



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 01:03 PM UTC

PDB ID : 6ENU / pdb_00006enu
EMDB ID : EMD-3903
Title : Polyproline-stalled ribosome in the presence of elongation-factor P (EF-P)
Authors : Huter, P.; Arenz, S.; Wilson, D.N.
Deposited on : 2017-10-06
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

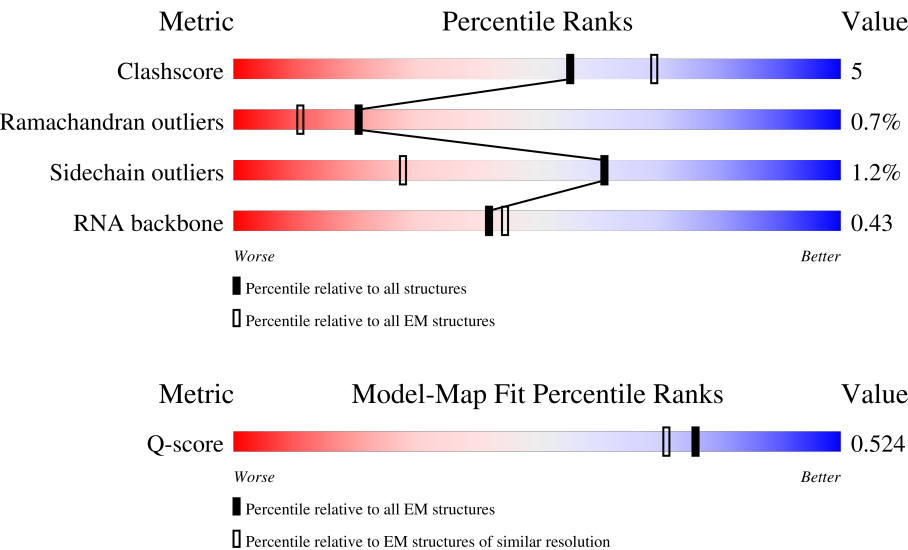
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	a	1539	
2	b	218	
3	c	206	

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Mol	Chain	Length	Quality of chain
4	d	205	
5	e	157	
6	f	100	
7	g	151	
8	h	129	
9	i	127	
10	j	98	
11	k	116	
12	l	123	
13	m	114	
14	n	101	
15	o	88	
16	p	82	
17	q	80	
18	r	65	
19	s	79	
20	t	85	
21	u	65	
22	v	6	
23	A	2903	
24	B	120	
25	C	271	
26	D	209	
27	E	201	
28	F	177	

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Mol	Chain	Length	Quality of chain
29	G	176	
30	H	149	
31	J	142	
32	K	122	
33	L	143	
34	M	136	
35	N	120	
36	O	116	
37	P	114	
38	Q	117	
39	R	103	
40	S	110	
41	T	93	
42	U	102	
43	V	94	
44	W	78	
45	X	77	
46	Y	63	
47	Z	58	
48	0	56	
49	1	50	
50	2	46	
51	3	64	
52	4	38	
53	6	66	

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Mol	Chain	Length	Quality of chain
54	x	77	13% 45% 36% 17%
55	7	224	100% 70% 23% 6%
56	w	188	74% 76% 19%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 146475 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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1539	Total	C	N	O	P	0	0
			33016	14725	6052	10700	1539		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	v	6	Total	C	N	O	P	0	0
			126	56	22	42	6		

- Molecule 23 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A	2871	Total	C	N	O	P	0	0
			61641	27498	11350	19922	2871		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	C	U	conflict	GB 802133627
A	1847	G	A	conflict	GB 802133627
A	2069	A	G	conflict	GB 802133627
A	2104	U	C	conflict	GB 802133627

- Molecule 24 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 1213441078

- Molecule 25 is a protein called 50S ribosomal protein L2.

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

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 27 is a protein called 50S ribosomal protein L4.

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

- Molecule 28 is a protein called 50S ribosomal protein L5.

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

- Molecule 29 is a protein called 50S ribosomal protein L6.

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

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 34 is a protein called 50S ribosomal protein L16.

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

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 36 is a protein called 50S ribosomal protein L18.

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

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

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

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	U	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	W	78	Total	C	N	O	S	0	0
			592	365	119	107	1		

- Molecule 45 is a protein called 50S ribosomal protein L28.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	1	50	Total	C	N	O	0	0
			409	263	75	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 53 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 54 is a RNA chain called Proline tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	x	77	Total	C	N	O	P	0	0
			1646	733	295	541	77		

- Molecule 55 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	7	224	Total	C	N	O	S	0	0
			1663	1039	303	315	6		

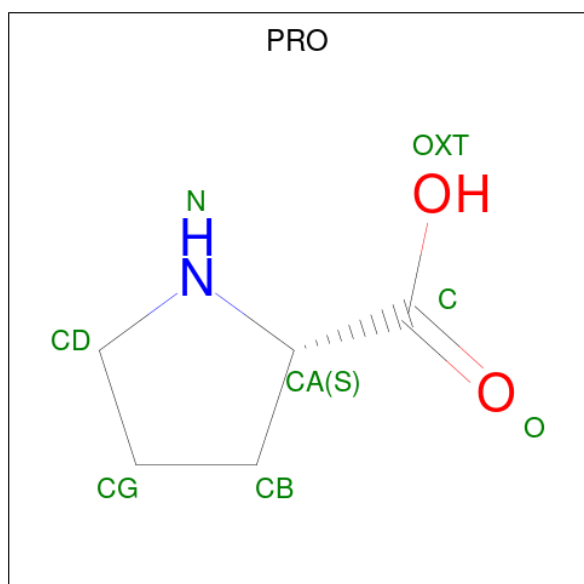
- Molecule 56 is a protein called Elongation factor P.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	w	188	Total	C	N	O	S	0	0
			1461	928	242	286	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
w	34	KEO	LYS	engineered mutation	UNP P0A6N4

- Molecule 57 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).

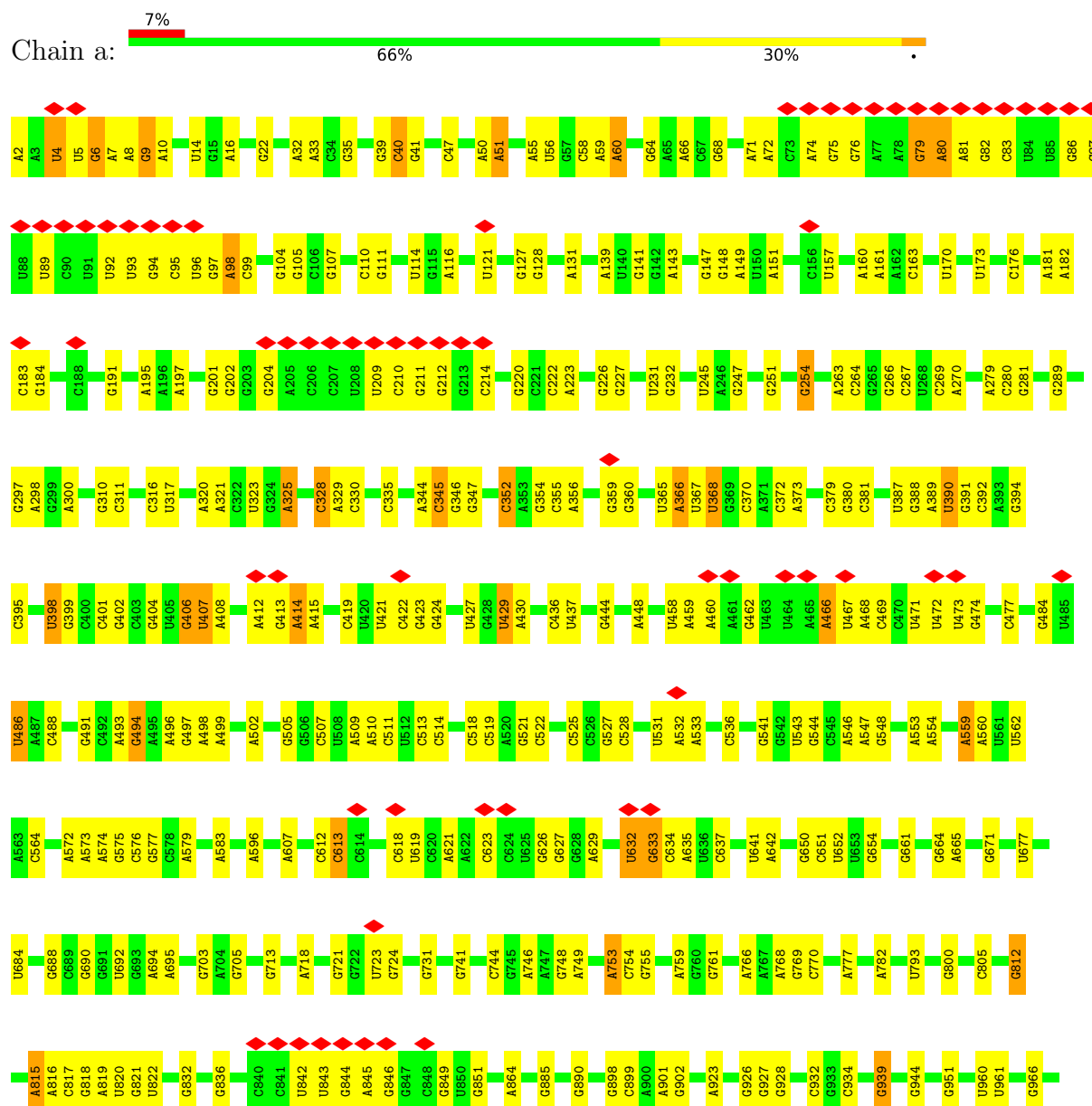


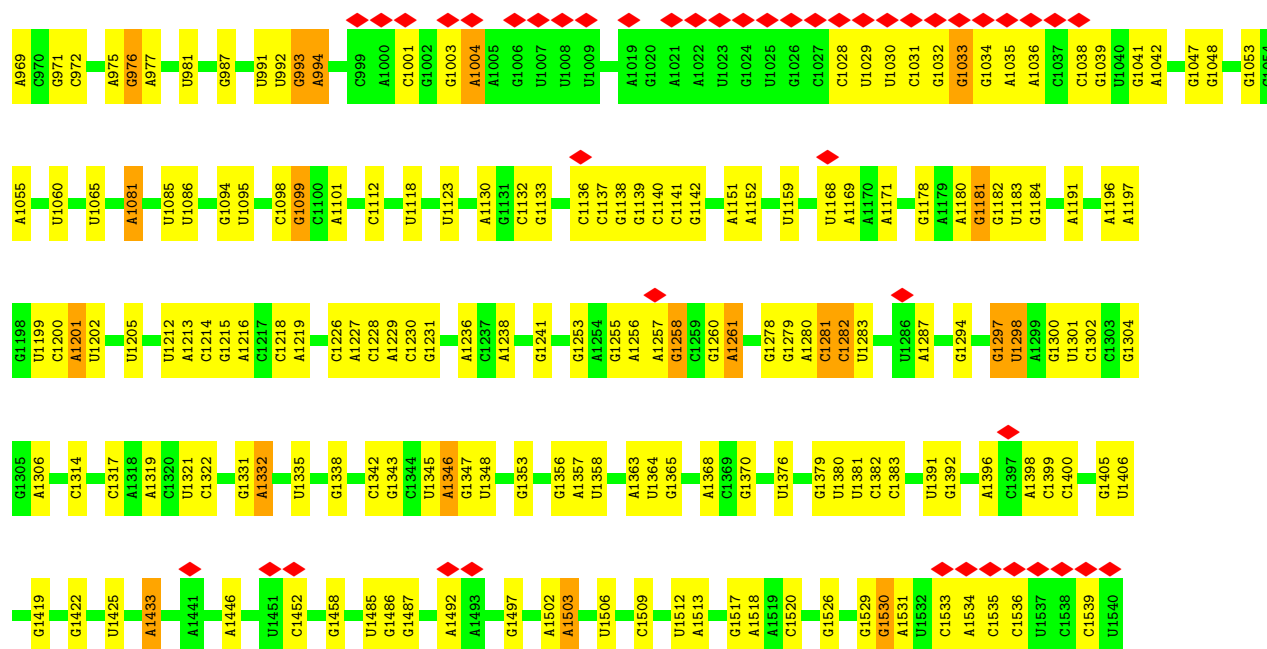
Mol	Chain	Residues	Atoms				AltConf
57	A	1	Total	C	N	O	0
			7	5	1	1	
57	x	1	Total	C	N	O	0
			7	5	1	1	

3 Residue-property plots

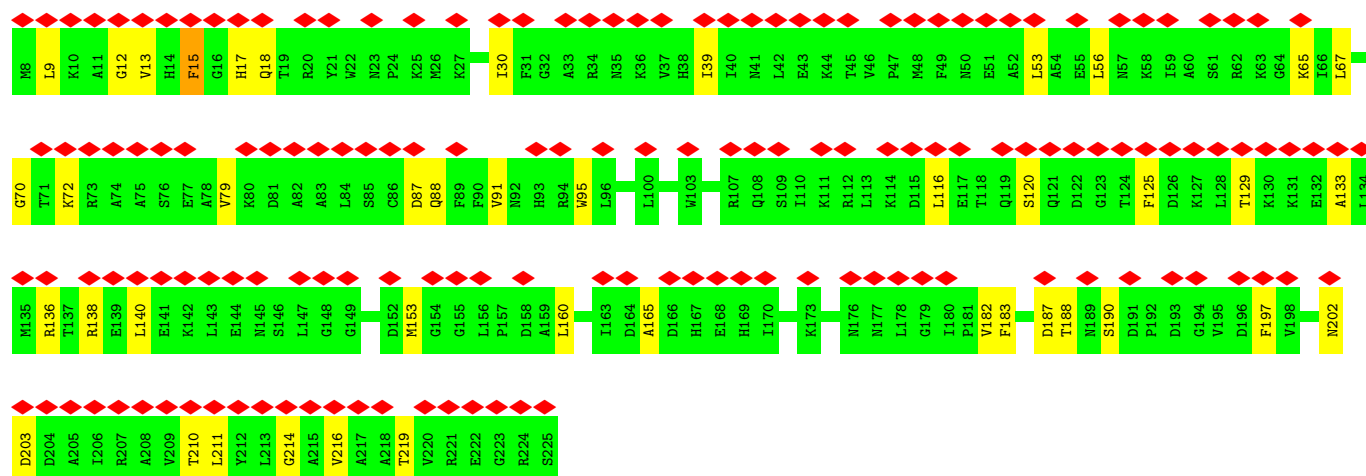
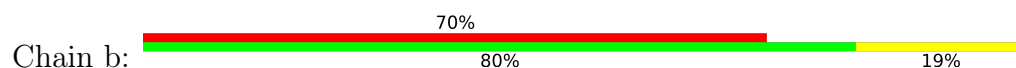
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S ribosomal RNA

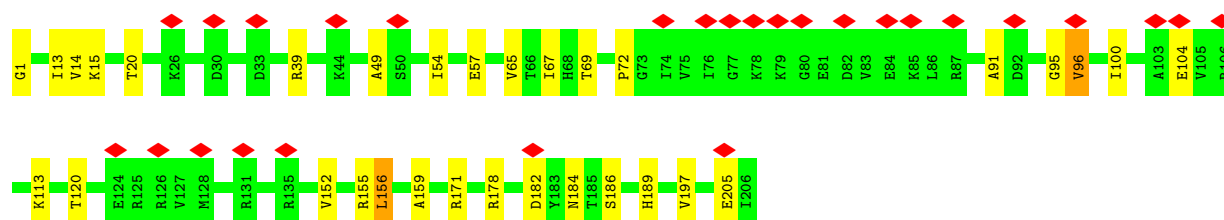
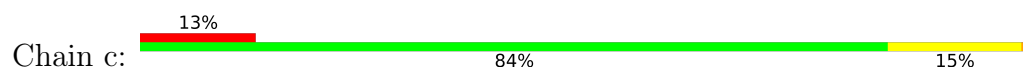




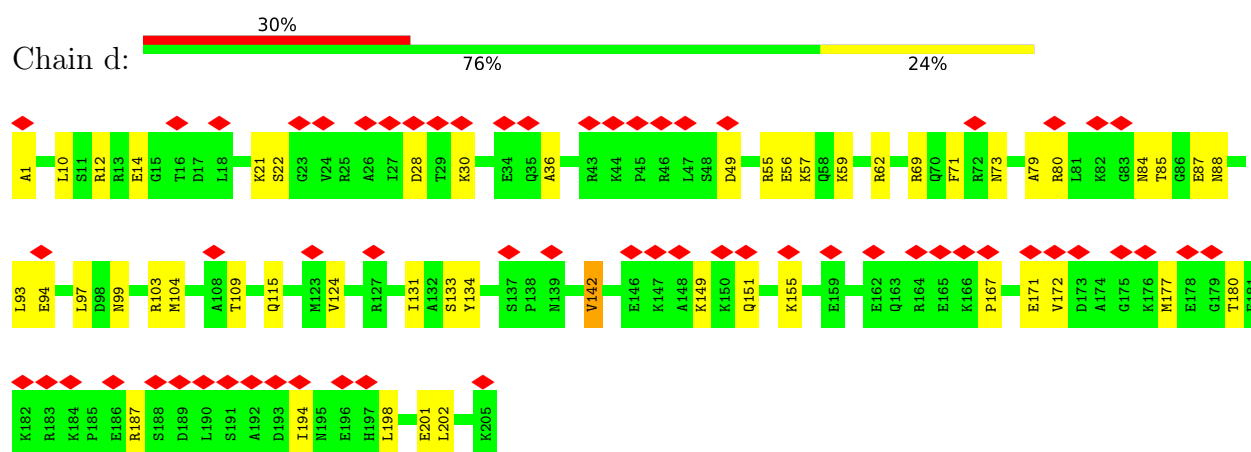
• Molecule 2: 30S ribosomal protein S2



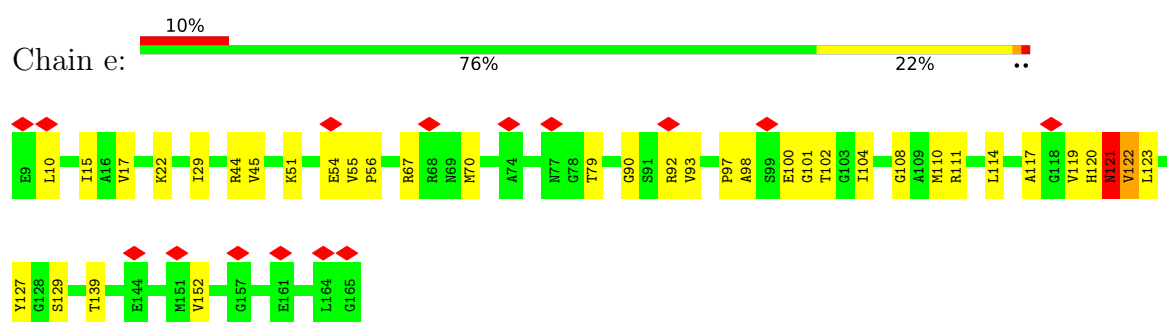
• Molecule 3: 30S ribosomal protein S3



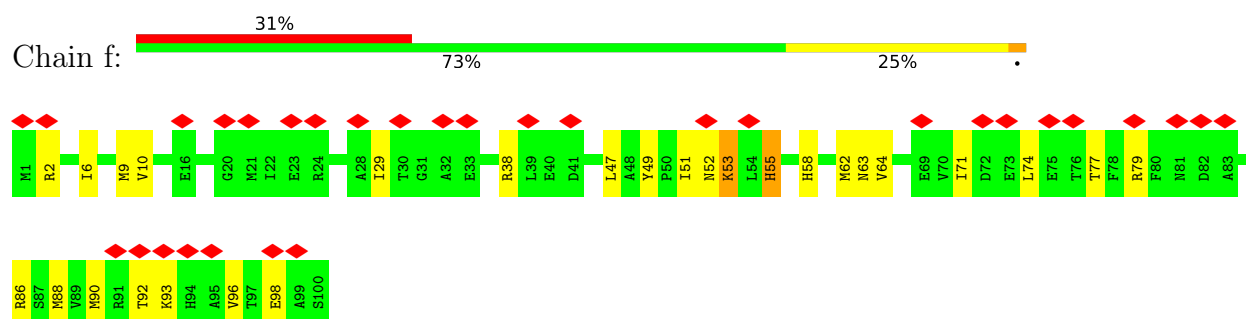
• Molecule 4: 30S ribosomal protein S4



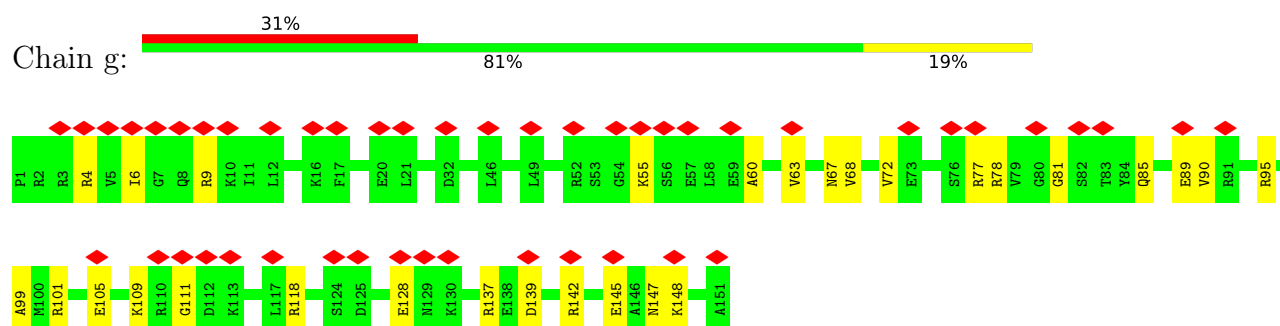
• Molecule 5: 30S ribosomal protein S5



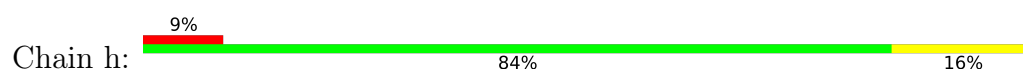
• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7

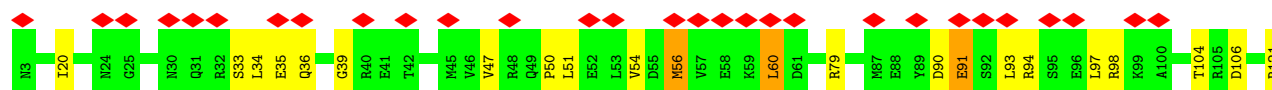
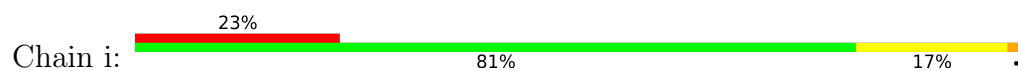


• Molecule 8: 30S ribosomal protein S8

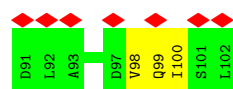
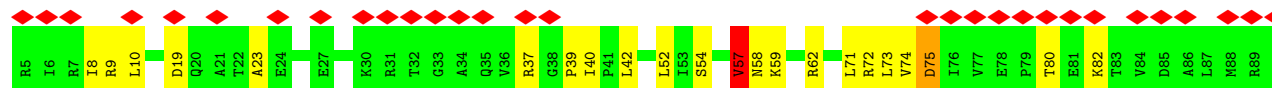
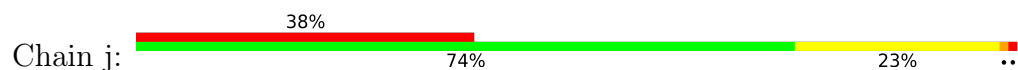




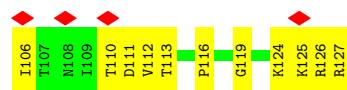
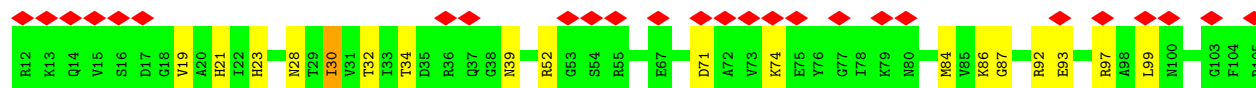
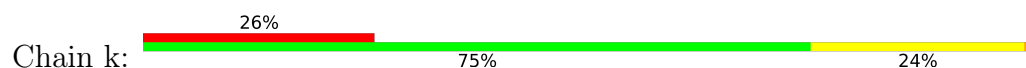
• Molecule 9: 30S ribosomal protein S9



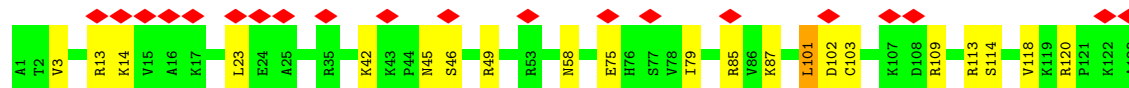
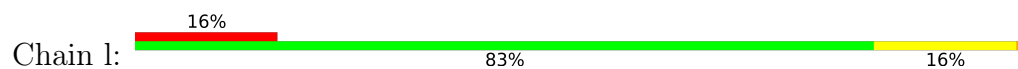
• Molecule 10: 30S ribosomal protein S10



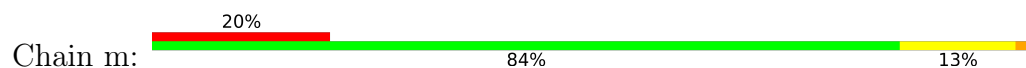
• Molecule 11: 30S ribosomal protein S11

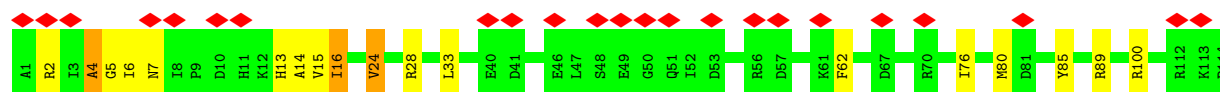


• Molecule 12: 30S ribosomal protein S12

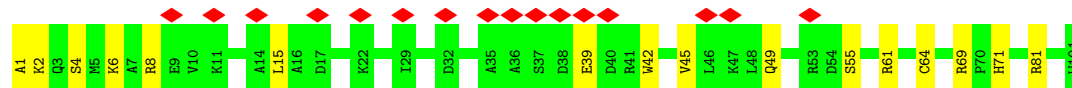
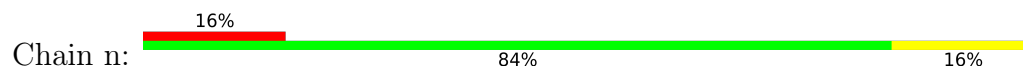


• Molecule 13: 30S ribosomal protein S13

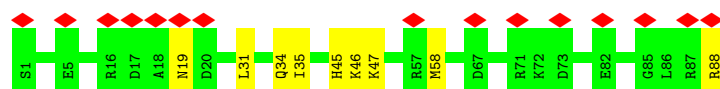




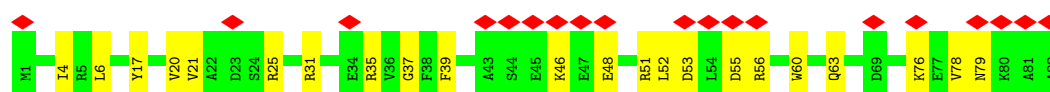
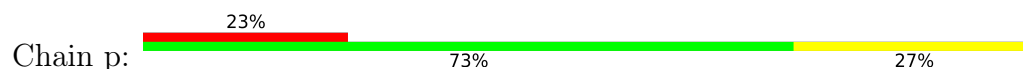
- Molecule 14: 30S ribosomal protein S14



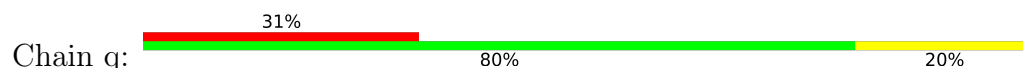
- Molecule 15: 30S ribosomal protein S15



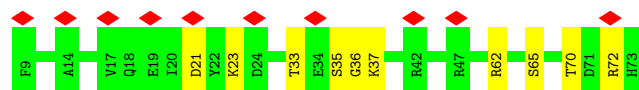
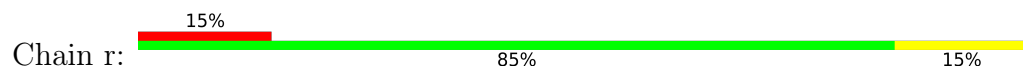
- Molecule 16: 30S ribosomal protein S16



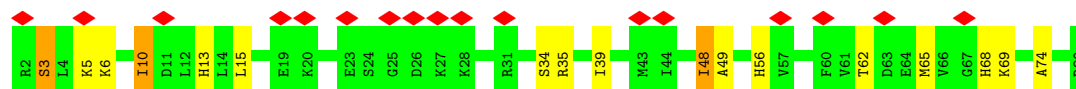
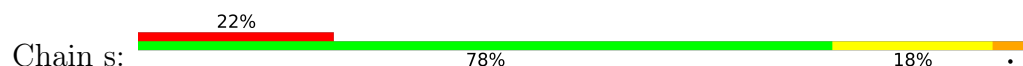
- Molecule 17: 30S ribosomal protein S17



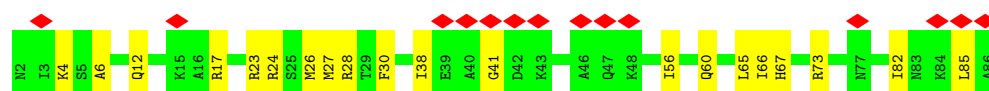
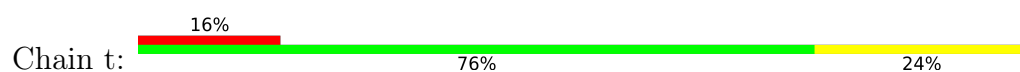
- Molecule 18: 30S ribosomal protein S18



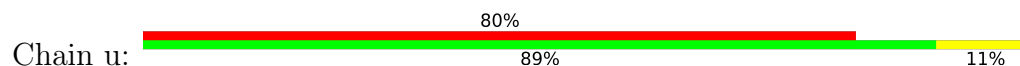
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



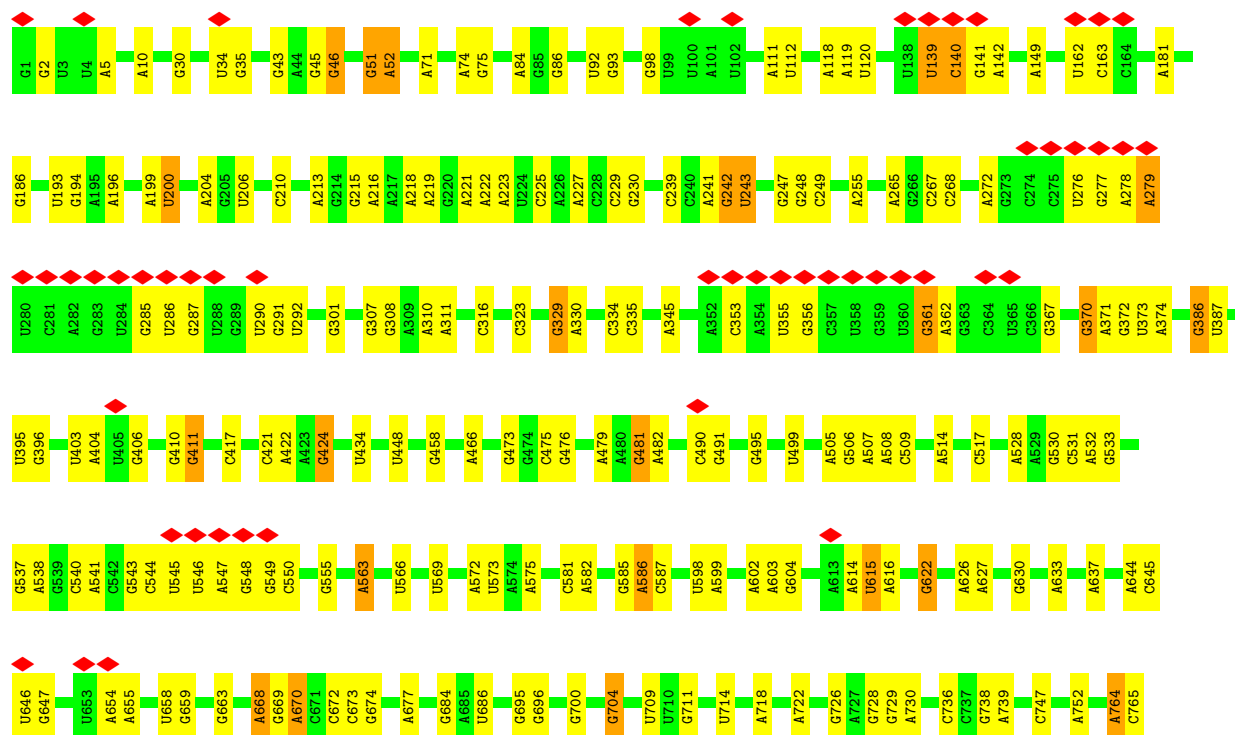
• Molecule 21: 30S ribosomal protein S21

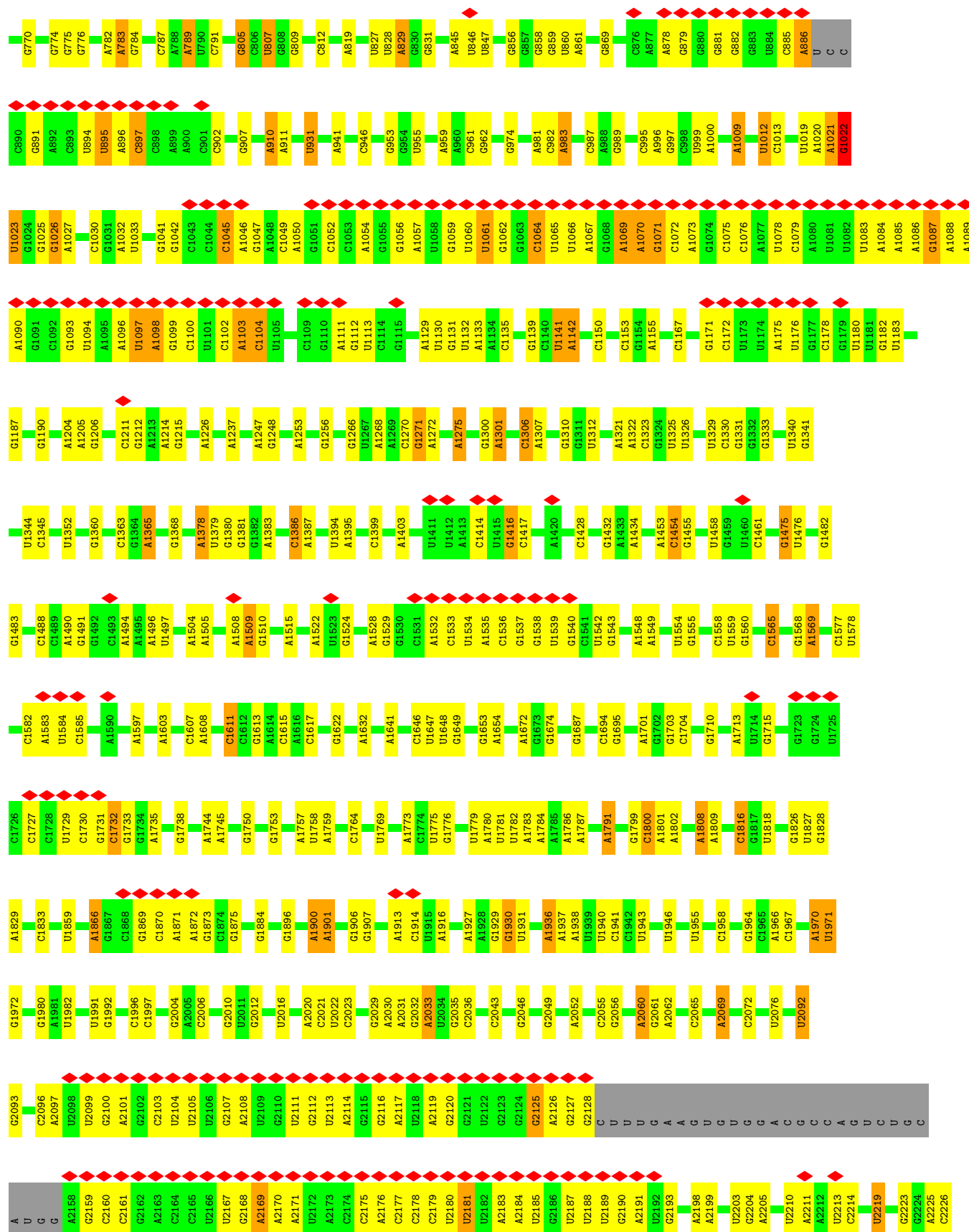


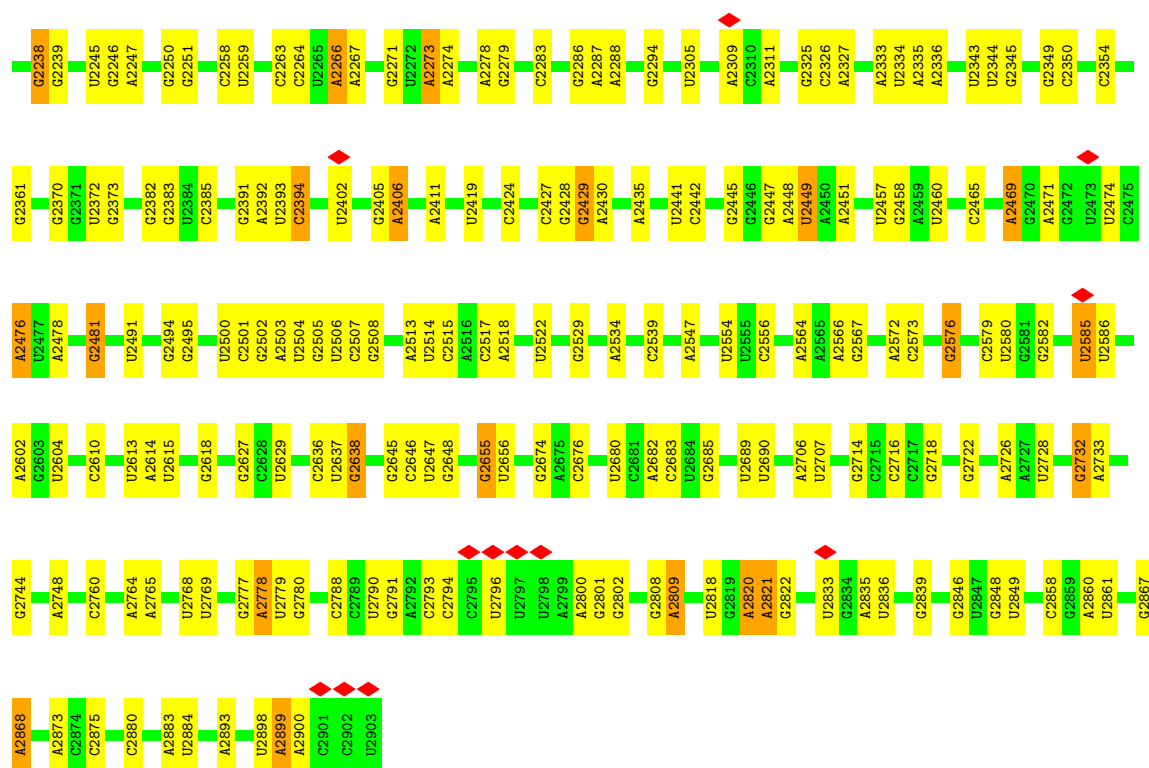
• Molecule 22: mRNA



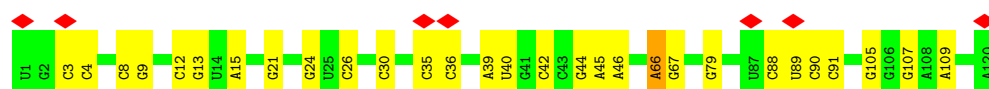
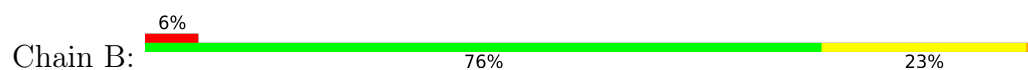
• Molecule 23: 23S Ribosomal RNA



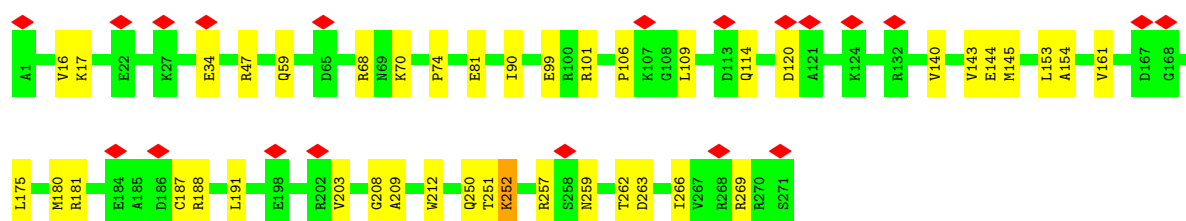
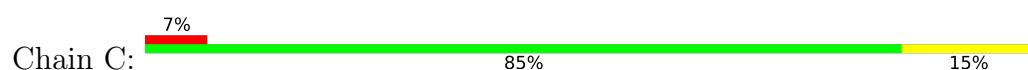




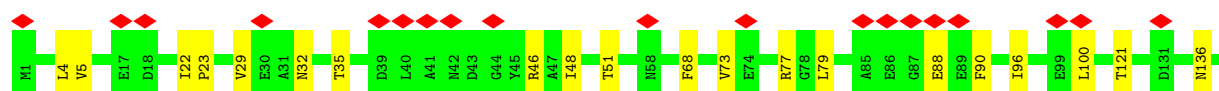
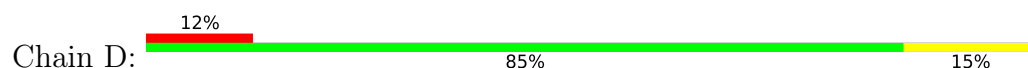
• Molecule 24: 5S Ribosomal RNA

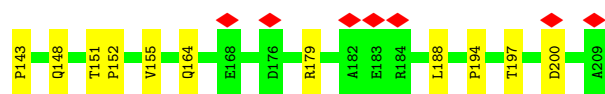


• Molecule 25: 50S ribosomal protein L2

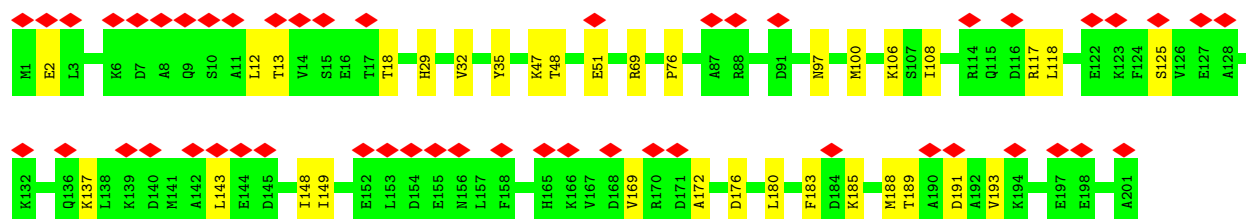
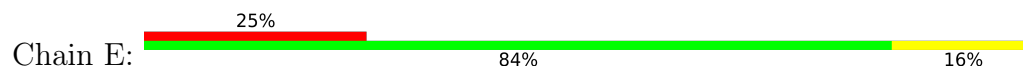


• Molecule 26: 50S ribosomal protein L3

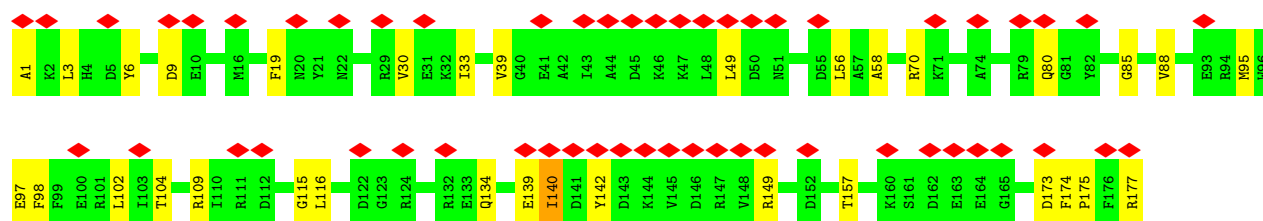
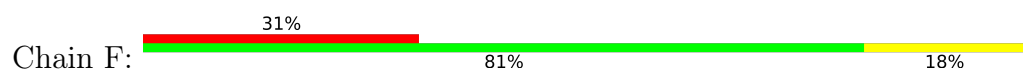




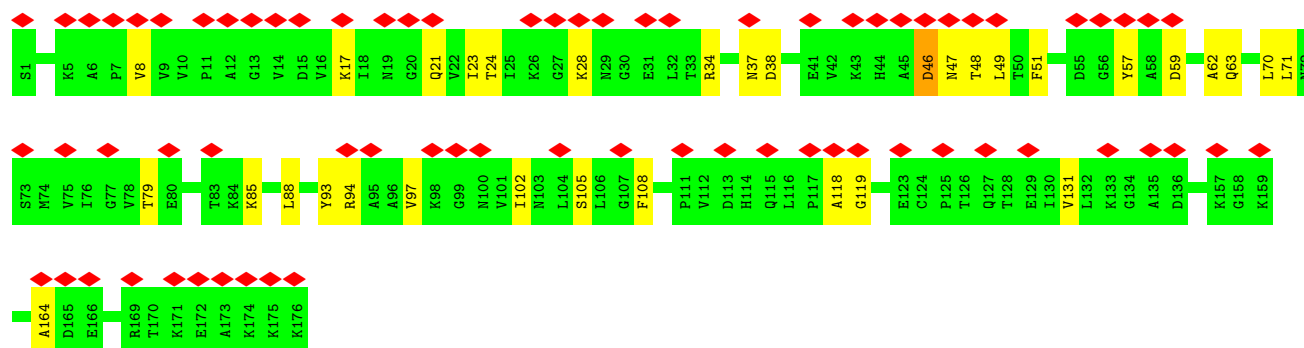
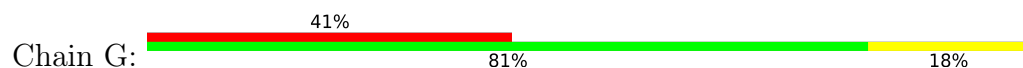
- Molecule 27: 50S ribosomal protein L4



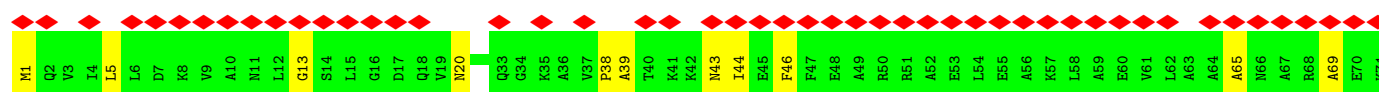
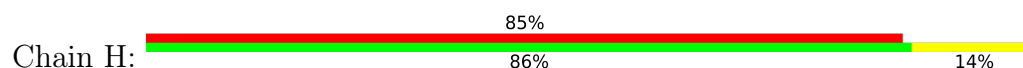
- Molecule 28: 50S ribosomal protein L5

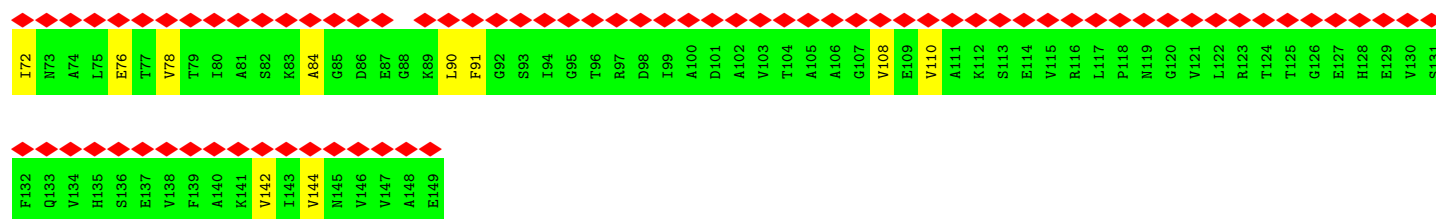


- Molecule 29: 50S ribosomal protein L6

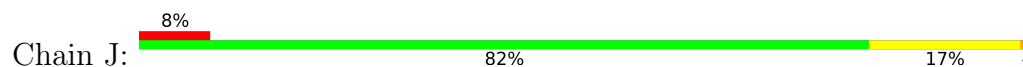


- Molecule 30: 50S ribosomal protein L9

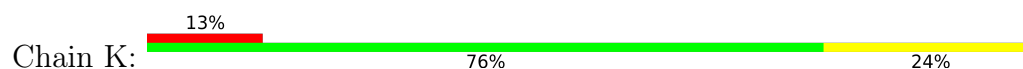




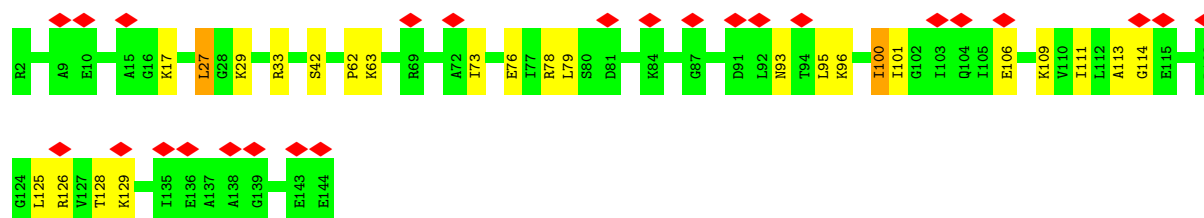
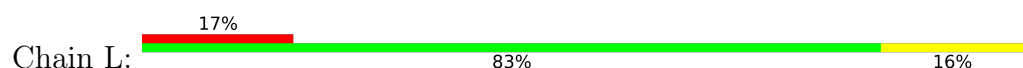
• Molecule 31: 50S ribosomal protein L13



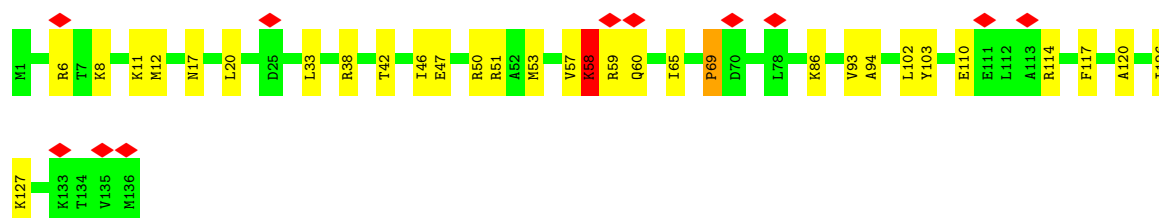
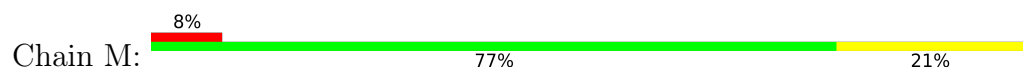
• Molecule 32: 50S ribosomal protein L14



• Molecule 33: 50S ribosomal protein L15

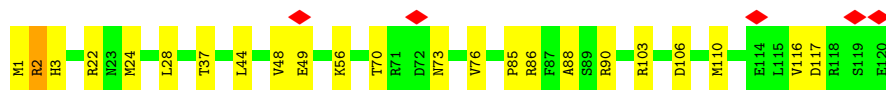


• Molecule 34: 50S ribosomal protein L16



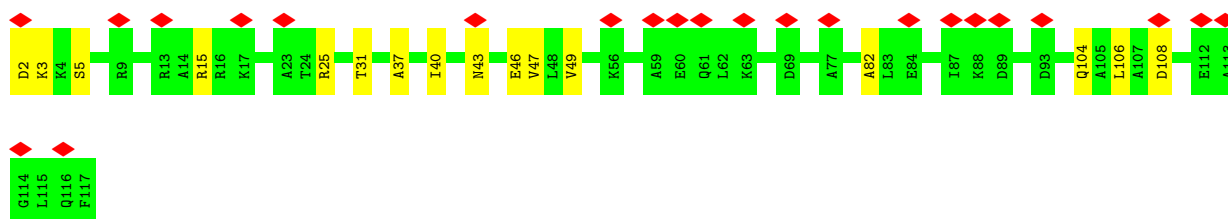
• Molecule 35: 50S ribosomal protein L17

Chain N:  81% 18% .



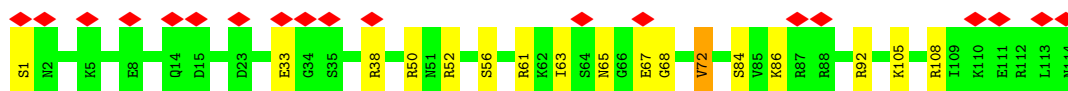
- Molecule 36: 50S ribosomal protein L18

Chain O:  20% 86% 14%



- Molecule 37: 50S ribosomal protein L19

Chain P:  17% 85% 14% .



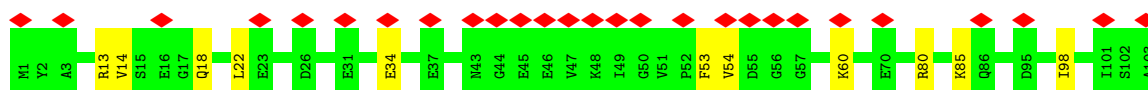
- Molecule 38: 50S ribosomal protein L20

Chain Q:  6% 85% 14% .



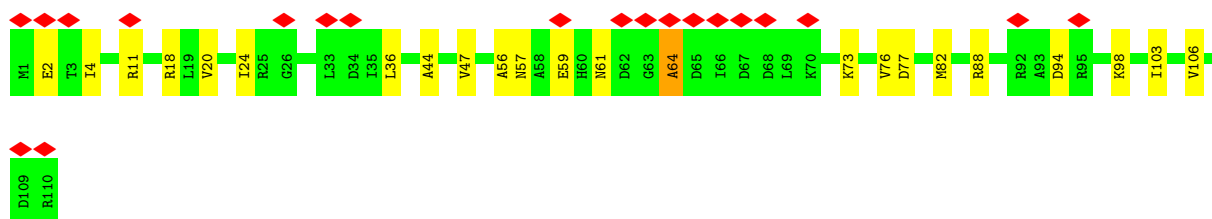
- Molecule 39: 50S ribosomal protein L21

Chain R:  26% 89% 11%

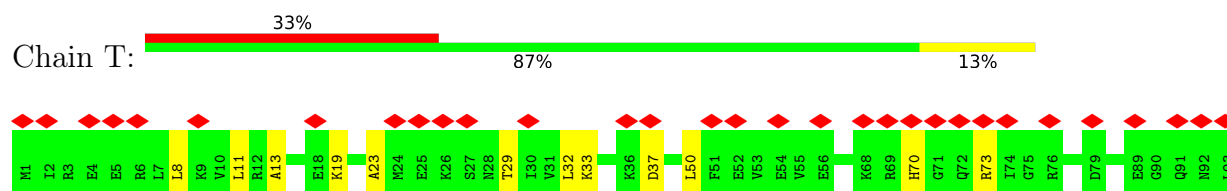


- Molecule 40: 50S ribosomal protein L22

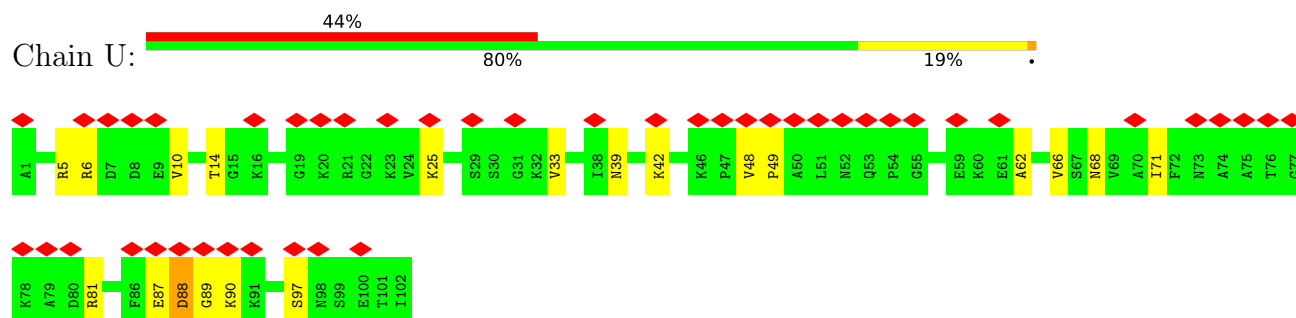
Chain S:  18% 79% 20% .



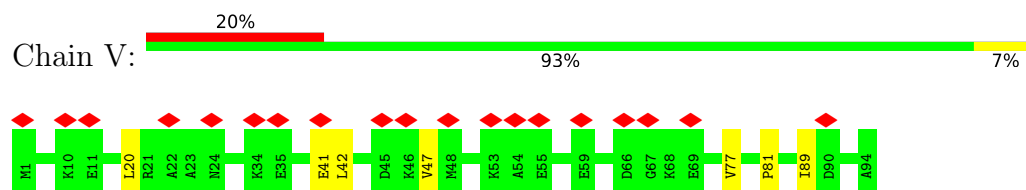
- Molecule 41: 50S ribosomal protein L23



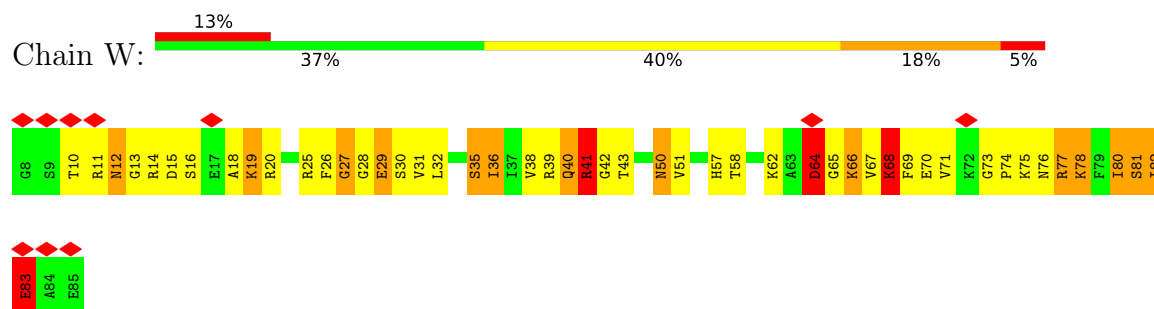
- Molecule 42: 50S ribosomal protein L24



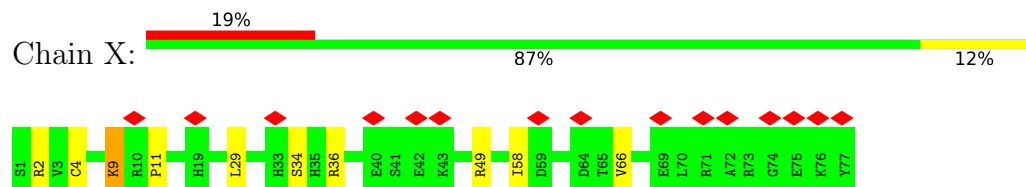
- Molecule 43: 50S ribosomal protein L25



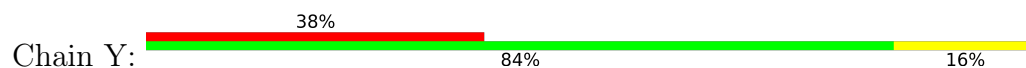
- Molecule 44: 50S ribosomal protein L27

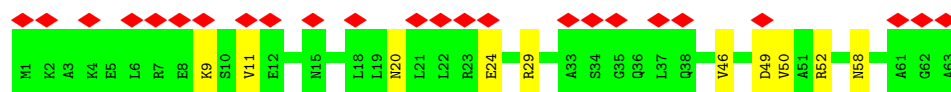


- Molecule 45: 50S ribosomal protein L28

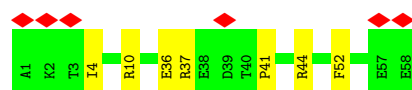
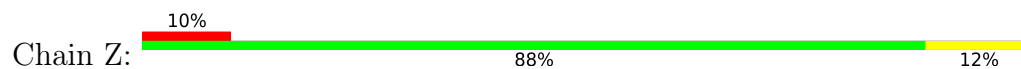


- Molecule 46: 50S ribosomal protein L29

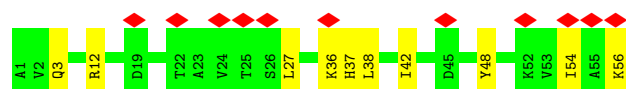
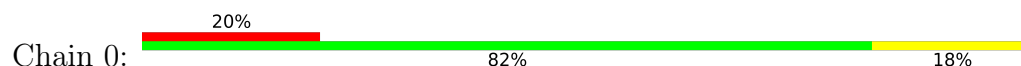




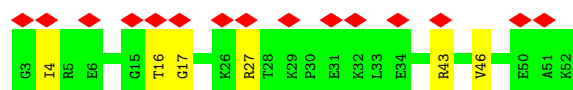
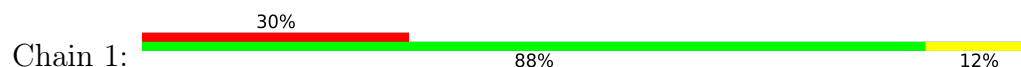
- Molecule 47: 50S ribosomal protein L30



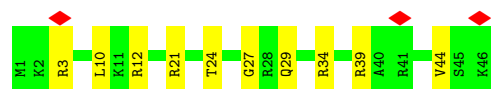
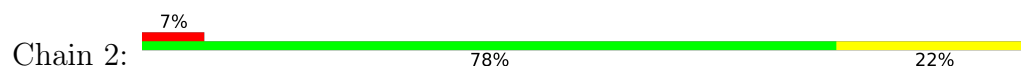
- Molecule 48: 50S ribosomal protein L32



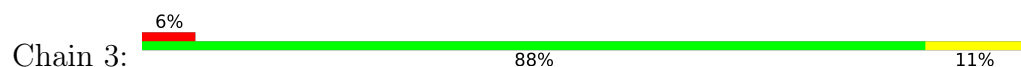
- Molecule 49: 50S ribosomal protein L33



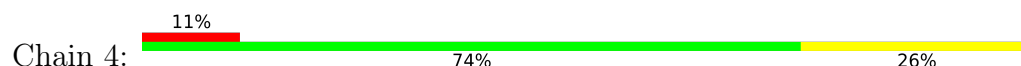
- Molecule 50: 50S ribosomal protein L34



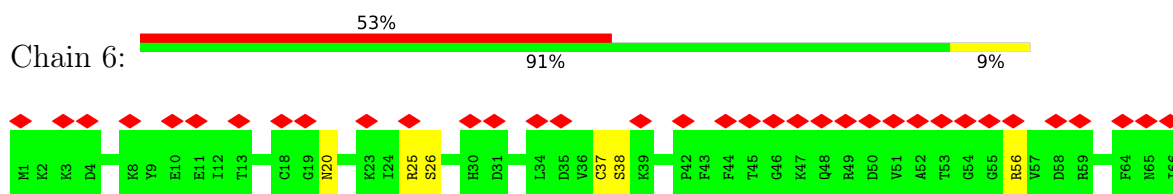
- Molecule 51: 50S ribosomal protein L35



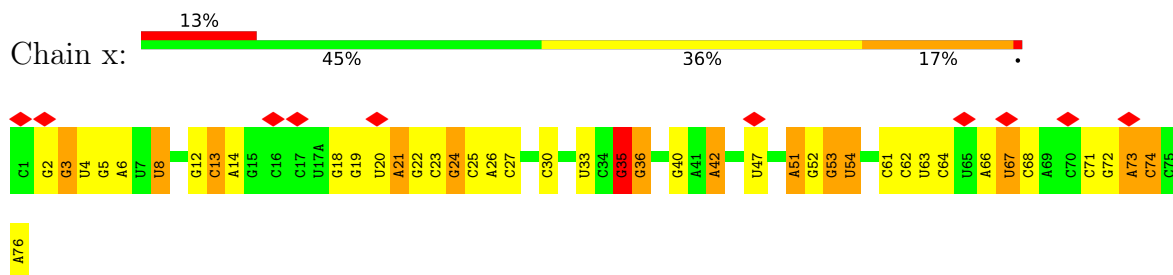
- Molecule 52: 50S ribosomal protein L36



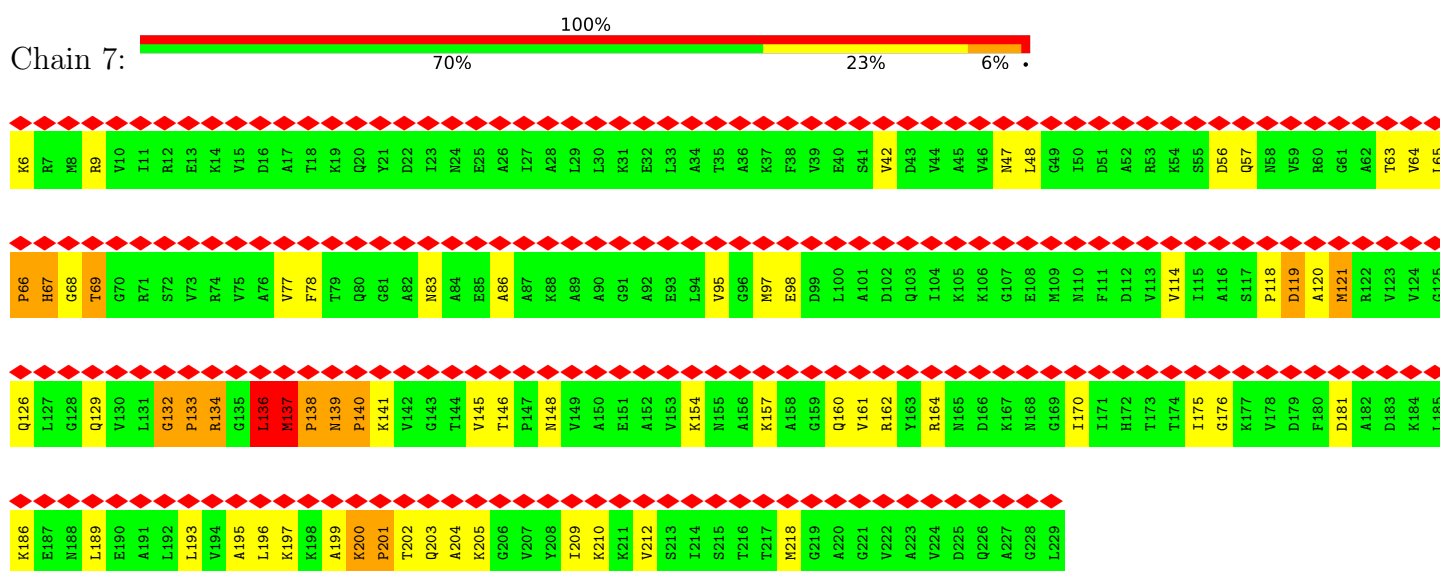
- Molecule 53: 50S ribosomal protein L31



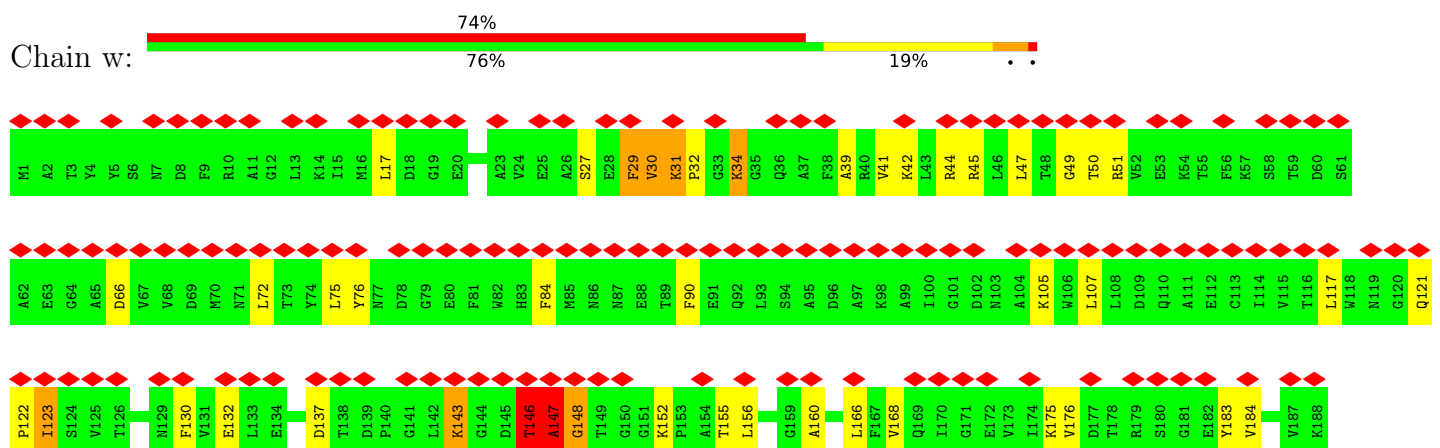
• Molecule 54: Proline tRNA



• Molecule 55: 50S ribosomal protein L1



• Molecule 56: Elongation factor P



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63665	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.669	Depositor
Minimum map value	-0.326	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.108	Depositor
Map size (Å)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality

5.1 Standard geometry

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

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	a	0.39	0/36967	0.44	0/57666
2	b	0.30	0/1735	0.67	0/2338
3	c	0.37	0/1651	0.65	0/2225
4	d	0.39	0/1665	0.77	0/2227
5	e	0.42	0/1154	0.83	2/1554 (0.1%)
6	f	0.35	0/835	0.79	1/1128 (0.1%)
7	g	0.34	0/1195	0.77	2/1602 (0.1%)
8	h	0.40	0/989	0.70	0/1326
9	i	0.38	0/1034	0.73	0/1375
10	j	0.38	0/796	0.85	2/1077 (0.2%)
11	k	0.38	0/885	0.72	0/1195
12	l	0.43	0/969	0.82	2/1300 (0.2%)
13	m	0.36	0/892	0.79	0/1193
14	n	0.40	0/811	0.69	0/1081
15	o	0.36	0/722	0.67	0/964
16	p	0.43	0/659	0.76	0/884
17	q	0.39	0/657	0.70	0/881
18	r	0.38	0/511	0.71	0/689
19	s	0.47	1/652 (0.2%)	0.71	0/877
20	t	0.36	0/671	0.70	0/888
21	u	0.35	0/500	0.90	0/668
22	v	0.46	0/139	0.69	0/214
23	A	0.39	0/69039	0.44	6/107701 (0.0%)
24	B	0.33	0/2876	0.44	0/4483
25	C	0.46	0/2121	0.71	0/2852
26	D	0.40	0/1586	0.67	0/2134
27	E	0.36	0/1571	0.61	0/2113
28	F	0.36	0/1434	0.74	2/1926 (0.1%)
29	G	0.34	0/1343	0.60	0/1816
30	H	0.23	0/1122	0.60	0/1515
31	J	0.36	0/1152	0.59	0/1551
32	K	0.43	0/947	0.71	0/1268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	L	0.39	0/1054	0.81	4/1403 (0.3%)
34	M	0.43	0/1093	0.72	0/1460
35	N	0.40	0/973	0.84	3/1301 (0.2%)
36	O	0.35	0/902	0.69	1/1209 (0.1%)
37	P	0.39	0/929	0.66	0/1242
38	Q	0.42	0/960	0.69	0/1278
39	R	0.35	0/829	0.71	0/1107
40	S	0.40	0/864	0.68	0/1156
41	T	0.31	0/744	0.64	0/994
42	U	0.34	0/787	0.71	0/1051
43	V	0.33	0/766	0.57	0/1025
44	W	0.87	0/599	1.22	4/792 (0.5%)
45	X	0.47	1/635 (0.2%)	0.60	0/848
46	Y	0.27	0/510	0.56	0/677
47	Z	0.36	0/453	0.63	0/605
48	0	0.39	0/450	0.67	0/599
49	1	0.34	0/416	0.62	0/554
50	2	0.47	0/380	0.73	0/498
51	3	0.48	0/513	0.84	1/676 (0.1%)
52	4	0.43	0/303	0.86	2/397 (0.5%)
53	6	0.28	0/531	0.64	0/709
54	x	0.44	1/1839 (0.1%)	0.78	11/2866 (0.4%)
55	7	0.25	0/1678	0.72	4/2262 (0.2%)
56	w	0.41	1/1470 (0.1%)	0.84	1/1992 (0.1%)
All	All	0.39	4/158958 (0.0%)	0.54	48/237412 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	b	0	3
3	c	0	2
5	e	0	1
6	f	0	1
7	g	0	1
9	i	0	1
11	k	0	1
12	l	0	2
13	m	0	1
17	q	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
19	s	0	1
21	u	0	1
28	F	0	2
29	G	0	2
31	J	0	1
34	M	0	2
39	R	0	1
42	U	0	4
51	3	0	1
55	7	0	1
56	w	0	3
All	All	0	35

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	x	74	C	O3'-P	-8.95	1.47	1.61
56	w	147	ALA	N-CA	8.12	1.56	1.46
19	s	39	ILE	C-N	-7.79	1.22	1.33
45	X	9	LYS	C-N	-7.32	1.20	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	x	73	A	OP1-P-O3'	-11.30	74.09	108.00
54	x	73	A	OP2-P-O3'	-10.69	75.92	108.00
55	7	132	GLY	C-N-CD	-9.65	85.44	125.00
55	7	139	ASN	C-N-CD	-9.47	86.17	125.00
55	7	134	ARG	N-CA-C	-8.20	102.28	111.14
54	x	74	C	OP1-P-OP2	7.43	141.90	119.60
5	e	121	ASN	CA-C-N	7.36	135.22	121.97
5	e	121	ASN	C-N-CA	7.36	135.22	121.97
54	x	74	C	C4'-C3'-O3'	-6.56	103.16	113.00
56	w	146	THR	O-C-N	-6.51	113.94	122.59
52	4	36	ARG	CA-C-N	6.50	133.95	121.54
52	4	36	ARG	C-N-CA	6.50	133.95	121.54
44	W	83	GLU	CA-C-N	-6.46	113.93	123.11
44	W	83	GLU	C-N-CA	-6.46	113.93	123.11
12	l	75	GLU	CA-C-N	6.38	131.21	120.81
12	l	75	GLU	C-N-CA	6.38	131.21	120.81
51	3	31	ILE	N-CA-C	6.23	122.31	109.34
54	x	73	A	P-O3'-C3'	5.97	129.16	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	x	73	A	C2'-C3'-O3'	5.94	122.61	113.70
54	x	35	G	C2'-C3'-O3'	5.77	122.35	113.70
36	O	31	THR	N-CA-C	-5.69	101.65	108.25
44	W	19	LYS	N-CA-C	5.67	119.94	113.19
28	F	19	PHE	CA-C-N	5.62	130.39	122.46
28	F	19	PHE	C-N-CA	5.62	130.39	122.46
55	7	137	MET	C-N-CD	-5.51	102.41	125.00
23	A	1378	A	P-O3'-C3'	5.46	128.39	120.20
33	L	93	ASN	CA-C-N	5.40	131.86	121.54
33	L	93	ASN	C-N-CA	5.40	131.86	121.54
54	x	35	G	C3'-C2'-O2'	5.37	118.75	110.70
54	x	24	G	P-O3'-C3'	5.35	128.22	120.20
6	f	53	LYS	N-CA-C	5.32	122.12	110.80
23	A	1930	G	P-O3'-C3'	5.24	128.06	120.20
7	g	128	GLU	CA-C-N	5.19	131.45	121.54
7	g	128	GLU	C-N-CA	5.19	131.45	121.54
35	N	2	ARG	N-CA-C	5.16	118.32	111.30
54	x	3	G	P-O3'-C3'	5.16	127.94	120.20
23	A	1378	A	C4'-C3'-O3'	5.15	117.12	109.40
33	L	100	ILE	CA-C-N	-5.13	117.68	122.66
33	L	100	ILE	C-N-CA	-5.13	117.68	122.66
44	W	39	ARG	N-CA-C	-5.11	100.20	108.52
23	A	242	G	P-O3'-C3'	5.10	127.84	120.20
10	j	57	VAL	CA-C-N	5.09	131.26	121.54
10	j	57	VAL	C-N-CA	5.09	131.26	121.54
23	A	1022	G	P-O3'-C3'	5.08	127.81	120.20
35	N	1	MET	CA-C-N	5.03	129.55	122.46
35	N	1	MET	C-N-CA	5.03	129.55	122.46
23	A	2655	G	P-O3'-C3'	5.02	127.73	120.20
54	x	67	U	P-O3'-C3'	5.01	127.72	120.20

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	3	30	HIS	Peptide
55	7	66	PRO	Peptide
28	F	173	ASP	Peptide
28	F	174	PHE	Peptide
29	G	118	ALA	Peptide
29	G	46	ASP	Peptide
31	J	81	ILE	Peptide

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Mol	Chain	Res	Type	Group
34	M	57	VAL	Peptide
34	M	58	LYS	Peptide
39	R	53	PHE	Peptide
42	U	5	ARG	Peptide
42	U	87	GLU	Peptide
42	U	88	ASP	Peptide
42	U	97	SER	Peptide
2	b	15	PHE	Peptide
2	b	18	GLN	Peptide
2	b	30	ILE	Peptide
3	c	95	GLY	Peptide
3	c	96	VAL	Peptide
5	e	120	HIS	Peptide
6	f	52	ASN	Peptide
7	g	63	VAL	Peptide
9	i	56	MET	Peptide
11	k	124	LYS	Peptide
12	l	101	LEU	Peptide
12	l	42	LYS	Peptide
13	m	4	ALA	Peptide
17	q	48	GLU	Peptide
17	q	67	SER	Peptide
17	q	69	THR	Peptide
19	s	3	SER	Peptide
21	u	33	ARG	Peptide
56	w	105	LYS	Peptide
56	w	123	ILE	Peptide
56	w	66	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	33016	0	16617	165	0
2	b	1704	0	1732	22	0
3	c	1624	0	1699	19	0
4	d	1643	0	1710	35	0
5	e	1141	0	1170	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	f	817	0	808	15	0
7	g	1181	0	1240	17	0
8	h	979	0	1034	11	0
9	i	1022	0	1070	16	0
10	j	786	0	828	18	0
11	k	869	0	878	21	0
12	l	955	0	1019	13	0
13	m	883	0	944	13	0
14	n	799	0	841	13	0
15	o	714	0	737	7	0
16	p	649	0	666	17	0
17	q	648	0	691	9	0
18	r	504	0	502	7	0
19	s	637	0	665	10	0
20	t	665	0	714	14	0
21	u	495	0	486	6	0
22	v	126	0	67	1	0
23	A	61641	0	31003	254	0
24	B	2572	0	1302	8	0
25	C	2082	0	2157	27	0
26	D	1565	0	1616	21	0
27	E	1552	0	1619	21	0
28	F	1410	0	1447	20	0
29	G	1323	0	1374	16	0
30	H	1111	0	1148	13	0
31	J	1129	0	1162	19	0
32	K	938	0	1012	21	0
33	L	1045	0	1117	20	0
34	M	1074	0	1157	18	0
35	N	960	0	1000	15	0
36	O	892	0	923	9	0
37	P	917	0	965	13	0
38	Q	947	0	1022	13	0
39	R	816	0	839	6	0
40	S	857	0	922	16	0
41	T	738	0	807	7	0
42	U	779	0	834	9	0
43	V	753	0	780	4	0
44	W	592	0	607	55	0
45	X	625	0	655	7	0
46	Y	509	0	543	7	0
47	Z	449	0	491	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	0	444	0	461	7	0
49	1	409	0	440	4	0
50	2	377	0	418	10	0
51	3	504	0	574	5	0
52	4	302	0	343	8	0
53	6	522	0	522	5	0
54	x	1646	0	830	22	0
55	7	1663	0	1742	124	0
56	w	1461	0	1421	38	0
57	A	7	0	7	2	0
57	x	7	0	7	1	0
All	All	146475	0	99385	1105	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 5.

All (1105) 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)
55:7:139:ASN:HB3	55:7:145:VAL:CG1	1.34	1.50
55:7:139:ASN:CB	55:7:145:VAL:CG1	1.91	1.44
55:7:139:ASN:HB2	55:7:145:VAL:CB	1.61	1.28
55:7:139:ASN:CB	55:7:145:VAL:HG11	1.57	1.21
55:7:137:MET:N	55:7:138:PRO:HD3	1.52	1.16
23:A:2169:A:O2'	55:7:134:ARG:NE	1.79	1.14
55:7:139:ASN:CB	55:7:145:VAL:CB	2.22	1.13
56:w:27:SER:OG	56:w:29:PHE:HE1	1.31	1.13
55:7:57:GLN:HA	55:7:202:THR:HG21	1.28	1.13
55:7:118:PRO:HD2	55:7:148:ASN:OD1	1.45	1.13
55:7:137:MET:H	55:7:138:PRO:CD	1.63	1.11
55:7:66:PRO:O	55:7:189:LEU:HD21	1.49	1.10
44:W:77:ARG:O	44:W:78:LYS:C	1.92	1.09
44:W:25:ARG:HD3	44:W:29:GLU:OE2	1.51	1.09
55:7:139:ASN:CB	55:7:145:VAL:HB	1.79	1.09
55:7:137:MET:N	55:7:138:PRO:CD	2.16	1.08
55:7:65:LEU:O	55:7:160:GLN:OE1	1.70	1.08
44:W:40:GLN:NE2	44:W:57:HIS:O	1.86	1.07
55:7:121:MET:CE	55:7:146:THR:HG21	1.83	1.07
55:7:121:MET:HE2	55:7:146:THR:HG21	1.31	1.07
23:A:2169:A:H1'	55:7:134:ARG:NH1	1.70	1.07
55:7:56:ASP:O	55:7:202:THR:HB	1.53	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:x:51:A:N1	54:x:63:U:N3	2.05	1.04
55:7:201:PRO:CB	55:7:205:LYS:HE3	1.88	1.02
23:A:2169:A:O2'	55:7:134:ARG:CD	2.11	0.99
55:7:121:MET:CE	55:7:139:ASN:ND2	2.25	0.99
23:A:2169:A:H1'	55:7:134:ARG:CZ	1.92	0.98
44:W:66:LYS:O	44:W:82:ILE:HD13	1.62	0.98
55:7:57:GLN:CA	55:7:202:THR:HG21	1.93	0.98
55:7:139:ASN:HB2	55:7:145:VAL:HB	0.98	0.97
55:7:137:MET:H	55:7:138:PRO:HD3	0.79	0.95
55:7:121:MET:HE1	55:7:139:ASN:ND2	1.82	0.95
55:7:78:PHE:O	55:7:120:ALA:HB3	1.66	0.93
55:7:139:ASN:CB	55:7:145:VAL:HG12	1.95	0.93
55:7:66:PRO:O	55:7:189:LEU:CD2	2.19	0.90
44:W:68:LYS:HB2	44:W:68:LYS:NZ	1.84	0.90
55:7:57:GLN:HA	55:7:202:THR:CG2	2.00	0.90
44:W:41:ARG:HA	44:W:41:ARG:NE	1.87	0.90
54:x:51:A:N6	54:x:63:U:O4	2.04	0.89
44:W:41:ARG:HA	44:W:41:ARG:HE	1.36	0.89
55:7:78:PHE:O	55:7:120:ALA:CB	2.21	0.88
44:W:77:ARG:O	44:W:78:LYS:O	1.92	0.88
55:7:132:GLY:O	55:7:138:PRO:HD3	1.73	0.87
55:7:121:MET:HB3	56:w:90:PHE:CE2	2.09	0.87
24:B:12:C:C2	44:W:73:GLY:O	2.28	0.86
44:W:36:ILE:HG23	44:W:58:THR:HG22	1.58	0.86
23:A:2169:A:O2'	55:7:134:ARG:CZ	2.24	0.86
56:w:27:SER:OG	56:w:29:PHE:CE1	2.13	0.86
44:W:67:VAL:O	44:W:81:SER:O	1.95	0.84
55:7:201:PRO:HB3	55:7:205:LYS:HE3	1.58	0.84
55:7:121:MET:HE2	55:7:146:THR:CG2	2.07	0.83
55:7:133:PRO:HG3	55:7:138:PRO:CG	2.08	0.83
55:7:57:GLN:C	55:7:202:THR:HG21	2.04	0.83
55:7:65:LEU:HD21	55:7:193:LEU:HD21	1.59	0.83
23:A:2169:A:C1'	55:7:134:ARG:CZ	2.58	0.82
44:W:26:PHE:O	44:W:27:GLY:O	1.98	0.82
55:7:121:MET:HE2	55:7:139:ASN:ND2	1.91	0.82
44:W:50:ASN:O	44:W:62:LYS:HB2	1.78	0.81
55:7:133:PRO:HG3	55:7:138:PRO:HG2	1.63	0.80
55:7:139:ASN:CG	55:7:145:VAL:HG12	2.08	0.78
23:A:2169:A:C2'	55:7:134:ARG:CZ	2.62	0.78
54:x:71:C:O2'	56:w:30:VAL:HG13	1.83	0.78
54:x:52:G:N1	54:x:62:C:N3	2.30	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:7:67:HIS:N	55:7:160:GLN:OE1	2.17	0.77
55:7:139:ASN:HB2	55:7:145:VAL:CG1	1.89	0.77
1:a:128:G:H5'	17:q:5:ARG:HH22	1.50	0.76
26:D:5:VAL:H	26:D:32:ASN:HD21	1.33	0.76
44:W:36:ILE:HG23	44:W:58:THR:CG2	2.15	0.76
44:W:40:GLN:HE21	44:W:57:HIS:HB3	1.50	0.76
44:W:68:LYS:HB2	44:W:68:LYS:HZ3	1.48	0.76
44:W:40:GLN:HG3	44:W:42:GLY:O	1.85	0.75
11:k:87:GLY:H	11:k:113:THR:HG22	1.53	0.74
55:7:139:ASN:CG	55:7:145:VAL:CG1	2.61	0.74
1:a:76:G:H1	1:a:93:U:H3	1.36	0.73
55:7:201:PRO:HB3	55:7:205:LYS:CE	2.18	0.73
23:A:585:G:N7	38:Q:5:ARG:NH1	2.36	0.73
55:7:114:VAL:HB	55:7:137:MET:O	1.89	0.72
44:W:25:ARG:CD	44:W:29:GLU:OE2	2.35	0.72
55:7:132:GLY:O	55:7:137:MET:N	2.23	0.72
55:7:121:MET:O	56:w:90:PHE:CZ	2.43	0.72
22:v:14:C:O2	56:w:146:THR:O	2.07	0.71
1:a:618:C:N4	1:a:621:A:N7	2.39	0.71
1:a:1200:C:H5''	1:a:1201:A:H3'	1.73	0.70
29:G:34:ARG:HE	29:G:70:LEU:HD13	1.58	0.68
44:W:68:LYS:O	44:W:68:LYS:HG3	1.93	0.67
55:7:140:PRO:HB3	56:w:90:PHE:O	1.94	0.67
56:w:143:LYS:O	56:w:146:THR:OG1	2.11	0.67
23:A:774:G:H5''	25:C:47:ARG:HH21	1.59	0.67
55:7:119:ASP:OD1	55:7:119:ASP:N	2.26	0.67
55:7:121:MET:O	56:w:90:PHE:CE1	2.47	0.67
15:o:34:GLN:HB3	15:o:58:MET:HE1	1.77	0.66
44:W:36:ILE:CG2	44:W:58:THR:CG2	2.73	0.66
44:W:40:GLN:HE21	44:W:57:HIS:CB	2.08	0.66
1:a:664:G:H22	1:a:741:G:H1	1.42	0.66
9:i:33:SER:H	9:i:36:GLN:HE21	1.44	0.66
19:s:5:LYS:HG3	19:s:6:LYS:HG2	1.77	0.66
55:7:133:PRO:HG3	55:7:138:PRO:HG3	1.76	0.66
10:j:37:ARG:HB2	10:j:75:ASP:HB2	1.77	0.65
55:7:68:GLY:N	55:7:160:GLN:HE22	1.93	0.65
55:7:133:PRO:HA	55:7:136:LEU:HA	1.76	0.65
5:e:92:ARG:HB2	5:e:127:TYR:HB2	1.78	0.65
26:D:4:LEU:HD23	26:D:29:VAL:HG11	1.79	0.65
23:A:1310:G:H1'	23:A:1611:C:H5''	1.79	0.65
44:W:30:SER:HA	44:W:65:GLY:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:S:82:MET:HB2	40:S:98:LYS:HB2	1.78	0.65
55:7:140:PRO:CB	56:w:90:PHE:O	2.45	0.64
56:w:117:LEU:HA	56:w:122:PRO:HA	1.77	0.64
16:p:4:ILE:HG12	16:p:21:VAL:HG22	1.79	0.64
23:A:1901:A:H4'	25:C:252:LYS:HD3	1.80	0.64
55:7:57:GLN:HA	55:7:202:THR:CB	2.27	0.64
4:d:104:MET:HE1	4:d:172:VAL:HA	1.80	0.64
1:a:671:G:O2'	6:f:79:ARG:NH2	2.30	0.64
30:H:1:MET:N	30:H:20:ASN:OD1	2.31	0.64
56:w:152:LYS:HE3	56:w:166:LEU:HA	1.79	0.64
44:W:31:VAL:O	44:W:64:ASP:HA	1.97	0.64
19:s:62:THR:H	19:s:65:MET:HE3	1.63	0.63
23:A:2169:A:O2'	55:7:134:ARG:HD3	1.98	0.63
1:a:1086:U:H3	1:a:1099:G:H22	1.46	0.63
48:0:42:ILE:HG22	48:0:48:TYR:HB2	1.80	0.63
55:7:139:ASN:HB3	55:7:145:VAL:HG11	0.65	0.63
55:7:201:PRO:HB2	55:7:205:LYS:HE3	1.80	0.63
5:e:93:VAL:HG11	5:e:139:THR:HG22	1.79	0.63
10:j:80:THR:HG22	10:j:82:LYS:H	1.63	0.63
12:l:23:LEU:HB2	12:l:58:ASN:HD22	1.63	0.63
55:7:56:ASP:OD1	56:w:121:GLN:NE2	2.32	0.63
1:a:612:C:H42	1:a:629:A:H61	1.44	0.63
44:W:70:GLU:O	44:W:78:LYS:HA	1.98	0.62
4:d:103:ARG:HD2	4:d:167:PRO:HG2	1.81	0.62
34:M:50:ARG:HD3	34:M:65:ILE:HD11	1.82	0.62
12:l:113:ARG:HB2	12:l:118:VAL:HB	1.81	0.62
23:A:1093:G:O2'	23:A:1098:A:N6	2.32	0.62
6:f:10:VAL:HB	6:f:58:HIS:HB3	1.80	0.62
23:A:2108:A:H61	23:A:2181:U:H3	1.48	0.62
6:f:6:ILE:HB	6:f:62:MET:HB2	1.82	0.62
1:a:939:G:OP1	7:g:101:ARG:NH1	2.31	0.62
23:A:2032:G:N2	26:D:151:THR:OG1	2.33	0.61
54:x:53:G:HO2'	54:x:54:U:P	2.23	0.61
23:A:2469:A:N6	23:A:2481:G:O2'	2.33	0.61
23:A:243:U:OP1	51:3:7:ARG:NH1	2.33	0.61
30:H:39:ALA:HA	30:H:43:ASN:HB2	1.82	0.61
4:d:131:ILE:HG22	4:d:133:SER:H	1.63	0.61
41:T:23:ALA:HB1	41:T:29:THR:HB	1.82	0.61
23:A:2683:C:OP1	37:P:50:ARG:NH2	2.34	0.61
23:A:2585:U:O4	57:A:3001:PRO:HB3	2.00	0.61
44:W:40:GLN:CD	44:W:57:HIS:O	2.44	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:w:27:SER:CB	56:w:29:PHE:HE1	2.13	0.61
16:p:53:ASP:OD2	16:p:56:ARG:N	2.33	0.60
20:t:4:LYS:HG3	20:t:6:ALA:H	1.65	0.60
47:Z:10:ARG:NH2	47:Z:52:PHE:O	2.34	0.60
52:4:2:LYS:NZ	52:4:32:LYS:O	2.34	0.60
8:h:42:GLU:HG2	8:h:100:ILE:HG12	1.82	0.60
55:7:65:LEU:HD12	55:7:162:ARG:HD2	1.83	0.60
1:a:1081:A:OP2	5:e:51:LYS:NZ	2.34	0.60
23:A:910:A:H62	34:M:12:MET:HA	1.65	0.60
23:A:1907:G:N2	54:x:13:C:OP1	2.35	0.60
31:J:102:GLU:HG3	31:J:119:PHE:HZ	1.66	0.60
19:s:35:ARG:NH2	19:s:74:ALA:O	2.34	0.60
15:o:88:ARG:NH2	23:A:714:U:OP2	2.35	0.60
23:A:1326:U:HO2'	23:A:2010:G:HO2'	1.41	0.60
30:H:72:ILE:HB	30:H:108:VAL:HG22	1.84	0.60
55:7:129:GLN:HB3	56:w:75:LEU:HB2	1.84	0.60
1:a:1376:U:O4	7:g:9:ARG:NH1	2.35	0.60
28:F:134:GLN:NE2	28:F:149:ARG:O	2.35	0.60
43:V:42:LEU:HD13	43:V:47:VAL:HG21	1.83	0.60
55:7:56:ASP:O	55:7:202:THR:CB	2.40	0.60
10:j:40:ILE:HB	10:j:73:LEU:HB2	1.83	0.59
54:x:8:U:O2'	54:x:21:A:N1	2.33	0.59
23:A:1153:C:OP1	38:Q:91:ARG:NH2	2.34	0.59
50:2:24:THR:HG23	50:2:27:GLY:H	1.67	0.59
23:A:1475:G:O2'	23:A:1732:C:N4	2.35	0.59
44:W:40:GLN:CG	44:W:42:GLY:O	2.50	0.59
1:a:1279:G:OP1	10:j:9:ARG:NH2	2.33	0.59
11:k:23:HIS:HB3	11:k:30:ILE:HG23	1.83	0.59
44:W:69:PHE:CE1	44:W:80:ILE:HD13	2.37	0.59
23:A:370:G:O2'	23:A:424:G:OP1	2.19	0.59
25:C:70:LYS:NZ	25:C:99:GLU:OE1	2.36	0.59
28:F:116:LEU:HD13	28:F:175:PRO:HD2	1.83	0.59
48:0:27:LEU:HD23	48:0:36:LYS:HB3	1.84	0.59
1:a:311:C:OP1	16:p:31:ARG:NH1	2.35	0.59
1:a:345:C:OP1	37:P:38:ARG:NH2	2.36	0.59
25:C:145:MET:SD	25:C:181:ARG:NH2	2.75	0.59
55:7:68:GLY:O	55:7:69:THR:C	2.46	0.59
55:7:201:PRO:CG	55:7:205:LYS:HE3	2.33	0.59
1:a:40:C:H42	1:a:402:G:H1	1.51	0.58
1:a:993:G:O2'	1:a:994:A:N7	2.36	0.58
6:f:63:ASN:HD21	6:f:96:VAL:HG23	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:W:82:ILE:HG22	44:W:82:ILE:O	2.03	0.58
55:7:121:MET:HE1	55:7:139:ASN:O	2.02	0.58
2:b:9:LEU:HD21	2:b:13:VAL:HG22	1.85	0.58
23:A:1012:U:OP2	38:Q:69:ARG:NH1	2.35	0.58
1:a:264:C:H4'	17:q:64:ARG:HD2	1.84	0.58
19:s:10:ILE:HD13	19:s:15:LEU:HB2	1.85	0.58
36:O:40:ILE:HG12	36:O:47:VAL:HG12	1.85	0.58
44:W:71:VAL:HG23	44:W:71:VAL:O	2.04	0.58
23:A:563:A:N3	38:Q:36:GLN:NE2	2.51	0.58
23:A:1936:A:H2	23:A:1943:U:H3	1.52	0.58
44:W:36:ILE:CG2	44:W:58:THR:HG22	2.31	0.58
56:w:39:ALA:O	56:w:41:VAL:HG23	2.04	0.58
26:D:148:GLN:HB2	26:D:152:PRO:HG2	1.86	0.58
27:E:117:ARG:NH2	27:E:183:PHE:O	2.36	0.58
32:K:69:VAL:HG21	32:K:104:THR:HG21	1.85	0.58
16:p:48:GLU:HG2	16:p:51:ARG:HE	1.67	0.58
44:W:25:ARG:HD2	44:W:31:VAL:HG12	1.86	0.58
3:c:171:ARG:NH2	3:c:205:GLU:OE2	2.37	0.58
1:a:462:G:N2	1:a:471:U:O2	2.37	0.57
4:d:155:LYS:NZ	4:d:177:MET:SD	2.73	0.57
9:i:35:GLU:HA	9:i:39:GLY:HA3	1.85	0.57
53:6:20:ASN:ND2	53:6:37:CYS:SG	2.73	0.57
2:b:91:VAL:HG11	2:b:95:TRP:HD1	1.69	0.57
23:A:2478:A:H5'	52:4:32:LYS:HE3	1.84	0.57
54:x:53:G:O2'	54:x:54:U:P	2.62	0.57
55:7:121:MET:HE1	55:7:139:ASN:CG	2.28	0.57
1:a:263:A:OP1	20:t:73:ARG:NH1	2.37	0.57
23:A:1533:C:O2	23:A:1538:G:N2	2.36	0.57
32:K:43:ILE:HD12	32:K:56:ASP:HB2	1.84	0.57
44:W:38:VAL:O	44:W:58:THR:HA	2.03	0.57
50:2:34:ARG:HE	50:2:39:ARG:HD2	1.70	0.57
1:a:1319:A:H5''	19:s:69:LYS:HE3	1.87	0.57
23:A:2168:G:N1	23:A:2171:A:OP2	2.38	0.57
28:F:104:THR:HA	53:6:38:SER:HB3	1.86	0.57
55:7:200:LYS:C	55:7:200:LYS:HE2	2.30	0.57
30:H:38:PRO:O	30:H:43:ASN:ND2	2.36	0.57
30:H:78:VAL:HB	30:H:144:VAL:HA	1.86	0.57
1:a:176:C:OP1	20:t:23:ARG:NH1	2.34	0.57
23:A:704:G:O2'	23:A:726:G:N2	2.37	0.57
44:W:29:GLU:HG2	44:W:29:GLU:O	2.03	0.57
55:7:121:MET:CE	55:7:139:ASN:O	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:0:37:HIS:ND1	48:0:38:LEU:O	2.34	0.57
3:c:13:ILE:HG22	3:c:14:VAL:HG23	1.87	0.57
3:c:39:ARG:HG3	3:c:54:ILE:HD11	1.86	0.56
27:E:148:ILE:HB	27:E:169:VAL:HG22	1.87	0.56
35:N:22:ARG:HG3	35:N:70:THR:HA	1.87	0.56
39:R:14:VAL:HG23	39:R:18:GLN:HE21	1.70	0.56
2:b:12:GLY:H	2:b:211:LEU:HD22	1.70	0.56
21:u:40:PRO:HA	21:u:43:GLU:HG2	1.87	0.56
23:A:355:U:H2'	23:A:356:G:H8	1.71	0.56
23:A:1056:G:O2'	23:A:1103:A:N6	2.37	0.56
56:w:34:KEO:O02	56:w:34:KEO:N02	2.38	0.56
8:h:28:SER:HB3	8:h:56:PRO:HB2	1.87	0.56
23:A:2199:A:OP1	45:X:36:ARG:NH2	2.38	0.56
31:J:31:GLU:HG2	31:J:142:ILE:HG12	1.87	0.56
23:A:1171:G:N2	23:A:1178:C:N3	2.54	0.56
23:A:1607:C:N4	23:A:1622:G:OP2	2.32	0.56
25:C:106:PRO:HD2	25:C:109:LEU:HD22	1.87	0.56
1:a:429:U:O2'	4:d:21:LYS:NZ	2.38	0.56
1:a:692:U:H5''	11:k:126:ARG:HH22	1.69	0.56
15:o:31:LEU:HD22	15:o:58:MET:HB2	1.86	0.56
23:A:2:G:O6	23:A:2900:A:N6	2.38	0.56
23:A:2263:C:N4	44:W:15:ASP:OD1	2.36	0.56
1:a:559:A:H4'	1:a:560:A:H3'	1.87	0.56
1:a:1405:G:H21	1:a:1518:A:H8	1.54	0.56
1:a:448:A:H62	1:a:486:U:H3	1.51	0.56
27:E:97:ASN:ND2	27:E:100:MET:SD	2.79	0.56
55:7:67:HIS:C	55:7:160:GLN:HE22	2.13	0.56
20:t:30:PHE:HD2	20:t:56:ILE:HG21	1.70	0.56
1:a:1180:A:OP2	9:i:98:ARG:NH2	2.39	0.56
23:A:475:C:O2	23:A:479:A:N6	2.34	0.56
23:A:775:G:H4'	23:A:776:G:H5'	1.88	0.56
1:a:406:G:H21	4:d:115:GLN:HE22	1.54	0.55
23:A:2539:C:H5'	52:4:3:VAL:HG21	1.88	0.55
30:H:65:ALA:O	30:H:69:ALA:N	2.39	0.55
4:d:14:GLU:OE2	4:d:55:ARG:NH1	2.39	0.55
23:A:2029:G:N1	23:A:2033:A:OP2	2.33	0.55
33:L:95:LEU:HD11	33:L:125:LEU:HD21	1.88	0.55
34:M:102:LEU:HD11	34:M:126:ILE:HD11	1.87	0.55
55:7:118:PRO:HD2	55:7:148:ASN:CG	2.27	0.55
55:7:139:ASN:HB3	55:7:145:VAL:CB	2.04	0.55
55:7:181:ASP:HB2	55:7:186:LYS:HE3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:356:A:N3	1:a:368:U:O2'	2.34	0.55
5:e:79:THR:HA	5:e:121:ASN:HD22	1.71	0.55
13:m:15:VAL:HG23	13:m:16:ILE:HD12	1.88	0.55
23:A:227:A:H61	23:A:410:G:H21	1.54	0.55
4:d:84:ASN:O	4:d:88:ASN:ND2	2.39	0.55
14:n:45:VAL:O	14:n:49:GLN:NE2	2.40	0.55
16:p:52:LEU:HD22	16:p:78:VAL:HG13	1.89	0.55
23:A:466:A:OP1	50:2:34:ARG:NH1	2.39	0.55
55:7:65:LEU:O	55:7:160:GLN:CB	2.55	0.55
44:W:51:VAL:HG23	44:W:82:ILE:HG13	1.88	0.55
1:a:1003:G:N2	1:a:1004:A:O2'	2.40	0.55
1:a:1458:G:H5'	20:t:26:MET:HB3	1.88	0.55
10:j:8:ILE:HG12	10:j:100:ILE:HG22	1.89	0.55
13:m:24:VAL:HG23	13:m:28:ARG:HB3	1.89	0.55
15:o:35:ILE:HG13	15:o:58:MET:HE2	1.88	0.55
33:L:62:PRO:HB2	51:3:29:ARG:HH11	1.71	0.55
34:M:20:LEU:HD23	43:V:81:PRO:HG2	1.89	0.55
23:A:112:U:H5'	46:Y:58:ASN:HD21	1.72	0.55
23:A:2169:A:C1'	55:7:134:ARG:NH2	2.70	0.55
1:a:297:G:N2	1:a:300:A:OP2	2.39	0.55
23:A:2069:A:H61	23:A:2442:C:H42	1.55	0.55
24:B:12:C:N3	44:W:73:GLY:O	2.39	0.55
44:W:68:LYS:HD3	44:W:70:GLU:HG3	1.88	0.54
4:d:171:GLU:HB3	4:d:180:THR:HB	1.89	0.54
7:g:68:VAL:HG23	7:g:99:ALA:HB1	1.89	0.54
23:A:1866:A:N6	23:A:1875:G:O2'	2.40	0.54
23:A:2266:A:N6	23:A:2273:A:OP2	2.39	0.54
44:W:66:LYS:HD3	44:W:66:LYS:N	2.21	0.54
1:a:9:G:H4'	5:e:108:GLY:H	1.71	0.54
1:a:522:C:H41	12:l:49:ARG:HH22	1.55	0.54
1:a:684:U:H1'	11:k:39:ASN:HB2	1.88	0.54
1:a:1178:G:N2	1:a:1181:G:OP2	2.39	0.54
23:A:2820:A:OP2	23:A:2821:A:N6	2.33	0.54
42:U:6:ARG:NH2	42:U:25:LYS:O	2.40	0.54
56:w:29:PHE:N	56:w:29:PHE:CD1	2.73	0.54
6:f:2:ARG:HD2	6:f:92:THR:HG21	1.88	0.54
14:n:69:ARG:NH1	14:n:71:HIS:O	2.41	0.54
23:A:2076:U:OP2	23:A:2238:G:N2	2.35	0.54
1:a:195:A:N3	1:a:222:C:O2'	2.39	0.54
1:a:379:C:N4	1:a:380:G:O6	2.40	0.54
3:c:72:PRO:HG3	3:c:104:GLU:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:84:ASN:ND2	4:d:87:GLU:OE1	2.40	0.54
23:A:476:G:N1	23:A:479:A:OP2	2.39	0.54
25:C:257:ARG:NH1	25:C:263:ASP:OD1	2.41	0.54
55:7:121:MET:HB3	56:w:90:PHE:CD2	2.43	0.54
56:w:75:LEU:HD12	56:w:76:TYR:HB2	1.89	0.54
20:t:38:ILE:HD11	20:t:82:ILE:HG22	1.89	0.54
23:A:2848:G:O2'	23:A:2868:A:N6	2.41	0.54
24:B:66:A:H61	24:B:107:G:H2'	1.73	0.54
28:F:115:GLY:HA3	28:F:177:ARG:HB2	1.90	0.54
26:D:35:THR:HG22	26:D:73:VAL:HG21	1.89	0.54
52:4:30:GLU:HG3	52:4:32:LYS:H	1.72	0.54
1:a:544:G:OP1	4:d:55:ARG:NH2	2.40	0.53
23:A:2032:G:N2	26:D:151:THR:HG1	2.05	0.53
23:A:2682:A:H61	23:A:2728:U:H1'	1.72	0.53
30:H:43:ASN:HA	30:H:46:PHE:HB2	1.89	0.53
55:7:48:LEU:HD11	55:7:197:LYS:HD3	1.90	0.53
56:w:44:ARG:NH1	56:w:50:THR:O	2.39	0.53
5:e:54:GLU:HG2	5:e:56:PRO:HD2	1.89	0.53
36:O:43:ASN:HD21	36:O:46:GLU:HG2	1.72	0.53
11:k:84:MET:SD	11:k:110:THR:OG1	2.60	0.53
23:A:1980:G:O2'	23:A:1982:U:OP2	2.26	0.53
1:a:254:G:O2'	17:q:17:GLU:O	2.25	0.53
21:u:16:ARG:HH21	21:u:19:LYS:HG2	1.72	0.53
23:A:200:U:O2	23:A:386:G:N2	2.41	0.53
23:A:495:G:O2'	40:S:57:ASN:ND2	2.41	0.53
44:W:77:ARG:C	44:W:78:LYS:O	2.50	0.53
1:a:1098:C:OP1	2:b:138:ARG:NH2	2.42	0.53
5:e:79:THR:OG1	5:e:97:PRO:O	2.26	0.53
13:m:76:ILE:HG22	13:m:80:MET:HE2	1.90	0.53
16:p:46:LYS:NZ	16:p:48:GLU:O	2.34	0.53
23:A:1032:A:H1'	52:4:23:ILE:HD13	1.90	0.53
54:x:62:C:H2'	54:x:63:U:C6	2.44	0.53
1:a:2:A:N3	1:a:613:C:O2'	2.40	0.53
2:b:15:PHE:HB2	2:b:39:ILE:HG12	1.91	0.53
17:q:30:HIS:HD2	17:q:33:TYR:H	1.54	0.53
31:J:17:VAL:HG23	31:J:137:PRO:HB2	1.90	0.53
32:K:102:PRO:HB3	32:K:121:GLU:HB3	1.91	0.53
55:7:121:MET:HE2	55:7:146:THR:CB	2.38	0.53
6:f:92:THR:OG1	6:f:93:LYS:N	2.38	0.53
11:k:71:ASP:HA	11:k:74:LYS:HG3	1.91	0.53
3:c:152:VAL:HG12	3:c:197:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:52:LEU:HB2	14:n:81:ARG:HD2	1.91	0.53
23:A:2458:G:O2'	23:A:2460:U:O4	2.27	0.53
26:D:179:ARG:HB3	26:D:188:LEU:HD12	1.91	0.53
55:7:67:HIS:H	55:7:160:GLN:CD	2.16	0.53
1:a:10:A:HO2'	1:a:507:C:HO2'	1.57	0.53
1:a:692:U:O2'	1:a:694:A:N7	2.35	0.53
1:a:951:G:OP2	13:m:100:ARG:NH2	2.38	0.53
23:A:1019:U:O2'	23:A:1021:A:N7	2.38	0.53
24:B:8:C:O3'	36:O:25:ARG:NH1	2.42	0.53
55:7:6:LYS:HD2	55:7:9:ARG:HB2	1.90	0.53
1:a:8:A:N6	4:d:201:GLU:O	2.38	0.52
13:m:2:ARG:HH11	28:F:109:ARG:HH22	1.57	0.52
23:A:674:G:H1'	27:E:69:ARG:HD3	1.91	0.52
23:A:1365:A:OP1	45:X:2:ARG:NH1	2.39	0.52
23:A:2016:U:O2	48:O:3:GLN:NE2	2.40	0.52
7:g:55:LYS:HB2	7:g:60:ALA:HB2	1.90	0.52
23:A:955:U:H5	23:A:962:G:H1	1.58	0.52
31:J:99:ARG:HA	31:J:102:GLU:HB3	1.91	0.52
33:L:78:ARG:HE	33:L:113:ALA:HB1	1.74	0.52
54:x:53:G:H8	54:x:53:G:H5''	1.73	0.52
55:7:129:GLN:O	55:7:133:PRO:HD2	2.08	0.52
32:K:13:ASN:HB3	32:K:100:PHE:HE2	1.74	0.52
32:K:88:ASN:ND2	32:K:93:GLN:O	2.42	0.52
33:L:17:LYS:HE3	33:L:27:LEU:HD22	1.91	0.52
34:M:53:MET:HB2	34:M:120:ALA:HB2	1.90	0.52
23:A:1064:C:N4	23:A:1069:A:OP2	2.43	0.52
23:A:2676:C:OP1	32:K:31:ARG:NH2	2.43	0.52
28:F:39:VAL:HG11	28:F:49:LEU:HD13	1.90	0.52
1:a:1380:U:O2	1:a:1382:C:N4	2.37	0.52
27:E:149:ILE:HD11	27:E:172:ALA:HA	1.92	0.52
31:J:35:ARG:HB2	31:J:54:ILE:HD11	1.92	0.52
44:W:18:ALA:O	44:W:20:ARG:NH1	2.40	0.52
55:7:121:MET:HG3	56:w:90:PHE:CD2	2.44	0.52
1:a:1123:U:O2'	10:j:39:PRO:O	2.27	0.52
23:A:2205:A:H61	23:A:2219:U:H3	1.57	0.52
33:L:95:LEU:HD22	33:L:100:ILE:HD11	1.92	0.52
16:p:35:ARG:NH2	16:p:37:GLY:O	2.43	0.52
23:A:1496:A:N3	23:A:1577:C:O2'	2.40	0.52
23:A:2125:G:H4'	55:7:218:MET:HE1	1.92	0.52
28:F:30:VAL:HG23	28:F:157:THR:HG22	1.91	0.52
2:b:187:ASP:OD1	2:b:188:THR:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:73:SER:OG	8:h:75:GLN:NE2	2.43	0.52
15:o:45:HIS:O	15:o:47:LYS:N	2.43	0.52
24:B:9:G:OP2	36:O:15:ARG:NH1	2.43	0.52
42:U:14:THR:OG1	42:U:68:ASN:ND2	2.42	0.52
56:w:45:ARG:HB2	56:w:49:GLY:HA2	1.91	0.52
56:w:152:LYS:NZ	56:w:168:VAL:O	2.39	0.52
1:a:127:G:O2'	17:q:5:ARG:NH2	2.43	0.52
1:a:460:A:H61	1:a:472:U:H3	1.57	0.52
1:a:972:C:OP2	10:j:59:LYS:NZ	2.40	0.52
44:W:12:ASN:OD1	44:W:12:ASN:N	2.43	0.52
1:a:1029:U:O2'	1:a:1033:G:N2	2.43	0.51
9:i:50:PRO:HD3	9:i:79:ARG:HG3	1.91	0.51
20:t:24:ARG:HG2	20:t:28:ARG:HH21	1.76	0.51
29:G:85:LYS:HG3	29:G:131:VAL:HG22	1.92	0.51
42:U:33:VAL:HG13	42:U:66:VAL:HG22	1.91	0.51
52:4:1:MET:HE3	52:4:34:LYS:HG2	1.92	0.51
2:b:53:LEU:HB3	2:b:219:THR:HG21	1.91	0.51
7:g:78:ARG:NH1	56:w:143:LYS:O	2.43	0.51
23:A:672:C:OP2	33:L:42:SER:OG	2.26	0.51
23:A:30:G:O2'	23:A:1214:A:N3	2.41	0.51
25:C:68:ARG:O	25:C:188:ARG:NH1	2.44	0.51
1:a:981:U:OP1	14:n:8:ARG:NH1	2.42	0.51
23:A:481:G:O2'	23:A:506:G:N2	2.43	0.51
25:C:120:ASP:HB2	30:H:91:PHE:HE1	1.76	0.51
34:M:33:LEU:HD13	34:M:117:PHE:HB3	1.91	0.51
54:x:51:A:N1	54:x:63:U:C4	2.78	0.51
23:A:1779:U:OP2	23:A:1784:A:N6	2.40	0.51
23:A:2768:U:O2'	31:J:95:ARG:NH2	2.43	0.51
4:d:59:LYS:HE3	4:d:194:ILE:HG22	1.91	0.51
6:f:29:ILE:HD13	6:f:64:VAL:HG21	1.93	0.51
8:h:45:ILE:HD13	8:h:60:LEU:HD22	1.93	0.51
14:n:39:GLU:HA	14:n:42:TRP:HB3	1.91	0.51
18:r:33:THR:HG23	18:r:35:SER:H	1.76	0.51
23:A:1275:A:OP2	23:A:1646:C:N4	2.43	0.51
54:x:53:G:O2'	54:x:54:U:OP1	2.27	0.51
55:7:68:GLY:N	55:7:160:GLN:NE2	2.59	0.51
1:a:766:A:OP2	1:a:812:G:N2	2.41	0.51
1:a:816:A:OP1	1:a:1526:G:O2'	2.28	0.51
1:a:842:U:O2'	1:a:845:A:OP1	2.26	0.51
3:c:91:ALA:HB1	3:c:96:VAL:HB	1.93	0.51
10:j:9:ARG:NH2	10:j:99:GLN:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:247:G:OP2	23:A:249:C:N4	2.44	0.51
23:A:1800:C:OP1	25:C:257:ARG:NH2	2.44	0.51
23:A:2394:C:H5''	33:L:63:LYS:HE3	1.93	0.51
38:Q:93:ILE:HD12	39:R:13:ARG:HB2	1.93	0.51
40:S:73:LYS:HB2	40:S:106:VAL:HB	1.92	0.51
7:g:67:ASN:O	7:g:137:ARG:NE	2.40	0.51
23:A:2638:G:O2'	23:A:2778:A:N6	2.43	0.51
26:D:77:ARG:NH2	26:D:200:ASP:OD1	2.43	0.51
28:F:9:ASP:OD1	28:F:9:ASP:N	2.44	0.51
44:W:40:GLN:O	44:W:40:GLN:HG2	2.09	0.51
3:c:120:THR:HG1	3:c:186:SER:HG	1.54	0.51
4:d:56:GLU:HG2	4:d:198:LEU:HB2	1.93	0.51
12:l:85:ARG:HH21	12:l:87:LYS:HA	1.76	0.51
23:A:910:A:N3	23:A:2264:C:O2'	2.41	0.51
23:A:1744:A:H3'	23:A:1745:A:H8	1.75	0.51
40:S:24:ILE:HD13	40:S:36:LEU:HD11	1.93	0.51
23:A:668:A:H2'	23:A:670:A:H62	1.75	0.51
34:M:110:GLU:OE2	34:M:114:ARG:NH1	2.43	0.51
35:N:90:ARG:HH12	35:N:116:VAL:HG11	1.76	0.51
49:1:4:ILE:HG23	49:1:27:ARG:HH21	1.75	0.51
1:a:7:A:H2'	5:e:123:LEU:HB3	1.93	0.50
1:a:201:G:O2'	1:a:469:C:O2'	2.23	0.50
1:a:1346:A:OP1	9:i:121:ARG:NH1	2.42	0.50
23:A:514:A:N3	23:A:581:C:O2'	2.40	0.50
23:A:770:G:H5''	50:2:10:LEU:HD23	1.93	0.50
23:A:764:A:H5''	25:C:208:GLY:HA3	1.93	0.50
25:C:143:VAL:HB	25:C:153:LEU:HB2	1.93	0.50
35:N:24:MET:HE3	35:N:44:LEU:HD22	1.93	0.50
46:Y:20:ASN:HB3	46:Y:50:VAL:HG22	1.93	0.50
1:a:51:A:N7	1:a:114:U:O2'	2.44	0.50
4:d:71:PHE:HE1	4:d:93:LEU:HD11	1.77	0.50
4:d:79:ALA:HA	4:d:85:THR:HG23	1.92	0.50
4:d:187:ARG:O	4:d:187:ARG:NH1	2.39	0.50
17:q:22:VAL:HG11	17:q:60:ILE:HD11	1.94	0.50
18:r:70:THR:HG23	18:r:72:ARG:H	1.75	0.50
23:A:301:G:OP2	42:U:81:ARG:NH1	2.44	0.50
55:7:65:LEU:CD1	55:7:162:ARG:HD2	2.41	0.50
40:S:59:GLU:HA	40:S:64:ALA:HA	1.94	0.50
41:T:8:LEU:HD23	41:T:50:LEU:HD21	1.92	0.50
52:4:25:VAL:HG21	52:4:35:GLN:HE21	1.77	0.50
55:7:137:MET:N	55:7:138:PRO:HD2	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:437:U:OP1	4:d:151:GLN:NE2	2.44	0.50
23:A:1380:G:O2'	23:A:1569:A:N6	2.44	0.50
23:A:2822:G:H5''	26:D:164:GLN:HE22	1.76	0.50
52:4:25:VAL:HB	52:4:35:GLN:HG2	1.93	0.50
1:a:768:A:N3	1:a:1512:U:O2'	2.44	0.50
1:a:976:G:OP2	1:a:1358:U:O2'	2.27	0.50
1:a:1055:A:N3	3:c:155:ARG:NH1	2.58	0.50
10:j:71:LEU:O	10:j:72:ARG:NH1	2.43	0.50
16:p:53:ASP:OD2	16:p:55:ASP:N	2.42	0.50
23:A:249:C:O2'	33:L:63:LYS:NZ	2.35	0.50
23:A:2722:G:O2'	35:N:3:HIS:O	2.28	0.50
29:G:51:PHE:HZ	29:G:71:LEU:HD22	1.77	0.50
37:P:105:LYS:O	37:P:108:ARG:NH2	2.44	0.50
49:l:27:ARG:O	55:7:141:LYS:NZ	2.40	0.50
1:a:927:G:O2'	1:a:1503:A:N7	2.42	0.50
12:l:109:ARG:HB2	12:l:118:VAL:HG21	1.94	0.50
14:n:64:CYS:HB3	14:n:69:ARG:H	1.77	0.50
20:t:23:ARG:HH21	20:t:60:GLN:HE22	1.59	0.50
23:A:210:C:OP1	50:2:29:GLN:NE2	2.45	0.50
23:A:1799:G:N2	23:A:1818:U:O2'	2.44	0.50
23:A:2508:G:H1	23:A:2580:U:H5	1.59	0.50
1:a:1381:U:H1'	7:g:77:ARG:HH22	1.76	0.50
23:A:2618:G:H21	26:D:155:VAL:HG21	1.76	0.50
27:E:189:THR:HG22	27:E:191:ASP:H	1.77	0.50
29:G:8:VAL:HB	29:G:49:LEU:HD12	1.94	0.50
1:a:35:G:O2'	12:l:114:SER:O	2.28	0.50
11:k:127:ARG:HB2	21:u:34:ARG:HH22	1.76	0.50
28:F:58:ALA:HB1	28:F:139:GLU:HB3	1.94	0.50
54:x:23:C:H2'	54:x:24:G:C8	2.47	0.50
23:A:1030:C:OP2	34:M:127:LYS:NZ	2.45	0.49
25:C:81:GLU:HB2	25:C:90:ILE:HG13	1.94	0.49
44:W:26:PHE:C	44:W:27:GLY:O	2.52	0.49
55:7:66:PRO:C	55:7:160:GLN:OE1	2.55	0.49
23:A:663:G:H5''	33:L:17:LYS:HD3	1.94	0.49
23:A:981:A:OP2	23:A:982:C:N4	2.43	0.49
23:A:1129:A:O2'	23:A:2515:C:O2	2.27	0.49
1:a:690:G:O6	11:k:52:ARG:NH2	2.45	0.49
23:A:2169:A:C2'	55:7:134:ARG:NE	2.71	0.49
29:G:88:LEU:HD23	29:G:93:TYR:HB3	1.94	0.49
38:Q:49:ARG:O	38:Q:53:LYS:NZ	2.44	0.49
1:a:151:A:H62	1:a:170:U:H3	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:165:ALA:HB3	2:b:190:SER:HB3	1.93	0.49
4:d:57:LYS:HD3	4:d:202:LEU:HD22	1.94	0.49
23:A:882:G:N2	23:A:895:U:O2'	2.44	0.49
23:A:2471:A:N6	23:A:2476:A:O2'	2.46	0.49
1:a:493:A:N6	1:a:494:G:H21	2.10	0.49
1:a:690:G:OP2	11:k:28:ASN:ND2	2.33	0.49
1:a:1216:A:H5''	14:n:4:SER:HB3	1.93	0.49
1:a:1281:C:H5''	1:a:1282:C:H5	1.77	0.49
23:A:987:C:O2'	23:A:1000:A:N3	2.39	0.49
23:A:1009:A:N3	23:A:1153:C:O2'	2.39	0.49
1:a:626:G:H2'	1:a:627:G:H8	1.77	0.49
2:b:70:GLY:HA3	2:b:79:VAL:HG21	1.93	0.49
23:A:139:U:H2'	23:A:140:C:H5	1.78	0.49
23:A:1187:G:OP1	39:R:85:LYS:NZ	2.37	0.49
32:K:105:ARG:NH2	37:P:33:GLU:OE2	2.46	0.49
1:a:509:A:N3	1:a:543:U:O2'	2.45	0.49
1:a:769:G:H4'	1:a:1513:A:H4'	1.94	0.49
23:A:2514:U:H5''	31:J:81:ILE:HD11	1.95	0.49
36:O:2:ASP:OD2	36:O:5:SER:N	2.39	0.49
44:W:25:ARG:HG2	44:W:25:ARG:HH11	1.77	0.49
55:7:68:GLY:O	55:7:69:THR:O	2.30	0.49
56:w:47:LEU:HG	56:w:123:ILE:HG21	1.94	0.49
4:d:69:ARG:O	4:d:73:ASN:ND2	2.46	0.49
4:d:201:GLU:OE1	5:e:111:ARG:NH2	2.30	0.49
6:f:38:ARG:NH1	6:f:98:GLU:OE2	2.46	0.49
9:i:20:ILE:HD11	9:i:60:LEU:HD13	1.95	0.49
12:l:101:LEU:O	12:l:103:CYS:N	2.45	0.49
17:q:8:GLN:NE2	17:q:59:GLU:OE2	2.44	0.49
19:s:68:HIS:HE1	53:6:56:ARG:HH22	1.60	0.49
56:w:156:LEU:HD23	56:w:160:ALA:HB3	1.94	0.49
1:a:1112:C:H1'	3:c:178:ARG:HE	1.76	0.49
2:b:120:SER:HA	2:b:125:PHE:HB3	1.95	0.49
11:k:93:GLU:OE2	11:k:97:ARG:NH1	2.46	0.49
31:J:118:MET:HA	31:J:121:LYS:HD3	1.94	0.49
34:M:42:THR:HG22	34:M:93:VAL:HG12	1.94	0.49
35:N:73:ASN:HA	35:N:76:VAL:HG12	1.95	0.49
55:7:6:LYS:HE3	55:7:9:ARG:HH21	1.78	0.49
10:j:59:LYS:HE2	10:j:62:ARG:HH21	1.78	0.49
23:A:2092:U:OP1	23:A:2199:A:O2'	2.27	0.49
23:A:2405:G:O2'	23:A:2411:A:N6	2.46	0.49
23:A:2627:G:N2	23:A:2777:G:OP2	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:45:G:H5'	23:A:46:G:H5'	1.95	0.48
23:A:2278:A:H8	44:W:12:ASN:HD22	1.61	0.48
23:A:2349:G:OP1	51:3:44:ARG:NH2	2.46	0.48
41:T:70:HIS:N	41:T:73:ARG:O	2.43	0.48
1:a:264:C:O2'	17:q:65:PRO:O	2.30	0.48
20:t:67:HIS:O	20:t:67:HIS:ND1	2.47	0.48
21:u:16:ARG:HB2	21:u:19:LYS:HD3	1.94	0.48
23:A:1826:G:O2'	23:A:1971:U:OP2	2.31	0.48
2:b:72:LYS:NZ	2:b:203:ASP:OD2	2.47	0.48
28:F:56:LEU:HD13	28:F:88:VAL:HG23	1.95	0.48
34:M:47:GLU:OE2	34:M:51:ARG:NE	2.46	0.48
40:S:56:ALA:HA	40:S:59:GLU:HG2	1.94	0.48
44:W:25:ARG:HG2	44:W:25:ARG:NH1	2.28	0.48
23:A:1021:A:H61	23:A:1142:A:H61	1.61	0.48
23:A:2175:C:H2'	23:A:2176:A:H8	1.78	0.48
32:K:76:VAL:H	37:P:72:VAL:HG22	1.77	0.48
4:d:12:ARG:NH1	4:d:36:ALA:O	2.47	0.48
5:e:110:MET:HG3	5:e:139:THR:HG21	1.95	0.48
10:j:8:ILE:HB	10:j:74:VAL:HB	1.94	0.48
11:k:92:ARG:NH2	11:k:111:ASP:OD1	2.46	0.48
23:A:239:C:HO2'	23:A:622:G:HO2'	1.61	0.48
23:A:286:U:H2'	23:A:287:G:H8	1.78	0.48
23:A:1653:G:H3'	35:N:2:ARG:HG2	1.95	0.48
33:L:76:GLU:HB2	33:L:111:ILE:HD13	1.94	0.48
37:P:63:ILE:HA	37:P:68:GLY:HA2	1.95	0.48
2:b:56:LEU:HD13	2:b:216:VAL:HG13	1.96	0.48
7:g:4:ARG:HB3	7:g:6:ILE:HG23	1.94	0.48
23:A:805:G:N2	23:A:829:A:OP1	2.46	0.48
31:J:60:ASP:OD1	31:J:60:ASP:N	2.45	0.48
40:S:88:ARG:NH2	40:S:94:ASP:OD2	2.46	0.48
54:x:12:G:O2'	54:x:13:C:O4'	2.32	0.48
55:7:67:HIS:CA	55:7:160:GLN:HE22	2.27	0.48
1:a:111:G:O2'	1:a:389:A:O2'	2.30	0.48
1:a:366:A:O2'	1:a:395:C:O2	2.30	0.48
1:a:770:C:O2'	1:a:899:C:N3	2.42	0.48
1:a:1218:C:H2'	1:a:1219:A:C8	2.49	0.48
26:D:51:THR:HB	26:D:79:LEU:HD23	1.95	0.48
32:K:80:ASP:OD2	37:P:61:ARG:NH1	2.44	0.48
34:M:50:ARG:HA	34:M:53:MET:HE2	1.93	0.48
55:7:66:PRO:HB2	55:7:189:LEU:HD21	1.96	0.48
23:A:279:A:N6	23:A:361:G:N3	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:569:U:O2'	23:A:983:A:N1	2.45	0.48
23:A:1750:G:O2'	23:A:2860:A:N1	2.44	0.48
27:E:47:LYS:HB2	27:E:51:GLU:HB2	1.96	0.48
5:e:10:LEU:HD13	5:e:67:ARG:HH22	1.78	0.48
23:A:2245:U:H5''	23:A:2246:G:H5'	1.95	0.48
23:A:2645:G:OP1	23:A:2732:G:N2	2.40	0.48
27:E:12:LEU:HD21	27:E:193:VAL:HG11	1.95	0.48
29:G:38:ASP:OD2	29:G:57:TYR:OH	2.31	0.48
32:K:12:ASP:HB2	32:K:96:GLY:HA3	1.94	0.48
33:L:27:LEU:H	33:L:27:LEU:HG	1.41	0.48
1:a:1048:G:H5''	14:n:2:LYS:HD2	1.96	0.48
1:a:1343:G:H4'	9:i:123:ARG:HB2	1.95	0.48
3:c:15:LYS:NZ	3:c:182:ASP:OD1	2.47	0.48
4:d:28:ASP:HB2	4:d:30:LYS:HB2	1.95	0.48
5:e:98:ALA:O	5:e:101:GLY:N	2.47	0.48
23:A:1022:G:N2	23:A:1023:U:O4	2.44	0.48
23:A:1270:C:H5''	23:A:1271:G:H5'	1.96	0.48
23:A:1323:C:OP1	40:S:98:LYS:NZ	2.46	0.48
23:A:1753:G:H5''	37:P:92:ARG:HD3	1.95	0.48
23:A:1827:U:O2'	23:A:1970:A:N3	2.43	0.48
23:A:2788:C:O2'	23:A:2809:A:N3	2.47	0.48
31:J:56:VAL:HB	31:J:124:VAL:HG12	1.96	0.48
34:M:11:LYS:HD2	34:M:86:LYS:HG2	1.95	0.48
1:a:4:U:O2'	1:a:6:G:OP1	2.32	0.47
11:k:112:VAL:HA	18:r:72:ARG:HH12	1.79	0.47
23:A:1537:G:N1	23:A:1538:G:N3	2.62	0.47
4:d:94:GLU:HA	4:d:99:ASN:HD22	1.79	0.47
23:A:673:C:H5''	27:E:76:PRO:HD2	1.95	0.47
23:A:1454:C:N4	35:N:73:ASN:OD1	2.47	0.47
1:a:1060:U:H5	3:c:1:GLY:HA2	1.79	0.47
11:k:86:LYS:HB2	11:k:112:VAL:HG23	1.94	0.47
23:A:538:A:H4'	31:J:7:LYS:HG2	1.96	0.47
23:A:1061:U:H4'	23:A:1070:A:C4	2.49	0.47
23:A:1613:G:HO2'	50:2:3:ARG:HH11	1.58	0.47
25:C:16:VAL:HB	25:C:203:VAL:HG22	1.95	0.47
3:c:20:THR:HB	3:c:57:GLU:HG2	1.95	0.47
3:c:113:LYS:HB2	3:c:184:ASN:HD22	1.78	0.47
5:e:22:LYS:HB3	5:e:29:ILE:HG23	1.95	0.47
9:i:91:GLU:HA	9:i:94:ARG:HB2	1.96	0.47
15:o:88:ARG:HH22	23:A:714:U:H5''	1.79	0.47
23:A:307:G:N1	23:A:310:A:OP2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:P:52:ARG:H	37:P:56:SER:HB3	1.79	0.47
1:a:1230:C:H5'	54:x:30:C:H5''	1.96	0.47
23:A:528:A:H5''	31:J:113:PRO:HG3	1.96	0.47
23:A:2636:C:H2'	23:A:2637:U:H6	1.79	0.47
1:a:1229:A:O2'	54:x:30:C:OP1	2.32	0.47
26:D:46:ARG:NH2	26:D:88:GLU:O	2.47	0.47
28:F:97:GLU:HG2	53:6:25:ARG:HB2	1.97	0.47
32:K:24:VAL:HG13	32:K:33:ALA:HB2	1.96	0.47
56:w:146:THR:O	56:w:148:GLY:N	2.47	0.47
1:a:110:C:O2'	16:p:25:ARG:O	2.30	0.47
1:a:323:U:H5'	20:t:17:ARG:HB3	1.95	0.47
4:d:97:LEU:HB2	4:d:134:TYR:HB3	1.96	0.47
5:e:152:VAL:HG21	8:h:98:LEU:HB2	1.96	0.47
6:f:9:MET:HE2	6:f:86:ARG:HB3	1.95	0.47
23:A:829:A:N7	23:A:2247:A:O2'	2.44	0.47
23:A:882:G:H1	23:A:894:U:H3	1.63	0.47
23:A:2447:G:H1	23:A:2451:A:H62	1.63	0.47
24:B:46:A:H5''	36:O:3:LYS:HE2	1.95	0.47
31:J:5:THR:HG23	31:J:45:THR:HG21	1.97	0.47
23:A:1085:A:O2'	23:A:1104:C:O2	2.27	0.47
23:A:1615:C:OP2	23:A:1617:C:N4	2.44	0.47
28:F:1:ALA:N	28:F:97:GLU:OE1	2.38	0.47
42:U:88:ASP:O	42:U:90:LYS:N	2.47	0.47
43:V:77:VAL:HG23	43:V:89:ILE:HG12	1.95	0.47
1:a:1422:G:H5'	32:K:48:PRO:HG3	1.97	0.47
23:A:290:U:H2'	23:A:291:G:C8	2.49	0.47
23:A:396:G:OP2	45:X:9:LYS:NZ	2.48	0.47
23:A:1613:G:H4'	50:2:3:ARG:HE	1.80	0.47
28:F:98:PHE:O	28:F:102:LEU:N	2.48	0.47
36:O:37:ALA:HB2	36:O:106:LEU:HD11	1.97	0.47
38:Q:109:VAL:HG12	38:Q:113:LYS:HE2	1.97	0.47
1:a:72:A:H61	1:a:98:A:H2	1.62	0.47
1:a:105:G:OP2	20:t:12:GLN:NE2	2.48	0.47
7:g:145:GLU:HA	7:g:148:LYS:HD3	1.96	0.47
23:A:959:A:N6	23:A:2495:G:O2'	2.45	0.47
23:A:2273:A:H2'	23:A:2274:A:C8	2.50	0.47
40:S:57:ASN:ND2	40:S:61:ASN:HD22	2.13	0.47
41:T:37:ASP:OD1	41:T:37:ASP:N	2.48	0.47
55:7:77:VAL:HG21	55:7:95:VAL:HG22	1.97	0.47
55:7:201:PRO:CB	55:7:205:LYS:CE	2.74	0.47
1:a:197:A:N1	1:a:220:G:O2'	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:111:GLY:HA2	7:g:118:ARG:HD3	1.97	0.46
23:A:495:G:H21	40:S:61:ASN:HD21	1.64	0.46
23:A:2169:A:O2'	55:7:134:ARG:CG	2.61	0.46
1:a:10:A:O2'	1:a:507:C:O2'	2.30	0.46
1:a:231:U:H2'	1:a:232:G:H8	1.80	0.46
1:a:1041:G:H2'	1:a:1042:A:C8	2.50	0.46
1:a:1236:A:H4'	1:a:1304:G:H4'	1.97	0.46
23:A:1266:G:O2'	23:A:2012:G:O6	2.29	0.46
27:E:29:HIS:HA	27:E:32:VAL:HG12	1.98	0.46
55:7:157:LYS:HG2	55:7:161:VAL:HG21	1.96	0.46
1:a:528:C:H41	12:l:45:ASN:ND2	2.14	0.46
6:f:49:TYR:OH	6:f:86:ARG:NH1	2.49	0.46
23:A:2271:G:OP1	44:W:18:ALA:HB1	2.15	0.46
25:C:140:VAL:HG12	25:C:191:LEU:HD23	1.97	0.46
28:F:33:ILE:HG13	28:F:95:MET:HE2	1.96	0.46
37:P:84:SER:OG	37:P:86:LYS:NZ	2.48	0.46
56:w:72:LEU:HB3	56:w:84:PHE:HB3	1.98	0.46
1:a:404:G:O6	4:d:1:ALA:N	2.49	0.46
2:b:67:LEU:HB2	2:b:160:LEU:HD12	1.96	0.46
28:F:140:ILE:HG22	28:F:142:TYR:H	1.81	0.46
2:b:65:LYS:HD2	2:b:153:MET:HG3	1.97	0.46
12:l:13:ARG:NH1	12:l:14:LYS:O	2.49	0.46
19:s:48:ILE:H	19:s:48:ILE:HG13	1.45	0.46
23:A:499:U:H5''	42:U:42:LYS:HE2	1.98	0.46
23:A:586:A:N1	23:A:809:G:O2'	2.46	0.46
23:A:1070:A:O2'	23:A:1097:U:O5'	2.28	0.46
55:7:209:ILE:HG22	55:7:210:LYS:HG3	1.96	0.46
23:A:1301:A:H62	23:A:1641:A:H61	1.63	0.46
23:A:1363:C:O2'	23:A:1809:A:N3	2.46	0.46
49:1:16:THR:OG1	49:1:17:GLY:N	2.48	0.46
23:A:517:C:OP1	48:0:12:ARG:NH2	2.49	0.46
23:A:886:A:H1'	23:A:891:G:H22	1.80	0.46
55:7:132:GLY:HA3	55:7:133:PRO:HD3	1.68	0.46
1:a:1297:G:N2	1:a:1298:U:O4	2.49	0.46
29:G:23:ILE:HG21	29:G:71:LEU:HD21	1.98	0.46
29:G:37:ASN:HD22	29:G:63:GLN:NE2	2.14	0.46
30:H:39:ALA:HB1	30:H:44:ILE:HG13	1.98	0.46
46:Y:9:LYS:HG2	46:Y:11:VAL:H	1.81	0.46
48:0:54:ILE:HG23	48:0:56:LYS:H	1.80	0.46
1:a:406:G:C2	1:a:407:U:H1'	2.51	0.46
23:A:1791:A:N6	23:A:1828:G:O2'	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1422:G:H4'	32:K:48:PRO:HB3	1.98	0.46
16:p:20:VAL:HG23	16:p:35:ARG:HB3	1.97	0.46
17:q:24:ILE:HD11	17:q:60:ILE:HD12	1.98	0.46
23:A:1509:A:H2'	23:A:1510:G:C8	2.51	0.46
1:a:427:U:O2'	1:a:541:G:OP1	2.32	0.45
1:a:1255:G:O2'	1:a:1258:G:N3	2.44	0.45
20:t:41:GLY:HA2	20:t:85:LEU:HD11	1.99	0.45
23:A:910:A:H2'	23:A:911:A:C8	2.51	0.45
28:F:3:LEU:HA	28:F:6:TYR:HB3	1.96	0.45
39:R:34:GLU:HG2	39:R:60:LYS:HG2	1.98	0.45
1:a:651:C:N4	1:a:753:A:OP2	2.46	0.45
2:b:160:LEU:HB3	2:b:182:VAL:HG12	1.98	0.45
10:j:59:LYS:HE2	10:j:62:ARG:NH2	2.31	0.45
23:A:700:G:O2'	23:A:1632:A:N3	2.39	0.45
23:A:881:G:N2	23:A:897:C:N3	2.64	0.45
23:A:1565:C:H5'	25:C:17:LYS:HE3	1.98	0.45
28:F:39:VAL:HG12	28:F:85:GLY:HA2	1.98	0.45
1:a:398:U:H2'	1:a:399:G:H8	1.81	0.45
23:A:2457:U:H5	23:A:2494:G:H1	1.64	0.45
45:X:34:SER:HA	45:X:49:ARG:HA	1.98	0.45
1:a:928:G:O2'	1:a:1533:C:OP1	2.31	0.45
7:g:85:GLN:HB2	7:g:147:ASN:HD22	1.81	0.45
18:r:37:LYS:NZ	21:u:22:CYS:SG	2.89	0.45
23:A:1026:G:H2'	23:A:1027:A:H8	1.82	0.45
23:A:1900:A:H1'	23:A:1970:A:H2'	1.97	0.45
26:D:121:THR:HG21	26:D:143:PRO:HB3	1.97	0.45
33:L:128:THR:OG1	33:L:129:LYS:N	2.48	0.45
35:N:85:PRO:HA	35:N:88:ALA:HB2	1.98	0.45
5:e:44:ARG:HH22	5:e:70:MET:HE3	1.82	0.45
6:f:88:MET:HG3	6:f:90:MET:HE2	1.99	0.45
23:A:2343:U:O2'	23:A:2373:G:O2'	2.35	0.45
31:J:14:ASP:OD2	31:J:138:GLN:NE2	2.45	0.45
11:k:116:PRO:HB2	11:k:119:GLY:H	1.80	0.45
23:A:729:G:H2'	23:A:1775:U:H1'	1.98	0.45
23:A:959:A:N3	23:A:2457:U:O2'	2.48	0.45
44:W:25:ARG:HA	44:W:29:GLU:OE2	2.15	0.45
55:7:162:ARG:NH1	55:7:175:ILE:O	2.48	0.45
1:a:815:A:N7	1:a:1509:C:O2'	2.46	0.45
4:d:28:ASP:OD1	4:d:28:ASP:N	2.50	0.45
23:A:861:A:N3	24:B:79:G:O2'	2.49	0.45
29:G:97:VAL:HG22	29:G:102:ILE:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:N:37:THR:HG22	35:N:110:MET:HE1	1.97	0.45
40:S:20:VAL:HG11	40:S:44:ALA:HA	1.99	0.45
46:Y:24:GLU:HB3	46:Y:46:VAL:HG21	1.98	0.45
55:7:64:VAL:HA	55:7:161:VAL:HG22	1.98	0.45
1:a:352:C:O2	1:a:355:C:N4	2.50	0.45
1:a:414:A:H3'	1:a:415:A:H8	1.82	0.45
1:a:971:G:OP2	1:a:1231:G:N2	2.41	0.45
1:a:1261:A:H1'	1:a:1283:U:H5''	1.99	0.45
1:a:1356:G:H2'	1:a:1357:A:C8	2.52	0.45
14:n:15:LEU:HD23	14:n:55:SER:HB3	1.98	0.45
41:T:13:ALA:HB3	41:T:33:LYS:HD3	1.99	0.45
55:7:47:ASN:HB3	55:7:170:ILE:HG22	1.99	0.45
23:A:2576:G:O2'	23:A:2579:C:OP2	2.30	0.45
33:L:73:ILE:HD12	33:L:106:GLU:HB2	1.98	0.45
41:T:11:LEU:O	46:Y:29:ARG:NH1	2.50	0.45
1:a:488:C:OP1	1:a:618:C:O2'	2.33	0.45
1:a:1205:U:H4'	3:c:189:HIS:HD2	1.82	0.45
1:a:1485:U:H2'	1:a:1486:G:H8	1.82	0.45
10:j:19:ASP:O	10:j:23:ALA:N	2.44	0.45
23:A:774:G:N2	23:A:787:C:O2'	2.47	0.45
23:A:783:A:O2'	23:A:1779:U:O2	2.35	0.45
23:A:2183:A:H2'	23:A:2184:A:H8	1.82	0.45
23:A:2579:C:O2'	26:D:136:ASN:OD1	2.36	0.45
56:w:143:LYS:H	56:w:143:LYS:HG3	1.44	0.45
1:a:14:U:O2'	1:a:16:A:N7	2.45	0.44
1:a:1342:C:H2'	1:a:1343:G:C8	2.51	0.44
9:i:129:ARG:NH1	54:x:33:U:OP2	2.42	0.44
23:A:482:A:OP2	23:A:507:A:N6	2.42	0.44
35:N:28:LEU:HD23	35:N:48:VAL:HG21	1.99	0.44
40:S:47:VAL:HG23	40:S:103:ILE:HG21	1.98	0.44
45:X:4:CYS:HB3	45:X:9:LYS:H	1.82	0.44
1:a:328:C:H4'	1:a:329:A:H5'	2.00	0.44
5:e:90:GLY:O	5:e:129:SER:N	2.41	0.44
5:e:104:ILE:HD11	5:e:114:LEU:HD23	1.99	0.44
16:p:56:ARG:O	16:p:60:TRP:N	2.44	0.44
44:W:69:PHE:CE1	44:W:80:ILE:CD1	3.00	0.44
6:f:6:ILE:HD11	6:f:71:ILE:HD11	2.00	0.44
12:l:113:ARG:HH12	12:l:120:ARG:HG3	1.82	0.44
23:A:572:A:OP2	39:R:80:ARG:NH2	2.49	0.44
23:A:602:A:O2'	23:A:604:G:O2'	2.31	0.44
23:A:1215:G:H5''	38:Q:7:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:O:104:GLN:O	36:O:108:ASP:N	2.48	0.44
55:7:42:VAL:HB	55:7:176:GLY:HA3	2.00	0.44
55:7:77:VAL:HG22	55:7:154:LYS:NZ	2.32	0.44
1:a:437:U:H5''	4:d:151:GLN:HB3	1.99	0.44
1:a:749:A:O2'	15:o:19:ASN:OD1	2.36	0.44
11:k:71:ASP:HB3	11:k:74:LYS:HE3	1.99	0.44
23:A:807:U:O2'	23:A:2060:A:N1	2.44	0.44
23:A:1049:C:H2'	23:A:1050:A:H8	1.81	0.44
23:A:2680:U:H5'	26:D:194:PRO:HA	1.99	0.44
29:G:46:ASP:O	29:G:48:THR:N	2.49	0.44
46:Y:49:ASP:OD1	46:Y:52:ARG:NH2	2.50	0.44
50:2:12:ARG:HE	50:2:44:VAL:HG21	1.83	0.44
55:7:132:GLY:N	55:7:133:PRO:CD	2.75	0.44
9:i:33:SER:HB3	9:i:36:GLN:HG2	1.99	0.44
23:A:1321:A:O2'	40:S:11:ARG:NH2	2.51	0.44
23:A:2278:A:H5''	44:W:12:ASN:HD21	1.83	0.44
1:a:677:U:H3	1:a:713:G:H22	1.64	0.44
11:k:19:VAL:N	11:k:34:THR:O	2.40	0.44
13:m:15:VAL:HG13	13:m:33:LEU:HD22	2.00	0.44
26:D:96:ILE:HG23	26:D:100:LEU:HD13	2.00	0.44
1:a:1038:C:H2'	1:a:1039:G:H8	1.83	0.44
7:g:105:GLU:OE2	7:g:109:LYS:NZ	2.45	0.44
23:A:411:G:OP2	23:A:2406:A:O2'	2.36	0.44
23:A:615:U:N3	27:E:35:TYR:O	2.45	0.44
23:A:1340:U:OP1	41:T:19:LYS:NZ	2.47	0.44
29:G:28:LYS:HE3	29:G:79:THR:HG23	2.00	0.44
32:K:40:LYS:HD2	32:K:57:VAL:HG12	1.99	0.44
35:N:86:ARG:NE	35:N:117:ASP:OD2	2.51	0.44
56:w:176:VAL:HG12	56:w:183:TYR:HA	2.00	0.44
1:a:107:G:OP1	1:a:325:A:N6	2.48	0.44
29:G:85:LYS:HB3	29:G:164:ALA:HB2	2.00	0.44
34:M:53:MET:HE2	34:M:53:MET:HB3	1.78	0.44
55:7:65:LEU:O	55:7:160:GLN:HB2	2.18	0.44
32:K:34:GLY:N	32:K:37:ASP:OD2	2.45	0.44
1:a:390:U:H2'	1:a:391:G:H8	1.82	0.43
1:a:782:A:H62	1:a:800:G:H21	1.66	0.43
3:c:156:LEU:H	3:c:156:LEU:HG	1.63	0.43
16:p:6:LEU:HD22	16:p:17:TYR:HB3	1.99	0.43
23:A:1568:G:H5'	25:C:59:GLN:HA	2.00	0.43
23:A:2065:C:O2	23:A:2449:U:N3	2.43	0.43
25:C:74:PRO:HB3	25:C:114:GLN:HE21	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:154:ALA:HB2	25:C:161:VAL:HG23	2.00	0.43
33:L:100:ILE:HG13	33:L:101:ILE:HG23	1.98	0.43
2:b:116:LEU:HD23	2:b:140:LEU:HD12	1.99	0.43
6:f:74:LEU:O	6:f:77:THR:OG1	2.36	0.43
9:i:51:LEU:HD13	9:i:56:MET:HG3	1.99	0.43
20:t:27:MET:HE1	20:t:66:ILE:HD11	2.00	0.43
23:A:2021:C:OP1	38:Q:24:TYR:OH	2.33	0.43
23:A:2615:U:C2	48:O:3:GLN:HA	2.54	0.43
23:A:2875:C:O3'	37:P:1:SER:N	2.51	0.43
56:w:130:PHE:HE1	56:w:184:VAL:HG11	1.82	0.43
1:a:60:A:N1	1:a:107:G:O2'	2.48	0.43
1:a:1306:A:N6	1:a:1331:G:H1'	2.32	0.43
7:g:72:VAL:HG12	7:g:89:GLU:HA	2.00	0.43
7:g:78:ARG:NH2	7:g:81:GLY:O	2.48	0.43
23:A:1322:A:N1	23:A:1333:G:O2'	2.44	0.43
25:C:180:MET:HE3	25:C:180:MET:HB3	1.92	0.43
25:C:209:ALA:HA	25:C:212:TRP:CE2	2.53	0.43
27:E:108:ILE:HD12	27:E:180:LEU:HB2	2.01	0.43
29:G:59:ASP:HB2	29:G:62:ALA:HB3	2.00	0.43
55:7:164:ARG:HH22	55:7:196:LEU:HB2	1.82	0.43
5:e:119:VAL:HB	5:e:121:ASN:ND2	2.33	0.43
16:p:53:ASP:CG	16:p:56:ARG:H	2.26	0.43
23:A:1056:G:H4'	23:A:1086:A:H8	1.84	0.43
23:A:1816:C:N4	25:C:34:GLU:OE2	2.46	0.43
32:K:108:ARG:HB2	32:K:116:ILE:HG21	2.00	0.43
42:U:10:VAL:HA	42:U:71:ILE:HA	2.00	0.43
54:x:23:C:H5''	56:w:130:PHE:HE2	1.84	0.43
55:7:65:LEU:O	55:7:160:GLN:HB3	2.18	0.43
3:c:54:ILE:HG22	3:c:67:ILE:HA	2.01	0.43
6:f:47:LEU:HD12	6:f:55:HIS:HA	2.01	0.43
23:A:931:U:O2	23:A:1167:C:O2'	2.33	0.43
23:A:2258:C:O2'	23:A:2427:C:OP2	2.33	0.43
27:E:18:THR:HA	27:E:106:LYS:HE3	1.99	0.43
35:N:106:ASP:N	35:N:106:ASP:OD1	2.52	0.43
42:U:39:ASN:HB3	42:U:62:ALA:HB3	2.00	0.43
44:W:13:GLY:O	44:W:14:ARG:HG3	2.18	0.43
56:w:132:GLU:HA	56:w:175:LYS:HA	2.01	0.43
9:i:104:THR:HG22	9:i:106:ASP:H	1.82	0.43
12:l:79:ILE:HG22	12:l:103:CYS:HB2	2.01	0.43
23:A:789:A:N1	50:2:3:ARG:NH1	2.66	0.43
23:A:1141:U:OP2	31:J:65:THR:OG1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:7:78:PHE:HB3	55:7:120:ALA:HB1	2.00	0.43
25:C:250:GLN:NE2	25:C:251:THR:O	2.49	0.43
1:a:96:U:H2'	1:a:97:G:C8	2.54	0.43
1:a:632:U:H3'	1:a:633:G:C8	2.54	0.43
18:r:21:ASP:OD1	18:r:23:LYS:NZ	2.49	0.43
23:A:869:G:H1'	34:M:8:LYS:HD2	1.99	0.43
23:A:1808:A:H3'	23:A:1809:A:C8	2.54	0.43
23:A:2449:U:O2'	23:A:2501:C:N4	2.52	0.43
25:C:153:LEU:HD13	25:C:175:LEU:HD21	2.01	0.43
28:F:70:ARG:O	28:F:80:GLN:NE2	2.45	0.43
33:L:63:LYS:O	51:3:29:ARG:NH1	2.51	0.43
35:N:103:ARG:HB2	35:N:110:MET:HE3	2.01	0.43
47:Z:36:GLU:O	47:Z:37:ARG:NH1	2.46	0.43
1:a:1314:C:H41	19:s:3:SER:HA	1.83	0.43
8:h:104:SER:HB2	8:h:125:ILE:HD11	2.01	0.43
23:A:373:U:H2'	23:A:374:A:H8	1.82	0.43
23:A:1070:A:H4'	23:A:1071:G:H5''	2.01	0.43
23:A:2780:G:N1	31:J:102:GLU:OE2	2.44	0.43
25:C:259:ASN:ND2	25:C:262:THR:OG1	2.51	0.43
27:E:176:ASP:N	27:E:176:ASP:OD1	2.52	0.43
40:S:77:ASP:OD1	40:S:77:ASP:N	2.51	0.43
55:7:77:VAL:HB	55:7:95:VAL:HA	2.01	0.43
1:a:143:A:H2	1:a:220:G:H1	1.66	0.43
1:a:310:G:H5''	16:p:31:ARG:HB2	2.00	0.43
1:a:944:G:N1	1:a:1338:G:OP2	2.39	0.43
10:j:54:SER:O	14:n:81:ARG:NH1	2.36	0.43
13:m:28:ARG:HH21	13:m:62:PHE:HB2	1.84	0.43
23:A:587:C:O2	33:L:33:ARG:NH1	2.52	0.43
34:M:33:LEU:HD23	34:M:103:TYR:HD2	1.82	0.43
34:M:69:PRO:HA	34:M:94:ALA:HB2	2.01	0.43
54:x:51:A:C2	54:x:64:C:C2	3.06	0.43
56:w:137:ASP:HB2	56:w:155:THR:HB	2.01	0.43
1:a:59:A:H5''	1:a:387:U:H5''	2.01	0.42
19:s:13:HIS:HE1	19:s:34:SER:HB2	1.85	0.42
26:D:22:ILE:HA	26:D:23:PRO:HD3	1.90	0.42
34:M:17:ASN:O	34:M:38:ARG:NH1	2.51	0.42
36:O:49:VAL:HG21	36:O:82:ALA:HA	2.01	0.42
44:W:68:LYS:HG2	44:W:83:GLU:OE1	2.19	0.42
55:7:63:THR:OG1	55:7:162:ARG:O	2.28	0.42
1:a:1530:G:H2'	1:a:1531:A:C8	2.55	0.42
8:h:4:ASP:OD2	8:h:76:ARG:NE	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:10:LEU:HB3	10:j:98:VAL:HG23	2.01	0.42
10:j:57:VAL:HG22	10:j:58:ASN:H	1.84	0.42
16:p:76:LYS:HA	16:p:79:ASN:HD21	1.83	0.42
23:A:1386:C:H2'	23:A:1387:A:C8	2.54	0.42
30:H:84:ALA:HA	30:H:90:LEU:HD12	2.01	0.42
47:Z:4:ILE:N	47:Z:37:ARG:O	2.52	0.42
1:a:1391:U:H2'	1:a:1392:G:C8	2.54	0.42
2:b:87:ASP:OD1	2:b:88:GLN:NE2	2.52	0.42
3:c:155:ARG:NE	3:c:159:ALA:O	2.39	0.42
31:J:114:LEU:HG	31:J:118:MET:HE3	2.02	0.42
42:U:48:VAL:HA	42:U:49:PRO:HD3	1.92	0.42
45:X:58:ILE:HG12	45:X:66:VAL:HG21	2.00	0.42
56:w:42:LYS:HD2	56:w:51:ARG:NH2	2.35	0.42
1:a:458:U:H2'	1:a:459:A:C8	2.54	0.42
1:a:1345:U:OP1	9:i:121:ARG:NH1	2.53	0.42
2:b:183:PHE:HB3	2:b:197:PHE:HB2	2.02	0.42
5:e:100:GLU:CD	5:e:102:THR:HG1	2.27	0.42
19:s:49:ALA:HB1	19:s:56:HIS:HB3	2.00	0.42
23:A:308:G:O2'	23:A:329:G:N2	2.52	0.42
23:A:1769:U:O2'	23:A:1958:C:OP1	2.37	0.42
38:Q:68:ALA:HB1	38:Q:73:ILE:HG23	2.01	0.42
39:R:14:VAL:HG21	39:R:98:ILE:HG13	2.00	0.42
1:a:335:C:O2'	1:a:1433:A:N3	2.49	0.42
1:a:923:A:O2'	1:a:1399:C:OP2	2.31	0.42
27:E:118:LEU:HD11	27:E:188:MET:HG3	2.02	0.42
27:E:125:SER:O	27:E:137:LYS:NZ	2.42	0.42
30:H:108:VAL:HG12	30:H:110:VAL:H	1.84	0.42
32:K:64:ARG:NE	37:P:67:GLU:OE2	2.53	0.42
56:w:31:LYS:HD2	56:w:31:LYS:O	2.18	0.42
1:a:553:A:H2'	1:a:554:A:C8	2.55	0.42
1:a:1141:C:H2'	1:a:1142:G:H8	1.84	0.42
2:b:129:THR:O	2:b:133:ALA:N	2.50	0.42
23:A:626:A:N3	33:L:78:ARG:NH2	2.67	0.42
23:A:2585:U:O4	57:A:3001:PRO:CB	2.68	0.42
1:a:519:C:OP2	12:l:46:SER:OG	2.31	0.42
14:n:1:ALA:HB3	14:n:6:LYS:HD2	2.02	0.42
23:A:51:G:H4'	23:A:52:A:H5'	2.01	0.42
23:A:1539:U:H2'	23:A:1540:G:H8	1.84	0.42
23:A:2427:C:H5'	23:A:2429:G:H5'	2.01	0.42
23:A:2820:A:N6	26:D:197:THR:O	2.52	0.42
29:G:94:ARG:HB2	29:G:105:SER:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Q:78:PHE:HE2	38:Q:94:LEU:HD21	1.85	0.42
47:Z:41:PRO:HA	47:Z:44:ARG:HB2	2.01	0.42
7:g:90:VAL:O	7:g:95:ARG:NH2	2.53	0.42
23:A:1042:G:H1	23:A:1113:U:H3	1.68	0.42
3:c:65:VAL:HB	3:c:100:ILE:HG22	2.02	0.42
20:t:24:ARG:HD3	20:t:65:LEU:HD11	2.01	0.42
24:B:39:A:O2'	24:B:46:A:N1	2.49	0.42
26:D:32:ASN:O	26:D:96:ILE:N	2.51	0.42
26:D:68:PHE:HE1	26:D:79:LEU:HD21	1.85	0.42
29:G:17:LYS:HB2	29:G:24:THR:HB	2.01	0.42
32:K:21:CYS:HA	32:K:41:ILE:HG22	2.02	0.42
4:d:22:SER:H	4:d:109:THR:HG22	1.85	0.42
4:d:84:ASN:OD1	4:d:85:THR:N	2.50	0.42
10:j:42:LEU:HD11	10:j:73:LEU:HG	2.02	0.42
23:A:2585:U:C4	57:x:101:PRO:HD2	2.54	0.42
29:G:21:GLN:NE2	29:G:37:ASN:O	2.53	0.42
54:x:53:G:C2'	54:x:54:U:O5'	2.68	0.42
55:7:66:PRO:HB2	55:7:189:LEU:CD2	2.49	0.42
1:a:1331:G:HO2'	1:a:1332:A:H8	1.68	0.41
5:e:121:ASN:CG	5:e:122:VAL:H	2.26	0.41
11:k:125:LYS:O	21:u:34:ARG:NE	2.48	0.41
13:m:14:ALA:HB3	13:m:33:LEU:HD21	2.01	0.41
23:A:1086:A:O2'	23:A:1087:G:N7	2.49	0.41
25:C:144:GLU:HB2	25:C:187:CYS:HB3	2.01	0.41
32:K:35:VAL:HG22	32:K:69:VAL:HG12	2.02	0.41
33:L:109:LYS:HG2	33:L:126:ARG:HB3	2.02	0.41
40:S:4:ILE:HG22	40:S:106:VAL:HG13	2.02	0.41
55:7:57:GLN:NE2	55:7:204:ALA:O	2.53	0.41
55:7:97:MET:HB3	55:7:98:GLU:H	1.75	0.41
2:b:210:THR:O	2:b:214:GLY:N	2.52	0.41
18:r:36:GLY:O	18:r:62:ARG:NH2	2.42	0.41
31:J:32:LEU:HD22	31:J:54:ILE:HG21	2.02	0.41
54:x:35:G:H2'	54:x:36:G:C8	2.56	0.41
1:a:437:U:H5''	4:d:151:GLN:HE21	1.84	0.41
16:p:17:TYR:O	16:p:39:PHE:N	2.44	0.41
23:A:658:U:O2'	27:E:97:ASN:OD1	2.37	0.41
44:W:69:PHE:CD2	44:W:69:PHE:N	2.89	0.41
55:7:47:ASN:HD22	55:7:212:VAL:HB	1.84	0.41
4:d:49:ASP:OD2	5:e:111:ARG:NH1	2.53	0.41
7:g:139:ASP:HA	7:g:142:ARG:HB2	2.03	0.41
23:A:2522:U:O2'	23:A:2647:U:OP1	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:2898:U:H2'	23:A:2899:A:C8	2.55	0.41
27:E:149:ILE:HG23	27:E:188:MET:HA	2.02	0.41
55:7:65:LEU:HD11	55:7:162:ARG:HB2	2.02	0.41
1:a:366:A:O2'	1:a:394:G:N2	2.53	0.41
13:m:6:ILE:HG13	13:m:7:ASN:H	1.84	0.41
34:M:58:LYS:O	34:M:60:GLN:N	2.53	0.41
38:Q:8:ILE:H	38:Q:8:ILE:HG13	1.71	0.41
1:a:1302:C:N4	13:m:13:HIS:HD2	2.19	0.41
11:k:87:GLY:O	11:k:92:ARG:NH1	2.51	0.41
23:A:1416:G:H1	23:A:1582:C:H42	1.68	0.41
23:A:1528:A:OP2	23:A:1543:G:N2	2.53	0.41
32:K:121:GLU:HB2	37:P:65:ASN:HD21	1.85	0.41
43:V:20:LEU:HD21	43:V:41:GLU:HG2	2.03	0.41
8:h:73:SER:HB3	8:h:129:ALA:HB3	2.03	0.41
9:i:51:LEU:HA	9:i:54:VAL:HG22	2.03	0.41
11:k:99:LEU:HB3	11:k:106:ILE:HD11	2.02	0.41
23:A:1226:A:OP1	38:Q:15:LYS:NZ	2.53	0.41
23:A:1827:U:OP1	23:A:1971:U:O2'	2.32	0.41
23:A:2500:U:O2	23:A:2504:U:N3	2.54	0.41
32:K:116:ILE:H	32:K:116:ILE:HG13	1.63	0.41
35:N:56:LYS:HE3	35:N:88:ALA:HA	2.01	0.41
1:a:269:C:H2'	1:a:270:A:C8	2.56	0.41
1:a:815:A:O2'	1:a:1526:G:N2	2.40	0.41
13:m:85:TYR:CZ	13:m:89:ARG:HD2	2.56	0.41
23:A:581:C:H2'	23:A:582:A:C8	2.56	0.41
23:A:1045:C:H1'	23:A:1047:G:C2	2.56	0.41
30:H:5:LEU:HD22	30:H:13:GLY:HA3	2.03	0.41
55:7:195:ALA:O	55:7:199:ALA:HB2	2.21	0.41
4:d:10:LEU:HD13	4:d:62:ARG:HG3	2.02	0.41
5:e:17:VAL:HG21	5:e:55:VAL:HG13	2.02	0.41
5:e:45:VAL:HG13	5:e:117:ALA:HB2	2.02	0.41
9:i:93:LEU:O	9:i:97:LEU:N	2.45	0.41
23:A:540:C:H2'	23:A:541:A:C8	2.56	0.41
23:A:566:U:H5''	33:L:29:LYS:HE3	2.03	0.41
23:A:598:U:H2'	23:A:599:A:C8	2.56	0.41
23:A:2839:G:O2'	35:N:49:GLU:OE1	2.39	0.41
25:C:266:ILE:HG21	25:C:269:ARG:HD2	2.03	0.41
33:L:79:LEU:HD12	33:L:114:GLY:H	1.86	0.41
56:w:146:THR:O	56:w:147:ALA:C	2.64	0.41
1:a:79:G:C2	1:a:80:A:H1'	2.55	0.41
1:a:202:G:H21	1:a:466:A:H61	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:626:G:H2'	1:a:627:G:C8	2.55	0.41
1:a:1338:G:O2'	54:x:42:A:OP1	2.34	0.41
4:d:124:VAL:HA	4:d:142:VAL:HA	2.03	0.41
8:h:39:LEU:HD21	8:h:128:VAL:HG21	2.03	0.41
14:n:2:LYS:HD2	14:n:2:LYS:HA	1.88	0.41
23:A:709:U:H3	23:A:722:A:H61	1.68	0.41
23:A:1306:C:H2'	23:A:1307:A:H8	1.86	0.41
23:A:1394:U:H4'	23:A:1603:A:H4'	2.03	0.41
23:A:2564:A:H5'	23:A:2648:G:H4'	2.02	0.41
55:7:126:GLN:HA	55:7:129:GLN:HE21	1.86	0.41
55:7:136:LEU:C	55:7:137:MET:HG2	2.45	0.41
1:a:398:U:H2'	1:a:399:G:C8	2.57	0.40
1:a:1226:C:OP2	13:m:89:ARG:NH2	2.39	0.40
2:b:116:LEU:HG	2:b:136:ARG:HH21	1.86	0.40
8:h:91:LEU:HB2	8:h:116:ARG:HE	1.86	0.40
11:k:71:ASP:N	11:k:71:ASP:OD1	2.48	0.40
23:A:684:G:OP1	50:2:21:ARG:NH2	2.54	0.40
23:A:1548:A:H2'	23:A:1549:A:C8	2.56	0.40
23:A:2370:G:H4'	49:1:43:ARG:HH11	1.86	0.40
26:D:48:ILE:HG21	26:D:90:PHE:HB2	2.03	0.40
27:E:143:LEU:HD22	27:E:185:LYS:HG3	2.03	0.40
44:W:32:LEU:O	44:W:35:SER:HB2	2.21	0.40
51:3:25:HIS:CE1	51:3:47:ALA:HB2	2.56	0.40
1:a:227:G:O2'	16:p:63:GLN:NE2	2.43	0.40
1:a:401:C:O2'	1:a:621:A:N3	2.50	0.40
1:a:981:U:H4'	14:n:61:ARG:HG2	2.02	0.40
4:d:104:MET:HE3	4:d:104:MET:HB3	1.86	0.40
5:e:100:GLU:OE1	5:e:102:THR:OG1	2.37	0.40
23:A:1779:U:O2	23:A:1783:A:N6	2.54	0.40
45:X:11:PRO:HB3	45:X:29:LEU:HD23	2.03	0.40
1:a:419:C:OP1	1:a:513:C:O2'	2.34	0.40
6:f:51:ILE:HD11	18:r:65:SER:HB2	2.02	0.40
8:h:27:PRO:O	8:h:32:LYS:NZ	2.53	0.40
25:C:99:GLU:OE2	25:C:101:ARG:NE	2.54	0.40
27:E:2:GLU:OE1	27:E:13:THR:OG1	2.32	0.40
40:S:18:ARG:NH2	40:S:76:VAL:O	2.53	0.40
1:a:522:C:N4	12:l:49:ARG:HH22	2.17	0.40
1:a:546:A:O2'	1:a:548:G:O2'	2.28	0.40
1:a:898:G:N2	1:a:901:A:OP2	2.50	0.40
1:a:1047:G:O2'	1:a:1215:G:O2'	2.33	0.40
2:b:17:HIS:CE1	2:b:202:ASN:HA	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:49:ALA:O	3:c:69:THR:OG1	2.39	0.40
7:g:6:ILE:H	7:g:6:ILE:HG13	1.73	0.40
9:i:34:LEU:HD11	9:i:47:VAL:HG21	2.04	0.40
13:m:2:ARG:NH1	28:F:109:ARG:HH22	2.18	0.40
23:A:111:A:O2'	46:Y:58:ASN:ND2	2.54	0.40
23:A:537:G:H4'	31:J:5:THR:HG21	2.03	0.40
23:A:1687:G:H21	23:A:1701:A:H62	1.70	0.40
23:A:1710:G:O2'	23:A:2858:C:N3	2.51	0.40
23:A:2169:A:O2'	55:7:134:ARG:HG2	2.21	0.40
23:A:2801:G:H2'	23:A:2802:G:C8	2.56	0.40
27:E:48:THR:OG1	27:E:51:GLU:OE1	2.31	0.40
30:H:76:GLU:HG2	30:H:142:VAL:HG22	2.03	0.40
44:W:65:GLY:C	44:W:66:LYS:HD3	2.46	0.40
11:k:21:HIS:N	11:k:32:THR:O	2.53	0.40
23:A:630:G:N2	23:A:633:A:OP2	2.49	0.40
28:F:139:GLU:OE2	53:6:26:SER:OG	2.36	0.40
55:7:83:ASN:HA	55:7:86:ALA:HB3	2.04	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	
2	b	216/218 (99%)	191 (88%)	25 (12%)	0	100	100
3	c	204/206 (99%)	189 (93%)	15 (7%)	0	100	100
4	d	203/205 (99%)	176 (87%)	27 (13%)	0	100	100
5	e	155/157 (99%)	132 (85%)	21 (14%)	2 (1%)	9	35
6	f	98/100 (98%)	82 (84%)	14 (14%)	2 (2%)	6	25
7	g	149/151 (99%)	130 (87%)	19 (13%)	0	100	100
8	h	127/129 (98%)	116 (91%)	11 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	i	125/127 (98%)	101 (81%)	22 (18%)	2 (2%)	7	30
10	j	96/98 (98%)	83 (86%)	12 (12%)	1 (1%)	12	41
11	k	114/116 (98%)	96 (84%)	18 (16%)	0	100	100
12	l	121/123 (98%)	90 (74%)	29 (24%)	2 (2%)	7	30
13	m	112/114 (98%)	97 (87%)	13 (12%)	2 (2%)	6	28
14	n	99/101 (98%)	86 (87%)	13 (13%)	0	100	100
15	o	86/88 (98%)	79 (92%)	6 (7%)	1 (1%)	10	37
16	p	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
17	q	78/80 (98%)	65 (83%)	12 (15%)	1 (1%)	9	35
18	r	63/65 (97%)	56 (89%)	7 (11%)	0	100	100
19	s	77/79 (98%)	72 (94%)	5 (6%)	0	100	100
20	t	83/85 (98%)	79 (95%)	4 (5%)	0	100	100
21	u	63/65 (97%)	47 (75%)	16 (25%)	0	100	100
25	C	269/271 (99%)	250 (93%)	19 (7%)	0	100	100
26	D	207/209 (99%)	191 (92%)	16 (8%)	0	100	100
27	E	199/201 (99%)	180 (90%)	19 (10%)	0	100	100
28	F	175/177 (99%)	157 (90%)	18 (10%)	0	100	100
29	G	174/176 (99%)	155 (89%)	16 (9%)	3 (2%)	7	30
30	H	147/149 (99%)	127 (86%)	20 (14%)	0	100	100
31	J	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
32	K	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
33	L	141/143 (99%)	120 (85%)	21 (15%)	0	100	100
34	M	134/136 (98%)	125 (93%)	6 (4%)	3 (2%)	5	24
35	N	118/120 (98%)	104 (88%)	14 (12%)	0	100	100
36	O	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
37	P	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
38	Q	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
39	R	101/103 (98%)	87 (86%)	13 (13%)	1 (1%)	12	41
40	S	108/110 (98%)	99 (92%)	7 (6%)	2 (2%)	6	27
41	T	91/93 (98%)	78 (86%)	13 (14%)	0	100	100
42	U	100/102 (98%)	83 (83%)	16 (16%)	1 (1%)	12	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
44	W	76/78 (97%)	55 (72%)	13 (17%)	8 (10%)	0	2
45	X	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
46	Y	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
47	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
48	0	54/56 (96%)	49 (91%)	5 (9%)	0	100	100
49	1	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
50	2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
51	3	62/64 (97%)	54 (87%)	6 (10%)	2 (3%)	3	18
52	4	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
53	6	64/66 (97%)	54 (84%)	10 (16%)	0	100	100
55	7	222/224 (99%)	181 (82%)	34 (15%)	7 (3%)	3	18
56	w	185/188 (98%)	153 (83%)	28 (15%)	4 (2%)	5	24
All	All	5989/6092 (98%)	5301 (88%)	644 (11%)	44 (1%)	20	49

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	f	53	LYS
17	q	70	LYS
29	G	47	ASN
42	U	89	GLY
44	W	27	GLY
51	3	31	ILE
55	7	69	THR
55	7	140	PRO
56	w	147	ALA
6	f	55	HIS
12	l	102	ASP
13	m	5	GLY
15	o	46	LYS
34	M	59	ARG
44	W	28	GLY
44	W	50	ASN
44	W	64	ASP
44	W	74	PRO
44	W	78	LYS

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Mol	Chain	Res	Type
51	3	32	LEU
55	7	133	PRO
55	7	201	PRO
29	G	108	PHE
56	w	32	PRO
56	w	148	GLY
5	e	122	VAL
9	i	90	ASP
9	i	91	GLU
34	M	58	LYS
39	R	54	VAL
40	S	2	GLU
40	S	64	ALA
44	W	41	ARG
44	W	68	LYS
5	e	121	ASN
13	m	4	ALA
29	G	119	GLY
55	7	67	HIS
55	7	138	PRO
12	l	3	VAL
55	7	136	LEU
56	w	146	THR
34	M	69	PRO
10	j	57	VAL

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	
2	b	180/180 (100%)	180 (100%)	0	100	100
3	c	170/170 (100%)	169 (99%)	1 (1%)	78	83
4	d	172/172 (100%)	169 (98%)	3 (2%)	53	74
5	e	114/119 (96%)	113 (99%)	1 (1%)	70	80
6	f	87/87 (100%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	g	124/124 (100%)	124 (100%)	0	100	100
8	h	104/104 (100%)	103 (99%)	1 (1%)	68	79
9	i	105/105 (100%)	104 (99%)	1 (1%)	68	79
10	j	86/86 (100%)	85 (99%)	1 (1%)	63	78
11	k	89/89 (100%)	88 (99%)	1 (1%)	65	78
12	l	103/103 (100%)	103 (100%)	0	100	100
13	m	92/92 (100%)	90 (98%)	2 (2%)	45	71
14	n	79/83 (95%)	79 (100%)	0	100	100
15	o	76/76 (100%)	76 (100%)	0	100	100
16	p	65/65 (100%)	65 (100%)	0	100	100
17	q	74/74 (100%)	73 (99%)	1 (1%)	59	76
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	70/70 (100%)	68 (97%)	2 (3%)	37	66
20	t	65/65 (100%)	65 (100%)	0	100	100
21	u	44/55 (80%)	44 (100%)	0	100	100
25	C	216/216 (100%)	215 (100%)	1 (0%)	81	85
26	D	164/164 (100%)	164 (100%)	0	100	100
27	E	165/165 (100%)	165 (100%)	0	100	100
28	F	148/148 (100%)	147 (99%)	1 (1%)	76	82
29	G	137/137 (100%)	137 (100%)	0	100	100
30	H	114/114 (100%)	114 (100%)	0	100	100
31	J	116/116 (100%)	116 (100%)	0	100	100
32	K	103/103 (100%)	103 (100%)	0	100	100
33	L	102/102 (100%)	100 (98%)	2 (2%)	48	72
34	M	109/109 (100%)	107 (98%)	2 (2%)	51	73
35	N	100/100 (100%)	100 (100%)	0	100	100
36	O	86/86 (100%)	86 (100%)	0	100	100
37	P	99/99 (100%)	98 (99%)	1 (1%)	68	79
38	Q	89/89 (100%)	88 (99%)	1 (1%)	65	78
39	R	84/84 (100%)	83 (99%)	1 (1%)	63	78
40	S	93/93 (100%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	T	80/80 (100%)	79 (99%)	1 (1%)	61	77
42	U	83/83 (100%)	83 (100%)	0	100	100
43	V	78/78 (100%)	78 (100%)	0	100	100
44	W	59/59 (100%)	38 (64%)	21 (36%)	0	0
45	X	67/67 (100%)	67 (100%)	0	100	100
46	Y	55/55 (100%)	55 (100%)	0	100	100
47	Z	48/48 (100%)	48 (100%)	0	100	100
48	0	47/47 (100%)	47 (100%)	0	100	100
49	1	45/45 (100%)	44 (98%)	1 (2%)	45	71
50	2	38/38 (100%)	38 (100%)	0	100	100
51	3	51/51 (100%)	50 (98%)	1 (2%)	48	72
52	4	34/34 (100%)	34 (100%)	0	100	100
53	6	59/59 (100%)	59 (100%)	0	100	100
55	7	173/173 (100%)	167 (96%)	6 (4%)	32	62
56	w	154/154 (100%)	148 (96%)	6 (4%)	28	60
All	All	4943/4971 (99%)	4884 (99%)	59 (1%)	61	78

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	156	LEU
4	d	80	ARG
4	d	142	VAL
4	d	149	LYS
5	e	15	ILE
8	h	120	LEU
9	i	60	LEU
10	j	75	ASP
11	k	30	ILE
13	m	16	ILE
13	m	24	VAL
17	q	18	LYS
19	s	10	ILE
19	s	48	ILE
25	C	252	LYS
28	F	140	ILE
33	L	27	LEU

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Mol	Chain	Res	Type
33	L	96	LYS
34	M	6	ARG
34	M	46	ILE
37	P	72	VAL
38	Q	8	ILE
39	R	22	LEU
41	T	32	LEU
44	W	10	THR
44	W	11	ARG
44	W	12	ASN
44	W	16	SER
44	W	19	LYS
44	W	29	GLU
44	W	35	SER
44	W	36	ILE
44	W	40	GLN
44	W	41	ARG
44	W	43	THR
44	W	64	ASP
44	W	66	LYS
44	W	68	LYS
44	W	75	LYS
44	W	76	ASN
44	W	77	ARG
44	W	80	ILE
44	W	81	SER
44	W	82	ILE
44	W	83	GLU
49	1	46	VAL
51	3	31	ILE
55	7	119	ASP
55	7	121	MET
55	7	136	LEU
55	7	137	MET
55	7	200	LYS
55	7	203	GLN
56	w	17	LEU
56	w	29	PHE
56	w	30	VAL
56	w	31	LYS
56	w	107	LEU
56	w	143	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	23	ASN
2	b	35	ASN
2	b	38	HIS
2	b	119	GLN
2	b	169	HIS
2	b	202	ASN
4	d	115	GLN
4	d	135	GLN
4	d	151	GLN
5	e	69	ASN
5	e	88	HIS
6	f	37	HIS
6	f	55	HIS
6	f	63	ASN
7	g	147	ASN
8	h	3	GLN
8	h	66	GLN
9	i	30	ASN
9	i	36	GLN
12	l	45	ASN
15	o	34	GLN
15	o	49	HIS
16	p	29	ASN
16	p	79	ASN
17	q	30	HIS
17	q	44	HIS
19	s	13	HIS
19	s	56	HIS
19	s	68	HIS
20	t	19	HIS
20	t	47	GLN
20	t	51	ASN
20	t	60	GLN
20	t	69	ASN
20	t	81	GLN
25	C	36	ASN
25	C	45	ASN
25	C	85	ASN
25	C	114	GLN
25	C	259	ASN
26	D	32	ASN

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Mol	Chain	Res	Type
26	D	49	GLN
26	D	150	GLN
26	D	164	GLN
27	E	90	GLN
27	E	92	HIS
27	E	136	GLN
27	E	156	ASN
29	G	63	GLN
29	G	115	GLN
29	G	138	GLN
30	H	66	ASN
30	H	145	ASN
31	J	40	HIS
31	J	58	ASN
32	K	5	GLN
35	N	31	HIS
37	P	11	GLN
38	Q	51	GLN
38	Q	71	ASN
39	R	18	GLN
39	R	43	ASN
39	R	91	GLN
40	S	7	HIS
40	S	57	ASN
41	T	15	HIS
42	U	68	ASN
42	U	73	ASN
43	V	80	HIS
44	W	40	GLN
45	X	33	HIS
46	Y	58	ASN
49	1	45	HIS
51	3	42	HIS
52	4	35	GLN
53	6	20	ASN
53	6	41	HIS
53	6	61	ASN
55	7	24	ASN
55	7	129	GLN
55	7	155	ASN
56	w	71	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1538/1539 (99%)	331 (21%)	0
22	v	5/6 (83%)	2 (40%)	0
23	A	2868/2903 (98%)	606 (21%)	27 (0%)
24	B	119/120 (99%)	21 (17%)	1 (0%)
54	x	76/77 (98%)	32 (42%)	0
All	All	4606/4645 (99%)	992 (21%)	28 (0%)

All (992) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	U
1	a	5	U
1	a	6	G
1	a	9	G
1	a	22	G
1	a	32	A
1	a	33	A
1	a	39	G
1	a	40	C
1	a	41	G
1	a	47	C
1	a	50	A
1	a	51	A
1	a	55	A
1	a	56	U
1	a	58	C
1	a	60	A
1	a	64	G
1	a	66	A
1	a	68	G
1	a	71	A
1	a	74	A
1	a	75	G
1	a	79	G
1	a	80	A
1	a	81	A
1	a	82	G
1	a	83	C
1	a	86	G
1	a	87	C
1	a	89	U

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Mol	Chain	Res	Type
1	a	92	U
1	a	94	G
1	a	95	C
1	a	98	A
1	a	99	C
1	a	104	G
1	a	116	A
1	a	121	U
1	a	131	A
1	a	139	A
1	a	141	G
1	a	147	G
1	a	148	G
1	a	149	A
1	a	157	U
1	a	160	A
1	a	161	A
1	a	163	C
1	a	173	U
1	a	181	A
1	a	182	A
1	a	183	C
1	a	184	G
1	a	191	G
1	a	204	G
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	214	C
1	a	223	A
1	a	226	G
1	a	245	U
1	a	247	G
1	a	251	G
1	a	254	G
1	a	266	G
1	a	267	C
1	a	279	A
1	a	280	C
1	a	281	G
1	a	289	G

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Mol	Chain	Res	Type
1	a	298	A
1	a	316	C
1	a	317	U
1	a	320	A
1	a	321	A
1	a	325	A
1	a	328	C
1	a	330	C
1	a	344	A
1	a	345	C
1	a	346	G
1	a	347	G
1	a	352	C
1	a	354	G
1	a	359	G
1	a	360	G
1	a	365	U
1	a	366	A
1	a	367	U
1	a	368	U
1	a	370	C
1	a	372	C
1	a	373	A
1	a	381	C
1	a	388	G
1	a	390	U
1	a	392	C
1	a	398	U
1	a	406	G
1	a	407	U
1	a	408	A
1	a	412	A
1	a	413	G
1	a	414	A
1	a	421	U
1	a	422	C
1	a	423	G
1	a	424	G
1	a	429	U
1	a	430	A
1	a	436	C
1	a	444	G

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Mol	Chain	Res	Type
1	a	466	A
1	a	467	U
1	a	468	A
1	a	473	U
1	a	474	G
1	a	477	C
1	a	484	G
1	a	486	U
1	a	491	G
1	a	494	G
1	a	496	A
1	a	497	G
1	a	498	A
1	a	499	A
1	a	502	A
1	a	505	G
1	a	510	A
1	a	511	C
1	a	514	C
1	a	518	C
1	a	521	G
1	a	525	C
1	a	527	G
1	a	531	U
1	a	532	A
1	a	533	A
1	a	536	C
1	a	547	A
1	a	559	A
1	a	562	U
1	a	564	C
1	a	572	A
1	a	573	A
1	a	574	A
1	a	575	G
1	a	576	C
1	a	577	G
1	a	579	A
1	a	583	A
1	a	596	A
1	a	607	A
1	a	613	C

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Mol	Chain	Res	Type
1	a	619	U
1	a	623	C
1	a	632	U
1	a	633	G
1	a	634	C
1	a	635	A
1	a	637	C
1	a	641	U
1	a	642	A
1	a	650	G
1	a	652	U
1	a	654	G
1	a	661	G
1	a	665	A
1	a	688	G
1	a	695	A
1	a	703	G
1	a	705	G
1	a	718	A
1	a	721	G
1	a	723	U
1	a	724	G
1	a	731	G
1	a	744	C
1	a	746	A
1	a	748	G
1	a	753	A
1	a	754	C
1	a	755	G
1	a	759	A
1	a	761	G
1	a	777	A
1	a	793	U
1	a	805	C
1	a	812	G
1	a	815	A
1	a	817	C
1	a	818	G
1	a	819	A
1	a	820	U
1	a	821	G
1	a	822	U

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Mol	Chain	Res	Type
1	a	832	G
1	a	836	G
1	a	843	U
1	a	844	G
1	a	846	G
1	a	849	G
1	a	851	G
1	a	864	A
1	a	885	G
1	a	890	G
1	a	902	G
1	a	926	G
1	a	932	C
1	a	934	C
1	a	939	G
1	a	960	U
1	a	961	U
1	a	966	G
1	a	969	A
1	a	975	A
1	a	976	G
1	a	977	A
1	a	987	G
1	a	991	U
1	a	992	U
1	a	993	G
1	a	994	A
1	a	1001	C
1	a	1004	A
1	a	1028	C
1	a	1030	U
1	a	1031	C
1	a	1032	G
1	a	1033	G
1	a	1034	G
1	a	1035	A
1	a	1036	A
1	a	1053	G
1	a	1065	U
1	a	1081	A
1	a	1085	U
1	a	1094	G

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Mol	Chain	Res	Type
1	a	1095	U
1	a	1099	G
1	a	1101	A
1	a	1118	U
1	a	1130	A
1	a	1132	C
1	a	1133	G
1	a	1136	C
1	a	1137	C
1	a	1138	G
1	a	1139	G
1	a	1140	C
1	a	1151	A
1	a	1152	A
1	a	1159	U
1	a	1168	U
1	a	1169	A
1	a	1171	A
1	a	1181	G
1	a	1182	G
1	a	1183	U
1	a	1184	G
1	a	1191	A
1	a	1196	A
1	a	1197	A
1	a	1199	U
1	a	1201	A
1	a	1202	U
1	a	1212	U
1	a	1213	A
1	a	1214	C
1	a	1227	A
1	a	1228	C
1	a	1238	A
1	a	1241	G
1	a	1253	G
1	a	1256	A
1	a	1257	A
1	a	1258	G
1	a	1260	G
1	a	1261	A
1	a	1278	G

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Mol	Chain	Res	Type
1	a	1280	A
1	a	1281	C
1	a	1282	C
1	a	1287	A
1	a	1294	G
1	a	1297	G
1	a	1298	U
1	a	1300	G
1	a	1301	U
1	a	1317	C
1	a	1321	U
1	a	1322	C
1	a	1332	A
1	a	1335	U
1	a	1346	A
1	a	1347	G
1	a	1348	U
1	a	1353	G
1	a	1363	A
1	a	1364	U
1	a	1365	G
1	a	1368	A
1	a	1370	G
1	a	1379	G
1	a	1383	C
1	a	1396	A
1	a	1398	A
1	a	1400	C
1	a	1406	U
1	a	1419	G
1	a	1425	U
1	a	1433	A
1	a	1446	A
1	a	1452	C
1	a	1487	G
1	a	1492	A
1	a	1497	G
1	a	1502	A
1	a	1503	A
1	a	1506	U
1	a	1517	G
1	a	1520	C

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Mol	Chain	Res	Type
1	a	1529	G
1	a	1530	G
1	a	1534	A
1	a	1535	C
1	a	1536	C
1	a	1539	C
22	v	17	C
22	v	18	G
23	A	5	A
23	A	10	A
23	A	34	U
23	A	35	G
23	A	43	G
23	A	46	G
23	A	51	G
23	A	52	A
23	A	71	A
23	A	74	A
23	A	75	G
23	A	84	A
23	A	86	G
23	A	92	U
23	A	93	G
23	A	98	G
23	A	118	A
23	A	119	A
23	A	120	U
23	A	139	U
23	A	140	C
23	A	141	G
23	A	142	A
23	A	149	A
23	A	162	U
23	A	163	C
23	A	181	A
23	A	186	G
23	A	193	U
23	A	194	G
23	A	196	A
23	A	199	A
23	A	200	U
23	A	204	A

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Mol	Chain	Res	Type
23	A	206	U
23	A	213	A
23	A	215	G
23	A	216	A
23	A	218	A
23	A	219	A
23	A	221	A
23	A	222	A
23	A	223	A
23	A	225	C
23	A	229	C
23	A	230	G
23	A	241	A
23	A	242	G
23	A	243	U
23	A	248	G
23	A	255	A
23	A	265	A
23	A	267	C
23	A	268	C
23	A	272	A
23	A	276	U
23	A	277	G
23	A	278	A
23	A	279	A
23	A	285	G
23	A	292	U
23	A	311	A
23	A	316	C
23	A	323	C
23	A	329	G
23	A	330	A
23	A	334	C
23	A	335	C
23	A	345	A
23	A	353	C
23	A	361	G
23	A	362	A
23	A	367	G
23	A	370	G
23	A	371	A
23	A	372	G

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Mol	Chain	Res	Type
23	A	386	G
23	A	387	U
23	A	395	U
23	A	403	U
23	A	404	A
23	A	406	G
23	A	411	G
23	A	417	C
23	A	421	C
23	A	422	A
23	A	424	G
23	A	434	U
23	A	448	U
23	A	458	G
23	A	473	G
23	A	481	G
23	A	491	G
23	A	505	A
23	A	508	A
23	A	509	C
23	A	530	G
23	A	531	C
23	A	532	A
23	A	533	G
23	A	543	G
23	A	544	C
23	A	545	U
23	A	546	U
23	A	547	A
23	A	548	G
23	A	549	G
23	A	550	C
23	A	555	G
23	A	563	A
23	A	573	U
23	A	575	A
23	A	586	A
23	A	603	A
23	A	614	A
23	A	615	U
23	A	616	A
23	A	622	G

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Mol	Chain	Res	Type
23	A	627	A
23	A	637	A
23	A	644	A
23	A	645	C
23	A	646	U
23	A	647	G
23	A	654	A
23	A	655	A
23	A	659	G
23	A	668	A
23	A	669	G
23	A	670	A
23	A	677	A
23	A	686	U
23	A	695	G
23	A	696	G
23	A	704	G
23	A	711	G
23	A	718	A
23	A	728	G
23	A	730	A
23	A	736	C
23	A	738	G
23	A	739	A
23	A	747	C
23	A	752	A
23	A	764	A
23	A	765	C
23	A	782	A
23	A	783	A
23	A	784	G
23	A	789	A
23	A	791	C
23	A	805	G
23	A	807	U
23	A	812	C
23	A	819	A
23	A	827	U
23	A	828	U
23	A	829	A
23	A	831	G
23	A	845	A

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Mol	Chain	Res	Type
23	A	846	U
23	A	847	U
23	A	856	G
23	A	858	G
23	A	860	U
23	A	878	A
23	A	879	G
23	A	885	C
23	A	886	A
23	A	895	U
23	A	896	A
23	A	897	C
23	A	902	C
23	A	907	G
23	A	910	A
23	A	931	U
23	A	941	A
23	A	946	C
23	A	953	G
23	A	961	C
23	A	974	G
23	A	983	A
23	A	989	G
23	A	995	C
23	A	996	A
23	A	997	G
23	A	999	U
23	A	1009	A
23	A	1012	U
23	A	1013	C
23	A	1021	A
23	A	1023	U
23	A	1025	G
23	A	1026	G
23	A	1033	U
23	A	1041	G
23	A	1045	C
23	A	1046	A
23	A	1052	C
23	A	1054	A
23	A	1057	A
23	A	1059	G

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Mol	Chain	Res	Type
23	A	1060	U
23	A	1061	U
23	A	1062	G
23	A	1064	C
23	A	1065	U
23	A	1066	U
23	A	1067	A
23	A	1069	A
23	A	1070	A
23	A	1071	G
23	A	1072	C
23	A	1073	A
23	A	1075	C
23	A	1076	C
23	A	1078	U
23	A	1079	C
23	A	1083	U
23	A	1084	A
23	A	1087	G
23	A	1088	A
23	A	1089	A
23	A	1090	A
23	A	1094	U
23	A	1096	A
23	A	1097	U
23	A	1098	A
23	A	1099	G
23	A	1100	C
23	A	1102	C
23	A	1103	A
23	A	1104	C
23	A	1111	A
23	A	1112	G
23	A	1130	U
23	A	1131	G
23	A	1132	U
23	A	1133	A
23	A	1135	C
23	A	1139	G
23	A	1142	A
23	A	1150	C
23	A	1155	A

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Mol	Chain	Res	Type
23	A	1172	C
23	A	1175	A
23	A	1176	U
23	A	1180	U
23	A	1183	U
23	A	1204	A
23	A	1205	A
23	A	1206	G
23	A	1211	C
23	A	1212	G
23	A	1237	A
23	A	1247	A
23	A	1248	G
23	A	1253	A
23	A	1256	G
23	A	1268	A
23	A	1271	G
23	A	1272	A
23	A	1275	A
23	A	1300	G
23	A	1301	A
23	A	1306	C
23	A	1312	U
23	A	1325	U
23	A	1329	U
23	A	1330	C
23	A	1341	G
23	A	1344	U
23	A	1345	C
23	A	1352	U
23	A	1360	G
23	A	1365	A
23	A	1368	G
23	A	1378	A
23	A	1379	U
23	A	1381	G
23	A	1383	A
23	A	1386	C
23	A	1395	A
23	A	1403	A
23	A	1414	C
23	A	1416	G

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Mol	Chain	Res	Type
23	A	1417	C
23	A	1428	C
23	A	1434	A
23	A	1453	A
23	A	1454	C
23	A	1455	G
23	A	1458	U
23	A	1461	C
23	A	1475	G
23	A	1476	U
23	A	1482	G
23	A	1483	G
23	A	1488	C
23	A	1490	A
23	A	1491	G
23	A	1494	A
23	A	1497	U
23	A	1504	A
23	A	1505	A
23	A	1508	A
23	A	1509	A
23	A	1515	A
23	A	1522	A
23	A	1524	G
23	A	1529	G
23	A	1532	A
23	A	1534	U
23	A	1535	A
23	A	1536	C
23	A	1542	U
23	A	1554	U
23	A	1555	G
23	A	1558	C
23	A	1559	U
23	A	1560	G
23	A	1565	C
23	A	1569	A
23	A	1578	U
23	A	1583	A
23	A	1584	U
23	A	1585	C
23	A	1597	A

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Mol	Chain	Res	Type
23	A	1608	A
23	A	1611	C
23	A	1647	U
23	A	1648	U
23	A	1649	G
23	A	1654	A
23	A	1672	A
23	A	1674	G
23	A	1694	C
23	A	1695	G
23	A	1703	G
23	A	1704	C
23	A	1713	A
23	A	1715	G
23	A	1727	C
23	A	1729	U
23	A	1730	C
23	A	1731	G
23	A	1732	C
23	A	1733	G
23	A	1735	A
23	A	1738	G
23	A	1757	A
23	A	1758	U
23	A	1759	A
23	A	1764	C
23	A	1773	A
23	A	1776	G
23	A	1780	A
23	A	1781	U
23	A	1782	U
23	A	1786	A
23	A	1787	A
23	A	1791	A
23	A	1800	C
23	A	1801	A
23	A	1802	A
23	A	1808	A
23	A	1816	C
23	A	1829	A
23	A	1833	C
23	A	1859	U

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Mol	Chain	Res	Type
23	A	1866	A
23	A	1869	G
23	A	1870	C
23	A	1871	A
23	A	1872	A
23	A	1873	G
23	A	1884	G
23	A	1896	G
23	A	1900	A
23	A	1901	A
23	A	1906	G
23	A	1913	A
23	A	1914	C
23	A	1916	A
23	A	1927	A
23	A	1929	G
23	A	1930	G
23	A	1931	U
23	A	1936	A
23	A	1937	A
23	A	1938	A
23	A	1940	U
23	A	1941	C
23	A	1946	U
23	A	1955	U
23	A	1964	G
23	A	1966	A
23	A	1967	C
23	A	1970	A
23	A	1971	U
23	A	1972	G
23	A	1991	U
23	A	1992	G
23	A	1996	C
23	A	1997	C
23	A	2004	G
23	A	2006	C
23	A	2020	A
23	A	2022	U
23	A	2023	C
23	A	2030	A
23	A	2031	A

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Mol	Chain	Res	Type
23	A	2033	A
23	A	2035	G
23	A	2036	C
23	A	2043	C
23	A	2046	G
23	A	2049	G
23	A	2052	A
23	A	2055	C
23	A	2056	G
23	A	2060	A
23	A	2061	G
23	A	2062	A
23	A	2069	A
23	A	2072	C
23	A	2092	U
23	A	2093	G
23	A	2096	C
23	A	2097	A
23	A	2099	U
23	A	2100	G
23	A	2101	A
23	A	2103	C
23	A	2104	U
23	A	2105	U
23	A	2107	G
23	A	2111	U
23	A	2112	G
23	A	2113	U
23	A	2114	A
23	A	2116	G
23	A	2117	A
23	A	2119	A
23	A	2120	G
23	A	2125	G
23	A	2126	A
23	A	2127	G
23	A	2128	G
23	A	2159	G
23	A	2160	C
23	A	2161	C
23	A	2167	U
23	A	2169	A

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Mol	Chain	Res	Type
23	A	2170	A
23	A	2177	C
23	A	2178	C
23	A	2179	C
23	A	2180	U
23	A	2181	U
23	A	2185	U
23	A	2187	U
23	A	2188	U
23	A	2189	U
23	A	2190	G
23	A	2191	A
23	A	2193	G
23	A	2198	A
23	A	2203	U
23	A	2204	G
23	A	2210	U
23	A	2211	A
23	A	2213	U
23	A	2214	C
23	A	2219	U
23	A	2223	G
23	A	2225	A
23	A	2226	C
23	A	2238	G
23	A	2239	G
23	A	2250	G
23	A	2251	G
23	A	2259	U
23	A	2266	A
23	A	2267	A
23	A	2273	A
23	A	2279	G
23	A	2283	C
23	A	2287	A
23	A	2288	A
23	A	2294	G
23	A	2305	U
23	A	2309	A
23	A	2311	A
23	A	2325	G
23	A	2327	A

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Mol	Chain	Res	Type
23	A	2333	A
23	A	2334	U
23	A	2335	A
23	A	2336	A
23	A	2344	U
23	A	2345	G
23	A	2350	C
23	A	2354	C
23	A	2361	G
23	A	2372	U
23	A	2382	G
23	A	2383	G
23	A	2385	C
23	A	2392	A
23	A	2393	U
23	A	2394	C
23	A	2402	U
23	A	2406	A
23	A	2419	U
23	A	2424	C
23	A	2428	G
23	A	2429	G
23	A	2430	A
23	A	2435	A
23	A	2441	U
23	A	2445	G
23	A	2448	A
23	A	2449	U
23	A	2465	C
23	A	2469	A
23	A	2474	U
23	A	2476	A
23	A	2481	G
23	A	2491	U
23	A	2502	G
23	A	2503	A
23	A	2505	G
23	A	2506	U
23	A	2507	C
23	A	2513	A
23	A	2517	C
23	A	2518	A

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Mol	Chain	Res	Type
23	A	2529	G
23	A	2534	A
23	A	2547	A
23	A	2554	U
23	A	2556	C
23	A	2566	A
23	A	2567	G
23	A	2572	A
23	A	2573	C
23	A	2576	G
23	A	2582	G
23	A	2585	U
23	A	2586	U
23	A	2602	A
23	A	2604	U
23	A	2610	C
23	A	2613	U
23	A	2614	A
23	A	2629	U
23	A	2638	G
23	A	2646	C
23	A	2655	G
23	A	2656	U
23	A	2674	G
23	A	2685	G
23	A	2689	U
23	A	2690	U
23	A	2706	A
23	A	2707	U
23	A	2714	G
23	A	2716	C
23	A	2718	G
23	A	2726	A
23	A	2732	G
23	A	2733	A
23	A	2744	G
23	A	2748	A
23	A	2760	C
23	A	2764	A
23	A	2765	A
23	A	2769	U
23	A	2778	A

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Mol	Chain	Res	Type
23	A	2779	U
23	A	2790	U
23	A	2791	G
23	A	2793	C
23	A	2794	C
23	A	2796	U
23	A	2800	A
23	A	2808	G
23	A	2809	A
23	A	2818	U
23	A	2820	A
23	A	2821	A
23	A	2833	U
23	A	2835	A
23	A	2836	U
23	A	2846	G
23	A	2849	U
23	A	2861	U
23	A	2867	G
23	A	2868	A
23	A	2873	A
23	A	2880	C
23	A	2883	A
23	A	2884	U
23	A	2893	A
23	A	2899	A
24	B	3	C
24	B	4	C
24	B	13	G
24	B	15	A
24	B	21	G
24	B	24	G
24	B	26	C
24	B	30	C
24	B	35	C
24	B	36	C
24	B	40	U
24	B	42	C
24	B	44	G
24	B	45	A
24	B	67	G
24	B	88	C

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Mol	Chain	Res	Type
24	B	89	U
24	B	90	C
24	B	91	C
24	B	105	G
24	B	109	A
54	x	2	G
54	x	3	G
54	x	4	U
54	x	5	G
54	x	6	A
54	x	8	U
54	x	13	C
54	x	14	A
54	x	18	G
54	x	19	G
54	x	20	U
54	x	21	A
54	x	22	G
54	x	25	C
54	x	26	A
54	x	27	C
54	x	35	G
54	x	36	G
54	x	40	G
54	x	42	A
54	x	47	U
54	x	51	A
54	x	53	G
54	x	54	U
54	x	61	C
54	x	66	A
54	x	67	U
54	x	68	C
54	x	72	G
54	x	73	A
54	x	74	C
54	x	76	A

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	A	51	G

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Mol	Chain	Res	Type
23	A	242	G
23	A	421	C
23	A	490	C
23	A	615	U
23	A	859	G
23	A	1020	A
23	A	1022	G
23	A	1070	A
23	A	1111	A
23	A	1141	U
23	A	1182	G
23	A	1190	G
23	A	1300	G
23	A	1331	G
23	A	1378	A
23	A	1399	C
23	A	1432	G
23	A	1730	C
23	A	1930	G
23	A	1940	U
23	A	2190	G
23	A	2286	G
23	A	2326	C
23	A	2391	G
23	A	2655	G
23	A	2808	G
24	B	66	A

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

1 non-standard protein/DNA/RNA residue is 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
56	KEO	w	34	-	16,18,19	1.46	2 (12%)	15,21,23	1.38	3 (20%)

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
56	KEO	w	34	-	-	10/19/20/22	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	34	KEO	C05-NZ	4.91	1.45	1.33
56	w	34	KEO	O02-C05	-2.33	1.18	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	34	KEO	CE-NZ-C05	-2.83	117.55	122.82
56	w	34	KEO	C06-C05-NZ	2.62	120.02	115.97
56	w	34	KEO	CB-CG-CD	-2.41	107.31	112.42

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	w	34	KEO	O-C-CA-CB
56	w	34	KEO	N-CA-CB-CG
56	w	34	KEO	C-CA-CB-CG
56	w	34	KEO	CA-CB-CG-O01
56	w	34	KEO	C05-C06-C07-C08
56	w	34	KEO	C05-C06-C07-N02
56	w	34	KEO	C06-C05-NZ-CE
56	w	34	KEO	O02-C05-NZ-CE
56	w	34	KEO	CA-CB-CG-CD
56	w	34	KEO	C06-C07-C08-C09

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	w	34	KEO	1	0

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	$\# Z > 2$
57	PRO	A	3001	-	6,7,8	0.74	0	7,8,10	1.25	1 (14%)
57	PRO	x	101	-	6,7,8	0.77	0	7,8,10	1.28	1 (14%)

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
57	PRO	A	3001	-	-	0/0/9/11	0/1/1/1
57	PRO	x	101	-	-	0/0/9/11	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A	3001	PRO	O-C-CA	-2.35	118.73	124.77
57	x	101	PRO	O-C-CA	-2.26	118.97	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	A	3001	PRO	2	0
57	x	101	PRO	1	0

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.

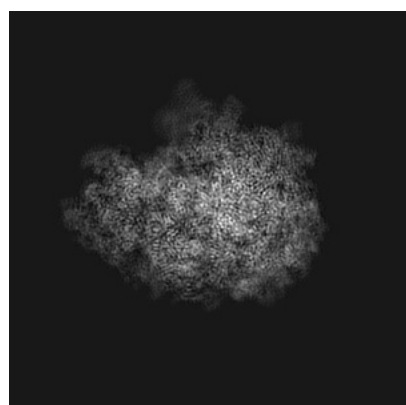
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3903. These allow visual inspection of the internal detail of the map and identification of artifacts.

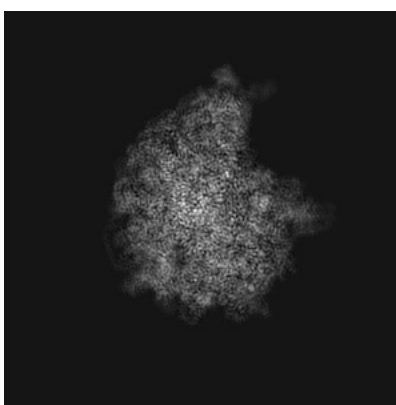
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

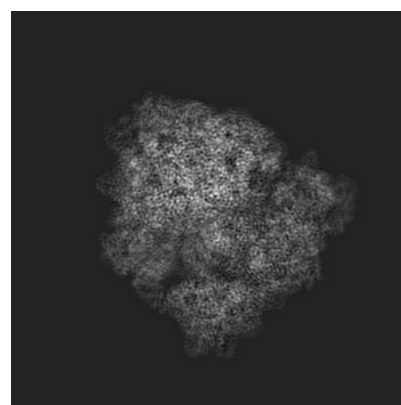
6.1.1 Primary map



X



Y

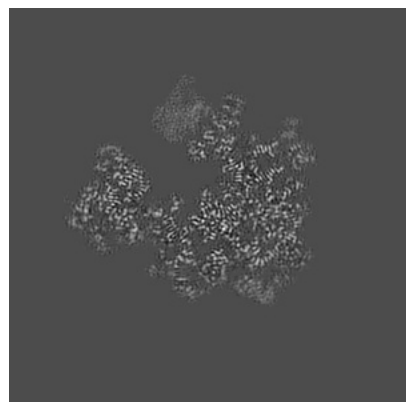


Z

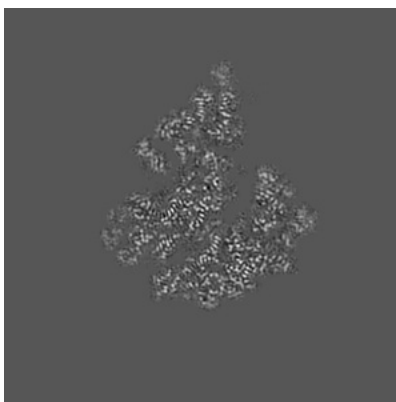
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

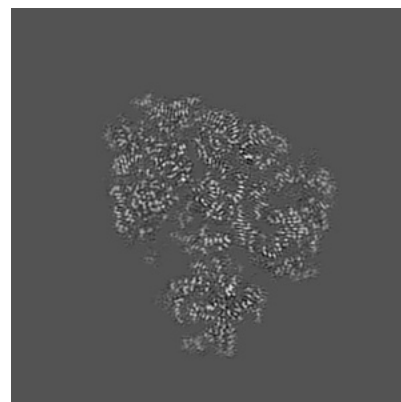
6.2.1 Primary map



X Index: 180



Y Index: 180

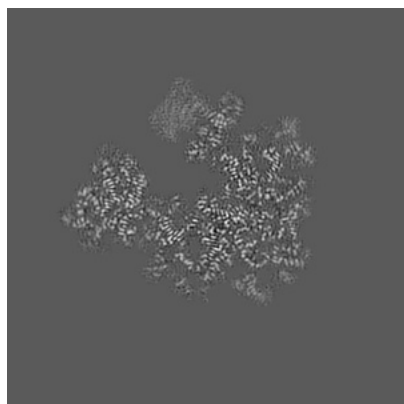


Z Index: 180

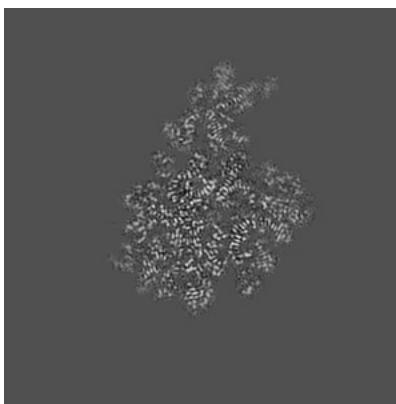
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

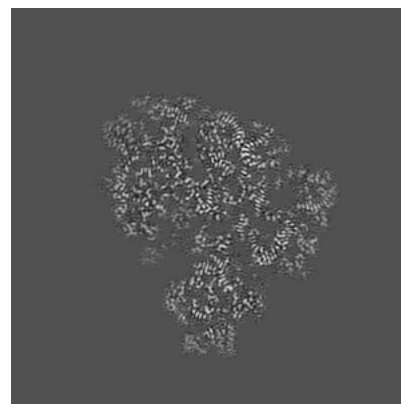
6.3.1 Primary map



X Index: 177



Y Index: 191

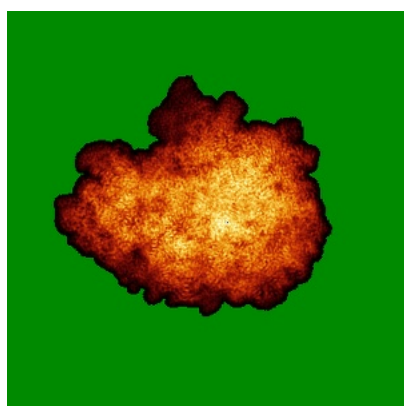


Z Index: 177

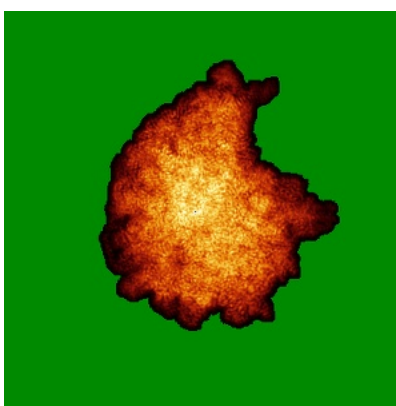
The images above show the largest variance slices of the map in three orthogonal directions.

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

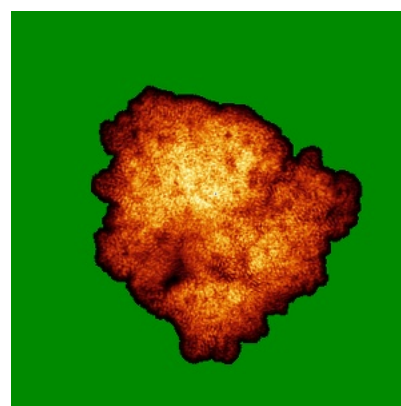
6.4.1 Primary map



X



Y

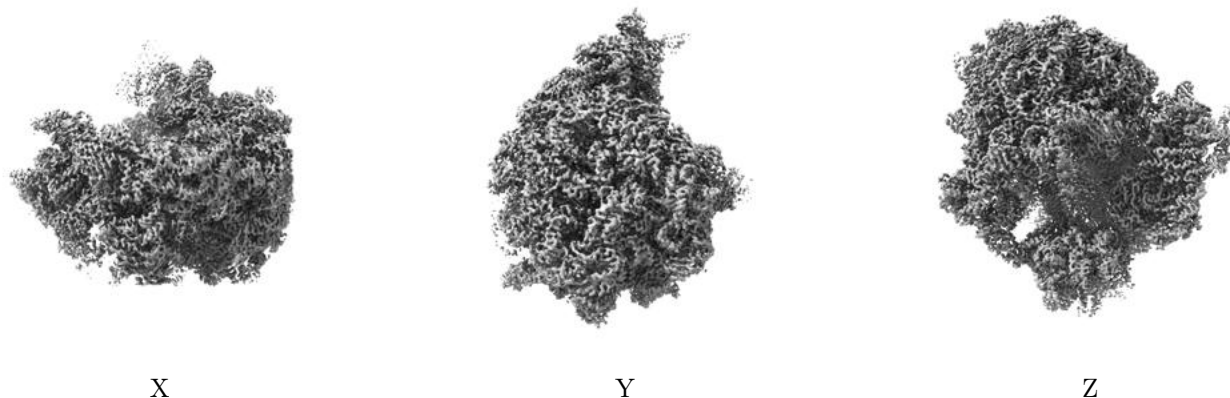


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.108. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

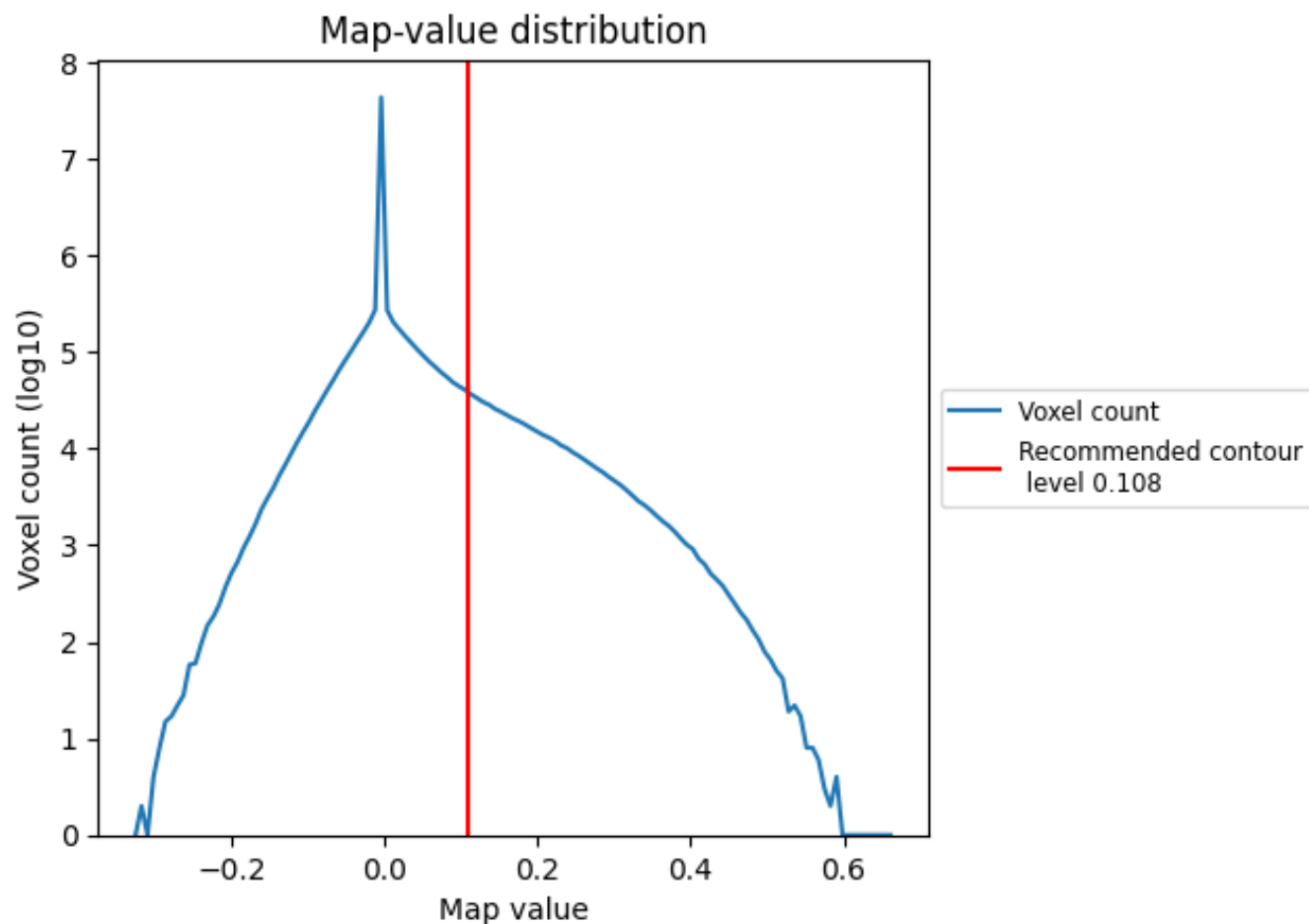
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

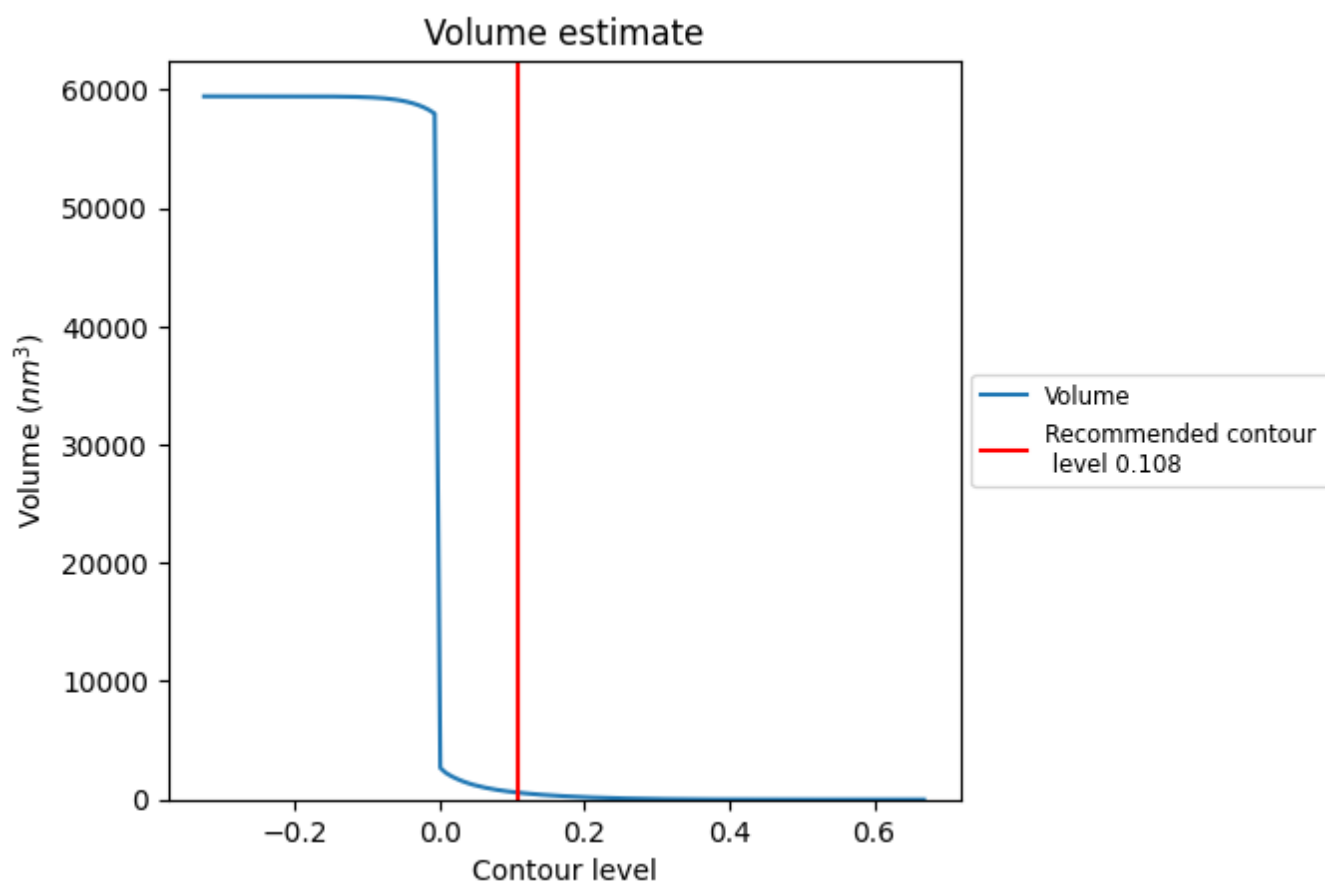
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

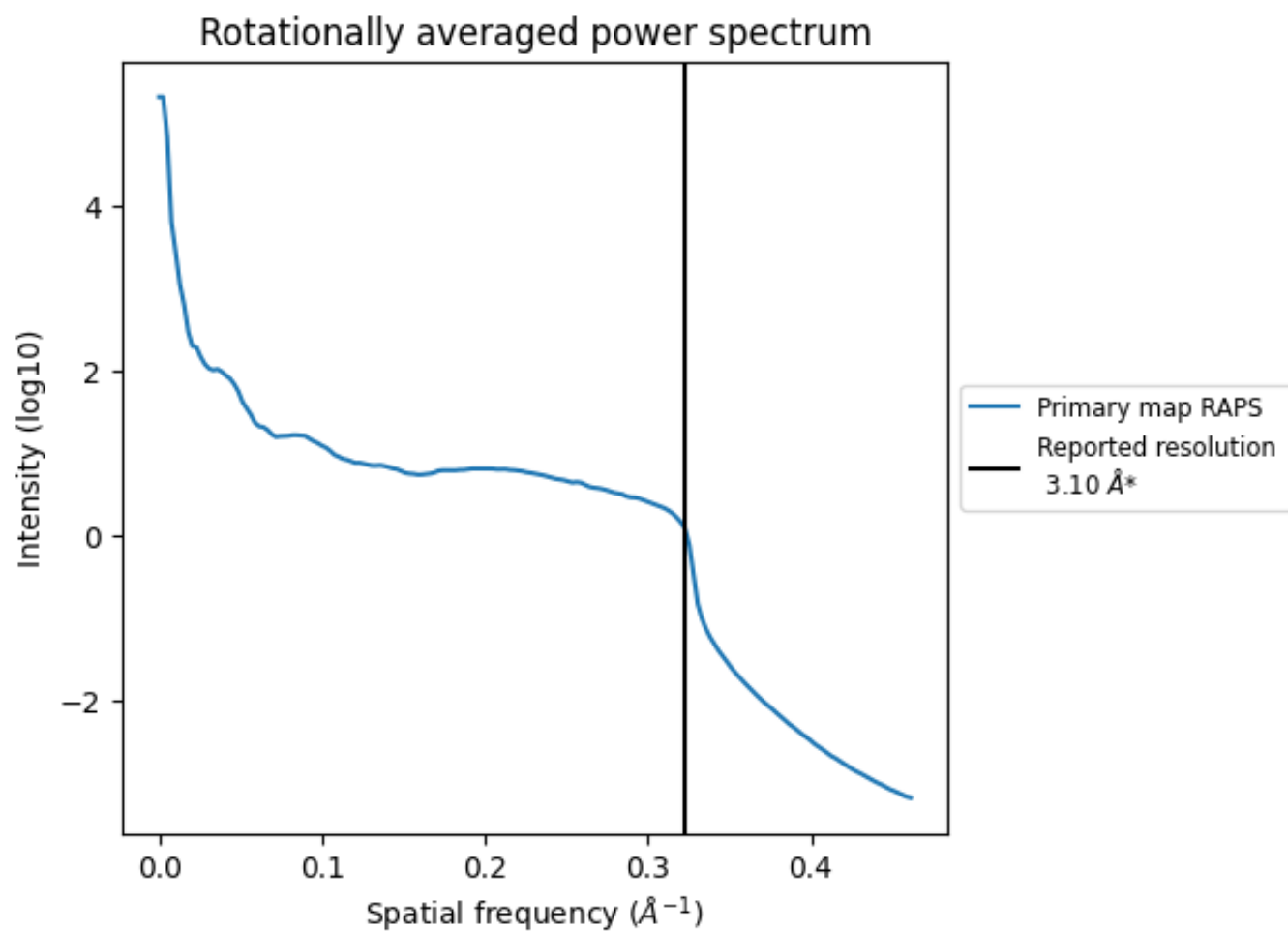
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 588 nm³; this corresponds to an approximate mass of 532 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 0.323 Å⁻¹

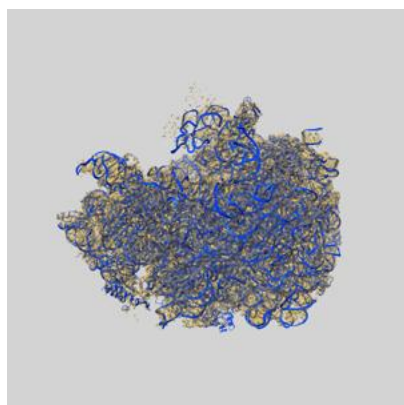
8 Fourier-Shell correlation

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

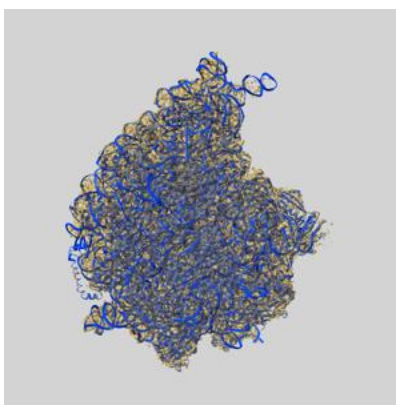
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3903 and PDB model 6ENU. Per-residue inclusion information can be found in section 3 on page 16.

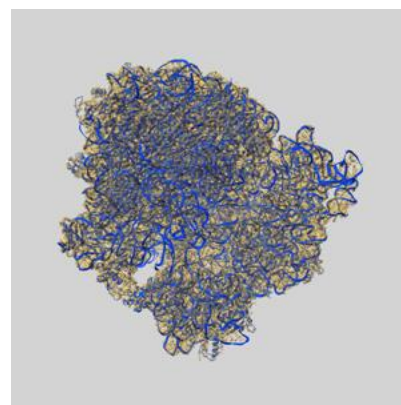
9.1 Map-model overlay [i](#)



X



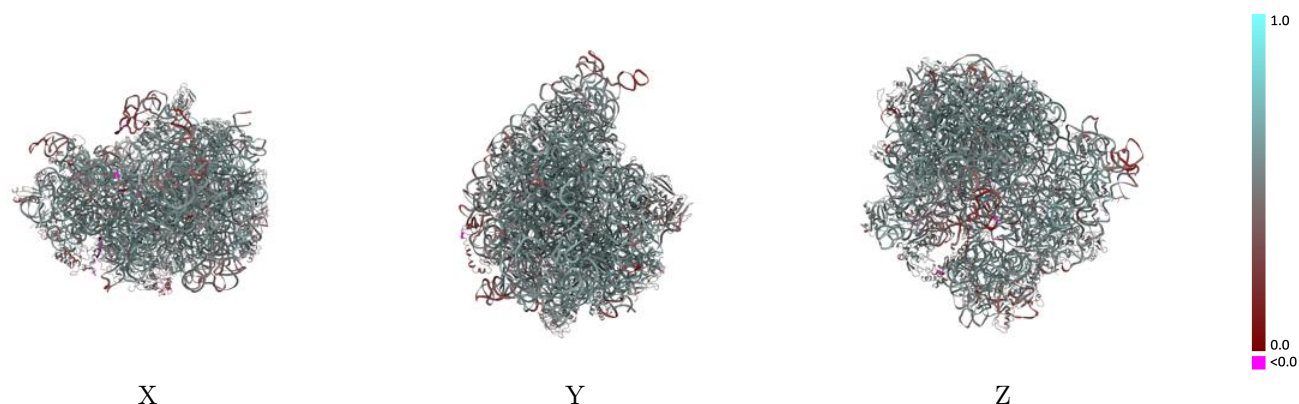
Y



Z

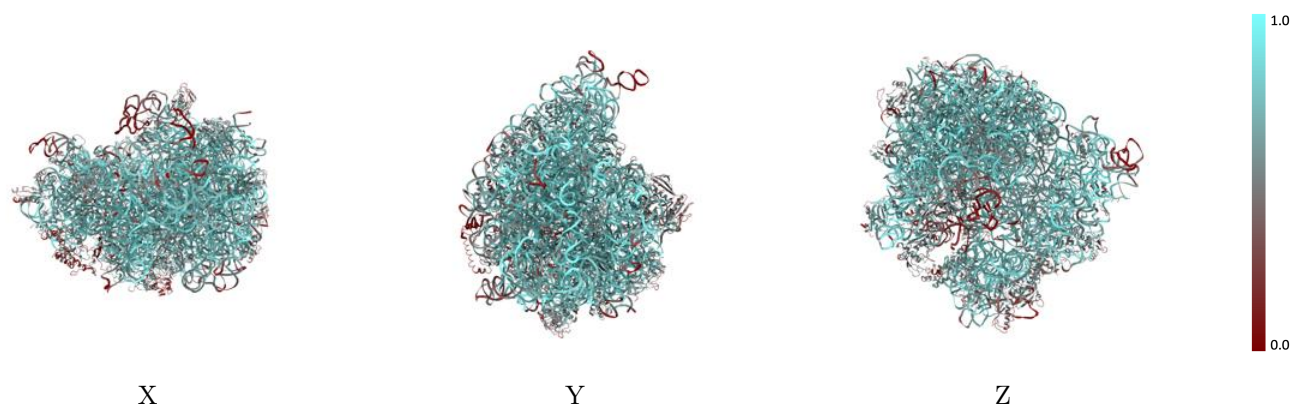
The images above show the 3D surface view of the map at the recommended contour level 0.108 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



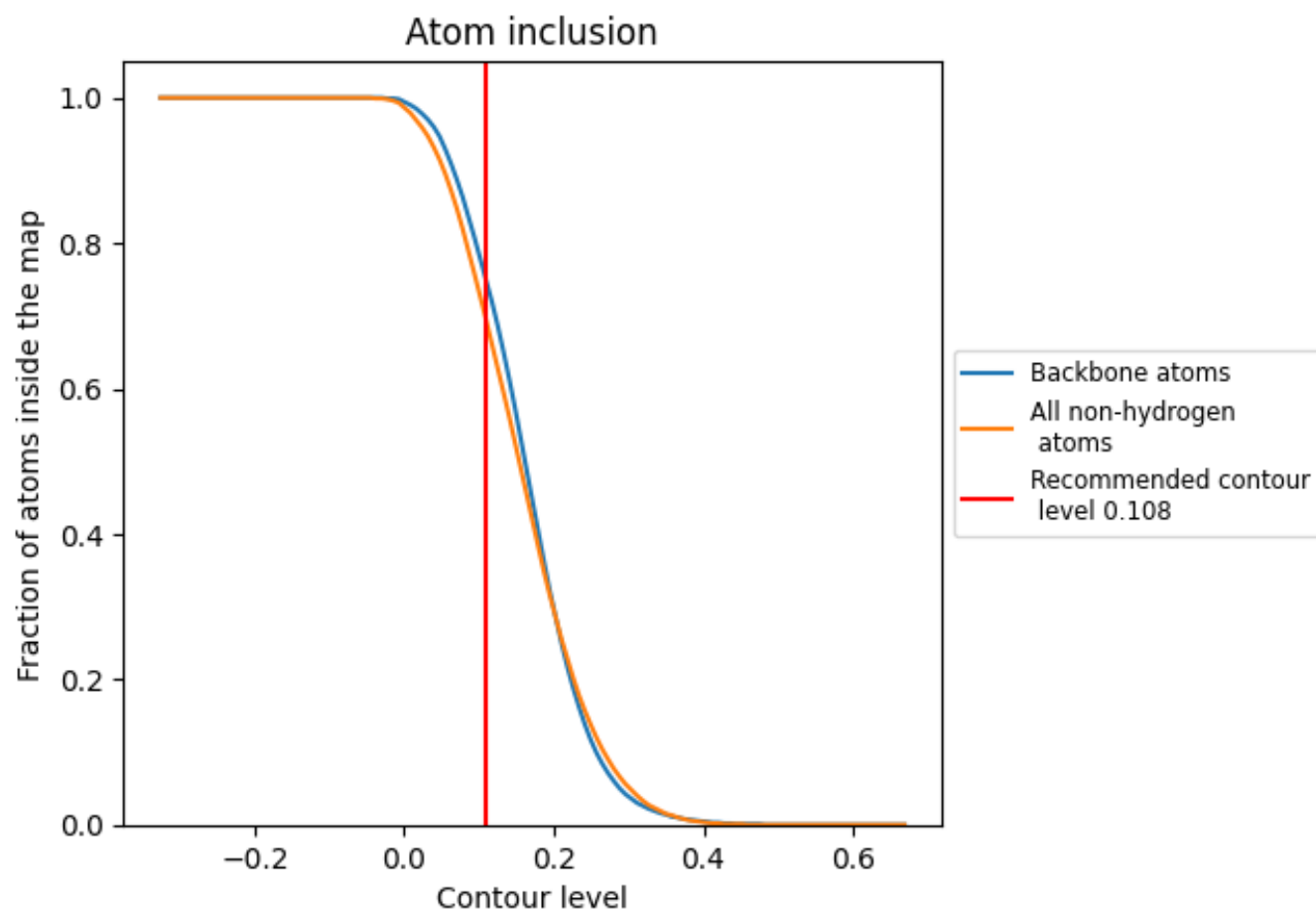
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.108).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 70% 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 (0.108) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7010	 0.5240
0	 0.6450	 0.5110
1	 0.5410	 0.5120
2	 0.7100	 0.5260
3	 0.6950	 0.5630
4	 0.6510	 0.5380
6	 0.3640	 0.4000
7	 0.0150	 0.2330
A	 0.7810	 0.5460
B	 0.7640	 0.5450
C	 0.6680	 0.5470
D	 0.6610	 0.5420
E	 0.5520	 0.5010
F	 0.5080	 0.4750
G	 0.4290	 0.4500
H	 0.1510	 0.2990
J	 0.6700	 0.5310
K	 0.6360	 0.5190
L	 0.6050	 0.5170
M	 0.6530	 0.5410
N	 0.6920	 0.5360
O	 0.6010	 0.5110
P	 0.5910	 0.5220
Q	 0.6950	 0.5470
R	 0.5660	 0.5040
S	 0.5960	 0.5150
T	 0.4940	 0.4830
U	 0.4300	 0.4670
V	 0.5800	 0.5120
W	 0.7010	 0.5680
X	 0.5910	 0.5160
Y	 0.4590	 0.4430
Z	 0.6270	 0.5260
a	 0.7860	 0.5430
b	 0.2910	 0.4060



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Chain	Atom inclusion	Q-score
c	 0.6280	 0.5090
d	 0.5190	 0.4650
e	 0.6420	 0.5080
f	 0.5000	 0.4660
g	 0.5050	 0.4770
h	 0.6490	 0.5250
i	 0.5490	 0.4680
j	 0.4990	 0.4560
k	 0.5230	 0.4900
l	 0.6220	 0.5050
m	 0.5700	 0.4820
n	 0.6340	 0.4950
o	 0.5900	 0.4970
p	 0.5690	 0.4690
q	 0.5220	 0.4810
r	 0.5960	 0.5030
s	 0.5730	 0.4790
t	 0.5830	 0.4880
u	 0.2580	 0.3250
v	 0.7780	 0.5620
w	 0.2770	 0.4440
x	 0.6410	 0.5170