100	100
31	e	199/201 (99%)	175 (88%)	24 (12%)	0	100	100
32	f	175/179 (98%)	158 (90%)	17 (10%)	0	100	100
33	g	174/177 (98%)	153 (88%)	20 (12%)	1 (1%)	22	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	i	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
35	j	121/123 (98%)	112 (93%)	9 (7%)	0	100	100
36	k	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
37	l	130/136 (96%)	124 (95%)	5 (4%)	1 (1%)	16	51
38	m	116/127 (91%)	108 (93%)	8 (7%)	0	100	100
39	n	114/117 (97%)	99 (87%)	15 (13%)	0	100	100
40	o	112/115 (97%)	101 (90%)	11 (10%)	0	100	100
41	p	52/118 (44%)	37 (71%)	15 (29%)	0	100	100
42	q	101/103 (98%)	90 (89%)	11 (11%)	0	100	100
43	s	90/100 (90%)	81 (90%)	9 (10%)	0	100	100
44	t	100/104 (96%)	93 (93%)	7 (7%)	0	100	100
45	u	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
46	v	76/85 (89%)	70 (92%)	6 (8%)	0	100	100
47	w	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
48	x	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
49	y	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
50	z	54/57 (95%)	47 (87%)	7 (13%)	0	100	100
All	All	5263/5654 (93%)	4828 (92%)	431 (8%)	4 (0%)	50	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	g	128	GLN
37	l	84	LYS
13	I	13	LYS
16	L	44	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	46 (100%)	0	100	100
2	1	38/38 (100%)	38 (100%)	0	100	100
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	55/62 (89%)	55 (100%)	0	100	100
6	B	186/199 (94%)	184 (99%)	2 (1%)	70	86
7	C	170/190 (90%)	169 (99%)	1 (1%)	84	92
8	D	172/173 (99%)	170 (99%)	2 (1%)	67	85
9	E	119/126 (94%)	117 (98%)	2 (2%)	56	78
10	F	90/116 (78%)	90 (100%)	0	100	100
11	G	125/147 (85%)	124 (99%)	1 (1%)	79	90
12	H	104/105 (99%)	104 (100%)	0	100	100
13	I	104/107 (97%)	104 (100%)	0	100	100
14	J	86/90 (96%)	86 (100%)	0	100	100
15	K	89/99 (90%)	88 (99%)	1 (1%)	70	86
16	L	101/104 (97%)	100 (99%)	1 (1%)	73	87
17	M	93/96 (97%)	92 (99%)	1 (1%)	70	86
18	N	83/84 (99%)	82 (99%)	1 (1%)	67	85
19	O	76/77 (99%)	76 (100%)	0	100	100
20	P	65/65 (100%)	65 (100%)	0	100	100
21	Q	73/78 (94%)	73 (100%)	0	100	100
22	R	57/65 (88%)	57 (100%)	0	100	100
23	S	72/79 (91%)	72 (100%)	0	100	100
24	T	65/66 (98%)	64 (98%)	1 (2%)	60	81
25	U	60/61 (98%)	60 (100%)	0	100	100
29	c	216/218 (99%)	216 (100%)	0	100	100
30	d	163/164 (99%)	161 (99%)	2 (1%)	67	85
31	e	165/165 (100%)	165 (100%)	0	100	100
32	f	148/150 (99%)	147 (99%)	1 (1%)	81	92
33	g	137/138 (99%)	135 (98%)	2 (2%)	60	81
34	i	115/116 (99%)	115 (100%)	0	100	100
35	j	104/104 (100%)	103 (99%)	1 (1%)	73	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	k	103/103 (100%)	102 (99%)	1 (1%)	73	87
37	l	107/109 (98%)	106 (99%)	1 (1%)	75	89
38	m	98/103 (95%)	98 (100%)	0	100	100
39	n	86/87 (99%)	86 (100%)	0	100	100
40	o	99/100 (99%)	99 (100%)	0	100	100
41	p	37/90 (41%)	37 (100%)	0	100	100
42	q	84/84 (100%)	83 (99%)	1 (1%)	67	85
43	s	79/84 (94%)	78 (99%)	1 (1%)	65	83
44	t	83/85 (98%)	83 (100%)	0	100	100
45	u	78/78 (100%)	78 (100%)	0	100	100
46	v	58/63 (92%)	57 (98%)	1 (2%)	56	78
47	w	67/68 (98%)	67 (100%)	0	100	100
48	x	51/55 (93%)	51 (100%)	0	100	100
49	y	48/49 (98%)	48 (100%)	0	100	100
50	z	47/48 (98%)	47 (100%)	0	100	100
All	All	4387/4623 (95%)	4363 (100%)	24 (0%)	85	93

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	94	HIS
6	B	153	ASP
7	C	176	HIS
8	D	30	THR
8	D	129	VAL
9	E	131	THR
9	E	141	ILE
11	G	12	ILE
15	K	59	THR
16	L	77	HIS
17	M	66	GLU
18	N	56	SER
24	T	32	ILE
30	d	126	ASN
30	d	129	THR
32	f	11	GLU
33	g	116	GLN

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Mol	Chain	Res	Type
33	g	131	ILE
35	j	118	LEU
36	k	80	SER
37	l	80	VAL
42	q	53	PHE
43	s	63	VAL
46	v	44	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	33	HIS
6	B	94	HIS
8	D	36	GLN
8	D	40	GLN
8	D	41	HIS
8	D	71	GLN
8	D	136	GLN
8	D	140	ASN
8	D	164	GLN
11	G	153	HIS
13	I	31	ASN
13	I	81	HIS
14	J	15	HIS
14	J	56	HIS
14	J	58	ASN
16	L	5	ASN
16	L	46	ASN
17	M	8	ASN
18	N	66	GLN
20	P	79	ASN
24	T	61	GLN
25	U	56	HIS
29	c	134	ASN
29	c	143	ASN
29	c	243	HIS
30	d	32	ASN
31	e	92	HIS
33	g	115	HIS
34	i	40	HIS
34	i	80	HIS
34	i	86	GLN

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Mol	Chain	Res	Type
37	l	3	GLN
37	l	13	HIS
38	m	3	HIS
38	m	31	HIS
39	n	116	GLN
42	q	66	HIS
42	q	91	GLN
45	u	88	HIS
46	v	50	ASN
47	w	34	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	X	2/28 (7%)	0	0
27	Z	75/76 (98%)	10 (13%)	0
28	b	118/120 (98%)	16 (13%)	0
51	A	1503/1542 (97%)	288 (19%)	9 (0%)
52	a	2711/2904 (93%)	357 (13%)	0
All	All	4409/4670 (94%)	671 (15%)	9 (0%)

All (671) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
27	Z	6	G
27	Z	9	G
27	Z	17(A)	U
27	Z	18	G
27	Z	19	G
27	Z	21	A
27	Z	43	A
27	Z	47	U
27	Z	48	C
27	Z	76	A
28	b	11	C
28	b	24	G
28	b	29	A
28	b	30	C
28	b	35	C
28	b	41	G
28	b	66	A

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Mol	Chain	Res	Type
28	b	67	G
28	b	88	C
28	b	89	U
28	b	90	C
28	b	99	A
28	b	105	G
28	b	109	A
28	b	111	U
28	b	115	A
51	A	5	U
51	A	6	G
51	A	7	A
51	A	8	A
51	A	9	G
51	A	31	G
51	A	32	A
51	A	33	A
51	A	39	G
51	A	41	G
51	A	43	C
51	A	47	C
51	A	48	C
51	A	49	U
51	A	50	A
51	A	51	A
51	A	66	A
51	A	71	A
51	A	73	C
51	A	74	A
51	A	81	A
51	A	83	C
51	A	84	U
51	A	85	U
51	A	86	G
51	A	87	C
51	A	88	U
51	A	91	U
51	A	92	U
51	A	93	U
51	A	95	C
51	A	106	C
51	A	121	U

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Mol	Chain	Res	Type
51	A	122	G
51	A	131	A
51	A	132	C
51	A	137	U
51	A	138	G
51	A	151	A
51	A	152	A
51	A	153	C
51	A	160	A
51	A	166	U
51	A	175	C
51	A	183	C
51	A	184	G
51	A	192	A
51	A	197	A
51	A	202	G
51	A	219	U
51	A	226	G
51	A	244	U
51	A	245	U
51	A	247	G
51	A	251	G
51	A	266	G
51	A	279	A
51	A	280	C
51	A	283	U
51	A	289	G
51	A	306	A
51	A	316	C
51	A	320	A
51	A	321	A
51	A	328	C
51	A	330	C
51	A	352	C
51	A	356	A
51	A	367	U
51	A	372	C
51	A	397	A
51	A	406	G
51	A	411	A
51	A	412	A
51	A	414	A

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Mol	Chain	Res	Type
51	A	415	A
51	A	418	C
51	A	420	U
51	A	421	U
51	A	422	C
51	A	423	G
51	A	429	U
51	A	435	A
51	A	444	G
51	A	446	G
51	A	459	A
51	A	460	A
51	A	461	A
51	A	463	U
51	A	464	U
51	A	465	A
51	A	466	A
51	A	467	U
51	A	468	A
51	A	470	C
51	A	478	A
51	A	481	G
51	A	482	A
51	A	486	U
51	A	493	A
51	A	494	G
51	A	495	A
51	A	496	A
51	A	497	G
51	A	518	C
51	A	519	C
51	A	520	A
51	A	524	G
51	A	526	C
51	A	530	G
51	A	531	U
51	A	532	A
51	A	533	A
51	A	534	U
51	A	547	A
51	A	559	A
51	A	564	C

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Mol	Chain	Res	Type
51	A	572	A
51	A	573	A
51	A	576	C
51	A	577	G
51	A	594	U
51	A	596	A
51	A	603	U
51	A	616	G
51	A	620	C
51	A	621	A
51	A	625	U
51	A	633	G
51	A	642	A
51	A	650	G
51	A	653	U
51	A	654	G
51	A	665	A
51	A	700	G
51	A	720	C
51	A	721	G
51	A	722	G
51	A	748	G
51	A	755	G
51	A	777	A
51	A	787	A
51	A	791	G
51	A	792	A
51	A	793	U
51	A	794	A
51	A	802	A
51	A	815	A
51	A	817	C
51	A	819	A
51	A	839	C
51	A	840	C
51	A	851	G
51	A	873	A
51	A	890	G
51	A	891	U
51	A	911	U
51	A	914	A
51	A	925	G

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Mol	Chain	Res	Type
51	A	934	C
51	A	935	A
51	A	960	U
51	A	969	A
51	A	972	C
51	A	975	A
51	A	976	G
51	A	977	A
51	A	982	U
51	A	984	C
51	A	987	G
51	A	992	U
51	A	993	G
51	A	994	A
51	A	999	C
51	A	1004	A
51	A	1006	G
51	A	1010	U
51	A	1011	C
51	A	1014	A
51	A	1017	U
51	A	1019	A
51	A	1023	U
51	A	1024	G
51	A	1027	C
51	A	1031	C
51	A	1039	G
51	A	1042	A
51	A	1043	G
51	A	1044	A
51	A	1053	G
51	A	1054	C
51	A	1065	U
51	A	1079	G
51	A	1092	A
51	A	1094	G
51	A	1095	U
51	A	1096	C
51	A	1101	A
51	A	1103	C
51	A	1106	G
51	A	1117	A

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Mol	Chain	Res	Type
51	A	1121	U
51	A	1130	A
51	A	1134	G
51	A	1137	C
51	A	1139	G
51	A	1146	A
51	A	1149	C
51	A	1151	A
51	A	1152	A
51	A	1159	U
51	A	1167	A
51	A	1169	A
51	A	1196	A
51	A	1197	A
51	A	1209	C
51	A	1212	U
51	A	1213	A
51	A	1214	C
51	A	1215	G
51	A	1216	A
51	A	1218	C
51	A	1226	C
51	A	1227	A
51	A	1238	A
51	A	1240	U
51	A	1241	G
51	A	1246	A
51	A	1248	A
51	A	1249	C
51	A	1252	A
51	A	1256	A
51	A	1257	A
51	A	1258	G
51	A	1259	C
51	A	1262	C
51	A	1267	C
51	A	1270	G
51	A	1278	G
51	A	1280	A
51	A	1284	C
51	A	1285	A
51	A	1286	U

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Mol	Chain	Res	Type
51	A	1287	A
51	A	1290	G
51	A	1291	U
51	A	1292	G
51	A	1294	G
51	A	1300	G
51	A	1303	C
51	A	1308	U
51	A	1309	G
51	A	1314	C
51	A	1315	U
51	A	1316	G
51	A	1317	C
51	A	1318	A
51	A	1320	C
51	A	1321	U
51	A	1323	G
51	A	1345	U
51	A	1361	G
51	A	1363	A
51	A	1373	G
51	A	1378	C
51	A	1379	G
51	A	1381	U
51	A	1394	A
51	A	1398	A
51	A	1399	C
51	A	1401	G
51	A	1441	A
51	A	1451	U
51	A	1453	G
51	A	1478	U
51	A	1491	G
51	A	1492	A
51	A	1494	G
51	A	1499	A
51	A	1503	A
51	A	1506	U
51	A	1507	A
51	A	1508	A
51	A	1517	G
51	A	1519	A

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Mol	Chain	Res	Type
51	A	1529	G
51	A	1530	G
51	A	1534	A
52	a	3	U
52	a	15	G
52	a	60	G
52	a	63	A
52	a	69	C
52	a	71	A
52	a	75	G
52	a	88	G
52	a	93	G
52	a	107	G
52	a	108	G
52	a	112	U
52	a	113	U
52	a	118	A
52	a	120	U
52	a	138	U
52	a	139	U
52	a	140	C
52	a	163	C
52	a	181	A
52	a	196	A
52	a	215	G
52	a	216	A
52	a	221	A
52	a	222	A
52	a	226	A
52	a	227	A
52	a	228	C
52	a	229	C
52	a	241	A
52	a	248	G
52	a	272	A
52	a	281	C
52	a	285	G
52	a	286	U
52	a	287	G
52	a	288	U
52	a	292	U
52	a	295	G

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Mol	Chain	Res	Type
52	a	299	A
52	a	305	C
52	a	311	A
52	a	321	U
52	a	327	G
52	a	329	G
52	a	330	A
52	a	345	A
52	a	356	G
52	a	358	U
52	a	361	G
52	a	362	A
52	a	365	U
52	a	383	C
52	a	386	G
52	a	396	G
52	a	405	U
52	a	406	G
52	a	411	G
52	a	416	U
52	a	424	G
52	a	425	G
52	a	448	U
52	a	449	A
52	a	456	C
52	a	481	G
52	a	491	G
52	a	504	A
52	a	505	A
52	a	508	A
52	a	509	C
52	a	530	G
52	a	531	C
52	a	532	A
52	a	533	G
52	a	543	G
52	a	546	U
52	a	547	A
52	a	557	C
52	a	559	G
52	a	560	C
52	a	562	U

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Mol	Chain	Res	Type
52	a	563	A
52	a	571	U
52	a	572	A
52	a	573	U
52	a	574	A
52	a	575	A
52	a	586	A
52	a	589	U
52	a	592	A
52	a	601	C
52	a	603	A
52	a	615	U
52	a	627	A
52	a	637	A
52	a	646	U
52	a	647	G
52	a	654	A
52	a	655	A
52	a	670	A
52	a	686	U
52	a	730	A
52	a	749	A
52	a	750	A
52	a	765	C
52	a	775	G
52	a	776	G
52	a	782	A
52	a	784	G
52	a	785	G
52	a	789	A
52	a	805	G
52	a	812	C
52	a	827	U
52	a	845	A
52	a	846	U
52	a	847	U
52	a	859	G
52	a	870	U
52	a	878	A
52	a	880	G
52	a	885	C
52	a	890	C

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Mol	Chain	Res	Type
52	a	893	C
52	a	896	A
52	a	897	C
52	a	905	A
52	a	907	G
52	a	910	A
52	a	914	G
52	a	915	C
52	a	919	U
52	a	931	U
52	a	932	U
52	a	945	A
52	a	946	C
52	a	959	A
52	a	961	C
52	a	974	G
52	a	983	A
52	a	994	C
52	a	995	C
52	a	996	A
52	a	1012	U
52	a	1013	C
52	a	1022	G
52	a	1026	G
52	a	1032	A
52	a	1033	U
52	a	1044	C
52	a	1046	A
52	a	1047	G
52	a	1048	A
52	a	1111	A
52	a	1112	G
52	a	1116	G
52	a	1130	U
52	a	1133	A
52	a	1135	C
52	a	1136	G
52	a	1141	U
52	a	1142	A
52	a	1151	A
52	a	1171	G
52	a	1206	G

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Mol	Chain	Res	Type
52	a	1212	G
52	a	1250	G
52	a	1253	A
52	a	1256	G
52	a	1271	G
52	a	1272	A
52	a	1299	G
52	a	1300	G
52	a	1302	A
52	a	1359	A
52	a	1365	A
52	a	1378	A
52	a	1379	U
52	a	1383	A
52	a	1394	U
52	a	1396	U
52	a	1413	A
52	a	1416	G
52	a	1417	C
52	a	1420	A
52	a	1428	C
52	a	1452	G
52	a	1453	A
52	a	1454	C
52	a	1482	G
52	a	1490	A
52	a	1497	U
52	a	1509	A
52	a	1510	G
52	a	1515	A
52	a	1524	G
52	a	1531	C
52	a	1534	U
52	a	1536	C
52	a	1537	G
52	a	1541	C
52	a	1566	A
52	a	1569	A
52	a	1578	U
52	a	1585	C
52	a	1608	A
52	a	1609	A

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Mol	Chain	Res	Type
52	a	1610	A
52	a	1644	C
52	a	1647	U
52	a	1648	U
52	a	1674	G
52	a	1713	A
52	a	1715	G
52	a	1729	U
52	a	1730	C
52	a	1732	C
52	a	1738	G
52	a	1757	A
52	a	1758	U
52	a	1764	C
52	a	1773	A
52	a	1800	C
52	a	1808	A
52	a	1816	C
52	a	1827	U
52	a	1829	A
52	a	1841	U
52	a	1848	A
52	a	1857	G
52	a	1866	A
52	a	1867	G
52	a	1868	C
52	a	1870	C
52	a	1872	A
52	a	1884	G
52	a	1906	G
52	a	1913	A
52	a	1914	C
52	a	1916	A
52	a	1926	U
52	a	1929	G
52	a	1930	G
52	a	1936	A
52	a	1938	A
52	a	1941	C
52	a	1951	U
52	a	1955	U
52	a	1964	G

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Mol	Chain	Res	Type
52	a	1966	A
52	a	1967	C
52	a	1970	A
52	a	1971	U
52	a	1972	G
52	a	1991	U
52	a	1993	U
52	a	1996	C
52	a	2006	C
52	a	2013	A
52	a	2014	A
52	a	2019	A
52	a	2023	C
52	a	2033	A
52	a	2034	U
52	a	2043	C
52	a	2052	A
52	a	2055	C
52	a	2056	G
52	a	2058	A
52	a	2060	A
52	a	2061	G
52	a	2062	A
52	a	2093	G
52	a	2192	U
52	a	2193	G
52	a	2198	A
52	a	2204	G
52	a	2211	A
52	a	2225	A
52	a	2238	G
52	a	2249	U
52	a	2264	C
52	a	2272	U
52	a	2273	A
52	a	2283	C
52	a	2287	A
52	a	2294	G
52	a	2303	G
52	a	2305	U
52	a	2308	G
52	a	2322	A

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Mol	Chain	Res	Type
52	a	2325	G
52	a	2345	G
52	a	2347	C
52	a	2361	G
52	a	2379	G
52	a	2383	G
52	a	2385	C
52	a	2402	U
52	a	2424	C
52	a	2425	A
52	a	2428	G
52	a	2429	G
52	a	2430	A
52	a	2431	U
52	a	2441	U
52	a	2448	A
52	a	2474	U
52	a	2476	A
52	a	2491	U
52	a	2502	G
52	a	2507	C
52	a	2518	A
52	a	2520	C
52	a	2533	U
52	a	2547	A
52	a	2554	U
52	a	2566	A
52	a	2567	G
52	a	2585	U
52	a	2586	U
52	a	2597	G
52	a	2602	A
52	a	2608	G
52	a	2609	U
52	a	2612	C
52	a	2613	U
52	a	2629	U
52	a	2630	G
52	a	2689	U
52	a	2690	U
52	a	2713	U
52	a	2714	G

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Mol	Chain	Res	Type
52	a	2726	A
52	a	2727	A
52	a	2729	G
52	a	2733	A
52	a	2748	A
52	a	2750	A
52	a	2765	A
52	a	2766	A
52	a	2778	A
52	a	2791	G
52	a	2793	C
52	a	2794	C
52	a	2795	C
52	a	2799	A
52	a	2818	U
52	a	2820	A
52	a	2821	A
52	a	2824	C
52	a	2850	A
52	a	2861	U
52	a	2863	C
52	a	2877	G
52	a	2880	C
52	a	2893	A

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
51	A	5	U
51	A	137	U
51	A	304	U
51	A	326	G
51	A	445	G
51	A	466	A
51	A	991	U
51	A	1299	A
51	A	1518	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	84G	A	1601	-	39,40,40	1.87	8 (20%)	48,57,57	1.21	5 (10%)
53	84G	a	3001	-	39,40,40	1.85	7 (17%)	48,57,57	1.13	6 (12%)

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	84G	A	1601	-	-	4/23/76/76	0/3/3/3
53	84G	a	3001	-	-	7/23/76/76	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	A	1601	84G	C3-N1	7.25	1.49	1.34
53	a	3001	84G	C3-N1	6.37	1.47	1.34
53	a	3001	84G	C21-C20	-4.56	1.47	1.53
53	A	1601	84G	C21-C20	-3.78	1.48	1.53
53	a	3001	84G	C19-C20	-3.66	1.48	1.53
53	A	1601	84G	O6-C16	3.42	1.50	1.41
53	a	3001	84G	O6-C16	3.35	1.50	1.41
53	A	1601	84G	C19-C20	-3.07	1.49	1.53
53	A	1601	84G	C11-C12	-2.79	1.46	1.52
53	a	3001	84G	O1-C3	-2.77	1.18	1.23

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	a	3001	84G	C11-C12	-2.69	1.46	1.52
53	A	1601	84G	C20-N5	2.52	1.51	1.47
53	A	1601	84G	O1-C3	-2.43	1.18	1.23
53	a	3001	84G	C20-N5	2.40	1.50	1.47
53	A	1601	84G	O-C2	-2.11	1.38	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A	1601	84G	C16-O5-C15	-3.71	109.17	117.98
53	A	1601	84G	C8-O2-C7	-3.26	110.25	117.98
53	a	3001	84G	O6-C17-C19	2.39	114.01	109.70
53	a	3001	84G	C-C1-C2	-2.39	109.26	112.52
53	a	3001	84G	C7-C14-C15	2.36	113.89	109.11
53	A	1601	84G	C-C1-C2	-2.27	109.41	112.52
53	a	3001	84G	C8-O2-C7	-2.18	112.81	117.98
53	a	3001	84G	C16-O5-C15	-2.17	112.83	117.98
53	A	1601	84G	C4-N1-C3	-2.10	119.60	123.25
53	A	1601	84G	C11-C9-C10	-2.06	108.90	112.83
53	a	3001	84G	C11-C9-C10	-2.05	108.92	112.83

There are no chirality outliers.

All (11) torsion outliers are listed below:

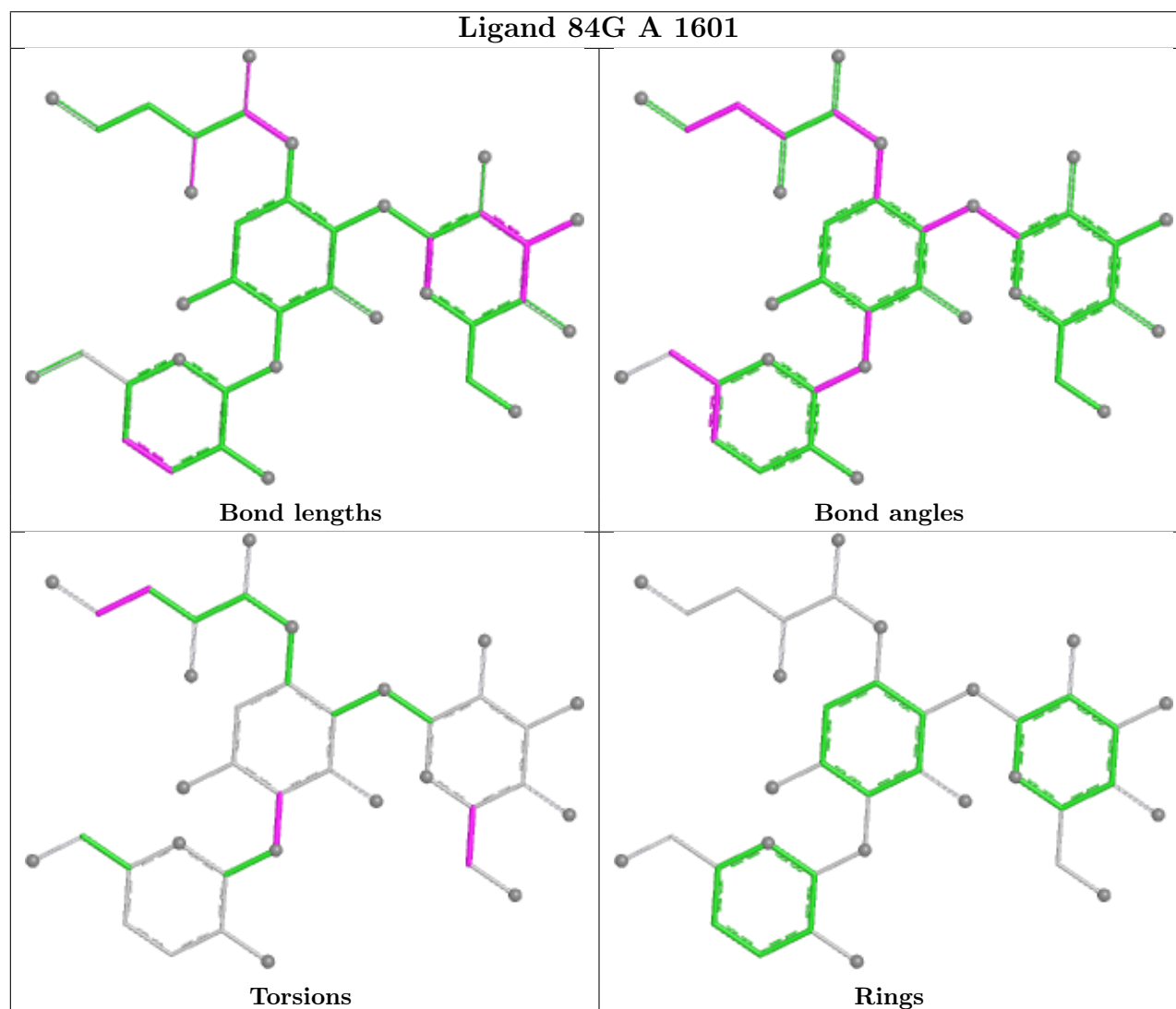
Mol	Chain	Res	Type	Atoms
53	a	3001	84G	C-C1-C2-O
53	a	3001	84G	N3-C10-C9-O3
53	a	3001	84G	N3-C10-C9-C11
53	a	3001	84G	O6-C17-C18-O7
53	A	1601	84G	C19-C17-C18-O7
53	A	1601	84G	O6-C17-C18-O7
53	A	1601	84G	C14-C7-O2-C8
53	a	3001	84G	C15-C4-N1-C3
53	a	3001	84G	C-C1-C2-C3
53	a	3001	84G	O-C2-C3-N1
53	A	1601	84G	N-C-C1-C2

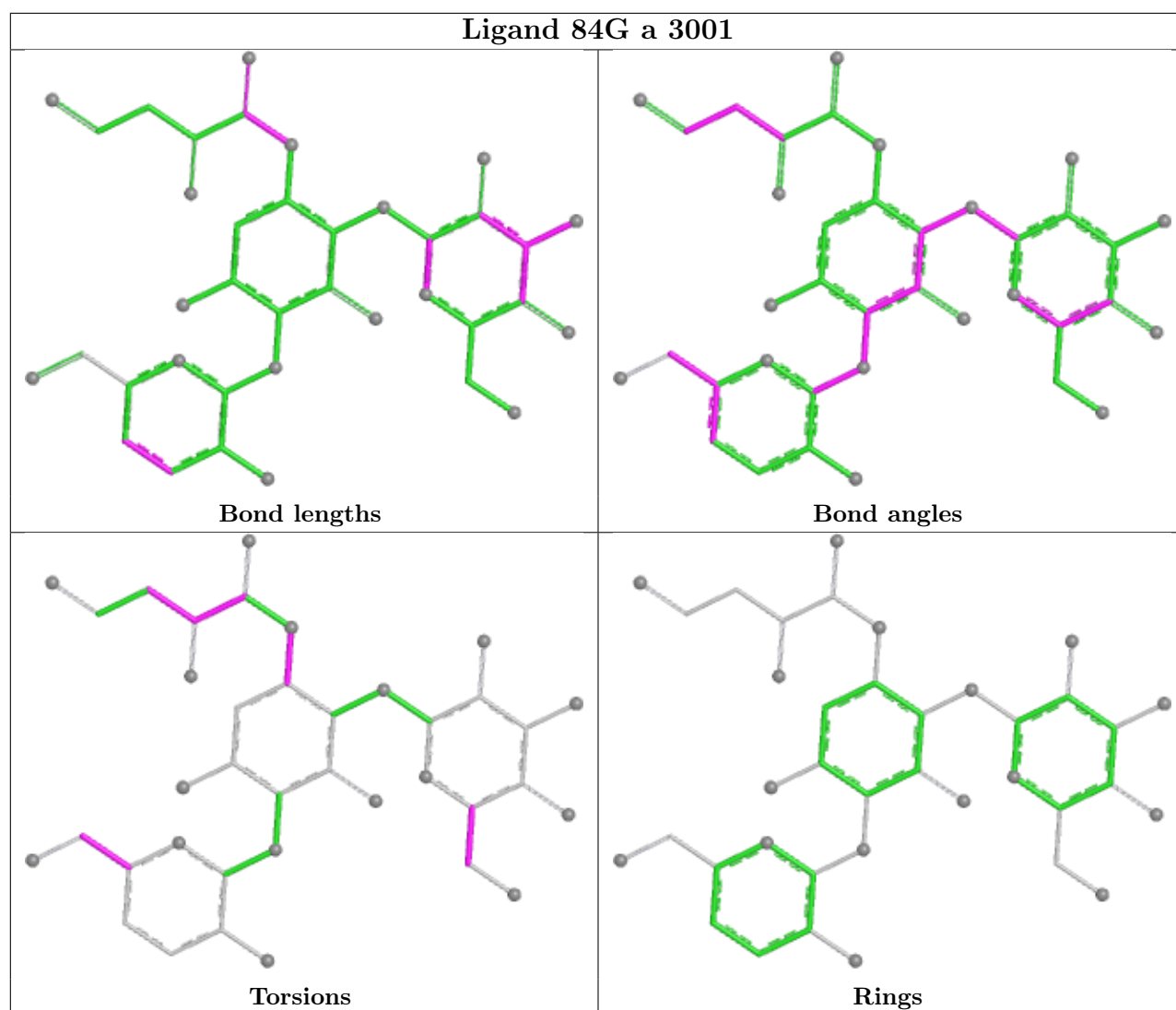
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	A	1601	84G	2	0
53	a	3001	84G	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

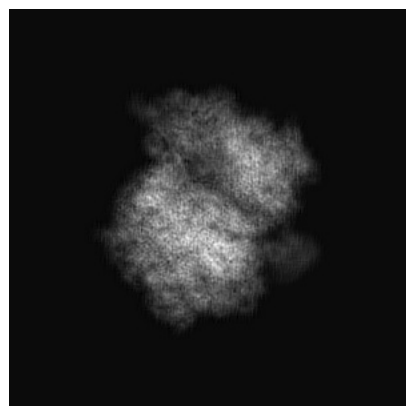
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48329. These allow visual inspection of the internal detail of the map and identification of artifacts.

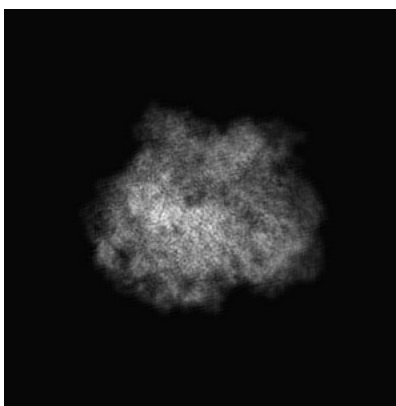
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

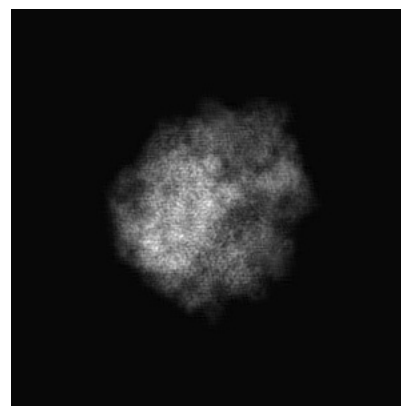
6.1.1 Primary map



X

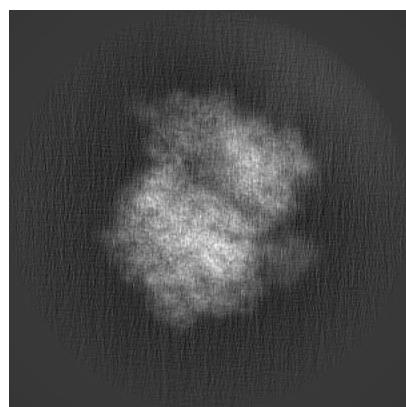


Y

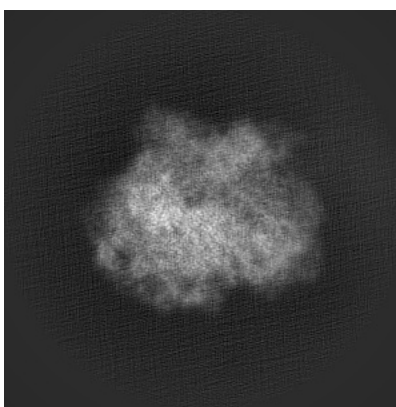


Z

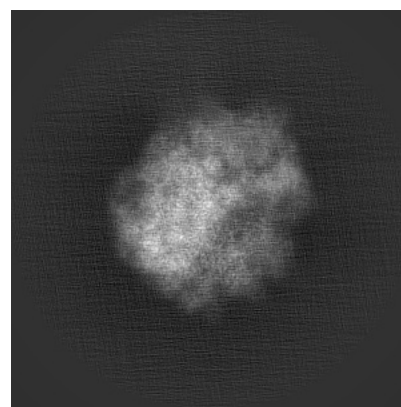
6.1.2 Raw map



X



Y

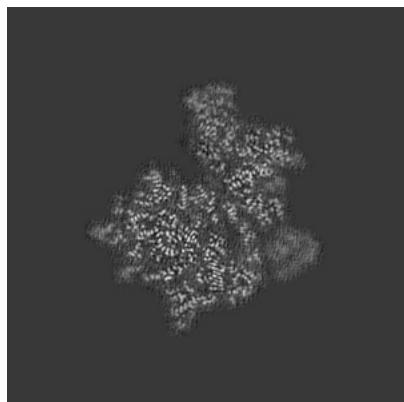


Z

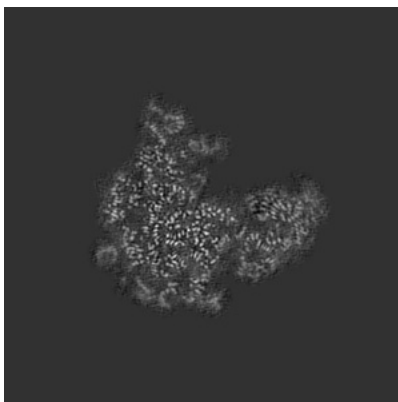
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

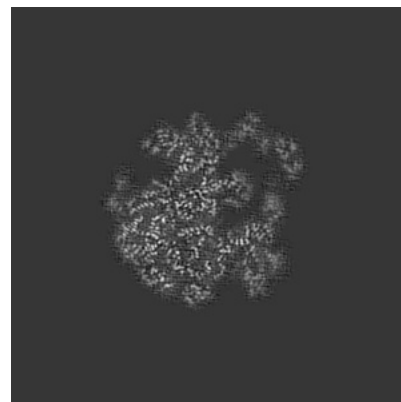
6.2.1 Primary map



X Index: 250

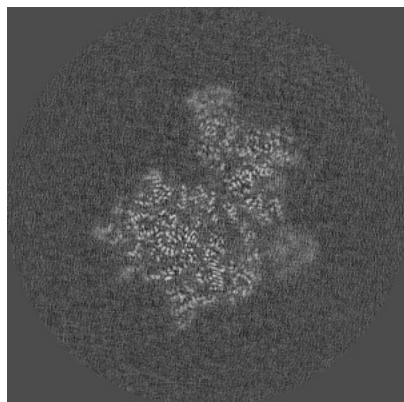


Y Index: 250

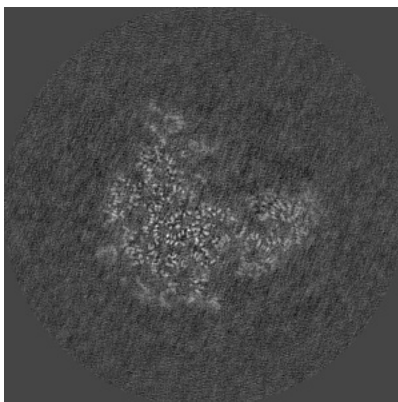


Z Index: 250

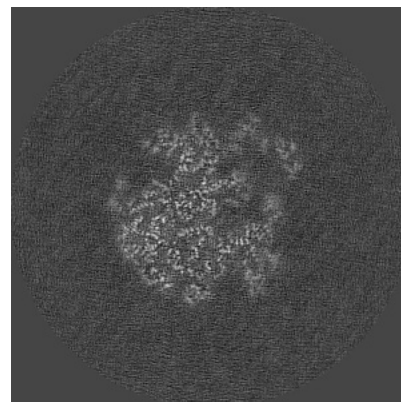
6.2.2 Raw map



X Index: 250



Y Index: 250

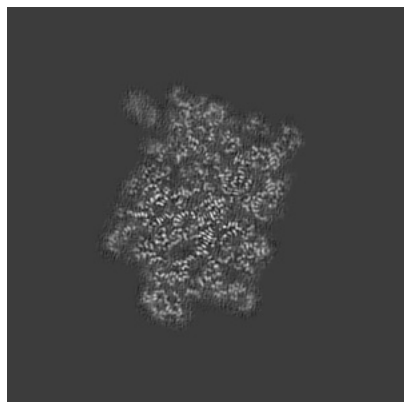


Z Index: 250

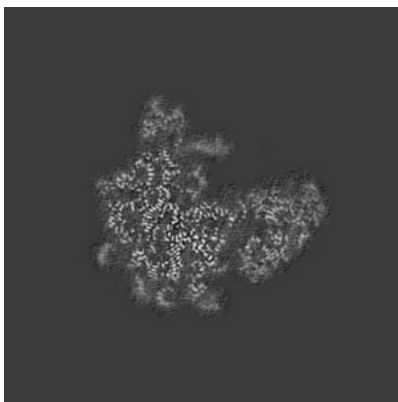
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

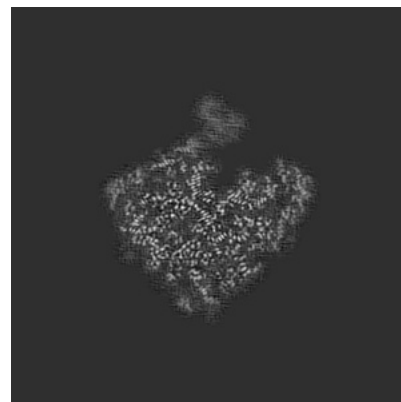
6.3.1 Primary map



X Index: 212

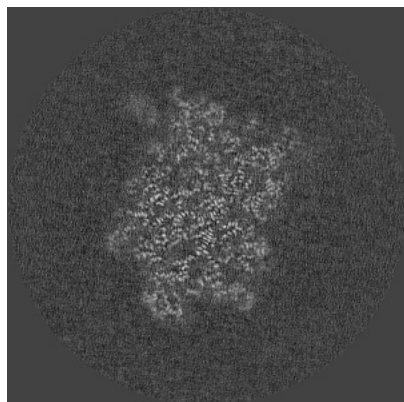


Y Index: 255

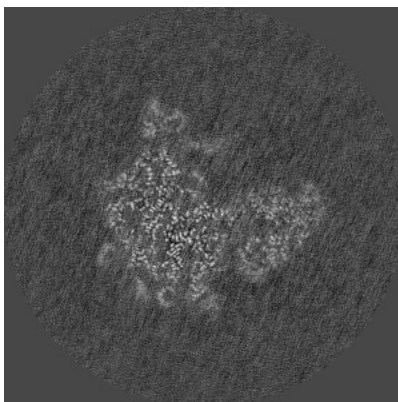


Z Index: 205

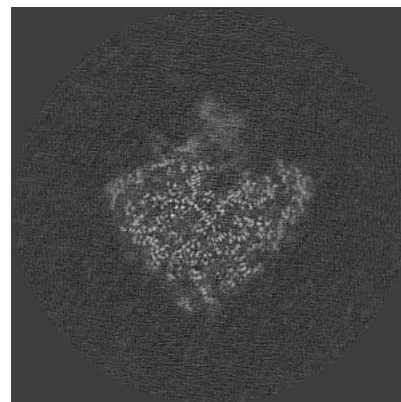
6.3.2 Raw map



X Index: 212



Y Index: 254

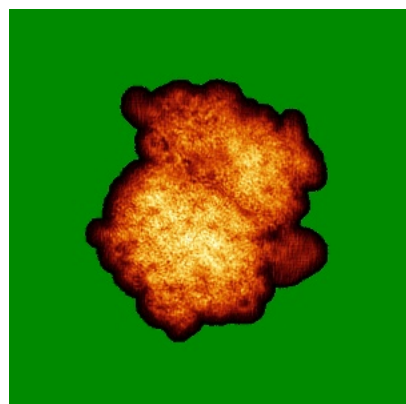


Z Index: 205

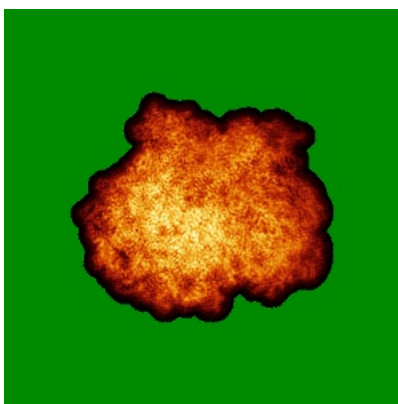
The images above show the largest variance slices of the map in three orthogonal directions.

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

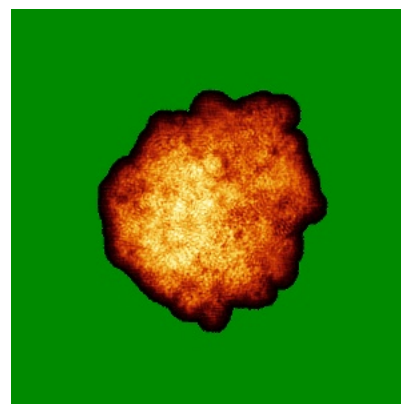
6.4.1 Primary map



X

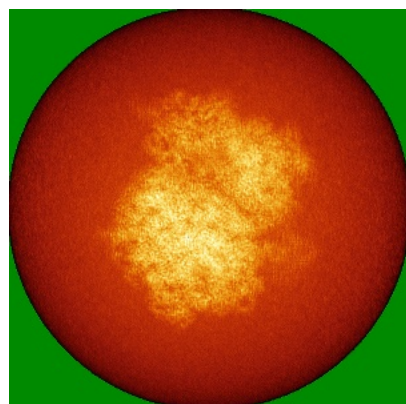


Y

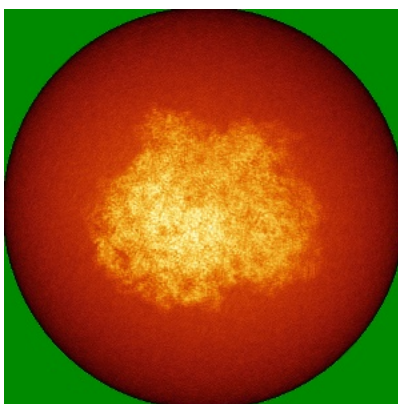


Z

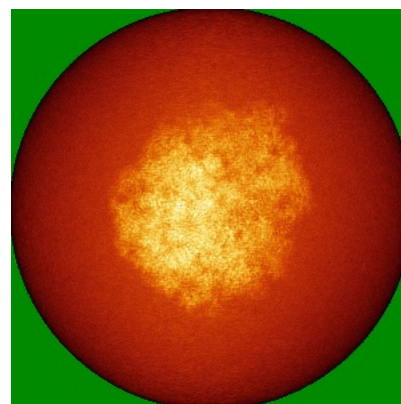
6.4.2 Raw map



X



Y

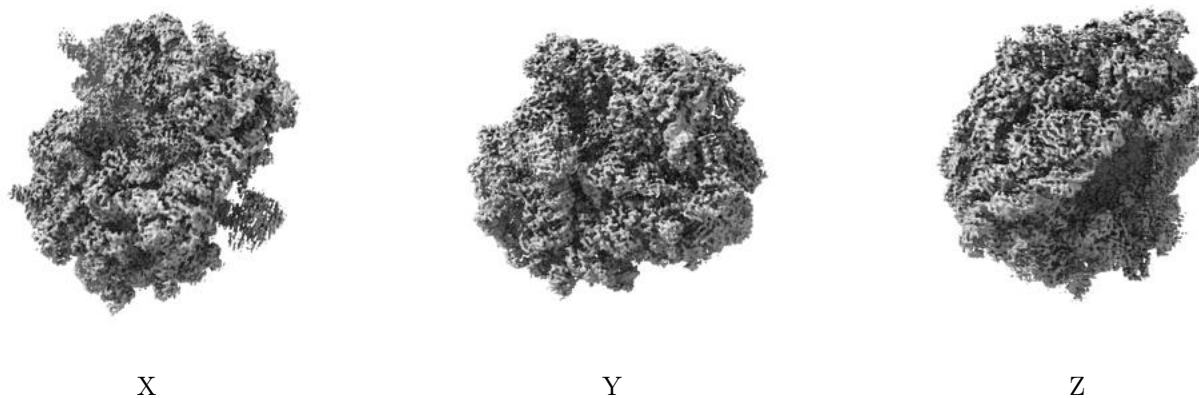


Z

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

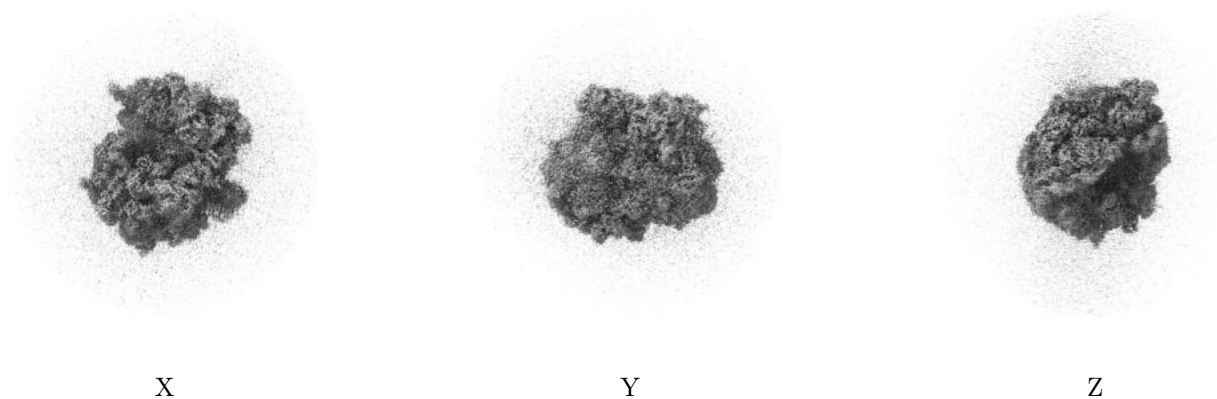
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

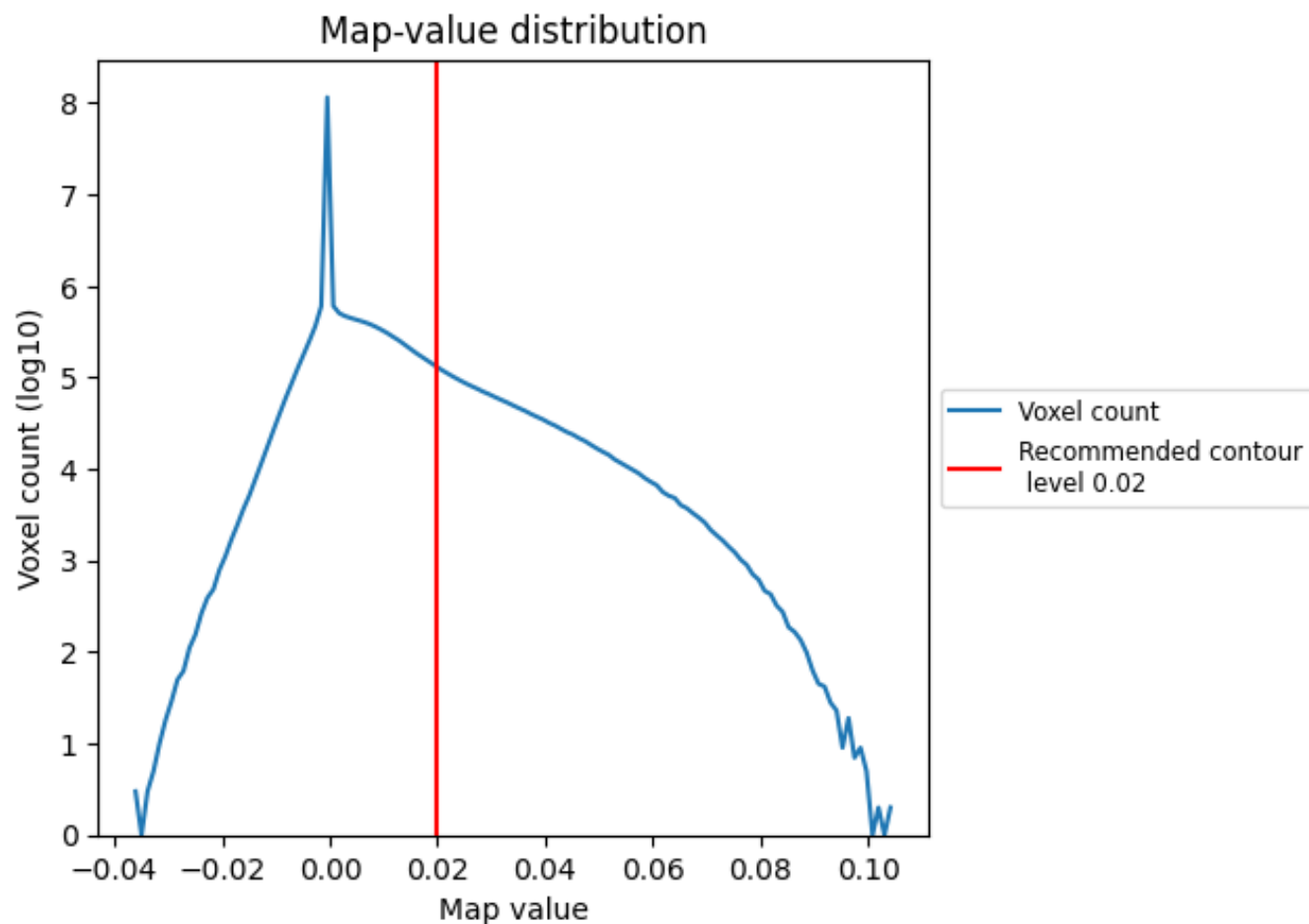
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

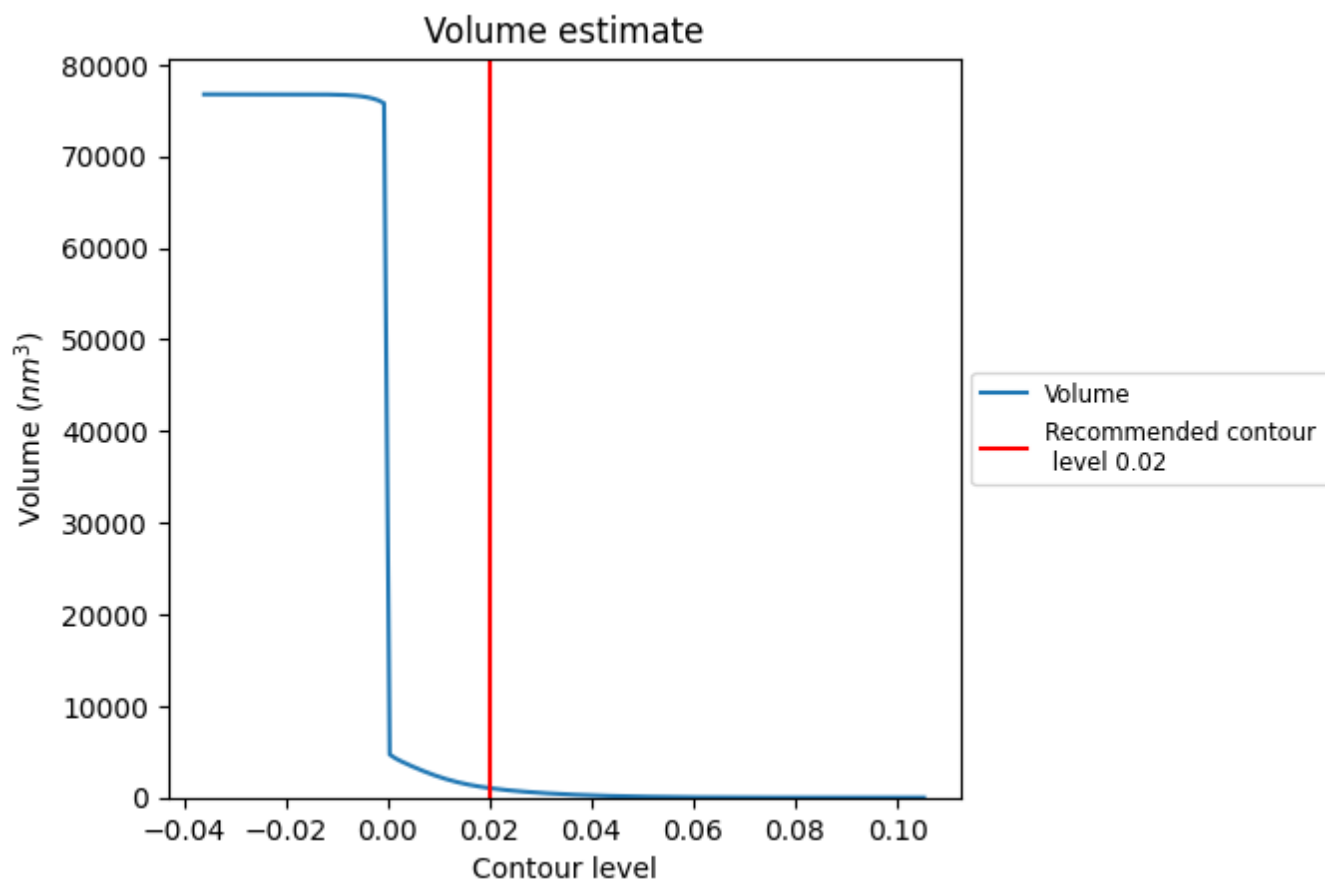
This section contains the results of statistical analysis of the map.

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.

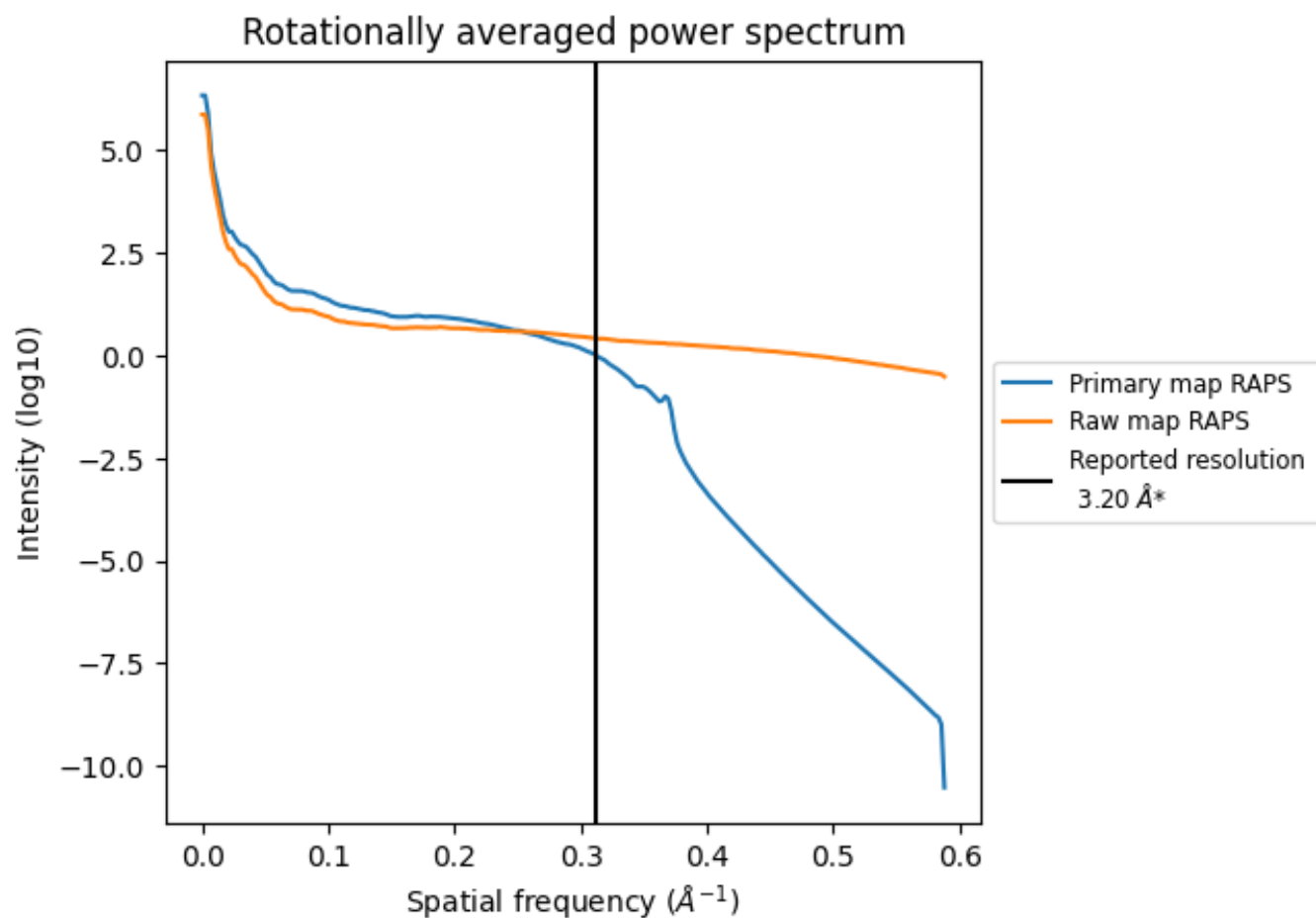
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1035 nm³; this corresponds to an approximate mass of 935 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 ⓘ

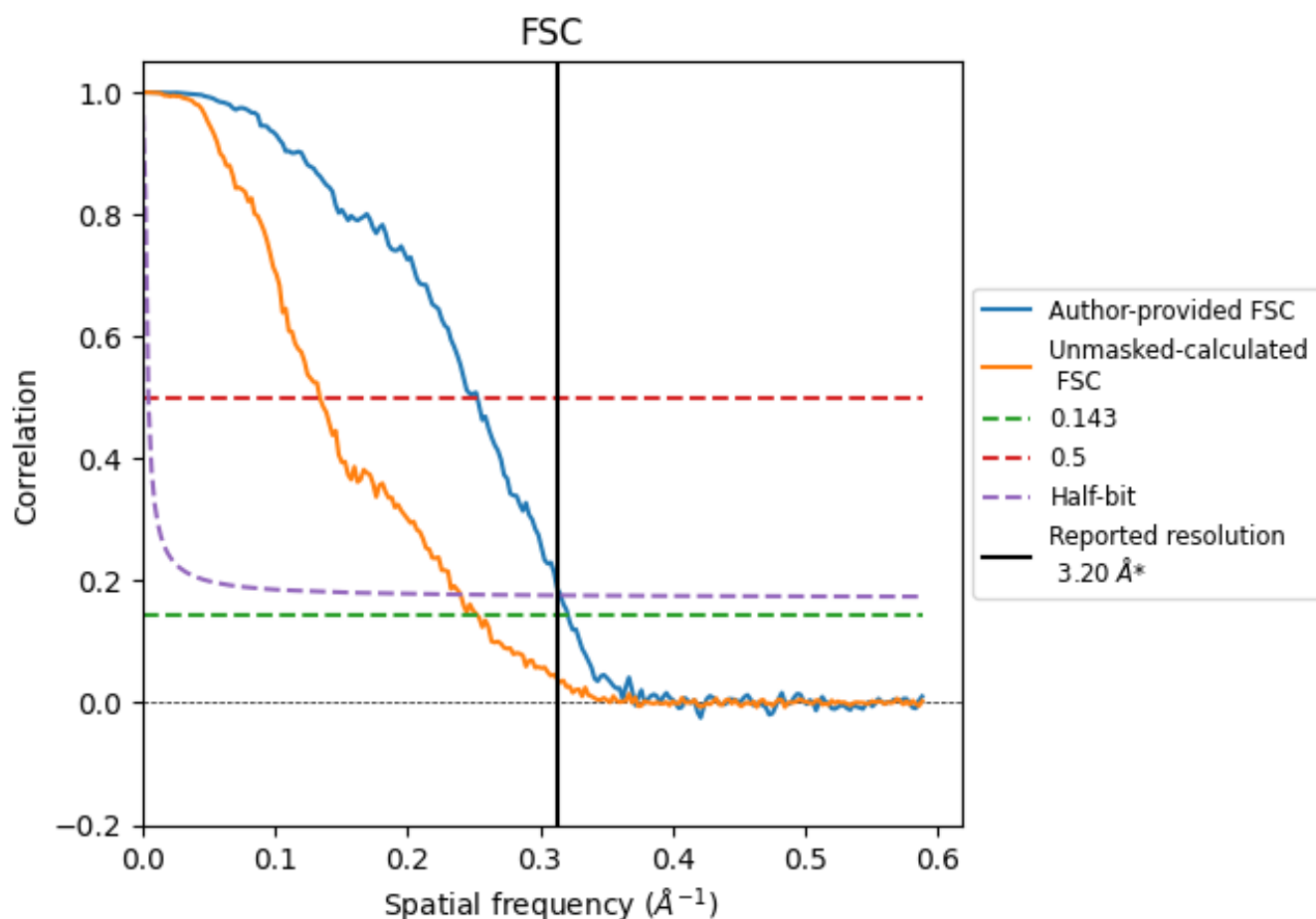


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

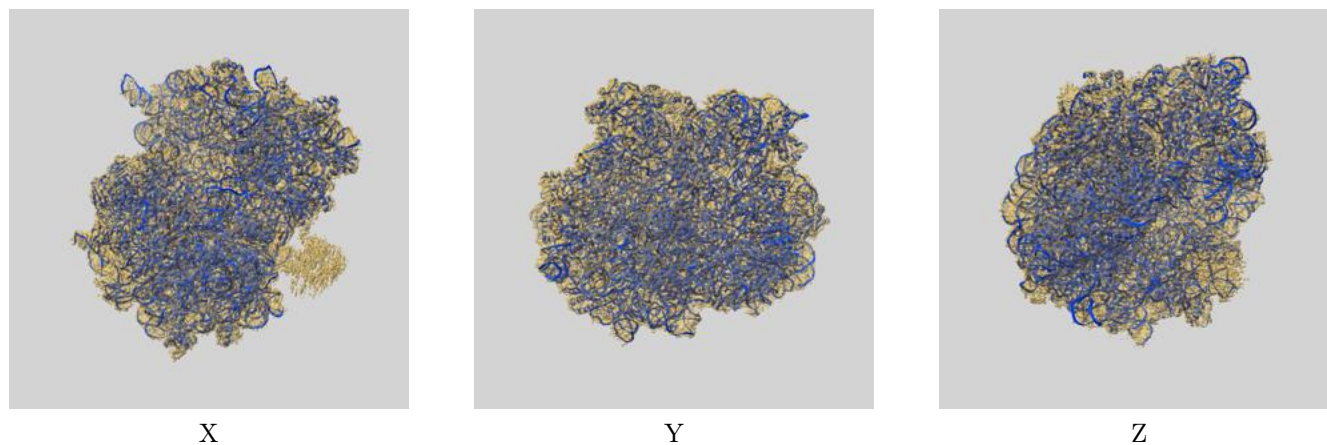
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.11	3.96	3.17
Unmasked-calculated*	3.96	7.46	4.16

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.96 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

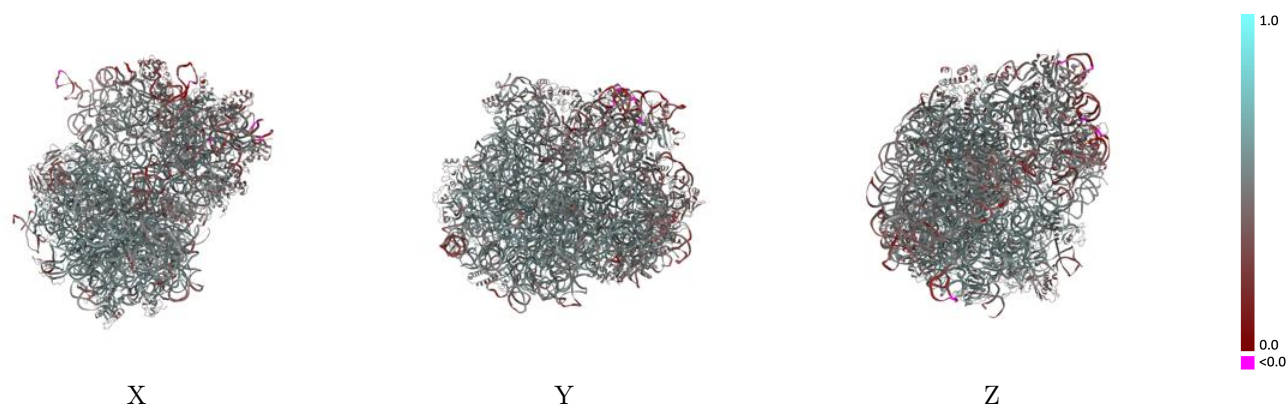
This section contains information regarding the fit between EMDB map EMD-48329 and PDB model 9MKK. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



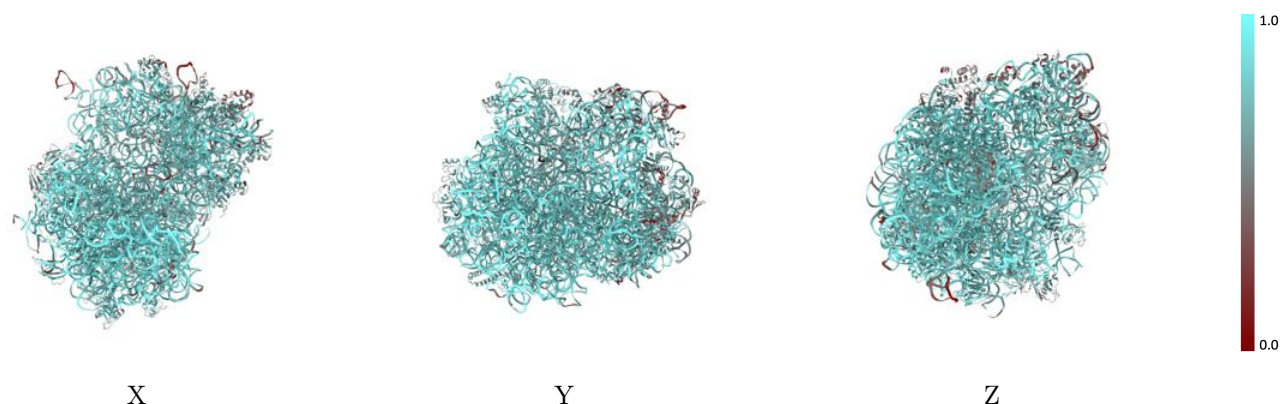
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



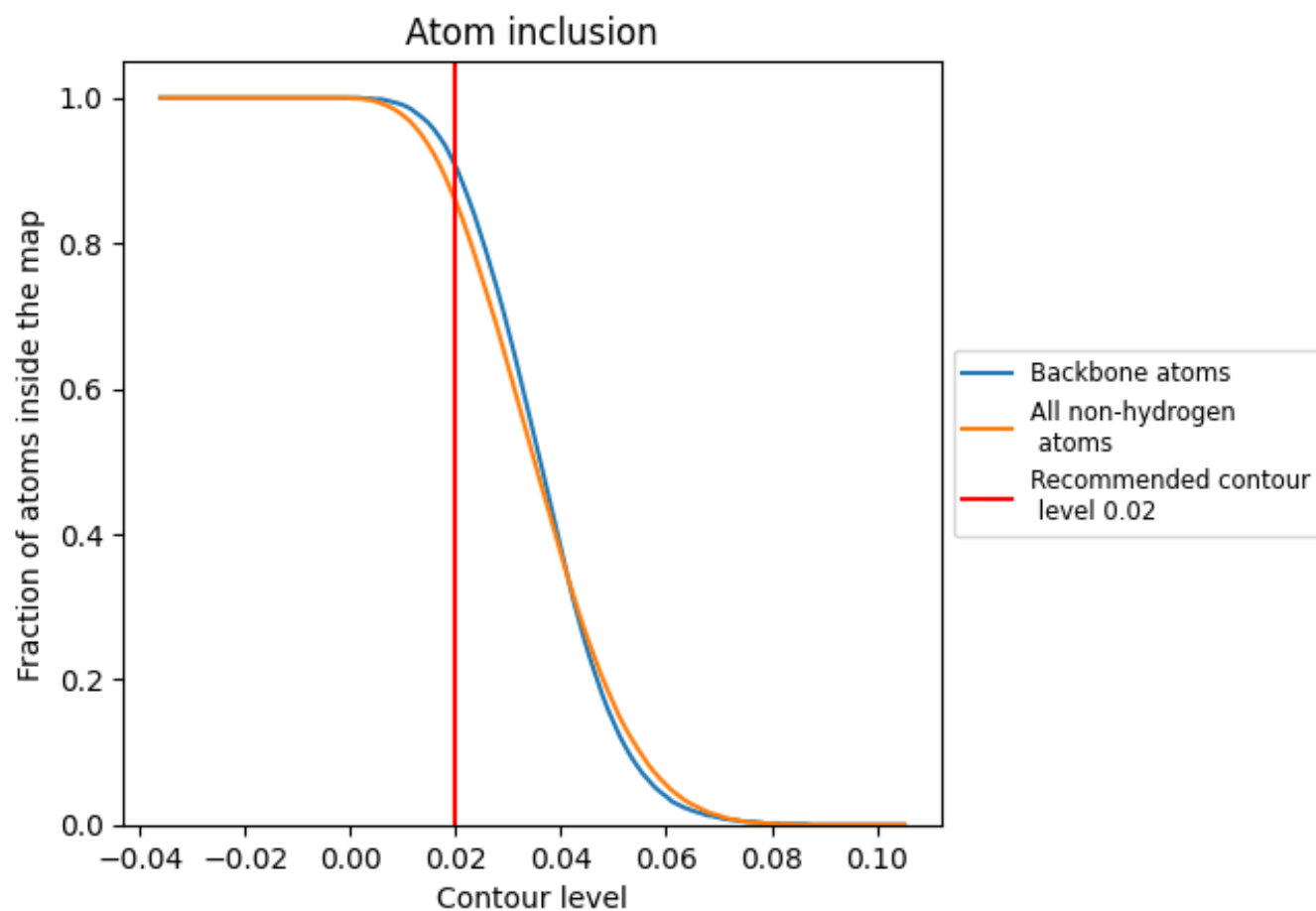
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8580	 0.5030
0	 0.7310	 0.4900
1	 0.8930	 0.5630
2	 0.8600	 0.5420
3	 0.8250	 0.5070
4	 0.5880	 0.4020
A	 0.8730	 0.4720
B	 0.4890	 0.4100
C	 0.7230	 0.4720
D	 0.6260	 0.4240
E	 0.7700	 0.5000
F	 0.6780	 0.4620
G	 0.6710	 0.4400
H	 0.7530	 0.4890
I	 0.6990	 0.4560
J	 0.6030	 0.4260
K	 0.7630	 0.4990
L	 0.7140	 0.4550
M	 0.6890	 0.4610
N	 0.7560	 0.4640
O	 0.7840	 0.5020
P	 0.7330	 0.4480
Q	 0.6640	 0.4350
R	 0.7210	 0.4720
S	 0.7120	 0.4560
T	 0.7050	 0.4420
U	 0.6300	 0.4310
X	 0.9540	 0.5530
Z	 0.7980	 0.4710
a	 0.9350	 0.5370
b	 0.9120	 0.5030
c	 0.8490	 0.5510
d	 0.8160	 0.5250
e	 0.7740	 0.5080
f	 0.6690	 0.4390



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Chain	Atom inclusion	Q-score
g	 0.6310	 0.4180
i	 0.8060	 0.5160
j	 0.7560	 0.5200
k	 0.7820	 0.5090
l	 0.8190	 0.5210
m	 0.8820	 0.5420
n	 0.7390	 0.4660
o	 0.7700	 0.5240
p	 0.8700	 0.4920
q	 0.7790	 0.4970
s	 0.7630	 0.4960
t	 0.7510	 0.4770
u	 0.7240	 0.4830
v	 0.8270	 0.5270
w	 0.8050	 0.4980
x	 0.7420	 0.4740
y	 0.7800	 0.5070
z	 0.7990	 0.5080