



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 11:03 PM UTC

PDB ID : 6VYS / pdb_00006vys
EMDB ID : EMD-21470
Title : Escherichia coli transcription-translation complex A1 (TTC-A1) containing a 21 nt long mRNA spacer, NusG, and fMet-tRNAs at E-site and P-site
Authors : Molodtsov, V.; Wang, C.; Su, M.; Ebright, R.H.
Deposited on : 2020-02-27
Resolution : 3.70 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:

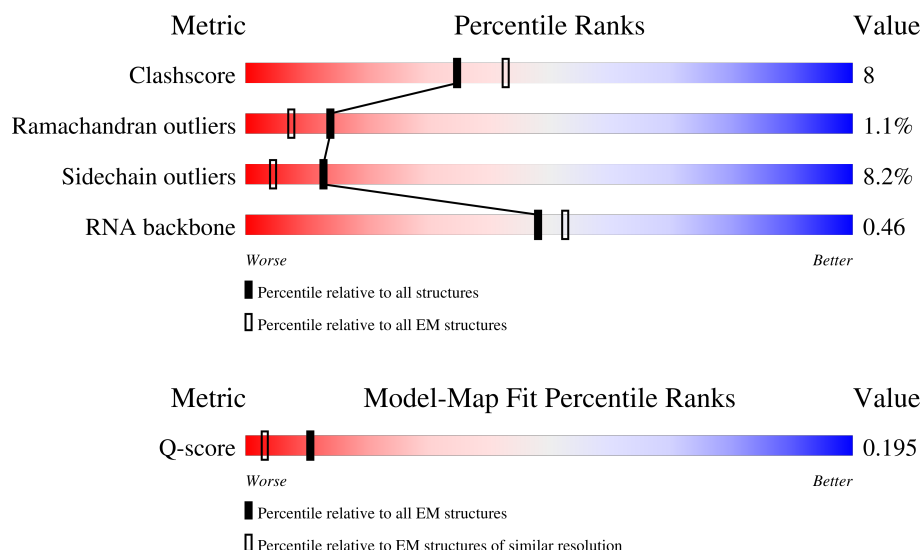
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

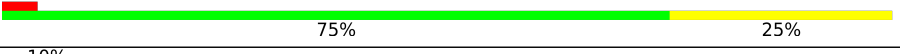
The reported resolution of this entry is 3.70 Å.

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	11569 (3.20 - 4.20)

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

Mol	Chain	Length	Quality of chain
1	0	103	
2	1	110	
3	2	100	

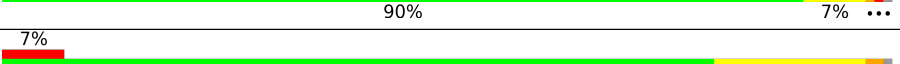
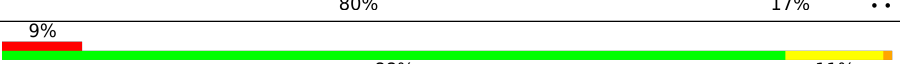
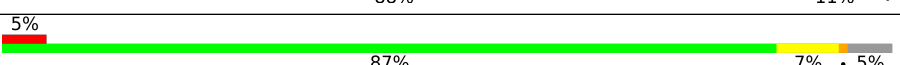
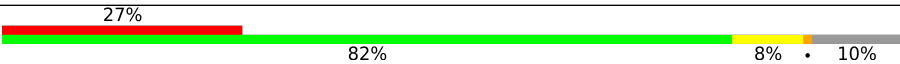
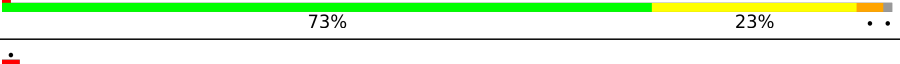
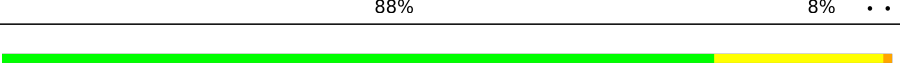
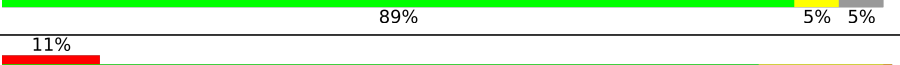
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Mol	Chain	Length	Quality of chain
4	3	104	
5	4	94	
6	5	36	
7	6	36	
8	7	37	
9	9	165	
10	A	76	
10	B	76	
11	AA	1342	
12	AB	181	
13	AC	329	
13	AD	329	
14	AE	1358	
15	C	75	
16	D	1542	
17	E	87	
18	F	71	
19	G	241	
20	H	557	
21	I	233	
22	J	206	
23	K	167	
24	L	135	
25	M	179	
26	N	130	

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Mol	Chain	Length	Quality of chain
27	O	130	
28	P	103	
29	Q	129	
30	R	124	
31	S	101	
32	T	89	
33	U	82	
34	V	84	
35	W	92	
36	X	118	
37	Y	142	
38	Z	121	
39	a	2904	
40	b	85	
41	c	78	
42	d	120	
43	e	63	
44	f	59	
45	g	70	
46	h	273	
47	i	57	
48	j	209	
49	k	55	
50	l	201	
51	m	46	

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Mol	Chain	Length	Quality of chain
52	n	179	
53	o	65	
54	p	177	
55	q	38	
56	r	149	
57	s	142	
58	t	123	
59	u	144	
60	v	136	
61	w	127	
62	x	117	
63	y	115	
64	z	118	

2 Entry composition

There are 66 unique types of molecules in this entry. The entry contains 300543 atoms, of which 124723 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	103	Total	C	H	N	O	S	0	0
			1655	516	839	153	145	2		

- Molecule 2 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1	110	Total	C	H	N	O	S	0	0
			1779	532	922	166	156	3		

- Molecule 3 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2	94	Total	C	H	N	O	S	0	0
			1557	470	811	140	134	2		

- Molecule 4 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	103	Total	C	H	N	O	0	0
			1632	498	844	148	142		

- Molecule 5 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4	94	Total	C	H	N	O	S	0	0
			1533	479	780	137	134	3		

- Molecule 6 is a DNA chain called NT DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	5	23	Total	C	H	N	O	P	0	0
			732	225	260	87	137	23		

- Molecule 7 is a DNA chain called T DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	6	27	Total	C	H	N	O	P	0	0
			847	259	305	89	167	27		

- Molecule 8 is a RNA chain called mRNA with 21 nt long spacer.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	7	26	Total	C	H	N	O	P	0	0
			644	244	97	82	195	26		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	148	Total	C	N	O	S	0	0
			1117	705	196	209	7		

- Molecule 10 is a RNA chain called E-site and P-site tRNA (fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
10	A	76	Total	C	H	N	O	P	0	0
			2446	723	826	295	527	75		
10	B	76	Total	C	H	N	O	P	0	0
			2433	723	813	295	527	75		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	AA	1322	Total	C	H	N	O	S	0	0
			20851	6539	10426	1817	2026	43		

- Molecule 12 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	AB	98	Total	C	H	N	O	S	0	0
			1573	505	783	139	140	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	AC	230	Total	C	H	N	O	S	0	0
			3599	1112	1813	317	351	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
13	AD	228	Total	C	H	N	O	S	0	0
			3556	1100	1789	312	349	6		

- Molecule 14 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	AE	1335	Total	C	H	N	O	S	0	0
			21000	6526	10612	1854	1958	50		

- Molecule 15 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	C	66	Total	C	H	N	O	S	0	0
			1103	344	559	102	97	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
16	D	1524	Total	C	H	N	O	P	0	0
			49126	14585	16423	6003	10591	1524		

- Molecule 17 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	E	86	Total	C	H	N	O	S	0	0
			1388	414	719	138	114	3		

- Molecule 18 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	F	70	Total	C	H	N	O	S	0	0
			1218	366	629	125	97	1		

- Molecule 19 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	G	225	Total	C	H	N	O	S	0	0
			3545	1113	1785	316	323	8		

- Molecule 20 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	H	259	Total	C	H	N	O	S	0	0
			3184	1073	1454	305	349	3		

- Molecule 21 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	I	208	Total	C	H	N	O	S	0	0
			3346	1036	1710	307	290	3		

- Molecule 22 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	J	205	Total	C	H	N	O	S	0	0
			3350	1026	1707	315	298	4		

- Molecule 23 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	K	156	Total	C	H	N	O	S	0	0
			2348	717	1196	217	212	6		

- Molecule 24 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	L	104	Total	C	H	N	O	S	0	0
			1694	536	846	153	152	7		

- Molecule 25 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	M	151	Total	C	H	N	O	S	0	0
			2416	735	1235	227	215	4		

- Molecule 26 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	N	129	Total	C	H	N	O	S	0	0
			2010	616	1031	173	184	6		

- Molecule 27 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	O	127	Total	C	H	N	O	S	0	0
			2092	634	1070	206	179	3		

- Molecule 28 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	P	99	Total	C	H	N	O	S	0	0
			1621	495	831	151	143	1		

- Molecule 29 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	Q	117	Total	C	H	N	O	S	0	0
			1764	540	887	174	160	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
30	R	121	Total	C	H	N	O	S	0	0
			1940	580	1001	194	161	4		

- Molecule 31 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	S	100	Total	C	H	N	O	S	0	0
			1649	499	844	164	139	3		

- Molecule 32 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	T	88	Total	C	H	N	O	S	0	0
			1448	439	734	144	130	1		

- Molecule 33 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	U	82	Total	C	H	N	O	S	0	0
			1315	406	666	128	114	1		

- Molecule 34 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	V	80	Total	C	H	N	O	S	0	0
			1339	411	691	121	113	3		

- Molecule 35 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	W	83	Total	C	H	N	O	S	0	0
			1351	424	688	126	111	2		

- Molecule 36 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	X	116	Total	C	H	N	O	S	0	0
			1864	558	964	181	158	3		

- Molecule 37 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Y	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 38 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Z	30	Total	C	N	O	S	0	0
			227	144	33	47	3		

- Molecule 39 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	a	2880	Total	C	H	N	O	P	0	0
			92918	27587	31077	11398	19976	2880		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	887	A	U	variant	GB 937521852

- Molecule 40 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	b	76	Total	C	H	N	O	S	0	0
			1181	360	599	117	104	1		

- Molecule 41 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	c	77	Total	C	H	N	O	S	0	0
			1277	388	652	129	106	2		

- Molecule 42 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	d	120	Total	C	H	N	O	P	0	0
			3870	1144	1301	468	837	120		

- Molecule 43 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	e	62	Total	C	H	N	O	S	0	0
			1032	308	531	98	94	1		

- Molecule 44 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	f	58	Total	C	H	N	O	S	0	0
			936	281	488	87	78	2		

- Molecule 45 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	g	66	Total	C	H	N	O	S	0	0
			1042	323	520	99	94	6		

- Molecule 46 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	h	271	Total	C	H	N	O	S	0	0
			4236	1288	2154	423	364	7		

- Molecule 47 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	i	56	Total	C	H	N	O	S	0	0
			903	269	459	94	80	1		

- Molecule 48 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	j	209	Total	C	H	N	O	S	0	0
			3182	979	1617	288	294	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
49	k	52	Total	C	H	N	O		0	0
			890	275	464	78	73			

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

Mol	Chain	Residues	Atoms						AltConf	Trace
50	l	201	Total	C	H	N	O	S	0	0
			3171	974	1619	283	290	5		

- Molecule 51 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	m	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

- Molecule 52 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	n	177	Total	C	H	N	O	S	0	0
			2853	899	1443	249	256	6		

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	o	64	Total	C	H	N	O	S	0	0
			1076	323	572	105	74	2		

- Molecule 54 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	p	175	Total	C	H	N	O	S	0	0
			2671	826	1358	241	244	2		

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	q	38	Total	C	H	N	O	S	0	0
			645	185	343	65	48	4		

- Molecule 56 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	r	149	Total	C	H	N	O	S	0	0
			2259	699	1148	197	214	1		

- Molecule 57 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	s	142	Total	C	H	N	O	S	0	0
			2291	714	1162	212	199	4		

- Molecule 58 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	t	123	Total	C	H	N	O	S	0	0
			1969	593	1023	181	166	6		

- Molecule 59 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	u	144	Total	C	H	N	O	S	0	0
			2182	654	1129	207	190	2		

- Molecule 60 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	v	136	Total	C	H	N	O	S	0	0
			2231	686	1157	205	177	6		

- Molecule 61 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	w	119	Total	C	H	N	O	S	0	0
			1945	588	994	195	163	5		

- Molecule 62 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	x	116	Total	C	H	N	O		0	0
			1815	552	923	178	162			

- Molecule 63 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	y	114	Total	C	H	N	O	S	0	0
			1879	574	962	179	163	1		

- Molecule 64 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	z	117	Total	C	H	N	O		0	0
			1967	604	1020	192	151			

- Molecule 65 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
65	AE	1	Total	Mg	0
			1	1	

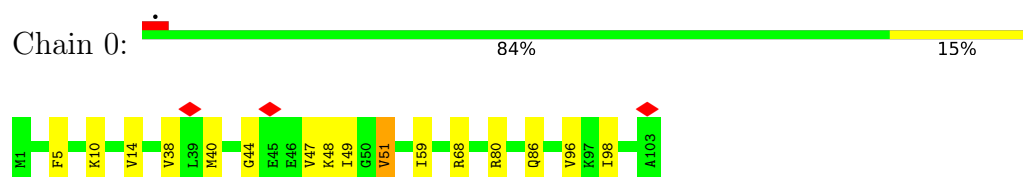
- Molecule 66 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
66	AE	2	Total	Zn	0
			2	2	

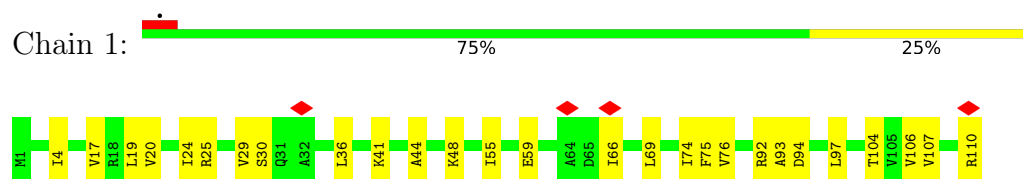
3 Residue-property plots [i](#)

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

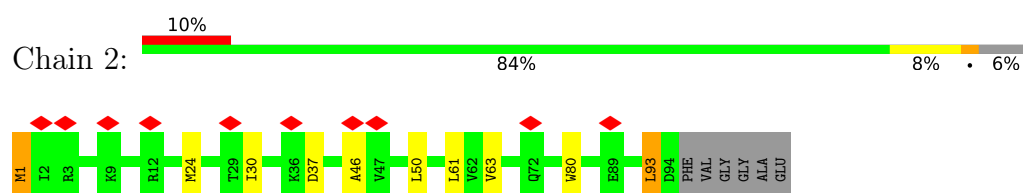
- Molecule 1: 50S ribosomal protein L21



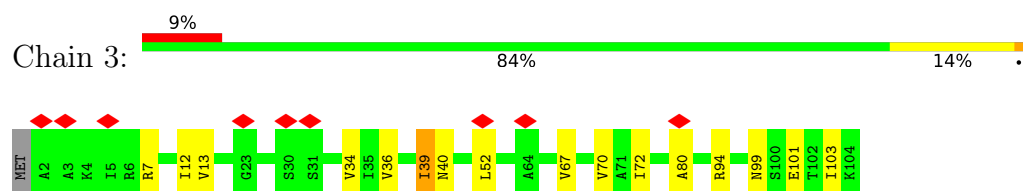
- Molecule 2: 50S ribosomal protein L22



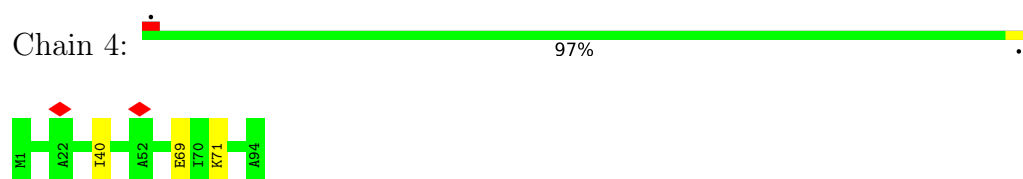
- Molecule 3: 50S ribosomal protein L23



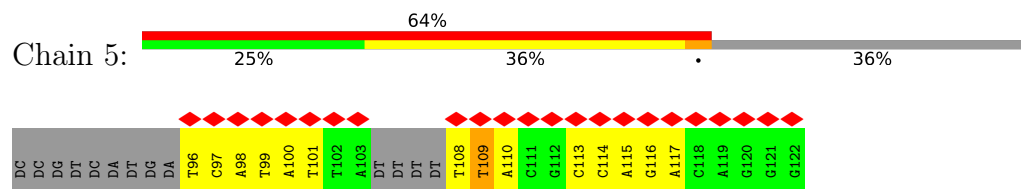
- Molecule 4: 50S ribosomal protein L24



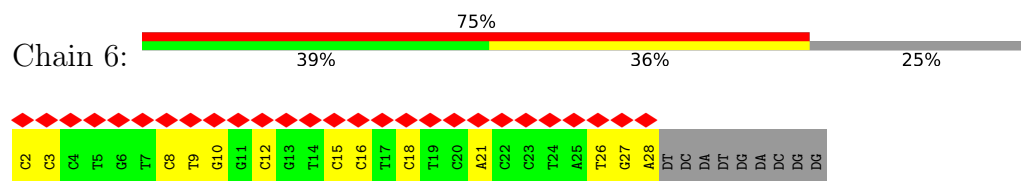
- Molecule 5: 50S ribosomal protein L25



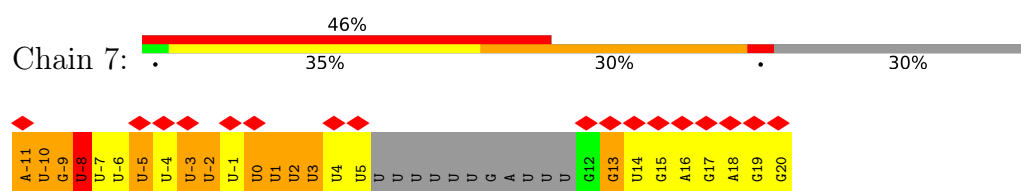
- Molecule 6: NT DNA



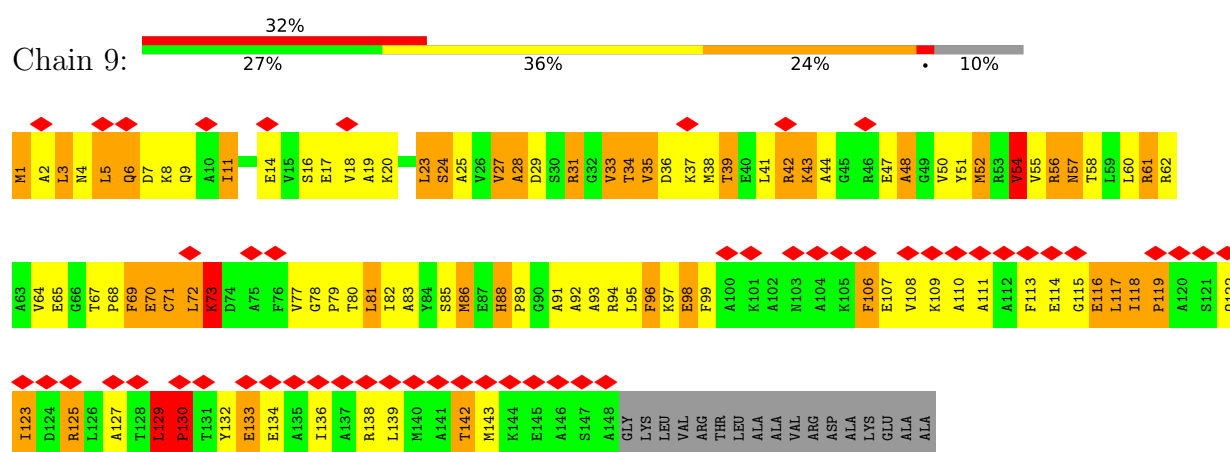
- Molecule 7: T DNA



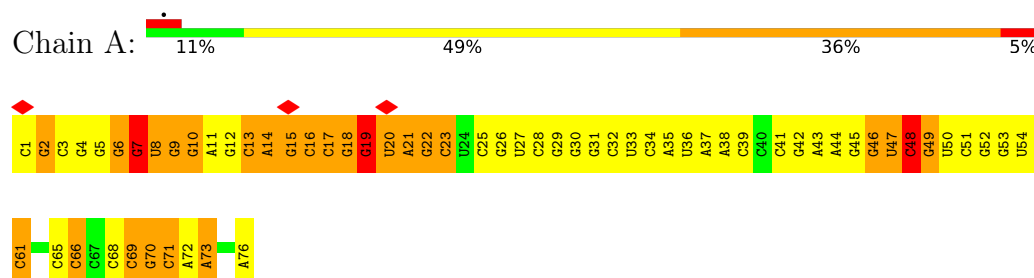
- Molecule 8: mRNA with 21 nt long spacer



- Molecule 9: 50S ribosomal protein L10

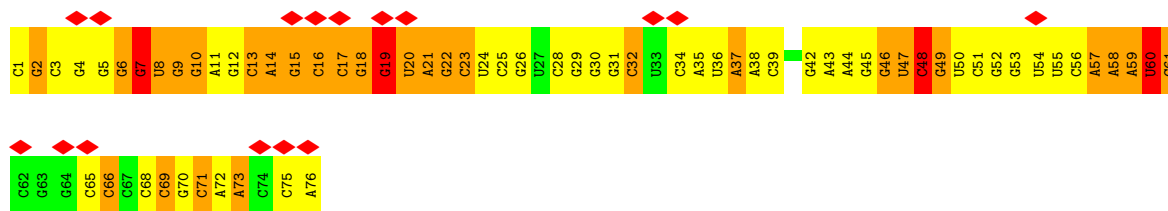


- Molecule 10: E-site and P-site tRNA (fMet)

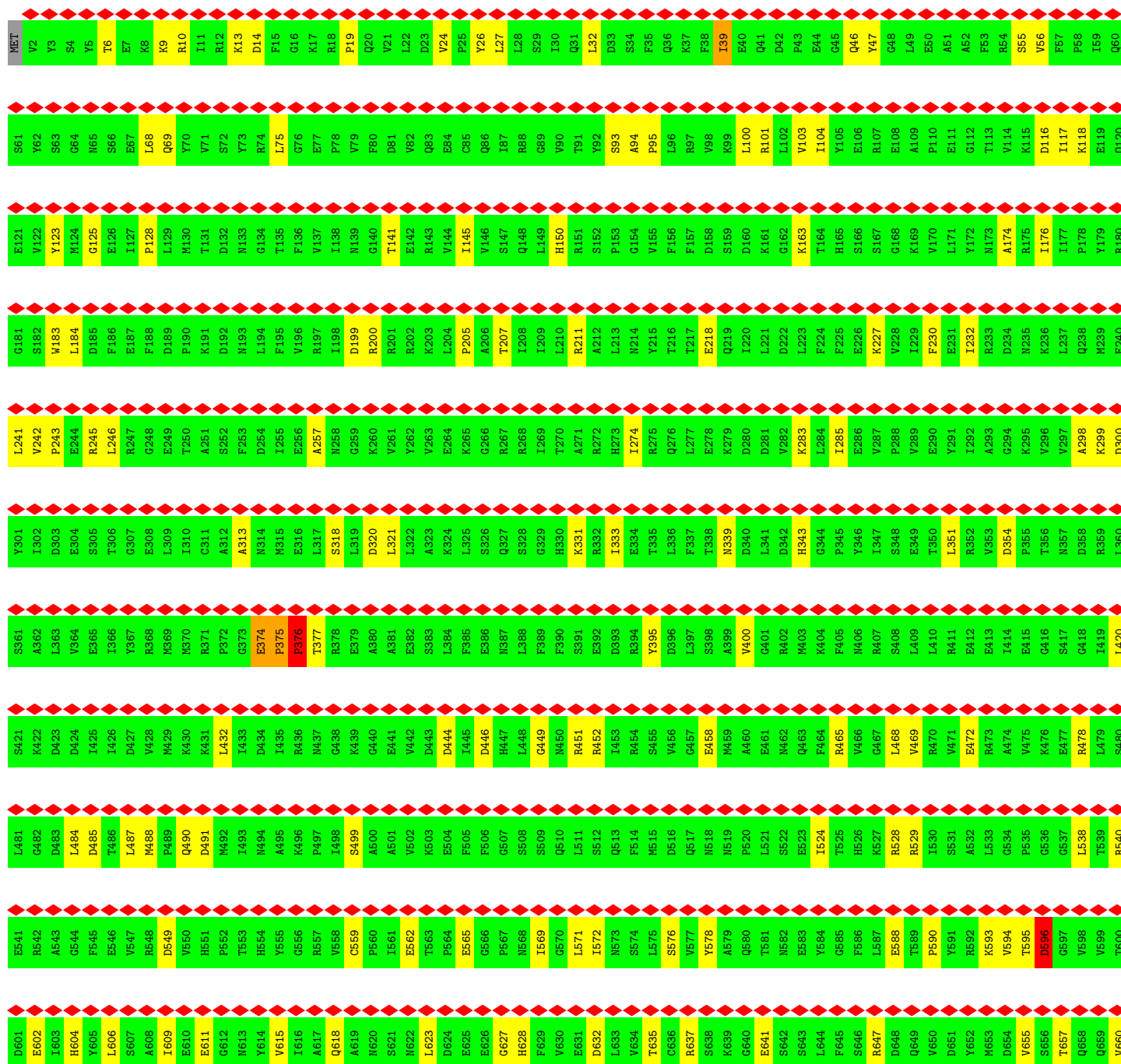


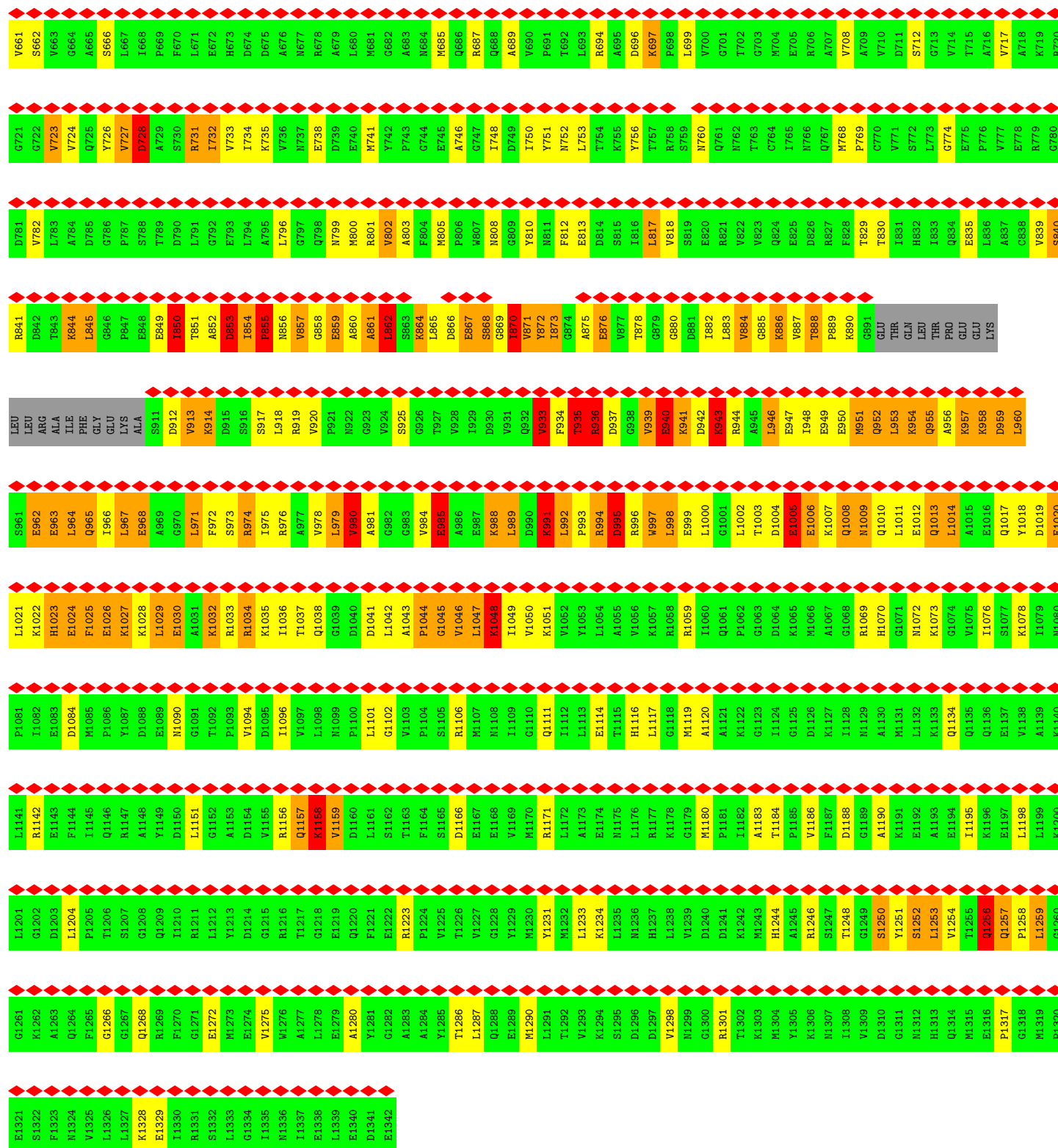
- Molecule 10: E-site and P-site tRNA (fMet)





● Molecule 11: DNA-directed RNA polymerase subunit beta



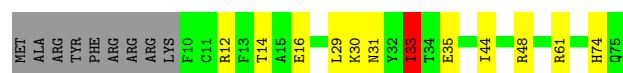


• Molecule 12: Transcription termination/antitermination protein NusG



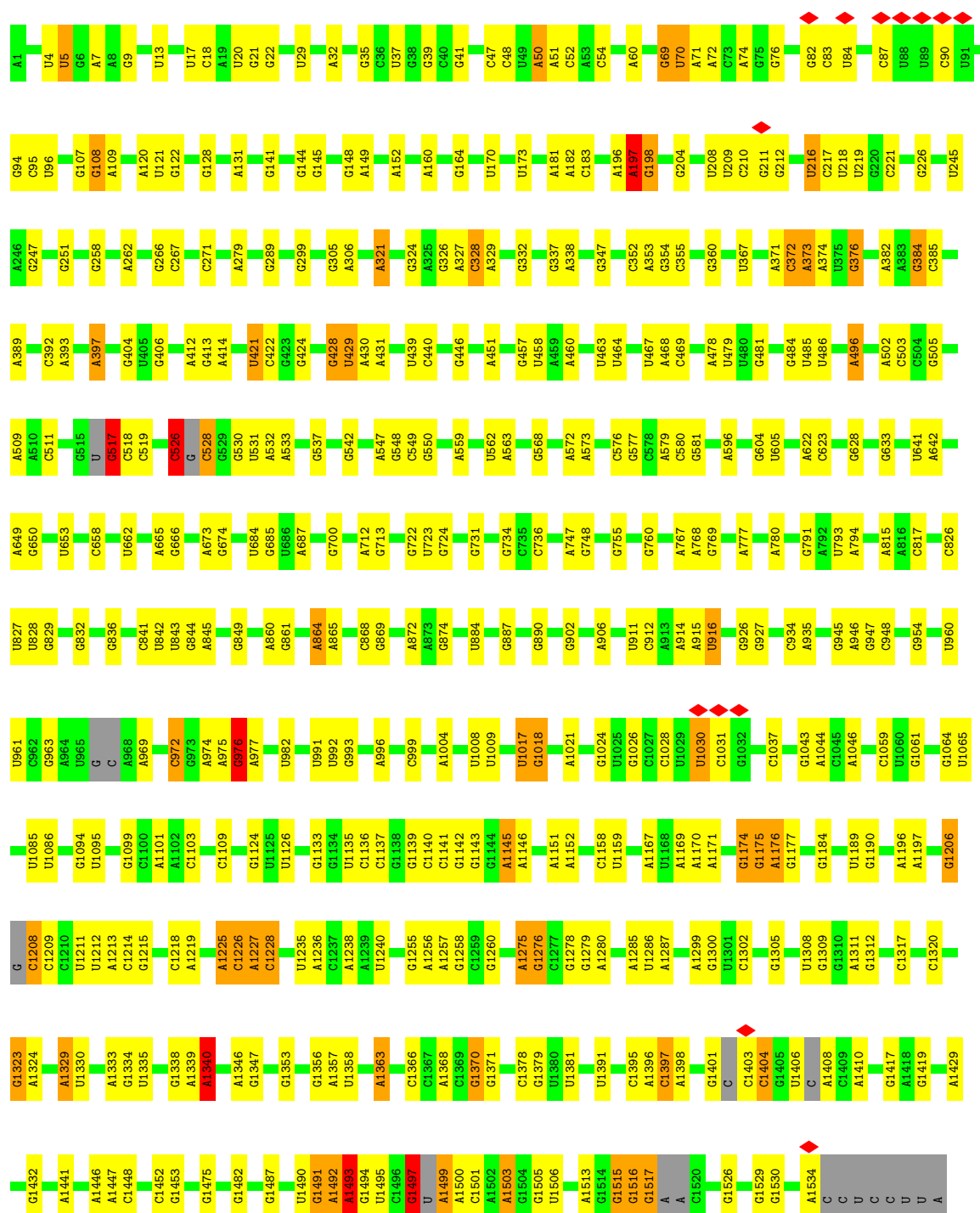
- Molecule 15: 30S ribosomal protein S18

Chain C:  72% 15% 12%

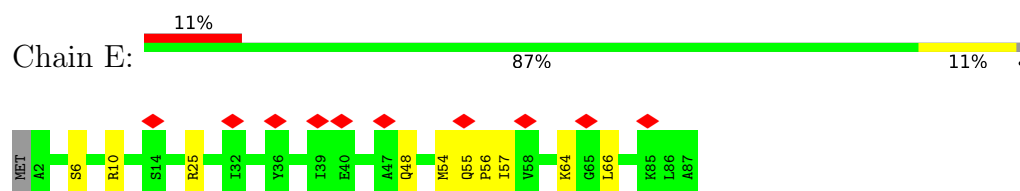


• Molecule 16: 16S rRNA

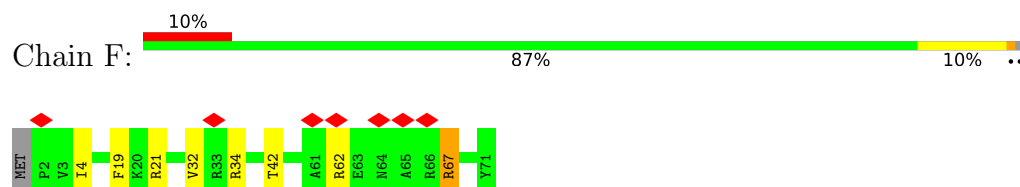
Chain D:  70% 25%



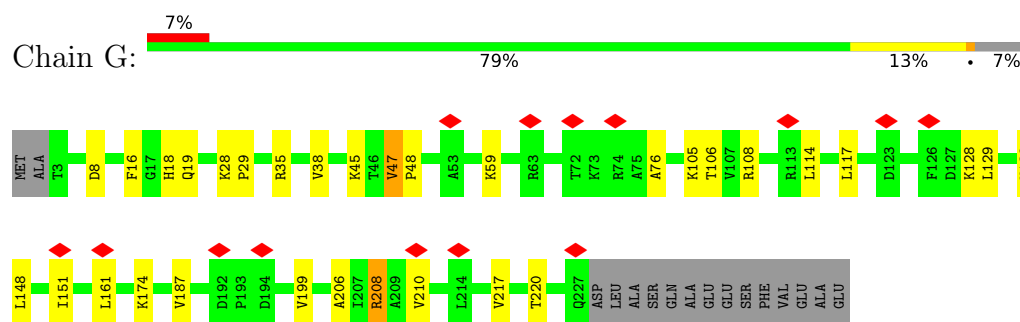
- Molecule 17: 30S ribosomal protein S20



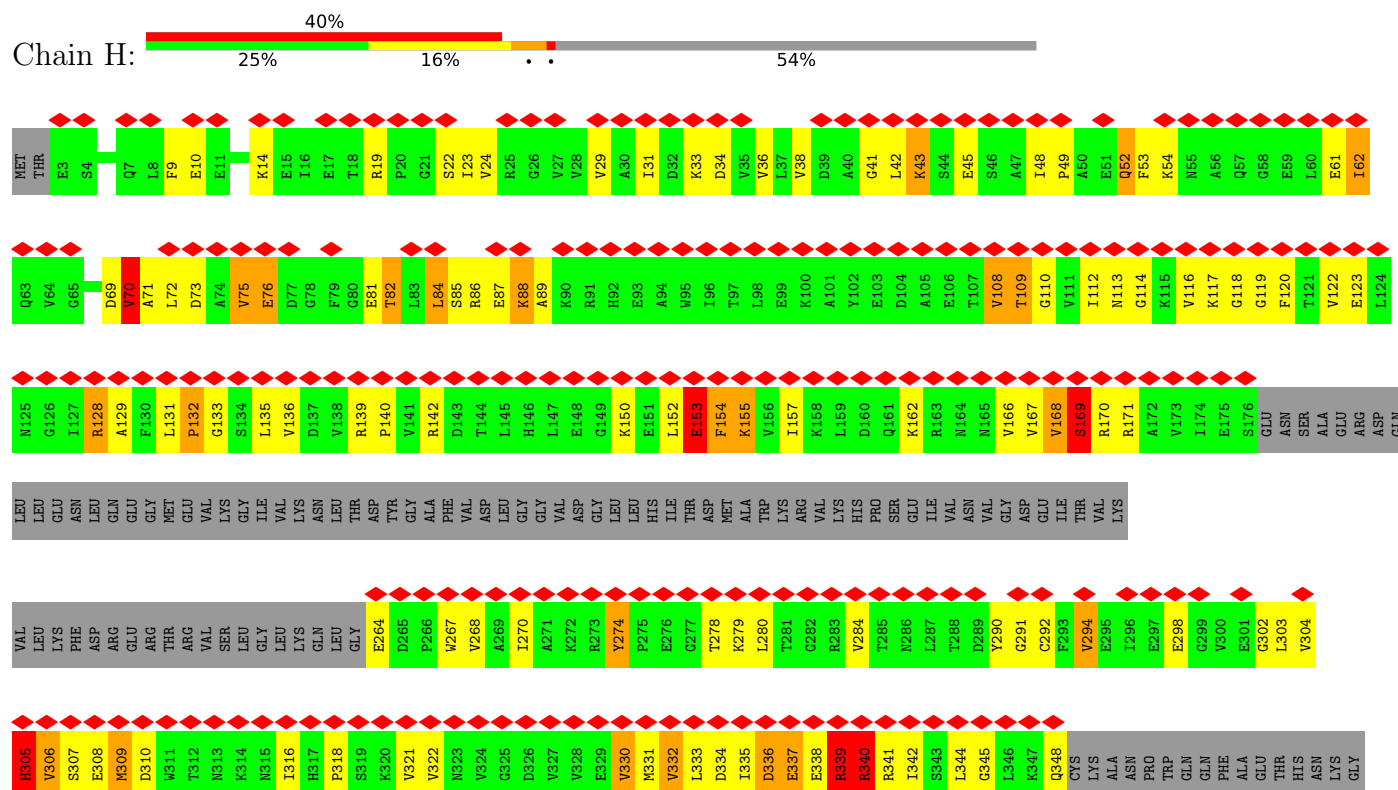
- Molecule 18: 30S ribosomal protein S21



- Molecule 19: 30S ribosomal protein S2



- Molecule 20: 30S ribosomal protein S1

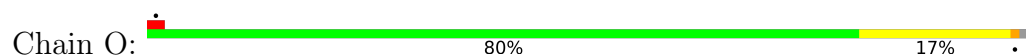




- Molecule 26: 30S ribosomal protein S8



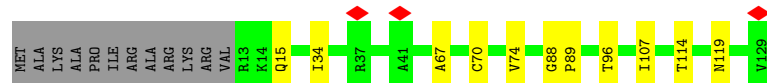
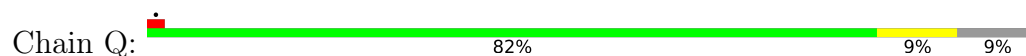
- Molecule 27: 30S ribosomal protein S9



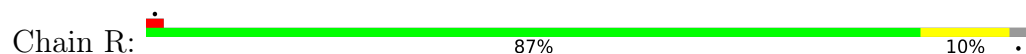
- Molecule 28: 30S ribosomal protein S10



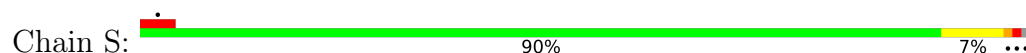
- Molecule 29: 30S ribosomal protein S11



- Molecule 30: 30S ribosomal protein S12

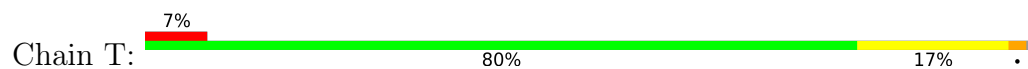


- Molecule 31: 30S ribosomal protein S14

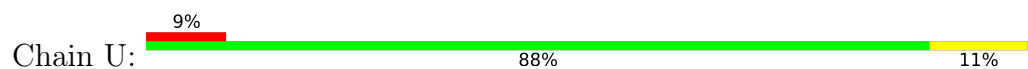




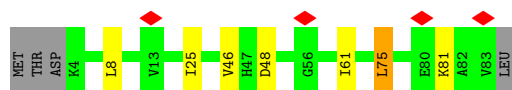
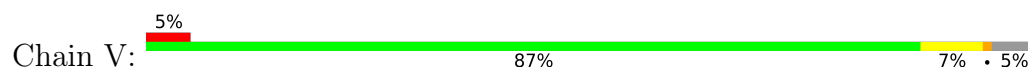
- Molecule 32: 30S ribosomal protein S15



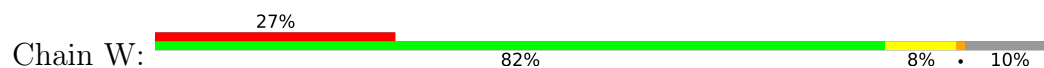
- Molecule 33: 30S ribosomal protein S16



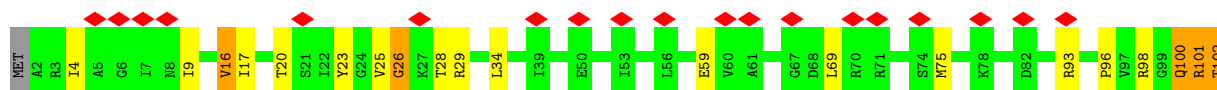
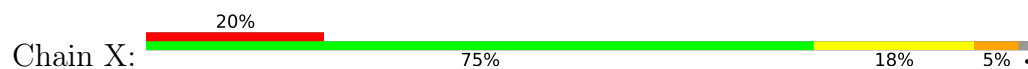
- Molecule 34: 30S ribosomal protein S17



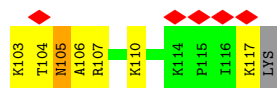
- Molecule 35: 30S ribosomal protein S19

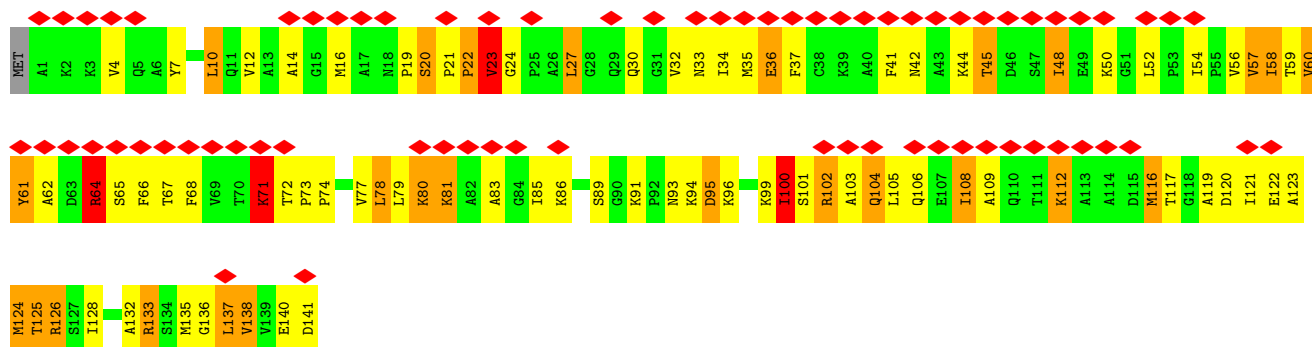


- Molecule 36: 30S ribosomal protein S13

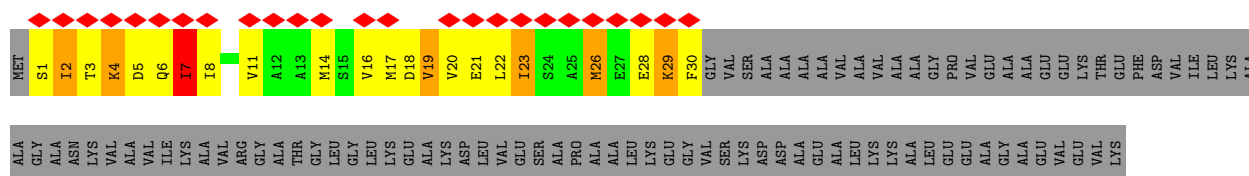


- Molecule 37: 50S ribosomal protein L11

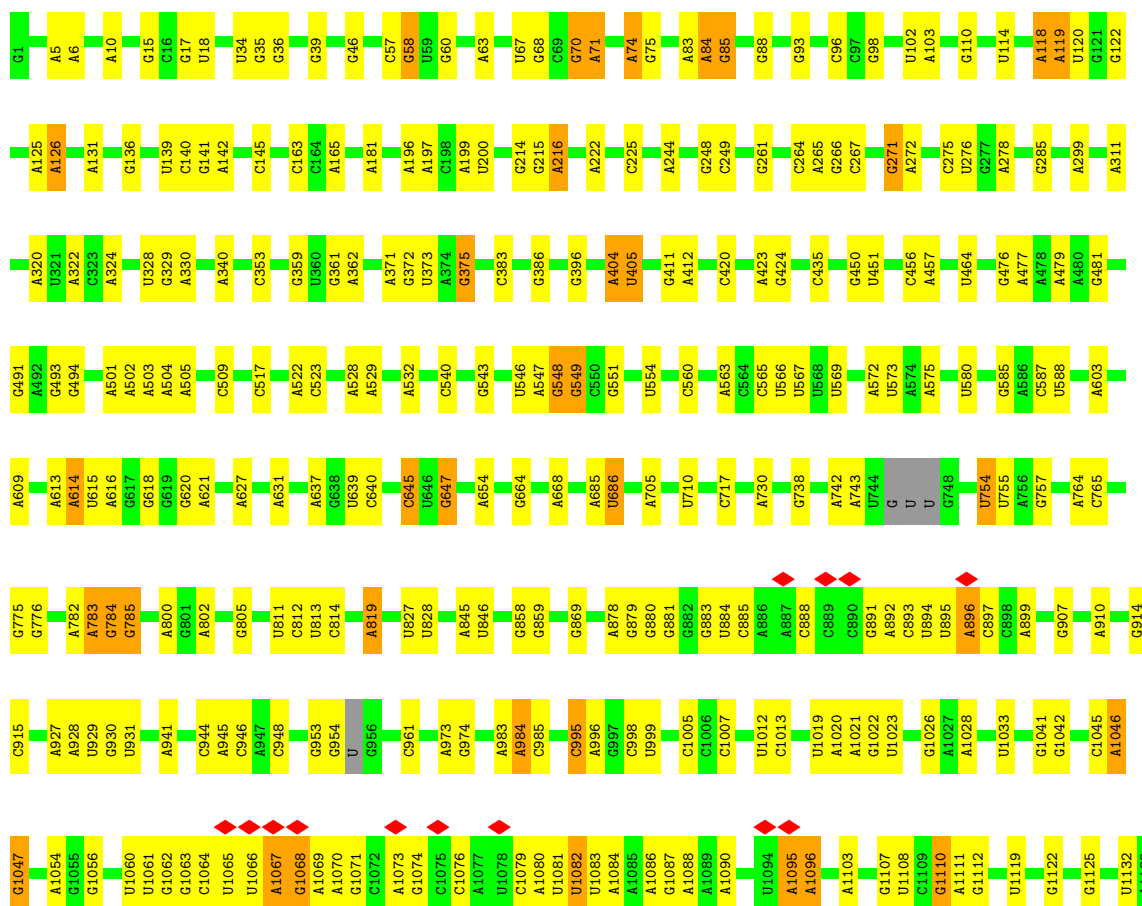


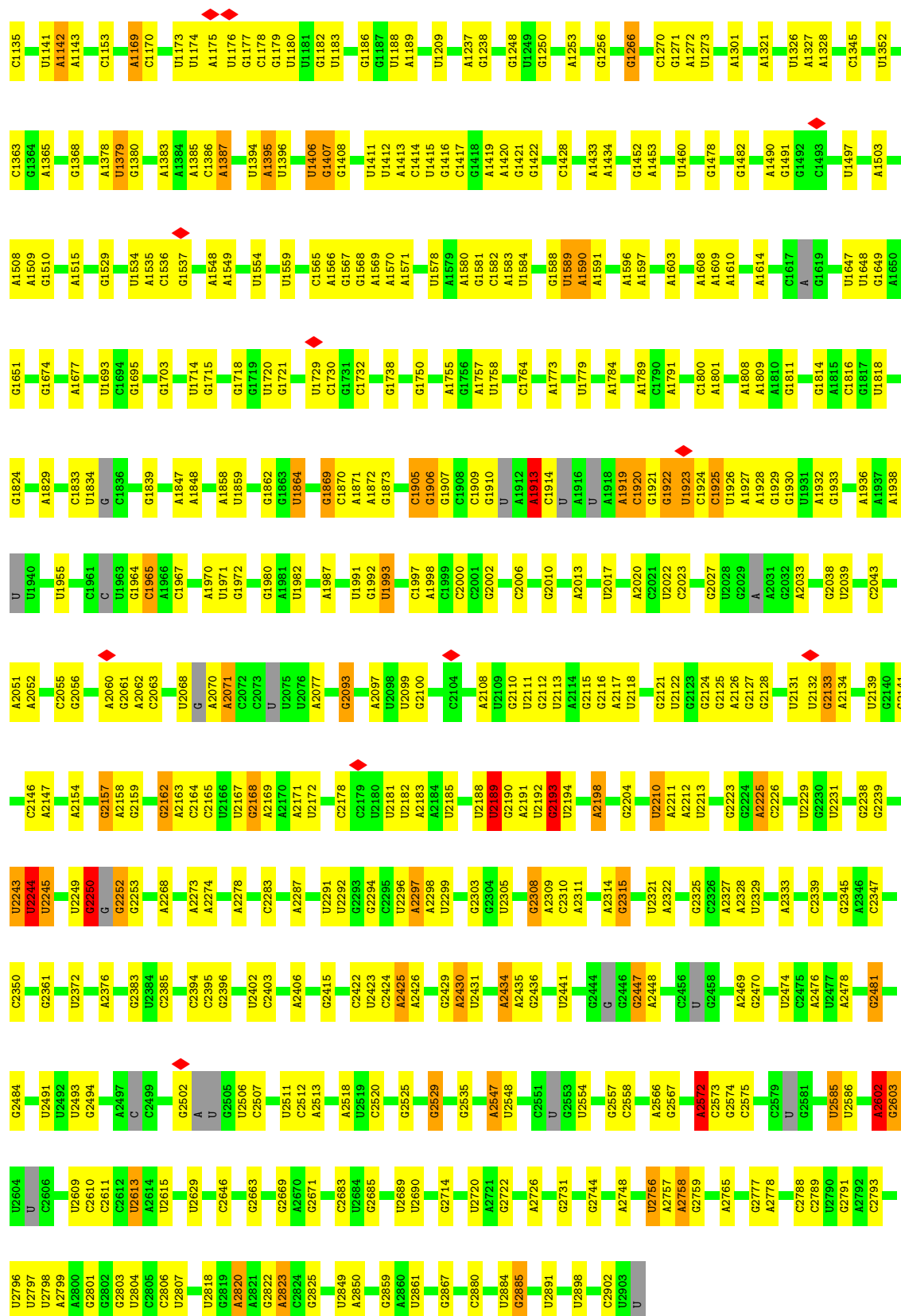


• Molecule 38: 50S ribosomal protein L7/L12

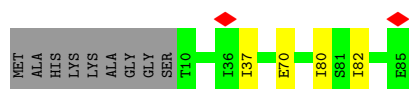
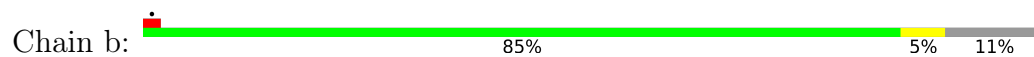


• Molecule 39: 23S rRNA

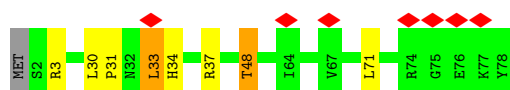
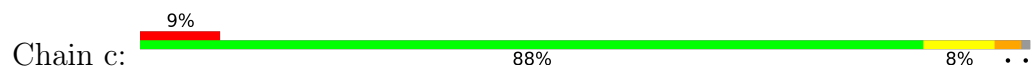




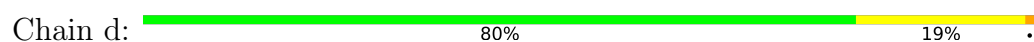
• Molecule 40: 50S ribosomal protein L27



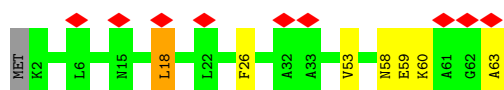
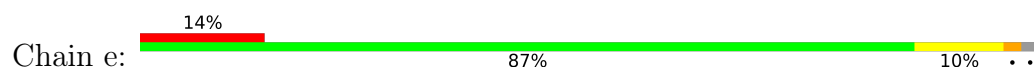
- Molecule 41: 50S ribosomal protein L28



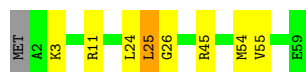
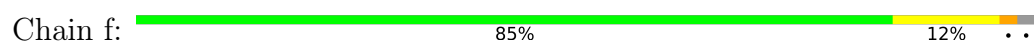
- Molecule 42: 5S rRNA



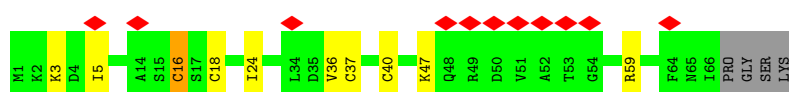
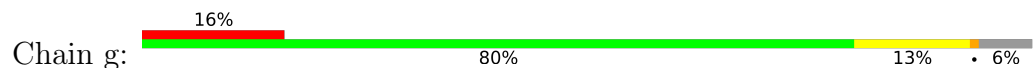
- Molecule 43: 50S ribosomal protein L29



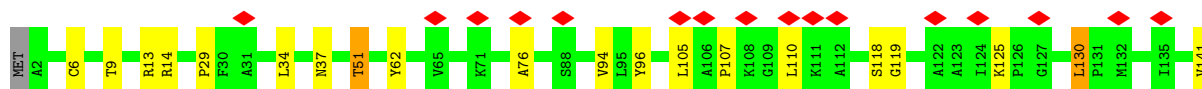
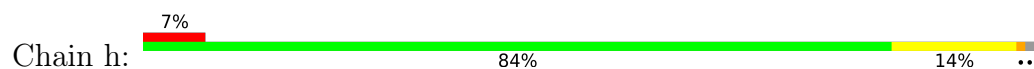
- Molecule 44: 50S ribosomal protein L30

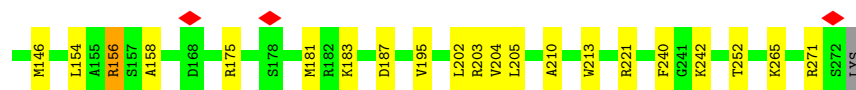


- Molecule 45: 50S ribosomal protein L31

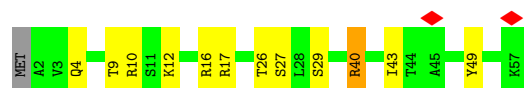
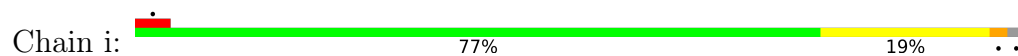


- Molecule 46: 50S ribosomal protein L2

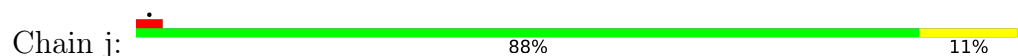




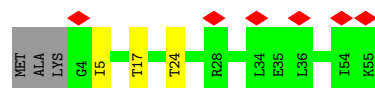
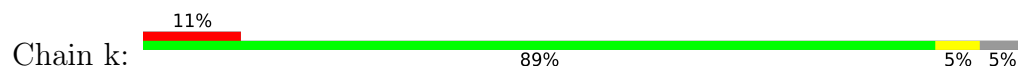
- Molecule 47: 50S ribosomal protein L32



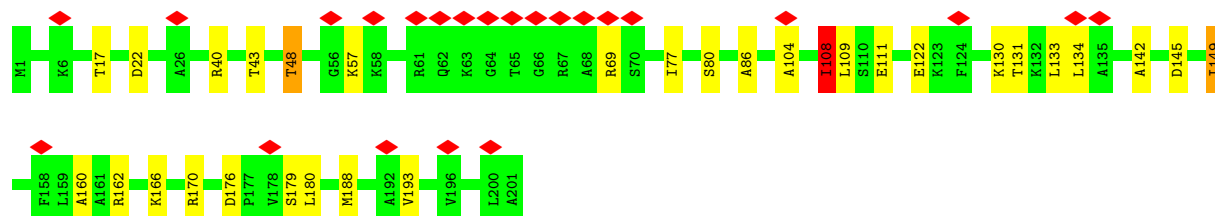
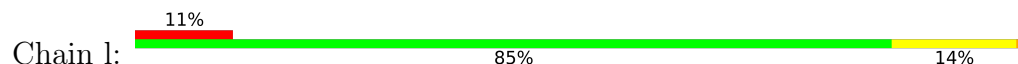
- Molecule 48: 50S ribosomal protein L3



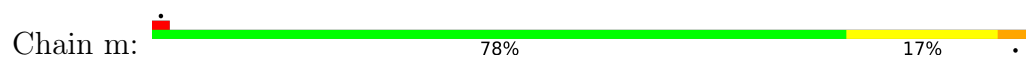
- Molecule 49: 50S ribosomal protein L33



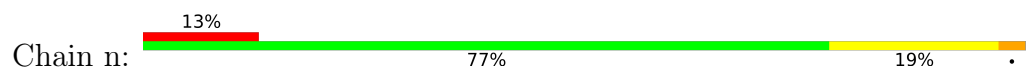
- Molecule 50: 50S ribosomal protein L4

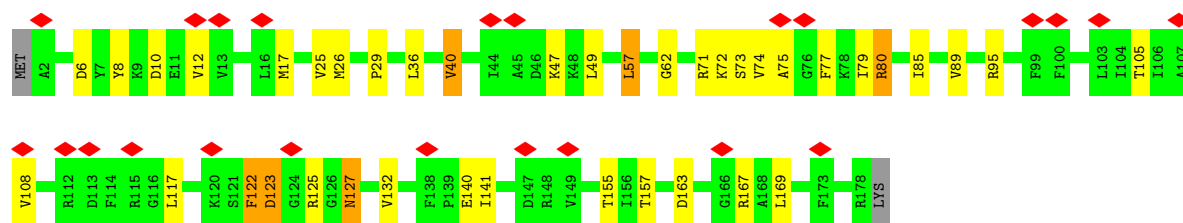


- Molecule 51: 50S ribosomal protein L34

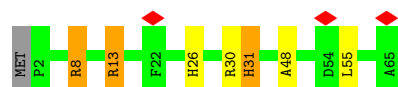
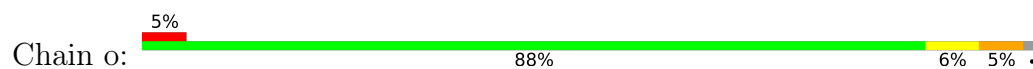


- Molecule 52: 50S ribosomal protein L5

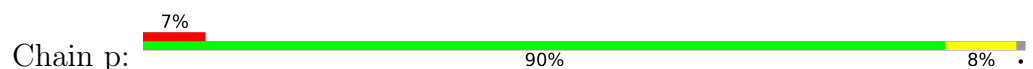




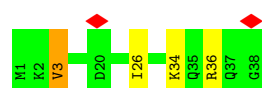
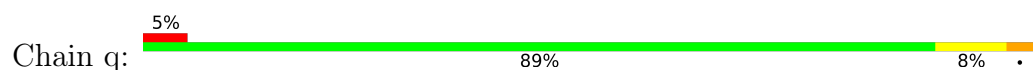
- Molecule 53: 50S ribosomal protein L35



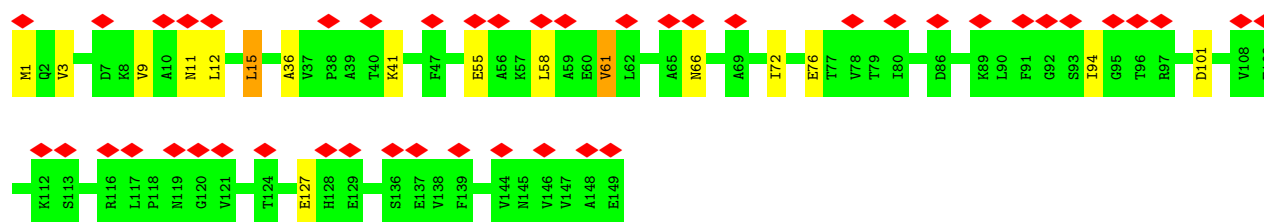
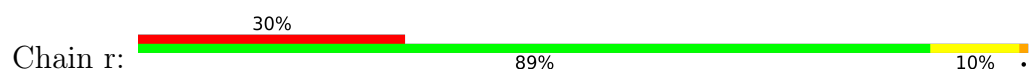
- Molecule 54: 50S ribosomal protein L6



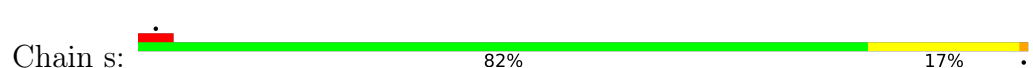
- Molecule 55: 50S ribosomal protein L36



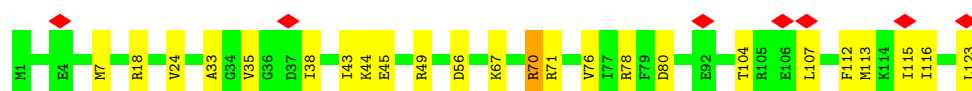
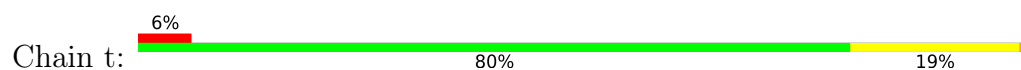
- Molecule 56: 50S ribosomal protein L9



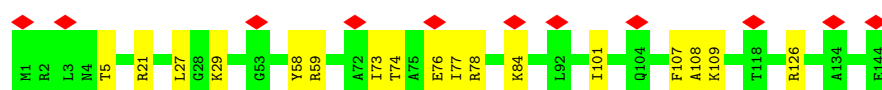
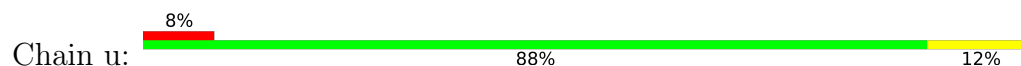
- Molecule 57: 50S ribosomal protein L13



- Molecule 58: 50S ribosomal protein L14



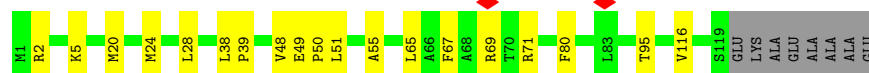
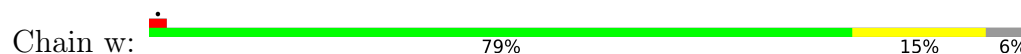
- Molecule 59: 50S ribosomal protein L15



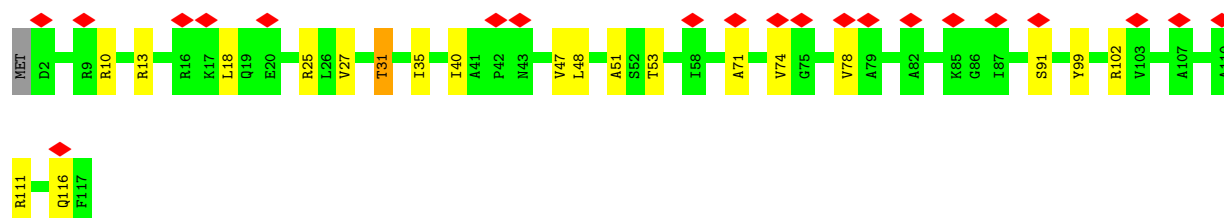
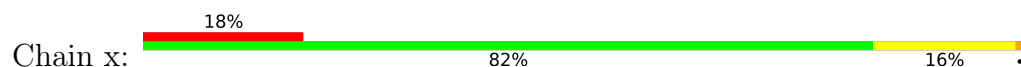
- Molecule 60: 50S ribosomal protein L16



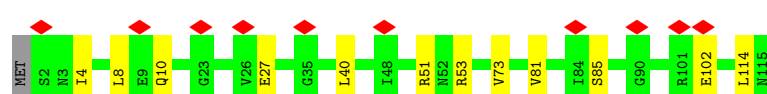
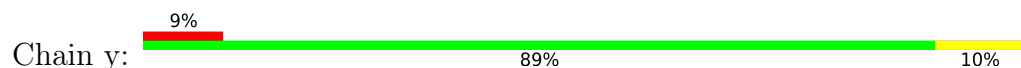
- Molecule 61: 50S ribosomal protein L17



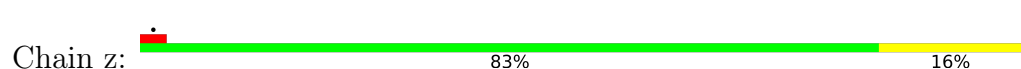
- Molecule 62: 50S ribosomal protein L18



- Molecule 63: 50S ribosomal protein L19



- Molecule 64: 50S ribosomal protein L20





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29704	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.010	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.00868	Depositor
Map size (Å)	520.0, 520.0, 520.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.50	0/829	0.73	0/1107
2	1	0.67	0/864	1.08	0/1156
3	2	0.54	0/752	0.90	0/1005
4	3	0.47	0/796	0.78	0/1062
5	4	0.52	0/766	0.88	0/1025
6	5	0.63	1/528 (0.2%)	0.55	0/810
7	6	0.55	1/603 (0.2%)	0.56	0/926
8	7	0.60	2/607 (0.3%)	0.84	2/940 (0.2%)
9	9	1.15	3/1131 (0.3%)	1.30	4/1524 (0.3%)
10	A	0.36	0/1810	0.72	2/2821 (0.1%)
10	B	0.43	0/1810	0.86	9/2821 (0.3%)
11	AA	0.67	13/10591 (0.1%)	0.96	54/14289 (0.4%)
12	AB	0.43	1/808 (0.1%)	0.70	2/1088 (0.2%)
13	AC	0.60	4/1808 (0.2%)	0.73	9/2450 (0.4%)
13	AD	0.40	0/1789	0.56	0/2425
14	AE	0.54	8/10545 (0.1%)	0.74	25/14236 (0.2%)
15	C	0.66	0/553	1.15	2/743 (0.3%)
16	D	0.40	9/36610 (0.0%)	0.75	39/57091 (0.1%)
17	E	0.76	0/675	1.32	0/895
18	F	0.71	0/597	1.20	0/792
19	G	0.65	0/1791	1.08	1/2413 (0.0%)
20	H	0.76	4/1746 (0.2%)	1.58	34/2382 (1.4%)
21	I	0.58	0/1663	0.98	0/2241
22	J	0.63	0/1665	1.08	0/2227
23	K	0.63	1/1165 (0.1%)	1.06	2/1568 (0.1%)
24	L	0.58	0/867	0.94	0/1171
25	M	0.68	0/1195	1.19	3/1602 (0.2%)
26	N	0.55	0/989	0.91	0/1326
27	O	0.59	0/1034	1.02	1/1375 (0.1%)
28	P	0.60	0/800	1.10	4/1082 (0.4%)
29	Q	0.55	0/893	0.91	0/1205
30	R	0.49	0/952	0.81	0/1274

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	S	0.64	0/817	1.11	1/1088 (0.1%)
32	T	0.69	0/722	1.21	0/964
33	U	0.57	0/659	0.99	0/884
34	V	0.45	0/657	0.73	0/881
35	W	0.51	0/680	0.83	0/915
36	X	0.67	0/909	1.21	3/1215 (0.2%)
37	Y	1.03	0/1046	1.08	0/1410
38	Z	1.03	0/227	1.12	0/304
39	a	0.40	3/69247 (0.0%)	0.75	55/107985 (0.1%)
40	b	0.51	0/589	0.76	0/779
41	c	0.63	0/635	0.97	0/848
42	d	0.37	0/2872	0.69	0/4478
43	e	0.69	0/502	1.19	0/667
44	f	0.62	0/452	1.02	0/605
45	g	0.55	0/531	0.99	1/709 (0.1%)
46	h	0.54	0/2121	0.85	0/2852
47	i	0.52	0/450	0.94	0/599
48	j	0.60	0/1586	0.87	0/2134
49	k	0.47	0/433	0.80	0/576
50	l	0.61	0/1571	1.03	1/2113 (0.0%)
51	m	0.68	0/380	1.21	0/498
52	n	0.62	0/1434	1.18	10/1926 (0.5%)
53	o	0.64	0/513	1.10	1/676 (0.1%)
54	p	0.58	0/1333	0.89	0/1805
55	q	0.50	0/303	0.88	0/397
56	r	0.63	0/1122	0.97	1/1515 (0.1%)
57	s	0.68	0/1152	1.02	2/1551 (0.1%)
58	t	0.57	0/955	0.88	0/1279
59	u	0.55	0/1062	0.96	1/1413 (0.1%)
60	v	0.60	0/1093	0.97	0/1460
61	w	0.67	0/964	1.13	0/1289
62	x	0.61	0/902	1.09	0/1209
63	y	0.53	0/929	0.79	0/1242
64	z	0.80	0/960	1.25	0/1278
All	All	0.50	50/189040 (0.0%)	0.84	269/278616 (0.1%)

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
10	A	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	B	0	2
11	AA	0	10
14	AE	0	5
20	H	0	3
36	X	0	1
All	All	0	23

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	9	130	PRO	N-CA	18.24	1.70	1.47
11	AA	374	GLU	C-N	17.62	1.54	1.33
11	AA	850	ILE	N-CA	-13.15	1.29	1.46
14	AE	93	THR	CA-C	12.13	1.69	1.52
20	H	169	SER	N-CA	11.81	1.61	1.46
16	D	1516	G	O3'-P	-10.83	1.44	1.61
14	AE	70	CYS	CA-CB	-8.71	1.41	1.53
16	D	1339	A	O3'-P	8.50	1.73	1.61
8	7	19	G	C1'-N9	-7.44	1.36	1.48
8	7	-10	U	C1'-N1	7.17	1.59	1.48
20	H	88	LYS	N-CA	7.03	1.55	1.46
6	5	109	DT	O3'-P	6.95	1.71	1.61
13	AC	76	GLU	N-CA	-6.85	1.37	1.46
16	D	145	G	O3'-P	6.71	1.71	1.61
16	D	196	A	O3'-P	6.62	1.71	1.61
20	H	168	VAL	C-N	6.41	1.42	1.33
13	AC	75	GLN	CA-C	-6.20	1.45	1.53
16	D	1275	A	O3'-P	6.20	1.70	1.61
39	a	2434	A	O3'-P	6.03	1.70	1.61
16	D	1395	C	O3'-P	5.83	1.69	1.61
16	D	1515	G	O3'-P	-5.83	1.52	1.61
20	H	88	LYS	CA-C	5.73	1.60	1.52
14	AE	90	VAL	CA-C	5.67	1.60	1.52
11	AA	885	GLY	C-O	-5.53	1.16	1.23
16	D	1490	U	O3'-P	5.42	1.69	1.61
7	6	10	DG	C1'-N9	-5.40	1.35	1.46
11	AA	996	ARG	N-CA	-5.27	1.38	1.45
11	AA	604	HIS	ND1-CE1	5.26	1.37	1.32
14	AE	1350	ASN	CG-ND2	-5.26	1.22	1.33
16	D	1492	A	O3'-P	5.26	1.69	1.61
12	AB	81	HIS	ND1-CE1	5.23	1.37	1.32
39	a	1905	C	O3'-P	5.22	1.69	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	1257	GLN	CD-OE1	5.21	1.33	1.23
13	AC	160	HIS	CD2-NE2	-5.21	1.32	1.37
11	AA	1256	GLN	CD-OE1	5.16	1.33	1.23
11	AA	604	HIS	CD2-NE2	-5.14	1.32	1.37
39	a	2167	U	O3'-P	5.14	1.68	1.61
9	9	129	LEU	C-N	5.14	1.45	1.33
11	AA	1157	GLN	CD-NE2	-5.13	1.22	1.33
9	9	116	GLU	N-CA	5.12	1.49	1.46
11	AA	1116	HIS	CD2-NE2	-5.12	1.32	1.37
14	AE	1108	GLN	CD-OE1	5.10	1.33	1.23
11	AA	1116	HIS	ND1-CE1	5.08	1.37	1.32
14	AE	424	ASN	CG-ND2	-5.08	1.22	1.33
14	AE	450	HIS	CD2-NE2	-5.07	1.32	1.37
11	AA	760	ASN	CG-ND2	-5.05	1.22	1.33
11	AA	1268	GLN	CD-NE2	-5.04	1.22	1.33
23	K	56	VAL	CA-CB	5.04	1.57	1.54
13	AC	23	HIS	CD2-NE2	-5.03	1.32	1.37
14	AE	777	HIS	CD2-NE2	-5.02	1.32	1.37

All (269) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	1516	G	O3'-P-O5'	17.48	130.22	104.00
11	AA	727	VAL	N-CA-C	-17.09	95.18	110.74
20	H	88	LYS	CA-C-N	16.96	143.61	120.38
20	H	88	LYS	C-N-CA	16.96	143.61	120.38
10	B	29	G	C3'-C2'-O2'	15.96	134.64	110.70
9	9	129	LEU	CA-C-N	15.80	139.59	119.84
9	9	129	LEU	C-N-CA	15.80	139.59	119.84
16	D	1516	G	P-O3'-C3'	-15.49	96.97	120.20
11	AA	1250	SER	CA-C-N	14.93	149.59	123.01
11	AA	1250	SER	C-N-CA	14.93	149.59	123.01
11	AA	374	GLU	CA-C-N	14.89	135.72	120.38
11	AA	374	GLU	C-N-CA	14.89	135.72	120.38
20	H	332	VAL	N-CA-C	13.61	124.50	110.62
20	H	169	SER	N-CA-C	12.73	137.91	110.80
20	H	330	VAL	N-CA-C	12.16	126.90	109.51
20	H	305	HIS	N-CA-C	11.96	131.10	111.37
14	AE	90	VAL	N-CA-C	9.92	122.23	107.75
11	AA	995	ASP	O-C-N	-9.82	109.52	122.59
39	a	2244	U	C1'-C2'-O2'	-9.79	93.71	108.40
11	AA	375	PRO	CA-N-CD	-9.59	98.58	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	1206	G	C4'-C3'-O3'	9.56	127.34	113.00
52	n	73	SER	N-CA-CB	-9.56	94.61	110.47
11	AA	935	THR	CA-CB-OG1	-9.47	95.40	109.60
28	P	54	SER	CA-C-N	9.37	129.06	118.85
28	P	54	SER	C-N-CA	9.37	129.06	118.85
39	a	2250	G	C4'-C3'-O3'	-9.21	95.59	109.40
11	AA	376	PRO	N-CA-CB	-9.18	93.61	103.25
11	AA	943	LYS	CA-C-O	-9.05	107.57	120.51
16	D	1401	G	C4'-C3'-O3'	8.89	126.34	113.00
16	D	428	G	C4'-C3'-O3'	8.70	122.46	109.40
9	9	130	PRO	CA-N-CD	-8.61	99.94	112.00
8	7	-11	A	O3'-P-O5'	-8.59	91.11	104.00
20	H	339	ARG	CA-C-N	8.54	137.86	121.54
20	H	339	ARG	C-N-CA	8.54	137.86	121.54
11	AA	375	PRO	N-CA-C	8.54	121.12	110.70
31	S	45	VAL	N-CA-CB	8.46	120.45	110.55
16	D	1515	G	O3'-P-O5'	-8.44	91.34	104.00
39	a	2296	U	C4'-C3'-O3'	8.42	122.03	109.40
11	AA	849	GLU	CA-C-N	8.40	137.09	121.97
11	AA	849	GLU	C-N-CA	8.40	137.09	121.97
39	a	404	A	C2'-C3'-O3'	8.36	122.04	109.50
28	P	57	VAL	N-CA-C	8.32	120.09	107.77
8	7	-8	U	C2'-C3'-O3'	8.32	121.97	109.50
16	D	197	A	C2'-C3'-O3'	8.14	121.72	109.50
39	a	2252	G	N9-C1'-C2'	-8.13	99.81	112.00
11	AA	1048	LYS	CA-C-N	-8.03	115.33	122.96
11	AA	1048	LYS	C-N-CA	-8.03	115.33	122.96
16	D	1401	G	N9-C1'-C2'	-7.90	100.14	112.00
39	a	2425	A	C2'-C3'-O3'	7.88	121.32	109.50
11	AA	855	PRO	N-CA-CB	-7.79	95.07	103.25
20	H	155	LYS	CA-C-N	-7.77	110.93	121.66
20	H	155	LYS	C-N-CA	-7.77	110.93	121.66
39	a	2071	A	C4'-C3'-O3'	-7.71	101.43	113.00
20	H	168	VAL	CA-C-N	7.66	136.18	121.54
20	H	168	VAL	C-N-CA	7.66	136.18	121.54
14	AE	903	LEU	CA-C-N	7.66	136.17	121.54
14	AE	903	LEU	C-N-CA	7.66	136.17	121.54
52	n	75	ALA	CA-C-N	7.66	129.71	120.14
52	n	75	ALA	C-N-CA	7.66	129.71	120.14
16	D	1499	A	N9-C1'-C2'	-7.64	100.55	112.00
16	D	1493	A	C2'-C3'-O3'	7.63	125.15	113.70
20	H	84	LEU	N-CA-C	7.62	120.99	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	52	GLN	N-CA-C	-7.62	104.13	113.50
36	X	102	THR	CB-CA-C	7.59	123.43	110.84
23	K	60	ILE	N-CA-CB	7.56	119.40	110.55
16	D	1339	A	P-O3'-C3'	7.54	131.51	120.20
11	AA	864	LYS	N-CA-C	-7.53	102.33	112.26
16	D	528	C	N1-C1'-C2'	-7.51	100.73	112.00
20	H	336	ASP	CB-CA-C	-7.46	98.63	110.79
52	n	73	SER	CB-CA-C	7.43	122.90	110.79
23	K	56	VAL	O-C-N	7.43	125.17	120.42
10	B	28	C	P-O3'-C3'	7.35	131.22	120.20
39	a	2602	A	C4'-C3'-O3'	7.34	120.40	109.40
52	n	108	VAL	O-C-N	7.34	125.28	120.07
11	AA	751	TYR	CA-C-N	7.26	132.25	121.72
11	AA	751	TYR	C-N-CA	7.26	132.25	121.72
39	a	783	A	C4'-C3'-O3'	7.26	123.90	113.00
16	D	196	A	P-O3'-C3'	7.20	131.00	120.20
19	G	47	VAL	O-C-N	7.18	125.02	120.42
10	B	29	G	N9-C1'-C2'	-7.15	101.28	112.00
11	AA	375	PRO	CB-CA-C	-7.12	102.23	110.92
16	D	1497	G	C1'-C2'-O2'	-7.10	97.75	108.40
39	a	2162	G	C4'-C3'-O3'	7.09	120.04	109.40
39	a	896	A	C4'-C3'-O3'	7.00	119.90	109.40
39	a	2225	A	C4'-C3'-O3'	7.00	119.89	109.40
39	a	1379	U	C2'-C3'-O3'	6.99	124.18	113.70
25	M	27	VAL	N-CA-CB	6.96	118.69	110.55
39	a	2244	U	C4'-C3'-O3'	6.92	123.37	113.00
20	H	140	PRO	N-CA-CB	6.86	110.46	103.25
11	AA	604	HIS	CB-CG-CD2	-6.83	122.32	131.20
20	H	340	ARG	CA-C-N	-6.81	112.54	123.23
20	H	340	ARG	C-N-CA	-6.81	112.54	123.23
13	AC	160	HIS	CB-CG-CD2	-6.78	122.38	131.20
11	AA	728	ASP	N-CA-C	6.76	125.19	110.80
39	a	2252	G	C4'-C3'-O3'	6.75	123.12	113.00
52	n	71	ARG	CA-C-N	6.72	133.94	122.37
52	n	71	ARG	C-N-CA	6.72	133.94	122.37
11	AA	855	PRO	CB-CA-C	-6.68	100.54	111.56
39	a	2243	U	C4'-C3'-O3'	6.67	123.00	113.00
20	H	170	ARG	N-CA-C	6.63	119.59	110.24
20	H	87	GLU	N-CA-C	-6.62	104.07	111.28
13	AC	117	HIS	CB-CA-C	-6.59	97.97	109.64
16	D	517	G	C5'-C4'-C3'	6.59	125.08	115.20
39	a	2189	U	C1'-C2'-O2'	-6.58	101.93	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	a	2167	U	P-O3'-C3'	6.57	130.05	120.20
11	AA	1116	HIS	CB-CG-CD2	-6.57	122.67	131.20
20	H	303	LEU	N-CA-C	6.56	121.12	112.13
16	D	526	C	C4'-C3'-O3'	6.55	122.83	113.00
20	H	132	PRO	N-CA-CB	6.55	110.26	103.38
27	O	72	ILE	N-CA-C	-6.54	105.34	111.48
39	a	894	U	C2'-C3'-O3'	6.52	119.28	109.50
20	H	155	LYS	N-CA-C	-6.51	98.29	108.90
52	n	127	ASN	CA-CB-CG	-6.51	106.09	112.60
52	n	127	ASN	CB-CA-C	6.51	121.64	110.77
20	H	112	ILE	N-CA-C	6.51	117.06	106.72
53	o	13	ARG	N-CA-C	6.48	121.02	113.18
56	r	61	VAL	N-CA-CB	6.48	118.13	110.55
39	a	754	U	N1-C1'-C2'	6.47	121.71	112.00
16	D	526	C	N1-C1'-C2'	-6.46	102.31	112.00
16	D	1340	A	C1'-C2'-O2'	6.45	118.08	108.40
13	AC	23	HIS	CB-CG-CD2	-6.37	122.92	131.20
11	AA	150	HIS	CB-CG-CD2	-6.36	122.93	131.20
12	AB	81	HIS	CB-CG-CD2	-6.36	122.93	131.20
16	D	69	G	C4'-C3'-O3'	-6.36	103.47	113.00
14	AE	93	THR	CA-C-N	6.33	132.97	121.06
14	AE	93	THR	C-N-CA	6.33	132.97	121.06
14	AE	61	ILE	CA-C-N	-6.33	114.04	121.64
14	AE	61	ILE	C-N-CA	-6.33	114.04	121.64
14	AE	450	HIS	CB-CG-CD2	-6.32	122.98	131.20
39	a	2434	A	P-O3'-C3'	6.30	129.65	120.20
11	AA	850	ILE	N-CA-CB	6.29	121.61	111.23
15	C	33	ILE	CA-C-O	-6.28	114.89	121.93
14	AE	777	HIS	CB-CG-CD2	-6.28	123.04	131.20
16	D	1208	C	N1-C1'-C2'	-6.27	102.60	112.00
20	H	153	GLU	N-CA-C	-6.25	97.48	110.80
10	B	28	C	O3'-P-O5'	-6.22	94.67	104.00
11	AA	888	THR	CB-CA-C	-6.22	99.40	108.91
39	a	2425	A	C4'-C3'-O3'	6.17	118.66	109.40
20	H	113	ASN	N-CA-C	6.15	118.07	111.36
16	D	1206	G	N9-C1'-C2'	-6.15	102.77	112.00
39	a	271	G	C4'-C3'-O3'	6.11	118.57	109.40
14	AE	70	CYS	CB-CA-C	6.10	120.29	110.29
11	AA	861	ALA	CA-C-N	6.07	133.14	121.54
11	AA	861	ALA	C-N-CA	6.07	133.14	121.54
16	D	1516	G	OP1-P-O3'	-6.04	89.87	108.00
39	a	2210	U	C4'-C3'-O3'	6.03	118.45	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AA	1004	ASP	CB-CA-C	5.99	122.35	110.42
13	AC	74	VAL	N-CA-C	5.98	117.45	108.96
16	D	1408	A	C4'-C3'-O3'	5.98	121.97	113.00
16	D	550	G	C3'-C2'-O2'	5.96	119.64	110.70
11	AA	869	GLY	CA-C-O	-5.96	117.81	122.52
39	a	1913	A	C2'-C3'-O3'	5.96	118.44	109.50
39	a	2820	A	C4'-C3'-O3'	-5.95	104.07	113.00
25	M	92	ARG	CA-C-N	5.91	125.39	119.24
25	M	92	ARG	C-N-CA	5.91	125.39	119.24
13	AC	75	GLN	N-CA-CB	5.90	119.34	110.19
14	AE	90	VAL	CA-C-O	-5.90	114.26	120.39
11	AA	604	HIS	CB-CG-ND1	5.89	131.53	122.70
20	H	109	THR	N-CA-C	-5.89	99.05	109.06
50	l	108	ILE	N-CA-CB	5.89	118.54	110.54
39	a	2308	G	C2'-C3'-O3'	-5.87	104.90	113.70
39	a	2756	U	C4'-C3'-O3'	5.86	118.19	109.40
13	AC	160	HIS	CB-CG-ND1	5.85	131.47	122.70
11	AA	936	ARG	CA-C-O	-5.84	113.99	120.70
11	AA	1116	HIS	CB-CG-ND1	5.84	131.46	122.70
39	a	1905	C	P-O3'-C3'	5.82	128.94	120.20
20	H	150	LYS	N-CA-C	5.82	118.20	110.53
52	n	72	LYS	N-CA-C	-5.82	99.17	109.06
39	a	70	G	C4'-C3'-O3'	5.80	118.11	109.40
20	H	75	VAL	N-CA-C	5.80	116.47	108.12
10	B	29	G	O5'-C5'-C4'	-5.79	102.81	111.50
11	AA	732	ILE	CB-CA-C	-5.78	103.64	111.15
36	X	26	GLY	N-CA-C	-5.77	104.40	112.13
16	D	1275	A	P-O3'-C3'	5.75	128.82	120.20
14	AE	91	GLU	N-CA-C	5.74	123.03	110.80
16	D	1492	A	P-O3'-C3'	5.74	128.81	120.20
13	AC	76	GLU	N-CA-C	-5.73	101.80	110.28
10	A	48	C	N1-C1'-C2'	5.73	120.59	112.00
16	D	1490	U	P-O3'-C3'	5.72	128.78	120.20
16	D	976	G	C4'-C3'-O3'	-5.71	104.44	113.00
10	B	48	C	N1-C1'-C2'	5.71	120.56	112.00
16	D	1406	U	N1-C1'-C2'	-5.70	103.45	112.00
16	D	1340	A	C5'-C4'-C3'	5.69	124.54	116.00
39	a	1757	A	C4'-C3'-O3'	-5.69	104.47	113.00
39	a	2168	G	C4'-C3'-O3'	-5.67	104.49	113.00
12	AB	81	HIS	CB-CG-ND1	5.66	131.19	122.70
39	a	2017	U	C2'-C3'-O3'	-5.61	105.28	113.70
11	AA	942	ASP	N-CA-C	-5.60	106.61	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AC	23	HIS	CB-CG-ND1	5.59	131.09	122.70
20	H	114	GLY	N-CA-C	5.59	121.20	111.14
16	D	780	A	C4'-C3'-O3'	-5.58	104.64	113.00
39	a	2447	G	C2'-C3'-O3'	-5.55	101.17	109.50
11	AA	996	ARG	N-CA-C	-5.55	101.36	109.63
39	a	1568	G	C4'-C3'-O3'	-5.53	104.70	113.00
11	AA	853	ASP	CA-C-N	5.52	130.31	120.70
11	AA	853	ASP	C-N-CA	5.52	130.31	120.70
14	AE	450	HIS	CB-CG-ND1	5.52	130.98	122.70
11	AA	940	GLU	CA-C-O	-5.50	112.64	120.51
11	AA	150	HIS	CB-CG-ND1	5.49	130.93	122.70
39	a	2731	G	C4'-C3'-O3'	-5.47	104.79	113.00
11	AA	872	TYR	CA-C-N	5.43	131.74	121.97
11	AA	872	TYR	C-N-CA	5.43	131.74	121.97
14	AE	93	THR	CB-CA-C	5.42	121.21	110.42
16	D	864	A	N9-C1'-C2'	5.40	120.09	112.00
39	a	2572	A	C4'-C3'-O3'	-5.39	101.32	109.40
39	a	944	C	C4'-C3'-O3'	-5.38	104.92	113.00
14	AE	69	GLU	CA-C-N	-5.38	113.92	121.72
14	AE	69	GLU	C-N-CA	-5.38	113.92	121.72
39	a	1270	C	C2'-C3'-O3'	-5.37	105.65	113.70
11	AA	375	PRO	N-CA-CB	5.37	108.29	103.08
16	D	1499	A	C4'-C3'-O3'	5.36	121.04	113.00
16	D	1145	A	C4'-C3'-O3'	-5.36	104.96	113.00
16	D	517	G	C4'-C3'-O3'	-5.36	101.36	109.40
10	B	35	A	P-O3'-C3'	5.35	128.23	120.20
14	AE	777	HIS	CB-CG-ND1	5.35	130.73	122.70
39	a	2481	G	C4'-C3'-O3'	-5.35	104.97	113.00
39	a	2068	U	C4'-C3'-O3'	-5.35	104.98	113.00
45	g	5	ILE	N-CA-C	5.34	117.72	111.05
14	AE	70	CYS	N-CA-C	-5.34	101.09	109.25
11	AA	1030	GLU	N-CA-C	-5.33	105.14	111.69
39	a	2231	U	C1'-C2'-O2'	5.32	116.38	108.40
39	a	375	G	C2'-C3'-O3'	5.31	121.66	113.70
36	X	102	THR	CA-C-O	-5.30	114.82	121.02
39	a	2020	A	C4'-C3'-O3'	-5.29	105.06	113.00
14	AE	73	GLY	N-CA-C	5.28	125.70	113.18
16	D	145	G	P-O3'-C3'	5.28	128.12	120.20
11	AA	1158	LYS	CA-C-N	5.27	131.46	121.97
11	AA	1158	LYS	C-N-CA	5.27	131.46	121.97
14	AE	90	VAL	O-C-N	-5.26	117.63	123.20
39	a	2529	G	C4'-C3'-O3'	-5.26	105.11	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AA	732	ILE	N-CA-CB	5.25	116.25	110.53
11	AA	934	PHE	N-CA-C	-5.25	103.73	111.81
16	D	1395	C	P-O3'-C3'	5.24	128.06	120.20
14	AE	88	CYS	N-CA-C	5.22	120.30	113.88
10	B	60	U	C2'-C3'-O3'	5.21	117.32	109.50
11	AA	870	ILE	CA-C-N	5.20	128.28	120.69
11	AA	870	ILE	C-N-CA	5.20	128.28	120.69
10	A	60	U	C2'-C3'-O3'	5.20	117.30	109.50
20	H	128	ARG	CA-C-N	-5.17	114.13	122.81
20	H	128	ARG	C-N-CA	-5.17	114.13	122.81
59	u	101	ILE	N-CA-C	5.16	116.46	112.12
39	a	1834	U	C4'-C3'-O3'	-5.16	105.26	113.00
39	a	2245	U	N1-C1'-C2'	-5.15	104.28	112.00
39	a	423	A	C2'-C3'-O3'	-5.14	105.98	113.70
39	a	528	A	C4'-C3'-O3'	-5.13	105.30	113.00
13	AC	117	HIS	N-CA-C	5.13	116.91	110.24
16	D	1335	U	C4'-C3'-O3'	-5.13	105.31	113.00
20	H	154	PHE	N-CA-C	-5.11	100.37	109.06
39	a	479	A	C4'-C3'-O3'	5.11	117.06	109.40
39	a	126	A	C4'-C3'-O3'	-5.10	105.34	113.00
14	AE	1184	ASP	N-CA-C	5.10	121.07	109.81
39	a	328	U	C4'-C3'-O3'	-5.09	105.37	113.00
9	9	115	GLY	CA-C-O	-5.07	118.18	122.29
28	P	25	ILE	N-CA-CB	5.06	117.43	110.54
39	a	614	A	C2'-C3'-O3'	5.06	117.10	109.50
15	C	35	GLU	N-CA-C	-5.05	105.96	111.82
14	AE	61	ILE	CA-C-O	-5.05	115.70	120.95
11	AA	377	THR	CA-C-N	5.05	127.00	120.44
11	AA	377	THR	C-N-CA	5.05	127.00	120.44
11	AA	943	LYS	N-CA-C	5.05	121.55	110.80
39	a	1864	U	C4'-C3'-O3'	-5.05	105.43	113.00
57	s	28	LEU	CA-C-N	5.04	126.99	120.44
57	s	28	LEU	C-N-CA	5.04	126.99	120.44
20	H	108	VAL	N-CA-C	-5.03	98.87	109.34
39	a	2193	G	C2'-C3'-O3'	5.03	121.25	113.70
10	B	19	G	N9-C1'-C2'	5.01	119.52	112.00
14	AE	89	GLY	CA-C-N	5.01	129.77	123.10
14	AE	89	GLY	C-N-CA	5.01	129.77	123.10
16	D	70	U	C2'-C3'-O3'	5.01	117.02	109.50

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	A	19	G	Sidechain
10	A	7	G	Sidechain
11	AA	1134	GLN	Peptide
11	AA	1157	GLN	Peptide
11	AA	1158	LYS	Peptide
11	AA	205	PRO	Peptide
11	AA	594	VAL	Peptide
11	AA	595	THR	Peptide
11	AA	596	ASP	Mainchain
11	AA	696	ASP	Peptide
11	AA	746	ALA	Peptide
11	AA	853	ASP	Mainchain
14	AE	1184	ASP	Peptide
14	AE	1326	GLN	Peptide
14	AE	313	GLY	Peptide
14	AE	416	ILE	Peptide
14	AE	804	ALA	Peptide
10	B	19	G	Sidechain
10	B	7	G	Sidechain
20	H	274	TYR	Peptide
20	H	81	GLU	Peptide
20	H	82	THR	Peptide
36	X	100	GLN	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	816	839	839	8	0
2	1	857	922	922	14	0
3	2	746	811	811	7	0
4	3	788	844	844	10	0
5	4	753	780	780	0	0
6	5	472	260	261	22	0
7	6	542	305	306	24	0
8	7	547	97	271	74	0
9	9	1117	0	1153	160	0
10	A	1620	826	826	171	0
10	B	1620	813	827	137	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	AA	10425	10426	10428	388	0
12	AB	790	783	783	8	0
13	AC	1786	1813	1813	78	0
13	AD	1767	1789	1789	48	0
14	AE	10388	10612	10611	373	0
15	C	544	559	560	23	0
16	D	32703	16423	16459	227	0
17	E	669	719	719	3	0
18	F	589	629	629	8	0
19	G	1760	1785	1785	47	0
20	H	1730	1454	1454	211	0
21	I	1636	1710	1710	39	0
22	J	1643	1707	1707	29	0
23	K	1152	1196	1196	22	0
24	L	848	846	846	3	0
25	M	1181	1235	1235	33	0
26	N	979	1031	1031	5	0
27	O	1022	1070	1070	12	0
28	P	790	831	831	37	0
29	Q	877	887	887	4	0
30	R	939	1001	1001	7	0
31	S	805	844	844	5	0
32	T	714	734	734	7	0
33	U	649	666	666	3	0
34	V	648	691	691	4	0
35	W	663	688	688	2	0
36	X	900	964	964	57	0
37	Y	1032	0	1088	88	0
38	Z	227	0	237	18	0
39	a	61841	31077	31123	293	0
40	b	582	599	599	2	0
41	c	625	652	652	4	0
42	d	2569	1301	1301	5	0
43	e	501	531	531	4	0
44	f	448	488	488	5	0
45	g	522	520	520	11	0
46	h	2082	2154	2154	20	0
47	i	444	459	458	6	0
48	j	1565	1617	1616	15	0
49	k	426	464	464	0	0
50	l	1552	1619	1619	14	0
51	m	377	418	418	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	n	1410	1443	1444	27	0
53	o	504	572	572	4	0
54	p	1313	1358	1358	7	0
55	q	302	343	343	1	0
56	r	1111	1148	1148	4	0
57	s	1129	1162	1162	14	0
58	t	946	1023	1023	12	0
59	u	1053	1129	1129	8	0
60	v	1074	1157	1157	5	0
61	w	951	994	994	7	0
62	x	892	923	923	10	0
63	y	917	962	962	4	0
64	z	947	1020	1019	13	0
65	AE	1	0	0	0	0
66	AE	2	0	0	0	0
All	All	175820	124723	127473	2425	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 8.

All (2425) 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)
20:H:131:LEU:CB	20:H:167:VAL:CA	1.78	1.58
15:C:12:ARG:HG3	20:H:264:GLU:CB	1.30	1.53
20:H:131:LEU:CB	20:H:167:VAL:HA	1.03	1.46
9:9:31:ARG:NE	39:a:1054:A:H5'	1.31	1.45
11:AA:1026:GLU:HG3	16:D:1030:U:C2	1.54	1.42
20:H:71:ALA:C	20:H:72:LEU:HD12	1.49	1.38
20:H:118:GLY:O	20:H:133:GLY:CA	1.74	1.35
9:9:130:PRO:N	9:9:130:PRO:CA	1.70	1.34
39:a:1839:G:H1'	39:a:1927:A:C8	1.62	1.33
9:9:57:ASN:OD1	9:9:62:ARG:CG	1.75	1.32
16:D:1358:U:O4	16:D:1363:A:N1	1.60	1.31
39:a:1021:A:N1	39:a:1141:U:O4	1.63	1.31
9:9:31:ARG:CZ	39:a:1054:A:H5'	1.63	1.29
16:D:1308:U:H3'	36:X:98:ARG:CZ	1.43	1.28
16:D:1308:U:H2'	36:X:98:ARG:NH2	1.48	1.27
8:7:17:G:OP2	11:AA:540:ARG:NH1	1.68	1.26
10:A:32:C:O4'	25:M:144:MET:HE1	1.09	1.25
15:C:12:ARG:CG	20:H:264:GLU:CB	2.15	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:948:C:OP2	36:X:105:ASN:OD1	1.53	1.23
20:H:118:GLY:O	20:H:133:GLY:HA3	1.27	1.22
16:D:1227:A:OP2	36:X:110:LYS:HE3	1.35	1.22
10:A:18:G:N7	10:A:57:A:N6	1.87	1.22
14:AE:87:LYS:HG3	22:J:20:PHE:CE1	1.73	1.22
16:D:1308:U:C2'	36:X:98:ARG:NH2	2.03	1.21
16:D:563:A:N1	16:D:884:U:O4	1.73	1.20
20:H:267:TRP:CZ2	20:H:340:ARG:HG2	1.75	1.20
10:B:18:G:N7	10:B:57:A:N6	1.87	1.20
9:9:88:HIS:HB3	9:9:89:PRO:CD	1.70	1.19
8:7:-9:G:H5''	16:D:1500:A:N6	1.61	1.16
13:AC:65:LEU:HA	21:I:80:LYS:HB3	1.26	1.16
9:9:31:ARG:NE	39:a:1054:A:C5'	2.07	1.15
16:D:1329:A:OP1	36:X:28:THR:HB	1.47	1.14
10:A:70:G:H2'	10:A:71:C:H5''	1.23	1.14
19:G:19:GLN:CD	20:H:76:GLU:CB	2.19	1.14
13:AC:65:LEU:HB3	21:I:80:LYS:HB2	1.16	1.13
20:H:135:LEU:CB	20:H:167:VAL:CB	2.27	1.13
10:A:32:C:O4'	25:M:144:MET:CE	1.98	1.12
20:H:267:TRP:CE2	20:H:340:ARG:HG2	1.84	1.12
9:9:142:THR:HG21	38:Z:7:ILE:HG12	1.21	1.12
11:AA:1026:GLU:HG3	16:D:1030:U:N1	1.65	1.11
14:AE:86:GLU:HA	22:J:166:GLU:CB	1.79	1.11
9:9:129:LEU:N	9:9:130:PRO:HD3	1.66	1.11
13:AC:119:GLY:H	28:P:90:LEU:HD23	1.01	1.11
19:G:19:GLN:CD	20:H:76:GLU:HB3	1.67	1.11
15:C:44:ILE:HD13	20:H:339:ARG:HG2	1.18	1.10
15:C:44:ILE:HD13	20:H:339:ARG:CG	1.78	1.10
14:AE:53:ARG:NH2	22:J:164:GLN:O	1.84	1.10
10:B:70:G:H2'	10:B:71:C:H5''	1.23	1.10
20:H:119:GLY:HA2	20:H:133:GLY:HA2	1.14	1.10
9:9:50:VAL:HG22	37:Y:119:ALA:CB	1.82	1.09
16:D:1308:U:C3'	36:X:98:ARG:CZ	2.31	1.09
22:J:162:ALA:HA	22:J:165:ARG:CZ	1.83	1.09
39:a:1839:G:C8	39:a:1927:A:H1'	1.87	1.08
9:9:88:HIS:CB	9:9:89:PRO:HD3	1.82	1.08
20:H:267:TRP:CH2	20:H:340:ARG:HG2	1.87	1.08
16:D:1308:U:C2'	36:X:98:ARG:HH21	1.63	1.08
19:G:19:GLN:CG	20:H:75:VAL:HG22	1.84	1.08
20:H:71:ALA:O	20:H:72:LEU:HD12	1.53	1.07
9:9:57:ASN:OD1	9:9:62:ARG:HG3	1.44	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:24:LEU:HG	14:AE:232:ASN:HD21	1.17	1.07
16:D:1308:U:C3'	36:X:98:ARG:NH2	2.16	1.06
10:A:56:C:H2'	10:A:57:A:H5''	1.39	1.05
9:9:129:LEU:H	9:9:130:PRO:HD3	0.90	1.05
10:A:18:G:N2	10:A:55:U:O2	1.90	1.04
20:H:19:ARG:O	20:H:72:LEU:HB2	1.58	1.04
10:B:18:G:N2	10:B:55:U:O2	1.90	1.03
20:H:162:LYS:CB	20:H:298:GLU:CD	2.30	1.03
16:D:1227:A:OP2	36:X:110:LYS:CE	2.06	1.02
14:AE:86:GLU:HA	22:J:166:GLU:HB3	1.35	1.02
10:B:56:C:O4'	52:n:80:ARG:NH2	1.91	1.02
13:AC:119:GLY:N	28:P:90:LEU:HD23	1.72	1.02
10:B:56:C:H5'	52:n:80:ARG:CZ	1.90	1.02
10:B:70:G:C2'	10:B:71:C:H5''	1.89	1.02
16:D:1329:A:OP1	36:X:28:THR:CB	2.07	1.02
8:7:2:U:O2'	23:K:57:PRO:HB3	1.58	1.01
10:B:56:C:H2'	10:B:57:A:H5''	1.39	1.01
20:H:290:TYR:O	20:H:305:HIS:O	1.77	1.01
8:7:-8:U:O2'	16:D:1403:C:O2	1.78	1.01
19:G:19:GLN:HG3	20:H:75:VAL:HG22	1.38	1.01
10:A:70:G:C2'	10:A:71:C:H5''	1.89	1.01
19:G:38:VAL:CG2	20:H:75:VAL:HG21	1.90	1.00
8:7:-9:G:C5'	16:D:1500:A:H62	1.73	1.00
13:AC:167:PRO:HB3	21:I:103:ILE:O	1.59	1.00
16:D:13:U:O4	16:D:20:U:O4	1.79	1.00
11:AA:992:LEU:HD22	11:AA:992:LEU:H	1.21	1.00
19:G:38:VAL:HG22	20:H:75:VAL:HG21	1.44	1.00
16:D:1308:U:H3'	36:X:98:ARG:NH2	1.76	1.00
8:7:-10:U:P	16:D:1505:G:H8	1.83	1.00
16:D:13:U:N3	16:D:915:A:C6	2.29	1.00
39:a:2297:A:N1	39:a:2321:U:C4	2.29	1.00
20:H:131:LEU:CB	20:H:167:VAL:CB	2.40	0.99
14:AE:111:THR:HG23	14:AE:300:GLN:CD	1.86	0.99
9:9:93:ALA:O	9:9:129:LEU:HD12	1.60	0.99
10:A:32:C:C4'	25:M:144:MET:HE1	1.93	0.99
9:9:31:ARG:CD	39:a:1054:A:H5'	1.94	0.98
20:H:118:GLY:O	20:H:133:GLY:HA2	1.63	0.98
39:a:1839:G:C1'	39:a:1927:A:C8	2.46	0.98
10:A:32:C:O2'	25:M:86:GLN:CG	2.12	0.97
9:9:129:LEU:H	9:9:130:PRO:CD	1.77	0.97
13:AC:118:ASP:HA	28:P:89:ARG:HB3	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:a:1839:G:O4'	39:a:1927:A:O4'	1.82	0.96
20:H:119:GLY:CA	20:H:133:GLY:HA2	1.95	0.96
9:9:142:THR:HG21	38:Z:7:ILE:CG1	1.95	0.96
9:9:57:ASN:OD1	9:9:62:ARG:HG2	1.64	0.95
10:A:72:A:H2'	10:A:73:A:H5''	1.49	0.95
8:7:-10:U:OP2	16:D:1505:G:C8	2.20	0.95
16:D:1308:U:H2'	36:X:98:ARG:HH21	1.06	0.95
7:6:15:DC:N4	7:6:16:DC:N4	2.15	0.95
9:9:88:HIS:CB	9:9:89:PRO:CD	2.41	0.95
13:AC:118:ASP:HB3	28:P:90:LEU:HD22	1.50	0.94
14:AE:68:TYR:O	14:AE:75:TYR:CE2	2.20	0.94
11:AA:878:THR:O	11:AA:920:VAL:HG11	1.68	0.94
11:AA:1026:GLU:CG	16:D:1030:U:C2	2.50	0.94
39:a:67:U:N3	39:a:74:A:C6	2.35	0.94
13:AC:158:ARG:HB3	13:AC:158:ARG:HH11	1.32	0.94
16:D:13:U:C4	16:D:915:A:N6	2.36	0.93
11:AA:768:MET:CE	13:AC:80:GLU:OE1	2.17	0.93
20:H:119:GLY:HA3	20:H:131:LEU:O	1.68	0.93
10:B:72:A:H2'	10:B:73:A:H5''	1.49	0.93
20:H:135:LEU:HA	20:H:157:ILE:CB	1.98	0.93
39:a:1839:G:O4'	39:a:1927:A:C1'	2.15	0.93
16:D:13:U:N3	16:D:915:A:N6	2.16	0.92
8:7:-10:U:P	16:D:1505:G:C8	2.62	0.92
10:B:75:C:OP1	39:a:2602:A:C8	2.22	0.92
39:a:2013:A:N6	39:a:2613:U:H3	1.68	0.92
10:B:68:C:H2'	10:B:69:C:H5''	1.50	0.92
9:9:50:VAL:HG22	37:Y:119:ALA:HB1	1.50	0.92
10:A:32:C:O2'	25:M:86:GLN:HG3	1.68	0.92
8:7:1:U:H5'	23:K:56:VAL:HG21	1.52	0.92
10:A:68:C:H2'	10:A:69:C:H5''	1.51	0.92
14:AE:86:GLU:CA	22:J:166:GLU:HB3	2.00	0.92
8:7:-9:G:C5'	16:D:1500:A:N6	2.31	0.91
13:AC:118:ASP:HB3	28:P:90:LEU:CD2	1.99	0.91
39:a:1406:U:O2'	39:a:1407:G:C5'	2.19	0.91
11:AA:868:SER:OG	11:AA:941:LYS:HG2	1.69	0.91
16:D:13:U:C4	16:D:20:U:O4	2.23	0.91
6:5:113:DC:OP2	11:AA:163:LYS:HD3	1.71	0.91
9:9:129:LEU:N	9:9:130:PRO:CD	2.34	0.91
9:9:88:HIS:HB3	9:9:89:PRO:HD3	0.92	0.90
11:AA:728:ASP:OD1	11:AA:769:PRO:HG2	1.71	0.90
14:AE:86:GLU:HA	22:J:166:GLU:HB2	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:109:DT:H2''	11:AA:200:ARG:HG3	1.54	0.90
14:AE:136:GLU:OE1	14:AE:312:ARG:NH1	2.04	0.90
10:B:18:G:N2	10:B:58:A:N7	2.19	0.90
11:AA:1030:GLU:CD	16:D:1030:U:O4	2.14	0.90
20:H:279:LYS:HA	20:H:331:MET:HB3	1.54	0.90
9:9:93:ALA:O	9:9:129:LEU:CD1	2.19	0.90
37:Y:21:PRO:HB2	37:Y:22:PRO:HD3	1.54	0.89
20:H:71:ALA:C	20:H:72:LEU:CD1	2.42	0.89
10:A:18:G:N2	10:A:58:A:N7	2.19	0.89
20:H:119:GLY:HA2	20:H:133:GLY:CA	2.01	0.89
10:A:56:C:H1'	39:a:2112:G:C6	2.06	0.89
6:5:114:DC:H5''	14:AE:1148:ARG:NH2	1.87	0.89
20:H:162:LYS:N	20:H:298:GLU:OE2	2.06	0.89
37:Y:104:GLN:HG2	37:Y:108:ILE:HD11	1.53	0.89
14:AE:202:ARG:HG2	14:AE:202:ARG:HH11	1.35	0.89
8:7:17:G:OP2	11:AA:540:ARG:CZ	2.21	0.89
39:a:2314:A:H1'	52:n:155:THR:HG21	1.54	0.89
14:AE:68:TYR:C	14:AE:75:TYR:HE2	1.80	0.88
14:AE:24:LEU:HB2	14:AE:232:ASN:OD1	1.71	0.88
20:H:131:LEU:CB	20:H:167:VAL:N	2.37	0.88
9:9:142:THR:CG2	38:Z:7:ILE:HG12	2.02	0.88
13:AC:65:LEU:HA	21:I:80:LYS:CB	2.02	0.88
12:AB:107:GLU:OE1	14:AE:288:PRO:HB3	1.72	0.88
12:AB:107:GLU:CD	14:AE:288:PRO:HB3	1.99	0.88
39:a:783:A:N3	39:a:783:A:H2'	1.89	0.88
13:AC:91:ARG:NE	13:AC:122:GLU:OE2	2.07	0.88
9:9:50:VAL:CG2	37:Y:119:ALA:HB3	2.04	0.87
6:5:110:DA:N7	11:AA:183:TRP:CH2	2.43	0.87
11:AA:1008:GLN:NE2	11:AA:1008:GLN:O	2.07	0.87
13:AC:65:LEU:CB	21:I:80:LYS:HB2	2.02	0.87
19:G:18:HIS:HA	20:H:43:LYS:HD2	1.55	0.87
11:AA:1026:GLU:CG	16:D:1030:U:N1	2.38	0.87
22:J:162:ALA:HB2	22:J:165:ARG:NH2	1.90	0.87
8:7:-3:U:C5	16:D:528:C:P	2.69	0.86
11:AA:1090:ASN:O	13:AC:182:ARG:NH1	2.09	0.86
14:AE:24:LEU:HG	14:AE:232:ASN:ND2	1.90	0.86
10:A:33:U:H5''	25:M:84:THR:HG21	1.55	0.86
20:H:332:VAL:HG11	20:H:335:ILE:HG13	1.57	0.86
45:g:16:CYS:CB	45:g:37:CYS:HB3	2.05	0.86
10:A:18:G:N7	10:A:57:A:C6	2.44	0.86
9:9:52:MET:C	9:9:52:MET:HE3	2.00	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:981:ALA:HB3	11:AA:1008:GLN:HG3	1.58	0.85
13:AC:167:PRO:CB	21:I:103:ILE:O	2.24	0.85
15:C:31:ASN:OD1	20:H:268:VAL:HG22	1.74	0.85
20:H:348:GLN:N	20:H:348:GLN:OE1	2.08	0.85
9:9:125:ARG:NH1	9:9:125:ARG:HA	1.92	0.85
37:Y:81:LYS:O	37:Y:81:LYS:HE3	1.75	0.85
10:B:18:G:N7	10:B:57:A:C6	2.44	0.85
16:D:197:A:C6	16:D:221:C:H4'	2.11	0.85
22:J:61:VAL:HG21	22:J:200:ILE:HD11	1.57	0.85
14:AE:26:SER:HB2	14:AE:236:TRP:CZ2	2.12	0.85
9:9:31:ARG:HH11	9:9:31:ARG:HG3	1.41	0.84
11:AA:967:LEU:O	11:AA:967:LEU:HD12	1.76	0.84
14:AE:68:TYR:HB3	14:AE:75:TYR:OH	1.76	0.84
15:C:12:ARG:HH22	20:H:268:VAL:CG2	1.90	0.84
39:a:67:U:N3	39:a:74:A:N6	2.25	0.84
20:H:135:LEU:CB	20:H:167:VAL:C	2.50	0.84
14:AE:425:ARG:NH1	14:AE:458:ASN:O	2.09	0.84
9:9:31:ARG:CD	39:a:1054:A:H4'	2.06	0.84
9:9:50:VAL:HG22	37:Y:119:ALA:HB3	1.60	0.84
10:A:16:C:O2	39:a:2181:U:H5'	1.76	0.84
10:B:68:C:C2'	10:B:69:C:H5''	2.08	0.84
20:H:131:LEU:CB	20:H:166:VAL:O	2.26	0.84
20:H:267:TRP:CD2	20:H:340:ARG:HG2	2.12	0.84
10:A:68:C:C2'	10:A:69:C:H5''	2.08	0.84
19:G:16:PHE:HB3	20:H:43:LYS:HA	1.60	0.84
20:H:267:TRP:CZ3	20:H:340:ARG:HG2	2.12	0.84
23:K:111:MET:HE2	23:K:125:ALA:HB1	1.59	0.84
16:D:1227:A:H5'	36:X:110:LYS:NZ	1.93	0.83
11:AA:975:ILE:HG13	11:AA:1014:LEU:HD23	1.57	0.83
11:AA:980:VAL:HA	11:AA:984:VAL:HB	1.58	0.83
10:B:56:C:H5'	52:n:80:ARG:NE	1.93	0.83
10:A:72:A:C2'	10:A:73:A:H5''	2.09	0.83
39:a:2303:G:C2	39:a:2314:A:C2	2.66	0.83
4:3:34:VAL:HG13	4:3:67:VAL:HG22	1.58	0.83
39:a:1021:A:N6	39:a:1141:U:H3	1.77	0.83
37:Y:20:SER:HB3	37:Y:21:PRO:HD3	1.59	0.83
7:6:21:DA:N1	8:7:15:G:N2	2.26	0.82
11:AA:883:LEU:HD11	11:AA:920:VAL:HG22	1.59	0.82
9:9:28:ALA:H	9:9:110:ALA:HA	1.44	0.82
10:B:54:U:H3	10:B:58:A:N6	1.77	0.82
9:9:62:ARG:HG2	9:9:62:ARG:HH21	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:141:PHE:HE2	14:AE:296:LYS:HB2	1.45	0.82
20:H:267:TRP:CH2	20:H:340:ARG:CG	2.61	0.82
11:AA:953:LEU:HA	11:AA:1036:ILE:HD13	1.59	0.82
9:9:31:ARG:CD	39:a:1054:A:C4'	2.56	0.82
9:9:3:LEU:HD13	9:9:5:LEU:HG	1.62	0.82
37:Y:60:VAL:HG13	37:Y:66:PHE:HB3	1.58	0.82
39:a:1839:G:C1'	39:a:1927:A:N9	2.43	0.82
9:9:57:ASN:OD1	9:9:62:ARG:CD	2.27	0.82
11:AA:1043:ALA:HB1	11:AA:1044:PRO:HD2	1.61	0.82
13:AD:86:LYS:CE	14:AE:528:THR:HB	2.09	0.82
9:9:31:ARG:CZ	39:a:1054:A:C5'	2.49	0.82
16:D:37:U:N3	16:D:397:A:N6	2.28	0.82
11:AA:886:LYS:HE3	11:AA:886:LYS:O	1.80	0.81
14:AE:68:TYR:O	14:AE:75:TYR:HE2	1.58	0.81
10:B:72:A:C2'	10:B:73:A:H5''	2.09	0.81
20:H:155:LYS:CB	20:H:169:SER:CB	2.58	0.81
20:H:162:LYS:CA	20:H:298:GLU:OE2	2.17	0.81
20:H:305:HIS:CD2	20:H:306:VAL:H	1.98	0.81
13:AC:65:LEU:HB3	21:I:80:LYS:CB	2.06	0.81
39:a:1019:U:H3	39:a:1142:A:H61	1.28	0.81
14:AE:1169:THR:OG1	14:AE:1192:LYS:NZ	2.13	0.81
10:B:76:A:H1'	39:a:2494:G:P	2.20	0.81
16:D:972:C:O2'	28:P:57:VAL:CG2	2.29	0.81
20:H:267:TRP:CZ3	20:H:340:ARG:CG	2.63	0.81
37:Y:102:ARG:HB3	37:Y:141:ASP:HA	1.61	0.81
39:a:585:G:N7	64:z:6:ARG:NH1	2.29	0.81
10:B:22:G:H2'	10:B:23:C:C6	2.16	0.81
15:C:12:ARG:CB	20:H:264:GLU:CB	2.59	0.81
39:a:1019:U:H3	39:a:1142:A:N6	1.77	0.81
7:6:18:DC:H42	8:7:17:G:H1	1.27	0.81
9:9:50:VAL:CG2	37:Y:119:ALA:CB	2.59	0.81
14:AE:141:PHE:CE2	14:AE:296:LYS:HB2	2.15	0.81
7:6:21:DA:N1	8:7:15:G:C2	2.49	0.80
9:9:43:LYS:HD2	9:9:43:LYS:C	2.05	0.80
14:AE:37:GLU:O	14:AE:61:ILE:HD11	1.81	0.80
6:5:110:DA:N7	11:AA:183:TRP:HH2	1.77	0.80
11:AA:724:VAL:CG1	11:AA:774:GLY:H	1.93	0.80
10:A:54:U:H3	10:A:58:A:N6	1.78	0.80
22:J:162:ALA:CB	22:J:165:ARG:NH2	2.44	0.80
37:Y:27:LEU:HD12	37:Y:27:LEU:O	1.81	0.80
11:AA:1026:GLU:HG3	16:D:1030:U:N3	1.94	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:123:GLU:HA	20:H:128:ARG:HA	1.63	0.80
10:A:22:G:H2'	10:A:23:C:C6	2.16	0.80
10:B:58:A:O2'	10:B:59:A:H3'	1.82	0.80
39:a:1406:U:O2'	39:a:1407:G:H5''	1.79	0.80
39:a:2298:A:C4	39:a:2321:U:C5	2.70	0.80
52:n:125:ARG:O	52:n:127:ASN:ND2	2.14	0.80
39:a:2297:A:N1	39:a:2321:U:O4	2.14	0.80
10:A:18:G:N2	10:A:58:A:C5	2.50	0.80
45:g:18:CYS:HB3	45:g:40:CYS:CB	2.12	0.80
10:A:56:C:C2'	10:A:57:A:H5''	2.10	0.80
11:AA:611:GLU:OE2	11:AA:637:ARG:NH2	2.13	0.80
10:A:58:A:O2'	10:A:59:A:H3'	1.81	0.80
14:AE:111:THR:HG23	14:AE:300:GLN:OE1	1.81	0.80
16:D:1397:C:OP1	16:D:1397:C:H2'	1.81	0.80
11:AA:118:LYS:NZ	11:AA:487:LEU:O	2.14	0.79
22:J:162:ALA:CA	22:J:165:ARG:NH2	2.44	0.79
9:9:39:THR:HA	9:9:42:ARG:HD2	1.64	0.79
10:B:18:G:N2	10:B:58:A:C5	2.50	0.79
22:J:162:ALA:HA	22:J:165:ARG:NH2	1.95	0.79
22:J:162:ALA:HB2	22:J:165:ARG:HH22	1.47	0.79
37:Y:72:THR:OG1	37:Y:73:PRO:HD2	1.81	0.79
39:a:2189:U:OP1	39:a:2189:U:O4'	2.00	0.79
9:9:31:ARG:HD2	39:a:1054:A:H4'	1.62	0.79
10:B:56:C:C2'	10:B:57:A:H5''	2.11	0.79
20:H:122:VAL:O	20:H:129:ALA:N	2.13	0.79
13:AC:119:GLY:H	28:P:90:LEU:CD2	1.89	0.79
14:AE:90:VAL:HG13	14:AE:90:VAL:O	1.82	0.79
20:H:270:ILE:CG2	20:H:337:GLU:HB3	2.12	0.79
45:g:16:CYS:HB2	45:g:37:CYS:HB3	1.63	0.79
14:AE:87:LYS:HA	14:AE:87:LYS:HE3	1.63	0.79
14:AE:144:TYR:HE1	14:AE:162:GLU:OE2	1.64	0.79
16:D:1329:A:P	36:X:28:THR:HB	2.22	0.79
11:AA:1007:LYS:O	11:AA:1007:LYS:HD2	1.83	0.78
19:G:35:ARG:HD2	20:H:14:LYS:HD3	1.66	0.78
39:a:1406:U:O2'	39:a:1407:G:P	2.41	0.78
9:9:3:LEU:H	9:9:3:LEU:HD12	1.47	0.78
9:9:78:GLY:N	9:9:79:PRO:HD2	1.97	0.78
10:B:7:G:H4'	10:B:8:U:OP1	1.81	0.78
8:7:-3:U:C5	16:D:528:C:OP2	2.37	0.78
11:AA:964:LEU:HD12	11:AA:964:LEU:O	1.84	0.78
10:A:5:G:H2'	10:A:6:G:H5'	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:16:PHE:CZ	20:H:41:GLY:O	2.37	0.78
14:AE:1075:ARG:NH2	14:AE:1168:GLU:OE2	2.17	0.78
9:9:11:ILE:HD11	9:9:62:ARG:HA	1.65	0.78
10:A:7:G:H4'	10:A:8:U:OP1	1.81	0.78
13:AC:167:PRO:HB3	21:I:103:ILE:C	2.09	0.78
10:B:5:G:H2'	10:B:6:G:H5'	1.66	0.77
10:B:15:G:N1	10:B:20:U:O2	2.17	0.77
10:B:18:G:C5	10:B:57:A:C6	2.72	0.77
8:7:-3:U:C6	16:D:528:C:OP1	2.38	0.77
10:A:33:U:O3'	25:M:84:THR:OG1	2.02	0.77
13:AC:76:GLU:CD	13:AC:131:CYS:HA	2.09	0.77
14:AE:186:GLN:HG3	14:AE:238:ILE:HG13	1.65	0.77
37:Y:32:VAL:HG13	37:Y:60:VAL:HG21	1.66	0.77
11:AA:1257:GLN:HE22	14:AE:345:LYS:HA	1.48	0.77
15:C:44:ILE:CD1	20:H:339:ARG:CG	2.62	0.77
39:a:2756:U:N3	39:a:2758:A:N6	2.32	0.77
10:A:70:G:H2'	10:A:71:C:C5'	2.11	0.77
20:H:19:ARG:HD3	20:H:73:ASP:CG	2.09	0.77
10:A:15:G:N1	10:A:20:U:O2	2.17	0.77
10:A:18:G:C5	10:A:57:A:C6	2.72	0.77
11:AA:1026:GLU:HA	11:AA:1026:GLU:OE2	1.84	0.77
20:H:305:HIS:CD2	20:H:306:VAL:N	2.53	0.77
9:9:31:ARG:NE	39:a:1054:A:C4'	2.48	0.77
11:AA:1257:GLN:OE1	14:AE:345:LYS:CG	2.32	0.77
16:D:1358:U:C4	16:D:1363:A:N1	2.53	0.77
9:9:31:ARG:CD	39:a:1054:A:C5'	2.58	0.77
14:AE:123:ARG:HG3	14:AE:1337:VAL:HG11	1.67	0.77
39:a:1021:A:H61	39:a:1141:U:H3	1.28	0.77
48:j:4:LEU:HD23	48:j:29:VAL:HG11	1.65	0.77
9:9:27:VAL:HG23	9:9:83:ALA:HB3	1.67	0.76
9:9:60:LEU:HD23	9:9:64:VAL:HG21	1.67	0.76
10:A:76:A:H2'	39:a:2394:C:H42	1.48	0.76
11:AA:1024:GLU:HA	11:AA:1027:LYS:HE3	1.66	0.76
39:a:2756:U:N3	39:a:2758:A:C6	2.53	0.76
7:6:15:DC:C4	7:6:16:DC:N4	2.53	0.76
10:A:68:C:C3'	10:A:69:C:H5''	2.15	0.76
10:B:68:C:C3'	10:B:69:C:H5''	2.15	0.76
11:AA:1026:GLU:CG	16:D:1030:U:C6	2.65	0.76
19:G:19:GLN:CD	20:H:76:GLU:HB2	2.08	0.76
8:7:-3:U:C5	16:D:528:C:OP1	2.39	0.76
9:9:97:LYS:HD3	9:9:127:ALA:HA	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:954:LYS:HZ2	11:AA:954:LYS:C	1.94	0.76
11:AA:871:VAL:N	11:AA:883:LEU:O	2.18	0.76
39:a:1406:U:O2'	39:a:1407:G:O5'	2.01	0.75
19:G:35:ARG:HG3	20:H:10:GLU:OE2	1.86	0.75
14:AE:110:PRO:HG2	14:AE:183:GLU:HG3	1.68	0.75
37:Y:74:PRO:HG2	37:Y:77:VAL:HB	1.67	0.75
11:AA:955:GLN:OE1	11:AA:955:GLN:HA	1.83	0.75
28:P:24:GLU:OE2	28:P:90:LEU:HD11	1.87	0.75
9:9:52:MET:HG3	9:9:95:LEU:HD11	1.68	0.75
11:AA:1272:GLU:OE2	14:AE:798:ARG:NH1	2.19	0.75
14:AE:86:GLU:CB	22:J:166:GLU:HB3	2.15	0.75
14:AE:87:LYS:CG	22:J:20:PHE:CE1	2.65	0.75
10:A:32:C:C1'	25:M:144:MET:HE1	2.16	0.75
13:AC:118:ASP:HA	28:P:89:ARG:CB	2.17	0.75
13:AC:120:ASP:HA	28:P:31:ARG:NH2	2.01	0.75
16:D:197:A:N6	16:D:221:C:H4'	2.01	0.75
45:g:18:CYS:CB	45:g:40:CYS:HB3	2.16	0.75
7:6:18:DC:N3	8:7:17:G:N2	2.31	0.75
11:AA:1246:ARG:HH11	11:AA:1266:GLY:HA2	1.50	0.75
14:AE:68:TYR:C	14:AE:75:TYR:CE2	2.65	0.75
13:AD:196:THR:HB	14:AE:443:GLU:HG3	1.68	0.75
4:3:36:VAL:HG11	4:3:39:ILE:HD12	1.68	0.74
8:7:14:U:H4'	14:AE:322:ARG:CD	2.17	0.74
10:A:41:C:O4'	25:M:143:ARG:NH1	2.20	0.74
10:B:70:G:C3'	10:B:71:C:H5''	2.17	0.74
20:H:131:LEU:CB	20:H:166:VAL:C	2.60	0.74
6:5:108:DT:H72	11:AA:199:ASP:HB3	1.67	0.74
9:9:78:GLY:N	9:9:79:PRO:CD	2.51	0.74
10:A:18:G:H1'	10:A:58:A:C2	2.23	0.74
13:AC:158:ARG:HB3	13:AC:158:ARG:NH1	2.02	0.74
10:B:76:A:H2'	10:B:76:A:N3	2.02	0.74
16:D:1228:C:OP1	36:X:107:ARG:NH1	2.21	0.74
19:G:19:GLN:OE1	20:H:75:VAL:O	1.85	0.74
20:H:109:THR:CA	20:H:153:GLU:HA	2.18	0.74
39:a:1021:A:N1	39:a:1141:U:C4	2.55	0.74
62:x:31:THR:O	62:x:102:ARG:NH1	2.19	0.74
10:B:18:G:H1'	10:B:58:A:C2	2.23	0.74
11:AA:998:LEU:HD13	11:AA:998:LEU:C	2.13	0.74
20:H:19:ARG:HB2	20:H:73:ASP:OD2	1.88	0.74
20:H:304:VAL:HG12	20:H:309:MET:SD	2.28	0.74
11:AA:956:ALA:HB1	11:AA:1032:LYS:HG3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:44:ILE:HD12	14:AE:252:LEU:CD2	2.18	0.74
11:AA:985:GLU:HG2	11:AA:988:LYS:HE3	1.69	0.74
10:B:76:A:H1'	39:a:2494:G:OP1	1.88	0.73
11:AA:979:LEU:HD21	11:AA:998:LEU:HD23	1.70	0.73
14:AE:107:LEU:HD11	14:AE:242:LEU:HB2	1.70	0.73
10:A:18:G:O2'	10:A:60:U:C2	2.41	0.73
11:AA:991:LYS:HD2	11:AA:991:LYS:N	2.03	0.73
16:D:517:G:O2'	16:D:530:G:H4'	1.88	0.73
10:A:41:C:H1'	25:M:143:ARG:HH12	1.52	0.73
11:AA:1253:LEU:HD12	14:AE:253:VAL:CG1	2.19	0.73
14:AE:211:GLU:HG2	14:AE:215:LYS:HE3	1.70	0.73
20:H:110:GLY:CA	20:H:153:GLU:O	2.36	0.73
39:a:1913:A:OP2	39:a:1913:A:H3'	1.89	0.73
11:AA:1034:ARG:HG2	11:AA:1034:ARG:HH11	1.52	0.73
14:AE:120:LEU:O	14:AE:1330:ARG:NH1	2.21	0.73
23:K:137:VAL:O	23:K:140:THR:OG1	2.04	0.73
39:a:2298:A:C4	39:a:2321:U:H5	2.04	0.73
10:A:6:G:O2'	10:A:7:G:O5'	2.05	0.73
10:A:33:U:H5''	25:M:84:THR:CG2	2.19	0.73
10:A:70:G:C3'	10:A:71:C:H5''	2.18	0.73
14:AE:157:GLN:OE1	14:AE:157:GLN:HA	1.89	0.73
15:C:44:ILE:HD13	20:H:339:ARG:HG3	1.70	0.73
8:7:-9:G:C4'	16:D:1500:A:H62	2.02	0.73
8:7:-9:G:C3'	16:D:1500:A:N6	2.51	0.73
11:AA:992:LEU:H	11:AA:992:LEU:CD2	1.95	0.73
13:AC:61:ILE:HB	13:AC:64:VAL:HG21	1.71	0.73
14:AE:210:SER:HB3	14:AE:213:LYS:HB2	1.70	0.73
11:AA:964:LEU:HD12	11:AA:964:LEU:C	2.13	0.73
10:B:18:G:O2'	10:B:60:U:C2	2.41	0.73
20:H:109:THR:HA	20:H:153:GLU:HA	1.69	0.73
39:a:1839:G:C1'	39:a:1927:A:C1'	2.67	0.73
11:AA:870:ILE:HG12	11:AA:884:VAL:HG12	1.71	0.73
11:AA:1043:ALA:HB1	11:AA:1044:PRO:CD	2.19	0.73
37:Y:85:ILE:H	37:Y:85:ILE:HD12	1.52	0.73
8:7:-10:U:OP1	16:D:1505:G:C8	2.42	0.72
19:G:19:GLN:CG	20:H:76:GLU:HB2	2.18	0.72
6:5:115:DA:OP1	14:AE:1148:ARG:NE	2.21	0.72
14:AE:44:ILE:HD12	14:AE:252:LEU:HD21	1.71	0.72
16:D:827:U:H3	16:D:872:A:N6	1.87	0.72
20:H:267:TRP:CE3	20:H:340:ARG:CG	2.72	0.72
7:6:21:DA:C6	8:7:15:G:N2	2.57	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:1308:U:C3'	36:X:98:ARG:HH21	1.92	0.72
14:AE:220:ARG:HG2	14:AE:220:ARG:HH11	1.55	0.72
15:C:12:ARG:HB2	20:H:264:GLU:CB	2.20	0.72
9:9:77:VAL:HG12	9:9:82:ILE:HG21	1.71	0.72
11:AA:972:PHE:HA	11:AA:975:ILE:HD12	1.70	0.72
10:B:70:G:H2'	10:B:71:C:C5'	2.11	0.72
14:AE:105:ILE:HD12	14:AE:242:LEU:HD22	1.71	0.72
10:B:6:G:O2'	10:B:7:G:O5'	2.05	0.72
10:B:46:G:H1'	10:B:47:U:C5	2.25	0.72
20:H:70:VAL:HA	20:H:85:SER:CB	2.20	0.72
10:A:72:A:C3'	10:A:73:A:H5''	2.20	0.72
19:G:16:PHE:CB	20:H:43:LYS:HA	2.20	0.72
20:H:267:TRP:CE3	20:H:340:ARG:HG2	2.25	0.72
39:a:67:U:C4	39:a:74:A:N6	2.57	0.72
9:9:18:VAL:HA	9:9:86:MET:HE2	1.71	0.71
14:AE:1143:ASP:OD1	14:AE:1148:ARG:NH1	2.21	0.71
39:a:1839:G:H1'	39:a:1927:A:N9	2.03	0.71
11:AA:207:THR:OG1	11:AA:354:ASP:OD2	2.08	0.71
45:g:18:CYS:CB	45:g:40:CYS:CB	2.69	0.71
11:AA:839:VAL:O	11:AA:886:LYS:HD3	1.90	0.71
10:B:76:A:H2'	39:a:2493:U:H5''	1.72	0.71
20:H:86:ARG:O	20:H:89:ALA:HB3	1.91	0.71
11:AA:1257:GLN:OE1	14:AE:345:LYS:HD3	1.89	0.71
10:B:72:A:C3'	10:B:73:A:H5''	2.20	0.71
37:Y:36:GLU:OE1	37:Y:36:GLU:HA	1.88	0.71
11:AA:878:THR:HA	11:AA:925:SER:HA	1.73	0.71
11:AA:1047:LEU:O	11:AA:1049:ILE:HD12	1.89	0.71
16:D:1308:U:O5'	36:X:98:ARG:HG3	1.90	0.71
9:9:3:LEU:HD12	9:9:3:LEU:N	2.05	0.71
27:O:84:THR:HG21	27:O:103:PHE:HB3	1.71	0.71
36:X:96:PRO:HG2	36:X:102:THR:CG2	2.21	0.71
8:7:-10:U:OP1	16:D:1505:G:H8	1.74	0.71
8:7:-9:G:H3'	16:D:1500:A:N6	2.04	0.71
10:A:46:G:H1'	10:A:47:U:C5	2.25	0.71
11:AA:1009:ASN:O	11:AA:1009:ASN:ND2	2.24	0.71
16:D:1309:G:H8	36:X:98:ARG:NH2	1.89	0.71
39:a:742:A:H2'	39:a:743:A:C8	2.26	0.70
13:AD:86:LYS:HE3	14:AE:528:THR:HB	1.72	0.70
10:A:18:G:C5	10:A:57:A:N6	2.59	0.70
10:B:18:G:C5	10:B:57:A:N6	2.59	0.70
30:R:86:ARG:HG3	30:R:86:ARG:O	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:14:U:H4'	14:AE:322:ARG:HD2	1.73	0.70
8:7:16:A:P	11:AA:540:ARG:HH21	2.15	0.70
10:A:15:G:H2'	10:A:15:G:N3	2.06	0.70
10:A:32:C:C1'	25:M:144:MET:CE	2.69	0.70
14:AE:128:LEU:HD11	14:AE:189:LEU:HG	1.74	0.70
10:A:41:C:C1'	25:M:143:ARG:NH1	2.55	0.70
14:AE:142:GLU:HG3	14:AE:142:GLU:O	1.89	0.70
39:a:2314:A:C1'	52:n:155:THR:HG21	2.21	0.70
10:A:32:C:C4'	25:M:144:MET:CE	2.66	0.70
11:AA:839:VAL:HA	11:AA:1048:LYS:O	1.91	0.70
9:9:50:VAL:HG13	37:Y:119:ALA:CB	2.22	0.70
39:a:1021:A:H3'	39:a:1021:A:N3	2.07	0.70
10:A:16:C:O2	39:a:2181:U:C5'	2.40	0.69
13:AC:65:LEU:CA	21:I:80:LYS:HB3	2.16	0.69
20:H:70:VAL:HA	20:H:85:SER:CA	2.22	0.69
8:7:-2:U:O4	16:D:1397:C:C5	2.45	0.69
11:AA:19:PRO:HA	11:AA:1156:ARG:HD3	1.73	0.69
13:AC:76:GLU:OE1	13:AC:131:CYS:HA	1.92	0.69
10:B:11:A:H2'	10:B:12:G:O4'	1.92	0.69
9:9:58:THR:HG21	9:9:81:LEU:HG	1.74	0.69
11:AA:1047:LEU:O	11:AA:1049:ILE:CD1	2.40	0.69
39:a:2310:C:O2'	52:n:74:VAL:CG1	2.40	0.69
10:A:6:G:HO2'	10:A:7:G:H8	1.39	0.69
20:H:19:ARG:HD3	20:H:73:ASP:OD1	1.92	0.69
16:D:972:C:O2'	28:P:57:VAL:HG23	1.92	0.69
14:AE:54:ASP:OD1	14:AE:54:ASP:N	2.24	0.69
16:D:915:A:N6	16:D:916:U:C4	2.60	0.69
8:7:-10:U:OP2	16:D:1505:G:H8	1.67	0.69
10:A:11:A:H2'	10:A:12:G:O4'	1.92	0.69
11:AA:802:VAL:HA	11:AA:1096:ILE:O	1.93	0.69
13:AC:167:PRO:HA	21:I:103:ILE:O	1.93	0.69
10:B:15:G:H2'	10:B:15:G:N3	2.06	0.69
20:H:19:ARG:HD3	20:H:73:ASP:OD2	1.92	0.69
39:a:927:A:H2'	39:a:928:A:C8	2.28	0.69
39:a:1839:G:C4	39:a:1927:A:C4	2.81	0.69
9:9:31:ARG:HD2	39:a:1054:A:C5'	2.22	0.69
11:AA:935:THR:HA	11:AA:1049:ILE:HD12	1.74	0.69
46:h:146:MET:HE3	46:h:154:LEU:HD21	1.74	0.69
8:7:2:U:O2'	23:K:57:PRO:CB	2.37	0.68
11:AA:883:LEU:HD11	11:AA:920:VAL:CG2	2.21	0.68
11:AA:958:LYS:HB3	11:AA:958:LYS:NZ	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Y:21:PRO:CB	37:Y:22:PRO:HD3	2.22	0.68
1:O:80:ARG:NH2	39:a:572:A:OP2	2.25	0.68
11:AA:868:SER:OG	11:AA:941:LYS:CG	2.41	0.68
11:AA:878:THR:O	11:AA:920:VAL:CG1	2.40	0.68
14:AE:94:GLN:HB2	14:AE:97:VAL:HG23	1.75	0.68
14:AE:202:ARG:HG2	14:AE:202:ARG:NH1	2.00	0.68
14:AE:832:LYS:C	14:AE:1242:ARG:HH12	2.01	0.68
16:D:37:U:H3	16:D:397:A:N6	1.90	0.68
39:a:2013:A:N6	39:a:2613:U:N3	2.33	0.68
13:AC:167:PRO:CA	21:I:103:ILE:O	2.41	0.68
10:B:5:G:H2'	10:B:6:G:C5'	2.24	0.68
9:9:118:ILE:HB	9:9:119:PRO:HD3	1.76	0.68
11:AA:768:MET:HE1	13:AC:80:GLU:CD	2.19	0.68
14:AE:39:LYS:O	14:AE:273:ILE:CG2	2.41	0.68
11:AA:872:TYR:HD2	21:I:78:GLY:O	1.75	0.68
16:D:1227:A:H5'	36:X:110:LYS:HZ1	1.57	0.68
7:6:8:DC:C6	7:6:9:DT:H72	2.29	0.68
16:D:13:U:O4	16:D:21:G:C2	2.46	0.68
11:AA:768:MET:HE1	13:AC:80:GLU:OE1	1.94	0.68
14:AE:141:PHE:CD2	14:AE:293:ARG:O	2.47	0.68
16:D:563:A:N1	16:D:884:U:C4	2.60	0.68
20:H:117:LYS:CB	20:H:279:LYS:O	2.41	0.68
20:H:267:TRP:CD2	20:H:340:ARG:CG	2.76	0.68
39:a:2310:C:O2'	52:n:74:VAL:HG12	1.94	0.68
19:G:16:PHE:HZ	20:H:41:GLY:O	1.77	0.67
36:X:96:PRO:CG	36:X:102:THR:CG2	2.71	0.67
39:a:1839:G:H8	39:a:1927:A:H1'	1.55	0.67
11:AA:992:LEU:HD22	11:AA:992:LEU:N	2.04	0.67
39:a:2756:U:C4	39:a:2758:A:N6	2.61	0.67
9:9:67:THR:N	9:9:68:PRO:CD	2.58	0.67
20:H:110:GLY:HA3	20:H:153:GLU:O	1.93	0.67
37:Y:116:MET:HB3	37:Y:124:MET:HG2	1.76	0.67
39:a:1596:A:H2'	39:a:1597:A:C8	2.28	0.67
8:7:-9:G:C4'	16:D:1500:A:N6	2.57	0.67
9:9:11:ILE:CD1	9:9:62:ARG:HD3	2.24	0.67
9:9:43:LYS:HD2	9:9:43:LYS:O	1.94	0.67
39:a:1153:C:OP1	64:z:92:ARG:NH1	2.27	0.67
39:a:1920:C:O5'	39:a:1920:C:H6	1.78	0.67
54:p:24:ILE:HD13	54:p:72:LEU:HD21	1.77	0.67
7:6:21:DA:C2	8:7:15:G:N2	2.62	0.67
10:A:66:C:H6	10:A:66:C:H5'	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:1005:GLU:OE1	11:AA:1005:GLU:HA	1.92	0.67
14:AE:111:THR:CG2	14:AE:300:GLN:CD	2.66	0.67
36:X:96:PRO:CG	36:X:102:THR:HG22	2.25	0.67
9:9:60:LEU:HA	9:9:64:VAL:HB	1.77	0.67
10:A:5:G:H2'	10:A:6:G:C5'	2.24	0.67
10:A:19:G:N2	39:a:2112:G:C8	2.62	0.67
11:AA:728:ASP:OD1	11:AA:769:PRO:CG	2.41	0.67
11:AA:963:GLU:HA	11:AA:966:ILE:HD12	1.77	0.67
13:AC:76:GLU:OE2	13:AC:131:CYS:HA	1.95	0.67
37:Y:58:ILE:HD13	37:Y:58:ILE:N	2.09	0.67
11:AA:1253:LEU:HD12	14:AE:253:VAL:HG11	1.77	0.67
14:AE:161:THR:HG22	14:AE:164:GLN:HB2	1.75	0.67
21:I:75:ILE:O	21:I:75:ILE:HD13	1.95	0.67
11:AA:339:ASN:HB3	11:AA:343:HIS:H	1.58	0.67
14:AE:1355:ARG:NH1	14:AE:1369:ARG:HH12	1.93	0.67
10:B:66:C:H5'	10:B:66:C:H6	1.60	0.67
20:H:110:GLY:H	20:H:153:GLU:CA	2.08	0.67
37:Y:14:ALA:HB2	37:Y:54:ILE:HD12	1.76	0.67
9:9:73:LYS:HB2	9:9:117:LEU:HD21	1.75	0.66
14:AE:108:ALA:HB3	14:AE:279:LEU:HD22	1.77	0.66
14:AE:978:ARG:HG2	14:AE:1197:ASN:HD21	1.60	0.66
10:B:56:C:H5'	52:n:80:ARG:NH2	2.10	0.66
10:A:56:C:C5	39:a:2168:G:C6	2.84	0.66
14:AE:117:LEU:HD12	14:AE:117:LEU:O	1.94	0.66
34:V:25:ILE:HD11	34:V:61:ILE:HD11	1.77	0.66
36:X:96:PRO:HG3	36:X:102:THR:HG22	1.77	0.66
39:a:1779:U:H5	39:a:1784:A:N7	1.93	0.66
11:AA:858:GLY:C	11:AA:860:ALA:H	2.03	0.66
13:AC:65:LEU:CA	21:I:80:LYS:CB	2.72	0.66
20:H:118:GLY:C	20:H:133:GLY:CA	2.67	0.66
11:AA:768:MET:HE3	13:AC:80:GLU:OE1	1.94	0.66
16:D:1358:U:O4	16:D:1363:A:C2	2.47	0.66
20:H:70:VAL:HA	20:H:85:SER:HA	1.77	0.66
11:AA:1251:TYR:C	11:AA:1259:LEU:CD1	2.69	0.66
13:AD:86:LYS:HE3	14:AE:528:THR:CG2	2.26	0.66
14:AE:108:ALA:CB	14:AE:279:LEU:HD22	2.25	0.66
14:AE:193:ASP:HB3	14:AE:196:GLN:HB2	1.78	0.66
10:B:21:A:H4'	10:B:21:A:OP1	1.95	0.66
20:H:267:TRP:CZ2	20:H:340:ARG:CG	2.68	0.66
20:H:270:ILE:HG23	20:H:337:GLU:HB3	1.78	0.66
31:S:47:LYS:O	31:S:50:THR:OG1	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:16:DC:H1'	14:AE:426:ALA:HB1	1.77	0.66
11:AA:1257:GLN:OE1	14:AE:345:LYS:HG2	1.96	0.66
14:AE:984:LEU:HB3	14:AE:993:GLU:HB2	1.76	0.66
14:AE:1037:PHE:HB3	14:AE:1040:MET:HB2	1.78	0.66
20:H:135:LEU:CA	20:H:157:ILE:CB	2.74	0.66
11:AA:964:LEU:HD21	11:AA:1022:LYS:HD2	1.77	0.66
10:B:37:A:H3'	10:B:37:A:OP2	1.96	0.66
11:AA:1257:GLN:OE1	14:AE:345:LYS:CD	2.44	0.65
20:H:110:GLY:N	20:H:153:GLU:C	2.53	0.65
10:A:18:G:C8	10:A:57:A:C6	2.85	0.65
11:AA:960:LEU:HD13	11:AA:1029:LEU:HB2	1.77	0.65
10:B:76:A:H1'	39:a:2493:U:O3'	1.96	0.65
20:H:19:ARG:O	20:H:72:LEU:CB	2.41	0.65
20:H:267:TRP:CE2	20:H:340:ARG:CG	2.73	0.65
9:9:61:ARG:NH1	39:a:1047:G:N7	2.44	0.65
9:9:142:THR:HG21	38:Z:7:ILE:CD1	2.26	0.65
11:AA:839:VAL:O	11:AA:886:LYS:CD	2.44	0.65
13:AC:118:ASP:CA	28:P:89:ARG:HB3	2.17	0.65
16:D:197:A:C6	16:D:221:C:C4'	2.80	0.65
39:a:1839:G:O4'	39:a:1927:A:H1'	1.97	0.65
9:9:50:VAL:CG1	37:Y:119:ALA:HB3	2.26	0.65
13:AC:118:ASP:HB3	28:P:90:LEU:HD23	1.78	0.65
57:s:114:LEU:HG	57:s:118:MET:HE3	1.78	0.65
9:9:78:GLY:H	9:9:79:PRO:CD	2.10	0.65
14:AE:975:ILE:HG22	14:AE:977:SER:H	1.62	0.65
11:AA:9:LYS:HG2	11:AA:1171:ARG:NH1	2.11	0.65
13:AD:102:LEU:HB2	13:AD:115:ILE:HG13	1.77	0.65
14:AE:67:ASP:OD1	14:AE:95:THR:OG1	2.15	0.65
14:AE:68:TYR:HB3	14:AE:75:TYR:CE2	2.32	0.65
14:AE:141:PHE:HD2	14:AE:293:ARG:O	1.80	0.65
20:H:52:GLN:O	20:H:53:PHE:CD1	2.50	0.65
10:A:21:A:H4'	10:A:21:A:OP1	1.95	0.65
11:AA:962:GLU:OE1	11:AA:962:GLU:HA	1.97	0.65
16:D:1308:U:H5''	36:X:98:ARG:HG2	1.78	0.65
53:o:26:HIS:CE1	53:o:48:ALA:HB2	2.32	0.65
22:J:162:ALA:CB	22:J:165:ARG:HH22	2.08	0.65
37:Y:116:MET:HE2	37:Y:116:MET:HA	1.79	0.65
14:AE:84:ILE:O	14:AE:84:ILE:HG13	1.96	0.65
10:B:18:G:C8	10:B:57:A:C6	2.85	0.65
39:a:1082:U:N3	39:a:1086:A:N6	2.45	0.65
39:a:1923:U:H2'	39:a:1923:U:OP2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:3:C:H2'	10:A:4:G:H8	1.62	0.64
10:A:22:G:H2'	10:A:23:C:H6	1.62	0.64
11:AA:9:LYS:HG2	11:AA:1171:ARG:HH12	1.61	0.64
20:H:85:SER:O	20:H:88:LYS:CB	2.45	0.64
9:9:29:ASP:HB2	9:9:56:ARG:HD3	1.79	0.64
10:A:41:C:C4'	25:M:143:ARG:NH1	2.60	0.64
20:H:162:LYS:CB	20:H:298:GLU:OE1	2.44	0.64
11:AA:529:ARG:HH11	11:AA:572:ILE:HG22	1.62	0.64
10:B:6:G:HO2'	10:B:7:G:H8	1.44	0.64
16:D:1227:A:OP2	36:X:110:LYS:NZ	2.29	0.64
16:D:1308:U:O5'	36:X:98:ARG:CG	2.45	0.64
19:G:19:GLN:CG	20:H:75:VAL:CG2	2.70	0.64
19:G:38:VAL:HG22	20:H:75:VAL:CG2	2.24	0.64
20:H:72:LEU:HD12	20:H:72:LEU:N	2.11	0.64
8:7:2:U:H4'	23:K:57:PRO:CD	2.18	0.64
14:AE:162:GLU:OE1	14:AE:162:GLU:HA	1.97	0.64
19:G:19:GLN:HG3	20:H:75:VAL:CG2	2.23	0.64
39:a:1839:G:C8	39:a:1927:A:C1'	2.74	0.64
39:a:1909:C:O5'	39:a:1909:C:H6	1.81	0.64
11:AA:118:LYS:NZ	11:AA:485:ASP:OD1	2.25	0.64
11:AA:852:ALA:O	11:AA:854:ILE:N	2.27	0.64
12:AB:93:ILE:HG22	14:AE:290:ILE:CG2	2.27	0.64
16:D:1329:A:P	36:X:28:THR:CB	2.83	0.64
20:H:332:VAL:HG12	20:H:334:ASP:H	1.62	0.64
9:9:11:ILE:HG13	9:9:65:GLU:HB3	1.79	0.64
20:H:267:TRP:CE3	20:H:340:ARG:HG3	2.32	0.64
1:0:40:MET:HE1	64:z:105:ALA:HB1	1.80	0.64
11:AA:1257:GLN:HE22	14:AE:345:LYS:CA	2.10	0.64
14:AE:136:GLU:CD	14:AE:312:ARG:HH22	2.06	0.64
10:A:50:U:H2'	10:A:51:C:C6	2.33	0.64
11:AA:872:TYR:CD2	21:I:78:GLY:O	2.51	0.64
6:5:101:DT:OP2	14:AE:275:ARG:NH2	2.31	0.63
10:A:31:G:O2'	25:M:144:MET:SD	2.56	0.63
11:AA:981:ALA:HB3	11:AA:1008:GLN:CG	2.28	0.63
14:AE:245:LEU:HG	14:AE:246:PRO:HD2	1.79	0.63
39:a:2303:G:N3	39:a:2314:A:C2	2.66	0.63
54:p:121:ILE:HD12	54:p:141:ILE:HG22	1.79	0.63
11:AA:978:VAL:HG21	11:AA:1010:GLN:HG3	1.79	0.63
11:AA:988:LYS:NZ	11:AA:988:LYS:HB3	2.13	0.63
14:AE:92:VAL:O	14:AE:92:VAL:HG12	1.99	0.63
10:B:3:C:H2'	10:B:4:G:H8	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:13:U:O4	16:D:20:U:C4	2.52	0.63
10:A:37:A:O2'	10:A:38:A:H5'	1.99	0.63
10:B:75:C:OP1	39:a:2602:A:N9	2.30	0.63
16:D:1309:G:C8	36:X:98:ARG:NH2	2.66	0.63
11:AA:867:GLU:HB3	21:I:75:ILE:HG13	1.80	0.63
16:D:1059:C:O2	28:P:55:PRO:HG3	1.99	0.63
16:D:1358:U:H3	16:D:1363:A:N6	1.96	0.63
37:Y:32:VAL:HA	37:Y:60:VAL:HG11	1.81	0.63
9:9:11:ILE:HD12	9:9:62:ARG:HD3	1.80	0.63
9:9:18:VAL:HG13	9:9:71:CYS:HB2	1.81	0.63
9:9:31:ARG:HD2	39:a:1054:A:H5'	1.80	0.63
10:A:56:C:O2	39:a:2112:G:C4	2.52	0.63
10:A:69:C:H2'	10:A:70:G:O4'	1.99	0.63
10:B:22:G:H2'	10:B:23:C:H6	1.62	0.63
16:D:1358:U:N3	16:D:1363:A:N6	2.46	0.63
10:B:50:U:H2'	10:B:51:C:C6	2.33	0.63
20:H:270:ILE:HG21	20:H:337:GLU:HB3	1.80	0.63
2:1:36:LEU:HD13	2:1:48:LYS:HA	1.80	0.63
10:B:69:C:H2'	10:B:70:G:O4'	1.99	0.63
13:AC:71:LYS:HZ1	13:AC:140:ILE:HB	1.64	0.62
16:D:37:U:O2	16:D:548:G:C2	2.52	0.62
19:G:35:ARG:HH21	20:H:10:GLU:HG2	1.62	0.62
20:H:110:GLY:N	20:H:153:GLU:O	2.32	0.62
39:a:1789:A:OP2	46:h:221:ARG:NH1	2.32	0.62
11:AA:992:LEU:N	11:AA:992:LEU:HD13	2.14	0.62
19:G:19:GLN:CG	20:H:76:GLU:CB	2.76	0.62
20:H:49:PRO:CD	20:H:84:LEU:HD11	2.29	0.62
11:AA:958:LYS:HB3	11:AA:958:LYS:HZ1	1.62	0.62
39:a:1998:A:OP2	48:j:141:ARG:NH2	2.32	0.62
11:AA:995:ASP:OD1	11:AA:995:ASP:N	2.29	0.62
13:AD:176:CYS:SG	14:AE:535:ARG:NH2	2.72	0.62
15:C:44:ILE:CD1	20:H:339:ARG:HG3	2.28	0.62
39:a:2189:U:O4'	39:a:2189:U:P	2.57	0.62
6:5:98:DA:C2'	6:5:99:DT:H72	2.28	0.62
8:7:16:A:P	11:AA:540:ARG:NH2	2.72	0.62
14:AE:44:ILE:CD1	14:AE:252:LEU:HD21	2.29	0.62
39:a:1839:G:N9	39:a:1927:A:N9	2.48	0.62
39:a:2297:A:C2	39:a:2321:U:C4	2.86	0.62
11:AA:13:LYS:HB2	11:AA:1180:MET:HE2	1.81	0.62
11:AA:850:ILE:O	11:AA:850:ILE:HG22	1.98	0.62
11:AA:868:SER:CB	11:AA:941:LYS:HG2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:1251:TYR:C	11:AA:1259:LEU:HD13	2.24	0.62
14:AE:128:LEU:HA	14:AE:192:MET:HE1	1.81	0.62
20:H:119:GLY:CA	20:H:131:LEU:O	2.46	0.62
10:A:65:C:H2'	10:A:66:C:H5'	1.82	0.62
28:P:57:VAL:O	28:P:58:ASN:CG	2.43	0.62
9:9:23:LEU:HB3	9:9:92:ALA:HA	1.81	0.62
10:B:42:G:H2'	10:B:43:A:H8	1.65	0.62
15:C:29:LEU:O	15:C:33:ILE:HG23	2.00	0.62
8:7:-5:U:H6	8:7:-5:U:H5''	1.65	0.62
9:9:57:ASN:CG	9:9:62:ARG:CG	2.68	0.62
10:B:65:C:H2'	10:B:66:C:H5'	1.82	0.62
9:9:57:ASN:OD1	9:9:62:ARG:HD2	1.98	0.62
11:AA:1328:LYS:HD2	14:AE:102:MET:SD	2.40	0.61
15:C:44:ILE:CD1	20:H:339:ARG:HG2	2.12	0.61
20:H:305:HIS:O	20:H:306:VAL:HB	2.00	0.61
39:a:754:U:H2'	39:a:755:U:C6	2.35	0.61
7:6:15:DC:C4	7:6:16:DC:C4	2.88	0.61
11:AA:660:VAL:HG13	11:AA:661:VAL:HG13	1.83	0.61
14:AE:1355:ARG:NH1	14:AE:1369:ARG:NH1	2.47	0.61
19:G:18:HIS:HA	20:H:43:LYS:CD	2.28	0.61
25:M:23:LEU:O	25:M:27:VAL:HG13	1.99	0.61
9:9:57:ASN:CG	9:9:62:ARG:HG2	2.25	0.61
11:AA:724:VAL:HG23	11:AA:734:ILE:HD13	1.80	0.61
14:AE:111:THR:CG2	14:AE:300:GLN:NE2	2.63	0.61
20:H:270:ILE:CG2	20:H:337:GLU:CB	2.77	0.61
36:X:101:ARG:O	36:X:101:ARG:HD3	2.00	0.61
39:a:2885:G:N7	47:i:40:ARG:NH2	2.46	0.61
11:AA:954:LYS:O	11:AA:954:LYS:NZ	2.33	0.61
19:G:19:GLN:HG3	20:H:76:GLU:HB2	1.82	0.61
20:H:304:VAL:HG12	20:H:304:VAL:O	1.99	0.61
23:K:107:ALA:HB2	23:K:125:ALA:HB3	1.82	0.61
33:U:21:VAL:HG21	33:U:60:TRP:CD1	2.36	0.61
39:a:2720:U:OP1	63:y:53:ARG:NH2	2.34	0.61
9:9:92:ALA:HB3	9:9:129:LEU:HB2	1.82	0.61
10:A:42:G:H2'	10:A:43:A:H8	1.65	0.61
16:D:13:U:C5	16:D:20:U:O4	2.53	0.61
16:D:1227:A:H5'	36:X:110:LYS:HZ3	1.62	0.61
20:H:84:LEU:HD22	20:H:84:LEU:N	2.16	0.61
39:a:84:A:N1	39:a:98:G:O2'	2.33	0.61
11:AA:858:GLY:O	11:AA:860:ALA:N	2.17	0.61
11:AA:978:VAL:HG11	11:AA:1010:GLN:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:1308:U:H2'	36:X:98:ARG:HH22	1.61	0.61
20:H:162:LYS:CB	20:H:298:GLU:OE2	2.45	0.61
9:9:77:VAL:HG12	9:9:77:VAL:O	2.01	0.61
14:AE:201:LEU:HB2	14:AE:221:ILE:HD13	1.80	0.61
14:AE:395:LYS:NZ	14:AE:399:LYS:HD3	2.15	0.61
10:B:54:U:N3	10:B:58:A:N6	2.47	0.61
9:9:136:ILE:HD12	9:9:139:LEU:HD12	1.83	0.61
10:A:54:U:N3	10:A:58:A:N6	2.48	0.61
14:AE:24:LEU:CG	14:AE:232:ASN:ND2	2.64	0.61
14:AE:154:LEU:HD21	14:AE:160:LEU:HD21	1.83	0.61
16:D:1218:C:H2'	16:D:1219:A:C8	2.36	0.61
20:H:280:LEU:N	20:H:330:VAL:O	2.32	0.61
37:Y:21:PRO:HB2	37:Y:22:PRO:CD	2.30	0.61
11:AA:981:ALA:CB	11:AA:1008:GLN:HG3	2.31	0.61
14:AE:416:ILE:HG13	14:AE:441:LEU:HD11	1.83	0.61
16:D:658:C:H1'	32:T:22:THR:HG21	1.83	0.61
19:G:18:HIS:CA	20:H:43:LYS:HD2	2.29	0.61
19:G:19:GLN:CD	20:H:75:VAL:HG22	2.25	0.61
3:2:50:LEU:HD23	43:e:26:PHE:CE1	2.35	0.60
44:f:24:LEU:HD11	44:f:54:MET:HE2	1.83	0.60
10:A:3:C:H2'	10:A:4:G:C8	2.36	0.60
10:A:33:U:H4'	25:M:84:THR:HB	1.82	0.60
10:A:34:C:P	25:M:84:THR:OG1	2.60	0.60
11:AA:374:GLU:HG3	11:AA:374:GLU:O	2.01	0.60
14:AE:67:ASP:OD1	14:AE:67:ASP:N	2.34	0.60
14:AE:1161:GLY:HA3	14:AE:1179:PRO:HA	1.82	0.60
10:B:3:C:H2'	10:B:4:G:C8	2.36	0.60
10:B:56:C:C4'	52:n:80:ARG:NH2	2.63	0.60
6:5:108:DT:O4	11:AA:199:ASP:OD2	2.18	0.60
9:9:6:GLN:OE1	9:9:6:GLN:HA	2.00	0.60
10:A:41:C:C1'	25:M:143:ARG:HH12	2.12	0.60
11:AA:872:TYR:CD2	21:I:74:GLY:HA2	2.37	0.60
14:AE:144:TYR:CE1	14:AE:162:GLU:OE2	2.51	0.60
20:H:305:HIS:CD2	20:H:307:SER:H	2.19	0.60
39:a:1021:A:C2	39:a:1141:U:O4	2.51	0.60
39:a:1921:G:O5'	39:a:1921:G:H8	1.84	0.60
51:m:31:LEU:HD22	51:m:42:LEU:HD13	1.84	0.60
20:H:117:LYS:CB	20:H:278:THR:HG23	2.32	0.60
11:AA:979:LEU:HD11	11:AA:998:LEU:HD23	1.84	0.60
14:AE:68:TYR:HB3	14:AE:75:TYR:CZ	2.35	0.60
14:AE:118:LYS:HD2	14:AE:312:ARG:NH2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:926:PRO:HG2	14:AE:1248:ILE:HD11	1.84	0.60
16:D:827:U:N3	16:D:872:A:N6	2.45	0.60
39:a:2297:A:C2	39:a:2321:U:C5	2.89	0.60
9:9:47:GLU:HG3	9:9:95:LEU:HD21	1.83	0.60
13:AD:86:LYS:HE3	14:AE:528:THR:CB	2.32	0.60
14:AE:90:VAL:O	14:AE:90:VAL:CG1	2.48	0.60
14:AE:342:LEU:HD23	14:AE:1352:ILE:HG23	1.83	0.60
7:6:15:DC:N4	7:6:16:DC:H41	1.96	0.60
11:AA:861:ALA:HA	11:AA:882:ILE:HD13	1.83	0.60
14:AE:223:LEU:HG	14:AE:223:LEU:O	2.00	0.60
14:AE:951:GLN:NE2	14:AE:1014:GLY:O	2.35	0.60
38:Z:7:ILE:HG23	38:Z:7:ILE:O	2.01	0.60
10:A:41:C:H4'	25:M:143:ARG:CZ	2.32	0.60
14:AE:201:LEU:HD11	14:AE:220:ARG:HH11	1.67	0.60
14:AE:412:LEU:HD22	14:AE:441:LEU:HD21	1.84	0.60
4:3:36:VAL:CG1	4:3:39:ILE:HD12	2.32	0.59
9:9:62:ARG:CG	9:9:62:ARG:HH21	2.14	0.59
11:AA:963:GLU:HA	11:AA:963:GLU:OE1	2.01	0.59
11:AA:1223:ARG:NH2	14:AE:721:SER:OG	2.34	0.59
14:AE:395:LYS:HZ2	14:AE:399:LYS:CD	2.15	0.59
11:AA:840:SER:O	11:AA:840:SER:OG	2.19	0.59
20:H:118:GLY:C	20:H:133:GLY:HA2	2.27	0.59
25:M:69:VAL:HG23	25:M:100:ALA:HB1	1.83	0.59
37:Y:54:ILE:O	37:Y:54:ILE:HG22	2.00	0.59
8:7:-3:U:C4	16:D:528:C:OP2	2.56	0.59
14:AE:87:LYS:HG3	22:J:20:PHE:HE1	1.56	0.59
16:D:1225:A:H4'	35:W:78:ARG:NH1	2.18	0.59
20:H:270:ILE:HG21	20:H:337:GLU:CB	2.32	0.59
11:AA:1030:GLU:OE1	16:D:1030:U:O4	2.20	0.59
20:H:331:MET:N	20:H:331:MET:SD	2.75	0.59
13:AD:81:ILE:HD13	13:AD:131:CYS:HB2	1.83	0.59
16:D:404:G:N7	22:J:2:ALA:HB3	2.17	0.59
16:D:1308:U:C5'	36:X:98:ARG:HG2	2.32	0.59
10:A:76:A:C2'	39:a:2394:C:H42	2.16	0.59
11:AA:888:THR:OG1	11:AA:889:PRO:HD2	2.02	0.59
10:B:58:A:H1'	10:B:60:U:C5	2.38	0.59
17:E:25:ARG:HA	17:E:66:LEU:HD21	1.85	0.59
10:A:35:A:H2'	10:A:36:U:C6	2.38	0.59
11:AA:478:ARG:NH1	11:AA:491:ASP:O	2.34	0.59
11:AA:528:ARG:NH2	11:AA:576:SER:O	2.34	0.59
10:B:47:U:O2'	10:B:50:U:P	2.60	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:13:U:C2	16:D:915:A:N6	2.70	0.59
16:D:439:U:O2	16:D:440:C:C6	2.56	0.59
38:Z:20:VAL:O	38:Z:20:VAL:HG12	2.02	0.59
9:9:19:ALA:HA	9:9:70:GLU:HG2	1.84	0.59
11:AA:974:ARG:HD2	11:AA:1014:LEU:HD11	1.85	0.59
14:AE:86:GLU:CA	22:J:166:GLU:CB	2.64	0.59
39:a:70:G:H4'	39:a:71:A:OP1	2.02	0.59
10:A:47:U:O2'	10:A:50:U:P	2.61	0.59
10:A:76:A:H2'	39:a:2394:C:N4	2.11	0.59
11:AA:1256:GLN:OE1	11:AA:1256:GLN:HA	2.03	0.59
13:AC:76:GLU:OE1	13:AC:131:CYS:CA	2.51	0.59
14:AE:99:ARG:HG3	14:AE:99:ARG:NH1	2.18	0.59
14:AE:275:ARG:NH1	14:AE:278:ARG:NH1	2.51	0.59
19:G:35:ARG:HD2	20:H:14:LYS:CD	2.32	0.59
39:a:1406:U:HO2'	39:a:1407:G:C5'	2.12	0.59
9:9:34:THR:HG22	9:9:38:MET:HE3	1.85	0.58
11:AA:1184:THR:HG23	11:AA:1190:ALA:H	1.67	0.58
14:AE:370:LYS:HG2	14:AE:441:LEU:HD23	1.84	0.58
39:a:2572:A:C8	48:j:149:ASN:OD1	2.56	0.58
11:AA:1014:LEU:HA	11:AA:1017:GLN:HG2	1.85	0.58
11:AA:1026:GLU:HG3	16:D:1030:U:C6	2.17	0.58
18:F:4:ILE:CD1	18:F:19:PHE:HA	2.33	0.58
20:H:119:GLY:HA3	20:H:132:PRO:C	2.28	0.58
39:a:2314:A:O2'	52:n:155:THR:CG2	2.52	0.58
7:6:18:DC:N4	8:7:17:G:H1	1.99	0.58
11:AA:862:LEU:HD12	21:I:72:ARG:NH2	2.19	0.58
11:AA:967:LEU:HD12	11:AA:967:LEU:C	2.25	0.58
14:AE:514:THR:HG21	14:AE:596:LEU:HD12	1.84	0.58
19:G:217:VAL:O	19:G:220:THR:HG22	2.02	0.58
39:a:1590:A:H2'	39:a:1591:A:C8	2.38	0.58
11:AA:376:PRO:O	11:AA:376:PRO:HG2	2.02	0.58
11:AA:979:LEU:HD13	11:AA:1011:LEU:HD21	1.84	0.58
11:AA:1008:GLN:HE21	11:AA:1008:GLN:C	2.11	0.58
11:AA:1034:ARG:NH1	11:AA:1034:ARG:O	2.37	0.58
48:j:33:ARG:NH1	48:j:53:GLY:O	2.36	0.58
9:9:54:VAL:O	9:9:54:VAL:HG22	2.03	0.58
16:D:1526:G:OP2	18:F:42:THR:HG23	2.04	0.58
11:AA:859:GLU:HB3	21:I:109:PRO:CG	2.33	0.58
12:AB:93:ILE:HG22	14:AE:290:ILE:HG22	1.85	0.58
14:AE:241:VAL:HG12	14:AE:241:VAL:O	2.04	0.58
16:D:496:A:N3	16:D:496:A:H2'	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:563:A:N6	16:D:884:U:N3	2.51	0.58
20:H:267:TRP:CH2	20:H:340:ARG:CB	2.86	0.58
20:H:284:VAL:HG12	20:H:294:VAL:HB	1.84	0.58
36:X:104:THR:O	36:X:104:THR:HG22	2.03	0.58
39:a:2683:C:OP1	63:y:51:ARG:NH2	2.32	0.58
6:5:99:DT:H2''	6:5:100:DA:H5''	1.86	0.58
8:7:-9:G:H5''	16:D:1501:C:N4	2.19	0.58
8:7:-5:U:H5''	8:7:-5:U:C6	2.39	0.58
9:9:61:ARG:CZ	39:a:1047:G:N7	2.67	0.58
33:U:4:ILE:HG12	33:U:21:VAL:HG22	1.84	0.58
37:Y:78:LEU:HD13	37:Y:108:ILE:HG22	1.85	0.58
6:5:115:DA:OP2	14:AE:1148:ARG:HG3	2.04	0.58
14:AE:97:VAL:HG11	14:AE:101:ARG:NH2	2.18	0.58
2:1:20:VAL:HG11	2:1:44:ALA:HA	1.86	0.58
11:AA:218:GLU:OE2	11:AA:300:ASP:N	2.28	0.58
11:AA:1142:ARG:NH2	11:AA:1166:ASP:OD1	2.36	0.58
20:H:291:GLY:HA2	20:H:305:HIS:HA	1.86	0.58
10:A:60:U:P	10:A:61:C:H41	2.27	0.58
11:AA:855:PRO:O	11:AA:855:PRO:HG2	2.04	0.58
14:AE:438:GLU:HG3	14:AE:485:MET:HE1	1.85	0.58
10:B:56:C:C5'	52:n:80:ARG:CZ	2.76	0.58
20:H:110:GLY:N	20:H:153:GLU:CA	2.67	0.58
39:a:1839:G:N9	39:a:1927:A:C4	2.72	0.58
8:7:-2:U:O4	16:D:1397:C:C4	2.57	0.57
10:A:58:A:H1'	10:A:60:U:C5	2.38	0.57
11:AA:870:ILE:HG12	11:AA:884:VAL:CG1	2.33	0.57
19:G:38:VAL:CG2	20:H:75:VAL:CG2	2.77	0.57
20:H:36:VAL:HB	20:H:48:ILE:HB	1.84	0.57
11:AA:1008:GLN:C	11:AA:1010:GLN:H	2.12	0.57
11:AA:1072:ASN:ND2	11:AA:1111:GLN:OE1	2.37	0.57
14:AE:37:GLU:O	14:AE:61:ILE:CD1	2.52	0.57
16:D:1329:A:P	36:X:28:THR:OG1	2.62	0.57
14:AE:161:THR:HG23	14:AE:164:GLN:H	1.68	0.57
14:AE:395:LYS:HZ2	14:AE:399:LYS:HD3	1.69	0.57
20:H:290:TYR:C	20:H:305:HIS:O	2.47	0.57
37:Y:7:TYR:HB2	37:Y:57:VAL:HG22	1.86	0.57
9:9:52:MET:HE3	9:9:52:MET:O	2.03	0.57
14:AE:638:SER:OG	14:AE:639:VAL:N	2.36	0.57
10:B:60:U:P	10:B:61:C:H41	2.27	0.57
20:H:332:VAL:CG1	20:H:335:ILE:HG13	2.33	0.57
10:A:34:C:P	25:M:84:THR:HG1	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:1006:GLU:OE1	11:AA:1006:GLU:HA	2.04	0.57
20:H:110:GLY:H	20:H:153:GLU:C	2.12	0.57
45:g:16:CYS:HB3	45:g:37:CYS:HB3	1.86	0.57
11:AA:10:ARG:NH1	11:AA:697:LYS:HD3	2.19	0.57
14:AE:903:LEU:HD21	14:AE:1249:ASN:HD22	1.70	0.57
37:Y:137:LEU:N	37:Y:137:LEU:HD23	2.19	0.57
32:T:5:THR:O	32:T:8:THR:OG1	2.18	0.57
10:A:50:U:H2'	10:A:51:C:H6	1.69	0.57
11:AA:400:VAL:HG11	11:AA:452:ARG:HD2	1.86	0.57
11:AA:914:LYS:H	11:AA:914:LYS:HD3	1.68	0.57
14:AE:124:ILE:HG22	14:AE:124:ILE:O	2.04	0.57
14:AE:130:MET:HE2	14:AE:135:ILE:HG12	1.87	0.57
14:AE:1046:ILE:HD12	14:AE:1059:LEU:HB3	1.86	0.57
13:AC:69:SER:OG	13:AC:70:THR:N	2.38	0.57
14:AE:160:LEU:HD22	14:AE:164:GLN:HB3	1.86	0.57
14:AE:198:CYS:HA	14:AE:221:ILE:HD11	1.86	0.57
14:AE:247:PRO:HA	14:AE:250:ARG:HG3	1.87	0.57
14:AE:510:LEU:HD22	14:AE:601:ILE:HD12	1.87	0.57
10:B:18:G:C8	10:B:57:A:N6	2.70	0.57
20:H:119:GLY:CA	20:H:133:GLY:CA	2.74	0.57
8:7:-11:A:H2'	8:7:-10:U:H6	1.70	0.56
9:9:17:GLU:HB3	9:9:86:MET:HB2	1.87	0.56
11:AA:818:VAL:HG22	11:AA:1096:ILE:HG12	1.86	0.56
11:AA:976:ARG:HG3	11:AA:989:LEU:HD13	1.85	0.56
10:B:11:A:H2'	10:B:12:G:C8	2.40	0.56
37:Y:59:THR:HG22	37:Y:61:TYR:HE1	1.69	0.56
10:B:56:C:C5'	52:n:80:ARG:NH2	2.67	0.56
37:Y:96:LYS:HE3	37:Y:136:GLY:HA3	1.87	0.56
59:u:77:ILE:HD11	59:u:108:ALA:HB1	1.87	0.56
2:1:93:ALA:HB2	39:a:1614:A:C2	2.40	0.56
10:A:11:A:H2'	10:A:12:G:C8	2.40	0.56
11:AA:39:ILE:HD12	11:AA:75:LEU:HD22	1.88	0.56
11:AA:227:LYS:NZ	11:AA:298:ALA:HB1	2.21	0.56
11:AA:855:PRO:CB	11:AA:913:VAL:HG21	2.36	0.56
11:AA:859:GLU:HB3	21:I:109:PRO:HG3	1.87	0.56
13:AC:120:ASP:CA	28:P:31:ARG:NH2	2.68	0.56
14:AE:99:ARG:HH11	14:AE:99:ARG:CG	2.18	0.56
14:AE:491:LEU:HB2	14:AE:904:ALA:HA	1.86	0.56
28:P:6:ILE:HG23	28:P:100:ILE:HG23	1.87	0.56
29:Q:67:ALA:HB2	29:Q:96:THR:HG23	1.86	0.56
39:a:2245:U:O2'	39:a:2436:G:OP2	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:g:16:CYS:CB	45:g:37:CYS:CB	2.82	0.56
7:6:21:DA:N6	8:7:15:G:H1	2.04	0.56
13:AD:81:ILE:HD11	13:AD:130:ILE:HG22	1.87	0.56
11:AA:880:GLY:O	11:AA:919:ARG:HD3	2.06	0.56
10:B:50:U:H2'	10:B:51:C:H6	1.69	0.56
20:H:49:PRO:HD3	20:H:84:LEU:HD11	1.87	0.56
20:H:330:VAL:HB	20:H:344:LEU:HD23	1.86	0.56
39:a:580:U:O3'	64:z:31:VAL:HG13	2.05	0.56
11:AA:1069:ARG:NH2	11:AA:1114:GLU:OE2	2.30	0.56
9:9:35:VAL:HA	9:9:38:MET:HB2	1.88	0.56
11:AA:1257:GLN:OE1	14:AE:345:LYS:HB3	2.05	0.56
19:G:19:GLN:NE2	20:H:75:VAL:HG22	2.19	0.56
19:G:148:LEU:HD22	19:G:151:ILE:HD11	1.86	0.56
11:AA:976:ARG:HG3	11:AA:976:ARG:HH11	1.71	0.56
13:AD:15:ASP:HB3	13:AD:27:THR:HB	1.87	0.56
14:AE:741:ALA:O	14:AE:762:ASN:ND2	2.38	0.56
23:K:56:VAL:O	23:K:60:ILE:HG23	2.04	0.56
41:c:31:PRO:HG2	41:c:33:LEU:HD13	1.87	0.56
11:AA:1084:ASP:OD1	13:AC:45:ARG:NH1	2.32	0.56
50:l:104:ALA:O	50:l:108:ILE:HG23	2.05	0.56
1:0:51:VAL:HG23	64:z:86:ALA:O	2.06	0.56
10:A:38:A:H2'	10:A:39:C:H5'	1.88	0.56
14:AE:74:LYS:HD2	14:AE:85:CYS:SG	2.45	0.56
10:B:32:C:OP2	27:O:130:ARG:NH2	2.38	0.56
20:H:267:TRP:CH2	20:H:340:ARG:HB3	2.41	0.56
39:a:1818:U:OP2	46:h:156:ARG:NH1	2.38	0.56
11:AA:801:ARG:HG2	11:AA:1094:VAL:HG23	1.87	0.55
11:AA:1246:ARG:NH1	11:AA:1266:GLY:HA2	2.20	0.55
13:AC:91:ARG:HD2	13:AC:122:GLU:HB3	1.88	0.55
14:AE:144:TYR:HE1	14:AE:162:GLU:CD	2.14	0.55
37:Y:77:VAL:O	37:Y:77:VAL:HG12	2.05	0.55
8:7:-2:U:H5''	8:7:-2:U:O2	2.07	0.55
11:AA:241:LEU:HD21	11:AA:246:LEU:HD11	1.88	0.55
11:AA:859:GLU:CB	21:I:109:PRO:HG2	2.36	0.55
11:AA:1046:VAL:HG22	11:AA:1049:ILE:HG13	1.88	0.55
14:AE:102:MET:HG2	14:AE:246:PRO:HG3	1.87	0.55
9:9:31:ARG:HG3	9:9:31:ARG:NH1	2.16	0.55
10:A:11:A:O5'	10:A:11:A:H8	1.89	0.55
26:N:10:MET:HE3	26:N:61:LEU:HD11	1.87	0.55
10:A:56:C:C6	39:a:2168:G:C6	2.94	0.55
11:AA:1257:GLN:NE2	14:AE:346:ARG:H	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AB:107:GLU:OE1	14:AE:288:PRO:CB	2.52	0.55
13:AC:118:ASP:CB	28:P:90:LEU:CD2	2.80	0.55
35:W:15:LEU:HD13	35:W:33:THR:HG21	1.88	0.55
37:Y:116:MET:HG3	37:Y:124:MET:HB3	1.89	0.55
39:a:2303:G:C4	39:a:2314:A:C2	2.95	0.55
14:AE:833:GLU:HB2	14:AE:1242:ARG:NH1	2.21	0.55
16:D:1227:A:P	36:X:110:LYS:HZ1	2.30	0.55
7:6:26:DT:H2''	7:6:27:DG:H5'	1.89	0.55
11:AA:991:LYS:HB2	11:AA:992:LEU:HD22	1.88	0.55
16:D:528:C:H6	16:D:528:C:H5''	1.71	0.55
16:D:1515:G:H2'	16:D:1516:G:H8	1.72	0.55
39:a:2314:A:O2'	52:n:155:THR:HG21	2.06	0.55
20:H:84:LEU:HD22	20:H:84:LEU:H	1.72	0.55
37:Y:112:LYS:HZ2	37:Y:112:LYS:HB3	1.71	0.55
39:a:2249:U:H3'	39:a:2250:G:C5'	2.36	0.55
50:l:108:ILE:HD11	50:l:180:LEU:HD13	1.89	0.55
9:9:31:ARG:HD2	39:a:1054:A:C4'	2.29	0.55
11:AA:1246:ARG:NH1	11:AA:1258:PRO:HB3	2.22	0.55
14:AE:343:LEU:HD11	14:AE:1324:SER:HB3	1.87	0.55
10:B:11:A:H8	10:B:11:A:O5'	1.89	0.55
16:D:769:G:H4'	16:D:1513:A:H4'	1.88	0.55
8:7:3:U:O2	8:7:3:U:H2'	2.06	0.55
11:AA:1252:SER:N	11:AA:1259:LEU:CD1	2.70	0.55
13:AD:215:GLU:OE1	13:AD:218:ARG:NH1	2.40	0.55
14:AE:171:GLU:HA	14:AE:171:GLU:OE1	2.05	0.55
37:Y:109:ALA:HB2	37:Y:128:ILE:HG13	1.89	0.55
11:AA:449:GLY:HA3	11:AA:609:ILE:HG23	1.87	0.55
16:D:961:U:O4	16:D:974:A:N1	2.40	0.55
20:H:154:PHE:CB	20:H:168:VAL:CB	2.85	0.55
23:K:99:ALA:HB1	23:K:103:THR:HG21	1.89	0.55
37:Y:57:VAL:O	37:Y:57:VAL:HG12	2.07	0.55
38:Z:2:ILE:HB	38:Z:5:ASP:HB3	1.89	0.55
11:AA:724:VAL:HG12	11:AA:774:GLY:H	1.72	0.54
11:AA:1034:ARG:HH11	11:AA:1034:ARG:CG	2.20	0.54
14:AE:136:GLU:OE1	14:AE:312:ARG:CZ	2.55	0.54
14:AE:759:ILE:HG23	14:AE:771:GLN:HB3	1.90	0.54
14:AE:1166:GLY:HA3	14:AE:1174:ARG:HB2	1.88	0.54
22:J:61:VAL:HG21	22:J:200:ILE:CD1	2.35	0.54
60:v:66:ARG:NH1	60:v:104:GLU:OE1	2.39	0.54
14:AE:111:THR:HG22	14:AE:300:GLN:NE2	2.23	0.54
3:2:50:LEU:HD23	43:e:26:PHE:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:18:G:C8	10:A:57:A:N6	2.69	0.54
28:P:8:ILE:HD12	28:P:25:ILE:HD11	1.89	0.54
9:9:51:TYR:CD1	9:9:51:TYR:C	2.85	0.54
11:AA:174:ALA:HB2	11:AA:432:LEU:HD13	1.88	0.54
11:AA:1251:TYR:C	11:AA:1259:LEU:HD11	2.31	0.54
13:AD:22:THR:OG1	13:AD:207:THR:O	2.26	0.54
13:AD:142:MET:N	13:AD:142:MET:SD	2.80	0.54
14:AE:39:LYS:O	14:AE:273:ILE:HG23	2.08	0.54
14:AE:46:TYR:CD1	14:AE:46:TYR:C	2.85	0.54
16:D:563:A:N6	16:D:884:U:H3	2.05	0.54
14:AE:53:ARG:NH2	22:J:164:GLN:C	2.61	0.54
14:AE:814:CYS:SG	14:AE:883:ARG:NH2	2.81	0.54
16:D:439:U:O2	16:D:440:C:C5	2.61	0.54
20:H:45:GLU:OE1	20:H:45:GLU:N	2.40	0.54
39:a:1839:G:N9	39:a:1927:A:H1'	2.23	0.54
62:x:35:ILE:HG21	62:x:71:ALA:HA	1.89	0.54
7:6:2:DC:H2''	7:6:3:DC:C5	2.43	0.54
10:A:12:G:H2'	10:A:13:C:OP1	2.08	0.54
11:AA:724:VAL:CG1	11:AA:774:GLY:N	2.68	0.54
20:H:305:HIS:HD2	20:H:306:VAL:H	1.49	0.54
8:7:-11:A:C4	8:7:-10:U:C5	2.95	0.54
11:AA:1253:LEU:HD12	14:AE:253:VAL:HG13	1.90	0.54
11:AA:1275:VAL:HG13	11:AA:1287:LEU:HD11	1.90	0.54
20:H:52:GLN:OE1	20:H:86:ARG:CB	2.55	0.54
37:Y:33:ASN:H	37:Y:66:PHE:HE1	1.56	0.54
16:D:945:G:C2	16:D:946:A:C8	2.96	0.54
20:H:279:LYS:HA	20:H:331:MET:CB	2.33	0.54
30:R:80:ILE:HD12	30:R:97:THR:HG22	1.89	0.54
39:a:811:U:H2'	59:u:21:ARG:HA	1.89	0.54
56:r:58:LEU:O	56:r:61:VAL:HG22	2.08	0.54
9:9:50:VAL:HG13	37:Y:119:ALA:HB3	1.88	0.54
11:AA:699:LEU:HG	11:AA:799:ASN:HD22	1.72	0.54
11:AA:985:GLU:HB2	11:AA:988:LYS:HB2	1.90	0.54
13:AC:140:ILE:HD11	13:AC:142:MET:HE3	1.89	0.54
14:AE:58:CYS:SG	14:AE:59:ALA:N	2.80	0.54
14:AE:785:ASP:O	14:AE:789:LYS:HB2	2.08	0.54
20:H:332:VAL:O	20:H:334:ASP:N	2.40	0.54
45:g:18:CYS:HB3	45:g:40:CYS:HB2	1.88	0.54
13:AC:65:LEU:HD22	21:I:80:LYS:O	2.08	0.54
20:H:22:SER:N	20:H:69:ASP:OD2	2.40	0.54
37:Y:12:VAL:HG12	37:Y:23:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:859:GLU:HB2	21:I:110:GLU:OE1	2.08	0.53
11:AA:870:ILE:HG23	11:AA:884:VAL:HG13	1.90	0.53
14:AE:145:VAL:HG23	14:AE:159:ILE:HG22	1.89	0.53
50:I:131:THR:HG22	50:I:160:ALA:O	2.08	0.53
9:9:123:ILE:O	9:9:123:ILE:HG12	2.08	0.53
11:AA:452:ARG:HH12	11:AA:458:GLU:CD	2.15	0.53
11:AA:946:LEU:HD23	11:AA:946:LEU:N	2.23	0.53
11:AA:994:ARG:HD2	11:AA:994:ARG:O	2.09	0.53
14:AE:39:LYS:O	14:AE:273:ILE:HG21	2.06	0.53
14:AE:87:LYS:HG3	22:J:20:PHE:CD1	2.35	0.53
14:AE:205:LEU:HG	14:AE:217:LEU:HB3	1.90	0.53
14:AE:746:LEU:HG	14:AE:758:PRO:HG3	1.90	0.53
14:AE:1175:LEU:HD22	14:AE:1190:ILE:HD11	1.88	0.53
37:Y:116:MET:HE2	37:Y:117:THR:H	1.73	0.53
39:a:1906:G:H5'	39:a:1906:G:H8	1.73	0.53
39:a:2192:U:H2'	39:a:2193:G:C8	2.43	0.53
9:9:71:CYS:HA	9:9:117:LEU:HD13	1.90	0.53
13:AC:65:LEU:CB	21:I:80:LYS:CB	2.76	0.53
16:D:13:U:C2	16:D:915:A:C6	2.95	0.53
20:H:19:ARG:O	20:H:72:LEU:HD22	2.09	0.53
40:b:37:ILE:HD11	40:b:82:ILE:HD11	1.90	0.53
50:I:130:LYS:HB2	50:I:133:LEU:HD12	1.89	0.53
9:9:58:THR:HG21	9:9:81:LEU:HA	1.90	0.53
10:A:56:C:C2	39:a:2112:G:C8	2.96	0.53
11:AA:835:GLU:OE2	11:AA:1051:LYS:HD3	2.08	0.53
11:AA:998:LEU:HD21	11:AA:1011:LEU:HD13	1.90	0.53
14:AE:26:SER:HB2	14:AE:236:TRP:CE2	2.42	0.53
4:3:13:VAL:CG2	4:3:39:ILE:HD13	2.39	0.53
11:AA:628:HIS:HB3	11:AA:647:ARG:HH21	1.73	0.53
11:AA:840:SER:HA	11:AA:886:LYS:HD2	1.90	0.53
14:AE:832:LYS:HB3	14:AE:1242:ARG:NH1	2.24	0.53
39:a:2315:G:O2'	52:n:125:ARG:HD3	2.09	0.53
58:t:7:MET:HE1	58:t:44:LYS:HD2	1.91	0.53
10:A:6:G:O2'	10:A:7:G:H8	1.92	0.53
10:A:16:C:O2	10:A:16:C:H2'	2.08	0.53
10:A:60:U:O2'	10:A:61:C:OP1	2.23	0.53
11:AA:808:ASN:H	14:AE:633:ALA:HB2	1.74	0.53
14:AE:209:ASN:HA	14:AE:214:ARG:HH21	1.74	0.53
10:B:12:G:H2'	10:B:13:C:OP1	2.08	0.53
16:D:13:U:C4	16:D:21:G:C2	2.96	0.53
16:D:1228:C:OP2	36:X:110:LYS:NZ	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:135:LEU:CB	20:H:167:VAL:CA	2.86	0.53
9:9:125:ARG:HA	9:9:125:ARG:CZ	2.38	0.53
13:AD:196:THR:HB	14:AE:443:GLU:CG	2.36	0.53
14:AE:124:ILE:HG23	14:AE:128:LEU:HD12	1.90	0.53
16:D:13:U:C4	16:D:915:A:C6	2.92	0.53
28:P:24:GLU:OE2	28:P:90:LEU:CD1	2.56	0.53
37:Y:37:PHE:CZ	37:Y:56:VAL:HG11	2.44	0.53
52:n:8:TYR:HA	52:n:12:VAL:HB	1.91	0.53
2:1:59:GLU:CG	2:1:66:ILE:HD11	2.38	0.53
8:7:15:G:H2'	8:7:16:A:C8	2.43	0.53
9:9:139:LEU:HD11	38:Z:11:VAL:HG13	1.90	0.53
10:A:18:G:C2	10:A:58:A:C5	2.96	0.53
13:AC:215:GLU:OE2	13:AC:219:ARG:NH2	2.41	0.53
14:AE:1155:ILE:HG13	14:AE:1210:ILE:HB	1.88	0.53
14:AE:1167:LYS:HZ2	14:AE:1170:LYS:HB2	1.73	0.53
10:B:16:C:O2	10:B:16:C:H2'	2.08	0.53
10:A:38:A:C2'	10:A:39:C:H5'	2.39	0.53
11:AA:1257:GLN:OE1	14:AE:345:LYS:CB	2.57	0.53
14:AE:30:ILE:HG21	14:AE:241:VAL:O	2.08	0.53
14:AE:56:LEU:CD1	14:AE:273:ILE:HD12	2.39	0.53
20:H:116:VAL:C	20:H:279:LYS:HB2	2.33	0.53
13:AD:109:PRO:HA	13:AD:132:HIS:HA	1.91	0.53
16:D:1329:A:OP1	36:X:28:THR:N	2.41	0.53
39:a:404:A:O2'	39:a:405:U:OP2	2.22	0.53
39:a:2298:A:C5	39:a:2321:U:O4	2.62	0.53
62:x:27:VAL:HG21	62:x:40:ILE:HD12	1.89	0.53
4:3:94:ARG:HB3	4:3:103:ILE:HD12	1.92	0.52
10:A:22:G:O2'	10:A:23:C:P	2.68	0.52
14:AE:78:LEU:O	14:AE:78:LEU:HD13	2.08	0.52
20:H:24:VAL:HG12	20:H:69:ASP:H	1.74	0.52
37:Y:19:PRO:HG2	37:Y:24:GLY:H	1.73	0.52
37:Y:59:THR:HG22	37:Y:61:TYR:CE1	2.44	0.52
39:a:1056:G:O2'	39:a:1103:A:N6	2.41	0.52
10:A:17:C:O2	10:A:17:C:H2'	2.08	0.52
14:AE:215:LYS:HA	14:AE:218:THR:HG22	1.91	0.52
10:B:18:G:C2	10:B:58:A:C5	2.97	0.52
10:A:32:C:O2'	25:M:86:GLN:CD	2.31	0.52
11:AA:726:TYR:HD2	11:AA:726:TYR:O	1.92	0.52
11:AA:953:LEU:HD13	11:AA:1036:ILE:HG21	1.91	0.52
13:AC:171:LEU:HD23	13:AC:171:LEU:N	2.24	0.52
13:AD:182:ARG:CD	14:AE:581:MET:HE1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:17:C:O2	10:B:17:C:H2'	2.08	0.52
16:D:673:A:H2'	16:D:674:G:C8	2.44	0.52
21:I:77:ILE:HA	21:I:84:VAL:HG23	1.91	0.52
8:7:17:G:H2'	8:7:18:A:C8	2.44	0.52
10:A:15:G:N3	10:A:15:G:C2'	2.73	0.52
11:AA:862:LEU:HD23	11:AA:862:LEU:H	1.74	0.52
11:AA:960:LEU:HB3	11:AA:1025:PHE:CE1	2.45	0.52
11:AA:984:VAL:O	11:AA:984:VAL:HG22	2.10	0.52
14:AE:99:ARG:HG3	14:AE:99:ARG:HH11	1.74	0.52
14:AE:975:ILE:HD11	14:AE:1003:LEU:HD11	1.90	0.52
11:AA:242:VAL:HB	11:AA:245:ARG:NH1	2.25	0.52
11:AA:738:GLU:HA	11:AA:741:MET:HE2	1.90	0.52
11:AA:884:VAL:HG11	11:AA:1050:VAL:HG11	1.91	0.52
11:AA:991:LYS:N	11:AA:991:LYS:CD	2.73	0.52
11:AA:1287:LEU:HD13	14:AE:1357:ILE:HD11	1.89	0.52
14:AE:112:ALA:HA	14:AE:238:ILE:HA	1.92	0.52
10:B:22:G:O2'	10:B:23:C:P	2.67	0.52
39:a:523:C:O2	39:a:554:U:O2'	2.25	0.52
8:7:20:G:O2'	14:AE:425:ARG:NH2	2.40	0.52
9:9:125:ARG:HG3	9:9:125:ARG:O	2.10	0.52
10:A:19:G:C5	39:a:2112:G:H4'	2.44	0.52
11:AA:876:GLU:HG2	13:AC:159:ILE:HD11	1.92	0.52
11:AA:1045:GLY:O	11:AA:1047:LEU:HD13	2.10	0.52
14:AE:68:TYR:CA	14:AE:75:TYR:HE2	2.21	0.52
15:C:61:ARG:NH2	16:D:736:C:OP1	2.43	0.52
16:D:864:A:C2	16:D:865:A:C2	2.98	0.52
10:B:6:G:O2'	10:B:7:G:H8	1.92	0.52
10:B:76:A:N3	39:a:2493:U:H4'	2.24	0.52
20:H:84:LEU:H	20:H:84:LEU:CD2	2.21	0.52
37:Y:138:VAL:HG12	37:Y:138:VAL:O	2.08	0.52
9:9:43:LYS:HG2	9:9:98:GLU:HG2	1.90	0.52
11:AA:813:GLU:HB2	14:AE:461:PHE:HD2	1.74	0.52
11:AA:1007:LYS:HD2	11:AA:1007:LYS:C	2.35	0.52
11:AA:1070:HIS:NE2	11:AA:1114:GLU:OE1	2.36	0.52
10:B:12:G:C2'	10:B:13:C:OP1	2.57	0.52
16:D:767:A:H2'	16:D:768:A:O4'	2.08	0.52
39:a:639:U:H2'	39:a:640:C:C6	2.45	0.52
39:a:1980:G:O2'	39:a:1982:U:OP2	2.28	0.52
39:a:2328:A:H2'	39:a:2329:U:C6	2.44	0.52
10:A:12:G:C2'	10:A:13:C:OP1	2.57	0.52
14:AE:99:ARG:HA	14:AE:248:ASP:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:390:LEU:N	14:AE:390:LEU:CD1	2.73	0.52
20:H:49:PRO:HD2	20:H:84:LEU:CD1	2.40	0.52
20:H:135:LEU:CB	20:H:157:ILE:CB	2.87	0.52
27:O:81:HIS:O	27:O:84:THR:OG1	2.23	0.52
27:O:98:LEU:HB3	27:O:104:VAL:HG13	1.91	0.52
39:a:523:C:H4'	39:a:540:C:O2	2.10	0.52
9:9:3:LEU:HD13	9:9:5:LEU:H	1.75	0.52
10:B:56:C:H2'	10:B:57:A:C5'	2.27	0.52
16:D:1404:C:H2'	16:D:1404:C:O2	2.10	0.52
42:d:106:G:H2'	42:d:107:G:O4'	2.10	0.52
8:7:-10:U:H2'	8:7:-9:G:C8	2.45	0.51
8:7:16:A:H2'	8:7:17:G:C8	2.45	0.51
13:AD:33:ARG:HD3	13:AD:197:ASP:HB2	1.91	0.51
14:AE:144:TYR:CE1	14:AE:162:GLU:CD	2.88	0.51
14:AE:683:ILE:HD12	14:AE:754:ILE:HG21	1.93	0.51
14:AE:850:LYS:HB2	14:AE:857:LEU:HB2	1.91	0.51
16:D:1308:U:P	36:X:98:ARG:HG3	2.50	0.51
20:H:71:ALA:O	20:H:72:LEU:CD1	2.42	0.51
48:j:4:LEU:HD23	48:j:29:VAL:CG1	2.39	0.51
13:AD:182:ARG:HD3	14:AE:581:MET:HE1	1.91	0.51
16:D:1499:A:O2'	16:D:1500:A:H5'	2.10	0.51
19:G:35:ARG:NH2	20:H:10:GLU:HG2	2.25	0.51
20:H:321:VAL:HG13	20:H:322:VAL:HG23	1.90	0.51
64:z:58:ARG:HA	64:z:61:TRP:CE3	2.45	0.51
11:AA:880:GLY:C	11:AA:919:ARG:HD3	2.36	0.51
39:a:2000:C:OP1	61:w:5:LYS:NZ	2.36	0.51
32:T:40:GLN:CA	32:T:40:GLN:HE21	2.23	0.51
39:a:1814:G:H4'	46:h:51:THR:HG21	1.92	0.51
39:a:1910:G:O5'	39:a:1910:G:H8	1.93	0.51
61:w:38:LEU:N	61:w:39:PRO:CD	2.73	0.51
2:1:93:ALA:HB2	39:a:1614:A:N1	2.25	0.51
9:9:11:ILE:CD1	9:9:11:ILE:N	2.73	0.51
10:A:56:C:H1'	39:a:2112:G:C5	2.46	0.51
10:A:56:C:C3'	10:A:57:A:H5''	2.40	0.51
11:AA:862:LEU:HD23	11:AA:862:LEU:N	2.25	0.51
23:K:94:VAL:HG13	23:K:111:MET:HE1	1.91	0.51
4:3:12:ILE:HG21	4:3:80:ALA:HB2	1.92	0.51
11:AA:524:ILE:HG21	11:AA:708:VAL:HG13	1.91	0.51
11:AA:1252:SER:HA	11:AA:1259:LEU:HD11	1.93	0.51
14:AE:804:ALA:O	14:AE:806:ASP:N	2.41	0.51
16:D:1228:C:OP1	36:X:107:ARG:CZ	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Y:112:LYS:NZ	37:Y:112:LYS:CB	2.73	0.51
10:A:48:C:H2'	10:A:48:C:O2	2.11	0.51
16:D:1276:G:O5'	16:D:1276:G:H8	1.93	0.51
37:Y:27:LEU:HD12	37:Y:27:LEU:C	2.35	0.51
39:a:1693:U:O2'	46:h:14:ARG:NH2	2.43	0.51
58:t:71:ARG:NH2	58:t:123:LEU:O	2.42	0.51
9:9:78:GLY:H	9:9:79:PRO:HD2	1.68	0.51
10:A:18:G:C2	10:A:58:A:C6	2.99	0.51
10:B:15:G:N3	10:B:15:G:C2'	2.73	0.51
10:B:56:C:C3'	10:B:57:A:H5''	2.40	0.51
20:H:49:PRO:HD2	20:H:84:LEU:HD11	1.92	0.51
23:K:81:LEU:HD13	23:K:123:VAL:HG12	1.92	0.51
39:a:587:C:OP2	59:u:21:ARG:NH1	2.43	0.51
39:a:1964:G:H4'	39:a:1965:C:OP2	2.11	0.51
42:d:5:U:OP1	42:d:61:G:O2'	2.26	0.51
54:p:121:ILE:HD12	54:p:141:ILE:CG2	2.41	0.51
2:1:24:ILE:HD13	2:1:36:LEU:HD11	1.93	0.51
11:AA:733:VAL:HG22	11:AA:750:ILE:HG12	1.93	0.51
18:F:4:ILE:HD12	18:F:19:PHE:HA	1.93	0.51
39:a:1141:U:O2	39:a:1142:A:N6	2.44	0.51
51:m:31:LEU:HD22	51:m:42:LEU:CD1	2.40	0.51
58:t:113:MET:O	58:t:116:ILE:HG13	2.11	0.51
2:1:59:GLU:HG3	2:1:66:ILE:HD11	1.92	0.51
6:5:101:DT:H72	14:AE:271:ARG:CZ	2.41	0.51
11:AA:988:LYS:NZ	11:AA:988:LYS:CB	2.73	0.51
10:B:24:U:O2'	39:a:1922:G:O3'	2.29	0.51
37:Y:80:LYS:HG3	37:Y:86:LYS:HA	1.93	0.51
37:Y:100:ILE:HB	37:Y:105:LEU:HD11	1.92	0.51
6:5:98:DA:N9	6:5:99:DT:H72	2.26	0.50
10:A:56:C:C5	39:a:2168:G:O6	2.64	0.50
11:AA:817:LEU:HD12	11:AA:1078:LYS:HB3	1.93	0.50
14:AE:88:CYS:HB3	14:AE:90:VAL:HG12	1.92	0.50
14:AE:201:LEU:HD12	14:AE:224:LEU:HD12	1.91	0.50
14:AE:972:LYS:HD2	14:AE:1004:ALA:HA	1.93	0.50
20:H:267:TRP:CZ3	20:H:340:ARG:HG3	2.43	0.50
57:s:30:THR:HG22	57:s:31:GLU:N	2.27	0.50
10:A:76:A:O2'	39:a:2395:C:C2	2.64	0.50
16:D:1410:A:C2	16:D:1491:G:C2	2.99	0.50
26:N:3:MET:HA	26:N:3:MET:HE3	1.94	0.50
39:a:118:A:C8	39:a:119:A:C8	2.99	0.50
39:a:1824:G:O2'	46:h:252:THR:HG21	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:a:1869:G:N2	39:a:1871:A:O2'	2.44	0.50
9:9:93:ALA:O	9:9:129:LEU:HD13	2.06	0.50
11:AA:1032:LYS:HZ1	11:AA:1036:ILE:HD11	1.76	0.50
10:B:48:C:O2	10:B:48:C:H2'	2.11	0.50
16:D:1356:G:H2'	16:D:1357:A:C8	2.47	0.50
61:w:55:ALA:HA	61:w:80:PHE:CE1	2.47	0.50
9:9:41:LEU:HD12	37:Y:117:THR:HG22	1.92	0.50
11:AA:14:ASP:HA	11:AA:1183:ALA:HB3	1.93	0.50
11:AA:657:THR:HG21	11:AA:1188:ASP:HB2	1.92	0.50
11:AA:1244:HIS:NE2	11:AA:1266:GLY:O	2.34	0.50
14:AE:421:VAL:O	14:AE:436:ALA:HA	2.11	0.50
15:C:30:LYS:HA	15:C:33:ILE:HD13	1.92	0.50
2:1:55:ILE:HG23	2:1:66:ILE:HD12	1.93	0.50
9:9:31:ARG:NH1	9:9:31:ARG:CG	2.73	0.50
10:A:15:G:H22	10:A:20:U:H3	1.59	0.50
11:AA:689:ALA:HB2	11:AA:1233:LEU:HD23	1.93	0.50
12:AB:71:VAL:HG12	12:AB:73:MET:HB2	1.93	0.50
14:AE:275:ARG:HH12	14:AE:278:ARG:NH1	2.09	0.50
10:B:18:G:C2	10:B:58:A:C6	2.99	0.50
20:H:332:VAL:C	20:H:334:ASP:H	2.18	0.50
39:a:929:U:H1'	44:f:26:GLY:O	2.10	0.50
39:a:2243:U:H2'	39:a:2244:U:C6	2.46	0.50
51:m:22:MET:O	51:m:28:ARG:NH1	2.45	0.50
10:A:59:A:H2'	10:A:60:U:H5'	1.94	0.50
11:AA:125:GLY:HA2	11:AA:499:SER:HB2	1.94	0.50
11:AA:632:ASP:HA	11:AA:647:ARG:HB2	1.94	0.50
11:AA:876:GLU:HA	11:AA:876:GLU:OE2	2.11	0.50
13:AD:100:LEU:O	13:AD:144:ILE:N	2.39	0.50
10:B:47:U:H2'	10:B:48:C:H4'	1.94	0.50
16:D:1499:A:H3'	16:D:1499:A:OP2	2.12	0.50
58:t:43:ILE:HD12	58:t:56:ASP:HB2	1.93	0.50
11:AA:1252:SER:CA	11:AA:1259:LEU:HD11	2.41	0.50
10:B:34:C:O2	10:B:34:C:H2'	2.11	0.50
16:D:1366:C:O2'	28:P:62:ARG:NH2	2.44	0.50
19:G:35:ARG:CD	20:H:14:LYS:HD3	2.40	0.50
20:H:308:GLU:O	20:H:310:ASP:N	2.43	0.50
32:T:21:ASP:O	32:T:22:THR:HG22	2.12	0.50
46:h:107:PRO:HD2	46:h:110:LEU:HD22	1.94	0.50
8:7:15:G:H2'	8:7:16:A:H8	1.75	0.50
10:A:28:C:H2'	10:A:29:G:H8	1.76	0.50
11:AA:935:THR:HA	11:AA:1049:ILE:CD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:31:ARG:HH11	9:9:31:ARG:CG	2.14	0.50
10:A:47:U:H2'	10:A:48:C:H4'	1.94	0.50
16:D:1208:C:H2'	16:D:1209:C:C6	2.47	0.50
57:s:17:VAL:HG23	57:s:137:PRO:HB2	1.93	0.50
6:5:96:DT:H2''	6:5:97:DC:C5	2.46	0.49
9:9:51:TYR:CG	9:9:89:PRO:HD2	2.47	0.49
10:A:11:A:H2'	10:A:12:G:C1'	2.42	0.49
11:AA:1008:GLN:C	11:AA:1010:GLN:N	2.70	0.49
14:AE:1371:ARG:HE	14:AE:1372:ARG:NH1	2.10	0.49
16:D:108:G:H5''	16:D:108:G:N3	2.27	0.49
20:H:120:PHE:CB	20:H:136:VAL:CB	2.91	0.49
32:T:4:SER:O	32:T:8:THR:HG23	2.12	0.49
39:a:1266:G:OP2	47:i:17:ARG:NE	2.43	0.49
48:j:25:THR:HG21	48:j:193:VAL:HG22	1.94	0.49
62:x:51:ALA:HB3	62:x:78:VAL:HB	1.94	0.49
8:7:0:U:H5''	8:7:0:U:O2	2.11	0.49
20:H:52:GLN:O	20:H:53:PHE:HD1	1.95	0.49
28:P:57:VAL:O	28:P:57:VAL:HG13	2.11	0.49
39:a:464:U:O3'	51:m:12:ARG:NH2	2.45	0.49
1:0:14:VAL:HG21	1:0:98:ILE:HG13	1.94	0.49
14:AE:749:LYS:HB3	14:AE:755:ILE:HD11	1.94	0.49
10:B:60:U:O2'	10:B:61:C:OP1	2.23	0.49
20:H:132:PRO:N	20:H:167:VAL:CB	2.75	0.49
39:a:2303:G:C6	39:a:2314:A:N1	2.81	0.49
39:a:2646:C:O5'	39:a:2646:C:H6	1.95	0.49
9:9:23:LEU:HA	9:9:118:ILE:HG13	1.92	0.49
13:AC:71:LYS:NZ	13:AC:140:ILE:CG1	2.76	0.49
13:AC:162:GLU:O	13:AC:162:GLU:HG2	2.04	0.49
14:AE:802:ASP:OD1	14:AE:1348:LYS:NZ	2.31	0.49
20:H:117:LYS:CB	20:H:278:THR:CG2	2.90	0.49
20:H:318:PRO:HA	20:H:321:VAL:HG12	1.95	0.49
37:Y:21:PRO:CB	37:Y:22:PRO:CD	2.90	0.49
39:a:742:A:C2	39:a:743:A:C6	3.00	0.49
41:c:3:ARG:HD2	41:c:30:LEU:HD22	1.95	0.49
64:z:47:TYR:CD1	64:z:47:TYR:C	2.90	0.49
9:9:44:ALA:HB1	9:9:52:MET:HB3	1.93	0.49
11:AA:694:ARG:NH2	13:AC:83:LEU:HD13	2.26	0.49
14:AE:395:LYS:NZ	14:AE:399:LYS:CD	2.74	0.49
36:X:17:ILE:O	36:X:20:THR:OG1	2.22	0.49
39:a:565:C:H2'	39:a:566:U:O4'	2.13	0.49
39:a:1433:A:H2'	39:a:1434:A:O4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:p:35:ARG:HD3	54:p:71:LEU:HD13	1.93	0.49
4:3:7:ARG:HB2	39:a:85:G:OP2	2.13	0.49
9:9:52:MET:HE3	9:9:52:MET:CA	2.42	0.49
9:9:62:ARG:CG	9:9:62:ARG:NH2	2.73	0.49
11:AA:859:GLU:HG3	21:I:109:PRO:HG2	1.94	0.49
13:AD:20:SER:OG	13:AD:21:SER:N	2.45	0.49
14:AE:437:PHE:HZ	14:AE:453:VAL:HG11	1.76	0.49
39:a:2297:A:C6	39:a:2321:U:O4	2.65	0.49
10:A:37:A:H2'	10:A:38:A:H8	1.77	0.49
10:A:41:C:H4'	25:M:143:ARG:NH1	2.25	0.49
11:AA:232:ILE:HD12	11:AA:331:LYS:HA	1.94	0.49
11:AA:845:LEU:HD23	11:AA:845:LEU:N	2.28	0.49
11:AA:1013:GLN:N	11:AA:1013:GLN:NE2	2.61	0.49
13:AC:158:ARG:NH1	13:AC:158:ARG:CB	2.73	0.49
16:D:5:U:O2	16:D:5:U:O4'	2.29	0.49
16:D:50:A:O2'	16:D:360:G:N2	2.45	0.49
16:D:1311:A:OP1	45:g:59:ARG:NH1	2.46	0.49
39:a:1412:U:C4	39:a:1413:A:N7	2.81	0.49
39:a:2038:G:H2'	39:a:2039:U:O4'	2.13	0.49
39:a:2298:A:N3	39:a:2321:U:C5	2.80	0.49
57:s:32:LEU:CD2	57:s:54:ILE:HG21	2.42	0.49
11:AA:991:LYS:HA	11:AA:991:LYS:HE3	1.95	0.49
10:B:39:C:O5'	10:B:39:C:H6	1.95	0.49
16:D:974:A:OP1	31:S:69:ARG:NH1	2.46	0.49
34:V:48:ASP:HB3	34:V:75:LEU:HD23	1.94	0.49
39:a:2557:G:H2'	39:a:2558:C:C6	2.47	0.49
10:A:72:A:H2'	10:A:73:A:C5'	2.32	0.49
10:B:25:C:H2'	10:B:26:G:H5'	1.94	0.49
24:L:18:VAL:N	24:L:19:PRO:CD	2.76	0.49
10:A:15:G:C2	10:A:20:U:O2	2.66	0.49
10:A:37:A:H2'	10:A:38:A:C8	2.48	0.49
11:AA:728:ASP:HA	11:AA:731:ARG:O	2.12	0.49
11:AA:958:LYS:NZ	11:AA:958:LYS:CB	2.73	0.49
11:AA:1102:GLY:HA2	11:AA:1106:ARG:NH1	2.28	0.49
14:AE:114:ILE:HG12	14:AE:311:ARG:HD2	1.95	0.49
14:AE:152:THR:HB	14:AE:172:PHE:CZ	2.48	0.49
14:AE:800:LEU:HB3	14:AE:920:ALA:HB1	1.95	0.49
10:B:49:G:O5'	10:B:49:G:H8	1.95	0.49
16:D:60:A:N1	16:D:107:G:O2'	2.42	0.49
16:D:872:A:H2'	16:D:872:A:N3	2.27	0.49
46:h:210:ALA:HA	46:h:213:TRP:CE3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:j:156:PHE:CE1	57:s:81:ILE:HD13	2.48	0.49
61:w:67:PHE:O	61:w:71:ARG:N	2.45	0.49
1:0:40:MET:HE3	1:0:49:ILE:CD1	2.43	0.48
13:AC:118:ASP:CB	28:P:90:LEU:HD23	2.42	0.48
13:AD:95:LYS:O	13:AD:148:ARG:NH2	2.42	0.48
16:D:1169:A:H2'	16:D:1170:A:C8	2.48	0.48
51:m:24:THR:HG23	51:m:27:GLY:H	1.78	0.48
10:A:25:C:H2'	10:A:26:G:H5'	1.95	0.48
11:AA:529:ARG:HH22	11:AA:687:ARG:NH1	2.11	0.48
14:AE:145:VAL:HG12	14:AE:184:ALA:HB1	1.94	0.48
10:B:11:A:C2'	10:B:12:G:O4'	2.60	0.48
52:n:127:ASN:ND2	52:n:127:ASN:N	2.60	0.48
9:9:23:LEU:HD22	9:9:92:ALA:HB1	1.95	0.48
11:AA:936:ARG:O	11:AA:936:ARG:HD3	2.14	0.48
11:AA:1101:LEU:HD21	14:AE:508:LEU:HD22	1.95	0.48
14:AE:102:MET:HG2	14:AE:246:PRO:HD3	1.95	0.48
14:AE:115:TRP:O	14:AE:1333:THR:HG21	2.13	0.48
14:AE:550:VAL:O	14:AE:569:LEU:HA	2.13	0.48
39:a:1209:U:O2'	39:a:1237:A:N1	2.40	0.48
1:0:14:VAL:CG2	1:0:98:ILE:HG13	2.43	0.48
14:AE:201:LEU:HD11	14:AE:220:ARG:HG2	1.94	0.48
14:AE:1027:VAL:HB	14:AE:1121:LEU:HB2	1.96	0.48
10:B:5:G:C2'	10:B:6:G:H5'	2.40	0.48
37:Y:77:VAL:HG13	37:Y:80:LYS:HE3	1.95	0.48
39:a:1839:G:N9	39:a:1927:A:C1'	2.77	0.48
2:1:25:ARG:NH1	2:1:74:ILE:O	2.46	0.48
11:AA:24:VAL:HG22	11:AA:578:TYR:HE1	1.78	0.48
11:AA:857:VAL:CG1	11:AA:861:ALA:HB2	2.44	0.48
10:B:14:A:N3	10:B:14:A:H2'	2.29	0.48
10:B:18:G:C5	10:B:57:A:C5	3.01	0.48
10:B:59:A:H2'	10:B:60:U:H5'	1.94	0.48
8:7:-5:U:C6	8:7:-5:U:C3'	2.97	0.48
10:A:18:G:C5	10:A:57:A:C5	3.01	0.48
11:AA:103:VAL:HG12	11:AA:117:ILE:HG22	1.94	0.48
13:AD:191:ARG:NH2	13:AD:193:GLU:O	2.47	0.48
14:AE:1146:GLU:OE2	14:AE:1310:THR:HG22	2.14	0.48
14:AE:1261:LEU:HD12	14:AE:1304:ARG:HH21	1.78	0.48
14:AE:1321:SER:OG	14:AE:1349:GLU:OE2	2.22	0.48
10:B:11:A:H2'	10:B:12:G:C1'	2.43	0.48
10:B:15:G:C2	10:B:20:U:O2	2.66	0.48
16:D:13:U:O4	16:D:21:G:N3	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:911:U:H2'	16:D:912:C:C6	2.49	0.48
20:H:33:LYS:HA	20:H:34:ASP:HA	1.61	0.48
56:r:3:VAL:HG22	56:r:36:ALA:HB1	1.95	0.48
8:7:-10:U:OP1	16:D:1505:G:O5'	2.31	0.48
10:A:41:C:H5'	25:M:143:ARG:HD2	1.96	0.48
10:A:49:G:H8	10:A:49:G:O5'	1.95	0.48
14:AE:968:ASN:HA	14:AE:1117:SER:HB2	1.96	0.48
16:D:1017:U:O2'	16:D:1018:G:O4'	2.31	0.48
16:D:1174:G:H2'	16:D:1175:G:H5'	1.95	0.48
23:K:99:ALA:CB	23:K:103:THR:HG21	2.43	0.48
23:K:114:VAL:HG21	23:K:141:ILE:HD12	1.94	0.48
28:P:6:ILE:HG23	28:P:100:ILE:CG2	2.43	0.48
34:V:75:LEU:C	34:V:75:LEU:HD12	2.38	0.48
39:a:2303:G:C2	39:a:2314:A:N3	2.82	0.48
40:b:37:ILE:HG21	40:b:80:ILE:HG21	1.95	0.48
48:j:121:THR:HB	48:j:127:PHE:CD2	2.49	0.48
3:2:61:LEU:C	3:2:61:LEU:HD12	2.39	0.48
13:AC:102:LEU:HB2	13:AC:115:ILE:HG12	1.95	0.48
37:Y:77:VAL:HG13	37:Y:80:LYS:CE	2.44	0.48
37:Y:133:ARG:O	37:Y:133:ARG:HG2	2.14	0.48
43:e:18:LEU:HB2	43:e:53:VAL:HG11	1.94	0.48
62:x:27:VAL:CG2	62:x:40:ILE:HD12	2.44	0.48
7:6:21:DA:N6	8:7:15:G:N1	2.61	0.48
10:A:76:A:N6	39:a:2422:C:O4'	2.46	0.48
11:AA:1280:ALA:HB1	14:AE:918:ILE:HG22	1.96	0.48
10:B:58:A:C8	10:B:58:A:OP2	2.67	0.48
20:H:23:ILE:N	20:H:69:ASP:OD2	2.46	0.48
39:a:686:U:O4	51:m:12:ARG:HB2	2.14	0.48
39:a:2685:G:OP1	58:t:78:ARG:NH2	2.47	0.48
1:0:5:PHE:HB3	1:0:59:ILE:HD12	1.96	0.48
9:9:51:TYR:CD1	9:9:88:HIS:HB2	2.49	0.48
10:A:11:A:C2'	10:A:12:G:O4'	2.60	0.48
10:A:68:C:C4	10:A:69:C:C5	3.02	0.48
11:AA:243:PRO:HB2	11:AA:274:ILE:HG23	1.96	0.48
13:AC:71:LYS:NZ	13:AC:140:ILE:HB	2.27	0.48
14:AE:47:ARG:CZ	14:AE:47:ARG:HB2	2.44	0.48
16:D:927:G:O2'	16:D:1503:A:N7	2.36	0.48
39:a:1993:U:H4'	48:j:133:THR:HG22	1.96	0.48
11:AA:562:GLU:OE1	11:AA:662:SER:OG	2.31	0.47
13:AD:48:LEU:HD22	14:AE:535:ARG:HG3	1.96	0.47
14:AE:103:GLY:H	14:AE:244:VAL:HG22	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:395:LYS:NZ	14:AE:399:LYS:CE	2.77	0.47
20:H:316:ILE:HD11	20:H:321:VAL:HG11	1.97	0.47
37:Y:71:LYS:HB3	37:Y:72:THR:H	1.58	0.47
39:a:1266:G:OP1	47:i:16:ARG:NE	2.45	0.47
10:A:18:G:N3	10:A:58:A:C6	2.82	0.47
10:A:33:U:H2'	10:A:35:A:OP2	2.14	0.47
11:AA:1029:LEU:C	11:AA:1029:LEU:HD23	2.39	0.47
13:AD:60:GLU:OE2	13:AD:170:ARG:NE	2.44	0.47
14:AE:108:ALA:HB1	14:AE:279:LEU:HD22	1.96	0.47
14:AE:128:LEU:HD21	14:AE:188:LEU:HB3	1.97	0.47
14:AE:1221:LEU:HD22	14:AE:1306:LEU:HB2	1.97	0.47
10:B:72:A:H2'	10:B:73:A:C5'	2.33	0.47
15:C:33:ILE:O	15:C:33:ILE:HG12	2.15	0.47
20:H:330:VAL:HG12	20:H:345:GLY:O	2.14	0.47
8:7:16:A:H2'	8:7:17:G:H8	1.79	0.47
9:9:48:ALA:HB3	9:9:51:TYR:CD2	2.50	0.47
11:AA:46:GLN:HA	11:AA:47:TYR:HA	1.77	0.47
13:AD:96:ASP:OD1	13:AD:96:ASP:N	2.46	0.47
14:AE:141:PHE:CE2	14:AE:296:LYS:CB	2.94	0.47
14:AE:809:VAL:HG21	14:AE:909:ILE:HG12	1.95	0.47
10:B:76:A:N3	10:B:76:A:C2'	2.74	0.47
16:D:13:U:O2	16:D:915:A:N7	2.47	0.47
28:P:6:ILE:CG2	28:P:100:ILE:HG23	2.43	0.47
39:a:1588:G:C6	39:a:1589:U:O4	2.67	0.47
11:AA:756:TYR:CD2	13:AC:68:TYR:O	2.68	0.47
16:D:371:A:H2'	16:D:372:C:O4'	2.14	0.47
44:f:24:LEU:HD11	44:f:54:MET:CE	2.42	0.47
9:9:1:MET:SD	9:9:2:ALA:N	2.88	0.47
9:9:8:LYS:NZ	39:a:1046:A:H61	2.11	0.47
11:AA:1119:MET:HG3	11:AA:1204:LEU:HD13	1.97	0.47
13:AC:43:LEU:O	13:AC:47:LEU:HB2	2.14	0.47
13:AD:199:ASP:N	13:AD:199:ASP:OD1	2.47	0.47
14:AE:220:ARG:HG2	14:AE:220:ARG:NH1	2.25	0.47
22:J:162:ALA:O	22:J:165:ARG:O	2.33	0.47
9:9:17:GLU:HG2	9:9:88:HIS:NE2	2.29	0.47
9:9:139:LEU:HD21	38:Z:11:VAL:HG22	1.97	0.47
10:A:14:A:H2'	10:A:14:A:N3	2.29	0.47
11:AA:618:GLN:HG3	14:AE:770:LEU:HD13	1.96	0.47
13:AD:104:LYS:HG2	13:AD:110:VAL:HB	1.97	0.47
10:B:18:G:N3	10:B:58:A:C6	2.82	0.47
16:D:321:A:N7	16:D:328:C:O2'	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:1308:U:OP1	36:X:100:GLN:OE1	2.23	0.47
20:H:309:MET:HE2	20:H:318:PRO:HB3	1.97	0.47
20:H:332:VAL:HG11	20:H:335:ILE:CG1	2.38	0.47
2:1:4:ILE:HG12	2:1:106:VAL:HG22	1.95	0.47
8:7:-6:U:C2	16:D:1493:A:C2	3.02	0.47
10:A:9:G:H5''	10:A:10:G:OP2	2.14	0.47
11:AA:93:SER:HA	11:AA:128:PRO:HA	1.97	0.47
11:AA:618:GLN:OE1	11:AA:635:THR:OG1	2.32	0.47
11:AA:829:THR:HG23	11:AA:1059:ARG:HA	1.97	0.47
11:AA:841:ARG:HB2	11:AA:841:ARG:NH1	2.30	0.47
11:AA:914:LYS:NZ	11:AA:914:LYS:HB2	2.29	0.47
11:AA:985:GLU:OE2	11:AA:1000:LEU:HD11	2.14	0.47
11:AA:1023:HIS:C	11:AA:1023:HIS:ND1	2.73	0.47
11:AA:1047:LEU:O	11:AA:1049:ILE:HD11	2.13	0.47
14:AE:86:GLU:CG	22:J:166:GLU:HB3	2.45	0.47
14:AE:117:LEU:HG	14:AE:118:LYS:HG3	1.95	0.47
14:AE:1060:VAL:HG13	14:AE:1106:ILE:HG12	1.96	0.47
10:B:18:G:C6	10:B:57:A:N7	2.83	0.47
16:D:526:C:P	30:R:88:LYS:HE3	2.54	0.47
16:D:604:G:H2'	16:D:605:U:O4'	2.14	0.47
16:D:1064:G:O2'	16:D:1190:G:N2	2.47	0.47
16:D:1103:C:O2	19:G:106:THR:HG21	2.15	0.47
16:D:1329:A:OP1	36:X:28:THR:OG1	2.31	0.47
17:E:54:MET:O	17:E:57:ILE:HG22	2.15	0.47
20:H:72:LEU:CD1	20:H:72:LEU:N	2.73	0.47
37:Y:20:SER:CB	37:Y:21:PRO:HD3	2.39	0.47
38:Z:4:LYS:O	38:Z:4:LYS:HD2	2.15	0.47
39:a:1020:A:C6	39:a:1141:U:O2	2.68	0.47
39:a:2168:G:H8	39:a:2168:G:OP1	1.97	0.47
39:a:2585:U:O2	39:a:2585:U:O4'	2.32	0.47
48:j:152:PRO:HG3	48:j:156:PHE:CZ	2.50	0.47
53:o:13:ARG:HD3	59:u:58:TYR:O	2.14	0.47
8:7:17:G:H2'	8:7:18:A:H8	1.80	0.47
9:9:27:VAL:HG22	9:9:99:PHE:HE2	1.80	0.47
10:A:29:G:H2'	10:A:30:G:O4'	2.15	0.47
11:AA:685:MET:SD	11:AA:1073:LYS:HG2	2.55	0.47
13:AD:109:PRO:HB3	13:AD:132:HIS:CD2	2.50	0.47
14:AE:24:LEU:CB	14:AE:232:ASN:OD1	2.54	0.47
14:AE:420:PRO:HA	14:AE:437:PHE:O	2.15	0.47
10:B:60:U:H4'	10:B:61:C:OP2	2.14	0.47
10:B:68:C:C4	10:B:69:C:C5	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:946:A:H2'	16:D:947:G:C8	2.50	0.47
16:D:1175:G:N3	16:D:1176:A:C8	2.83	0.47
36:X:16:VAL:HG23	36:X:17:ILE:HD12	1.97	0.47
37:Y:64:ARG:HE	37:Y:64:ARG:HB2	1.51	0.47
39:a:1363:C:O2'	39:a:1809:A:N3	2.46	0.47
57:s:84:ILE:HG23	57:s:84:ILE:O	2.14	0.47
9:9:50:VAL:CG1	37:Y:119:ALA:CB	2.88	0.47
10:A:60:U:H4'	10:A:61:C:OP2	2.14	0.47
11:AA:978:VAL:HG11	11:AA:1010:GLN:CB	2.45	0.47
11:AA:1034:ARG:NH1	11:AA:1034:ARG:C	2.73	0.47
11:AA:1257:GLN:CD	14:AE:345:LYS:HB3	2.40	0.47
14:AE:43:THR:HG22	14:AE:57:PHE:HE1	1.80	0.47
14:AE:891:ASP:OD2	14:AE:1290:ARG:NH2	2.47	0.47
14:AE:1036:ARG:HE	14:AE:1081:VAL:HG11	1.79	0.47
14:AE:1347:LEU:HG	14:AE:1357:ILE:HG23	1.96	0.47
1:0:51:VAL:HG22	1:0:51:VAL:O	2.15	0.47
8:7:-11:A:H2'	8:7:-10:U:C6	2.50	0.47
10:A:68:C:H3'	10:A:69:C:H5''	1.96	0.47
11:AA:549:ASP:OD2	14:AE:750:PRO:HB3	2.15	0.47
11:AA:641:GLU:OE2	14:AE:749:LYS:NZ	2.47	0.47
14:AE:198:CYS:HA	14:AE:221:ILE:CD1	2.45	0.47
14:AE:799:ARG:HG2	14:AE:1325:PHE:HZ	1.78	0.47
14:AE:902:ASP:OD2	14:AE:905:ARG:HB2	2.15	0.47
16:D:373:A:C2	16:D:374:A:C8	3.03	0.47
16:D:1228:C:P	36:X:107:ARG:HH12	2.38	0.47
24:L:67:PRO:O	24:L:70:VAL:HG22	2.15	0.47
38:Z:29:LYS:HE2	38:Z:29:LYS:HB2	1.45	0.47
2:1:29:VAL:HB	2:1:55:ILE:HD11	1.96	0.46
10:A:56:C:H2'	10:A:57:A:C5'	2.27	0.46
14:AE:1150:PRO:HG3	14:AE:1214:PRO:HB2	1.96	0.46
10:B:5:G:C2'	10:B:6:G:C5'	2.93	0.46
10:B:15:G:H22	10:B:20:U:H3	1.59	0.46
16:D:1308:U:P	36:X:98:ARG:CG	3.03	0.46
23:K:96:MET:CE	23:K:115:LEU:HD11	2.45	0.46
38:Z:18:ASP:HB3	38:Z:22:LEU:CD1	2.45	0.46
11:AA:735:LYS:HA	11:AA:748:ILE:HG22	1.96	0.46
11:AA:941:LYS:HD3	11:AA:941:LYS:HA	1.78	0.46
11:AA:1252:SER:N	11:AA:1259:LEU:HD11	2.30	0.46
13:AC:117:HIS:HB2	28:P:89:ARG:HD3	1.97	0.46
26:N:102:ALA:HB3	26:N:113:ASP:HB3	1.96	0.46
34:V:8:LEU:HD23	34:V:25:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Y:79:LEU:HD13	37:Y:132:ALA:HA	1.97	0.46
9:9:67:THR:H	9:9:68:PRO:HD3	1.80	0.46
13:AC:141:SER:O	13:AC:141:SER:OG	2.33	0.46
14:AE:99:ARG:NH1	14:AE:99:ARG:CG	2.76	0.46
14:AE:842:ARG:HH22	14:AE:1250:ASP:HB2	1.80	0.46
14:AE:1219:ASP:O	14:AE:1223:LEU:HB2	2.15	0.46
10:B:42:G:H2'	10:B:43:A:C8	2.47	0.46
16:D:915:A:C8	16:D:915:A:H3'	2.50	0.46
21:I:75:ILE:HD13	21:I:75:ILE:C	2.40	0.46
9:9:132:TYR:CE1	38:Z:19:VAL:HG22	2.50	0.46
10:A:5:G:C2'	10:A:6:G:H5'	2.40	0.46
10:A:58:A:OP2	10:A:58:A:C8	2.67	0.46
11:AA:724:VAL:HG13	11:AA:774:GLY:H	1.76	0.46
11:AA:994:ARG:C	11:AA:994:ARG:CD	2.89	0.46
11:AA:1010:GLN:C	11:AA:1010:GLN:NE2	2.73	0.46
14:AE:526:VAL:HG12	14:AE:549:LYS:HB2	1.96	0.46
14:AE:833:GLU:N	14:AE:1242:ARG:HH12	2.12	0.46
14:AE:847:ASP:OD1	14:AE:847:ASP:N	2.49	0.46
14:AE:1167:LYS:NZ	14:AE:1170:LYS:HB2	2.30	0.46
16:D:1225:A:OP1	36:X:101:ARG:HB2	2.15	0.46
19:G:114:LEU:HA	19:G:144:LEU:HD13	1.98	0.46
20:H:291:GLY:HA2	20:H:305:HIS:O	2.15	0.46
28:P:8:ILE:HD12	28:P:25:ILE:CD1	2.46	0.46
39:a:517:C:OP2	47:i:10:ARG:NH2	2.48	0.46
39:a:1814:G:C4'	46:h:51:THR:HG21	2.44	0.46
39:a:2756:U:C4	39:a:2759:G:C6	3.03	0.46
44:f:25:LEU:C	44:f:25:LEU:HD13	2.41	0.46
4:3:94:ARG:CB	4:3:103:ILE:HD12	2.45	0.46
11:AA:974:ARG:HD2	11:AA:1014:LEU:CD1	2.46	0.46
11:AA:988:LYS:HB3	11:AA:988:LYS:HZ2	1.80	0.46
20:H:332:VAL:HG13	20:H:342:ILE:HG23	1.98	0.46
39:a:560:C:O2	64:z:48:ARG:NH1	2.41	0.46
39:a:2168:G:OP1	39:a:2168:G:C8	2.68	0.46
39:a:2298:A:C6	39:a:2299:U:C2	3.04	0.46
46:h:76:ALA:HB2	46:h:96:TYR:CD1	2.51	0.46
6:5:113:DC:P	11:AA:163:LYS:HD3	2.55	0.46
9:9:43:LYS:HZ1	9:9:95:LEU:HD13	1.80	0.46
10:A:18:G:C6	10:A:57:A:N7	2.83	0.46
11:AA:855:PRO:HB3	11:AA:913:VAL:HG21	1.97	0.46
11:AA:948:ILE:HA	11:AA:951:MET:SD	2.55	0.46
11:AA:965:GLN:HA	11:AA:968:GLU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AC:73:GLY:HA3	13:AC:138:ALA:CB	2.46	0.46
15:C:12:ARG:CZ	20:H:264:GLU:HA	2.46	0.46
16:D:35:G:N3	30:R:115:SER:OG	2.47	0.46
16:D:1176:A:H2'	16:D:1177:G:O4'	2.16	0.46
18:F:67:ARG:HD3	18:F:67:ARG:N	2.31	0.46
20:H:69:ASP:O	20:H:85:SER:CB	2.63	0.46
39:a:1021:A:N3	39:a:1021:A:C3'	2.78	0.46
3:2:30:ILE:HD13	3:2:93:LEU:HD12	1.97	0.46
10:A:6:G:O2'	10:A:7:G:C5'	2.64	0.46
11:AA:1020:GLU:HA	11:AA:1023:HIS:HD2	1.81	0.46
13:AD:96:ASP:HB3	13:AD:148:ARG:HE	1.81	0.46
10:B:9:G:H5''	10:B:10:G:OP2	2.14	0.46
10:B:14:A:H1'	10:B:22:G:N2	2.31	0.46
15:C:61:ARG:HG2	24:L:88:MET:HE1	1.98	0.46
29:Q:34:ILE:HG12	29:Q:70:CYS:SG	2.56	0.46
37:Y:116:MET:CB	37:Y:124:MET:HG2	2.46	0.46
39:a:2291:U:H2'	39:a:2292:U:C6	2.51	0.46
57:s:30:THR:CG2	57:s:31:GLU:N	2.79	0.46
9:9:43:LYS:NZ	9:9:95:LEU:HD13	2.30	0.46
9:9:58:THR:HB	9:9:82:ILE:H	1.80	0.46
10:A:18:G:O2'	10:A:60:U:N3	2.48	0.46
16:D:526:C:OP2	30:R:88:LYS:HE3	2.15	0.46
16:D:868:C:H2'	16:D:869:G:O4'	2.16	0.46
36:X:106:ALA:HB3	36:X:110:LYS:HD2	1.98	0.46
52:n:36:LEU:HB3	52:n:57:LEU:HD21	1.97	0.46
9:9:24:SER:HB2	9:9:116:GLU:HG2	1.98	0.46
9:9:118:ILE:HB	9:9:119:PRO:CD	2.45	0.46
10:A:18:G:C8	10:A:57:A:N1	2.83	0.46
14:AE:109:SER:HB2	14:AE:296:LYS:HG2	1.98	0.46
14:AE:141:PHE:HE2	14:AE:296:LYS:CB	2.22	0.46
10:B:6:G:O2'	10:B:7:G:C5'	2.64	0.46
10:B:48:C:N4	10:B:59:A:C5	2.84	0.46
50:l:149:ILE:CD1	50:l:188:MET:HE3	2.46	0.46
6:5:114:DC:H5''	14:AE:1148:ARG:CZ	2.46	0.46
9:9:50:VAL:HG22	37:Y:119:ALA:C	2.41	0.46
9:9:106:PHE:CG	9:9:106:PHE:O	2.69	0.46
11:AA:559:CYS:HB2	11:AA:662:SER:HB3	1.97	0.46
11:AA:588:GLU:HA	11:AA:606:LEU:O	2.15	0.46
13:AC:228:LEU:HD11	13:AD:224:LEU:HD23	1.97	0.46
16:D:1517:G:H1'	39:a:1919:A:O2'	2.16	0.46
19:G:16:PHE:CD2	20:H:42:LEU:O	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:135:LEU:CB	20:H:167:VAL:O	2.63	0.46
28:P:99:GLN:O	28:P:99:GLN:HG2	2.16	0.46
7:6:15:DC:N3	7:6:16:DC:C4	2.84	0.45
11:AA:318:SER:H	11:AA:321:LEU:HD12	1.80	0.45
11:AA:914:LYS:HD3	11:AA:914:LYS:N	2.31	0.45
11:AA:976:ARG:HG3	11:AA:976:ARG:NH1	2.30	0.45
11:AA:1043:ALA:CB	11:AA:1044:PRO:CD	2.91	0.45
11:AA:1046:VAL:CG2	11:AA:1049:ILE:HG13	2.45	0.45
13:AC:166:ARG:HB3	13:AC:166:ARG:NH1	2.30	0.45
13:AD:212:ASP:O	13:AD:215:GLU:N	2.48	0.45
14:AE:385:LEU:HD23	14:AE:390:LEU:HB2	1.98	0.45
10:B:18:G:C8	10:B:57:A:N1	2.83	0.45
21:I:117:ALA:HB2	21:I:200:VAL:CG1	2.46	0.45
38:Z:7:ILE:HD12	38:Z:7:ILE:HA	1.77	0.45
39:a:784:G:H5'	39:a:785:G:OP1	2.15	0.45
46:h:6:CYS:SG	46:h:13:ARG:NH1	2.89	0.45
58:t:18:ARG:HB2	58:t:45:GLU:HB3	1.97	0.45
10:A:42:G:H2'	10:A:43:A:C8	2.47	0.45
10:A:60:U:OP2	10:A:61:C:N4	2.45	0.45
11:AA:318:SER:OG	11:AA:320:ASP:OD1	2.31	0.45
13:AC:120:ASP:HB3	28:P:31:ARG:HH21	1.81	0.45
39:a:1067:A:O2'	39:a:1068:G:O4'	2.31	0.45
39:a:1906:G:H4'	39:a:1906:G:OP1	2.17	0.45
60:v:96:ILE:HG21	60:v:126:ILE:HD12	1.97	0.45
11:AA:933:VAL:O	11:AA:933:VAL:HG12	2.16	0.45
11:AA:957:LYS:HA	11:AA:1029:LEU:HD12	1.97	0.45
14:AE:202:ARG:HH11	14:AE:202:ARG:CG	2.14	0.45
14:AE:209:ASN:HA	14:AE:214:ARG:NH2	2.31	0.45
10:B:58:A:C1'	10:B:60:U:C5	2.99	0.45
16:D:429:U:N3	16:D:431:A:N6	2.64	0.45
19:G:114:LEU:HD13	19:G:144:LEU:CB	2.46	0.45
21:I:155:GLY:HA2	21:I:163:ALA:HB1	1.99	0.45
37:Y:23:VAL:HB	37:Y:24:GLY:H	1.65	0.45
37:Y:95:ASP:OD2	37:Y:95:ASP:N	2.50	0.45
37:Y:125:THR:HA	37:Y:128:ILE:HG12	1.98	0.45
39:a:1394:U:H4'	39:a:1603:A:H4'	1.97	0.45
45:g:18:CYS:HB2	45:g:40:CYS:HB3	1.96	0.45
52:n:57:LEU:HD22	52:n:89:VAL:CG2	2.47	0.45
10:A:41:C:C5'	25:M:143:ARG:HD2	2.46	0.45
11:AA:1018:TYR:CD1	11:AA:1018:TYR:C	2.94	0.45
11:AA:1029:LEU:HD11	11:AA:1033:ARG:HH21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:1032:LYS:HA	11:AA:1032:LYS:CE	2.46	0.45
11:AA:1034:ARG:NH1	11:AA:1034:ARG:CG	2.77	0.45
13:AC:71:LYS:HZ1	13:AC:140:ILE:HD12	1.80	0.45
14:AE:1106:ILE:O	14:AE:1123:ARG:N	2.45	0.45
39:a:1007:C:OP1	57:s:37:ARG:NH2	2.50	0.45
39:a:2898:U:O2'	57:s:134:ALA:O	2.28	0.45
48:j:186:LEU:HD21	63:y:4:ILE:HG21	1.98	0.45
6:5:116:DG:OP1	14:AE:1311:LYS:NZ	2.46	0.45
9:9:127:ALA:O	9:9:130:PRO:HG2	2.16	0.45
10:A:5:G:C2'	10:A:6:G:C5'	2.93	0.45
11:AA:176:ILE:HD12	11:AA:184:LEU:HD23	1.99	0.45
11:AA:724:VAL:HG12	11:AA:774:GLY:N	2.31	0.45
14:AE:115:TRP:HB3	14:AE:1333:THR:CG2	2.47	0.45
14:AE:388:ARG:HG2	14:AE:388:ARG:NH1	2.32	0.45
16:D:1340:A:H8	16:D:1340:A:O5'	2.00	0.45
20:H:19:ARG:O	20:H:72:LEU:HD13	2.16	0.45
20:H:38:VAL:HG22	20:H:48:ILE:HD11	1.99	0.45
39:a:1095:A:O2'	39:a:1096:A:O4'	2.33	0.45
8:7:14:U:H2'	8:7:15:G:C8	2.52	0.45
10:A:49:G:C2'	10:A:50:U:H5'	2.47	0.45
11:AA:446:ASP:HA	11:AA:451:ARG:HH21	1.81	0.45
11:AA:976:ARG:NH2	11:AA:989:LEU:HB3	2.32	0.45
11:AA:1008:GLN:HE22	11:AA:1011:LEU:HG	1.82	0.45
13:AD:131:CYS:SG	13:AD:132:HIS:N	2.89	0.45
14:AE:395:LYS:NZ	14:AE:399:LYS:HE2	2.32	0.45
14:AE:1158:GLU:HA	14:AE:1223:LEU:HD21	1.99	0.45
16:D:1240:U:OP1	25:M:116:MET:HB2	2.16	0.45
39:a:1385:A:O2'	39:a:1396:U:O2	2.35	0.45
39:a:1695:G:N7	46:h:14:ARG:NH2	2.64	0.45
39:a:1720:U:H2'	39:a:1721:G:O4'	2.16	0.45
61:w:28:LEU:HD23	61:w:48:VAL:HG21	1.98	0.45
10:A:48:C:C5	10:A:59:A:C8	3.05	0.45
13:AC:59:VAL:O	13:AC:171:LEU:HG	2.16	0.45
13:AD:81:ILE:HD12	13:AD:81:ILE:HA	1.85	0.45
13:AD:211:ILE:HD11	13:AD:215:GLU:HG3	1.98	0.45
14:AE:926:PRO:HB2	14:AE:1241:TYR:HE1	1.82	0.45
14:AE:978:ARG:HD3	14:AE:999:TYR:H	1.82	0.45
16:D:17:U:H2'	16:D:18:C:C6	2.52	0.45
20:H:294:VAL:HG21	20:H:330:VAL:HG21	1.99	0.45
22:J:165:ARG:NH1	22:J:165:ARG:HB2	2.32	0.45
25:M:24:ALA:O	25:M:27:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:P:28:THR:HG21	28:P:87:LEU:CD1	2.46	0.45
39:a:1021:A:N6	39:a:1141:U:N3	2.47	0.45
39:a:2547:A:H2'	39:a:2548:U:C6	2.52	0.45
52:n:77:PHE:CD1	52:n:77:PHE:N	2.82	0.45
9:9:39:THR:HA	9:9:42:ARG:HH11	1.81	0.45
11:AA:227:LYS:HZ2	11:AA:298:ALA:HB1	1.79	0.45
11:AA:538:LEU:HD11	11:AA:571:LEU:HD22	1.98	0.45
13:AD:86:LYS:HE3	14:AE:528:THR:HG21	1.97	0.45
14:AE:76:LYS:HB3	14:AE:76:LYS:NZ	2.32	0.45
14:AE:201:LEU:CD1	14:AE:224:LEU:HD12	2.46	0.45
10:B:49:G:C2'	10:B:50:U:H5'	2.47	0.45
15:C:12:ARG:NH2	20:H:268:VAL:CG2	2.71	0.45
16:D:1493:A:C8	16:D:1493:A:OP1	2.70	0.45
17:E:55:GLN:N	17:E:56:PRO:HD2	2.32	0.45
39:a:340:A:O2'	50:l:162:ARG:NH1	2.50	0.45
39:a:954:G:OP2	60:v:16:ARG:NH2	2.50	0.45
9:9:111:ALA:HB3	9:9:114:GLU:HG3	1.98	0.45
9:9:139:LEU:CD2	38:Z:11:VAL:HG22	2.47	0.45
10:A:58:A:C1'	10:A:60:U:C5	2.99	0.45
11:AA:596:ASP:N	11:AA:596:ASP:OD1	2.49	0.45
11:AA:857:VAL:HG11	11:AA:861:ALA:HB2	1.99	0.45
11:AA:985:GLU:CG	11:AA:988:LYS:HE3	2.45	0.45
13:AD:64:VAL:HG11	13:AD:78:ILE:HG21	1.99	0.45
14:AE:126:LEU:HD12	14:AE:223:LEU:HD22	1.99	0.45
14:AE:161:THR:H	14:AE:164:GLN:HB2	1.82	0.45
14:AE:213:LYS:CA	14:AE:213:LYS:HE3	2.47	0.45
37:Y:140:GLU:OE1	37:Y:140:GLU:N	2.50	0.45
39:a:742:A:C2	39:a:755:U:N3	2.80	0.45
39:a:930:G:H1'	44:f:25:LEU:HD11	1.98	0.45
39:a:2315:G:H5'	52:n:157:THR:HG23	1.97	0.45
51:m:12:ARG:HG3	51:m:44:VAL:HG11	1.99	0.45
7:6:15:DC:C4	7:6:16:DC:C5	3.05	0.45
9:9:60:LEU:HB2	9:9:61:ARG:NH2	2.31	0.45
10:A:48:C:N4	10:A:59:A:C5	2.84	0.45
11:AA:27:LEU:O	11:AA:528:ARG:NH1	2.42	0.45
11:AA:850:ILE:HD12	11:AA:1048:LYS:HG2	1.99	0.45
11:AA:1029:LEU:HA	11:AA:1032:LYS:HB2	1.99	0.45
14:AE:1108:GLN:HG3	14:AE:1109:LEU:HD12	1.99	0.45
27:O:63:LEU:HD13	27:O:65:ILE:HD11	1.97	0.45
39:a:2006:C:O2'	39:a:2823:A:N3	2.47	0.45
9:9:50:VAL:CG2	37:Y:120:ASP:N	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:75:TYR:CD2	14:AE:75:TYR:O	2.70	0.44
10:B:48:C:C5	10:B:59:A:C8	3.05	0.44
16:D:397:A:H3'	16:D:397:A:N3	2.33	0.44
22:J:197:GLU:HA	22:J:200:ILE:HD12	1.99	0.44
25:M:27:VAL:HG12	25:M:43:VAL:HG11	1.98	0.44
36:X:96:PRO:HG2	36:X:102:THR:HG23	1.97	0.44
37:Y:34:ILE:HG22	37:Y:34:ILE:O	2.18	0.44
37:Y:37:PHE:CD2	37:Y:37:PHE:O	2.70	0.44
43:e:59:GLU:O	43:e:63:ALA:HB3	2.18	0.44
52:n:17:MET:HE2	52:n:25:VAL:HA	1.98	0.44
2:1:17:VAL:HG12	2:1:76:VAL:HG21	1.98	0.44
9:9:34:THR:HG22	9:9:38:MET:CE	2.47	0.44
10:A:25:C:C2'	10:A:26:G:H5'	2.48	0.44
14:AE:894:VAL:HG22	14:AE:1258:ARG:HH11	1.83	0.44
10:B:34:C:C5	10:B:34:C:OP1	2.70	0.44
16:D:1515:G:H2'	16:D:1516:G:C8	2.52	0.44
27:O:80:ARG:O	27:O:84:THR:HG23	2.17	0.44
39:a:1927:A:C8	39:a:1927:A:O5'	2.71	0.44
52:n:29:PRO:HB2	52:n:169:LEU:HD22	1.99	0.44
9:9:106:PHE:O	9:9:106:PHE:CD2	2.70	0.44
10:A:14:A:H1'	10:A:22:G:N2	2.31	0.44
11:AA:875:ALA:H	21:I:80:LYS:HE3	1.82	0.44
11:AA:933:VAL:HG22	11:AA:935:THR:CG2	2.47	0.44
11:AA:939:VAL:HG12	11:AA:939:VAL:O	2.17	0.44
11:AA:967:LEU:HD23	11:AA:1021:LEU:HD21	1.98	0.44
14:AE:50:LYS:HD3	14:AE:50:LYS:HA	1.71	0.44
14:AE:515:ARG:NH2	14:AE:718:SER:O	2.48	0.44
14:AE:850:LYS:HB3	14:AE:855:ASP:HB2	2.00	0.44
18:F:21:ARG:HH22	20:H:341:ARG:HD2	1.82	0.44
19:G:208:ARG:HH12	20:H:29:VAL:HG11	1.82	0.44
9:9:18:VAL:HA	9:9:86:MET:CE	2.44	0.44
10:A:76:A:C2	53:o:31:HIS:NE2	2.85	0.44
11:AA:803:ALA:HB2	11:AA:1094:VAL:HG21	1.99	0.44
13:AC:65:LEU:CD2	21:I:80:LYS:O	2.65	0.44
13:AC:92:VAL:HG12	13:AC:121:VAL:HG12	1.98	0.44
14:AE:67:ASP:CG	14:AE:95:THR:HG1	2.23	0.44
14:AE:128:LEU:CD2	14:AE:188:LEU:HB3	2.47	0.44
14:AE:1357:ILE:HG22	14:AE:1359:ALA:H	1.82	0.44
16:D:109:A:C6	16:D:326:G:C6	3.05	0.44
16:D:684:U:H2'	16:D:685:G:O4'	2.18	0.44
19:G:114:LEU:HD13	19:G:144:LEU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:J:61:VAL:CG2	22:J:200:ILE:HD11	2.39	0.44
36:X:106:ALA:HB3	36:X:110:LYS:CD	2.47	0.44
37:Y:37:PHE:CE1	37:Y:56:VAL:HG11	2.51	0.44
39:a:1589:U:C2	39:a:1590:A:C8	3.06	0.44
39:a:2093:G:O2'	39:a:2198:A:N1	2.41	0.44
39:a:2822:G:OP1	48:j:164:GLN:NE2	2.47	0.44
9:9:16:SER:HB2	9:9:20:LYS:NZ	2.33	0.44
11:AA:952:GLN:H	11:AA:952:GLN:HG3	1.66	0.44
11:AA:960:LEU:HB3	11:AA:1025:PHE:CD1	2.52	0.44
10:B:37:A:N3	10:B:37:A:H5''	2.32	0.44
16:D:198:G:OP2	16:D:198:G:C8	2.70	0.44
16:D:337:G:H2'	16:D:338:A:C8	2.52	0.44
16:D:1397:C:O5'	16:D:1397:C:C6	2.70	0.44
37:Y:7:TYR:CD2	37:Y:7:TYR:O	2.70	0.44
39:a:1327:A:H2'	39:a:1328:A:O4'	2.17	0.44
39:a:1925:C:C5	39:a:1925:C:OP2	2.71	0.44
9:9:106:PHE:CD2	9:9:106:PHE:C	2.95	0.44
10:A:57:A:O5'	10:A:58:A:P	2.76	0.44
14:AE:1024:THR:HG23	14:AE:1123:ARG:HA	2.00	0.44
36:X:75:MET:HA	36:X:75:MET:HE3	1.99	0.44
37:Y:42:ASN:HA	37:Y:45:THR:HB	1.98	0.44
39:a:645:C:H2'	39:a:647:G:C8	2.52	0.44
42:d:48:U:H2'	42:d:49:C:C6	2.52	0.44
6:5:115:DA:P	14:AE:1148:ARG:HG3	2.58	0.44
11:AA:1117:LEU:HD12	11:AA:1195:ILE:HG12	2.00	0.44
13:AC:71:LYS:NZ	13:AC:140:ILE:HG13	2.32	0.44
13:AC:145:LYS:HE3	13:AC:145:LYS:HB2	1.83	0.44
14:AE:211:GLU:CG	14:AE:215:LYS:HE3	2.44	0.44
14:AE:213:LYS:HE3	14:AE:213:LYS:HA	1.99	0.44
10:B:49:G:O5'	10:B:49:G:C8	2.71	0.44
16:D:376:G:C2	16:D:389:A:C2	3.05	0.44
19:G:76:ALA:CB	19:G:210:VAL:HG11	2.48	0.44
39:a:998:C:OP2	64:z:58:ARG:NH2	2.49	0.44
56:r:55:GLU:HA	56:r:58:LEU:HD12	1.99	0.44
9:9:72:LEU:HD22	9:9:72:LEU:C	2.42	0.44
11:AA:241:LEU:N	11:AA:283:LYS:O	2.51	0.44
11:AA:800:MET:HE3	11:AA:800:MET:HB2	1.60	0.44
14:AE:506:VAL:HG23	14:AE:628:GLY:HA3	1.98	0.44
10:B:57:A:O5'	10:B:58:A:P	2.76	0.44
19:G:206:ALA:O	19:G:210:VAL:HG23	2.18	0.44
39:a:57:C:H2'	39:a:58:G:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:a:1406:U:H3	39:a:1596:A:H2	1.59	0.44
39:a:2070:A:H2'	39:a:2071:A:O4'	2.16	0.44
9:9:86:MET:H	9:9:86:MET:HG2	1.59	0.44
10:A:49:G:O5'	10:A:49:G:C8	2.71	0.44
11:AA:95:PRO:HB3	11:AA:123:TYR:HE1	1.83	0.44
11:AA:1032:LYS:CE	11:AA:1032:LYS:CA	2.92	0.44
10:B:68:C:H3'	10:B:69:C:H5''	1.96	0.44
16:D:915:A:H8	16:D:915:A:O5'	2.00	0.44
20:H:84:LEU:N	20:H:84:LEU:CD2	2.78	0.44
23:K:156:LYS:HG2	26:N:71:VAL:HG13	2.00	0.44
27:O:84:THR:HG21	27:O:103:PHE:CB	2.45	0.44
32:T:21:ASP:OD1	32:T:22:THR:N	2.49	0.44
39:a:813:U:H2'	39:a:814:C:C6	2.53	0.44
39:a:1386:C:H2'	39:a:1387:A:C8	2.53	0.44
39:a:2133:G:O2'	39:a:2157:G:N2	2.51	0.44
57:s:73:VAL:HG11	57:s:75:TYR:CZ	2.53	0.44
8:7:-2:U:O2'	21:I:162:ILE:HG13	2.18	0.43
8:7:2:U:C2'	23:K:57:PRO:HB3	2.32	0.43
10:A:1:C:C5	10:A:2:G:N7	2.86	0.43
11:AA:524:ILE:HB	11:AA:712:SER:HB2	1.99	0.43
11:AA:1032:LYS:CA	11:AA:1032:LYS:HE2	2.47	0.43
14:AE:62:PHE:N	14:AE:62:PHE:CD1	2.86	0.43
14:AE:1227:HIS:HA	14:AE:1230:THR:HG22	1.99	0.43
10:B:26:G:N2	10:B:45:G:N2	2.66	0.43
21:I:50:ALA:HB2	21:I:75:ILE:HD12	2.00	0.43
38:Z:18:ASP:HB3	38:Z:22:LEU:HD12	2.00	0.43
41:c:37:ARG:HG2	41:c:48:THR:HG23	2.00	0.43
56:r:15:LEU:HD13	56:r:15:LEU:C	2.42	0.43
58:t:24:VAL:HG13	58:t:33:ALA:HB2	2.00	0.43
62:x:18:LEU:HD23	62:x:25:ARG:HD2	1.99	0.43
10:A:56:C:OP1	39:a:2168:G:C4	2.71	0.43
11:AA:717:VAL:HG22	11:AA:782:VAL:HG12	2.00	0.43
13:AD:16:ILE:HD13	13:AD:214:GLU:HG2	1.99	0.43
10:B:25:C:C2'	10:B:26:G:H5'	2.47	0.43
16:D:976:G:C8	16:D:1358:U:O2	2.71	0.43
6:5:116:DG:C6	6:5:117:DA:C6	3.06	0.43
10:A:18:G:N3	10:A:58:A:C5	2.87	0.43
11:AA:998:LEU:CD2	11:AA:1011:LEU:HD13	2.49	0.43
14:AE:26:SER:HB2	14:AE:236:TRP:CH2	2.51	0.43
14:AE:26:SER:CB	14:AE:236:TRP:CZ2	2.95	0.43
14:AE:1046:ILE:HG22	14:AE:1061:VAL:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:1079:LYS:HD3	14:AE:1098:GLN:HB3	2.00	0.43
10:B:34:C:O5'	10:B:34:C:C6	2.70	0.43
16:D:13:U:C2	16:D:915:A:C5	3.05	0.43
16:D:1499:A:O2'	16:D:1500:A:C5'	2.67	0.43
20:H:280:LEU:HB2	20:H:330:VAL:O	2.18	0.43
23:K:153:VAL:HG23	23:K:164:ILE:HD13	2.00	0.43
28:P:28:THR:HG21	28:P:87:LEU:HD12	1.99	0.43
37:Y:19:PRO:HG2	37:Y:24:GLY:N	2.32	0.43
39:a:214:G:N2	39:a:216:A:N3	2.66	0.43
39:a:2252:G:H2'	39:a:2253:G:H8	1.84	0.43
60:v:35:ALA:HB2	60:v:102:LEU:HD11	2.00	0.43
9:9:52:MET:HE1	9:9:85:SER:HB2	2.00	0.43
10:A:9:G:O2'	10:A:45:G:H2'	2.18	0.43
11:AA:469:VAL:HA	11:AA:472:GLU:HG2	2.00	0.43
11:AA:623:LEU:HD13	11:AA:627:GLY:HA2	2.01	0.43
11:AA:1010:GLN:C	11:AA:1010:GLN:CD	2.86	0.43
13:AC:58:GLU:HB3	13:AC:170:ARG:HG2	1.99	0.43
16:D:1417:G:C6	16:D:1482:G:C6	3.06	0.43
20:H:61:GLU:HG2	20:H:62:ILE:HG23	2.01	0.43
64:z:76:TYR:OH	64:z:92:ARG:NH1	2.51	0.43
11:AA:444:ASP:OD1	11:AA:444:ASP:N	2.46	0.43
13:AD:86:LYS:NZ	14:AE:528:THR:HB	2.33	0.43
14:AE:58:CYS:SG	14:AE:60:ARG:HG2	2.59	0.43
14:AE:515:ARG:HH12	14:AE:724:MET:HG2	1.84	0.43
14:AE:1033:GLY:HA3	14:AE:1081:VAL:O	2.18	0.43
10:B:1:C:C5	10:B:2:G:N7	2.86	0.43
10:B:22:G:H2'	10:B:23:C:C5	2.52	0.43
19:G:35:ARG:CG	20:H:10:GLU:OE2	2.63	0.43
20:H:109:THR:C	20:H:153:GLU:HA	2.43	0.43
11:AA:1329:GLU:HA	14:AE:245:LEU:HD13	2.01	0.43
14:AE:111:THR:CG2	14:AE:300:GLN:HA	2.48	0.43
14:AE:126:LEU:CD1	14:AE:223:LEU:HD22	2.49	0.43
14:AE:144:TYR:OH	14:AE:162:GLU:OE1	2.34	0.43
10:B:46:G:O2'	10:B:47:U:H5''	2.19	0.43
20:H:136:VAL:HA	20:H:168:VAL:O	2.18	0.43
37:Y:10:LEU:HD13	37:Y:10:LEU:HA	1.79	0.43
37:Y:121:ILE:HA	37:Y:124:MET:SD	2.58	0.43
39:a:39:G:H1'	50:l:43:THR:HG21	1.99	0.43
52:n:123:ASP:C	52:n:123:ASP:OD1	2.62	0.43
10:A:22:G:O2'	10:A:23:C:O5'	2.36	0.43
11:AA:300:ASP:OD1	11:AA:313:ALA:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:565:GLU:HA	11:AA:569:ILE:HG12	2.01	0.43
11:AA:726:TYR:O	11:AA:726:TYR:CD2	2.70	0.43
11:AA:959:ASP:HA	11:AA:962:GLU:HB2	2.01	0.43
13:AC:50:SER:HB3	13:AD:8:PHE:HZ	1.84	0.43
13:AC:118:ASP:HA	28:P:89:ARG:C	2.44	0.43
13:AD:57:THR:HG21	13:AD:147:GLN:HB2	1.99	0.43
14:AE:111:THR:HG21	14:AE:303:VAL:HB	1.99	0.43
14:AE:586:GLY:HA3	14:AE:612:LEU:HD11	2.01	0.43
10:B:9:G:O2'	10:B:45:G:H2'	2.18	0.43
10:B:18:G:N3	10:B:58:A:C5	2.87	0.43
10:B:22:G:O2'	10:B:23:C:O5'	2.36	0.43
39:a:68:G:N2	39:a:74:A:OP2	2.49	0.43
39:a:74:A:N7	39:a:88:G:C5	2.86	0.43
39:a:995:C:O2	57:s:3:THR:OG1	2.24	0.43
39:a:1095:A:H2'	39:a:1096:A:C8	2.54	0.43
39:a:2252:G:O2'	39:a:2253:G:H5'	2.18	0.43
48:j:172:VAL:HG11	48:j:175:LEU:HD21	2.00	0.43
54:p:24:ILE:CD1	54:p:72:LEU:HD21	2.44	0.43
8:7:-5:U:H6	8:7:-5:U:H3'	1.83	0.43
9:9:31:ARG:HE	39:a:1054:A:C5'	2.18	0.43
10:A:34:C:OP1	25:M:84:THR:OG1	2.35	0.43
11:AA:75:LEU:HD23	11:AA:94:ALA:HB3	2.00	0.43
11:AA:971:LEU:HG	11:AA:1014:LEU:HG	2.00	0.43
13:AC:159:ILE:HD13	13:AC:159:ILE:HA	1.69	0.43
14:AE:244:VAL:HA	14:AE:269:TYR:OH	2.19	0.43
16:D:842:U:H3'	16:D:843:U:C5'	2.48	0.43
36:X:23:TYR:CD2	36:X:69:LEU:HD23	2.53	0.43
39:a:1047:G:N2	39:a:1110:G:O2'	2.50	0.43
39:a:1921:G:C2'	39:a:1922:G:H5'	2.49	0.43
39:a:1932:A:H2'	39:a:1933:G:O4'	2.19	0.43
39:a:2511:U:O4	39:a:2575:C:N3	2.52	0.43
58:t:107:LEU:HD21	58:t:115:ILE:HG21	2.01	0.43
8:7:-6:U:C2	16:D:1493:A:H2	2.36	0.43
9:9:9:GLN:CD	9:9:9:GLN:C	2.85	0.43
9:9:71:CYS:CA	9:9:117:LEU:HD13	2.48	0.43
10:A:26:G:N2	10:A:45:G:N2	2.66	0.43
10:A:53:G:C2	10:A:54:U:C5	3.07	0.43
11:AA:230:PHE:HB2	11:AA:333:ILE:HB	2.01	0.43
11:AA:666:SER:HB2	11:AA:1186:VAL:HG21	2.01	0.43
11:AA:796:LEU:N	11:AA:1231:TYR:OH	2.52	0.43
11:AA:830:THR:HG22	11:AA:1234:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:839:VAL:O	11:AA:886:LYS:HD2	2.19	0.43
13:AC:47:LEU:HD23	13:AC:47:LEU:HA	1.88	0.43
14:AE:123:ARG:HA	14:AE:123:ARG:HD3	1.49	0.43
16:D:826:C:O2	26:N:16:ASN:ND2	2.52	0.43
20:H:76:GLU:HA	20:H:76:GLU:OE2	2.19	0.43
23:K:150:PRO:O	23:K:153:VAL:HG22	2.19	0.43
39:a:973:A:O4'	39:a:1188:U:C6	2.72	0.43
14:AE:824:PRO:HD3	14:AE:835:LEU:HD12	2.00	0.43
10:B:18:G:O2'	10:B:60:U:N3	2.48	0.43
15:C:12:ARG:HD3	15:C:16:GLU:OE1	2.18	0.43
16:D:429:U:O2	16:D:430:A:C8	2.72	0.43
16:D:1255:G:O2'	16:D:1258:G:N3	2.47	0.43
16:D:1371:G:O3'	27:O:71:GLY:HA3	2.19	0.43
19:G:208:ARG:NH1	20:H:29:VAL:HG11	2.34	0.43
20:H:19:ARG:CD	20:H:73:ASP:OD1	2.65	0.43
20:H:290:TYR:O	20:H:305:HIS:C	2.56	0.43
33:U:6:LEU:HG	33:U:17:TYR:HB3	2.00	0.43
45:g:37:CYS:N	45:g:40:CYS:SG	2.78	0.43
50:l:170:ARG:NH2	50:l:176:ASP:OD1	2.49	0.43
3:2:1:MET:N	39:a:142:A:O2'	2.48	0.42
4:3:12:ILE:CG2	4:3:80:ALA:HB2	2.49	0.42
7:6:18:DC:C2	8:7:17:G:N2	2.78	0.42
11:AA:484:LEU:HA	11:AA:485:ASP:HA	1.81	0.42
14:AE:201:LEU:HD11	14:AE:220:ARG:NH1	2.31	0.42
14:AE:394:ILE:O	14:AE:394:ILE:HG13	2.18	0.42
10:B:53:G:C2	10:B:54:U:C5	3.07	0.42
16:D:324:G:N2	16:D:327:A:C8	2.86	0.42
16:D:1126:U:OP1	28:P:7:ARG:NH2	2.51	0.42
16:D:1308:U:O5'	36:X:98:ARG:HG2	2.16	0.42
20:H:302:GLY:HA3	20:H:344:LEU:HD13	2.00	0.42
21:I:9:GLY:HA3	31:S:89:MET:HE3	2.01	0.42
37:Y:112:LYS:HB3	37:Y:112:LYS:NZ	2.34	0.42
38:Z:26:MET:HE2	38:Z:26:MET:HB2	1.71	0.42
39:a:1326:U:O2'	39:a:2010:G:O2'	2.35	0.42
39:a:2395:C:H2'	39:a:2396:G:O4'	2.18	0.42
9:9:125:ARG:NH1	9:9:125:ARG:CA	2.73	0.42
10:A:36:U:H2'	10:A:37:A:O4'	2.19	0.42
11:AA:55:SER:CB	11:AA:465:ARG:HH12	2.32	0.42
11:AA:68:LEU:HD11	11:AA:100:LEU:HB3	2.01	0.42
11:AA:400:VAL:HG21	11:AA:452:ARG:HE	1.84	0.42
11:AA:1018:TYR:HA	11:AA:1021:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:107:LEU:HA	14:AE:276:ASN:ND2	2.33	0.42
14:AE:319:SER:HA	14:AE:320:ASN:HA	1.64	0.42
16:D:384:G:H2'	16:D:385:C:C6	2.54	0.42
16:D:1329:A:OP1	36:X:28:THR:CA	2.67	0.42
19:G:16:PHE:CG	20:H:43:LYS:HA	2.53	0.42
20:H:110:GLY:H	20:H:153:GLU:N	2.17	0.42
20:H:152:LEU:CB	20:H:171:ARG:H	2.32	0.42
39:a:705:A:O4'	46:h:9:THR:HG21	2.19	0.42
39:a:819:A:C4	39:a:1189:A:C2	3.07	0.42
39:a:879:G:H2'	39:a:880:G:O4'	2.19	0.42
39:a:2602:A:H5''	39:a:2603:G:C5'	2.49	0.42
39:a:2683:C:O2	58:t:70:ARG:NH2	2.52	0.42
50:l:145:ASP:HA	50:l:166:LYS:HB3	2.01	0.42
9:9:72:LEU:HD22	9:9:72:LEU:O	2.19	0.42
10:A:56:C:C2	39:a:2112:G:C5	3.07	0.42
11:AA:395:TYR:HE2	11:AA:420:LEU:HG	1.84	0.42
11:AA:859:GLU:CG	21:I:110:GLU:OE1	2.67	0.42
14:AE:568:SER:HB3	14:AE:570:LYS:NZ	2.34	0.42
14:AE:609:TYR:HD2	14:AE:610:ARG:NH1	2.17	0.42
14:AE:1350:ASN:HA	14:AE:1353:VAL:HG12	2.01	0.42
16:D:537:G:OP1	30:R:110:ARG:NH2	2.48	0.42
18:F:67:ARG:HD3	18:F:67:ARG:H	1.85	0.42
20:H:119:GLY:CA	20:H:132:PRO:C	2.92	0.42
27:O:28:ILE:HD12	27:O:28:ILE:N	2.35	0.42
27:O:55:VAL:O	27:O:57:MET:N	2.52	0.42
29:Q:88:GLY:H	29:Q:114:THR:HG22	1.84	0.42
37:Y:123:ALA:HA	37:Y:126:ARG:HG3	2.00	0.42
39:a:567:U:OP2	59:u:29:LYS:NZ	2.53	0.42
39:a:631:A:N3	39:a:2415:G:O2'	2.48	0.42
64:z:65:ILE:CD1	64:z:92:ARG:HB2	2.49	0.42
8:7:13:G:H5''	8:7:13:G:H8	1.85	0.42
11:AA:998:LEU:C	11:AA:998:LEU:CD1	2.85	0.42
14:AE:271:ARG:HE	14:AE:271:ARG:HB2	1.58	0.42
14:AE:388:ARG:HG2	14:AE:388:ARG:HH11	1.84	0.42
14:AE:797:THR:HG22	14:AE:924:GLY:HA3	2.01	0.42
14:AE:820:ILE:HD11	14:AE:822:MET:HE2	2.02	0.42
16:D:662:U:O2'	16:D:836:G:OP1	2.32	0.42
16:D:1333:A:H2'	16:D:1334:G:O4'	2.19	0.42
7:6:21:DA:C6	8:7:15:G:C2	3.03	0.42
7:6:27:DG:H1'	7:6:28:DA:C5	2.55	0.42
10:A:22:G:H2'	10:A:23:C:C5	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:513:MET:HG3	14:AE:544:LEU:HD11	2.01	0.42
14:AE:616:PRO:HA	14:AE:619:ILE:HG22	2.02	0.42
14:AE:1272:SER:OG	14:AE:1273:ASP:N	2.53	0.42
15:C:44:ILE:HG21	20:H:339:ARG:HA	2.01	0.42
20:H:332:VAL:HG12	20:H:334:ASP:N	2.33	0.42
20:H:342:ILE:HG22	20:H:344:LEU:HD12	2.02	0.42
30:R:110:ARG:NH1	30:R:112:GLN:O	2.53	0.42
39:a:1020:A:C2	39:a:1141:U:C2	3.07	0.42
39:a:2615:U:C2	47:i:4:GLN:HA	2.55	0.42
46:h:240:PHE:CD2	46:h:240:PHE:O	2.73	0.42
50:l:134:LEU:HB2	50:l:160:ALA:HB1	2.02	0.42
58:t:113:MET:HE3	58:t:116:ILE:HD11	2.01	0.42
9:9:80:THR:O	39:a:1108:U:OP1	2.38	0.42
10:A:46:G:O2'	10:A:47:U:H5''	2.19	0.42
14:AE:220:ARG:NH1	14:AE:220:ARG:CG	2.82	0.42
14:AE:279:LEU:HD13	14:AE:299:LEU:HD13	2.02	0.42
39:a:1394:U:C4	39:a:1395:A:C6	3.07	0.42
46:h:37:ASN:HB2	46:h:62:TYR:HB2	2.01	0.42
62:x:99:TYR:OH	62:x:111:ARG:NH1	2.53	0.42
4:3:39:ILE:HG22	4:3:40:ASN:N	2.34	0.42
8:7:-8:U:C6	16:D:1403:C:H1'	2.55	0.42
11:AA:867:GLU:CB	21:I:75:ILE:HG13	2.49	0.42
14:AE:87:LYS:HE3	14:AE:87:LYS:CA	2.41	0.42
14:AE:820:ILE:HG12	14:AE:884:SER:HB2	2.02	0.42
15:C:12:ARG:O	15:C:16:GLU:HG3	2.19	0.42
16:D:197:A:C5	16:D:221:C:H4'	2.53	0.42
19:G:19:GLN:OE1	20:H:76:GLU:HB3	2.12	0.42
20:H:335:ILE:HG12	20:H:342:ILE:HG23	2.00	0.42
28:P:57:VAL:O	28:P:58:ASN:ND2	2.53	0.42
37:Y:102:ARG:H	37:Y:102:ARG:HG3	1.59	0.42
39:a:126:A:O5'	51:m:19:ARG:HG3	2.19	0.42
39:a:1925:C:OP2	39:a:1925:C:C6	2.73	0.42
55:q:3:VAL:HA	55:q:36:ARG:O	2.19	0.42
58:t:76:VAL:HG12	63:y:73:VAL:HB	2.01	0.42
11:AA:1026:GLU:HG3	16:D:1030:U:C4	2.48	0.42
14:AE:105:ILE:HD12	14:AE:242:LEU:CD2	2.44	0.42
14:AE:144:TYR:CE1	14:AE:162:GLU:OE1	2.73	0.42
14:AE:385:LEU:CD2	14:AE:390:LEU:HB2	2.50	0.42
14:AE:559:ALA:HB3	14:AE:562:GLU:HB3	2.01	0.42
10:B:58:A:OP2	10:B:58:A:H8	2.02	0.42
15:C:14:THR:CG2	15:C:48:ARG:HE	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:216:U:H2'	16:D:217:C:C6	2.55	0.42
20:H:274:TYR:HD1	20:H:335:ILE:HD12	1.85	0.42
23:K:136:VAL:O	23:K:140:THR:HG23	2.20	0.42
39:a:1082:U:N3	39:a:1086:A:C6	2.87	0.42
39:a:1142:A:N3	39:a:1142:A:H2'	2.34	0.42
47:i:43:ILE:HG22	47:i:49:TYR:HB2	2.01	0.42
59:u:109:LYS:HG2	59:u:126:ARG:HB2	2.01	0.42
7:6:12:DC:O5'	7:6:12:DC:H6	2.01	0.42
10:A:58:A:OP2	10:A:58:A:H8	2.02	0.42
11:AA:218:GLU:HG2	11:AA:299:LYS:HA	2.02	0.42
11:AA:888:THR:HG22	11:AA:914:LYS:HD2	2.02	0.42
11:AA:976:ARG:HA	11:AA:979:LEU:HB2	2.02	0.42
12:AB:7:LYS:HG2	12:AB:74:VAL:HG13	2.01	0.42
14:AE:47:ARG:HA	14:AE:47:ARG:NE	2.35	0.42
14:AE:839:VAL:HG12	14:AE:864:LEU:HD12	2.02	0.42
14:AE:930:LEU:HA	14:AE:1244:GLN:HG3	2.02	0.42
14:AE:1026:PRO:HB2	14:AE:1028:ILE:HG23	2.00	0.42
20:H:119:GLY:O	20:H:120:PHE:C	2.62	0.42
39:a:742:A:N1	39:a:755:U:O4	2.53	0.42
39:a:2469:A:N6	39:a:2481:G:O2'	2.52	0.42
58:t:38:ILE:HD11	58:t:112:PHE:CZ	2.54	0.42
61:w:49:GLU:HB2	61:w:50:PRO:HD3	2.01	0.42
9:9:96:PHE:HD1	9:9:96:PHE:HA	1.70	0.42
11:AA:812:PHE:HZ	14:AE:503:SER:HB2	1.85	0.42
11:AA:867:GLU:HB3	21:I:75:ILE:CG1	2.49	0.42
13:AC:79:LEU:HA	13:AC:79:LEU:HD23	1.86	0.42
14:AE:24:LEU:CD1	14:AE:232:ASN:ND2	2.82	0.42
14:AE:102:MET:HG2	14:AE:246:PRO:CG	2.49	0.42
14:AE:220:ARG:HH11	14:AE:220:ARG:CG	2.26	0.42
16:D:37:U:O2	16:D:548:G:N2	2.53	0.42
16:D:1061:G:H5'	28:P:61:ALA:HB2	2.02	0.42
16:D:1235:U:H2'	16:D:1236:A:O4'	2.20	0.42
37:Y:41:PHE:HA	37:Y:68:PHE:CE2	2.54	0.42
39:a:948:C:H1'	39:a:984:A:C8	2.55	0.42
39:a:2756:U:C4	39:a:2759:G:O6	2.72	0.42
11:AA:257:ALA:HB2	11:AA:285:ILE:HG22	2.02	0.41
11:AA:991:LYS:HD2	11:AA:991:LYS:H	1.80	0.41
14:AE:141:PHE:CD2	14:AE:297:ARG:HB2	2.54	0.41
14:AE:190:LYS:HB2	14:AE:190:LYS:HE3	1.42	0.41
10:B:60:U:OP2	10:B:61:C:N4	2.45	0.41
16:D:37:U:C4	16:D:397:A:N6	2.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:187:VAL:HG21	19:G:199:VAL:HG23	2.02	0.41
39:a:493:G:H2'	39:a:494:G:O4'	2.20	0.41
39:a:2311:A:C2	52:n:85:ILE:HD11	2.55	0.41
39:a:2803:G:H2'	39:a:2804:U:C5	2.55	0.41
2:1:92:ARG:NE	2:1:94:ASP:OD1	2.53	0.41
9:9:48:ALA:HB3	9:9:51:TYR:HD2	1.86	0.41
11:AA:69:GLN:HE21	11:AA:101:ARG:HD2	1.85	0.41
11:AA:488:MET:O	11:AA:490:GLN:N	2.47	0.41
11:AA:844:LYS:HD3	11:AA:844:LYS:HA	1.48	0.41
11:AA:914:LYS:C	11:AA:914:LYS:HE3	2.45	0.41
11:AA:1009:ASN:ND2	11:AA:1012:GLU:HB3	2.35	0.41
13:AC:231:PHE:HE2	13:AD:39:LEU:HD13	1.84	0.41
13:AD:207:THR:OG1	13:AD:208:ASN:N	2.52	0.41
10:B:26:G:C2	10:B:45:G:N2	2.89	0.41
31:S:41:ARG:O	31:S:45:VAL:HG12	2.20	0.41
39:a:1570:A:H2'	39:a:1571:A:C8	2.55	0.41
39:a:2788:C:H2'	39:a:2789:C:C6	2.55	0.41
46:h:119:GLY:O	46:h:130:LEU:HB3	2.20	0.41
54:p:52:PHE:CZ	54:p:72:LEU:HD22	2.56	0.41
6:5:98:DA:C2'	6:5:99:DT:C7	2.96	0.41
8:7:13:G:H8	8:7:13:G:C5'	2.33	0.41
9:9:31:ARG:HD3	39:a:1054:A:H4'	1.96	0.41
10:A:56:C:OP1	39:a:2168:G:N3	2.53	0.41
11:AA:933:VAL:O	11:AA:933:VAL:CG1	2.68	0.41
11:AA:1020:GLU:HA	11:AA:1023:HIS:CD2	2.56	0.41
13:AD:152:TYR:HE2	14:AE:535:ARG:HH21	1.68	0.41
14:AE:1050:THR:HG23	14:AE:1057:SER:HB3	2.03	0.41
16:D:946:A:O2'	16:D:1333:A:N3	2.51	0.41
18:F:32:VAL:HG11	29:Q:89:PRO:HG3	2.01	0.41
20:H:155:LYS:O	20:H:169:SER:CB	2.69	0.41
22:J:48:LEU:HD13	22:J:48:LEU:N	2.33	0.41
23:K:133:PRO:HA	23:K:136:VAL:HG12	2.02	0.41
32:T:43:PHE:CE2	32:T:56:LEU:HD22	2.55	0.41
37:Y:78:LEU:CD1	37:Y:108:ILE:HG22	2.50	0.41
38:Z:23:ILE:HD12	38:Z:23:ILE:HA	1.77	0.41
39:a:36:G:N3	39:a:450:G:O2'	2.53	0.41
39:a:244:A:OP2	53:o:8:ARG:NH2	2.50	0.41
39:a:299:A:N1	39:a:322:A:O2'	2.47	0.41
39:a:548:G:H3'	39:a:549:G:O4'	2.20	0.41
39:a:984:A:H2'	39:a:984:A:N3	2.35	0.41
9:9:61:ARG:C	9:9:65:GLU:HB2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:71:CYS:SG	9:9:117:LEU:HB2	2.60	0.41
10:A:34:C:H41	25:M:83:SER:HA	1.86	0.41
39:a:1548:A:H2'	39:a:1549:A:C8	2.55	0.41
39:a:2298:A:C5	39:a:2321:U:C4	3.09	0.41
46:h:76:ALA:HB2	46:h:96:TYR:CE1	2.56	0.41
8:7:-9:G:C5'	16:D:1501:C:H41	2.33	0.41
10:A:26:G:C2	10:A:45:G:N2	2.89	0.41
11:AA:211:ARG:HH21	11:AA:351:LEU:HD22	1.86	0.41
13:AC:120:ASP:OD1	28:P:90:LEU:HD21	2.20	0.41
14:AE:233:LYS:HA	14:AE:234:PRO:HD3	1.89	0.41
14:AE:239:LEU:N	14:AE:239:LEU:HD23	2.36	0.41
10:B:46:G:H2'	10:B:47:U:OP2	2.21	0.41
16:D:622:A:C8	16:D:623:C:C6	3.08	0.41
16:D:860:A:H2'	16:D:861:G:O4'	2.21	0.41
16:D:1323:G:H2'	16:D:1324:A:C8	2.54	0.41
16:D:1330:U:OP2	36:X:26:GLY:HA3	2.21	0.41
39:a:1028:A:N6	39:a:1125:G:H2'	2.34	0.41
39:a:1565:C:O2'	39:a:1567:G:N7	2.48	0.41
57:s:32:LEU:HD23	57:s:54:ILE:HD13	2.01	0.41
11:AA:452:ARG:NH1	11:AA:458:GLU:OE2	2.52	0.41
11:AA:529:ARG:HH22	11:AA:687:ARG:HH11	1.66	0.41
11:AA:953:LEU:HA	11:AA:953:LEU:HD13	1.83	0.41
13:AD:111:THR:OG1	13:AD:126:PRO:O	2.35	0.41
16:D:218:U:H2'	16:D:219:U:O4'	2.21	0.41
16:D:977:A:H1'	16:D:982:U:O4	2.20	0.41
19:G:47:VAL:N	19:G:48:PRO:HD2	2.34	0.41
39:a:1169:A:H5''	39:a:1169:A:N3	2.36	0.41
39:a:1406:U:C2'	39:a:1407:G:OP2	2.69	0.41
39:a:1839:G:C4	39:a:1927:A:C5	3.08	0.41
64:z:66:ASN:OD1	64:z:70:ARG:NE	2.54	0.41
9:9:25:ALA:HA	9:9:96:PHE:HE1	1.85	0.41
10:A:26:G:H1	10:A:44:A:N6	2.18	0.41
11:AA:960:LEU:HD21	11:AA:1028:LYS:HB3	2.02	0.41
11:AA:1252:SER:N	11:AA:1259:LEU:HD13	2.35	0.41
11:AA:1286:THR:O	11:AA:1290:MET:HB2	2.21	0.41
13:AC:158:ARG:HH12	13:AC:172:LEU:HD23	1.86	0.41
14:AE:47:ARG:NE	14:AE:47:ARG:CA	2.84	0.41
14:AE:245:LEU:CG	14:AE:246:PRO:HD2	2.47	0.41
14:AE:390:LEU:N	14:AE:390:LEU:HD13	2.35	0.41
14:AE:576:ARG:HD3	14:AE:593:ASN:HA	2.03	0.41
14:AE:1289:ASN:O	14:AE:1293:GLU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:15:G:H1	10:B:20:U:H3	1.68	0.41
16:D:429:U:O2	16:D:430:A:N7	2.53	0.41
16:D:502:A:H2'	16:D:503:C:O4'	2.20	0.41
16:D:580:C:H2'	16:D:581:G:O4'	2.21	0.41
20:H:292:CYS:SG	20:H:304:VAL:HB	2.60	0.41
23:K:144:LEU:HD23	23:K:144:LEU:HA	1.95	0.41
37:Y:35:MET:O	37:Y:35:MET:SD	2.79	0.41
39:a:2294:G:OP1	62:x:10:ARG:HD3	2.21	0.41
8:7:-2:U:O2	8:7:-2:U:H3'	2.20	0.41
10:A:15:G:N2	10:A:20:U:C2	2.89	0.41
14:AE:109:SER:CB	14:AE:296:LYS:HG2	2.51	0.41
10:B:7:G:O6	10:B:49:G:O6	2.39	0.41
16:D:548:G:C6	16:D:549:C:C4	3.08	0.41
37:Y:85:ILE:H	37:Y:85:ILE:CD1	2.28	0.41
39:a:17:G:H2'	39:a:18:U:C6	2.56	0.41
39:a:1082:U:H3	39:a:1086:A:N6	2.15	0.41
39:a:1182:G:H2'	39:a:1183:U:O4'	2.21	0.41
39:a:1250:G:OP2	59:u:21:ARG:NH2	2.52	0.41
42:d:8:C:O3'	62:x:25:ARG:NH1	2.50	0.41
6:5:108:DT:C7	11:AA:199:ASP:HB3	2.45	0.41
8:7:20:G:H21	14:AE:427:PRO:HD3	1.86	0.41
9:9:57:ASN:CG	9:9:62:ARG:HG3	2.30	0.41
10:A:8:U:OP2	10:A:8:U:H6	2.04	0.41
10:A:15:G:H1	10:A:20:U:H3	1.68	0.41
11:AA:56:VAL:HG11	11:AA:468:LEU:HD13	2.02	0.41
11:AA:593:LYS:HB3	11:AA:602:GLU:HG3	2.02	0.41
11:AA:1034:ARG:HG2	11:AA:1034:ARG:NH1	2.25	0.41
11:AA:1251:TYR:CE2	11:AA:1301:ARG:NH1	2.88	0.41
14:AE:68:TYR:CB	14:AE:75:TYR:HE2	2.34	0.41
14:AE:136:GLU:OE1	14:AE:312:ARG:NH2	2.53	0.41
14:AE:201:LEU:CB	14:AE:221:ILE:HD13	2.47	0.41
14:AE:242:LEU:C	14:AE:242:LEU:HD23	2.44	0.41
14:AE:395:LYS:HB3	14:AE:395:LYS:HE3	1.45	0.41
14:AE:848:VAL:HB	14:AE:858:VAL:HG22	2.02	0.41
14:AE:923:ILE:O	14:AE:1241:TYR:OH	2.31	0.41
16:D:152:A:N6	16:D:170:U:C2	2.89	0.41
16:D:421:U:O2	16:D:421:U:O4'	2.36	0.41
16:D:712:A:H2'	16:D:713:G:O4'	2.21	0.41
21:I:112:ASP:HB3	21:I:115:LEU:HD12	2.03	0.41
25:M:22:LEU:HD13	25:M:97:ASN:ND2	2.35	0.41
36:X:16:VAL:HG13	36:X:34:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Y:100:ILE:HB	37:Y:101:SER:H	1.71	0.41
39:a:67:U:C2	39:a:74:A:N6	2.89	0.41
39:a:126:A:OP1	51:m:45:SER:OG	2.38	0.41
39:a:1082:U:C4	39:a:1086:A:N6	2.88	0.41
39:a:2314:A:O2'	52:n:155:THR:HG22	2.21	0.41
50:l:149:ILE:HD11	50:l:188:MET:HE3	2.02	0.41
10:A:46:G:H2'	10:A:47:U:OP2	2.21	0.41
11:AA:26:TYR:HE2	11:AA:32:LEU:HD12	1.86	0.41
11:AA:936:ARG:HH21	11:AA:936:ARG:HG3	1.86	0.41
14:AE:144:TYR:N	14:AE:144:TYR:CD1	2.88	0.41
16:D:915:A:C8	16:D:915:A:C3'	3.04	0.41
16:D:1189:U:OP1	31:S:98:LYS:NZ	2.55	0.41
16:D:1225:A:H2'	16:D:1226:C:C5	2.56	0.41
20:H:110:GLY:N	20:H:153:GLU:HA	2.36	0.41
27:O:10:GLY:HA3	27:O:78:ALA:O	2.21	0.41
37:Y:72:THR:OG1	37:Y:73:PRO:CD	2.62	0.41
37:Y:122:GLU:O	37:Y:122:GLU:HG2	2.21	0.41
37:Y:133:ARG:HG3	37:Y:136:GLY:HA2	2.03	0.41
39:a:320:A:H2'	50:l:131:THR:HG21	2.01	0.41
39:a:1921:G:O5'	39:a:1921:G:C8	2.70	0.41
2:1:75:PHE:CZ	2:1:104:THR:HG21	2.56	0.40
7:6:21:DA:H5''	11:AA:141:THR:HG21	2.03	0.40
9:9:8:LYS:NZ	39:a:1046:A:N6	2.69	0.40
9:9:118:ILE:H	9:9:119:PRO:HD2	1.85	0.40
10:A:7:G:O6	10:A:49:G:O6	2.39	0.40
11:AA:805:MET:HE3	11:AA:805:MET:HB2	1.87	0.40
11:AA:855:PRO:O	11:AA:857:VAL:N	2.55	0.40
11:AA:968:GLU:HG3	11:AA:972:PHE:CZ	2.56	0.40
12:AB:8:ARG:HH11	12:AB:8:ARG:HD3	1.75	0.40
14:AE:137:ARG:HA	14:AE:142:GLU:HG2	2.02	0.40
14:AE:950:ILE:HB	14:AE:1018:ALA:HB3	2.01	0.40
10:B:8:U:OP2	10:B:8:U:H6	2.04	0.40
10:B:37:A:H5''	10:B:37:A:C4	2.56	0.40
16:D:915:A:C6	16:D:916:U:C4	3.09	0.40
16:D:1370:G:C2	16:D:1371:G:C8	3.09	0.40
46:h:29:PRO:HG2	46:h:34:LEU:HD11	2.03	0.40
46:h:175:ARG:NH1	46:h:181:MET:HE2	2.36	0.40
48:j:175:LEU:CD1	48:j:193:VAL:HG12	2.51	0.40
61:w:67:PHE:O	61:w:71:ARG:HG2	2.21	0.40
64:z:83:LEU:HD23	64:z:83:LEU:HA	1.92	0.40
3:2:46:ALA:O	3:2:50:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:31:ARG:HD3	9:9:31:ARG:HA	1.92	0.40
11:AA:104:ILE:HD11	11:AA:116:ASP:HB2	2.02	0.40
11:AA:801:ARG:HH12	11:AA:1119:MET:HE1	1.86	0.40
11:AA:958:LYS:NZ	11:AA:962:GLU:HG2	2.36	0.40
13:AD:111:THR:OG1	13:AD:112:ALA:N	2.54	0.40
14:AE:647:PRO:HG3	14:AE:697:MET:HB3	2.02	0.40
10:B:26:G:H1	10:B:44:A:N6	2.18	0.40
16:D:890:G:O2'	16:D:906:A:N6	2.55	0.40
16:D:1368:A:OP1	27:O:113:ARG:NH2	2.54	0.40
23:K:150:PRO:HA	23:K:153:VAL:HG22	2.03	0.40
36:X:4:ILE:CG1	36:X:9:ILE:HD12	2.50	0.40
37:Y:7:TYR:HB2	37:Y:57:VAL:CG2	2.51	0.40
39:a:476:G:H4'	39:a:502:A:N1	2.35	0.40
39:a:2223:G:O2'	46:h:265:LYS:NZ	2.49	0.40
50:l:48:THR:HG23	50:l:86:ALA:HB3	2.02	0.40
51:m:12:ARG:CG	51:m:44:VAL:HG11	2.50	0.40
54:p:25:THR:HG22	54:p:34:THR:HG23	2.02	0.40
62:x:53:THR:HG23	62:x:74:VAL:HG21	2.03	0.40
9:9:67:THR:N	9:9:68:PRO:HD2	2.36	0.40
11:AA:590:PRO:HB2	11:AA:655:VAL:HG21	2.04	0.40
11:AA:867:GLU:N	21:l:75:ILE:CG1	2.85	0.40
11:AA:978:VAL:HG11	11:AA:1010:GLN:CG	2.51	0.40
11:AA:1029:LEU:HD21	11:AA:1033:ARG:CZ	2.51	0.40
13:AC:43:LEU:HD23	13:AC:43:LEU:HA	1.95	0.40
13:AD:228:LEU:HA	13:AD:228:LEU:HD23	1.89	0.40
14:AE:113:HIS:ND1	14:AE:115:TRP:HB2	2.37	0.40
14:AE:390:LEU:HD13	14:AE:390:LEU:H	1.86	0.40
14:AE:442:ILE:HA	14:AE:442:ILE:HD13	1.88	0.40
14:AE:515:ARG:HH21	14:AE:717:VAL:HG23	1.87	0.40
16:D:563:A:C2	16:D:884:U:O4	2.62	0.40
16:D:1526:G:P	18:F:42:THR:HG23	2.61	0.40
19:G:28:LYS:N	19:G:29:PRO:CD	2.85	0.40
37:Y:102:ARG:HD2	37:Y:103:ALA:N	2.36	0.40
39:a:5:A:H2'	39:a:6:A:C8	2.56	0.40
39:a:125:A:OP2	51:m:19:ARG:NH2	2.50	0.40
39:a:2602:A:H5''	39:a:2603:G:H5''	2.03	0.40
39:a:2806:C:H2'	39:a:2807:U:O4'	2.22	0.40
3:2:63:VAL:HG21	3:2:80:TRP:CZ2	2.57	0.40
8:7:-9:G:C5'	16:D:1501:C:N4	2.83	0.40
9:9:73:LYS:CB	9:9:117:LEU:HD11	2.51	0.40
11:AA:6:THR:HA	11:AA:9:LYS:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:1253:LEU:CD1	14:AE:253:VAL:CG1	2.95	0.40
13:AD:97:GLU:HG3	13:AD:147:GLN:HG2	2.03	0.40
13:AD:154:PRO:HG2	13:AD:157:THR:HG22	2.04	0.40
14:AE:111:THR:HG23	14:AE:300:GLN:HA	2.03	0.40
14:AE:182:ALA:HB1	14:AE:238:ILE:CG2	2.52	0.40
22:J:100:ASN:OD1	22:J:111:ARG:NH1	2.54	0.40
28:P:22:THR:HA	28:P:25:ILE:HG22	2.04	0.40
37:Y:128:ILE:N	37:Y:128:ILE:HD13	2.37	0.40
39:a:2273:A:H2'	39:a:2274:A:C8	2.55	0.40
39:a:2572:A:N7	48:j:150:GLN:NE2	2.69	0.40
42:d:89:U:O2	42:d:89:U:O4'	2.40	0.40
50:l:188:MET:HE2	50:l:193:VAL:HA	2.03	0.40
52:n:122:PHE:CZ	52:n:167:ARG:HA	2.56	0.40
57:s:104:ALA:O	57:s:108:MET:HG3	2.22	0.40
59:u:74:THR:HG22	59:u:107:PHE:HB2	2.04	0.40
60:v:73:ILE:HG21	60:v:91:TYR:CZ	2.55	0.40
10:A:26:G:H2'	10:A:27:U:C6	2.57	0.40
11:AA:810:TYR:CE1	11:AA:1078:LYS:HD2	2.57	0.40
11:AA:839:VAL:HG12	11:AA:1048:LYS:O	2.22	0.40
11:AA:868:SER:OG	11:AA:941:LYS:HB2	2.21	0.40
11:AA:940:GLU:O	11:AA:940:GLU:CG	2.69	0.40
11:AA:1120:ALA:HB1	11:AA:1198:LEU:HG	2.04	0.40
14:AE:68:TYR:O	14:AE:75:TYR:CD2	2.70	0.40
16:D:791:G:N2	16:D:1497:G:O3'	2.53	0.40
39:a:197:A:N6	39:a:2430:A:H2'	2.36	0.40
39:a:1406:U:O2'	39:a:1407:G:OP2	2.39	0.40
39:a:1421:G:C2	39:a:1422:G:C8	3.09	0.40
41:c:33:LEU:O	41:c:34:HIS:CG	2.75	0.40
57:s:114:LEU:HA	57:s:114:LEU:HD12	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	12	43
2	1	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
3	2	92/100 (92%)	90 (98%)	2 (2%)	0	100	100
4	3	101/104 (97%)	96 (95%)	4 (4%)	1 (1%)	12	43
5	4	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
9	9	146/165 (88%)	95 (65%)	37 (25%)	14 (10%)	0	7
11	AA	1318/1342 (98%)	1149 (87%)	137 (10%)	32 (2%)	4	29
12	AB	94/181 (52%)	88 (94%)	6 (6%)	0	100	100
13	AC	228/329 (69%)	215 (94%)	11 (5%)	2 (1%)	14	45
13	AD	226/329 (69%)	212 (94%)	13 (6%)	1 (0%)	30	60
14	AE	1329/1358 (98%)	1200 (90%)	120 (9%)	9 (1%)	18	50
15	C	64/75 (85%)	63 (98%)	1 (2%)	0	100	100
17	E	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
18	F	68/71 (96%)	68 (100%)	0	0	100	100
19	G	223/241 (92%)	210 (94%)	13 (6%)	0	100	100
20	H	255/557 (46%)	188 (74%)	55 (22%)	12 (5%)	2	18
21	I	206/233 (88%)	196 (95%)	9 (4%)	1 (0%)	24	56
22	J	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
23	K	154/167 (92%)	146 (95%)	7 (4%)	1 (1%)	21	52
24	L	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	12	43
25	M	149/179 (83%)	144 (97%)	4 (3%)	1 (1%)	18	50
26	N	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	16	48
27	O	125/130 (96%)	115 (92%)	9 (7%)	1 (1%)	16	48
28	P	97/103 (94%)	88 (91%)	8 (8%)	1 (1%)	12	43
29	Q	115/129 (89%)	104 (90%)	9 (8%)	2 (2%)	7	34
30	R	117/124 (94%)	116 (99%)	1 (1%)	0	100	100
31	S	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
32	T	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
33	U	80/82 (98%)	76 (95%)	3 (4%)	1 (1%)	9	38
34	V	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
35	W	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
36	X	114/118 (97%)	107 (94%)	5 (4%)	2 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	Y	139/142 (98%)	102 (73%)	25 (18%)	12 (9%)	0	8
38	Z	28/121 (23%)	19 (68%)	7 (25%)	2 (7%)	1	12
40	b	74/85 (87%)	69 (93%)	5 (7%)	0	100	100
41	c	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
43	e	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
44	f	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
45	g	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
46	h	269/273 (98%)	259 (96%)	9 (3%)	1 (0%)	30	60
47	i	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
48	j	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
49	k	50/55 (91%)	50 (100%)	0	0	100	100
50	l	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	24	56
51	m	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
52	n	175/179 (98%)	162 (93%)	11 (6%)	2 (1%)	11	42
53	o	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
54	p	173/177 (98%)	161 (93%)	12 (7%)	0	100	100
55	q	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
56	r	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
57	s	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
58	t	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
59	u	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
60	v	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
61	w	117/127 (92%)	107 (92%)	10 (8%)	0	100	100
62	x	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
63	y	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
64	z	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	14	45
All	All	9368/10437 (90%)	8605 (92%)	660 (7%)	103 (1%)	14	42

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	9	88	HIS
11	AA	596	ASP

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Mol	Chain	Res	Type
11	AA	853	ASP
11	AA	859	GLU
11	AA	862	LEU
11	AA	873	ILE
11	AA	937	ASP
11	AA	993	PRO
20	H	139	ARG
20	H	153	GLU
20	H	169	SER
20	H	306	VAL
20	H	340	ARG
27	O	56	ASP
36	X	103	LYS
37	Y	48	ILE
9	9	33	VAL
9	9	119	PRO
11	AA	375	PRO
11	AA	856	ASN
11	AA	870	ILE
11	AA	940	GLU
11	AA	985	GLU
11	AA	1003	THR
11	AA	1158	LYS
14	AE	175	GLU
20	H	108	VAL
20	H	309	MET
20	H	333	LEU
37	Y	93	ASN
46	h	158	ALA
50	l	142	ALA
64	z	3	ARG
9	9	48	ALA
9	9	91	ALA
9	9	118	ILE
9	9	130	PRO
11	AA	376	PRO
11	AA	723	VAL
11	AA	728	ASP
11	AA	935	THR
11	AA	980	VAL
11	AA	1005	GLU
11	AA	1045	GLY

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Mol	Chain	Res	Type
13	AC	164	ASP
14	AE	51	PRO
14	AE	805	GLN
20	H	76	GLU
20	H	142	ARG
28	P	58	ASN
29	Q	119	ASN
36	X	105	ASN
37	Y	20	SER
37	Y	64	ARG
37	Y	106	GLN
9	9	69	PHE
9	9	73	LYS
9	9	108	VAL
9	9	129	LEU
9	9	133	GLU
11	AA	850	ILE
11	AA	943	LYS
11	AA	995	ASP
13	AC	165	GLU
14	AE	174	ASP
14	AE	193	ASP
21	I	80	LYS
25	M	130	ASN
37	Y	83	ALA
38	Z	21	GLU
52	n	40	VAL
11	AA	917	SER
11	AA	991	LYS
11	AA	997	TRP
11	AA	1044	PRO
14	AE	91	GLU
20	H	70	VAL
20	H	82	THR
37	Y	22	PRO
37	Y	71	LYS
37	Y	89	SER
38	Z	7	ILE
4	3	39	ILE
9	9	28	ALA
13	AD	210	THR
14	AE	49	PHE

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Mol	Chain	Res	Type
14	AE	73	GLY
14	AE	904	ALA
37	Y	62	ALA
24	L	96	VAL
37	Y	23	VAL
37	Y	100	ILE
1	0	44	GLY
11	AA	697	LYS
11	AA	1159	VAL
11	AA	1317	PRO
23	K	44	GLY
29	Q	74	VAL
33	U	64	GLY
9	9	54	VAL
52	n	62	GLY
11	AA	933	VAL
26	N	75	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	84/84 (100%)	76 (90%)	8 (10%)	8	31
2	1	93/93 (100%)	86 (92%)	7 (8%)	12	39
3	2	81/84 (96%)	77 (95%)	4 (5%)	22	48
4	3	84/85 (99%)	79 (94%)	5 (6%)	17	44
5	4	78/78 (100%)	75 (96%)	3 (4%)	29	53
9	9	112/123 (91%)	63 (56%)	49 (44%)	0	0
11	AA	1140/1157 (98%)	1027 (90%)	113 (10%)	7	30
12	AB	86/158 (54%)	85 (99%)	1 (1%)	63	72
13	AC	198/286 (69%)	183 (92%)	15 (8%)	12	38
13	AD	196/286 (68%)	193 (98%)	3 (2%)	57	68
14	AE	1120/1134 (99%)	1046 (93%)	74 (7%)	15	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	C	57/65 (88%)	55 (96%)	2 (4%)	32	54
17	E	65/66 (98%)	61 (94%)	4 (6%)	16	44
18	F	60/61 (98%)	57 (95%)	3 (5%)	22	48
19	G	187/199 (94%)	174 (93%)	13 (7%)	14	41
20	H	137/461 (30%)	124 (90%)	13 (10%)	8	31
21	I	171/190 (90%)	163 (95%)	8 (5%)	23	48
22	J	172/173 (99%)	164 (95%)	8 (5%)	23	48
23	K	119/126 (94%)	111 (93%)	8 (7%)	15	42
24	L	91/116 (78%)	84 (92%)	7 (8%)	12	38
25	M	124/147 (84%)	113 (91%)	11 (9%)	9	33
26	N	104/105 (99%)	101 (97%)	3 (3%)	37	57
27	O	105/107 (98%)	99 (94%)	6 (6%)	18	45
28	P	86/90 (96%)	77 (90%)	9 (10%)	6	28
29	Q	90/99 (91%)	88 (98%)	2 (2%)	45	63
30	R	101/104 (97%)	95 (94%)	6 (6%)	18	44
31	S	83/84 (99%)	79 (95%)	4 (5%)	23	48
32	T	76/77 (99%)	65 (86%)	11 (14%)	3	17
33	U	65/65 (100%)	60 (92%)	5 (8%)	12	38
34	V	74/78 (95%)	71 (96%)	3 (4%)	27	52
35	W	72/79 (91%)	66 (92%)	6 (8%)	10	35
36	X	94/96 (98%)	87 (93%)	7 (7%)	13	39
37	Y	109/110 (99%)	69 (63%)	40 (37%)	0	1
38	Z	26/85 (31%)	10 (38%)	16 (62%)	0	0
40	b	58/63 (92%)	57 (98%)	1 (2%)	53	67
41	c	67/68 (98%)	64 (96%)	3 (4%)	24	49
43	e	54/55 (98%)	51 (94%)	3 (6%)	19	46
44	f	48/49 (98%)	43 (90%)	5 (10%)	7	28
45	g	59/62 (95%)	54 (92%)	5 (8%)	10	35
46	h	216/218 (99%)	199 (92%)	17 (8%)	11	37
47	i	47/48 (98%)	41 (87%)	6 (13%)	4	21
48	j	164/164 (100%)	156 (95%)	8 (5%)	22	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	k	47/49 (96%)	44 (94%)	3 (6%)	16	43
50	l	165/165 (100%)	151 (92%)	14 (8%)	10	35
51	m	38/38 (100%)	36 (95%)	2 (5%)	20	46
52	n	148/150 (99%)	130 (88%)	18 (12%)	5	22
53	o	51/52 (98%)	47 (92%)	4 (8%)	11	37
54	p	136/138 (99%)	130 (96%)	6 (4%)	25	50
55	q	34/34 (100%)	31 (91%)	3 (9%)	9	33
56	r	114/114 (100%)	102 (90%)	12 (10%)	6	28
57	s	116/116 (100%)	106 (91%)	10 (9%)	10	34
58	t	104/104 (100%)	98 (94%)	6 (6%)	18	45
59	u	103/103 (100%)	96 (93%)	7 (7%)	14	42
60	v	109/109 (100%)	105 (96%)	4 (4%)	30	54
61	w	99/103 (96%)	91 (92%)	8 (8%)	11	36
62	x	86/87 (99%)	80 (93%)	6 (7%)	14	41
63	y	99/100 (99%)	91 (92%)	8 (8%)	11	36
64	z	89/90 (99%)	85 (96%)	4 (4%)	24	49
All	All	7791/8630 (90%)	7151 (92%)	640 (8%)	13	36

All (640) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	10	LYS
1	0	38	VAL
1	0	47	VAL
1	0	48	LYS
1	0	51	VAL
1	0	68	ARG
1	0	86	GLN
1	0	96	VAL
2	1	19	LEU
2	1	30	SER
2	1	41	LYS
2	1	69	LEU
2	1	97	LEU
2	1	107	VAL
2	1	110	ARG

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Mol	Chain	Res	Type
3	2	1	MET
3	2	24	MET
3	2	37	ASP
3	2	93	LEU
4	3	52	LEU
4	3	70	VAL
4	3	72	ILE
4	3	99	ASN
4	3	101	GLU
5	4	40	ILE
5	4	69	GLU
5	4	71	LYS
9	9	1	MET
9	9	3	LEU
9	9	4	ASN
9	9	5	LEU
9	9	6	GLN
9	9	7	ASP
9	9	11	ILE
9	9	14	GLU
9	9	23	LEU
9	9	24	SER
9	9	27	VAL
9	9	31	ARG
9	9	33	VAL
9	9	34	THR
9	9	35	VAL
9	9	36	ASP
9	9	37	LYS
9	9	39	THR
9	9	42	ARG
9	9	43	LYS
9	9	52	MET
9	9	54	VAL
9	9	55	VAL
9	9	56	ARG
9	9	57	ASN
9	9	61	ARG
9	9	69	PHE
9	9	70	GLU
9	9	71	CYS
9	9	72	LEU

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Mol	Chain	Res	Type
9	9	73	LYS
9	9	81	LEU
9	9	86	MET
9	9	94	ARG
9	9	96	PHE
9	9	98	GLU
9	9	106	PHE
9	9	107	GLU
9	9	109	LYS
9	9	113	PHE
9	9	117	LEU
9	9	122	GLN
9	9	123	ILE
9	9	125	ARG
9	9	133	GLU
9	9	134	GLU
9	9	138	ARG
9	9	142	THR
9	9	143	MET
11	AA	39	ILE
11	AA	145	ILE
11	AA	376	PRO
11	AA	615	VAL
11	AA	723	VAL
11	AA	727	VAL
11	AA	728	ASP
11	AA	731	ARG
11	AA	732	ILE
11	AA	752	ASN
11	AA	753	LEU
11	AA	802	VAL
11	AA	817	LEU
11	AA	840	SER
11	AA	844	LYS
11	AA	845	LEU
11	AA	851	THR
11	AA	854	ILE
11	AA	855	PRO
11	AA	857	VAL
11	AA	862	LEU
11	AA	864	LYS
11	AA	865	LEU

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Mol	Chain	Res	Type
11	AA	866	ASP
11	AA	867	GLU
11	AA	868	SER
11	AA	871	VAL
11	AA	873	ILE
11	AA	876	GLU
11	AA	884	VAL
11	AA	886	LYS
11	AA	887	VAL
11	AA	890	LYS
11	AA	912	ASP
11	AA	913	VAL
11	AA	914	LYS
11	AA	918	LEU
11	AA	933	VAL
11	AA	936	ARG
11	AA	939	VAL
11	AA	941	LYS
11	AA	943	LYS
11	AA	944	ARG
11	AA	946	LEU
11	AA	947	GLU
11	AA	949	GLU
11	AA	950	GLU
11	AA	951	MET
11	AA	952	GLN
11	AA	953	LEU
11	AA	954	LYS
11	AA	955	GLN
11	AA	957	LYS
11	AA	958	LYS
11	AA	959	ASP
11	AA	960	LEU
11	AA	962	GLU
11	AA	963	GLU
11	AA	964	LEU
11	AA	965	GLN
11	AA	967	LEU
11	AA	968	GLU
11	AA	971	LEU
11	AA	973	SER
11	AA	974	ARG

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Mol	Chain	Res	Type
11	AA	979	LEU
11	AA	980	VAL
11	AA	985	GLU
11	AA	988	LYS
11	AA	989	LEU
11	AA	991	LYS
11	AA	992	LEU
11	AA	994	ARG
11	AA	995	ASP
11	AA	997	TRP
11	AA	998	LEU
11	AA	999	GLU
11	AA	1002	LEU
11	AA	1005	GLU
11	AA	1006	GLU
11	AA	1008	GLN
11	AA	1009	ASN
11	AA	1013	GLN
11	AA	1014	LEU
11	AA	1019	ASP
11	AA	1020	GLU
11	AA	1023	HIS
11	AA	1024	GLU
11	AA	1025	PHE
11	AA	1026	GLU
11	AA	1027	LYS
11	AA	1029	LEU
11	AA	1032	LYS
11	AA	1034	ARG
11	AA	1035	LYS
11	AA	1037	THR
11	AA	1038	GLN
11	AA	1041	ASP
11	AA	1042	LEU
11	AA	1046	VAL
11	AA	1047	LEU
11	AA	1048	LYS
11	AA	1076	ILE
11	AA	1151	LEU
11	AA	1159	VAL
11	AA	1248	THR
11	AA	1250	SER

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Mol	Chain	Res	Type
11	AA	1252	SER
11	AA	1253	LEU
11	AA	1254	VAL
11	AA	1256	GLN
11	AA	1259	LEU
11	AA	1298	VAL
12	AB	47	GLU
13	AC	62	ASP
13	AC	65	LEU
13	AC	72	GLU
13	AC	91	ARG
13	AC	134	THR
13	AC	158	ARG
13	AC	159	ILE
13	AC	160	HIS
13	AC	162	GLU
13	AC	163	GLU
13	AC	165	GLU
13	AC	166	ARG
13	AC	168	ILE
13	AC	170	ARG
13	AC	171	LEU
13	AD	110	VAL
13	AD	187	VAL
13	AD	208	ASN
14	AE	40	LYS
14	AE	42	GLU
14	AE	44	ILE
14	AE	46	TYR
14	AE	47	ARG
14	AE	49	PHE
14	AE	50	LYS
14	AE	52	GLU
14	AE	53	ARG
14	AE	54	ASP
14	AE	56	LEU
14	AE	60	ARG
14	AE	66	LYS
14	AE	67	ASP
14	AE	70	CYS
14	AE	74	LYS
14	AE	76	LYS

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Mol	Chain	Res	Type
14	AE	78	LEU
14	AE	80	HIS
14	AE	81	ARG
14	AE	87	LYS
14	AE	88	CYS
14	AE	91	GLU
14	AE	94	GLN
14	AE	95	THR
14	AE	96	LYS
14	AE	99	ARG
14	AE	100	GLU
14	AE	114	ILE
14	AE	117	LEU
14	AE	119	SER
14	AE	123	ARG
14	AE	132	LEU
14	AE	135	ILE
14	AE	142	GLU
14	AE	144	TYR
14	AE	145	VAL
14	AE	146	VAL
14	AE	147	ILE
14	AE	152	THR
14	AE	154	LEU
14	AE	157	GLN
14	AE	159	ILE
14	AE	175	GLU
14	AE	180	MET
14	AE	190	LYS
14	AE	193	ASP
14	AE	196	GLN
14	AE	210	SER
14	AE	212	THR
14	AE	216	LYS
14	AE	222	LYS
14	AE	223	LEU
14	AE	227	PHE
14	AE	233	LYS
14	AE	237	MET
14	AE	238	ILE
14	AE	239	LEU
14	AE	240	THR

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Mol	Chain	Res	Type
14	AE	244	VAL
14	AE	271	ARG
14	AE	324	LEU
14	AE	385	LEU
14	AE	386	GLU
14	AE	387	LEU
14	AE	390	LEU
14	AE	393	THR
14	AE	394	ILE
14	AE	395	LYS
14	AE	506	VAL
14	AE	514	THR
14	AE	839	VAL
14	AE	1172	LYS
14	AE	1233	ILE
15	C	33	ILE
15	C	74	HIS
17	E	6	SER
17	E	10	ARG
17	E	48	GLN
17	E	64	LYS
18	F	34	ARG
18	F	62	ARG
18	F	67	ARG
19	G	8	ASP
19	G	45	LYS
19	G	59	LYS
19	G	105	LYS
19	G	108	ARG
19	G	117	LEU
19	G	128	LYS
19	G	129	LEU
19	G	132	LYS
19	G	135	LEU
19	G	161	LEU
19	G	174	LYS
19	G	208	ARG
20	H	9	PHE
20	H	31	ILE
20	H	43	LYS
20	H	54	LYS
20	H	62	ILE

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Mol	Chain	Res	Type
20	H	70	VAL
20	H	294	VAL
20	H	305	HIS
20	H	336	ASP
20	H	337	GLU
20	H	338	GLU
20	H	339	ARG
20	H	340	ARG
21	I	14	ILE
21	I	21	THR
21	I	33	LEU
21	I	75	ILE
21	I	89	LYS
21	I	175	LEU
21	I	178	LEU
21	I	200	VAL
22	J	47	ARG
22	J	48	LEU
22	J	95	GLU
22	J	104	ARG
22	J	105	MET
22	J	116	GLN
22	J	138	SER
22	J	143	VAL
23	K	10	GLU
23	K	15	LEU
23	K	60	ILE
23	K	114	VAL
23	K	115	LEU
23	K	138	ARG
23	K	141	ILE
23	K	162	GLU
24	L	7	VAL
24	L	16	GLU
24	L	24	ARG
24	L	36	ILE
24	L	38	ARG
24	L	54	LEU
24	L	86	ARG
25	M	7	ILE
25	M	17	LYS
25	M	21	GLU

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Mol	Chain	Res	Type
25	M	23	LEU
25	M	27	VAL
25	M	50	LEU
25	M	79	ARG
25	M	91	VAL
25	M	109	ARG
25	M	130	ASN
25	M	146	GLU
26	N	96	MET
26	N	104	VAL
26	N	117	ARG
27	O	27	LYS
27	O	60	LYS
27	O	61	LEU
27	O	63	LEU
27	O	116	VAL
27	O	118	LEU
28	P	17	LEU
28	P	18	ILE
28	P	24	GLU
28	P	25	ILE
28	P	27	GLU
28	P	37	ARG
28	P	87	LEU
28	P	90	LEU
28	P	102	LEU
29	Q	15	GLN
29	Q	107	ILE
30	R	5	ASN
30	R	12	ARG
30	R	24	LEU
30	R	62	GLU
30	R	74	LEU
30	R	102	LEU
31	S	45	VAL
31	S	46	LEU
31	S	89	MET
31	S	92	GLU
32	T	10	LYS
32	T	22	THR
32	T	39	LEU
32	T	40	GLN

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Mol	Chain	Res	Type
32	T	64	ARG
32	T	66	LEU
32	T	67	LEU
32	T	70	LEU
32	T	73	LYS
32	T	84	ARG
32	T	85	LEU
33	U	1	MET
33	U	2	VAL
33	U	6	LEU
33	U	19	VAL
33	U	50	THR
34	V	46	VAL
34	V	75	LEU
34	V	81	LYS
35	W	21	LYS
35	W	33	THR
35	W	49	ILE
35	W	58	VAL
35	W	79	THR
35	W	81	ARG
36	X	16	VAL
36	X	25	VAL
36	X	29	ARG
36	X	59	GLU
36	X	93	ARG
36	X	101	ARG
36	X	117	LYS
37	Y	4	VAL
37	Y	10	LEU
37	Y	16	MET
37	Y	23	VAL
37	Y	27	LEU
37	Y	30	GLN
37	Y	36	GLU
37	Y	44	LYS
37	Y	45	THR
37	Y	48	ILE
37	Y	50	LYS
37	Y	52	LEU
37	Y	57	VAL
37	Y	58	ILE

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Mol	Chain	Res	Type
37	Y	60	VAL
37	Y	61	TYR
37	Y	64	ARG
37	Y	65	SER
37	Y	67	THR
37	Y	71	LYS
37	Y	78	LEU
37	Y	80	LYS
37	Y	81	LYS
37	Y	91	LYS
37	Y	94	LYS
37	Y	95	ASP
37	Y	99	LYS
37	Y	100	ILE
37	Y	102	ARG
37	Y	104	GLN
37	Y	108	ILE
37	Y	112	LYS
37	Y	116	MET
37	Y	124	MET
37	Y	125	THR
37	Y	126	ARG
37	Y	133	ARG
37	Y	135	MET
37	Y	137	LEU
37	Y	138	VAL
38	Z	1	SER
38	Z	2	ILE
38	Z	3	THR
38	Z	4	LYS
38	Z	6	GLN
38	Z	7	ILE
38	Z	8	ILE
38	Z	14	MET
38	Z	16	VAL
38	Z	17	MET
38	Z	19	VAL
38	Z	23	ILE
38	Z	26	MET
38	Z	28	GLU
38	Z	29	LYS
38	Z	30	PHE

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Mol	Chain	Res	Type
40	b	70	GLU
41	c	33	LEU
41	c	48	THR
41	c	71	LEU
43	e	18	LEU
43	e	58	ASN
43	e	60	LYS
44	f	3	LYS
44	f	11	ARG
44	f	25	LEU
44	f	45	ARG
44	f	55	VAL
45	g	3	LYS
45	g	16	CYS
45	g	24	ILE
45	g	36	VAL
45	g	47	LYS
46	h	51	THR
46	h	94	VAL
46	h	105	LEU
46	h	118	SER
46	h	125	LYS
46	h	130	LEU
46	h	141	VAL
46	h	156	ARG
46	h	183	LYS
46	h	187	ASP
46	h	195	VAL
46	h	202	LEU
46	h	203	ARG
46	h	204	VAL
46	h	205	LEU
46	h	242	LYS
46	h	271	ARG
47	i	9	THR
47	i	12	LYS
47	i	26	THR
47	i	27	SER
47	i	29	SER
47	i	40	ARG
48	j	13	ARG
48	j	18	ASP

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Mol	Chain	Res	Type
48	j	91	THR
48	j	99	GLU
48	j	104	VAL
48	j	177	VAL
48	j	189	VAL
48	j	193	VAL
49	k	5	ILE
49	k	17	THR
49	k	24	THR
50	l	17	THR
50	l	22	ASP
50	l	40	ARG
50	l	48	THR
50	l	57	LYS
50	l	69	ARG
50	l	77	ILE
50	l	80	SER
50	l	108	ILE
50	l	109	LEU
50	l	111	GLU
50	l	122	GLU
50	l	149	ILE
50	l	179	SER
51	m	22	MET
51	m	42	LEU
52	n	6	ASP
52	n	10	ASP
52	n	26	MET
52	n	40	VAL
52	n	47	LYS
52	n	49	LEU
52	n	57	LEU
52	n	79	ILE
52	n	80	ARG
52	n	95	ARG
52	n	105	THR
52	n	117	LEU
52	n	122	PHE
52	n	123	ASP
52	n	132	VAL
52	n	140	GLU
52	n	141	ILE

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Mol	Chain	Res	Type
52	n	163	ASP
53	o	8	ARG
53	o	30	ARG
53	o	31	HIS
53	o	55	LEU
54	p	11	VAL
54	p	85	LYS
54	p	95	ARG
54	p	125	CYS
54	p	168	VAL
54	p	171	THR
55	q	3	VAL
55	q	26	ILE
55	q	34	LYS
56	r	1	MET
56	r	9	VAL
56	r	11	ASN
56	r	12	LEU
56	r	15	LEU
56	r	41	LYS
56	r	66	ASN
56	r	72	ILE
56	r	76	GLU
56	r	94	ILE
56	r	101	ASP
56	r	127	GLU
57	s	1	MET
57	s	30	THR
57	s	31	GLU
57	s	43	GLU
57	s	57	LEU
57	s	123	LYS
57	s	124	VAL
57	s	139	VAL
57	s	140	LEU
57	s	142	ILE
58	t	35	VAL
58	t	49	ARG
58	t	67	LYS
58	t	70	ARG
58	t	80	ASP
58	t	104	THR

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Mol	Chain	Res	Type
59	u	5	THR
59	u	27	LEU
59	u	59	ARG
59	u	73	ILE
59	u	76	GLU
59	u	78	ARG
59	u	84	LYS
60	v	110	GLU
60	v	126	ILE
60	v	127	LYS
60	v	128	THR
61	w	2	ARG
61	w	20	MET
61	w	24	MET
61	w	51	LEU
61	w	65	LEU
61	w	69	ARG
61	w	95	THR
61	w	116	VAL
62	x	13	ARG
62	x	31	THR
62	x	47	VAL
62	x	48	LEU
62	x	91	SER
62	x	116	GLN
63	y	8	LEU
63	y	10	GLN
63	y	27	GLU
63	y	40	LEU
63	y	81	VAL
63	y	85	SER
63	y	102	GLU
63	y	114	LEU
64	z	18	LEU
64	z	51	ARG
64	z	109	LEU
64	z	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	86	GLN

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Mol	Chain	Res	Type
2	1	61	ASN
3	2	28	ASN
3	2	59	ASN
4	3	54	GLN
5	4	12	GLN
9	9	103	ASN
9	9	122	GLN
11	AA	69	GLN
11	AA	193	ASN
11	AA	273	HIS
11	AA	761	GLN
11	AA	808	ASN
11	AA	965	GLN
11	AA	1157	GLN
11	AA	1236	ASN
13	AC	41	ASN
13	AC	132	HIS
13	AD	41	ASN
13	AD	93	GLN
13	AD	103	ASN
14	AE	196	GLN
14	AE	424	ASN
14	AE	469	HIS
14	AE	865	HIS
14	AE	1195	GLN
14	AE	1238	GLN
14	AE	1249	ASN
17	E	3	ASN
17	E	55	GLN
17	E	61	GLN
19	G	18	HIS
19	G	58	ASN
19	G	94	HIS
21	I	6	HIS
21	I	25	ASN
21	I	123	GLN
22	J	36	GLN
22	J	40	GLN
22	J	41	HIS
23	K	97	GLN
24	L	11	HIS
24	L	63	ASN

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Mol	Chain	Res	Type
24	L	94	HIS
25	M	97	ASN
25	M	148	ASN
27	O	81	HIS
28	P	58	ASN
29	Q	15	GLN
30	R	6	GLN
30	R	72	HIS
32	T	40	GLN
33	U	59	HIS
36	X	12	HIS
36	X	105	ASN
45	g	33	ASN
45	g	65	ASN
46	h	70	ASN
46	h	260	ASN
47	i	5	GLN
49	k	26	ASN
52	n	63	GLN
53	o	28	ASN
54	p	48	ASN
54	p	88	GLN
55	q	35	GLN
56	r	20	ASN
56	r	133	GLN
58	t	88	ASN
63	y	15	GLN
63	y	66	ASN
63	y	77	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	75/76 (98%)	29 (38%)	6 (8%)
10	B	75/76 (98%)	35 (46%)	6 (8%)
16	D	1515/1542 (98%)	289 (19%)	35 (2%)
39	a	2859/2904 (98%)	541 (18%)	0
42	d	119/120 (99%)	17 (14%)	0
8	7	24/37 (64%)	15 (62%)	3 (12%)
All	All	4667/4755 (98%)	926 (19%)	50 (1%)

All (926) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	-9	G
8	7	-8	U
8	7	-7	U
8	7	-5	U
8	7	-4	U
8	7	-3	U
8	7	-2	U
8	7	-1	U
8	7	0	U
8	7	1	U
8	7	2	U
8	7	3	U
8	7	4	U
8	7	5	U
8	7	13	G
10	A	2	G
10	A	6	G
10	A	7	G
10	A	8	U
10	A	10	G
10	A	13	C
10	A	14	A
10	A	15	G
10	A	16	C
10	A	17	C
10	A	18	G
10	A	19	G
10	A	20	U
10	A	21	A
10	A	22	G
10	A	23	C
10	A	46	G
10	A	47	U
10	A	48	C
10	A	49	G
10	A	52	G
10	A	57	A
10	A	58	A
10	A	59	A
10	A	61	C
10	A	66	C
10	A	69	C
10	A	71	C

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Mol	Chain	Res	Type
10	A	73	A
10	B	2	G
10	B	6	G
10	B	7	G
10	B	8	U
10	B	10	G
10	B	13	C
10	B	14	A
10	B	15	G
10	B	16	C
10	B	17	C
10	B	18	G
10	B	19	G
10	B	20	U
10	B	21	A
10	B	22	G
10	B	23	C
10	B	30	G
10	B	31	G
10	B	32	C
10	B	36	U
10	B	37	A
10	B	38	A
10	B	46	G
10	B	47	U
10	B	48	C
10	B	49	G
10	B	52	G
10	B	57	A
10	B	58	A
10	B	59	A
10	B	61	C
10	B	66	C
10	B	69	C
10	B	71	C
10	B	73	A
16	D	4	U
16	D	5	U
16	D	9	G
16	D	22	G
16	D	29	U
16	D	32	A

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Mol	Chain	Res	Type
16	D	39	G
16	D	41	G
16	D	47	C
16	D	48	C
16	D	50	A
16	D	51	A
16	D	52	C
16	D	54	C
16	D	69	G
16	D	70	U
16	D	71	A
16	D	72	A
16	D	74	A
16	D	76	G
16	D	82	G
16	D	83	C
16	D	84	U
16	D	87	C
16	D	90	C
16	D	94	G
16	D	95	C
16	D	96	U
16	D	108	G
16	D	120	A
16	D	122	G
16	D	128	G
16	D	131	A
16	D	141	G
16	D	144	G
16	D	148	G
16	D	149	A
16	D	160	A
16	D	164	G
16	D	173	U
16	D	181	A
16	D	182	A
16	D	197	A
16	D	198	G
16	D	204	G
16	D	208	U
16	D	209	U
16	D	210	C

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Mol	Chain	Res	Type
16	D	211	G
16	D	212	G
16	D	216	U
16	D	226	G
16	D	245	U
16	D	247	G
16	D	251	G
16	D	258	G
16	D	262	A
16	D	266	G
16	D	267	C
16	D	271	C
16	D	279	A
16	D	289	G
16	D	299	G
16	D	306	A
16	D	321	A
16	D	328	C
16	D	329	A
16	D	332	G
16	D	347	G
16	D	352	C
16	D	353	A
16	D	354	G
16	D	355	C
16	D	367	U
16	D	372	C
16	D	373	A
16	D	376	G
16	D	382	A
16	D	384	G
16	D	392	C
16	D	393	A
16	D	397	A
16	D	406	G
16	D	412	A
16	D	413	G
16	D	414	A
16	D	421	U
16	D	422	C
16	D	424	G
16	D	429	U

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Mol	Chain	Res	Type
16	D	446	G
16	D	451	A
16	D	457	G
16	D	458	U
16	D	460	A
16	D	463	U
16	D	464	U
16	D	467	U
16	D	468	A
16	D	469	C
16	D	478	A
16	D	479	U
16	D	481	G
16	D	484	G
16	D	485	U
16	D	486	U
16	D	505	G
16	D	509	A
16	D	511	C
16	D	518	C
16	D	519	C
16	D	526	C
16	D	531	U
16	D	532	A
16	D	533	A
16	D	542	G
16	D	547	A
16	D	559	A
16	D	562	U
16	D	568	G
16	D	572	A
16	D	573	A
16	D	576	C
16	D	577	G
16	D	579	A
16	D	596	A
16	D	628	G
16	D	633	G
16	D	641	U
16	D	642	A
16	D	649	A
16	D	650	G

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Mol	Chain	Res	Type
16	D	653	U
16	D	665	A
16	D	666	G
16	D	687	A
16	D	700	G
16	D	723	U
16	D	724	G
16	D	731	G
16	D	734	G
16	D	747	A
16	D	748	G
16	D	755	G
16	D	760	G
16	D	777	A
16	D	793	U
16	D	794	A
16	D	815	A
16	D	817	C
16	D	828	U
16	D	829	G
16	D	832	G
16	D	841	C
16	D	844	G
16	D	845	A
16	D	849	G
16	D	874	G
16	D	887	G
16	D	902	G
16	D	914	A
16	D	916	U
16	D	926	G
16	D	934	C
16	D	935	A
16	D	954	G
16	D	960	U
16	D	963	G
16	D	969	A
16	D	972	C
16	D	975	A
16	D	976	G
16	D	991	U
16	D	992	U

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Mol	Chain	Res	Type
16	D	993	G
16	D	996	A
16	D	999	C
16	D	1004	A
16	D	1008	U
16	D	1009	U
16	D	1017	U
16	D	1018	G
16	D	1021	A
16	D	1024	G
16	D	1026	G
16	D	1028	C
16	D	1030	U
16	D	1031	C
16	D	1037	C
16	D	1043	G
16	D	1044	A
16	D	1046	A
16	D	1065	U
16	D	1085	U
16	D	1086	U
16	D	1094	G
16	D	1095	U
16	D	1099	G
16	D	1101	A
16	D	1124	G
16	D	1133	G
16	D	1135	U
16	D	1136	C
16	D	1137	C
16	D	1139	G
16	D	1140	C
16	D	1141	C
16	D	1142	G
16	D	1143	G
16	D	1145	A
16	D	1146	A
16	D	1151	A
16	D	1152	A
16	D	1158	C
16	D	1159	U
16	D	1167	A

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Mol	Chain	Res	Type
16	D	1171	A
16	D	1174	G
16	D	1175	G
16	D	1176	A
16	D	1184	G
16	D	1196	A
16	D	1197	A
16	D	1206	G
16	D	1211	U
16	D	1212	U
16	D	1213	A
16	D	1214	C
16	D	1215	G
16	D	1226	C
16	D	1227	A
16	D	1228	C
16	D	1238	A
16	D	1256	A
16	D	1257	A
16	D	1260	G
16	D	1275	A
16	D	1276	G
16	D	1278	G
16	D	1279	G
16	D	1280	A
16	D	1285	A
16	D	1286	U
16	D	1287	A
16	D	1299	A
16	D	1300	G
16	D	1302	C
16	D	1305	G
16	D	1312	G
16	D	1317	C
16	D	1320	C
16	D	1323	G
16	D	1329	A
16	D	1338	G
16	D	1340	A
16	D	1346	A
16	D	1347	G
16	D	1353	G

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Mol	Chain	Res	Type
16	D	1363	A
16	D	1370	G
16	D	1378	C
16	D	1379	G
16	D	1381	U
16	D	1391	U
16	D	1396	A
16	D	1397	C
16	D	1398	A
16	D	1404	C
16	D	1419	G
16	D	1429	A
16	D	1441	A
16	D	1446	A
16	D	1447	A
16	D	1448	C
16	D	1452	C
16	D	1453	G
16	D	1475	G
16	D	1487	G
16	D	1492	A
16	D	1493	A
16	D	1494	G
16	D	1495	U
16	D	1497	G
16	D	1503	A
16	D	1506	U
16	D	1517	G
16	D	1529	G
16	D	1530	G
16	D	1534	A
39	a	10	A
39	a	15	G
39	a	34	U
39	a	35	G
39	a	46	G
39	a	58	G
39	a	60	G
39	a	63	A
39	a	71	A
39	a	74	A
39	a	75	G

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Mol	Chain	Res	Type
39	a	83	A
39	a	84	A
39	a	85	G
39	a	93	G
39	a	96	C
39	a	102	U
39	a	103	A
39	a	110	G
39	a	114	U
39	a	118	A
39	a	119	A
39	a	120	U
39	a	122	G
39	a	131	A
39	a	136	G
39	a	139	U
39	a	140	C
39	a	141	G
39	a	145	C
39	a	163	C
39	a	165	A
39	a	181	A
39	a	196	A
39	a	199	A
39	a	200	U
39	a	215	G
39	a	216	A
39	a	222	A
39	a	225	C
39	a	248	G
39	a	249	C
39	a	261	G
39	a	264	C
39	a	265	A
39	a	266	G
39	a	267	C
39	a	271	G
39	a	272	A
39	a	275	C
39	a	276	U
39	a	278	A
39	a	285	G

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Mol	Chain	Res	Type
39	a	311	A
39	a	324	A
39	a	329	G
39	a	330	A
39	a	353	C
39	a	359	G
39	a	361	G
39	a	362	A
39	a	371	A
39	a	372	G
39	a	373	U
39	a	375	G
39	a	383	C
39	a	386	G
39	a	396	G
39	a	405	U
39	a	411	G
39	a	412	A
39	a	420	C
39	a	424	G
39	a	435	C
39	a	451	U
39	a	456	C
39	a	457	A
39	a	477	A
39	a	481	G
39	a	491	G
39	a	501	A
39	a	503	A
39	a	504	A
39	a	505	A
39	a	509	C
39	a	522	A
39	a	529	A
39	a	532	A
39	a	543	G
39	a	546	U
39	a	547	A
39	a	548	G
39	a	549	G
39	a	551	G
39	a	563	A

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Mol	Chain	Res	Type
39	a	569	U
39	a	573	U
39	a	575	A
39	a	588	U
39	a	603	A
39	a	609	A
39	a	613	A
39	a	614	A
39	a	615	U
39	a	616	A
39	a	618	G
39	a	620	G
39	a	621	A
39	a	627	A
39	a	637	A
39	a	645	C
39	a	647	G
39	a	654	A
39	a	664	G
39	a	668	A
39	a	685	A
39	a	686	U
39	a	710	U
39	a	717	C
39	a	730	A
39	a	738	G
39	a	757	G
39	a	764	A
39	a	765	C
39	a	775	G
39	a	776	G
39	a	782	A
39	a	784	G
39	a	785	G
39	a	800	A
39	a	802	A
39	a	805	G
39	a	812	C
39	a	819	A
39	a	827	U
39	a	828	U
39	a	845	A

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Mol	Chain	Res	Type
39	a	846	U
39	a	858	G
39	a	859	G
39	a	869	G
39	a	878	A
39	a	881	G
39	a	883	G
39	a	884	U
39	a	885	C
39	a	888	C
39	a	891	G
39	a	892	A
39	a	893	C
39	a	895	U
39	a	896	A
39	a	897	C
39	a	899	A
39	a	907	G
39	a	910	A
39	a	914	G
39	a	915	C
39	a	931	U
39	a	941	A
39	a	945	A
39	a	946	C
39	a	953	G
39	a	961	C
39	a	974	G
39	a	983	A
39	a	984	A
39	a	985	C
39	a	995	C
39	a	996	A
39	a	999	U
39	a	1005	C
39	a	1012	U
39	a	1013	C
39	a	1022	G
39	a	1023	U
39	a	1026	G
39	a	1033	U
39	a	1041	G

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Mol	Chain	Res	Type
39	a	1042	G
39	a	1045	C
39	a	1046	A
39	a	1047	G
39	a	1060	U
39	a	1061	U
39	a	1062	G
39	a	1063	G
39	a	1064	C
39	a	1065	U
39	a	1066	U
39	a	1067	A
39	a	1068	G
39	a	1069	A
39	a	1070	A
39	a	1071	G
39	a	1073	A
39	a	1074	G
39	a	1076	C
39	a	1079	C
39	a	1080	A
39	a	1081	U
39	a	1082	U
39	a	1083	U
39	a	1084	A
39	a	1087	G
39	a	1088	A
39	a	1090	A
39	a	1095	A
39	a	1096	A
39	a	1107	G
39	a	1110	G
39	a	1111	A
39	a	1112	G
39	a	1119	U
39	a	1122	G
39	a	1132	U
39	a	1134	A
39	a	1135	C
39	a	1142	A
39	a	1143	A
39	a	1169	A

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Mol	Chain	Res	Type
39	a	1170	C
39	a	1173	U
39	a	1174	U
39	a	1175	A
39	a	1176	U
39	a	1177	G
39	a	1178	C
39	a	1179	G
39	a	1180	U
39	a	1186	G
39	a	1238	G
39	a	1248	G
39	a	1253	A
39	a	1256	G
39	a	1266	G
39	a	1271	G
39	a	1272	A
39	a	1273	U
39	a	1301	A
39	a	1321	A
39	a	1345	C
39	a	1352	U
39	a	1365	A
39	a	1368	G
39	a	1378	A
39	a	1379	U
39	a	1380	G
39	a	1383	A
39	a	1387	A
39	a	1395	A
39	a	1406	U
39	a	1407	G
39	a	1408	G
39	a	1411	U
39	a	1414	C
39	a	1415	U
39	a	1416	G
39	a	1417	C
39	a	1419	A
39	a	1420	A
39	a	1428	C
39	a	1452	G

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Mol	Chain	Res	Type
39	a	1453	A
39	a	1460	U
39	a	1478	G
39	a	1482	G
39	a	1490	A
39	a	1491	G
39	a	1497	U
39	a	1503	A
39	a	1508	A
39	a	1509	A
39	a	1510	G
39	a	1515	A
39	a	1529	G
39	a	1534	U
39	a	1535	A
39	a	1536	C
39	a	1537	G
39	a	1554	U
39	a	1559	U
39	a	1566	A
39	a	1569	A
39	a	1578	U
39	a	1580	A
39	a	1581	G
39	a	1582	C
39	a	1583	A
39	a	1584	U
39	a	1589	U
39	a	1590	A
39	a	1608	A
39	a	1609	A
39	a	1610	A
39	a	1647	U
39	a	1648	U
39	a	1649	G
39	a	1651	G
39	a	1674	G
39	a	1677	A
39	a	1703	G
39	a	1714	U
39	a	1715	G
39	a	1718	G

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Mol	Chain	Res	Type
39	a	1729	U
39	a	1730	C
39	a	1732	C
39	a	1738	G
39	a	1750	G
39	a	1755	A
39	a	1758	U
39	a	1764	C
39	a	1773	A
39	a	1791	A
39	a	1800	C
39	a	1801	A
39	a	1808	A
39	a	1811	G
39	a	1816	C
39	a	1829	A
39	a	1833	C
39	a	1847	A
39	a	1848	A
39	a	1858	A
39	a	1859	U
39	a	1862	G
39	a	1864	U
39	a	1869	G
39	a	1870	C
39	a	1872	A
39	a	1873	G
39	a	1905	C
39	a	1906	G
39	a	1907	G
39	a	1913	A
39	a	1914	C
39	a	1919	A
39	a	1920	C
39	a	1922	G
39	a	1923	U
39	a	1924	C
39	a	1925	C
39	a	1926	U
39	a	1928	A
39	a	1929	G
39	a	1930	G

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Mol	Chain	Res	Type
39	a	1936	A
39	a	1938	A
39	a	1955	U
39	a	1965	C
39	a	1967	C
39	a	1970	A
39	a	1971	U
39	a	1972	G
39	a	1987	A
39	a	1991	U
39	a	1992	G
39	a	1993	U
39	a	1997	C
39	a	2002	G
39	a	2022	U
39	a	2023	C
39	a	2027	G
39	a	2033	A
39	a	2043	C
39	a	2051	A
39	a	2052	A
39	a	2055	C
39	a	2056	G
39	a	2060	A
39	a	2061	G
39	a	2062	A
39	a	2063	C
39	a	2077	A
39	a	2093	G
39	a	2097	A
39	a	2099	U
39	a	2100	G
39	a	2108	A
39	a	2110	G
39	a	2111	U
39	a	2113	U
39	a	2115	G
39	a	2116	G
39	a	2117	A
39	a	2118	U
39	a	2121	G
39	a	2122	U

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Mol	Chain	Res	Type
39	a	2124	G
39	a	2125	G
39	a	2126	A
39	a	2127	G
39	a	2128	G
39	a	2131	U
39	a	2132	U
39	a	2133	G
39	a	2134	A
39	a	2139	U
39	a	2141	G
39	a	2146	C
39	a	2147	A
39	a	2154	A
39	a	2157	G
39	a	2158	A
39	a	2159	G
39	a	2162	G
39	a	2163	A
39	a	2164	C
39	a	2165	C
39	a	2169	A
39	a	2171	A
39	a	2172	U
39	a	2178	C
39	a	2182	U
39	a	2183	A
39	a	2185	U
39	a	2188	U
39	a	2189	U
39	a	2190	G
39	a	2191	A
39	a	2193	G
39	a	2194	U
39	a	2198	A
39	a	2204	G
39	a	2210	U
39	a	2211	A
39	a	2212	A
39	a	2213	U
39	a	2225	A
39	a	2226	C

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Mol	Chain	Res	Type
39	a	2229	U
39	a	2238	G
39	a	2239	G
39	a	2244	U
39	a	2250	G
39	a	2268	A
39	a	2278	A
39	a	2283	C
39	a	2287	A
39	a	2297	A
39	a	2305	U
39	a	2308	G
39	a	2309	A
39	a	2315	G
39	a	2322	A
39	a	2325	G
39	a	2327	A
39	a	2333	A
39	a	2339	C
39	a	2345	G
39	a	2347	C
39	a	2350	C
39	a	2361	G
39	a	2372	U
39	a	2376	A
39	a	2383	G
39	a	2385	C
39	a	2402	U
39	a	2403	C
39	a	2406	A
39	a	2423	U
39	a	2424	C
39	a	2425	A
39	a	2426	A
39	a	2429	G
39	a	2430	A
39	a	2431	U
39	a	2434	A
39	a	2435	A
39	a	2441	U
39	a	2447	G
39	a	2448	A

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Mol	Chain	Res	Type
39	a	2470	G
39	a	2474	U
39	a	2476	A
39	a	2478	A
39	a	2484	G
39	a	2491	U
39	a	2502	G
39	a	2506	U
39	a	2507	C
39	a	2512	C
39	a	2513	A
39	a	2518	A
39	a	2520	C
39	a	2525	G
39	a	2529	G
39	a	2535	G
39	a	2547	A
39	a	2554	U
39	a	2566	A
39	a	2567	G
39	a	2572	A
39	a	2573	C
39	a	2574	G
39	a	2585	U
39	a	2586	U
39	a	2602	A
39	a	2603	G
39	a	2609	U
39	a	2610	C
39	a	2611	C
39	a	2613	U
39	a	2629	U
39	a	2663	G
39	a	2669	G
39	a	2671	G
39	a	2689	U
39	a	2690	U
39	a	2714	G
39	a	2722	G
39	a	2726	A
39	a	2744	G
39	a	2748	A

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Mol	Chain	Res	Type
39	a	2757	A
39	a	2758	A
39	a	2765	A
39	a	2777	G
39	a	2778	A
39	a	2791	G
39	a	2793	C
39	a	2796	U
39	a	2797	U
39	a	2798	U
39	a	2799	A
39	a	2801	G
39	a	2818	U
39	a	2820	A
39	a	2823	A
39	a	2825	G
39	a	2849	U
39	a	2850	A
39	a	2859	G
39	a	2861	U
39	a	2867	G
39	a	2880	C
39	a	2884	U
39	a	2885	G
39	a	2891	U
39	a	2902	C
42	d	2	G
42	d	9	G
42	d	13	G
42	d	16	G
42	d	17	C
42	d	35	C
42	d	36	C
42	d	45	A
42	d	51	G
42	d	56	G
42	d	64	G
42	d	66	A
42	d	88	C
42	d	89	U
42	d	90	C
42	d	99	A

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Mol	Chain	Res	Type
42	d	109	A

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	7	-8	U
8	7	-5	U
8	7	-3	U
10	A	6	G
10	A	7	G
10	A	9	G
10	A	22	G
10	A	60	U
10	A	70	G
10	B	6	G
10	B	7	G
10	B	9	G
10	B	22	G
10	B	37	A
10	B	60	U
16	D	7	A
16	D	70	U
16	D	121	U
16	D	181	A
16	D	183	C
16	D	197	A
16	D	209	U
16	D	305	G
16	D	328	C
16	D	428	G
16	D	496	A
16	D	517	G
16	D	531	U
16	D	532	A
16	D	562	U
16	D	641	U
16	D	722	G
16	D	793	U
16	D	991	U
16	D	992	U
16	D	1109	C
16	D	1145	A

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Mol	Chain	Res	Type
16	D	1196	A
16	D	1211	U
16	D	1212	U
16	D	1213	A
16	D	1214	C
16	D	1225	A
16	D	1299	A
16	D	1396	A
16	D	1432	G
16	D	1447	A
16	D	1491	G
16	D	1492	A
16	D	1493	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

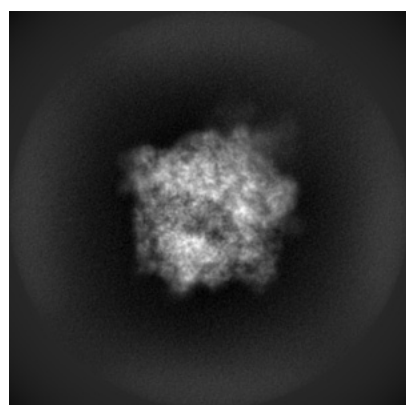
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21470. These allow visual inspection of the internal detail of the map and identification of artifacts.

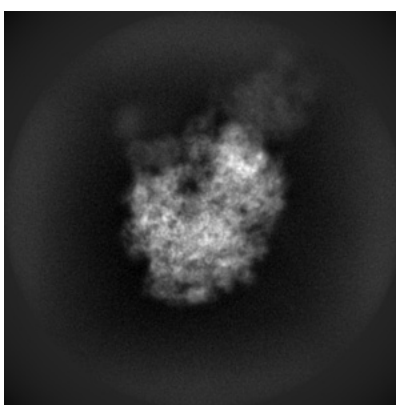
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

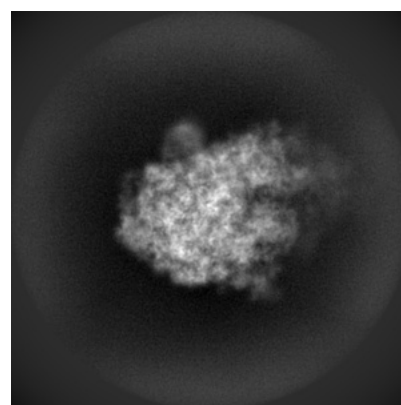
6.1.1 Primary map



X



Y

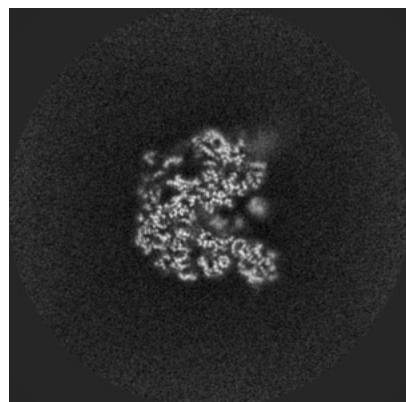


Z

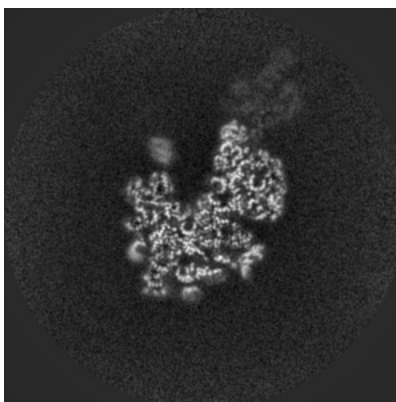
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

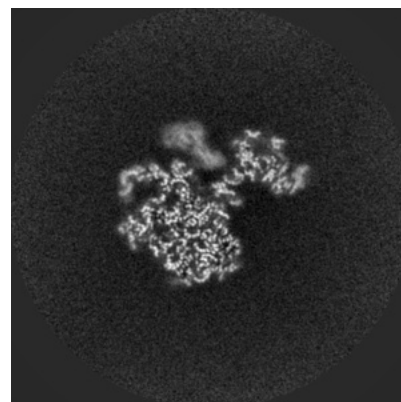
6.2.1 Primary map



X Index: 250



Y Index: 250

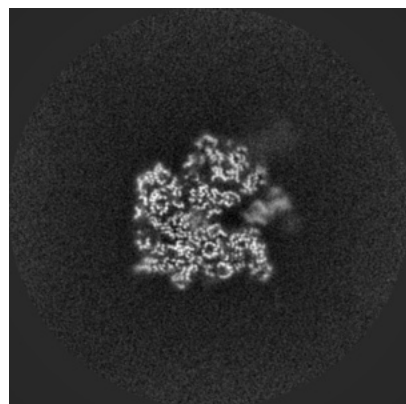


Z Index: 250

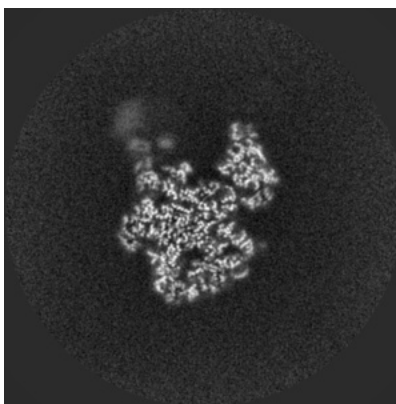
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

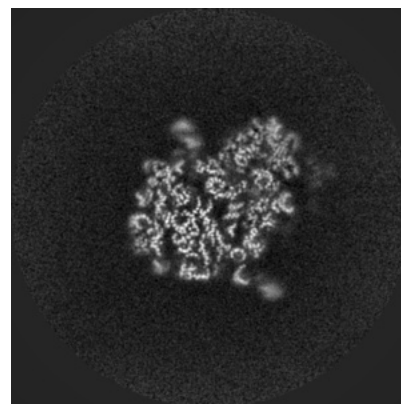
6.3.1 Primary map



X Index: 238



Y Index: 213

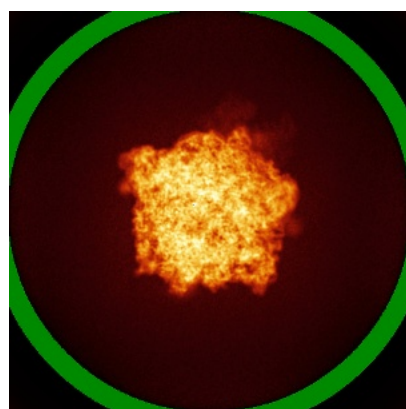


Z Index: 276

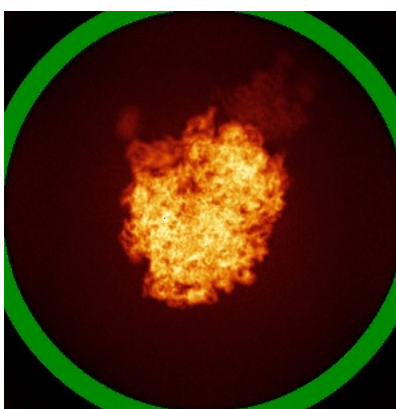
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.00868. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

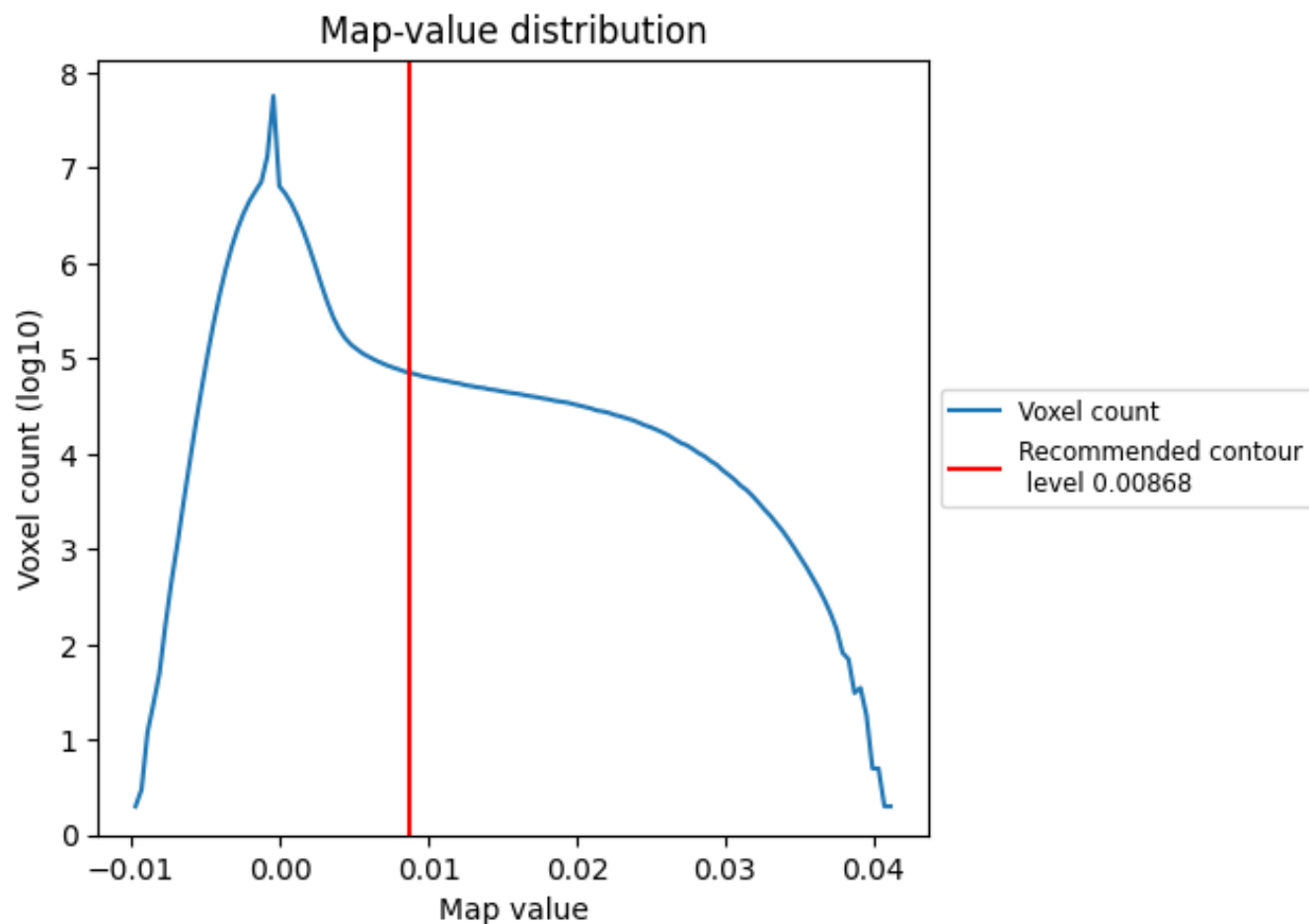
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

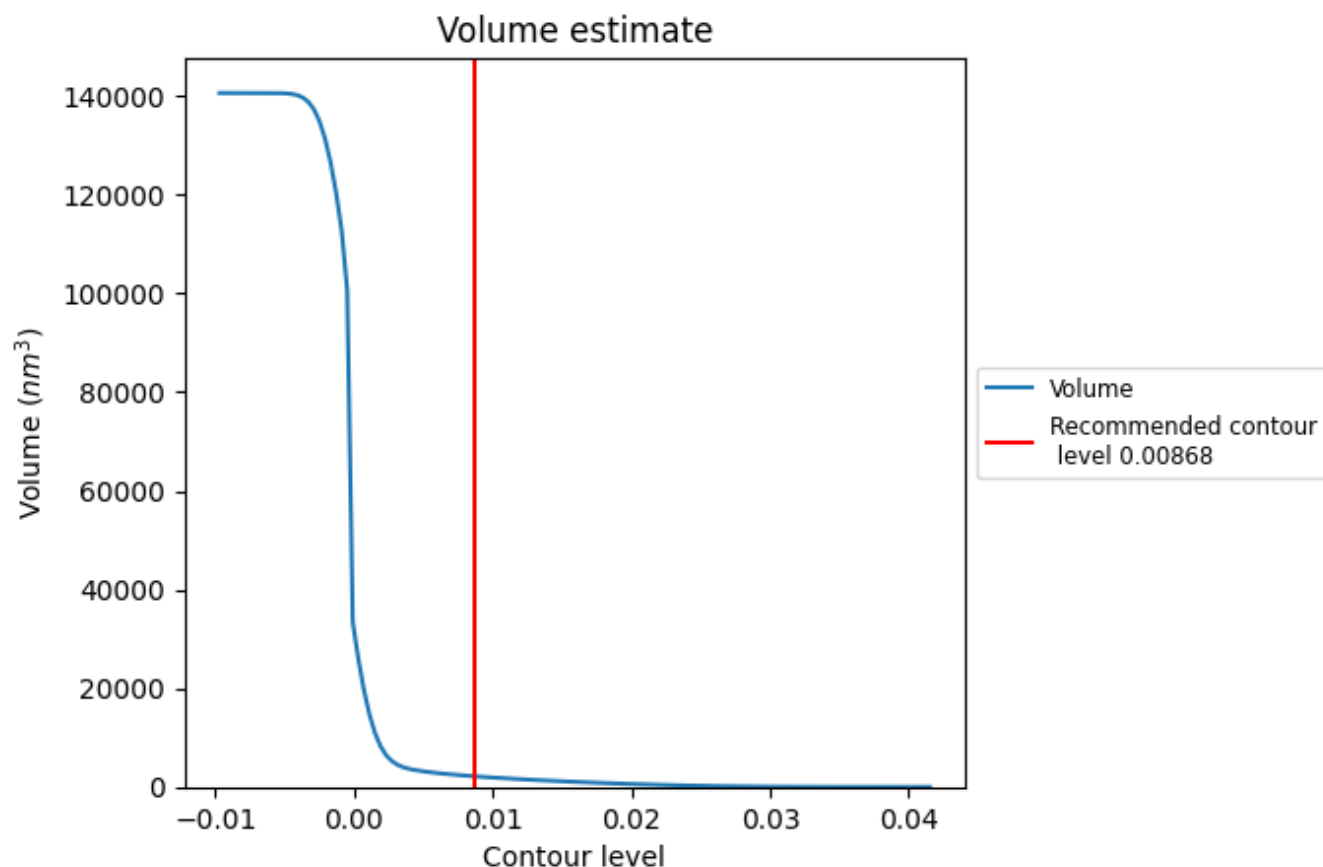
This section contains the results of statistical analysis of the map.

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.

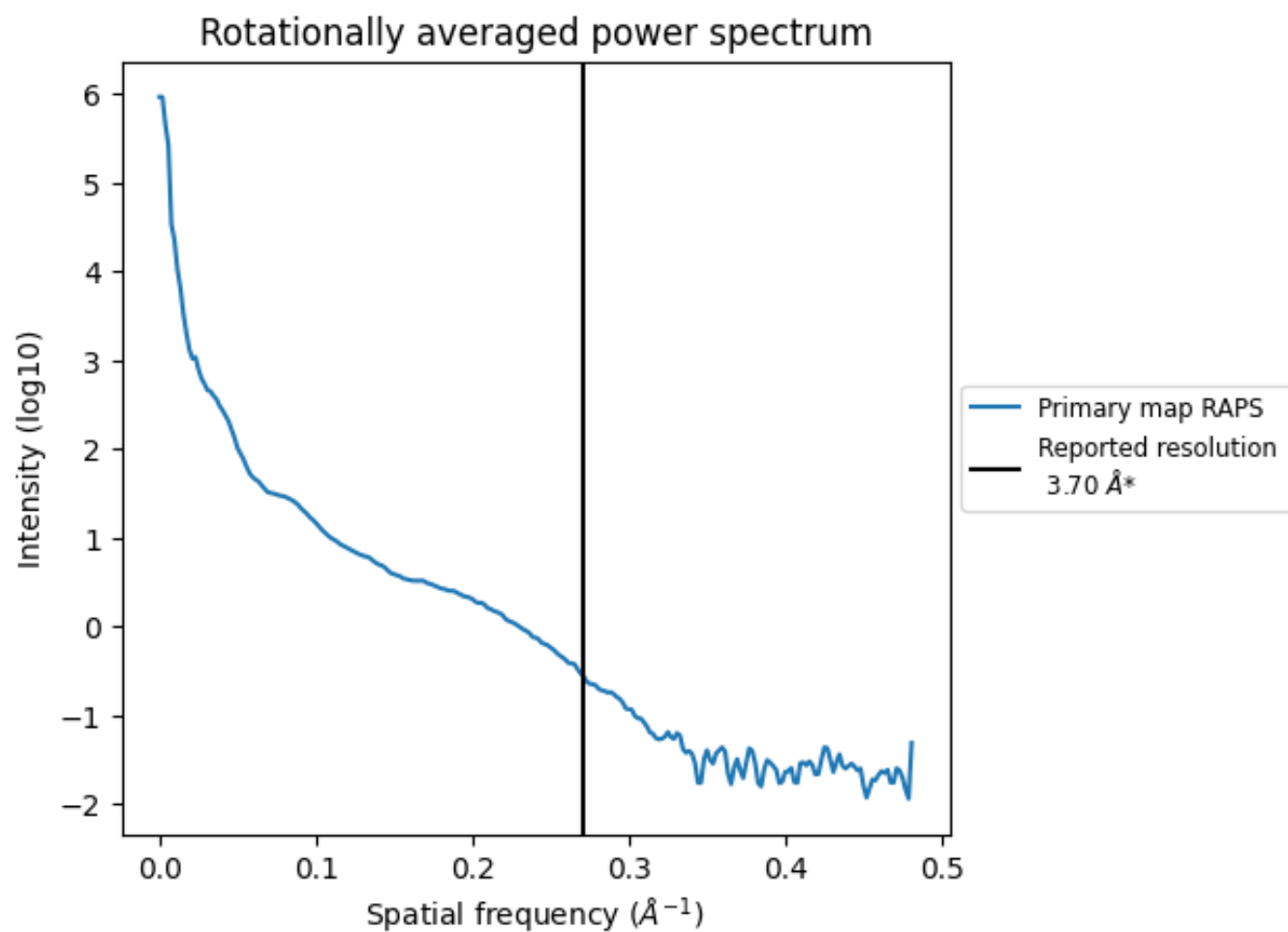
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2155 nm^3 ; this corresponds to an approximate mass of 1947 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 0.270 Å⁻¹

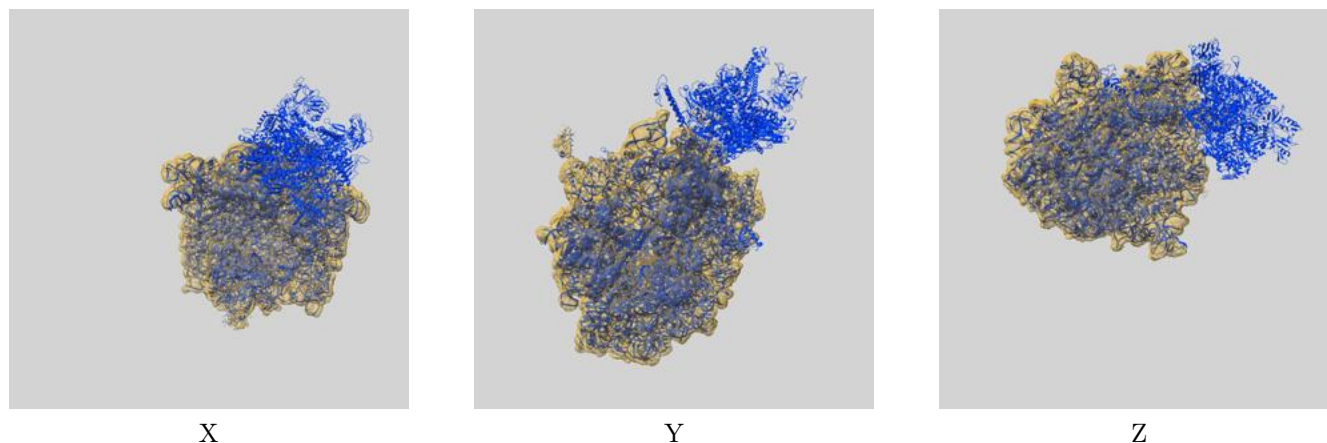
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

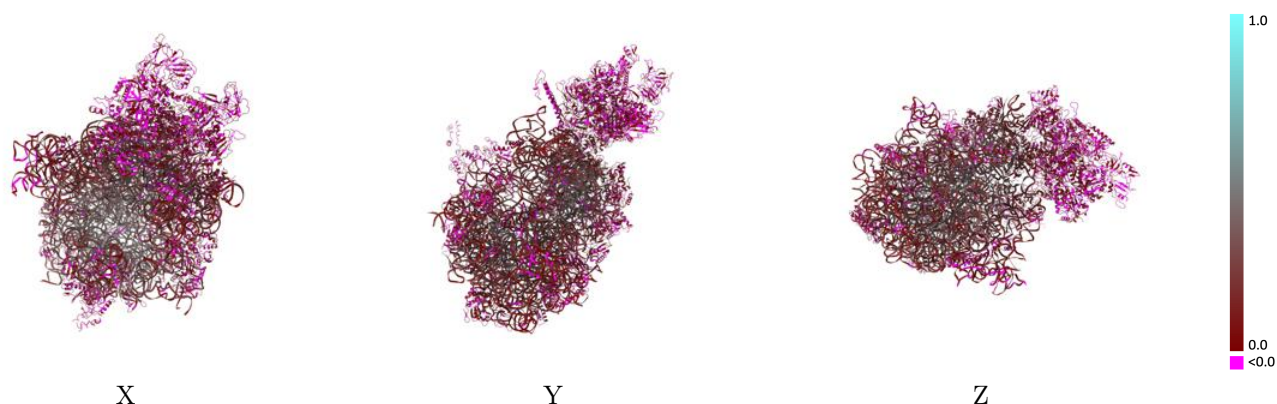
This section contains information regarding the fit between EMDB map EMD-21470 and PDB model 6VYS. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



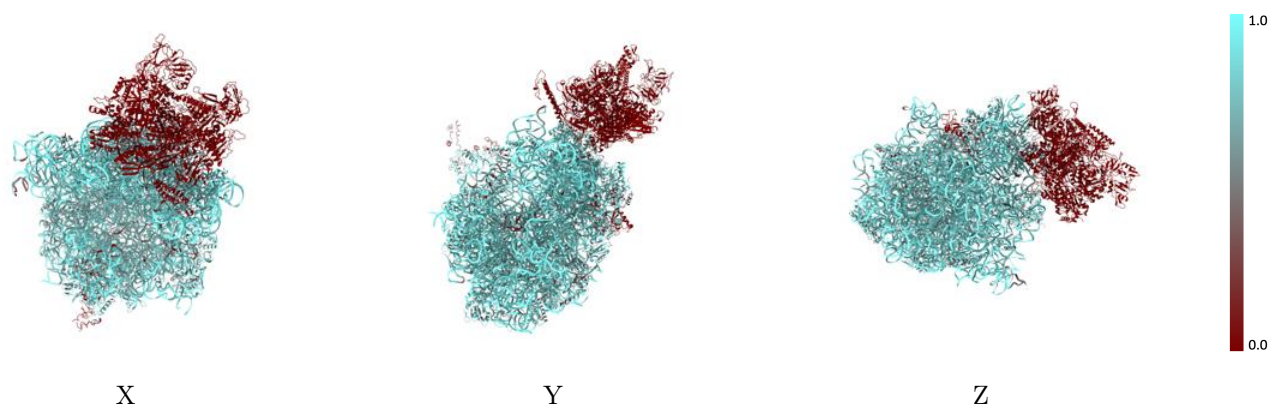
The images above show the 3D surface view of the map at the recommended contour level 0.00868 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



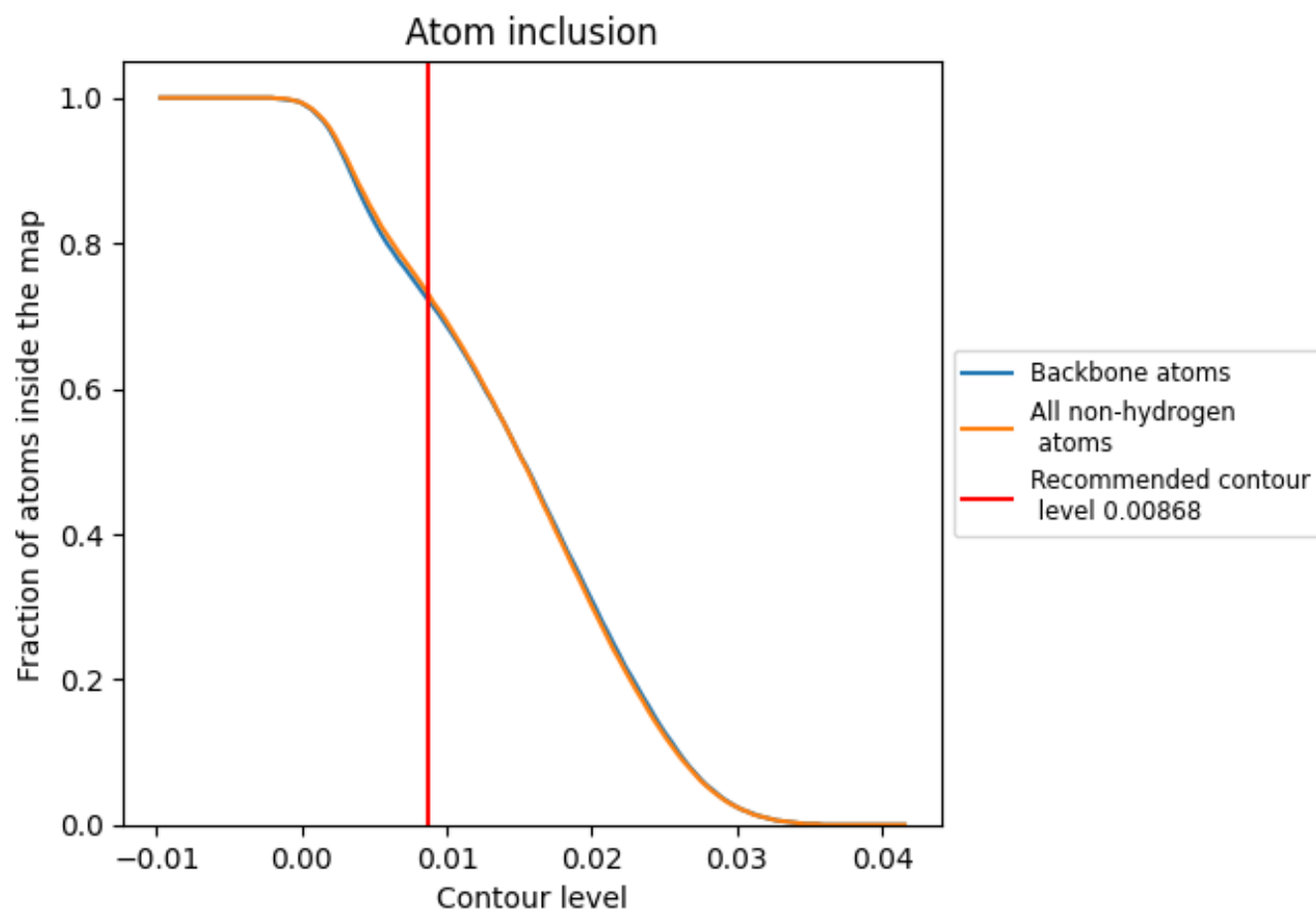
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00868).

9.4 Atom inclusion ⓘ



At the recommended contour level, 72% of all backbone atoms, 73% 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 (0.00868) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7320	 0.1950
0	 0.8140	 0.1990
1	 0.7810	 0.2550
2	 0.7000	 0.1110
3	 0.7650	 0.0900
4	 0.8100	 0.1990
5	 0.0000	 0.0130
6	 0.0180	 0.1500
7	 0.3070	 0.1010
9	 0.5580	 0.0400
A	 0.8900	 0.1870
AA	 0.0080	 0.0770
AB	 0.0000	 0.0340
AC	 0.0180	 0.1010
AD	 0.0000	 0.0460
AE	 0.0010	 0.0650
B	 0.6520	 0.0930
C	 0.7840	 0.1820
D	 0.9470	 0.2610
E	 0.7200	 0.0870
F	 0.7080	 0.2360
G	 0.7490	 0.1920
H	 0.1450	 0.0410
I	 0.7550	 0.2330
J	 0.7790	 0.1880
K	 0.8300	 0.3220
L	 0.7150	 0.1180
M	 0.7510	 0.1930
N	 0.8120	 0.2400
O	 0.8210	 0.1920
P	 0.7490	 0.1880
Q	 0.7690	 0.2140
R	 0.8290	 0.3250
S	 0.7930	 0.1770
T	 0.7800	 0.1690



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Chain	Atom inclusion	Q-score
U	 0.7370	 0.1070
V	 0.7780	 0.2040
W	 0.6270	 0.0470
X	 0.6820	 0.1050
Y	 0.4350	 0.0490
Z	 0.1760	 0.0610
a	 0.9340	 0.2370
b	 0.7900	 0.1940
c	 0.7390	 0.1720
d	 0.9290	 0.1880
e	 0.7490	 0.0770
f	 0.8100	 0.2460
g	 0.6970	 0.0790
h	 0.7390	 0.1500
i	 0.8110	 0.2560
j	 0.7950	 0.2150
k	 0.7030	 0.1200
l	 0.7300	 0.1640
m	 0.8280	 0.2680
n	 0.7170	 0.1030
o	 0.7430	 0.2070
p	 0.7690	 0.1100
q	 0.7980	 0.1930
r	 0.5710	 0.0620
s	 0.8150	 0.2330
t	 0.7320	 0.2060
u	 0.7800	 0.1890
v	 0.7810	 0.2590
w	 0.7930	 0.1840
x	 0.7520	 0.0520
y	 0.7420	 0.1430
z	 0.8410	 0.2700