



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 01:48 AM UTC

PDB ID : 5O61 / pdb_00005o61
EMDB ID : EMD-3751
Title : The complete structure of the Mycobacterium smegmatis 70S ribosome
Authors : Hentschel, J.; Burnside, C.; Mignot, I.; Leibundgut, M.; Boehringer, D.; Ban, N.
Deposited on : 2017-06-03
Resolution : 3.31 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

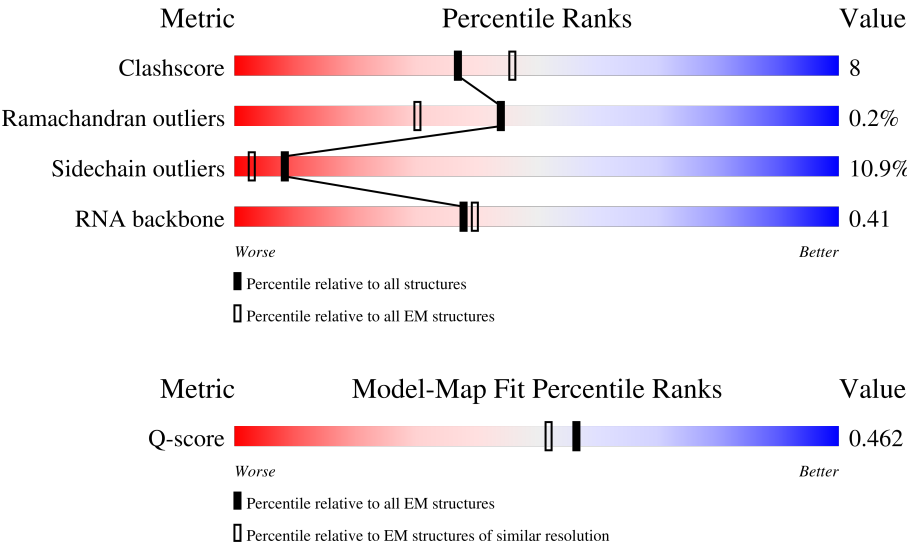
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.31 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	14550 (2.81 - 3.81)

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	3	24	
2	A	3120	
3	B	118	

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Mol	Chain	Length	Quality of chain
4	C	278	
5	D	217	
6	E	215	
7	F	187	
8	G	179	
9	H	151	
10	I	175	
11	J	142	
12	K	147	
13	L	122	
14	M	147	
15	N	138	
16	O	199	
17	P	127	
18	Q	113	
19	R	129	
20	S	103	
21	T	153	
22	U	100	
23	V	105	
24	W	215	
25	X	88	
26	Y	64	
27	Z	77	
28	a	61	

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Mol	Chain	Length	Quality of chain
29	b	57	
30	c	55	
31	d	47	
32	e	64	
33	f	37	
34	g	75	
35	BA	1528	
36	BB	33	
37	BC	275	
38	BD	201	
39	BE	214	
40	BF	96	
41	BG	156	
42	BH	132	
43	BI	150	
44	BJ	101	
45	BK	138	
46	BL	124	
47	BM	124	
48	BN	61	
49	BO	89	
50	BP	156	
51	BQ	98	
52	BR	84	
53	BS	93	

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Mol	Chain	Length	Quality of chain
54	BT	86	15% 69% 24% 6%
55	BV	277	82% 51% 26% 5% 18%
56	BW	76	78% 53% 38% 9%
57	BX	6	67% 17% 67% 17%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 151463 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein bL37.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 26 is a protein called LSU ribosomal protein L28P.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	59	Total	C	N	O	S	0	0
			458	284	84	85	5		

- Molecule 35 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BA	1511	Total	C	N	O	P	0	0
			32439	14448	5930	10550	1511		

- Molecule 36 is a protein called Conserved domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BB	32	Total	C	N	O	S	0	0
			280	172	71	36	1		

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BC	208	Total	C	N	O	S	0	0
			1660	1036	322	298	4		

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BD	200	Total	C	N	O	S	0	0
			1641	1028	316	295	2		

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BE	180	Total	C	N	O	S	0	0
			1296	812	245	235	4		

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BF	96	Total	C	N	O	S	0	0
			771	486	138	145	2		

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BG	155	Total	C	N	O	S	0	0
			1232	768	241	221	2		

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BH	131	Total	C	N	O	S	0	0
			1010	633	189	187	1		

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BI	126	Total	C	N	O	S	0	0
			994	630	194	170			

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BJ	99	Total	C	N	O	S	0	0
			788	495	146	144	3		

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BK	115	Total	C	N	O	S	0	0
			855	528	170	156	1		

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BL	122	Total	C	N	O	S	0	0
			958	594	197	165	2		

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BM	116	Total	C	N	O	S	0	0
			935	572	191	169	3		

- Molecule 48 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BN	60	Total	C	N	O	S	0	0
			477	302	97	73	5		

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	BO	88	Total	C	N	O	0	0
			720	449	147	124		

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	BP	113	Total	C	N	O	0	0
			891	570	162	159		

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BQ	94	Total	C	N	O	S	0	0
			748	469	142	135	2		

- Molecule 52 is a protein called 30S ribosomal protein S18 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BR	65	Total	C	N	O	S	0	0
			513	318	102	90	3		

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BS	82	Total	C	N	O	S	0	0
			662	425	124	112	1		

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	BT	85	Total	C	N	O	0	0
			660	402	139	119		

- Molecule 55 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BV	228	Total	C	N	O	S	0	0
			1793	1132	322	330	9		

- Molecule 56 is a RNA chain called P/P-site Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BW	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

- Molecule 57 is a RNA chain called mRNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BX	6	Total	C	N	O	P	0	0
			117	54	13	45	5		

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	A	390	Total	Mg	0
			390	390	
58	B	9	Total	Mg	0
			9	9	
58	C	4	Total	Mg	0
			4	4	
58	F	1	Total	Mg	0
			1	1	
58	M	1	Total	Mg	0
			1	1	
58	N	1	Total	Mg	0
			1	1	
58	T	1	Total	Mg	0
			1	1	
58	c	1	Total	Mg	0
			1	1	
58	BA	215	Total	Mg	0
			215	215	
58	BF	1	Total	Mg	0
			1	1	
58	BR	1	Total	Mg	0
			1	1	

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

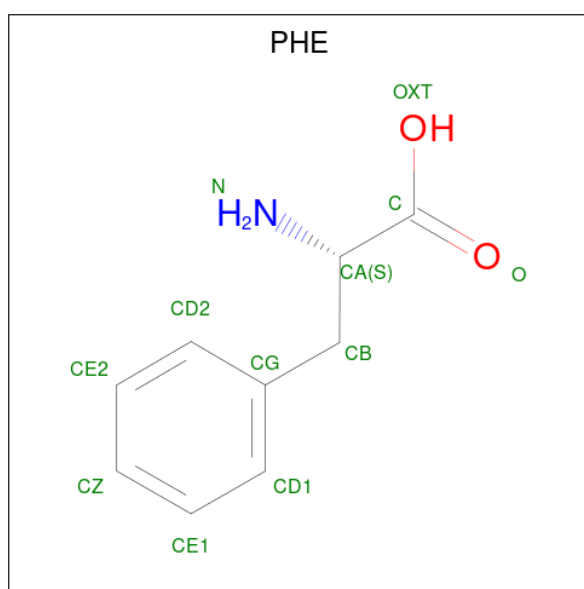
Mol	Chain	Residues	Atoms		AltConf
59	Y	1	Total	Zn	0
			1	1	
59	c	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
59	f	1	Total	Zn	0
			1	1	
59	g	1	Total	Zn	0
			1	1	
59	BN	1	Total	Zn	0
			1	1	
59	BR	1	Total	Zn	0
			1	1	

- Molecule 60 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).

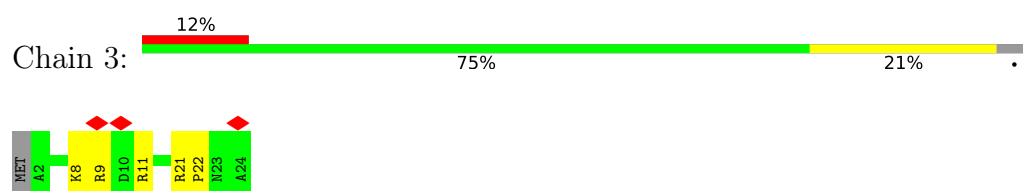


Mol	Chain	Residues	Atoms				AltConf
60	BW	1	Total	C	N	O	0
			11	9	1	1	

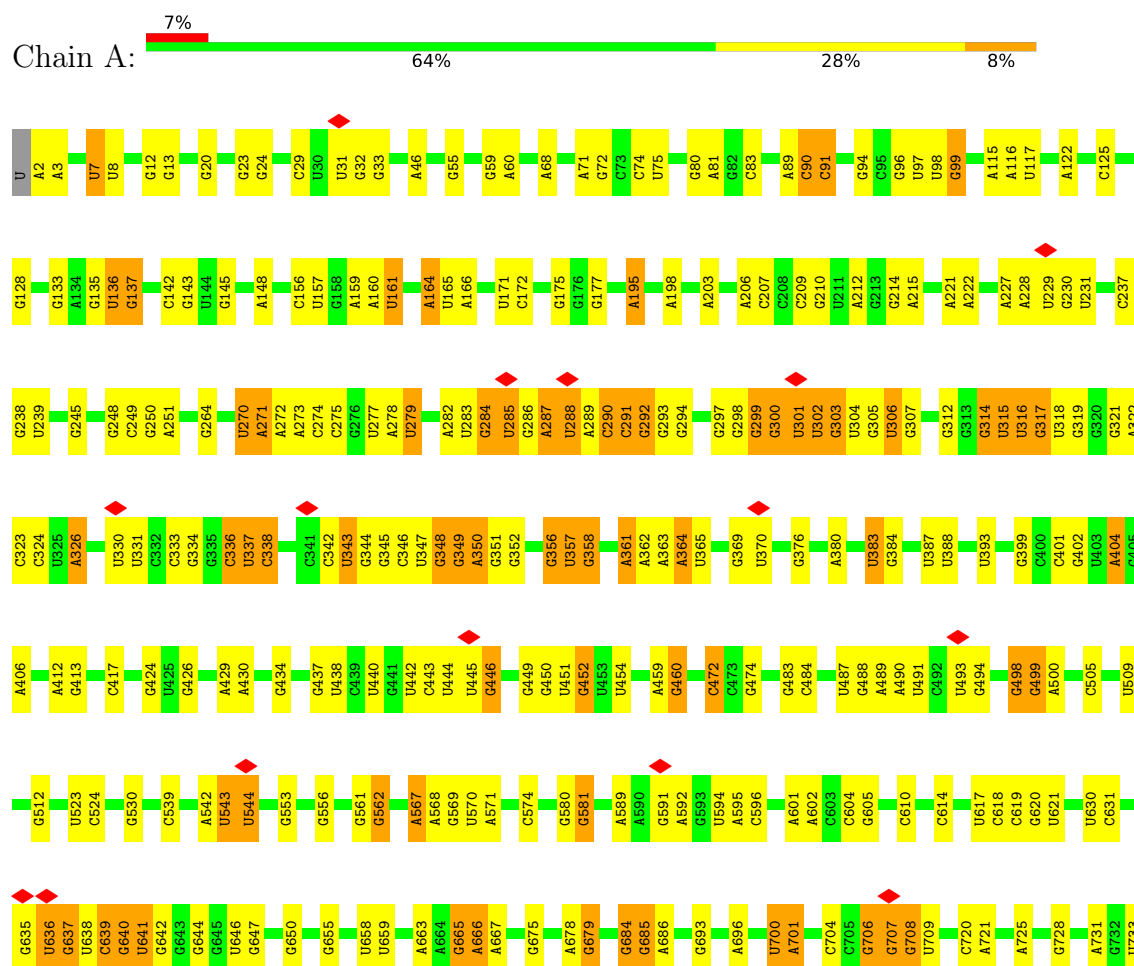
3 Residue-property plots

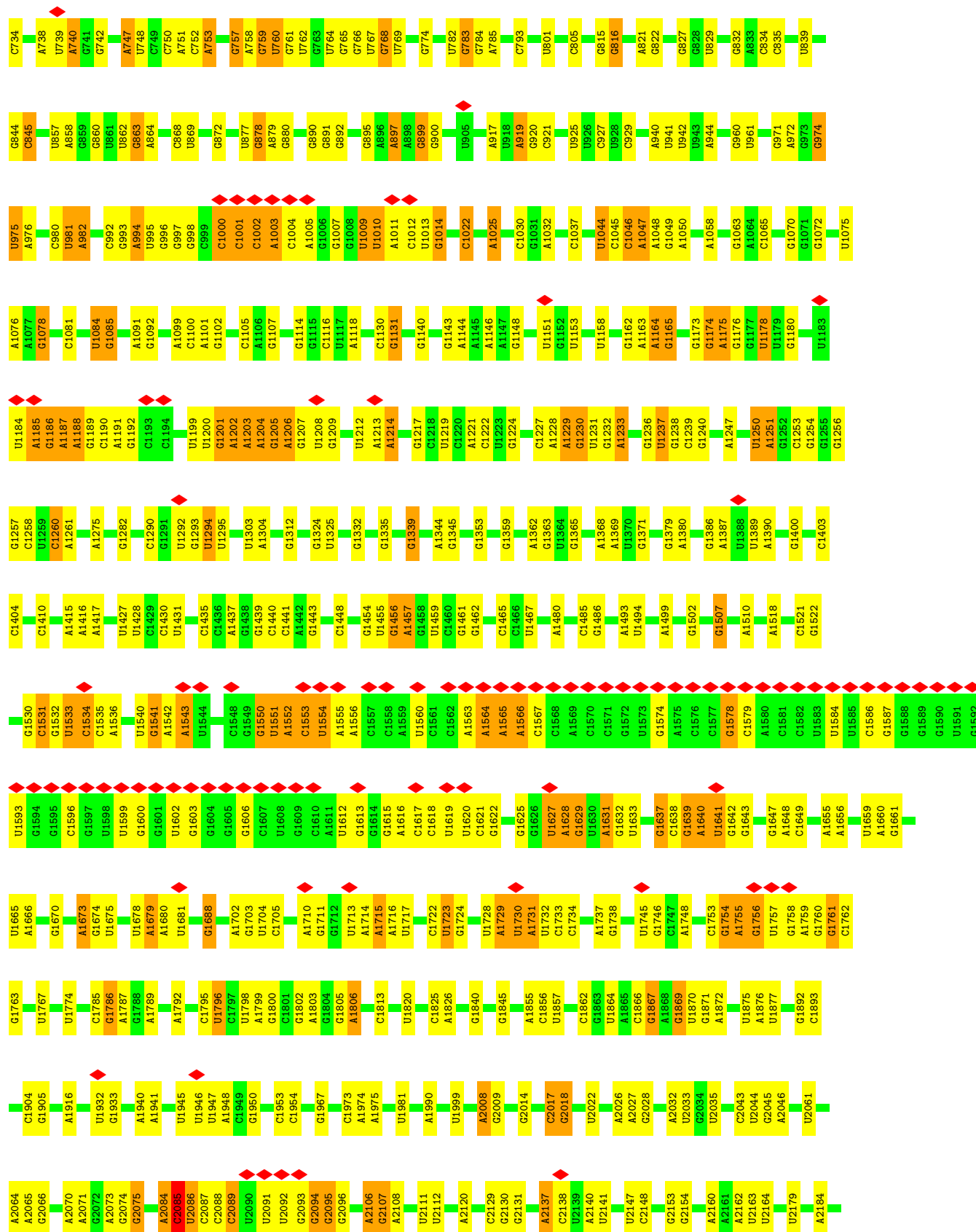
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

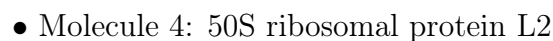
- Molecule 1: 50S ribosomal protein bL37

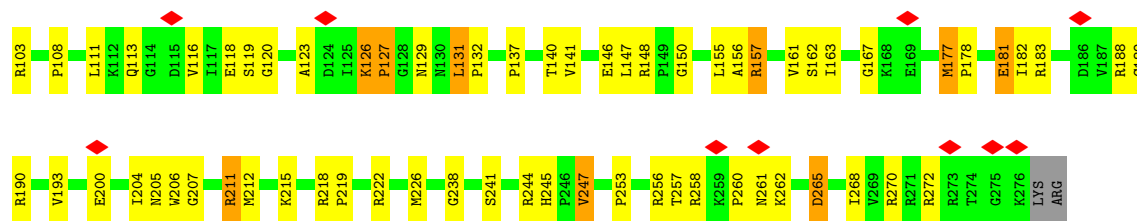


- Molecule 2: 23S rRNA

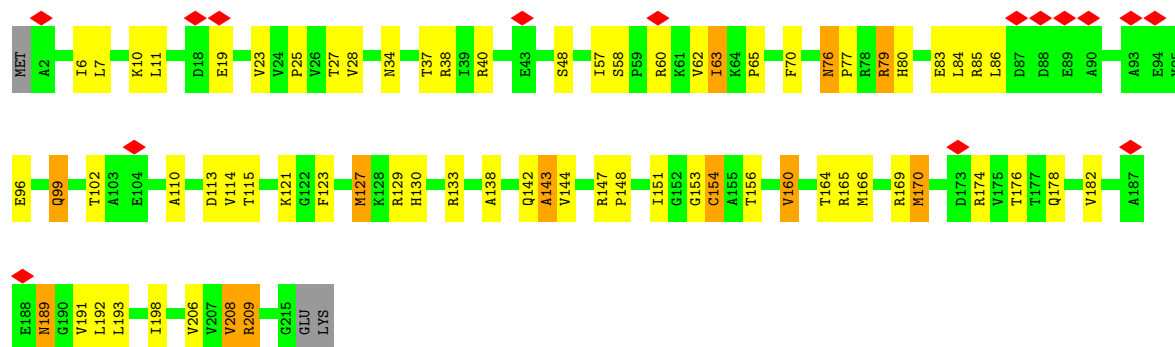




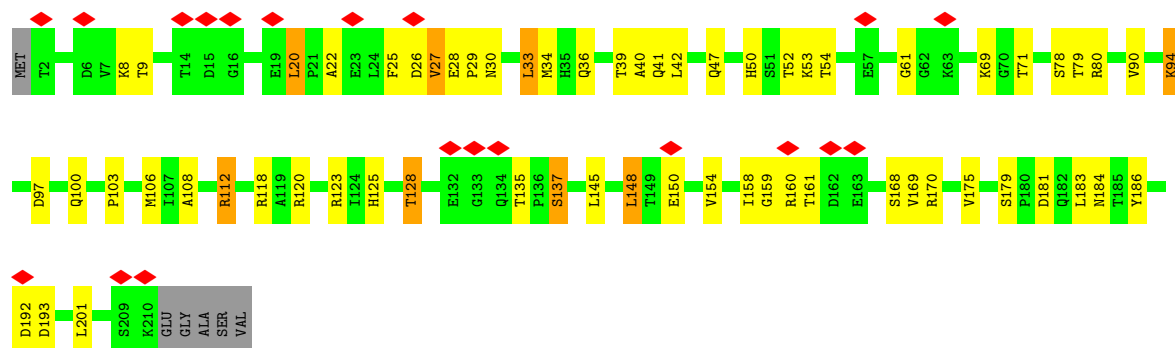




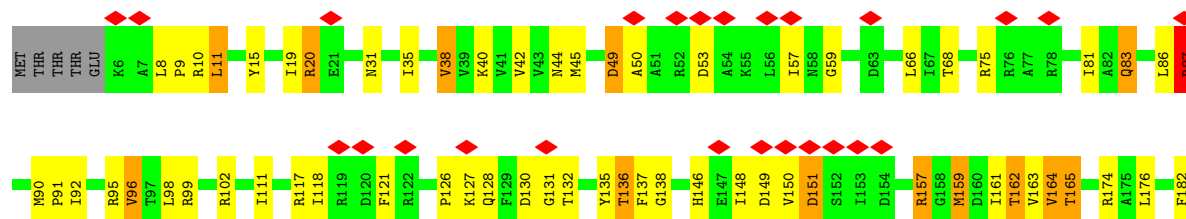
• Molecule 5: 50S ribosomal protein L3



• Molecule 6: 50S ribosomal protein L4

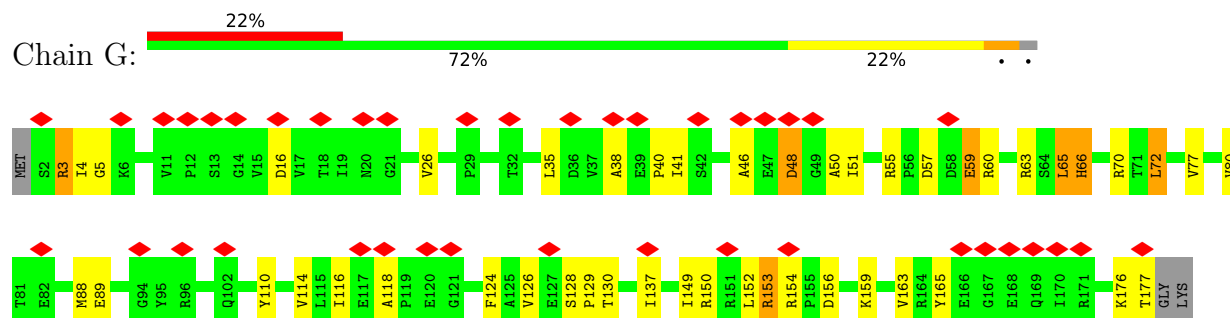


• Molecule 7: 50S ribosomal protein L5

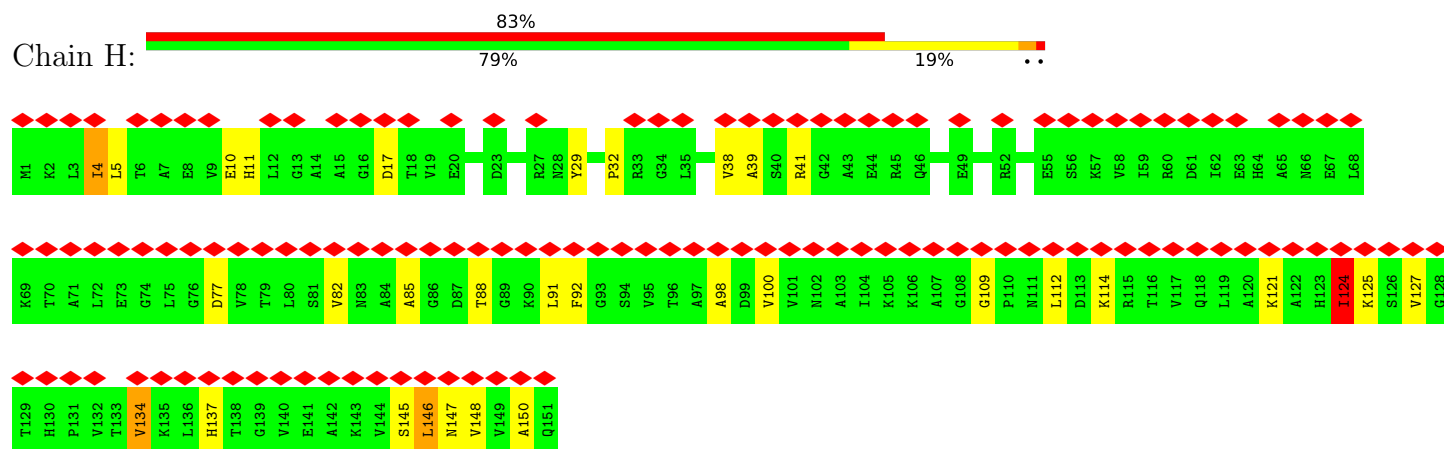




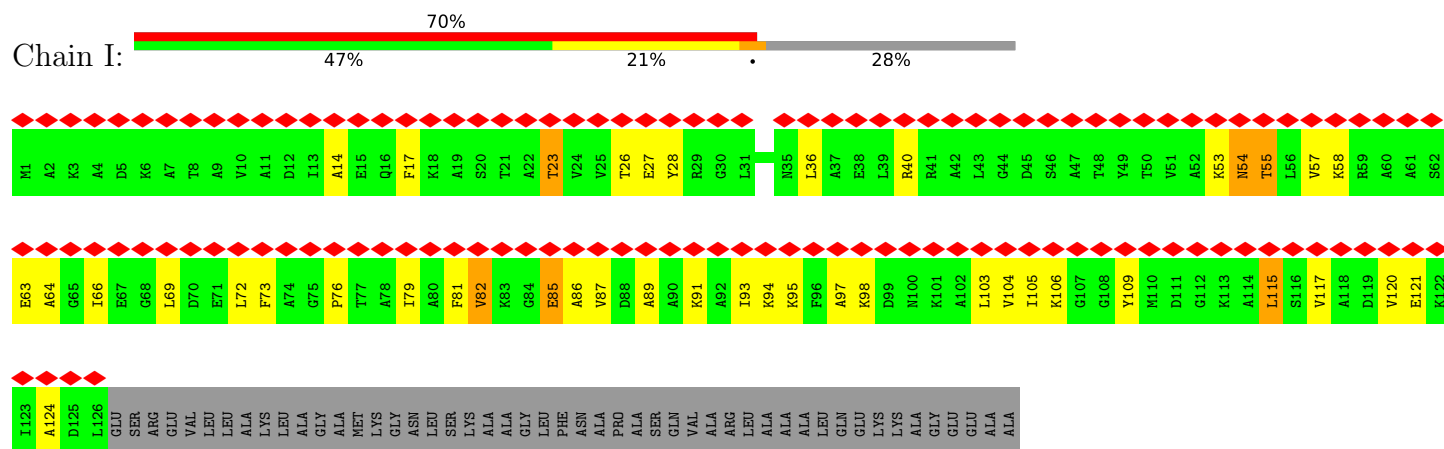
• Molecule 8: 50S ribosomal protein L6



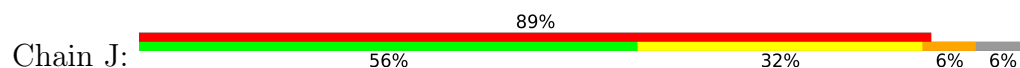
• Molecule 9: 50S ribosomal protein L9

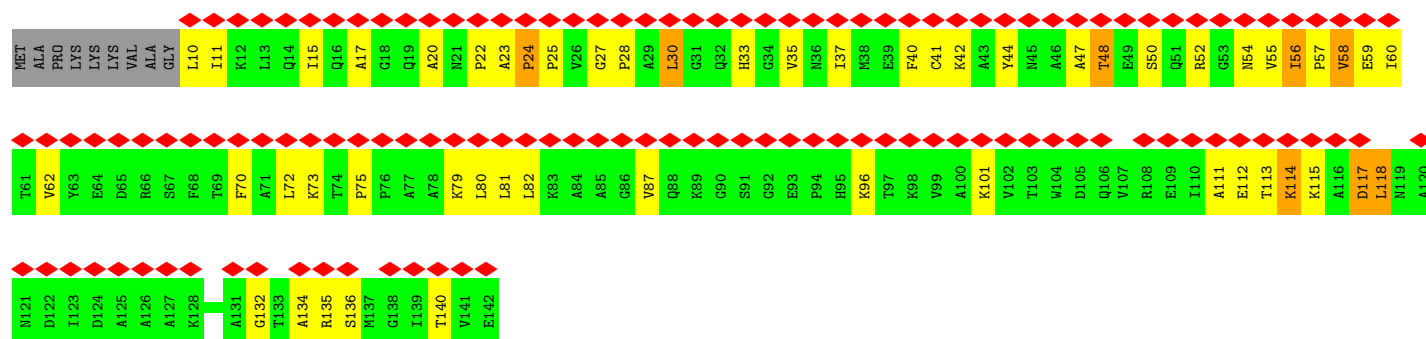


• Molecule 10: 50S ribosomal protein L10

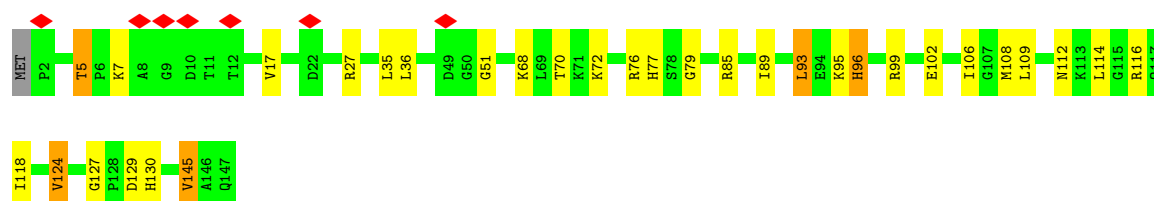
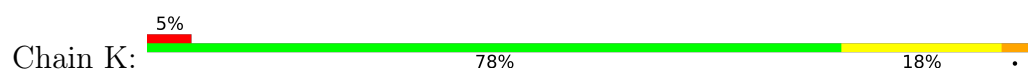


• Molecule 11: 50S ribosomal protein L11

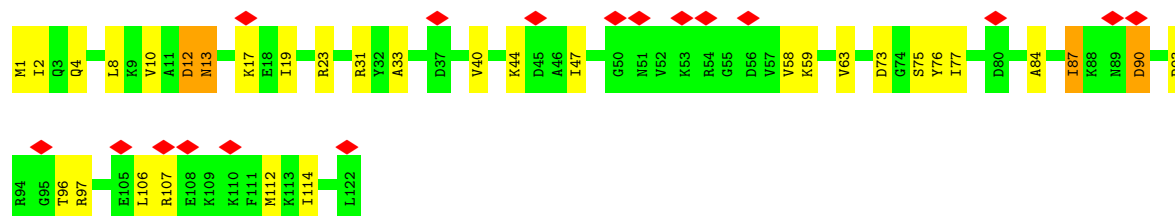
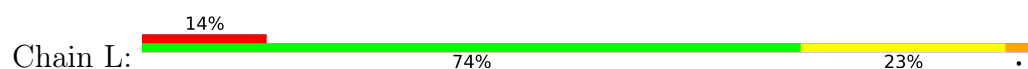




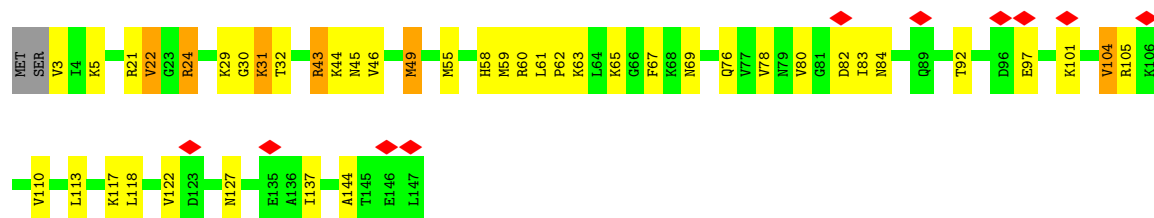
• Molecule 12: 50S ribosomal protein L13



• Molecule 13: 50S ribosomal protein L14



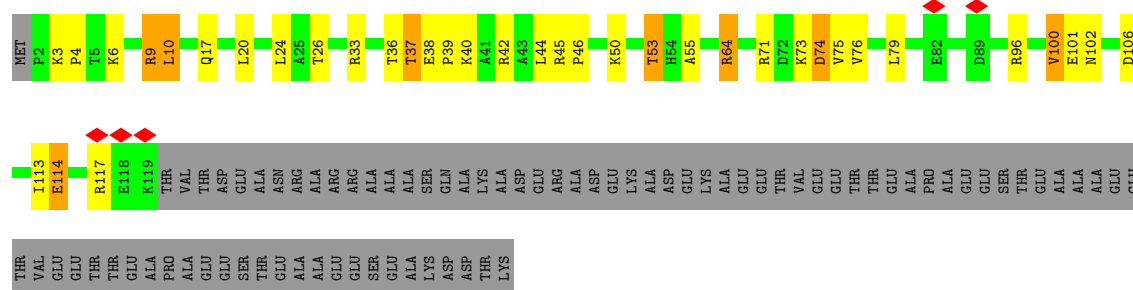
• Molecule 14: 50S ribosomal protein L15



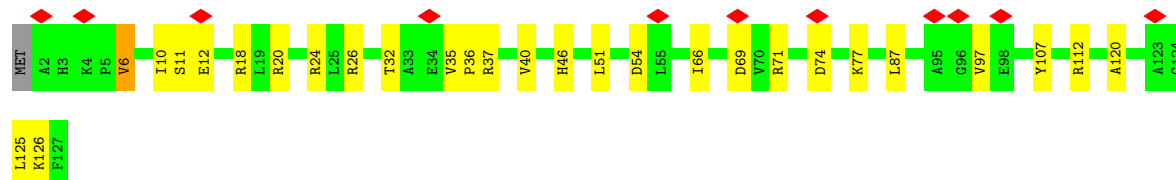
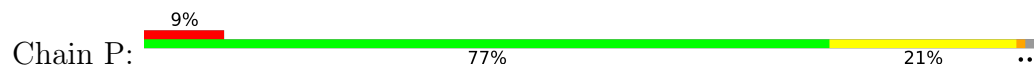
• Molecule 15: 50S ribosomal protein L16



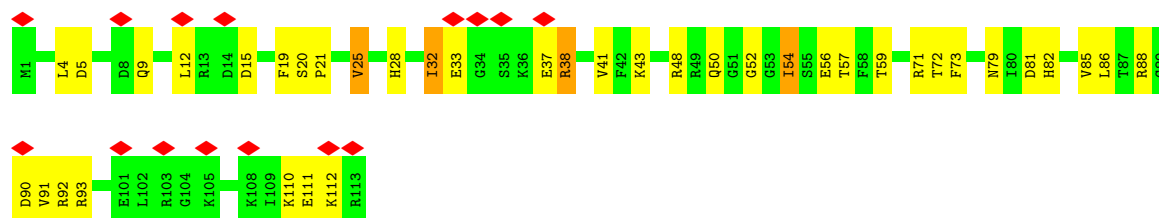
- Molecule 16: 50S ribosomal protein L17



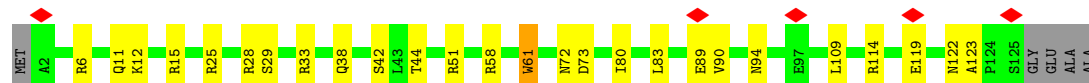
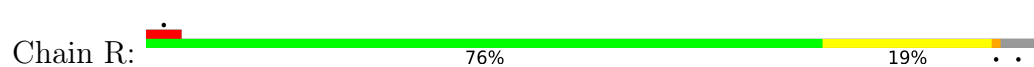
- Molecule 17: 50S ribosomal protein L18



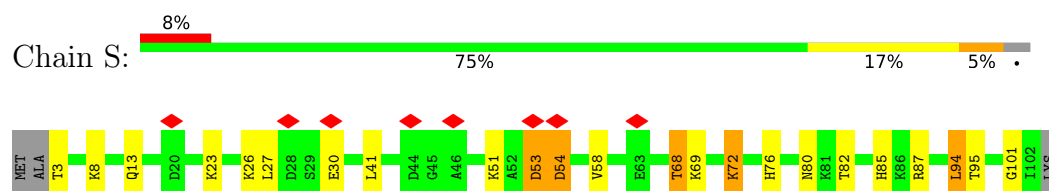
- Molecule 18: 50S ribosomal protein L19



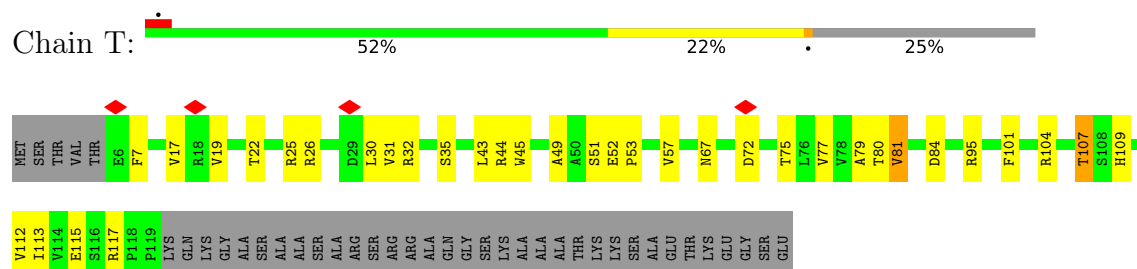
- Molecule 19: 50S ribosomal protein L20



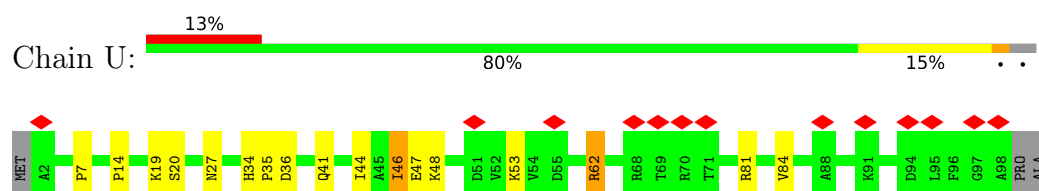
- Molecule 20: 50S ribosomal protein L21



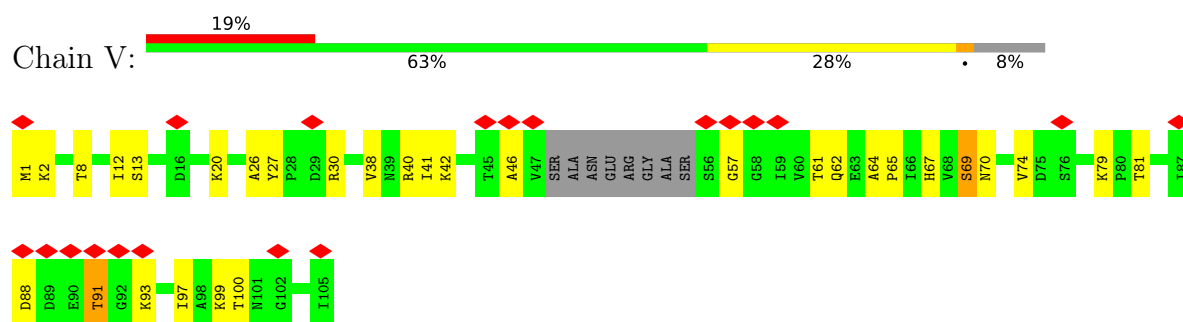
- Molecule 21: 50S ribosomal protein L22



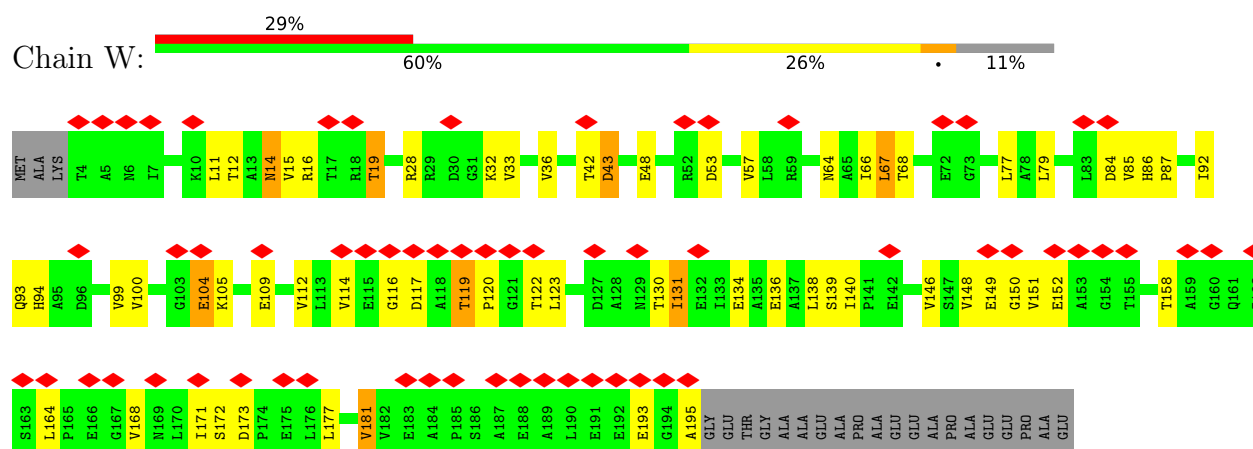
- Molecule 22: 50S ribosomal protein L23



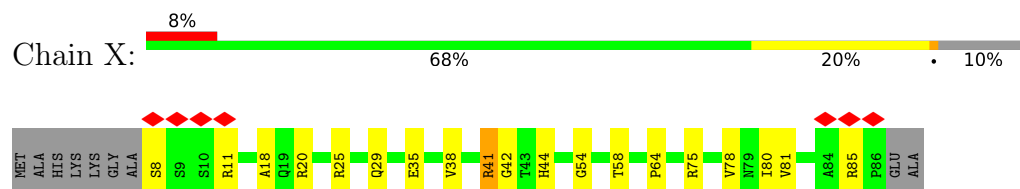
- Molecule 23: 50S ribosomal protein L24



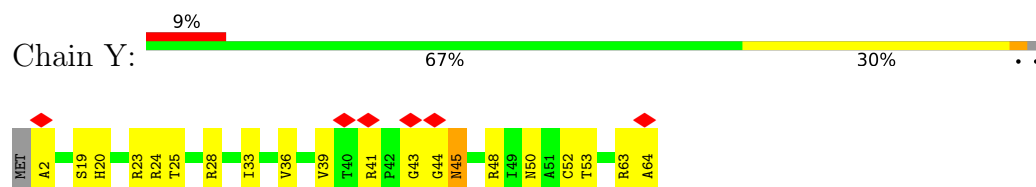
- Molecule 24: 50S ribosomal protein L25



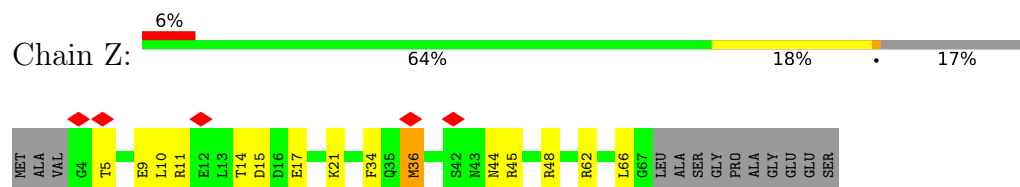
- Molecule 25: 50S ribosomal protein L27



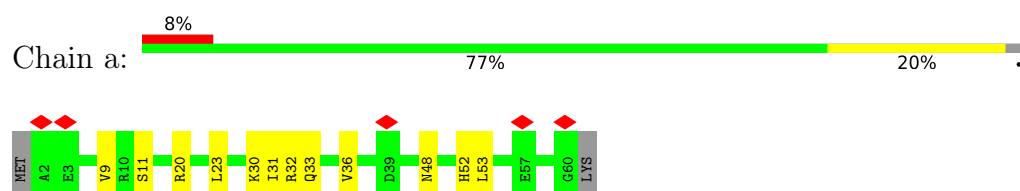
- Molecule 26: LSU ribosomal protein L28P



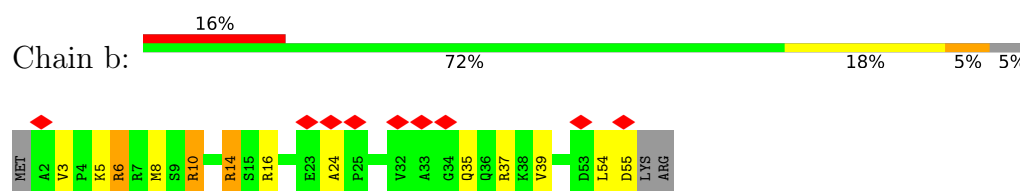
- Molecule 27: 50S ribosomal protein L29



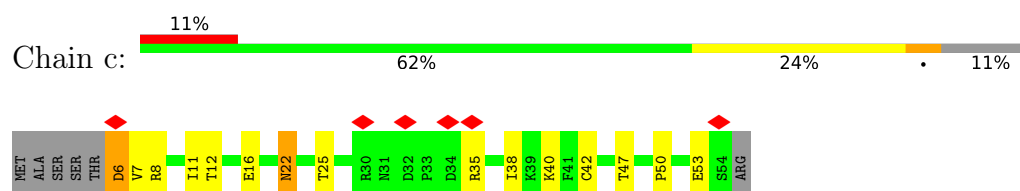
- Molecule 28: 50S ribosomal protein L30



- Molecule 29: 50S ribosomal protein L32

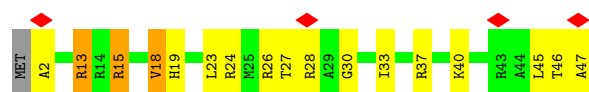


- Molecule 30: 50S ribosomal protein L33 1

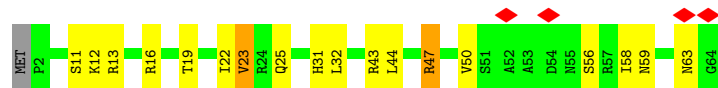


- Molecule 31: 50S ribosomal protein L34

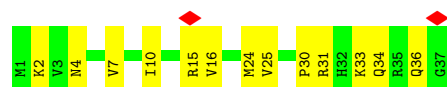




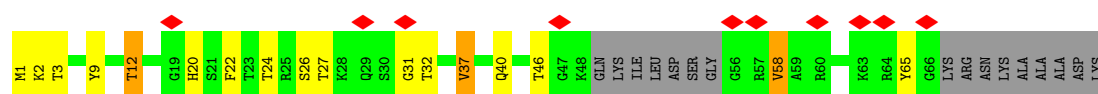
- Molecule 32: 50S ribosomal protein L35



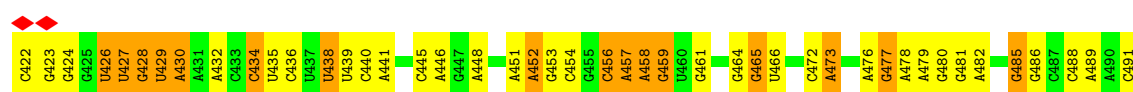
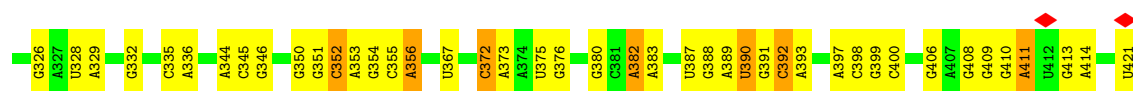
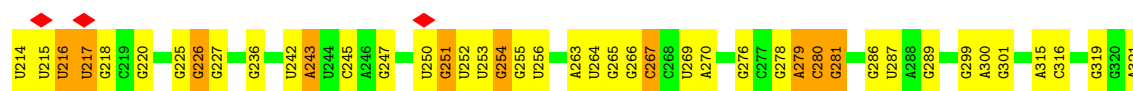
- Molecule 33: 50S ribosomal protein L36

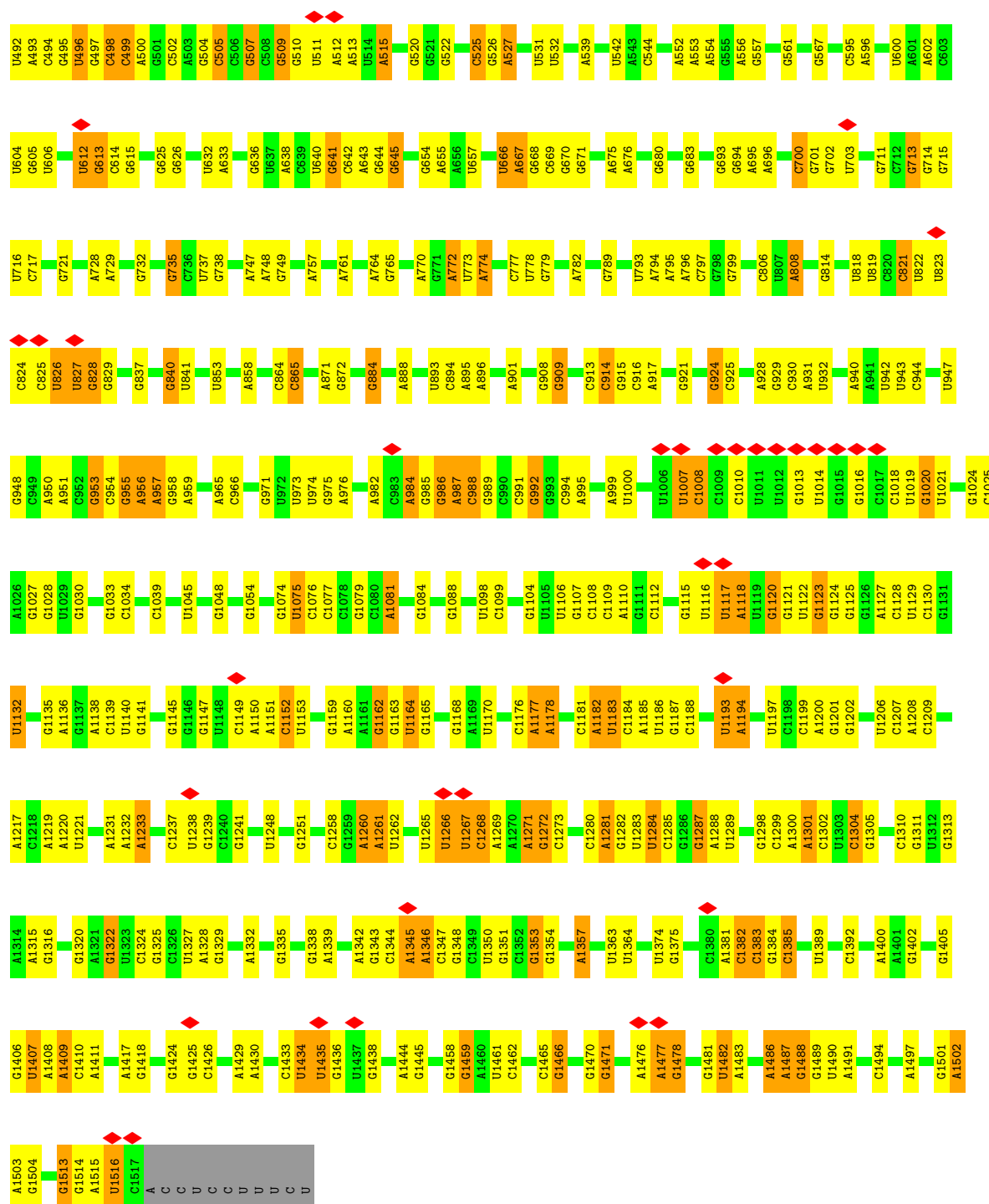


- Molecule 34: 50S ribosomal protein L31

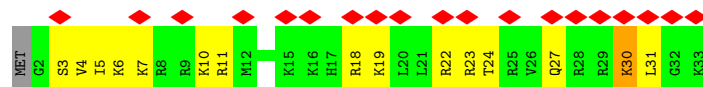


- Molecule 35: 16S rRNA

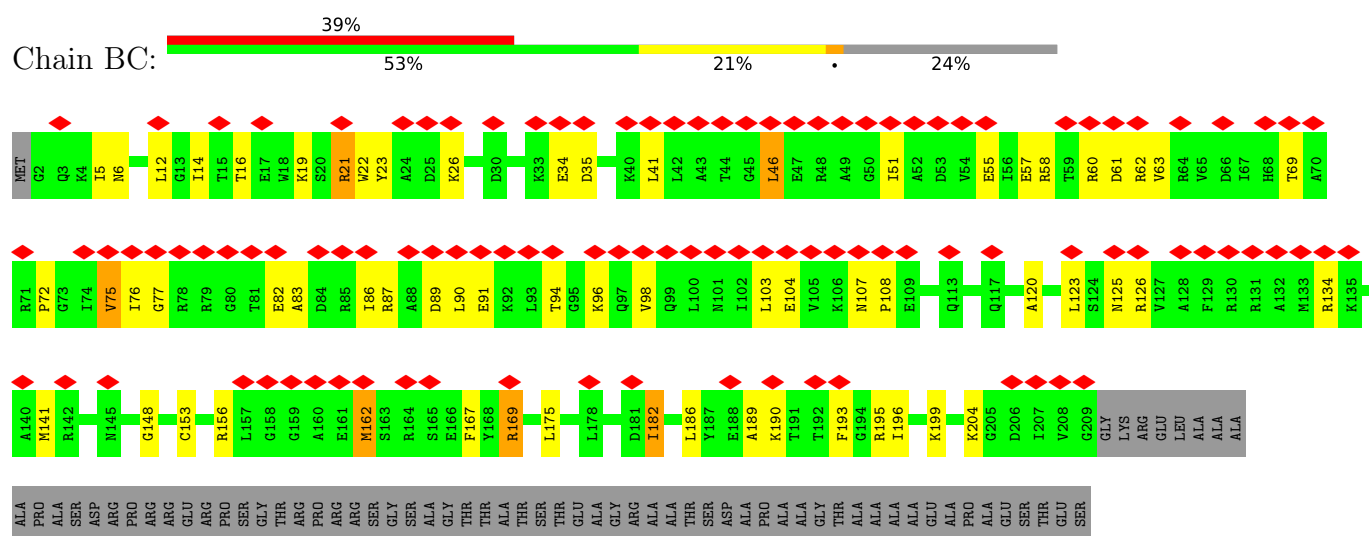




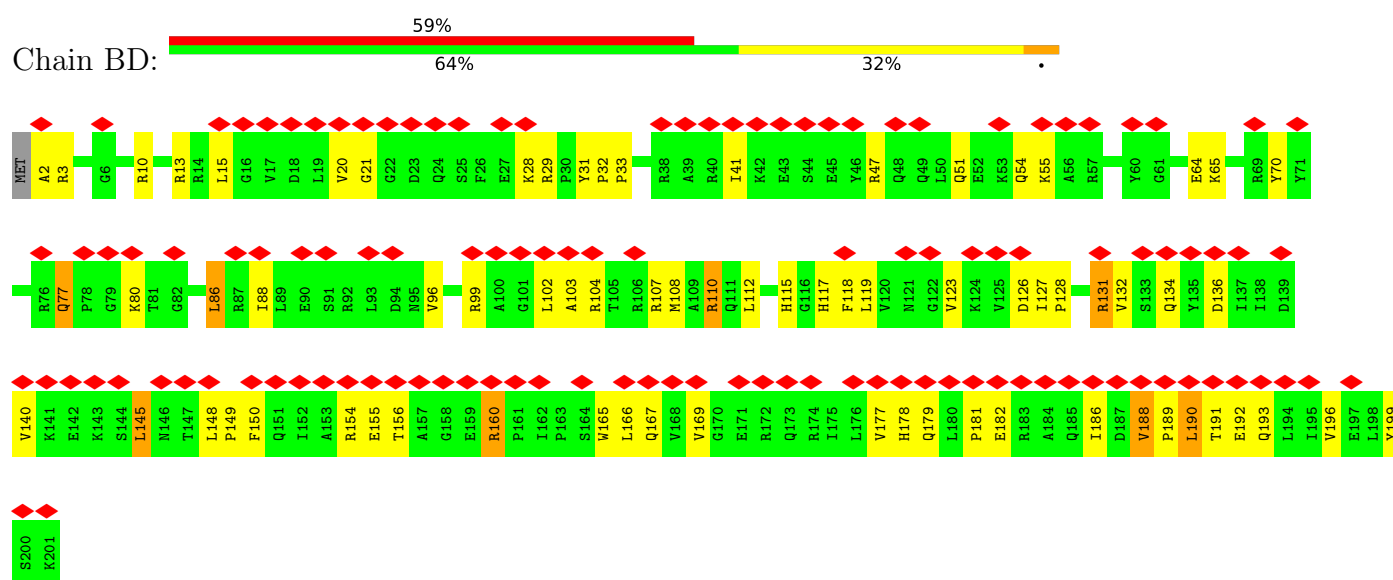
- Molecule 36: Conserved domain protein



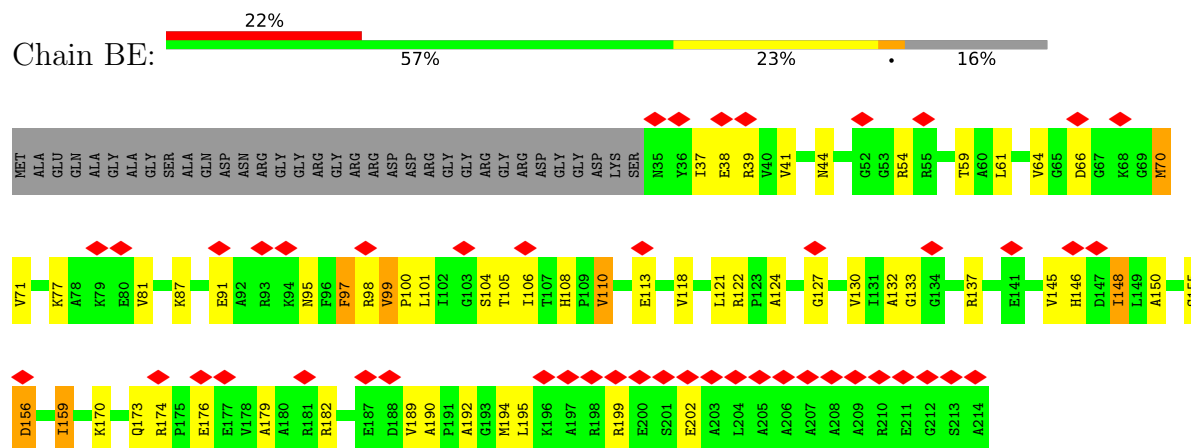
- Molecule 37: 30S ribosomal protein S3



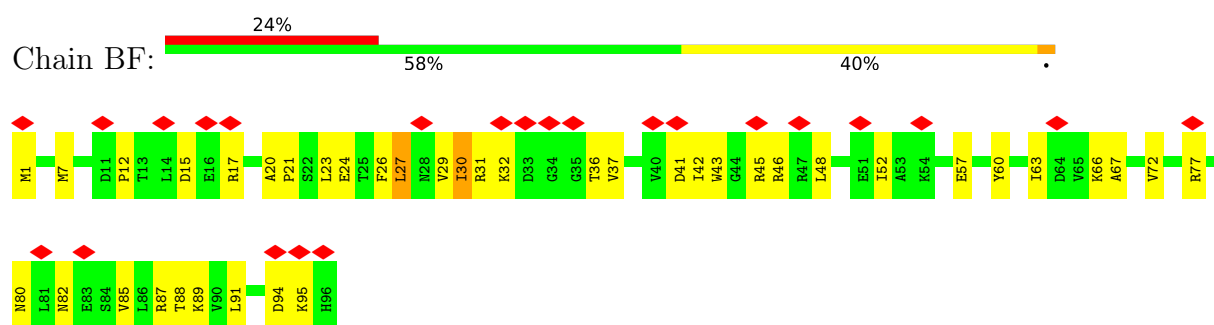
• Molecule 38: 30S ribosomal protein S4



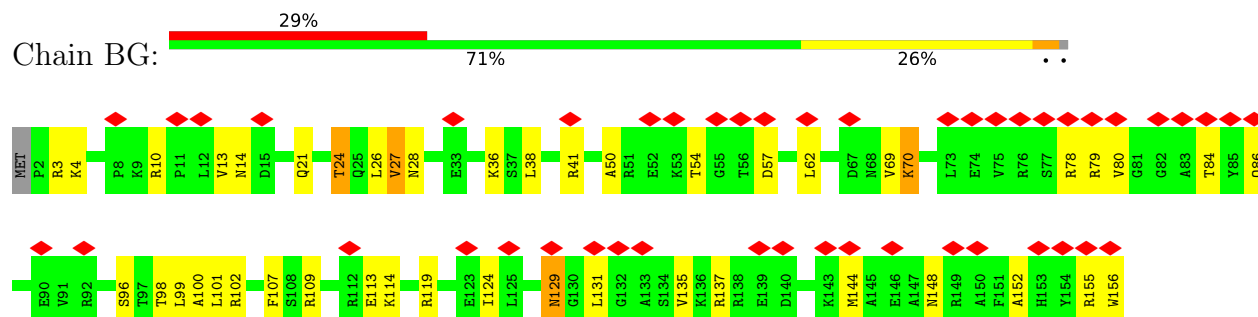
• Molecule 39: 30S ribosomal protein S5



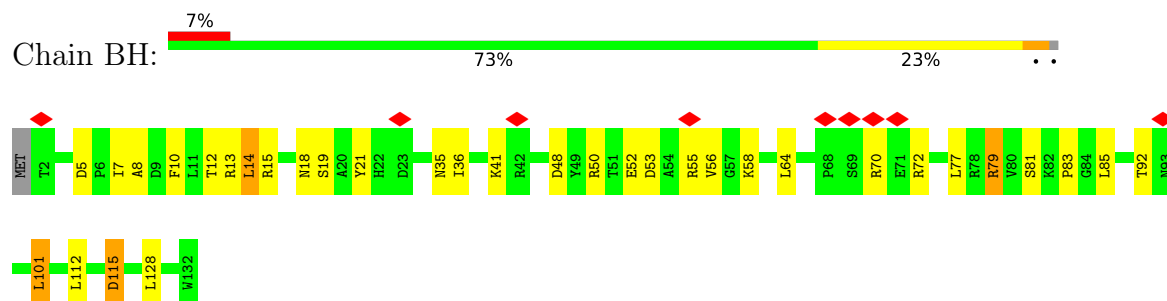
• Molecule 40: 30S ribosomal protein S6



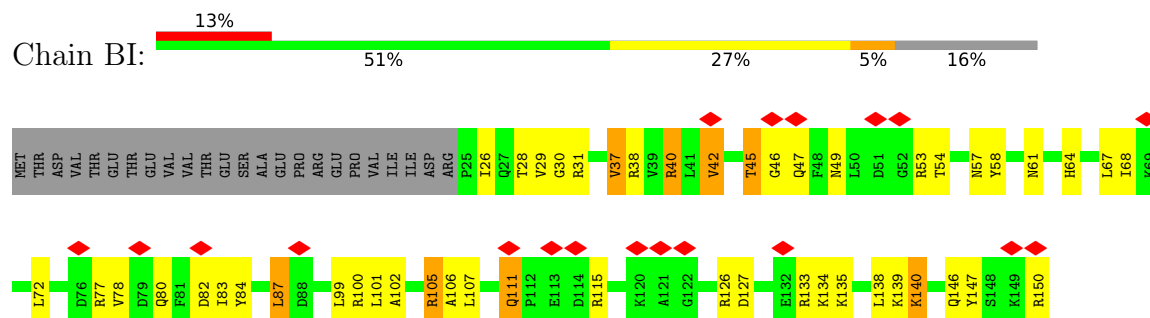
• Molecule 41: 30S ribosomal protein S7



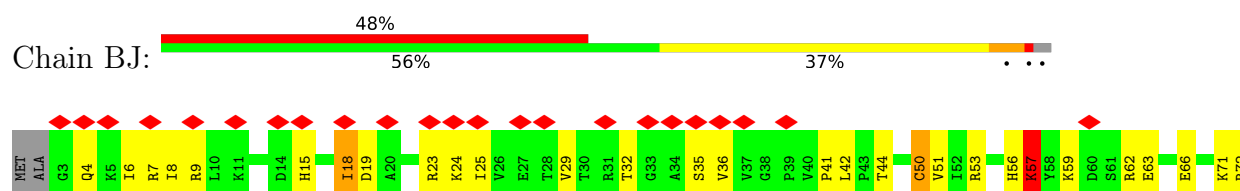
• Molecule 42: 30S ribosomal protein S8



• Molecule 43: 30S ribosomal protein S9

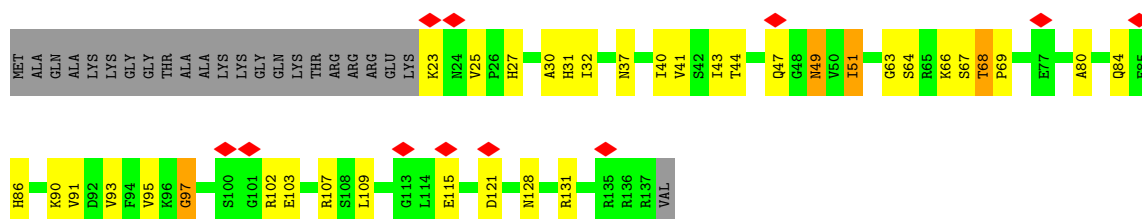


• Molecule 44: 30S ribosomal protein S10

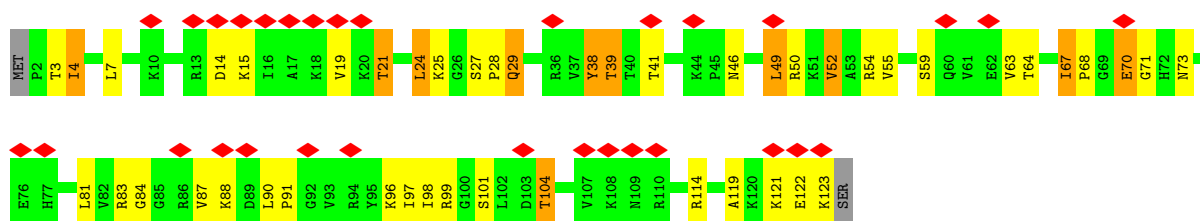




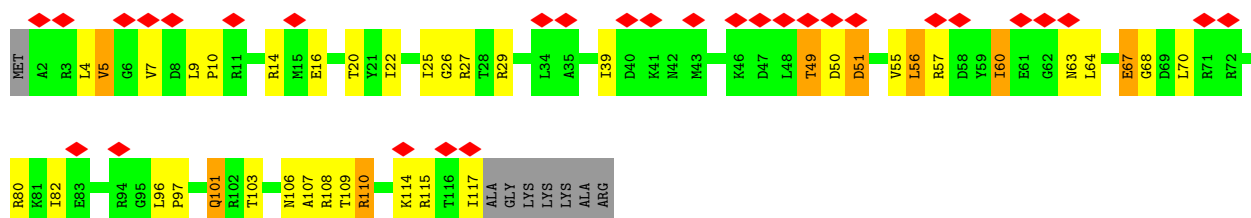
- Molecule 45: 30S ribosomal protein S11



- Molecule 46: 30S ribosomal protein S12



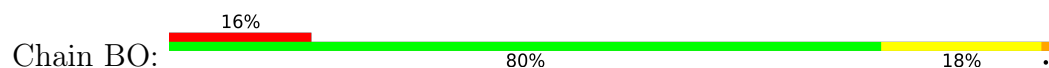
- Molecule 47: 30S ribosomal protein S13

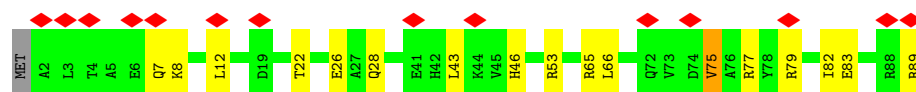


- Molecule 48: 30S ribosomal protein S14 type Z

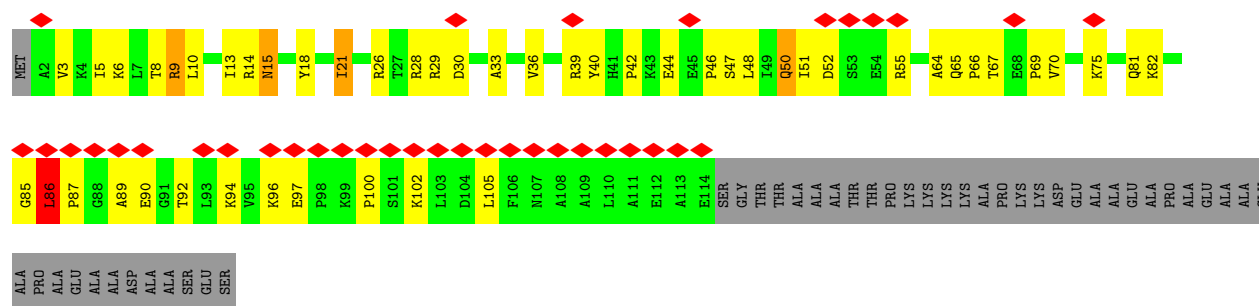
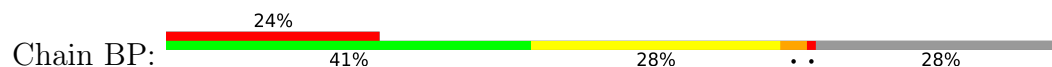


- Molecule 49: 30S ribosomal protein S15

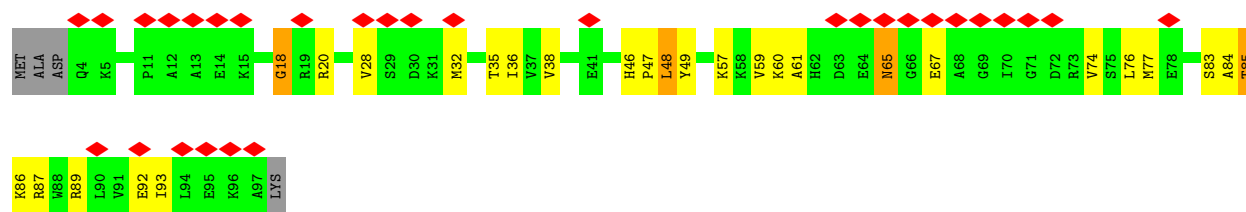




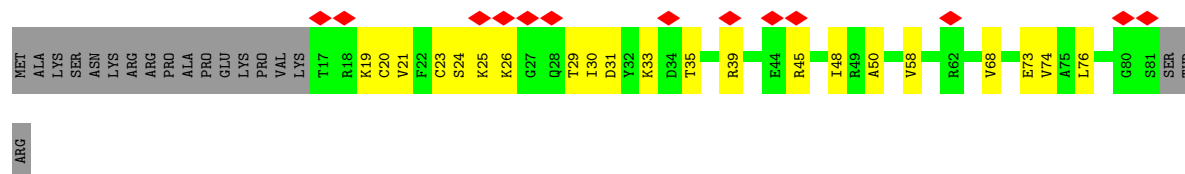
- Molecule 50: 30S ribosomal protein S16



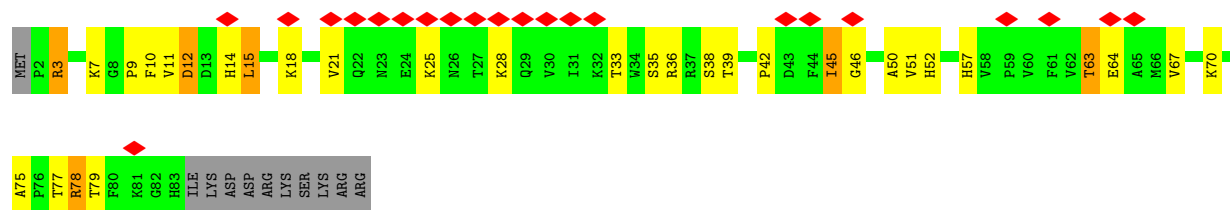
- Molecule 51: 30S ribosomal protein S17



- Molecule 52: 30S ribosomal protein S18 2

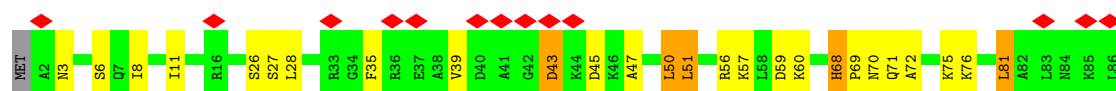


- Molecule 53: 30S ribosomal protein S19



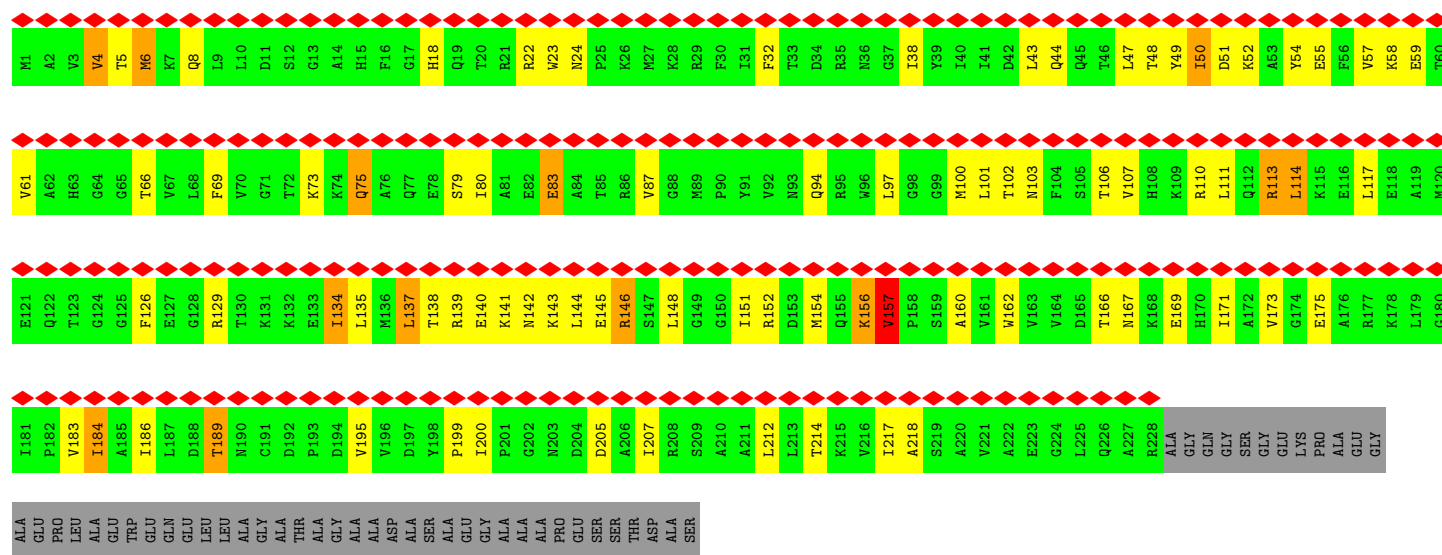
- Molecule 54: 30S ribosomal protein S20

Chain BT: 



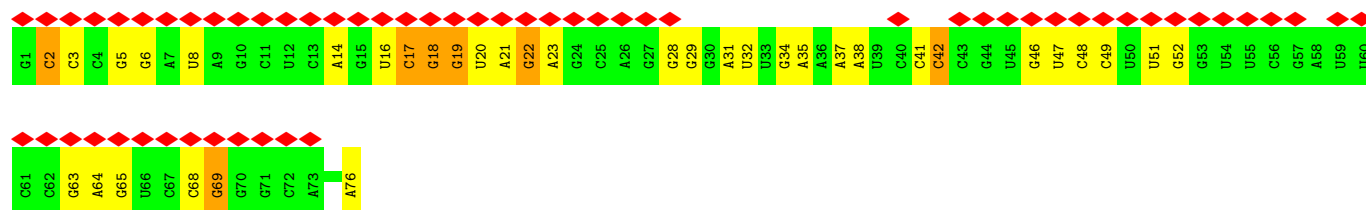
• Molecule 55: 30S ribosomal protein S2

Chain BV: 



• Molecule 56: P/P-site Phe-tRNA(Phe)

Chain BW: 



• Molecule 57: mRNA fragment

Chain BX: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	224584	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF correction in Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	100719	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.437	Depositor
Minimum map value	-0.187	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	300.24, 300.24, 300.24	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.39, 1.39, 1.39	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	3	0.58	0/191	0.85	0/247
2	A	0.37	0/75001	0.42	1/117027 (0.0%)
3	B	0.25	0/2821	0.36	0/4396
4	C	0.64	0/2153	1.00	4/2895 (0.1%)
5	D	0.64	0/1609	0.96	3/2165 (0.1%)
6	E	0.53	0/1592	0.95	4/2153 (0.2%)
7	F	0.47	0/1467	0.93	2/1973 (0.1%)
8	G	0.48	0/1369	0.90	2/1848 (0.1%)
9	H	0.64	0/1027	0.89	1/1398 (0.1%)
10	I	0.90	0/925	0.95	2/1246 (0.2%)
11	J	0.98	1/1006 (0.1%)	1.06	5/1364 (0.4%)
12	K	0.58	0/1157	0.98	8/1567 (0.5%)
13	L	0.59	0/946	0.90	1/1268 (0.1%)
14	M	0.57	0/1091	1.08	0/1457
15	N	0.62	0/1118	1.05	9/1506 (0.6%)
16	O	0.57	0/945	0.94	0/1267
17	P	0.47	0/966	0.91	3/1298 (0.2%)
18	Q	0.55	0/921	0.97	1/1236 (0.1%)
19	R	0.73	1/1000 (0.1%)	0.92	5/1341 (0.4%)
20	S	0.55	0/764	0.98	1/1030 (0.1%)
21	T	0.87	5/887 (0.6%)	1.03	6/1204 (0.5%)
22	U	0.56	0/766	0.93	0/1030
23	V	0.47	0/738	0.89	2/987 (0.2%)
24	W	0.50	0/1443	0.91	3/1970 (0.2%)
25	X	0.63	0/595	0.97	4/798 (0.5%)
26	Y	0.63	0/478	0.98	1/641 (0.2%)
27	Z	0.51	0/534	0.81	0/713
28	a	0.59	0/477	0.94	1/640 (0.2%)
29	b	0.60	0/427	0.85	0/572
30	c	0.53	0/413	1.02	2/553 (0.4%)
31	d	0.63	0/380	0.96	1/500 (0.2%)
32	e	0.56	0/507	0.88	0/672

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	f	0.62	0/303	1.06	1/401 (0.2%)
34	g	0.49	0/467	0.92	1/626 (0.2%)
35	BA	0.30	0/36309	0.41	1/56657 (0.0%)
36	BB	0.49	0/280	0.82	0/359
37	BC	0.49	0/1684	0.91	2/2261 (0.1%)
38	BD	0.74	4/1672 (0.2%)	1.02	10/2251 (0.4%)
39	BE	0.50	0/1312	0.97	4/1772 (0.2%)
40	BF	0.50	0/782	0.90	1/1059 (0.1%)
41	BG	0.52	0/1252	0.84	2/1690 (0.1%)
42	BH	0.46	0/1025	0.89	0/1385
43	BI	0.55	0/1012	0.88	4/1362 (0.3%)
44	BJ	0.59	0/802	0.93	2/1086 (0.2%)
45	BK	0.50	0/873	0.94	2/1180 (0.2%)
46	BL	0.53	0/969	0.95	3/1294 (0.2%)
47	BM	0.47	0/942	0.84	2/1260 (0.2%)
48	BN	0.40	0/488	0.97	3/650 (0.5%)
49	BO	0.45	0/729	0.82	0/977
50	BP	0.53	0/908	1.08	4/1226 (0.3%)
51	BQ	0.49	0/759	0.94	1/1016 (0.1%)
52	BR	0.52	0/518	0.90	1/693 (0.1%)
53	BS	0.71	3/680 (0.4%)	0.87	0/915
54	BT	0.52	0/663	0.90	2/882 (0.2%)
55	BV	0.77	1/1822 (0.1%)	0.88	0/2457
56	BW	0.36	0/1809	0.42	0/2819
57	BX	0.38	0/128	0.39	0/196
All	All	0.43	15/163902 (0.0%)	0.60	118/245436 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
21	T	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	BD	115	HIS	ND1-CE1	-13.58	1.19	1.32
21	T	109	HIS	CG-ND1	8.41	1.47	1.38
21	T	109	HIS	CE1-NE2	7.79	1.40	1.32
21	T	109	HIS	ND1-CE1	-7.78	1.24	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	BD	115	HIS	CG-CD2	7.22	1.43	1.35
53	BS	14	HIS	ND1-CE1	-6.95	1.25	1.32
53	BS	14	HIS	CG-ND1	6.18	1.45	1.38
21	T	109	HIS	CD2-NE2	-6.12	1.31	1.37
19	R	61	TRP	CD2-CE2	5.93	1.51	1.41
38	BD	115	HIS	CG-ND1	5.85	1.44	1.38
11	J	24	PRO	CA-C	5.79	1.57	1.52
53	BS	14	HIS	CE1-NE2	5.64	1.38	1.32
38	BD	115	HIS	CB-CG	-5.54	1.42	1.50
55	BV	157	VAL	CA-CB	5.51	1.61	1.54
21	T	109	HIS	CB-CG	-5.24	1.42	1.50

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	20	LEU	CA-C-N	9.70	129.79	119.90
6	E	20	LEU	C-N-CA	9.70	129.79	119.90
19	R	61	TRP	CG-CD2-CE3	9.34	143.24	133.90
30	c	42	CYS	CA-C-N	9.27	128.61	118.97
30	c	42	CYS	C-N-CA	9.27	128.61	118.97
12	K	130	HIS	CA-C-N	8.77	128.42	119.82
12	K	130	HIS	C-N-CA	8.77	128.42	119.82
15	N	125	LEU	CA-C-N	8.64	128.28	119.82
15	N	125	LEU	C-N-CA	8.64	128.28	119.82
44	BJ	57	LYS	CB-CA-C	-8.16	105.12	115.89
38	BD	115	HIS	ND1-CG-CD2	-7.90	98.20	106.10
11	J	27	GLY	CA-C-N	7.66	127.55	119.05
11	J	27	GLY	C-N-CA	7.66	127.55	119.05
6	E	94	LYS	CA-C-N	-7.55	111.97	119.90
6	E	94	LYS	C-N-CA	-7.55	111.97	119.90
4	C	245	HIS	CA-C-N	7.46	127.51	119.90
4	C	245	HIS	C-N-CA	7.46	127.51	119.90
5	D	160	VAL	N-CA-C	7.43	120.19	112.83
38	BD	32	PRO	CA-C-N	7.39	127.35	120.03
38	BD	32	PRO	C-N-CA	7.39	127.35	120.03
21	T	109	HIS	CG-CD2-NE2	7.35	114.55	107.20
48	BN	53	LEU	CA-C-N	7.27	128.92	119.84
48	BN	53	LEU	C-N-CA	7.27	128.92	119.84
15	N	72	ARG	CA-C-N	7.25	127.82	120.14
15	N	72	ARG	C-N-CA	7.25	127.82	120.14
50	BP	92	THR	N-CA-C	-7.20	104.10	113.17
21	T	109	HIS	ND1-CG-CD2	-7.18	98.92	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	BP	86	LEU	CA-C-N	-7.17	110.88	119.84
50	BP	86	LEU	C-N-CA	-7.17	110.88	119.84
33	f	10	ILE	N-CA-C	7.05	118.66	110.62
11	J	117	ASP	N-CA-C	7.01	122.00	113.17
19	R	61	TRP	CE2-CD2-CE3	-6.99	111.81	118.80
12	K	96	HIS	CA-C-N	6.66	126.91	119.32
12	K	96	HIS	C-N-CA	6.66	126.91	119.32
43	BI	42	VAL	CA-C-N	6.61	126.30	119.82
43	BI	42	VAL	C-N-CA	6.61	126.30	119.82
9	H	109	GLY	N-CA-C	6.58	125.77	112.34
38	BD	190	LEU	CB-CA-C	-6.45	107.31	116.34
31	d	18	VAL	N-CA-C	6.26	116.90	110.82
41	BG	57	ASP	CA-C-N	6.26	125.48	118.97
41	BG	57	ASP	C-N-CA	6.26	125.48	118.97
11	J	24	PRO	N-CA-C	6.22	118.28	110.70
38	BD	190	LEU	N-CA-C	6.18	117.14	108.00
19	R	123	ALA	CA-C-N	6.17	125.87	119.82
19	R	123	ALA	C-N-CA	6.17	125.87	119.82
51	BQ	18	GLY	N-CA-C	6.14	119.09	112.33
25	X	81	VAL	CA-C-N	6.13	127.50	119.84
25	X	81	VAL	C-N-CA	6.13	127.50	119.84
12	K	127	GLY	CA-C-N	6.08	125.70	119.56
12	K	127	GLY	C-N-CA	6.08	125.70	119.56
38	BD	77	GLN	CA-C-N	6.08	126.25	119.32
38	BD	77	GLN	C-N-CA	6.08	126.25	119.32
15	N	62	GLY	N-CA-C	-6.07	102.30	110.56
46	BL	67	ILE	CA-C-N	6.00	126.50	120.14
46	BL	67	ILE	C-N-CA	6.00	126.50	120.14
45	BK	97	GLY	CA-C-N	5.97	125.99	119.90
45	BK	97	GLY	C-N-CA	5.97	125.99	119.90
25	X	44	HIS	N-CA-C	-5.95	104.74	112.23
10	I	85	GLU	CB-CA-C	-5.93	108.06	115.89
7	F	87	ARG	NE-CZ-NH2	5.90	124.51	119.20
52	BR	25	LYS	N-CA-C	-5.81	106.19	113.28
7	F	92	ILE	N-CA-C	5.75	117.67	111.58
48	BN	24	CYS	N-CA-C	5.72	118.36	110.35
39	BE	99	VAL	CA-C-N	5.71	126.97	119.84
39	BE	99	VAL	C-N-CA	5.71	126.97	119.84
21	T	72	ASP	CA-C-N	5.70	125.38	119.05
21	T	72	ASP	C-N-CA	5.70	125.38	119.05
37	BC	77	GLY	N-CA-C	-5.67	104.83	112.14
5	D	76	ASN	CA-C-N	5.66	125.66	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	76	ASN	C-N-CA	5.66	125.66	119.89
8	G	156	ASP	CA-C-N	5.66	126.91	119.84
8	G	156	ASP	C-N-CA	5.66	126.91	119.84
39	BE	99	VAL	N-CA-C	5.63	114.03	107.89
43	BI	111	GLN	CA-C-N	5.60	125.70	119.32
43	BI	111	GLN	C-N-CA	5.60	125.70	119.32
37	BC	162	MET	N-CA-C	-5.59	98.89	110.80
24	W	116	GLY	N-CA-C	5.58	118.31	110.38
23	V	27	TYR	CA-C-N	5.57	125.93	119.47
23	V	27	TYR	C-N-CA	5.57	125.93	119.47
40	BF	67	ALA	N-CA-C	5.54	115.86	108.38
28	a	9	VAL	N-CA-C	5.52	116.17	110.82
34	g	3	THR	N-CA-C	5.49	116.95	110.97
11	J	118	LEU	N-CA-C	5.46	118.41	110.17
39	BE	81	VAL	CB-CA-C	-5.43	108.54	113.70
15	N	108	TYR	CA-C-N	5.40	124.86	119.24
15	N	108	TYR	C-N-CA	5.40	124.86	119.24
38	BD	160	ARG	CA-C-N	5.39	125.69	119.92
38	BD	160	ARG	C-N-CA	5.39	125.69	119.92
12	K	5	THR	CA-C-N	5.38	125.39	119.90
12	K	5	THR	C-N-CA	5.38	125.39	119.90
10	I	54	ASN	N-CA-C	5.37	116.94	111.14
25	X	42	GLY	N-CA-C	-5.29	104.47	112.41
46	BL	55	VAL	N-CA-C	5.27	115.55	108.17
2	A	2085	C	C2'-C3'-O3'	5.26	117.39	109.50
4	C	167	GLY	N-CA-C	5.26	119.17	110.55
54	BT	68	HIS	CA-C-N	5.21	125.26	119.32
54	BT	68	HIS	C-N-CA	5.21	125.26	119.32
19	R	61	TRP	CD2-CE3-CZ3	5.20	125.36	118.60
47	BM	67	GLU	N-CA-C	5.20	115.69	108.00
17	P	35	VAL	CA-C-N	5.15	125.13	120.03
17	P	35	VAL	C-N-CA	5.15	125.13	120.03
26	Y	44	GLY	N-CA-C	5.13	122.39	115.00
50	BP	13	ILE	N-CA-C	5.12	115.85	110.62
15	N	69	PHE	CA-C-N	5.10	126.21	119.84
15	N	69	PHE	C-N-CA	5.10	126.21	119.84
20	S	101	GLY	N-CA-C	5.09	118.53	111.10
24	W	173	ASP	CA-C-N	5.09	125.16	119.87
24	W	173	ASP	C-N-CA	5.09	125.16	119.87
44	BJ	57	LYS	N-CA-C	5.08	117.55	109.02
35	BA	1482	U	P-O3'-C3'	5.07	127.80	120.20
21	T	31	VAL	N-CA-C	5.06	117.84	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	12	ASP	N-CA-C	5.05	117.22	109.95
18	Q	5	ASP	N-CA-C	5.04	117.43	111.33
47	BM	67	GLU	CB-CA-C	-5.03	109.30	116.34
17	P	46	HIS	N-CA-C	5.01	114.91	108.34
38	BD	169	VAL	N-CA-C	5.01	117.79	112.83
4	C	238	GLY	N-CA-C	-5.01	103.30	110.46
21	T	109	HIS	CB-CG-CD2	5.00	137.70	131.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	T	117	ARG	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	189	0	205	4	0
2	A	66981	0	33699	520	0
3	B	2522	0	1285	13	0
4	C	2110	0	2165	75	0
5	D	1587	0	1630	41	0
6	E	1569	0	1607	43	0
7	F	1445	0	1476	44	0
8	G	1348	0	1399	32	0
9	H	1018	0	988	20	0
10	I	918	0	959	38	0
11	J	990	0	1021	30	0
12	K	1130	0	1167	24	0
13	L	938	0	1000	20	0
14	M	1078	0	1151	44	0
15	N	1092	0	1128	38	0
16	O	928	0	972	31	0
17	P	956	0	991	11	0
18	Q	907	0	938	27	0
19	R	988	0	1038	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	S	754	0	802	17	0
21	T	873	0	909	22	0
22	U	756	0	802	12	0
23	V	732	0	782	20	0
24	W	1428	0	1443	29	0
25	X	586	0	601	12	0
26	Y	470	0	480	15	0
27	Z	531	0	541	18	0
28	a	474	0	500	6	0
29	b	423	0	463	20	0
30	c	405	0	407	6	0
31	d	377	0	411	16	0
32	e	502	0	541	12	0
33	f	299	0	321	7	0
34	g	458	0	443	9	0
35	BA	32439	0	16320	337	0
36	BB	280	0	342	9	0
37	BC	1660	0	1707	39	0
38	BD	1641	0	1668	57	0
39	BE	1296	0	1360	37	0
40	BF	771	0	797	27	0
41	BG	1232	0	1282	30	0
42	BH	1010	0	1046	25	0
43	BI	994	0	1050	35	0
44	BJ	788	0	819	32	0
45	BK	855	0	863	19	0
46	BL	958	0	1045	32	0
47	BM	935	0	986	24	0
48	BN	477	0	499	15	0
49	BO	720	0	760	10	0
50	BP	891	0	935	35	0
51	BQ	748	0	795	17	0
52	BR	513	0	537	16	0
53	BS	662	0	677	22	0
54	BT	660	0	712	15	0
55	BV	1793	0	1839	54	0
56	BW	1619	0	821	23	0
57	BX	117	0	63	3	0
58	A	390	0	0	0	0
58	B	9	0	0	0	0
58	BA	215	0	0	0	0
58	BF	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	BR	1	0	0	0	0
58	C	4	0	0	0	0
58	F	1	0	0	0	0
58	M	1	0	0	0	0
58	N	1	0	0	0	0
58	T	1	0	0	0	0
58	c	1	0	0	0	0
59	BN	1	0	0	0	0
59	BR	1	0	0	0	0
59	Y	1	0	0	0	0
59	c	1	0	0	0	0
59	f	1	0	0	0	0
59	g	1	0	0	0	0
60	BW	11	0	8	0	0
All	All	151463	0	101196	1890	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 (1890) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BA:531:U:O2'	46:BL:83:ARG:NH1	1.92	1.01
2:A:1786:G:OP1	4:C:211:ARG:NH1	1.97	0.98
2:A:2509:C:OP2	30:c:8:ARG:NH1	1.97	0.98
2:A:2772:G:H1'	13:L:23:ARG:HH12	1.29	0.96
2:A:2279:C:OP1	29:b:5:LYS:NZ	1.98	0.96
2:A:142:C:H5''	22:U:41:GLN:HE21	1.32	0.94
37:BC:169:ARG:HH11	37:BC:169:ARG:HB2	1.31	0.94
2:A:2245:C:OP1	19:R:25:ARG:NH1	2.02	0.92
6:E:112:ARG:HG2	6:E:112:ARG:HH11	1.33	0.92
6:E:192:ASP:OD1	14:M:5:LYS:NZ	2.05	0.90
35:BA:1350:U:H5'	44:BJ:62:ARG:HH11	1.37	0.90
32:e:47:ARG:HH11	32:e:47:ARG:HB2	1.35	0.89
44:BJ:66:GLU:HB2	48:BN:59:SER:HB2	1.56	0.88
39:BE:132:ALA:O	39:BE:137:ARG:NH1	2.08	0.87
2:A:2343:G:O6	2:A:2399:A:N6	2.07	0.87
2:A:1612:U:H1'	40:BF:17:ARG:HH12	1.38	0.86
2:A:301:U:H5'	2:A:302:U:H5''	1.55	0.86
1:3:8:LYS:NZ	2:A:2253:A:OP2	2.08	0.85
40:BF:24:GLU:OE2	40:BF:31:ARG:NH1	2.09	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BA:1350:U:H5'	44:BJ:62:ARG:NH1	1.94	0.83
2:A:1730:U:H5''	2:A:1731:A:H8	1.43	0.83
35:BA:1301:A:OP1	53:BS:70:LYS:NZ	2.11	0.83
2:A:2357:A:H1'	2:A:2382:G:H21	1.41	0.83
2:A:1730:U:H5''	2:A:1731:A:C8	2.14	0.82
2:A:1552:A:H1'	2:A:1618:C:H42	1.45	0.81
2:A:2358:A:N6	2:A:2379:G:O2'	2.12	0.81
5:D:121:LYS:HG3	5:D:170:MET:HE3	1.60	0.81
10:I:40:ARG:HH11	10:I:40:ARG:HG3	1.46	0.81
2:A:1578:G:H22	2:A:1593:U:H3	1.24	0.81
35:BA:427:U:OP2	38:BD:29:ARG:NH1	2.15	0.80
2:A:2363:A:H61	2:A:2374:U:H3	1.27	0.80
2:A:2234:G:H5''	21:T:49:ALA:HB2	1.61	0.80
45:BK:90:LYS:HG3	45:BK:115:GLU:HB2	1.63	0.80
2:A:1365:G:OP2	14:M:24:ARG:NH1	2.16	0.79
47:BM:20:THR:HG23	47:BM:26:GLY:HA2	1.65	0.79
35:BA:986:G:N1	35:BA:1016:G:O6	2.16	0.78
29:b:37:ARG:HH11	29:b:54:LEU:HB3	1.45	0.78
35:BA:644:G:H22	35:BA:721:G:H1	1.30	0.78
35:BA:1287:G:HO2'	35:BA:1288:A:H8	1.32	0.78
29:b:10:ARG:HG2	29:b:14:ARG:NH1	1.99	0.78
40:BF:12:PRO:O	40:BF:45:ARG:NH1	2.17	0.78
44:BJ:63:GLU:OE1	48:BN:45:ARG:NH1	2.15	0.78
35:BA:393:A:OP1	50:BP:14:ARG:NH2	2.16	0.77
29:b:10:ARG:HG2	29:b:14:ARG:HH12	1.50	0.77
2:A:160:A:H3'	2:A:161:U:H5''	1.66	0.77
2:A:2032:A:OP2	4:C:54:LYS:NZ	2.18	0.77
49:BO:26:GLU:OE2	49:BO:77:ARG:NH1	2.17	0.77
41:BG:10:ARG:HH11	41:BG:10:ARG:HG3	1.50	0.77
3:B:41:U:O4	34:g:1:MET:N	2.16	0.77
2:A:1541:G:OP2	2:A:1629:G:N2	2.17	0.77
19:R:114:ARG:HG3	19:R:114:ARG:HH11	1.50	0.77
13:L:17:LYS:HE3	13:L:47:ILE:HG22	1.67	0.76
2:A:1825:C:N4	2:A:1840:G:OP2	2.18	0.76
2:A:2386:U:OP1	2:A:2393:A:O2'	2.03	0.76
1:3:21:ARG:HG2	1:3:22:PRO:HD2	1.67	0.76
23:V:88:ASP:HB2	23:V:93:LYS:HB2	1.67	0.76
54:BT:35:PHE:HA	54:BT:50:LEU:HD21	1.67	0.76
35:BA:392:C:OP1	50:BP:9:ARG:NH2	2.18	0.76
2:A:249:C:O2	32:e:12:LYS:NZ	2.17	0.76
19:R:28:ARG:NH1	19:R:38:GLN:OE1	2.18	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:290:C:H42	2:A:298:G:H22	1.35	0.75
27:Z:5:THR:HG21	27:Z:21:LYS:HZ1	1.51	0.75
35:BA:1177:A:O2'	35:BA:1178:A:OP1	2.02	0.75
2:A:1530:G:H22	2:A:1805:G:H1	1.35	0.75
2:A:543:U:H3'	2:A:544:U:H5''	1.69	0.74
2:A:2044:U:OP2	4:C:222:ARG:NH1	2.19	0.74
4:C:80:ALA:O	4:C:113:GLN:NE2	2.20	0.74
8:G:55:ARG:HH12	8:G:63:ARG:HG3	1.49	0.74
26:Y:36:VAL:HG12	26:Y:63:ARG:HH21	1.50	0.74
2:A:2587:U:OP2	32:e:43:ARG:NH2	2.20	0.74
14:M:43:ARG:HG3	14:M:43:ARG:HH11	1.53	0.74
19:R:73:ASP:O	19:R:114:ARG:NH2	2.20	0.74
15:N:18:ARG:O	15:N:98:LYS:NZ	2.18	0.73
41:BG:69:VAL:HG23	41:BG:100:ALA:HB1	1.70	0.73
35:BA:413:G:N7	38:BD:28:LYS:NZ	2.31	0.73
56:BW:49:C:H42	56:BW:65:G:H1	1.35	0.73
7:F:75:ARG:HH21	7:F:95:ARG:NH1	1.86	0.73
2:A:556:G:OP2	31:d:40:LYS:NZ	2.21	0.73
20:S:76:HIS:HE1	20:S:85:HIS:HB3	1.54	0.73
53:BS:3:ARG:NH1	53:BS:10:PHE:HB2	2.04	0.73
2:A:679:G:OP2	14:M:24:ARG:NH2	2.21	0.72
43:BI:126:ARG:NH1	43:BI:127:ASP:O	2.22	0.72
29:b:6:ARG:HH11	29:b:6:ARG:HG3	1.54	0.72
2:A:1612:U:H2'	2:A:1613:G:C8	2.24	0.72
26:Y:41:ARG:HG2	26:Y:43:GLY:H	1.55	0.72
2:A:2332:U:H1'	2:A:2404:G:H21	1.52	0.72
14:M:84:ASN:HD21	14:M:118:LEU:HA	1.52	0.72
47:BM:5:VAL:HG21	47:BM:60:ILE:HD11	1.70	0.72
55:BV:18:HIS:HB3	55:BV:22:ARG:HD2	1.71	0.72
2:A:383:U:O4	23:V:79:LYS:NZ	2.22	0.72
35:BA:1332:A:OP2	43:BI:140:LYS:NZ	2.16	0.71
2:A:860:G:HO2'	2:A:863:G:HO2'	1.38	0.71
2:A:1551:U:H3	2:A:1619:U:H3	1.39	0.71
37:BC:141:MET:HE1	37:BC:148:GLY:HA2	1.73	0.71
2:A:2975:G:H4'	8:G:4:ILE:HD11	1.73	0.71
2:A:1257:G:H5''	12:K:72:LYS:NZ	2.06	0.70
6:E:112:ARG:HH11	6:E:112:ARG:CG	2.05	0.70
4:C:247:VAL:HG12	4:C:253:PRO:HA	1.73	0.70
19:R:89:GLU:OE1	20:S:8:LYS:NZ	2.22	0.70
35:BA:531:U:HO2'	46:BL:83:ARG:NH1	1.89	0.70
43:BI:135:LYS:HB2	43:BI:138:LEU:HD12	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BA:819:U:H3	35:BA:829:G:H1	1.39	0.70
2:A:2914:A:OP1	16:O:9:ARG:NH1	2.24	0.70
21:T:81:VAL:HG13	21:T:112:VAL:HG22	1.74	0.70
4:C:126:LYS:HD3	4:C:127:PRO:HD2	1.72	0.70
38:BD:10:ARG:HD2	38:BD:33:PRO:HG3	1.72	0.70
10:I:17:PHE:CE2	10:I:64:ALA:HB3	2.27	0.70
2:A:2348:G:O2'	2:A:2396:A:N6	2.22	0.69
10:I:94:LYS:NZ	10:I:121:GLU:HA	2.07	0.69
20:S:87:ARG:HH11	20:S:87:ARG:HG3	1.57	0.69
39:BE:70:MET:HE1	39:BE:98:ARG:HG3	1.72	0.69
2:A:753:A:H61	2:A:762:U:H3	1.40	0.69
2:A:2529:A:H5''	7:F:138:GLY:HA3	1.72	0.69
29:b:6:ARG:HH11	29:b:6:ARG:CG	2.06	0.69
50:BP:44:GLU:HB3	50:BP:47:SER:HA	1.72	0.69
50:BP:48:LEU:HB2	50:BP:96:LYS:HE3	1.73	0.69
50:BP:46:PRO:HG3	50:BP:96:LYS:HA	1.73	0.69
35:BA:772:A:O2'	35:BA:774:A:N7	2.25	0.69
2:A:1187:A:H5''	2:A:1188:A:C8	2.27	0.69
2:A:2343:G:N2	2:A:2401:U:O2	2.23	0.69
2:A:2862:G:O2'	2:A:3002:A:N6	2.26	0.69
39:BE:61:LEU:HD22	39:BE:159:ILE:HD13	1.75	0.69
35:BA:1375:G:H21	35:BA:1486:A:H8	1.41	0.69
37:BC:58:ARG:HG2	37:BC:63:VAL:HG22	1.74	0.69
2:A:1493:A:OP1	31:d:13:ARG:NH2	2.25	0.68
2:A:2276:G:H4'	5:D:153:GLY:O	1.93	0.68
10:I:23:THR:HG23	10:I:109:TYR:HB3	1.75	0.68
55:BV:6:MET:HG2	55:BV:47:LEU:HD11	1.76	0.68
41:BG:129:ASN:HB2	41:BG:131:LEU:HG	1.73	0.68
55:BV:114:LEU:HD13	55:BV:152:ARG:HH11	1.56	0.68
2:A:1187:A:H5''	2:A:1188:A:H8	1.59	0.68
7:F:136:THR:HG23	7:F:162:THR:HB	1.74	0.68
35:BA:700:C:H5'	52:BR:50:ALA:HA	1.74	0.68
35:BA:1300:A:OP1	53:BS:3:ARG:NH2	2.27	0.68
2:A:290:C:N4	2:A:298:G:H22	1.90	0.68
35:BA:184:U:H5''	54:BT:81:LEU:HD13	1.76	0.68
46:BL:54:ARG:HH11	46:BL:64:THR:HG23	1.56	0.68
14:M:137:ILE:HG21	14:M:144:ALA:HB2	1.76	0.67
35:BA:953:G:O2'	35:BA:1348:G:O2'	2.06	0.67
2:A:1673:A:O2'	2:A:2926:A:OP2	2.12	0.67
11:J:40:PHE:HE1	11:J:58:VAL:HG21	1.59	0.67
35:BA:1304:C:OP1	53:BS:78:ARG:NH2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:51:ARG:NH2	24:W:193:GLU:O	2.27	0.67
35:BA:821:C:H42	35:BA:826:U:H3	1.42	0.67
2:A:553:G:OP1	31:d:15:ARG:NH2	2.27	0.67
35:BA:1486:A:H2	35:BA:1489:G:H1	1.42	0.67
4:C:132:PRO:HD3	4:C:190:ARG:HH11	1.60	0.67
27:Z:10:LEU:HD21	27:Z:21:LYS:NZ	2.10	0.67
2:A:997:G:H1	2:A:1010:U:H3	1.43	0.67
2:A:2618:C:H5''	14:M:63:LYS:HD2	1.77	0.67
39:BE:113:GLU:HG2	39:BE:118:VAL:HG22	1.77	0.67
40:BF:29:VAL:HA	40:BF:32:LYS:HE2	1.76	0.67
2:A:639:C:HO2'	2:A:640:G:H8	1.41	0.66
2:A:706:G:O2'	6:E:160:ARG:NH2	2.28	0.66
2:A:1456:G:OP1	2:A:1820:U:O2'	2.13	0.66
42:BH:79:ARG:NE	42:BH:81:SER:O	2.28	0.66
2:A:994:A:N6	2:A:1014:G:O2'	2.26	0.66
2:A:2882:C:H5''	8:G:159:LYS:HD2	1.78	0.66
2:A:2862:G:OP1	5:D:85:ARG:NH1	2.28	0.66
44:BJ:59:LYS:HE2	44:BJ:62:ARG:NH2	2.11	0.66
11:J:96:LYS:HE2	24:W:120:PRO:HB2	1.78	0.66
2:A:2626:U:H4'	2:A:2627:C:OP2	1.96	0.66
3:B:76:G:H5''	24:W:19:THR:HG21	1.77	0.66
35:BA:1289:U:H5''	47:BM:101:GLN:HE22	1.60	0.66
2:A:75:U:H5'	27:Z:11:ARG:HH22	1.60	0.66
35:BA:1160:A:OP2	43:BI:115:ARG:NH2	2.29	0.66
35:BA:984:A:H61	35:BA:1018:C:H42	1.43	0.66
2:A:164:A:O2'	26:Y:41:ARG:NH1	2.29	0.65
35:BA:507:G:O6	46:BL:46:ASN:ND2	2.28	0.65
35:BA:1018:C:H2'	35:BA:1019:U:C6	2.30	0.65
37:BC:76:ILE:HG22	37:BC:83:ALA:HB2	1.77	0.65
56:BW:35:A:H61	57:BX:5:C:H42	1.44	0.65
2:A:164:A:H4'	26:Y:41:ARG:HH12	1.62	0.65
2:A:2735:U:O2'	5:D:148:PRO:O	2.14	0.65
3:B:81:U:OP1	15:N:18:ARG:NH2	2.26	0.65
4:C:19:SER:HB2	4:C:204:ILE:HD11	1.77	0.65
38:BD:55:LYS:HB2	38:BD:190:LEU:HD11	1.78	0.65
40:BF:26:PHE:HZ	40:BF:82:ASN:HD22	1.43	0.65
41:BG:26:LEU:HD13	41:BG:101:LEU:HD22	1.77	0.65
2:A:1551:U:H3'	2:A:1552:A:H8	1.62	0.65
35:BA:11:G:H1	39:BE:122:ARG:HH11	1.45	0.65
35:BA:315:A:N7	35:BA:328:U:H5	1.95	0.65
35:BA:1117:U:H1'	35:BA:1118:A:H5''	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:BE:179:ALA:HA	39:BE:189:VAL:HG21	1.79	0.65
56:BW:51:U:H3	56:BW:63:G:H1	1.44	0.65
2:A:333:C:H2'	2:A:334:G:H8	1.61	0.65
39:BE:101:LEU:HD21	39:BE:145:VAL:HG22	1.77	0.65
2:A:659:U:OP2	14:M:31:LYS:NZ	2.28	0.65
10:I:36:LEU:O	10:I:40:ARG:HG2	1.97	0.65
35:BA:1434:U:O2'	35:BA:1435:U:H5''	1.95	0.65
2:A:1072:G:OP1	15:N:87:LYS:NZ	2.25	0.65
37:BC:90:LEU:HD13	37:BC:98:VAL:HG11	1.79	0.65
47:BM:14:ARG:NH2	47:BM:16:GLU:OE2	2.30	0.65
2:A:1084:U:O2'	2:A:1085:G:OP1	2.14	0.65
6:E:118:ARG:HH12	14:M:3:VAL:HG13	1.62	0.65
2:A:3113:A:H4'	2:A:3114:A:OP2	1.98	0.64
18:Q:32:ILE:HG22	18:Q:37:GLU:HG2	1.79	0.64
2:A:2708:G:OP1	15:N:45:ARG:NH1	2.29	0.64
2:A:1875:U:H4'	5:D:143:ALA:HB1	1.79	0.64
37:BC:72:PRO:HD3	37:BC:104:GLU:HB3	1.79	0.64
38:BD:112:LEU:HB3	38:BD:118:PHE:HE1	1.62	0.64
2:A:1002:C:H2'	2:A:1003:A:H5''	1.79	0.64
35:BA:525:C:OP2	38:BD:54:GLN:NE2	2.25	0.64
39:BE:70:MET:HE3	39:BE:98:ARG:NH1	2.13	0.64
2:A:2795:C:O2'	5:D:156:THR:O	2.16	0.64
7:F:130:ASP:O	7:F:132:THR:N	2.26	0.64
12:K:76:ARG:HB3	12:K:85:ARG:NH1	2.12	0.64
35:BA:481:G:H2'	35:BA:482:A:C8	2.32	0.64
2:A:1457:A:O2'	2:A:1459:U:OP2	2.15	0.64
8:G:35:LEU:HD11	8:G:72:LEU:HB3	1.79	0.64
43:BI:150:ARG:NH1	56:BW:35:A:OP2	2.31	0.64
35:BA:436:C:H5''	38:BD:148:LEU:HD12	1.79	0.64
35:BA:858:A:H1'	42:BH:12:THR:HG21	1.80	0.64
2:A:1260:C:H6	12:K:27:ARG:HH12	1.46	0.64
2:A:2424:C:OP1	26:Y:48:ARG:NH2	2.31	0.64
14:M:43:ARG:HH11	14:M:43:ARG:CG	2.10	0.64
31:d:37:ARG:NH1	31:d:45:LEU:O	2.29	0.64
34:g:37:VAL:HG22	47:BM:57:ARG:HH12	1.62	0.64
35:BA:1400:A:H5'	36:BB:31:LEU:HD21	1.79	0.63
38:BD:47:ARG:HG2	38:BD:47:ARG:HH11	1.63	0.63
2:A:2350:G:O2'	2:A:2351:A:O4'	2.13	0.63
2:A:2404:G:H2'	2:A:2405:A:C8	2.34	0.63
2:A:2412:U:H2'	2:A:2413:G:C8	2.32	0.63
35:BA:1130:C:OP1	43:BI:31:ARG:NH1	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BA:438:U:P	38:BD:117:HIS:HE2	2.21	0.63
35:BA:1471:G:OP1	36:BB:23:ARG:NH2	2.32	0.63
55:BV:117:LEU:HB3	55:BV:141:LYS:HE3	1.80	0.63
55:BV:162:TRP:HH2	55:BV:214:THR:HG22	1.62	0.63
2:A:3014:A:O2'	2:A:3015:C:H5''	1.98	0.63
35:BA:390:U:O3'	50:BP:29:ARG:NH2	2.32	0.63
51:BQ:20:ARG:HB2	51:BQ:77:MET:HE2	1.79	0.63
2:A:1403:C:H5	2:A:1441:C:N3	1.96	0.63
2:A:2374:U:H2'	2:A:2375:G:C8	2.34	0.63
13:L:10:VAL:HG12	13:L:12:ASP:H	1.64	0.63
35:BA:1220:A:H62	35:BA:1281:A:H62	1.46	0.63
2:A:543:U:H3'	2:A:544:U:C5'	2.29	0.63
6:E:40:ALA:HA	6:E:100:GLN:HE21	1.63	0.63
20:S:87:ARG:HG3	20:S:87:ARG:NH1	2.12	0.63
39:BE:145:VAL:HG11	39:BE:148:ILE:HD12	1.81	0.63
2:A:2557:A:OP1	25:X:75:ARG:NH2	2.32	0.62
2:A:2772:G:H1'	13:L:23:ARG:NH1	2.08	0.62
9:H:127:VAL:HG21	9:H:150:ALA:HB2	1.81	0.62
31:d:27:THR:OG1	31:d:28:ARG:N	2.31	0.62
39:BE:38:GLU:HG2	39:BE:64:VAL:HG22	1.80	0.62
2:A:292:G:N2	2:A:343:U:O2	2.31	0.62
2:A:1554:U:H3	2:A:1617:C:H42	1.46	0.62
35:BA:448:A:OP2	35:BA:465:G:N2	2.31	0.62
41:BG:107:PHE:HZ	41:BG:137:ARG:NH1	1.96	0.62
2:A:567:A:H4'	2:A:568:A:H5'	1.80	0.62
42:BH:85:LEU:HB2	46:BL:4:ILE:HD12	1.81	0.62
55:BV:4:VAL:HG13	55:BV:8:GLN:HB3	1.81	0.62
2:A:1201:G:N2	2:A:1203:A:H3'	2.14	0.62
2:A:2369:C:H5''	2:A:2370:A:C8	2.35	0.62
14:M:110:VAL:H	14:M:127:ASN:HD22	1.45	0.62
42:BH:50:ARG:NH1	42:BH:52:GLU:OE2	2.33	0.62
53:BS:33:THR:HG22	53:BS:35:SER:H	1.64	0.62
2:A:1675:U:O2	16:O:64:ARG:NH1	2.32	0.62
9:H:112:LEU:HD13	9:H:134:VAL:HG11	1.82	0.62
18:Q:90:ASP:HB2	18:Q:110:LYS:HB2	1.81	0.62
19:R:114:ARG:HG3	19:R:114:ARG:NH1	2.15	0.62
2:A:899:G:H5'	2:A:899:G:H8	1.64	0.62
35:BA:254:G:H4'	51:BQ:35:THR:HG21	1.82	0.62
35:BA:438:U:OP1	38:BD:117:HIS:NE2	2.29	0.62
2:A:380:A:P	23:V:99:LYS:HZ1	2.22	0.62
2:A:2404:G:H2'	2:A:2405:A:H8	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BJ:6:ILE:HB	44:BJ:76:ILE:HG23	1.82	0.62
47:BM:4:LEU:HG	47:BM:5:VAL:HG23	1.82	0.62
2:A:1869:G:OP1	16:O:40:LYS:NZ	2.33	0.62
2:A:2089:C:O2	2:A:2094:G:N2	2.33	0.62
2:A:2340:A:H61	2:A:2389:U:H3	1.48	0.62
35:BA:612:U:H5'	35:BA:613:G:C8	2.34	0.62
10:I:94:LYS:HD3	10:I:121:GLU:HG2	1.80	0.61
35:BA:1265:U:H5''	35:BA:1266:U:H4'	1.82	0.61
37:BC:169:ARG:HB2	37:BC:169:ARG:NH1	2.09	0.61
38:BD:51:GLN:HB3	38:BD:55:LYS:HE3	1.82	0.61
25:X:18:ALA:HB3	25:X:20:ARG:NH1	2.15	0.61
35:BA:987:A:H8	35:BA:1007:U:H1'	1.63	0.61
35:BA:1382:C:H4'	35:BA:1383:C:H5''	1.81	0.61
11:J:20:ALA:HB1	11:J:41:CYS:HB3	1.82	0.61
35:BA:1515:A:H2'	35:BA:1516:U:O4'	2.00	0.61
55:BV:114:LEU:HD21	55:BV:145:GLU:HG3	1.82	0.61
35:BA:193:C:N4	51:BQ:18:GLY:O	2.33	0.61
35:BA:1220:A:H62	35:BA:1281:A:N6	1.98	0.61
43:BI:53:ARG:HB3	43:BI:57:ASN:HD22	1.66	0.61
15:N:37:LEU:O	15:N:99:PRO:HB3	2.01	0.61
22:U:46:ILE:HD12	22:U:84:VAL:HG21	1.83	0.61
29:b:37:ARG:NH1	29:b:54:LEU:HB3	2.15	0.61
45:BK:30:ALA:HB3	45:BK:93:VAL:HG12	1.81	0.61
55:BV:111:LEU:HD13	55:BV:148:LEU:HD23	1.82	0.61
2:A:333:C:H2'	2:A:334:G:C8	2.35	0.61
2:A:604:C:O2'	21:T:25:ARG:NH2	2.34	0.61
2:A:752:C:H2'	2:A:753:A:C8	2.35	0.61
4:C:108:PRO:HG2	4:C:111:LEU:HB2	1.82	0.61
35:BA:561:G:OP1	49:BO:65:ARG:NH2	2.33	0.61
2:A:2351:A:N3	2:A:2396:A:O2'	2.34	0.61
4:C:96:HIS:CD2	4:C:102:LYS:HG2	2.35	0.61
24:W:16:ARG:HG2	24:W:48:GLU:HG3	1.81	0.61
35:BA:956:A:OP2	48:BN:41:ARG:NH1	2.33	0.61
2:A:1551:U:H3'	2:A:1552:A:C8	2.34	0.61
10:I:69:LEU:HD22	10:I:72:LEU:HD12	1.82	0.61
51:BQ:65:ASN:OD1	51:BQ:65:ASN:N	2.34	0.61
26:Y:19:SER:OG	26:Y:20:HIS:N	2.34	0.61
38:BD:96:VAL:HG13	38:BD:166:LEU:HD21	1.81	0.61
2:A:142:C:H5''	22:U:41:GLN:NE2	2.11	0.60
3:B:31:C:H5'	17:P:11:SER:HB3	1.83	0.60
35:BA:1170:U:H5''	37:BC:5:ILE:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BD:15:LEU:HD22	38:BD:55:LYS:HG3	1.83	0.60
38:BD:103:ALA:HA	38:BD:108:MET:HE2	1.83	0.60
2:A:292:G:H1	2:A:343:U:H3	1.47	0.60
2:A:1153:U:H4'	8:G:60:ARG:CZ	2.32	0.60
2:A:1722:C:OP1	4:C:78:LYS:NZ	2.20	0.60
2:A:2274:C:H1'	5:D:166:MET:HE3	1.83	0.60
35:BA:11:G:H1	39:BE:122:ARG:NH1	1.99	0.60
35:BA:808:A:H62	35:BA:840:G:H21	1.49	0.60
47:BM:97:PRO:HB2	47:BM:101:GLN:HG3	1.84	0.60
35:BA:216:U:O2'	35:BA:217:U:H5'	2.02	0.60
55:BV:162:TRP:CH2	55:BV:214:THR:HG22	2.36	0.60
56:BW:17:C:H3'	56:BW:18:G:H5''	1.84	0.60
8:G:116:ILE:HD13	8:G:149:ILE:HG12	1.82	0.60
16:O:33:ARG:HB3	16:O:114:GLU:HG3	1.84	0.60
5:D:130:HIS:CD2	5:D:165:ARG:HB3	2.37	0.60
50:BP:40:TYR:CE2	50:BP:42:PRO:HG3	2.37	0.60
2:A:1455:U:OP2	22:U:62:ARG:NH1	2.32	0.60
9:H:124:ILE:HG22	9:H:125:LYS:H	1.67	0.60
13:L:90:ASP:N	13:L:90:ASP:OD1	2.33	0.60
43:BI:61:ASN:HD22	43:BI:64:HIS:CD2	2.19	0.60
2:A:733:U:H2'	2:A:734:C:H6	1.66	0.60
2:A:1621:C:H2'	2:A:1622:G:C8	2.37	0.60
13:L:76:TYR:HB2	18:Q:72:THR:HB	1.84	0.60
18:Q:19:PHE:HA	18:Q:88:ARG:HH12	1.67	0.60
20:S:54:ASP:N	20:S:54:ASP:OD1	2.35	0.60
2:A:897:A:C6	4:C:226:MET:HE2	2.37	0.59
2:A:1174:G:O2'	2:A:1221:A:N6	2.34	0.59
41:BG:107:PHE:HZ	41:BG:137:ARG:HH11	1.50	0.59
2:A:1158:U:H3	2:A:1233:A:H61	1.49	0.59
7:F:128:GLN:HB2	7:F:135:TYR:CE1	2.37	0.59
35:BA:382:A:H2'	35:BA:383:A:H8	1.66	0.59
38:BD:21:GLY:HA3	38:BD:160:ARG:HH22	1.67	0.59
2:A:1530:G:N2	2:A:1805:G:H1	2.01	0.59
35:BA:481:G:H2'	35:BA:482:A:H8	1.66	0.59
41:BG:79:ARG:HA	41:BG:84:THR:HA	1.84	0.59
55:BV:97:LEU:HG	55:BV:100:MET:HE3	1.84	0.59
2:A:759:G:H1	25:X:64:PRO:HB3	1.66	0.59
2:A:1146:A:N3	2:A:2710:G:O2'	2.33	0.59
2:A:2381:A:H4'	2:A:2382:G:O5'	2.00	0.59
2:A:2580:G:H2'	2:A:2581:G:O4'	2.02	0.59
22:U:34:HIS:ND1	22:U:36:ASP:OD1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1164:A:H4'	10:I:55:THR:HB	1.84	0.59
40:BF:89:LYS:NZ	52:BR:73:GLU:OE1	2.36	0.59
48:BN:21:TYR:HE1	48:BN:23:ARG:HE	1.50	0.59
2:A:451:U:H2'	2:A:452:G:C8	2.38	0.59
12:K:77:HIS:CD2	12:K:79:GLY:H	2.20	0.59
24:W:43:ASP:OD1	24:W:43:ASP:N	2.34	0.59
31:d:15:ARG:HE	31:d:47:ALA:HB1	1.68	0.59
44:BJ:25:ILE:HD11	44:BJ:92:LEU:HD11	1.84	0.59
2:A:13:G:H5''	29:b:14:ARG:HB3	1.85	0.59
2:A:858:A:O2'	2:A:1877:U:OP1	2.19	0.59
40:BF:27:LEU:O	40:BF:30:ILE:HG13	2.03	0.59
31:d:27:THR:HG23	31:d:30:GLY:H	1.68	0.59
2:A:1410:C:H5''	16:O:71:ARG:HH11	1.67	0.59
6:E:52:THR:O	6:E:94:LYS:NZ	2.36	0.58
10:I:72:LEU:HD22	10:I:106:LYS:HB3	1.84	0.58
46:BL:121:LYS:HG3	46:BL:122:GLU:N	2.18	0.58
52:BR:20:CYS:HB3	52:BR:23:CYS:HB2	1.86	0.58
2:A:1647:G:N7	4:C:31:LYS:NZ	2.43	0.58
10:I:14:ALA:HB1	10:I:63:GLU:HG3	1.84	0.58
35:BA:600:U:H1'	38:BD:127:ILE:HG21	1.85	0.58
35:BA:1199:C:H2'	35:BA:1200:A:C8	2.39	0.58
43:BI:40:ARG:HG2	43:BI:84:TYR:HB2	1.85	0.58
35:BA:502:C:H41	46:BL:50:ARG:HH12	1.51	0.58
35:BA:1261:A:P	44:BJ:9:ARG:HH22	2.26	0.58
38:BD:188:VAL:HG22	38:BD:189:PRO:HD2	1.86	0.58
42:BH:12:THR:HG22	42:BH:15:ARG:HH12	1.68	0.58
44:BJ:24:LYS:HD2	44:BJ:92:LEU:HD23	1.85	0.58
2:A:2137:A:N6	35:BA:1392:C:O2	2.36	0.58
4:C:155:LEU:HD13	4:C:177:MET:HE1	1.85	0.58
35:BA:1267:U:H3'	35:BA:1268:C:H5'	1.86	0.58
24:W:105:LYS:NZ	24:W:136:GLU:OE2	2.27	0.58
37:BC:41:LEU:HD13	37:BC:89:ASP:HB3	1.85	0.58
40:BF:80:ASN:HD21	40:BF:88:THR:HG22	1.68	0.58
9:H:32:PRO:HB3	26:Y:64:ALA:HA	1.85	0.58
11:J:79:LYS:HD3	11:J:82:LEU:HD12	1.86	0.58
39:BE:100:PRO:HB3	39:BE:174:ARG:HG2	1.85	0.58
40:BF:7:MET:HE2	52:BR:33:LYS:NZ	2.19	0.58
46:BL:83:ARG:HH21	46:BL:96:LYS:HD2	1.68	0.58
2:A:2009:G:H5'	4:C:205:ASN:ND2	2.19	0.58
5:D:6:ILE:HG22	5:D:208:VAL:HG22	1.85	0.58
25:X:8:SER:N	56:BW:2:C:H4'	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:752:C:H2'	2:A:753:A:H8	1.68	0.57
2:A:2304:C:H4'	26:Y:25:THR:HG21	1.86	0.57
10:I:27:GLU:HG3	10:I:76:PRO:HG2	1.86	0.57
54:BT:39:VAL:HG22	54:BT:47:ALA:HB1	1.85	0.57
2:A:1427:U:H4'	2:A:1428:U:O5'	2.04	0.57
5:D:154:CYS:C	5:D:156:THR:H	2.11	0.57
15:N:91:GLU:HB3	15:N:92:TRP:CE3	2.39	0.57
35:BA:500:A:H62	35:BA:509:G:H8	1.53	0.57
46:BL:121:LYS:HG3	46:BL:122:GLU:H	1.67	0.57
2:A:2936:C:OP1	2:A:2938:G:H4'	2.04	0.57
15:N:63:LYS:HD3	15:N:65:TRP:CZ2	2.40	0.57
37:BC:46:LEU:HD13	37:BC:75:VAL:HG13	1.86	0.57
40:BF:30:ILE:HG22	40:BF:36:THR:HG21	1.85	0.57
2:A:273:A:H61	2:A:314:G:H1'	1.69	0.57
2:A:3023:G:H2'	2:A:3024:A:O4'	2.03	0.57
35:BA:452:A:H62	50:BP:94:LYS:H	1.52	0.57
35:BA:1077:C:H5''	55:BV:143:LYS:NZ	2.20	0.57
2:A:1203:A:O2'	2:A:1222:C:O2'	2.22	0.57
49:BO:43:LEU:HD13	49:BO:53:ARG:HG2	1.85	0.57
51:BQ:32:MET:HB2	51:BQ:35:THR:OG1	2.05	0.57
2:A:1640:A:H3'	2:A:1641:U:H5''	1.87	0.57
18:Q:28:HIS:ND1	18:Q:41:VAL:HG12	2.19	0.57
38:BD:3:ARG:HD2	38:BD:110:ARG:HH11	1.70	0.57
55:BV:18:HIS:NE2	55:BV:205:ASP:OD2	2.35	0.57
2:A:571:A:H5''	23:V:46:ALA:HB2	1.86	0.57
25:X:41:ARG:NE	25:X:41:ARG:HA	2.19	0.57
35:BA:1145:G:H1	35:BA:1153:U:H3	1.52	0.57
38:BD:86:LEU:HD13	38:BD:186:ILE:HG21	1.87	0.57
40:BF:23:LEU:HD13	40:BF:63:ILE:HD11	1.86	0.57
4:C:132:PRO:HA	4:C:190:ARG:HA	1.87	0.57
24:W:11:LEU:HD12	24:W:67:LEU:HD13	1.87	0.57
2:A:356:G:H21	2:A:362:A:H62	1.53	0.57
5:D:114:VAL:HG12	5:D:208:VAL:HG12	1.87	0.57
43:BI:77:ARG:HH22	43:BI:111:GLN:HG2	1.70	0.57
56:BW:14:A:N1	56:BW:22:G:H1'	2.19	0.56
2:A:1410:C:H5''	16:O:71:ARG:NH1	2.20	0.56
10:I:94:LYS:HZ1	10:I:124:ALA:CB	2.18	0.56
11:J:101:LYS:HG3	11:J:140:THR:HB	1.86	0.56
14:M:30:GLY:O	14:M:32:THR:N	2.31	0.56
47:BM:97:PRO:HG2	47:BM:103:THR:HG22	1.87	0.56
4:C:141:VAL:HG13	4:C:162:SER:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:56:ILE:HD11	11:J:72:LEU:HB3	1.86	0.56
12:K:102:GLU:HG3	12:K:124:VAL:HG11	1.86	0.56
14:M:84:ASN:ND2	14:M:117:LYS:O	2.39	0.56
21:T:44:ARG:NH1	29:b:55:ASP:OD2	2.39	0.56
24:W:14:ASN:OD1	24:W:14:ASN:N	2.38	0.56
35:BA:243:A:N1	35:BA:281:G:O2'	2.37	0.56
35:BA:526:G:OP1	38:BD:65:LYS:HG2	2.05	0.56
35:BA:958:G:H22	35:BA:1345:A:H5'	1.69	0.56
35:BA:1106:U:P	44:BJ:7:ARG:HH22	2.27	0.56
41:BG:50:ALA:O	41:BG:54:THR:HG22	2.04	0.56
10:I:94:LYS:HZ1	10:I:124:ALA:HB2	1.71	0.56
35:BA:956:A:P	48:BN:41:ARG:HH12	2.28	0.56
42:BH:7:ILE:HB	42:BH:79:ARG:NH1	2.21	0.56
43:BI:54:THR:HG23	43:BI:57:ASN:H	1.69	0.56
51:BQ:83:SER:OG	51:BQ:84:ALA:O	2.22	0.56
2:A:314:G:H5'	2:A:315:U:OP2	2.05	0.56
2:A:1875:U:H5''	5:D:143:ALA:O	2.06	0.56
2:A:2900:C:OP1	13:L:31:ARG:NH2	2.37	0.56
2:A:2950:C:H4'	13:L:1:MET:HE1	1.87	0.56
2:A:3032:G:H5''	5:D:63:ILE:HD12	1.87	0.56
2:A:2491:A:H5''	2:A:2492:A:H5'	1.86	0.56
4:C:258:ARG:HH12	4:C:268:ILE:CD1	2.18	0.56
7:F:20:ARG:HD3	7:F:35:ILE:HG21	1.87	0.56
8:G:55:ARG:NH1	8:G:63:ARG:HG3	2.20	0.56
35:BA:925:C:H1'	43:BI:146:GLN:HE22	1.70	0.56
35:BA:931:A:O2'	35:BA:1346:A:OP2	2.23	0.56
2:A:380:A:P	23:V:99:LYS:NZ	2.79	0.56
2:A:860:G:O2'	2:A:863:G:O2'	2.15	0.56
5:D:115:THR:HG21	5:D:174:ARG:HE	1.70	0.56
21:T:32:ARG:HH11	21:T:32:ARG:HG3	1.71	0.56
35:BA:372:C:N4	35:BA:388:G:OP2	2.39	0.56
47:BM:39:ILE:HD12	47:BM:56:LEU:HD13	1.87	0.56
4:C:262:LYS:O	4:C:265:ASP:HB2	2.05	0.56
14:M:110:VAL:H	14:M:127:ASN:ND2	2.04	0.56
17:P:26:ARG:NH1	17:P:54:ASP:OD2	2.34	0.56
24:W:66:ILE:HD11	24:W:77:LEU:HD21	1.88	0.56
31:d:18:VAL:O	31:d:23:LEU:HD22	2.06	0.56
44:BJ:50:CYS:SG	44:BJ:62:ARG:HD3	2.46	0.56
44:BJ:51:VAL:HG11	48:BN:44:LEU:HD23	1.88	0.56
4:C:206:TRP:CH2	4:C:215:LYS:HE3	2.39	0.56
44:BJ:29:VAL:HG11	44:BJ:36:VAL:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:37:THR:HG21	5:D:70:PHE:HE1	1.70	0.56
6:E:118:ARG:NH1	14:M:3:VAL:HG13	2.20	0.56
45:BK:27:HIS:HD2	45:BK:90:LYS:HB3	1.70	0.56
2:A:733:U:H2'	2:A:734:C:C6	2.41	0.55
19:R:90:VAL:HG21	20:S:41:LEU:HD22	1.87	0.55
35:BA:1458:G:H2'	35:BA:1459:G:O4'	2.06	0.55
55:BV:111:LEU:HD11	55:BV:152:ARG:HA	1.87	0.55
2:A:2571:C:OP1	30:c:40:LYS:NZ	2.39	0.55
18:Q:52:GLY:H	18:Q:56:GLU:HB2	1.71	0.55
35:BA:1202:G:O3'	53:BS:77:THR:HG21	2.05	0.55
37:BC:12:LEU:HA	37:BC:16:THR:HG23	1.88	0.55
2:A:2018:G:H22	2:A:2028:G:P	2.29	0.55
35:BA:382:A:H2'	35:BA:383:A:C8	2.42	0.55
48:BN:32:SER:O	48:BN:32:SER:OG	2.20	0.55
51:BQ:65:ASN:HB2	51:BQ:67:GLU:HG3	1.88	0.55
35:BA:439:U:O2'	38:BD:126:ASP:OD2	2.24	0.55
43:BI:101:LEU:HG	43:BI:105:ARG:HD2	1.88	0.55
2:A:639:C:O2'	2:A:640:G:H8	1.89	0.55
2:A:3014:A:N6	2:A:3112:A:H2'	2.21	0.55
4:C:26:ARG:HG2	4:C:28:THR:H	1.70	0.55
14:M:67:PHE:HD2	14:M:69:ASN:H	1.55	0.55
24:W:119:THR:HG23	24:W:150:GLY:HA2	1.87	0.55
35:BA:21:U:OP1	39:BE:44:ASN:ND2	2.34	0.55
2:A:363:A:H2'	2:A:364:A:O4'	2.06	0.55
2:A:1552:A:H2	2:A:1617:C:H5	1.53	0.55
4:C:147:LEU:HD21	4:C:155:LEU:HD11	1.88	0.55
35:BA:458:A:OP1	35:BA:459:G:H1'	2.07	0.55
46:BL:14:ASP:OD1	46:BL:15:LYS:N	2.39	0.55
53:BS:36:ARG:NH2	53:BS:77:THR:OG1	2.39	0.55
2:A:1756:G:N3	2:A:1756:G:H2'	2.22	0.55
10:I:94:LYS:NZ	10:I:120:VAL:O	2.39	0.55
15:N:10:ARG:HH12	56:BW:64:A:H4'	1.72	0.55
27:Z:62:ARG:HH21	27:Z:66:LEU:HD21	1.71	0.55
2:A:1722:C:H2'	2:A:1723:U:O4'	2.07	0.55
2:A:3021:A:H4'	2:A:3022:G:C8	2.42	0.55
11:J:11:ILE:HG21	11:J:33:HIS:CD2	2.42	0.55
35:BA:452:A:N6	50:BP:94:LYS:H	2.05	0.55
53:BS:15:LEU:HD23	53:BS:33:THR:HG21	1.89	0.55
55:BV:114:LEU:HD13	55:BV:152:ARG:NH1	2.22	0.55
2:A:316:U:O2'	2:A:317:G:OP1	2.20	0.55
2:A:998:G:H22	2:A:1009:U:H3	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1564:A:H2'	2:A:1565:A:C8	2.42	0.55
6:E:192:ASP:HA	14:M:5:LYS:HZ3	1.71	0.55
38:BD:99:ARG:HH22	38:BD:188:VAL:HG23	1.71	0.55
47:BM:96:LEU:O	47:BM:110:ARG:NH1	2.39	0.55
2:A:857:U:H2'	2:A:858:A:C8	2.42	0.54
15:N:72:ARG:NH1	15:N:72:ARG:HB3	2.22	0.54
35:BA:987:A:C8	35:BA:1007:U:H1'	2.42	0.54
53:BS:3:ARG:HH11	53:BS:10:PHE:HB2	1.72	0.54
4:C:26:ARG:HG2	4:C:27:SER:N	2.22	0.54
15:N:62:GLY:HA2	24:W:123:LEU:HD11	1.89	0.54
37:BC:22:TRP:CE2	48:BN:54:PRO:HG3	2.42	0.54
39:BE:130:VAL:O	39:BE:137:ARG:NH2	2.41	0.54
9:H:82:VAL:HG11	9:H:91:LEU:HD13	1.89	0.54
14:M:65:LYS:HG2	32:e:25:GLN:HE22	1.72	0.54
15:N:65:TRP:HB2	15:N:105:GLU:HB2	1.88	0.54
35:BA:1110:A:H4'	43:BI:40:ARG:NH1	2.22	0.54
10:I:82:VAL:HG13	10:I:89:ALA:HB2	1.90	0.54
35:BA:108:G:OP2	50:BP:28:ARG:NH2	2.40	0.54
35:BA:1298:G:N7	53:BS:7:LYS:NZ	2.55	0.54
55:BV:75:GLN:HG3	55:BV:207:ILE:HB	1.89	0.54
55:BV:110:ARG:HD3	55:BV:144:LEU:HD11	1.89	0.54
11:J:114:LYS:O	11:J:118:LEU:N	2.41	0.54
16:O:26:THR:HG23	16:O:75:VAL:HG21	1.90	0.54
23:V:41:ILE:O	23:V:61:THR:HA	2.06	0.54
35:BA:924:G:H21	43:BI:146:GLN:NE2	2.05	0.54
37:BC:186:LEU:HD13	37:BC:199:LYS:HG2	1.90	0.54
38:BD:77:GLN:NE2	38:BD:88:ILE:HD11	2.22	0.54
45:BK:23:LYS:HE3	45:BK:86:HIS:CD2	2.42	0.54
2:A:539:C:H4'	6:E:53:LYS:NZ	2.23	0.54
2:A:2761:U:H2'	2:A:2762:C:C6	2.43	0.54
3:B:15:U:OP2	3:B:71:C:O2'	2.26	0.54
7:F:57:ILE:HD13	7:F:91:PRO:HB2	1.89	0.54
16:O:33:ARG:NH2	16:O:114:GLU:OE2	2.40	0.54
18:Q:71:ARG:HG2	18:Q:73:PHE:CZ	2.42	0.54
35:BA:1201:G:H1'	53:BS:52:HIS:HD2	1.73	0.54
35:BA:1237:C:H3'	37:BC:26:LYS:HZ2	1.73	0.54
37:BC:46:LEU:HD12	37:BC:51:ILE:HD11	1.88	0.54
38:BD:165:TRP:CE3	38:BD:181:PRO:HB3	2.43	0.54
40:BF:37:VAL:HB	40:BF:66:LYS:HB2	1.90	0.54
47:BM:56:LEU:O	47:BM:60:ILE:HG23	2.06	0.54
2:A:1627:U:H2'	2:A:1628:A:H8	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1640:A:H3'	2:A:1641:U:C5'	2.37	0.54
35:BA:299:G:H2'	35:BA:300:A:C8	2.43	0.54
35:BA:1470:G:H2'	35:BA:1471:G:O4'	2.08	0.54
54:BT:68:HIS:ND1	54:BT:69:PRO:HD2	2.22	0.54
2:A:1162:G:O2'	2:A:1229:A:N6	2.41	0.54
2:A:2422:A:O2'	26:Y:63:ARG:NH1	2.41	0.54
10:I:40:ARG:HG3	10:I:40:ARG:NH1	2.17	0.54
29:b:10:ARG:CG	29:b:14:ARG:HH12	2.19	0.54
13:L:13:ASN:OD1	13:L:13:ASN:N	2.41	0.54
23:V:67:HIS:HD2	23:V:69:SER:H	1.56	0.54
39:BE:110:VAL:HG12	39:BE:121:LEU:HB2	1.90	0.54
2:A:288:U:H4'	2:A:289:A:O5'	2.07	0.54
2:A:336:C:N4	2:A:337:U:O4	2.41	0.54
2:A:2343:G:H2'	2:A:2344:G:C8	2.43	0.54
9:H:4:ILE:HG13	9:H:39:ALA:HB2	1.89	0.54
45:BK:103:GLU:HB3	45:BK:107:ARG:NH2	2.22	0.54
2:A:1679:A:OP1	2:A:1679:A:H4'	2.08	0.53
2:A:2147:U:H2'	2:A:2148:C:C6	2.43	0.53
9:H:124:ILE:O	9:H:125:LYS:HB2	2.08	0.53
18:Q:28:HIS:CD2	18:Q:82:HIS:HB2	2.42	0.53
20:S:80:ASN:C	20:S:82:THR:H	2.15	0.53
35:BA:1232:A:H2'	35:BA:1233:A:O4'	2.08	0.53
2:A:1533:U:H3'	2:A:1534:C:H5''	1.91	0.53
39:BE:105:THR:HG21	39:BE:124:ALA:H	1.74	0.53
2:A:2864:G:H5'	12:K:99:ARG:HH22	1.73	0.53
4:C:68:ARG:NH1	4:C:150:GLY:O	2.41	0.53
17:P:77:LYS:HB3	17:P:112:ARG:HD3	1.90	0.53
30:c:35:ARG:NH2	30:c:53:GLU:O	2.41	0.53
35:BA:793:U:H5''	35:BA:796:A:N6	2.22	0.53
35:BA:954:C:O3'	44:BJ:59:LYS:HD2	2.08	0.53
47:BM:7:VAL:HG21	47:BM:22:ILE:HG12	1.90	0.53
56:BW:28:G:H1	56:BW:42:C:H42	1.56	0.53
2:A:574:C:O2'	21:T:67:ASN:ND2	2.40	0.53
10:I:54:ASN:ND2	10:I:73:PHE:O	2.42	0.53
13:L:2:ILE:HG13	13:L:8:LEU:HD21	1.90	0.53
21:T:30:LEU:HD22	29:b:24:ALA:HB2	1.91	0.53
35:BA:269:U:H2'	35:BA:270:A:C8	2.43	0.53
43:BI:58:TYR:HE2	43:BI:87:LEU:HD12	1.72	0.53
2:A:442:U:H2'	2:A:443:C:C6	2.44	0.53
2:A:1260:C:H6	12:K:27:ARG:NH1	2.04	0.53
4:C:108:PRO:HD2	4:C:111:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:19:PHE:HA	18:Q:88:ARG:NH1	2.23	0.53
25:X:41:ARG:HA	25:X:41:ARG:HE	1.74	0.53
2:A:1206:A:H62	11:J:136:SER:HB3	1.74	0.53
2:A:2387:U:H3'	2:A:2388:G:H8	1.74	0.53
11:J:132:GLY:HA2	11:J:135:ARG:HD2	1.91	0.53
12:K:116:ARG:HH11	12:K:116:ARG:HG3	1.73	0.53
35:BA:1513:G:N7	36:BB:7:LYS:HE3	2.23	0.53
6:E:112:ARG:CG	6:E:112:ARG:NH1	2.66	0.53
24:W:28:ARG:HH21	24:W:93:GLN:HB3	1.74	0.53
55:BV:151:ILE:HA	55:BV:154:MET:HB2	1.90	0.53
2:A:302:U:H1'	2:A:303:G:C8	2.44	0.53
2:A:2334:U:H4'	2:A:2341:U:O2'	2.08	0.53
8:G:116:ILE:HD11	8:G:152:LEU:HD11	1.91	0.53
55:BV:23:TRP:HA	55:BV:189:THR:HG23	1.91	0.53
2:A:380:A:N1	2:A:404:A:O2'	2.40	0.53
2:A:1756:G:H1'	2:A:1758:G:N1	2.23	0.53
16:O:36:THR:OG1	16:O:37:THR:N	2.42	0.53
17:P:26:ARG:HD3	17:P:37:ARG:NH1	2.24	0.53
35:BA:645:G:H1'	35:BA:713:G:H1'	1.91	0.53
2:A:210:G:OP2	31:d:28:ARG:NH2	2.42	0.53
2:A:3052:A:O2'	2:A:3105:C:OP1	2.23	0.53
13:L:13:ASN:HD21	13:L:97:ARG:N	2.06	0.53
35:BA:252:U:H2'	35:BA:253:U:C6	2.44	0.53
35:BA:482:A:OP1	46:BL:114:ARG:N	2.42	0.53
40:BF:20:ALA:HB3	40:BF:21:PRO:HD3	1.91	0.53
54:BT:8:ILE:HA	54:BT:11:ILE:HD12	1.91	0.53
2:A:306:U:H5''	9:H:41:ARG:HG2	1.90	0.52
5:D:79:ARG:HG2	5:D:80:HIS:CE1	2.44	0.52
6:E:154:VAL:HG12	6:E:175:VAL:HG22	1.91	0.52
9:H:77:ASP:HB3	9:H:147:ASN:HD21	1.73	0.52
11:J:114:LYS:HB3	11:J:118:LEU:HG	1.91	0.52
2:A:337:U:H5'	2:A:338:C:O5'	2.09	0.52
15:N:1:MET:SD	15:N:45:ARG:HG2	2.49	0.52
40:BF:1:MET:HE1	40:BF:37:VAL:HG23	1.91	0.52
46:BL:21:THR:HG22	46:BL:24:LEU:HG	1.91	0.52
46:BL:71:GLY:O	46:BL:99:ARG:NH2	2.35	0.52
52:BR:35:THR:O	52:BR:39:ARG:HG2	2.09	0.52
53:BS:50:ALA:HB1	53:BS:57:HIS:HB3	1.91	0.52
8:G:38:ALA:HB1	8:G:40:PRO:HD2	1.92	0.52
9:H:100:VAL:HG22	9:H:146:LEU:HD21	1.90	0.52
11:J:111:ALA:O	11:J:115:LYS:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BA:488:C:H1'	35:BA:489:A:H2	1.74	0.52
2:A:7:U:H5	2:A:2853:C:N3	2.06	0.52
2:A:1257:G:OP2	12:K:72:LYS:NZ	2.37	0.52
2:A:2356:G:H2'	2:A:2380:G:H22	1.74	0.52
5:D:110:ALA:O	5:D:182:VAL:HG12	2.09	0.52
13:L:63:VAL:HG12	13:L:106:LEU:HD11	1.91	0.52
17:P:66:ILE:HG23	17:P:71:ARG:HH21	1.74	0.52
33:f:16:VAL:HG22	33:f:25:VAL:HG22	1.90	0.52
56:BW:49:C:N4	56:BW:65:G:H1	2.05	0.52
2:A:1312:G:O2'	19:R:12:LYS:NZ	2.42	0.52
10:I:17:PHE:CZ	10:I:64:ALA:HB3	2.45	0.52
35:BA:928:A:H2'	35:BA:929:G:C8	2.45	0.52
44:BJ:56:HIS:C	44:BJ:57:LYS:HG3	2.35	0.52
11:J:114:LYS:HE3	11:J:117:ASP:HB3	1.92	0.52
35:BA:23:C:OP1	39:BE:155:SER:OG	2.28	0.52
35:BA:411:A:C4	35:BA:413:G:H1'	2.45	0.52
35:BA:909:G:O2'	35:BA:1487:A:N7	2.40	0.52
35:BA:994:C:H2'	35:BA:995:A:C8	2.45	0.52
37:BC:94:THR:C	37:BC:96:LYS:H	2.17	0.52
38:BD:29:ARG:HD3	38:BD:31:TYR:OH	2.10	0.52
38:BD:134:GLN:HG2	38:BD:179:GLN:HA	1.92	0.52
2:A:2:A:H2'	2:A:3:A:C8	2.45	0.52
10:I:26:THR:HG22	10:I:105:ILE:HA	1.91	0.52
27:Z:14:THR:HG23	27:Z:17:GLU:H	1.75	0.52
35:BA:1477:A:H4'	35:BA:1478:G:OP1	2.09	0.52
50:BP:100:PRO:HB2	50:BP:105:LEU:HD21	1.91	0.52
2:A:460:G:O2'	2:A:488:G:O6	2.28	0.52
4:C:26:ARG:HD3	4:C:28:THR:O	2.10	0.52
11:J:40:PHE:CD1	11:J:60:ILE:HD11	2.44	0.52
17:P:18:ARG:HD2	17:P:107:TYR:CZ	2.45	0.52
23:V:40:ARG:HA	23:V:62:GLN:O	2.10	0.52
27:Z:5:THR:HG21	27:Z:21:LYS:NZ	2.24	0.52
35:BA:1267:U:H3'	35:BA:1268:C:C5'	2.39	0.52
45:BK:32:ILE:HG12	45:BK:41:VAL:HG12	1.92	0.52
2:A:444:U:H5'	2:A:446:G:H4'	1.91	0.52
2:A:523:U:H2'	2:A:524:C:H5'	1.92	0.52
2:A:2704:C:H5'	2:A:2705:G:OP2	2.10	0.52
10:I:94:LYS:HZ3	10:I:121:GLU:HA	1.73	0.52
35:BA:821:C:N4	35:BA:826:U:H3	2.08	0.52
50:BP:21:ILE:HD13	50:BP:33:ALA:HB2	1.91	0.52
2:A:1107:G:OP2	28:a:11:SER:OG	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2495:G:OP1	25:X:18:ALA:HB1	2.10	0.51
4:C:200:GLU:OE1	4:C:200:GLU:N	2.40	0.51
7:F:117:ARG:HD2	7:F:146:HIS:CE1	2.45	0.51
21:T:32:ARG:HG3	21:T:32:ARG:NH1	2.26	0.51
35:BA:440:C:H2'	35:BA:441:A:H8	1.75	0.51
35:BA:1502:A:H5'	36:BB:19:LYS:NZ	2.25	0.51
45:BK:97:GLY:O	45:BK:102:ARG:NH2	2.43	0.51
2:A:287:A:C6	2:A:300:G:C6	2.98	0.51
7:F:20:ARG:HH11	7:F:20:ARG:HG3	1.75	0.51
35:BA:638:A:H1'	49:BO:22:THR:HG21	1.91	0.51
35:BA:695:A:H2'	35:BA:696:A:C8	2.45	0.51
39:BE:66:ASP:OD1	39:BE:70:MET:HB2	2.10	0.51
45:BK:64:SER:O	45:BK:67:SER:OG	2.28	0.51
7:F:42:VAL:HB	7:F:162:THR:HG23	1.90	0.51
26:Y:2:ALA:HA	26:Y:33:ILE:HD11	1.91	0.51
35:BA:376:G:H5''	50:BP:6:LYS:HB3	1.92	0.51
35:BA:440:C:H2'	35:BA:441:A:C8	2.45	0.51
39:BE:77:LYS:O	39:BE:87:LYS:NZ	2.32	0.51
43:BI:68:ILE:HD13	43:BI:99:LEU:HD23	1.91	0.51
2:A:164:A:H2'	2:A:165:U:C6	2.46	0.51
2:A:635:G:H1'	2:A:636:U:H5'	1.91	0.51
2:A:1455:U:OP1	22:U:19:LYS:NZ	2.40	0.51
2:A:1619:U:H2'	2:A:1620:U:O4'	2.10	0.51
2:A:1755:A:H2	2:A:1759:A:N6	2.09	0.51
10:I:14:ALA:CB	10:I:63:GLU:HG3	2.40	0.51
23:V:91:THR:HB	23:V:93:LYS:HG3	1.91	0.51
35:BA:492:U:H2'	35:BA:493:A:C8	2.45	0.51
2:A:80:G:N2	2:A:99:G:H1'	2.26	0.51
2:A:1000:C:H3'	2:A:1001:C:H5''	1.92	0.51
2:A:2306:A:H61	2:A:2460:U:H3	1.59	0.51
2:A:2552:A:H2'	2:A:2553:G:C8	2.45	0.51
2:A:2636:A:H2'	2:A:2637:G:O4'	2.09	0.51
12:K:76:ARG:HB3	12:K:85:ARG:HH12	1.74	0.51
22:U:7:PRO:HG3	22:U:48:LYS:HD3	1.93	0.51
35:BA:495:G:H2'	35:BA:496:U:C6	2.44	0.51
35:BA:1273:C:OP1	41:BG:41:ARG:NH1	2.44	0.51
2:A:334:G:N2	2:A:347:U:O2	2.44	0.51
2:A:1044:U:H5'	2:A:1045:C:OP2	2.11	0.51
2:A:1224:G:O2'	10:I:28:TYR:OH	2.12	0.51
4:C:146:GLU:HB2	4:C:189:CYS:HB2	1.93	0.51
18:Q:43:LYS:HZ2	18:Q:86:LEU:HD12	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BA:1237:C:H2'	37:BC:26:LYS:NZ	2.26	0.51
56:BW:14:A:C2	56:BW:22:G:H1'	2.46	0.51
15:N:75:THR:HG22	15:N:90:PRO:HA	1.91	0.51
27:Z:10:LEU:HD21	27:Z:21:LYS:HZ3	1.76	0.51
35:BA:928:A:O2'	35:BA:1315:A:N3	2.39	0.51
38:BD:64:GLU:OE2	38:BD:199:TYR:OH	2.27	0.51
39:BE:156:ASP:OD1	39:BE:156:ASP:N	2.42	0.51
40:BF:94:ASP:OD1	40:BF:95:LYS:N	2.35	0.51
50:BP:15:ASN:OD1	50:BP:15:ASN:N	2.43	0.51
56:BW:2:C:H2'	56:BW:3:C:C6	2.46	0.51
5:D:7:LEU:H	5:D:34:ASN:ND2	2.09	0.51
5:D:142:GLN:O	5:D:143:ALA:HB3	2.10	0.51
27:Z:45:ARG:NH1	27:Z:48:ARG:HE	2.08	0.51
55:BV:113:ARG:NH1	55:BV:117:LEU:HD21	2.26	0.51
2:A:357:U:H4'	2:A:358:G:O5'	2.11	0.51
44:BJ:35:SER:HB2	44:BJ:77:LEU:HB2	1.92	0.51
4:C:68:ARG:HH12	4:C:150:GLY:CA	2.24	0.51
5:D:28:VAL:HG22	5:D:193:LEU:HD22	1.92	0.51
8:G:5:GLY:HA3	8:G:66:HIS:CD2	2.46	0.51
43:BI:37:VAL:HG21	43:BI:99:LEU:HA	1.92	0.51
56:BW:51:U:O2	56:BW:63:G:N2	2.43	0.51
2:A:925:U:C4	14:M:31:LYS:O	2.64	0.50
2:A:1250:U:H3'	2:A:1251:A:H5''	1.93	0.50
2:A:1552:A:H2	2:A:1617:C:C5	2.29	0.50
5:D:57:ILE:HG21	5:D:62:VAL:HG13	1.93	0.50
32:e:16:ARG:HG2	32:e:22:ILE:HD13	1.93	0.50
35:BA:399:G:H2'	35:BA:400:C:C6	2.47	0.50
35:BA:956:A:P	48:BN:41:ARG:NH1	2.84	0.50
38:BD:47:ARG:HG2	38:BD:47:ARG:NH1	2.25	0.50
2:A:404:A:OP1	6:E:170:ARG:HD2	2.10	0.50
15:N:72:ARG:HB3	15:N:72:ARG:HH11	1.76	0.50
34:g:37:VAL:HG22	47:BM:57:ARG:NH1	2.27	0.50
35:BA:409:G:OP1	38:BD:104:ARG:NH2	2.43	0.50
38:BD:70:TYR:HE1	38:BD:131:ARG:HE	1.58	0.50
50:BP:86:LEU:HB2	50:BP:87:PRO:CD	2.41	0.50
55:BV:69:PHE:HB3	55:BV:80:ILE:HG23	1.93	0.50
56:BW:17:C:O2'	56:BW:18:G:H3'	2.11	0.50
2:A:1178:U:C2	2:A:1180:G:H5'	2.46	0.50
2:A:1542:A:N6	2:A:1628:A:O2'	2.44	0.50
2:A:2338:G:H4'	2:A:2388:G:H22	1.76	0.50
11:J:23:ALA:HB3	11:J:24:PRO:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BA:642:C:H2'	35:BA:643:A:C8	2.46	0.50
35:BA:955:G:OP1	44:BJ:59:LYS:HE3	2.11	0.50
55:BV:129:ARG:CZ	55:BV:137:LEU:HD11	2.42	0.50
2:A:2463:G:OP1	4:C:244:ARG:NH2	2.29	0.50
8:G:55:ARG:HH11	8:G:63:ARG:HA	1.76	0.50
35:BA:872:G:O2'	35:BA:888:A:N6	2.44	0.50
35:BA:893:U:H2'	35:BA:894:C:H6	1.75	0.50
53:BS:42:PRO:HA	53:BS:45:ILE:HG13	1.92	0.50
55:BV:50:ILE:O	55:BV:54:TYR:HB2	2.10	0.50
2:A:725:A:OP1	14:M:65:LYS:HE3	2.12	0.50
35:BA:427:U:P	38:BD:13:ARG:HH22	2.34	0.50
2:A:1187:A:H4'	2:A:1188:A:H5''	1.93	0.50
35:BA:826:U:H2'	35:BA:828:G:H5'	1.94	0.50
55:BV:162:TRP:CD1	55:BV:217:ILE:HD13	2.45	0.50
56:BW:68:C:H2'	56:BW:69:G:O4'	2.12	0.50
2:A:561:G:H2'	2:A:562:G:H5'	1.93	0.50
2:A:2515:U:H2'	2:A:2516:U:C6	2.47	0.50
4:C:76:ASN:ND2	4:C:118:GLU:HB3	2.27	0.50
11:J:75:PRO:HG2	11:J:80:LEU:HD21	1.94	0.50
35:BA:498:C:H5	35:BA:509:G:H3'	1.77	0.50
35:BA:837:G:OP2	35:BA:853:U:N3	2.40	0.50
35:BA:1076:C:O2'	35:BA:1151:A:O2'	2.28	0.50
2:A:1612:U:H1'	40:BF:17:ARG:NH1	2.17	0.50
2:A:1729:A:H2'	2:A:1731:A:C8	2.47	0.50
27:Z:10:LEU:HD21	27:Z:21:LYS:HZ2	1.76	0.50
35:BA:1375:G:N2	35:BA:1486:A:H8	2.09	0.50
2:A:289:A:C5	2:A:290:C:H5	2.30	0.50
2:A:1037:C:O2'	25:X:29:GLN:NE2	2.45	0.50
2:A:2350:G:H21	2:A:2396:A:H1'	1.76	0.50
14:M:78:VAL:HG23	14:M:104:VAL:HG13	1.93	0.50
16:O:44:LEU:HD23	16:O:113:ILE:HD13	1.94	0.50
35:BA:1027:G:OP1	48:BN:4:LYS:NZ	2.31	0.50
42:BH:14:LEU:HD21	42:BH:64:LEU:HD21	1.93	0.50
44:BJ:41:PRO:HB3	44:BJ:72:ARG:NH1	2.27	0.50
47:BM:51:ASP:O	47:BM:55:VAL:HG23	2.12	0.50
2:A:1001:C:H4'	2:A:1001:C:OP1	2.12	0.49
4:C:43:ARG:NH2	4:C:49:ILE:HD11	2.27	0.49
7:F:130:ASP:C	7:F:132:THR:H	2.17	0.49
16:O:37:THR:HG23	16:O:40:LYS:HD2	1.94	0.49
16:O:45:ARG:HB2	16:O:46:PRO:HD3	1.95	0.49
35:BA:958:G:N2	35:BA:1345:A:H5'	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BD:112:LEU:HB3	38:BD:118:PHE:CE1	2.43	0.49
2:A:919:A:H8	2:A:919:A:H5''	1.76	0.49
2:A:1754:G:C6	2:A:1755:A:C2	2.99	0.49
2:A:1940:A:H2'	2:A:1941:A:O4'	2.12	0.49
2:A:2022:U:O2	4:C:50:THR:HB	2.12	0.49
2:A:2707:C:N3	15:N:124:LYS:NZ	2.53	0.49
6:E:137:SER:O	6:E:168:SER:OG	2.26	0.49
35:BA:1122:U:H2'	35:BA:1123:G:H8	1.77	0.49
40:BF:7:MET:HE2	52:BR:33:LYS:HZ2	1.77	0.49
41:BG:28:ASN:HD21	41:BG:36:LYS:NZ	2.10	0.49
42:BH:35:ASN:HB2	42:BH:112:LEU:HD12	1.94	0.49
54:BT:27:SER:HB3	54:BT:57:LYS:HZ1	1.77	0.49
55:BV:54:TYR:HE1	55:BV:58:LYS:HE3	1.77	0.49
4:C:76:ASN:O	4:C:98:LEU:HG	2.13	0.49
7:F:87:ARG:NH1	56:BW:19:G:N1	2.60	0.49
11:J:60:ILE:HD13	11:J:70:PHE:HB3	1.94	0.49
21:T:17:VAL:O	21:T:107:THR:OG1	2.24	0.49
32:e:31:HIS:CD2	32:e:32:LEU:HG	2.47	0.49
56:BW:29:G:H1	56:BW:41:C:H42	1.59	0.49
2:A:992:C:H2'	2:A:993:G:O4'	2.12	0.49
2:A:1805:G:H2'	2:A:1806:A:H8	1.76	0.49
4:C:68:ARG:HH12	4:C:150:GLY:HA2	1.77	0.49
7:F:49:ASP:OD1	7:F:49:ASP:N	2.45	0.49
10:I:53:LYS:O	10:I:57:VAL:HG23	2.12	0.49
20:S:76:HIS:CE1	20:S:85:HIS:HB3	2.41	0.49
29:b:14:ARG:NH1	29:b:14:ARG:HG2	2.26	0.49
49:BO:8:LYS:O	49:BO:12:LEU:HB2	2.12	0.49
54:BT:56:ARG:O	54:BT:60:LYS:HG2	2.12	0.49
2:A:760:U:H2'	2:A:761:G:C8	2.48	0.49
2:A:1678:U:H5'	2:A:1679:A:OP2	2.13	0.49
11:J:30:LEU:HA	11:J:33:HIS:HD2	1.76	0.49
32:e:47:ARG:HB2	32:e:47:ARG:NH1	2.15	0.49
35:BA:749:G:H4'	35:BA:1497:A:H4'	1.94	0.49
2:A:287:A:N6	2:A:299:G:O2'	2.46	0.49
9:H:77:ASP:OD1	9:H:145:SER:OG	2.28	0.49
35:BA:770:A:OP1	56:BW:38:A:O2'	2.30	0.49
38:BD:154:ARG:HG2	38:BD:155:GLU:HG3	1.94	0.49
2:A:658:U:H5'	14:M:31:LYS:NZ	2.28	0.49
2:A:1867:G:O2'	16:O:106:ASP:OD2	2.26	0.49
6:E:118:ARG:HH12	14:M:3:VAL:CG1	2.25	0.49
14:M:84:ASN:ND2	14:M:118:LEU:HA	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:BE:104:SER:HA	39:BE:146:HIS:HD2	1.78	0.49
43:BI:72:LEU:HD23	43:BI:107:LEU:HD11	1.95	0.49
50:BP:102:LYS:HA	50:BP:105:LEU:HD12	1.94	0.49
2:A:574:C:H4'	21:T:67:ASN:ND2	2.27	0.49
2:A:1702:A:H61	2:A:1732:U:H3	1.60	0.49
2:A:2342:A:C2	2:A:2392:A:H2'	2.48	0.49
14:M:104:VAL:HG11	14:M:110:VAL:HG22	1.95	0.49
16:O:20:LEU:HD21	16:O:40:LYS:HE3	1.95	0.49
21:T:43:LEU:O	21:T:51:SER:OG	2.30	0.49
35:BA:335:C:H2'	35:BA:336:A:C8	2.48	0.49
35:BA:636:G:O2'	49:BO:28:GLN:NE2	2.46	0.49
38:BD:110:ARG:HE	38:BD:128:PRO:HB2	1.77	0.49
41:BG:10:ARG:HH11	41:BG:10:ARG:CG	2.22	0.49
55:BV:166:THR:HG23	55:BV:173:VAL:HG21	1.94	0.49
2:A:270:U:H2'	2:A:271:A:H5'	1.93	0.49
2:A:639:C:O2'	2:A:640:G:O5'	2.31	0.49
11:J:48:THR:HG21	11:J:56:ILE:HG21	1.94	0.49
17:P:36:PRO:HG2	17:P:97:VAL:HG11	1.94	0.49
35:BA:1186:U:H5''	37:BC:195:ARG:HH21	1.78	0.49
56:BW:5:G:H1'	56:BW:69:G:N2	2.27	0.49
2:A:349:G:H2'	2:A:350:A:H8	1.77	0.49
2:A:1639:G:H5'	2:A:1640:A:OP1	2.13	0.49
4:C:79:VAL:HG21	4:C:111:LEU:HD21	1.94	0.49
5:D:40:ARG:O	5:D:48:SER:HA	2.13	0.49
14:M:78:VAL:HG11	14:M:83:ILE:HD11	1.95	0.49
28:a:52:HIS:CD2	28:a:53:LEU:HG	2.48	0.49
35:BA:146:A:H2'	35:BA:147:U:C6	2.48	0.49
2:A:610:C:O2	2:A:646:U:O2'	2.31	0.48
2:A:1550:G:O2'	2:A:1551:U:OP2	2.29	0.48
4:C:96:HIS:HD2	4:C:102:LYS:HG2	1.78	0.48
4:C:182:ILE:HB	4:C:270:ARG:NH1	2.28	0.48
6:E:9:THR:HG22	6:E:128:THR:HG21	1.95	0.48
8:G:118:ALA:HB2	8:G:124:PHE:CE2	2.46	0.48
21:T:80:THR:OG1	21:T:113:ILE:HB	2.13	0.48
42:BH:8:ALA:O	42:BH:12:THR:HG23	2.12	0.48
54:BT:43:ASP:OD1	54:BT:43:ASP:N	2.45	0.48
2:A:90:C:H2'	2:A:91:C:O4'	2.13	0.48
2:A:365:U:H3	2:A:437:G:H1	1.61	0.48
23:V:20:LYS:HZ2	23:V:74:VAL:HG21	1.78	0.48
41:BG:10:ARG:HG3	41:BG:10:ARG:NH1	2.26	0.48
2:A:273:A:N6	2:A:314:G:H1'	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:284:G:H5''	2:A:285:U:OP2	2.14	0.48
7:F:81:ILE:HG22	7:F:86:LEU:HD23	1.94	0.48
19:R:51:ARG:HG3	19:R:51:ARG:HH11	1.77	0.48
19:R:94:ASN:HD21	20:S:13:GLN:HB2	1.78	0.48
35:BA:1417:A:H2'	35:BA:1418:G:O4'	2.14	0.48
2:A:2975:G:C4	8:G:3:ARG:HD3	2.48	0.48
16:O:101:GLU:HG3	16:O:102:ASN:N	2.27	0.48
35:BA:1357:A:OP1	41:BG:36:LYS:NZ	2.46	0.48
35:BA:1476:A:H2'	35:BA:1477:A:H2'	1.95	0.48
39:BE:132:ALA:HB2	39:BE:150:ALA:HB3	1.94	0.48
41:BG:152:ALA:HB1	41:BG:155:ARG:NH2	2.28	0.48
42:BH:41:LYS:NZ	42:BH:48:ASP:OD1	2.44	0.48
43:BI:77:ARG:O	43:BI:80:GLN:HG2	2.13	0.48
2:A:80:G:H22	2:A:99:G:H1'	1.77	0.48
2:A:621:U:H5'	19:R:42:SER:OG	2.13	0.48
2:A:760:U:H2'	2:A:761:G:H8	1.78	0.48
2:A:2221:A:H5''	5:D:127:MET:HE1	1.96	0.48
5:D:147:ARG:HB2	5:D:148:PRO:HD2	1.94	0.48
34:g:20:HIS:ND1	34:g:40:GLN:HG3	2.28	0.48
38:BD:55:LYS:CB	38:BD:190:LEU:HD11	2.42	0.48
39:BE:192:ALA:HA	39:BE:195:LEU:HD12	1.95	0.48
40:BF:30:ILE:HB	40:BF:36:THR:OG1	2.13	0.48
2:A:273:A:N1	2:A:321:G:O2'	2.43	0.48
2:A:2043:C:O2'	2:A:2195:U:OP2	2.32	0.48
30:c:6:ASP:OD1	30:c:6:ASP:N	2.47	0.48
35:BA:612:U:H5'	35:BA:613:G:H8	1.77	0.48
35:BA:1322:G:HO2'	56:BW:31:A:HO2'	1.61	0.48
38:BD:80:LYS:HB2	39:BE:127:GLY:HA3	1.95	0.48
2:A:1260:C:O2'	12:K:27:ARG:NH2	2.47	0.48
2:A:2199:G:H4'	36:BB:30:LYS:HG2	1.94	0.48
4:C:206:TRP:CG	4:C:212:MET:HE3	2.49	0.48
5:D:27:THR:HG21	5:D:198:ILE:HG12	1.95	0.48
13:L:59:LYS:HB3	13:L:87:ILE:HG22	1.95	0.48
15:N:63:LYS:HD3	15:N:65:TRP:CH2	2.48	0.48
18:Q:48:ARG:HD2	18:Q:50:GLN:HE21	1.78	0.48
35:BA:737:U:H2'	35:BA:738:G:O4'	2.13	0.48
35:BA:1284:U:O4	47:BM:14:ARG:HD3	2.14	0.48
38:BD:126:ASP:OD1	38:BD:126:ASP:N	2.47	0.48
41:BG:70:LYS:HD2	41:BG:96:SER:HB3	1.96	0.48
46:BL:122:GLU:HG2	46:BL:123:LYS:H	1.78	0.48
2:A:7:U:H3'	2:A:8:U:H6	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1753:C:N4	2:A:1754:G:O6	2.47	0.48
2:A:1760:G:H2'	2:A:1761:G:C8	2.49	0.48
10:I:94:LYS:NZ	10:I:124:ALA:HB3	2.28	0.48
15:N:34:ILE:HD12	15:N:104:PHE:HB2	1.95	0.48
16:O:55:ALA:HB2	16:O:79:LEU:HD22	1.96	0.48
19:R:51:ARG:HG3	19:R:51:ARG:NH1	2.29	0.48
29:b:14:ARG:HG2	29:b:14:ARG:HH11	1.79	0.48
35:BA:372:C:H41	35:BA:387:U:H2'	1.79	0.48
35:BA:476:A:H5'	35:BA:477:G:OP2	2.13	0.48
35:BA:988:C:H4'	35:BA:1018:C:H1'	1.95	0.48
35:BA:1280:C:H2'	41:BG:114:LYS:NZ	2.29	0.48
37:BC:61:ASP:HB2	37:BC:96:LYS:HD3	1.96	0.48
55:BV:162:TRP:HD1	55:BV:184:ILE:HB	1.79	0.48
2:A:159:A:C6	2:A:160:A:C6	3.02	0.48
2:A:2356:G:H2'	2:A:2380:G:H1	1.78	0.48
6:E:27:VAL:O	6:E:120:ARG:NH2	2.47	0.48
14:M:44:LYS:HG3	14:M:45:ASN:H	1.77	0.48
15:N:69:PHE:HA	15:N:70:PRO:HD3	1.72	0.48
23:V:1:MET:O	23:V:2:LYS:HB2	2.14	0.48
44:BJ:83:THR:O	44:BJ:87:LEU:HG	2.14	0.48
2:A:1704:U:H2'	2:A:1705:C:C6	2.49	0.48
2:A:2569:G:H4'	2:A:2570:A:H5''	1.96	0.48
7:F:117:ARG:HH11	7:F:146:HIS:CE1	2.31	0.48
11:J:54:ASN:HB3	11:J:75:PRO:HB3	1.96	0.48
35:BA:1488:G:OP1	35:BA:1491:A:H4'	2.14	0.48
38:BD:99:ARG:HB3	38:BD:166:LEU:HD11	1.96	0.48
2:A:356:G:H4'	2:A:358:G:N1	2.30	0.47
2:A:1282:G:OP1	20:S:26:LYS:NZ	2.46	0.47
2:A:1560:U:O2	40:BF:17:ARG:HD3	2.14	0.47
7:F:149:ASP:HB3	7:F:151:ASP:OD1	2.14	0.47
10:I:97:ALA:HB2	10:I:103:LEU:HD22	1.94	0.47
11:J:44:TYR:HD2	11:J:72:LEU:HD21	1.79	0.47
25:X:25:ARG:NH2	25:X:35:GLU:OE2	2.47	0.47
29:b:6:ARG:CG	29:b:6:ARG:NH1	2.70	0.47
35:BA:826:U:OP1	52:BR:24:SER:OG	2.22	0.47
35:BA:1109:C:H1'	35:BA:1127:A:H61	1.78	0.47
36:BB:22:ARG:HG2	36:BB:22:ARG:HH11	1.79	0.47
42:BH:77:LEU:HA	42:BH:77:LEU:HD12	1.67	0.47
46:BL:70:GLU:H	46:BL:70:GLU:CD	2.21	0.47
55:BV:48:THR:O	55:BV:51:ASP:HB3	2.14	0.47
2:A:2780:C:H2'	2:A:2781:G:O4'	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3055:G:H2'	2:A:3100:A:H61	1.79	0.47
4:C:258:ARG:HH12	4:C:268:ILE:HD12	1.79	0.47
14:M:110:VAL:N	14:M:127:ASN:HD22	2.10	0.47
18:Q:38:ARG:NH2	35:BA:346:G:OP1	2.47	0.47
35:BA:100:G:H2'	35:BA:101:G:H5''	1.96	0.47
35:BA:456:C:H6	35:BA:456:C:H2'	1.45	0.47
35:BA:1132:U:H5''	44:BJ:44:THR:HG23	1.96	0.47
35:BA:1342:A:OP2	48:BN:35:ARG:NH2	2.47	0.47
54:BT:68:HIS:CG	54:BT:69:PRO:HD2	2.48	0.47
2:A:1400:G:H21	2:A:1443:G:H5''	1.79	0.47
2:A:2445:A:H4'	4:C:188:ARG:HH12	1.79	0.47
2:A:2977:A:O2'	33:f:15:ARG:NH1	2.47	0.47
2:A:2997:C:H2'	2:A:2998:C:H6	1.80	0.47
24:W:14:ASN:HD21	24:W:32:LYS:NZ	2.13	0.47
35:BA:263:A:H2'	35:BA:264:U:C6	2.49	0.47
42:BH:18:ASN:O	42:BH:72:ARG:NH1	2.47	0.47
50:BP:9:ARG:O	50:BP:10:LEU:HD23	2.15	0.47
56:BW:2:C:H2'	56:BW:3:C:H6	1.79	0.47
2:A:750:C:H2'	2:A:751:A:C8	2.49	0.47
2:A:929:C:H1'	2:A:1339:G:H21	1.79	0.47
2:A:1535:C:H2'	2:A:1536:A:O4'	2.14	0.47
2:A:1762:C:H2'	2:A:1763:G:O4'	2.14	0.47
14:M:58:HIS:O	32:e:13:ARG:HD3	2.14	0.47
30:c:16:GLU:HG2	30:c:50:PRO:O	2.13	0.47
50:BP:86:LEU:HB2	50:BP:87:PRO:HD3	1.96	0.47
2:A:543:U:H5	2:A:561:G:H5'	1.80	0.47
2:A:805:C:O2'	2:A:895:G:OP1	2.31	0.47
2:A:1542:A:H2'	2:A:1543:A:C8	2.48	0.47
6:E:108:ALA:O	6:E:112:ARG:HG3	2.14	0.47
24:W:11:LEU:HD21	24:W:57:VAL:HG21	1.95	0.47
35:BA:279:A:H4'	35:BA:280:C:H5'	1.96	0.47
35:BA:413:G:O2'	35:BA:428:G:N2	2.48	0.47
35:BA:428:G:OP2	38:BD:10:ARG:NH1	2.35	0.47
11:J:23:ALA:O	11:J:28:PRO:HD2	2.15	0.47
35:BA:436:C:O2'	38:BD:149:PRO:HG3	2.15	0.47
37:BC:87:ARG:O	37:BC:91:GLU:HG2	2.14	0.47
2:A:707:G:N3	2:A:707:G:H2'	2.29	0.47
2:A:1250:U:H2'	2:A:1251:A:C8	2.50	0.47
2:A:1258:C:P	12:K:68:LYS:HZ2	2.38	0.47
2:A:1555:A:H2'	2:A:1556:A:O4'	2.15	0.47
2:A:1875:U:H2'	2:A:1876:A:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2394:A:O2'	2:A:2396:A:OP1	2.32	0.47
5:D:63:ILE:CG2	5:D:65:PRO:HD2	2.44	0.47
6:E:22:ALA:O	6:E:26:ASP:HB2	2.15	0.47
18:Q:25:VAL:HG23	18:Q:85:VAL:HA	1.97	0.47
18:Q:43:LYS:NZ	18:Q:86:LEU:HD12	2.30	0.47
20:S:26:LYS:HE2	20:S:26:LYS:HB3	1.71	0.47
21:T:79:ALA:HB2	21:T:115:GLU:HG2	1.97	0.47
35:BA:409:G:H2'	35:BA:410:G:O4'	2.14	0.47
35:BA:1120:G:H4'	35:BA:1121:G:H5'	1.97	0.47
35:BA:1465:C:C2'	35:BA:1466:G:H5'	2.44	0.47
51:BQ:46:HIS:HD2	51:BQ:49:TYR:H	1.62	0.47
2:A:2543:U:H4'	2:A:2544:U:H5'	1.97	0.47
35:BA:255:G:H2'	35:BA:256:U:C6	2.50	0.47
35:BA:502:C:H41	46:BL:50:ARG:NH1	2.13	0.47
38:BD:192:GLU:O	38:BD:196:VAL:HG23	2.15	0.47
42:BH:115:ASP:OD1	42:BH:115:ASP:N	2.42	0.47
53:BS:63:THR:HG22	53:BS:64:GLU:H	1.79	0.47
2:A:270:U:C2'	2:A:271:A:H5'	2.45	0.47
2:A:1552:A:H1'	2:A:1618:C:N4	2.22	0.47
2:A:1554:U:H3	2:A:1617:C:N4	2.13	0.47
2:A:2588:C:H2'	2:A:2589:G:O4'	2.14	0.47
3:B:110:G:H2'	3:B:111:C:C6	2.50	0.47
8:G:128:SER:HB3	8:G:129:PRO:HD2	1.97	0.47
19:R:11:GLN:HB3	19:R:15:ARG:NH2	2.30	0.47
35:BA:495:G:H2'	35:BA:496:U:H6	1.79	0.47
35:BA:1266:U:H2'	35:BA:1267:U:H5''	1.97	0.47
42:BH:21:TYR:CE2	42:BH:70:ARG:HG3	2.50	0.47
46:BL:28:PRO:C	46:BL:29:GLN:HE21	2.22	0.47
55:BV:140:GLU:O	55:BV:144:LEU:HB2	2.15	0.47
2:A:739:U:O3'	2:A:740:A:H2'	2.15	0.47
2:A:1116:C:O2	28:a:32:ARG:NH2	2.47	0.47
2:A:1660:A:H2'	2:A:1661:G:O4'	2.15	0.47
4:C:126:LYS:HB2	4:C:126:LYS:HE3	1.58	0.47
4:C:260:PRO:O	4:C:261:ASN:HB2	2.15	0.47
6:E:61:GLY:HA3	6:E:80:ARG:HG2	1.96	0.47
40:BF:48:LEU:HD13	40:BF:52:ILE:HD12	1.96	0.47
2:A:665:G:O2'	2:A:666:A:H3'	2.14	0.46
2:A:1003:A:OP1	2:A:1003:A:H2'	2.15	0.46
2:A:1904:C:H2'	2:A:1905:G:O4'	2.14	0.46
2:A:2801:A:H5''	2:A:2802:G:H5'	1.97	0.46
4:C:73:ASP:C	4:C:75:VAL:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:182:ILE:HD12	4:C:270:ARG:NH1	2.30	0.46
7:F:20:ARG:HG3	7:F:20:ARG:NH1	2.29	0.46
10:I:69:LEU:HD21	10:I:109:TYR:HB2	1.97	0.46
12:K:114:LEU:HD12	12:K:114:LEU:HA	1.73	0.46
35:BA:675:A:H2'	35:BA:676:A:C8	2.50	0.46
35:BA:827:U:OP1	52:BR:19:LYS:HB2	2.15	0.46
35:BA:1159:G:N2	35:BA:1162:G:OP2	2.30	0.46
39:BE:159:ILE:H	39:BE:159:ILE:HG12	1.61	0.46
39:BE:190:ALA:HB1	39:BE:194:MET:HE2	1.97	0.46
46:BL:49:LEU:HA	46:BL:49:LEU:HD12	1.72	0.46
2:A:137:G:H8	2:A:137:G:OP1	1.98	0.46
2:A:238:G:H2'	2:A:239:U:O4'	2.16	0.46
2:A:571:A:O2'	23:V:57:GLY:HA3	2.16	0.46
2:A:1201:G:H4'	10:I:40:ARG:NH1	2.30	0.46
2:A:2362:C:H2'	2:A:2363:A:C8	2.50	0.46
4:C:137:PRO:O	4:C:140:THR:HG23	2.15	0.46
7:F:40:LYS:HD3	7:F:99:ARG:NH2	2.30	0.46
16:O:10:LEU:HB2	16:O:17:GLN:HE21	1.80	0.46
26:Y:33:ILE:HD12	26:Y:50:ASN:HB3	1.95	0.46
35:BA:429:U:O4'	35:BA:430:A:H8	1.98	0.46
35:BA:614:C:H2'	35:BA:615:G:C8	2.50	0.46
35:BA:1280:C:H2'	41:BG:114:LYS:HZ2	1.80	0.46
37:BC:21:ARG:HG2	37:BC:57:GLU:HG2	1.97	0.46
38:BD:55:LYS:HD3	38:BD:190:LEU:HD21	1.97	0.46
2:A:195:A:N3	2:A:195:A:H2'	2.29	0.46
2:A:277:U:H2'	2:A:278:A:C8	2.50	0.46
10:I:58:LYS:HE3	10:I:73:PHE:HB2	1.97	0.46
15:N:1:MET:HG2	15:N:48:GLU:HG3	1.96	0.46
15:N:51:ARG:NH1	24:W:195:ALA:HB2	2.30	0.46
35:BA:606:U:H4'	50:BP:39:ARG:CZ	2.45	0.46
35:BA:1163:G:H4'	35:BA:1164:U:H5'	1.98	0.46
37:BC:60:ARG:HA	37:BC:60:ARG:HD3	1.84	0.46
37:BC:134:ARG:HD2	37:BC:134:ARG:HA	1.73	0.46
37:BC:156:ARG:NH1	37:BC:193:PHE:HB3	2.31	0.46
43:BI:134:LYS:HE3	43:BI:139:LYS:O	2.15	0.46
55:BV:135:LEU:O	55:BV:139:ARG:HG2	2.14	0.46
2:A:650:G:H5''	12:K:112:ASN:ND2	2.30	0.46
3:B:17:G:N2	3:B:70:G:H1'	2.30	0.46
3:B:41:U:H2'	34:g:2:LYS:HE3	1.98	0.46
7:F:40:LYS:HG3	7:F:164:VAL:HG13	1.96	0.46
35:BA:522:G:OP1	38:BD:10:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BD:15:LEU:HD13	38:BD:55:LYS:HA	1.97	0.46
42:BH:70:ARG:HD2	42:BH:70:ARG:HA	1.60	0.46
2:A:747:A:H2'	2:A:748:U:O4'	2.15	0.46
35:BA:464:G:H4'	35:BA:465:G:H4'	1.98	0.46
35:BA:640:U:H2'	35:BA:641:G:O4'	2.16	0.46
35:BA:1075:U:H2'	35:BA:1076:C:O4'	2.15	0.46
40:BF:21:PRO:O	40:BF:24:GLU:HB3	2.15	0.46
41:BG:113:GLU:HG3	41:BG:119:ARG:HA	1.96	0.46
43:BI:37:VAL:HB	43:BI:87:LEU:HD22	1.97	0.46
43:BI:45:THR:HG22	43:BI:46:GLY:H	1.80	0.46
2:A:976:A:C2	2:A:1032:A:C4	3.03	0.46
4:C:218:ARG:HB3	4:C:219:PRO:HD2	1.98	0.46
7:F:8:LEU:HD23	7:F:9:PRO:HD2	1.98	0.46
31:d:24:ARG:HH11	31:d:24:ARG:HG3	1.81	0.46
35:BA:85:C:H4'	35:BA:86:G:C8	2.50	0.46
35:BA:236:G:H5''	51:BQ:57:LYS:NZ	2.30	0.46
35:BA:472:C:H2'	35:BA:473:A:C8	2.51	0.46
35:BA:1237:C:H2'	37:BC:26:LYS:HZ1	1.79	0.46
51:BQ:85:THR:H	51:BQ:87:ARG:NH1	2.14	0.46
2:A:74:C:O2'	27:Z:11:ARG:NH2	2.48	0.46
2:A:2567:U:H2'	2:A:2568:U:C6	2.51	0.46
2:A:2672:A:H4'	2:A:2673:U:OP2	2.15	0.46
2:A:2778:U:H2'	2:A:2779:U:C6	2.51	0.46
7:F:15:TYR:HA	7:F:19:ILE:HD12	1.98	0.46
14:M:43:ARG:CG	14:M:43:ARG:NH1	2.70	0.46
17:P:126:LYS:HA	17:P:126:LYS:HD3	1.76	0.46
35:BA:1099:C:OP2	43:BI:31:ARG:NH2	2.49	0.46
35:BA:1123:G:C2	35:BA:1124:G:H1'	2.51	0.46
39:BE:97:PHE:CZ	39:BE:170:LYS:HG2	2.51	0.46
55:BV:57:VAL:HG21	55:BV:217:ILE:HD11	1.98	0.46
5:D:84:LEU:HB3	5:D:209:ARG:CZ	2.46	0.46
5:D:198:ILE:HD12	5:D:206:VAL:HG11	1.98	0.46
7:F:118:ILE:HB	7:F:121:PHE:HB2	1.98	0.46
18:Q:9:GLN:HA	18:Q:12:LEU:HD12	1.98	0.46
35:BA:278:G:H5'	35:BA:279:A:OP1	2.16	0.46
43:BI:49:ASN:HD22	43:BI:84:TYR:HD1	1.64	0.46
45:BK:80:ALA:O	45:BK:84:GLN:HG2	2.15	0.46
50:BP:9:ARG:HB2	50:BP:29:ARG:NH1	2.30	0.46
2:A:81:A:N1	2:A:96:G:O2'	2.36	0.46
2:A:284:G:H1'	2:A:303:G:C6	2.51	0.46
2:A:1022:C:O2'	15:N:101:ARG:NH2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1081:C:O2'	2:A:2497:A:N3	2.43	0.46
2:A:3116:C:H2'	2:A:3117:U:H6	1.81	0.46
4:C:118:GLU:H	4:C:129:ASN:ND2	2.14	0.46
4:C:212:MET:HE2	4:C:212:MET:HA	1.97	0.46
19:R:11:GLN:HB3	19:R:15:ARG:HH21	1.80	0.46
35:BA:352:C:O2	35:BA:355:C:N4	2.49	0.46
35:BA:914:C:H5'	41:BG:4:LYS:HE2	1.98	0.46
35:BA:957:A:N3	35:BA:957:A:H5'	2.30	0.46
35:BA:1197:U:H5''	48:BN:5:ALA:HB2	1.97	0.46
1:3:21:ARG:NH2	2:A:1100:C:N3	2.64	0.46
2:A:356:G:H5''	2:A:357:U:OP1	2.16	0.46
2:A:1454:G:OP2	22:U:62:ARG:NH2	2.49	0.46
2:A:1530:G:N2	2:A:1805:G:H22	2.14	0.46
8:G:129:PRO:HG2	8:G:130:THR:HG23	1.98	0.46
9:H:82:VAL:HG11	9:H:91:LEU:HD22	1.97	0.46
27:Z:14:THR:HG22	27:Z:17:GLU:HB2	1.98	0.46
32:e:50:VAL:HG11	32:e:58:ILE:HD12	1.98	0.46
35:BA:225:G:H2'	35:BA:226:G:O4'	2.16	0.46
35:BA:375:U:OP1	50:BP:69:PRO:HB3	2.16	0.46
35:BA:814:G:H5''	52:BR:58:VAL:HG21	1.98	0.46
54:BT:72:ALA:O	54:BT:76:LYS:HG3	2.16	0.46
2:A:2558:C:H5''	17:P:20:ARG:HH21	1.80	0.45
14:M:55:MET:O	14:M:60:ARG:NH1	2.48	0.45
35:BA:265:G:H2'	35:BA:267:C:H5	1.81	0.45
35:BA:694:G:H2'	35:BA:695:A:C8	2.50	0.45
35:BA:1494:C:OP1	36:BB:11:ARG:HB2	2.16	0.45
2:A:1065:C:H1'	2:A:1102:G:C8	2.51	0.45
2:A:2959:A:H61	2:A:2993:U:H3	1.64	0.45
4:C:155:LEU:HB3	4:C:177:MET:HE1	1.97	0.45
7:F:127:LYS:HA	7:F:127:LYS:HD3	1.78	0.45
12:K:89:ILE:O	12:K:93:LEU:HB2	2.17	0.45
21:T:35:SER:HA	21:T:77:VAL:HA	1.99	0.45
35:BA:1039:C:OP2	37:BC:199:LYS:NZ	2.47	0.45
35:BA:1084:G:O5'	55:BV:110:ARG:HD2	2.16	0.45
2:A:708:G:N2	6:E:184:ASN:HD21	2.15	0.45
2:A:1001:C:C5	2:A:1002:C:H1'	2.52	0.45
7:F:81:ILE:HG22	7:F:86:LEU:HB3	1.98	0.45
35:BA:58:C:O2'	35:BA:59:A:H5''	2.16	0.45
46:BL:81:LEU:HB3	46:BL:98:ILE:HG22	1.99	0.45
2:A:530:G:O4'	6:E:47:GLN:NE2	2.50	0.45
2:A:571:A:H4'	23:V:46:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2394:A:O2'	2:A:2395:U:H3'	2.15	0.45
2:A:2702:A:OP1	33:f:31:ARG:NH1	2.49	0.45
2:A:2937:G:H3'	2:A:2938:G:H5''	1.99	0.45
4:C:156:ALA:HB2	4:C:163:ILE:HG13	1.99	0.45
12:K:35:LEU:HD23	12:K:35:LEU:HA	1.74	0.45
12:K:36:LEU:O	12:K:51:GLY:HA3	2.16	0.45
14:M:82:ASP:N	14:M:82:ASP:OD1	2.49	0.45
35:BA:567:G:OP1	42:BH:83:PRO:HB3	2.16	0.45
35:BA:1338:G:H2'	35:BA:1339:A:C8	2.52	0.45
37:BC:34:GLU:HB3	37:BC:58:ARG:HH22	1.81	0.45
44:BJ:19:ASP:O	44:BJ:23:ARG:HG2	2.16	0.45
47:BM:27:ARG:NH1	47:BM:27:ARG:HB2	2.31	0.45
56:BW:28:G:H1	56:BW:42:C:N4	2.14	0.45
2:A:1755:A:C2	2:A:1758:G:O6	2.70	0.45
2:A:2014:G:O2'	4:C:257:THR:OG1	2.20	0.45
2:A:2922:U:H2'	2:A:2923:C:C6	2.52	0.45
4:C:177:MET:HG3	4:C:181:GLU:HG2	1.98	0.45
26:Y:45:ASN:HD22	26:Y:45:ASN:HA	1.52	0.45
35:BA:480:G:H2'	35:BA:481:G:C8	2.51	0.45
35:BA:944:C:H1'	35:BA:1182:A:N6	2.32	0.45
35:BA:1076:C:H2'	35:BA:1077:C:C6	2.51	0.45
35:BA:1444:A:H2'	35:BA:1445:G:O4'	2.17	0.45
44:BJ:4:GLN:O	44:BJ:79:PRO:HD3	2.17	0.45
2:A:498:G:H5'	2:A:499:G:O5'	2.17	0.45
2:A:899:G:H5'	2:A:899:G:C8	2.49	0.45
2:A:1236:G:H2'	2:A:1237:U:O4'	2.16	0.45
2:A:1875:U:H2'	2:A:1876:A:C8	2.52	0.45
2:A:2457:U:H2'	2:A:2458:G:C8	2.52	0.45
5:D:142:GLN:O	5:D:143:ALA:CB	2.64	0.45
10:I:91:LYS:HG2	10:I:95:LYS:HE3	1.99	0.45
27:Z:62:ARG:NH2	27:Z:66:LEU:HD21	2.30	0.45
35:BA:146:A:H2'	35:BA:147:U:H6	1.82	0.45
35:BA:666:U:H2'	35:BA:667:A:C8	2.52	0.45
2:A:877:U:H4'	2:A:878:G:O5'	2.16	0.45
2:A:1799:A:H2'	2:A:1800:G:O4'	2.16	0.45
2:A:2137:A:H2	35:BA:1478:G:C8	2.35	0.45
8:G:55:ARG:NH1	8:G:63:ARG:HA	2.32	0.45
13:L:19:ILE:HD11	13:L:84:ALA:HB3	1.99	0.45
16:O:101:GLU:OE1	21:T:45:TRP:HZ3	1.99	0.45
22:U:14:PRO:HD3	27:Z:34:PHE:CD1	2.51	0.45
28:a:11:SER:N	28:a:31:ILE:HD11	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BA:196:G:C2	35:BA:197:G:C5	3.05	0.45
35:BA:505:C:H5'	46:BL:88:LYS:HE3	1.99	0.45
35:BA:1266:U:O2'	35:BA:1267:U:OP1	2.30	0.45
50:BP:9:ARG:HG2	50:BP:18:TYR:CE1	2.51	0.45
2:A:23:G:C6	2:A:24:G:N1	2.84	0.45
2:A:1202:A:O2'	2:A:1203:A:O4'	2.22	0.45
2:A:1566:A:H2'	2:A:1567:C:C5	2.51	0.45
2:A:2061:U:H5''	4:C:256:ARG:HG2	1.99	0.45
20:S:53:ASP:N	20:S:53:ASP:OD1	2.49	0.45
26:Y:33:ILE:HA	26:Y:52:CYS:HA	1.99	0.45
37:BC:69:THR:HG21	37:BC:75:VAL:HG21	1.98	0.45
51:BQ:46:HIS:CD2	51:BQ:48:LEU:H	2.34	0.45
2:A:974:G:O2'	2:A:975:U:P	2.75	0.45
2:A:2106:A:H3'	2:A:2107:G:H5''	1.97	0.45
4:C:270:ARG:HG2	4:C:270:ARG:HH11	1.82	0.45
12:K:95:LYS:HA	12:K:95:LYS:HD2	1.63	0.45
35:BA:632:U:O4	35:BA:732:G:O2'	2.23	0.45
35:BA:976:A:C8	35:BA:1197:U:H4'	2.52	0.45
39:BE:97:PHE:CE1	39:BE:170:LYS:HG2	2.52	0.45
48:BN:42:ILE:O	48:BN:46:GLU:HG2	2.17	0.45
50:BP:29:ARG:HD2	50:BP:30:ASP:OD1	2.16	0.45
2:A:636:U:H5''	2:A:637:G:C4	2.52	0.45
2:A:2315:U:P	26:Y:63:ARG:HH12	2.40	0.45
2:A:2421:A:C2	9:H:29:TYR:HB2	2.52	0.45
2:A:2800:G:O2'	2:A:2803:C:OP2	2.31	0.45
3:B:81:U:H2'	3:B:82:A:C8	2.52	0.45
4:C:147:LEU:HA	4:C:147:LEU:HD23	1.84	0.45
10:I:17:PHE:HB2	10:I:81:PHE:CE1	2.52	0.45
16:O:74:ASP:OD1	16:O:74:ASP:N	2.47	0.45
21:T:43:LEU:HA	21:T:43:LEU:HD23	1.59	0.45
35:BA:625:G:H2'	35:BA:626:G:H8	1.82	0.45
2:A:347:U:H2'	2:A:348:G:C8	2.52	0.44
2:A:1260:C:HO2'	12:K:27:ARG:NH2	2.15	0.44
2:A:1733:C:H2'	2:A:1734:C:C6	2.52	0.44
2:A:2251:G:N2	2:A:2261:U:C2	2.85	0.44
6:E:42:LEU:HD21	6:E:186:TYR:CE1	2.52	0.44
7:F:83:GLN:H	7:F:83:GLN:HG2	1.32	0.44
35:BA:1110:A:H4'	43:BI:40:ARG:HH12	1.82	0.44
35:BA:1170:U:OP1	44:BJ:53:ARG:NH2	2.46	0.44
41:BG:101:LEU:HD23	41:BG:101:LEU:HA	1.72	0.44
42:BH:5:ASP:OD1	42:BH:79:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BJ:85:ASP:O	44:BJ:89:ARG:HG3	2.17	0.44
55:BV:126:PHE:HD1	55:BV:134:ILE:HG23	1.81	0.44
2:A:863:G:OP1	21:T:95:ARG:NH1	2.49	0.44
2:A:1174:G:H5'	2:A:1175:A:O4'	2.16	0.44
7:F:111:ILE:HD11	7:F:182:PHE:CD2	2.52	0.44
16:O:100:VAL:HB	16:O:101:GLU:H	1.67	0.44
33:f:25:VAL:HB	33:f:34:GLN:HG2	1.99	0.44
35:BA:492:U:H2'	35:BA:493:A:H8	1.81	0.44
35:BA:991:C:H2'	35:BA:992:G:O4'	2.18	0.44
35:BA:1408:A:H2'	35:BA:1409:A:O4'	2.17	0.44
38:BD:15:LEU:HB3	38:BD:55:LYS:HG2	1.98	0.44
50:BP:51:ILE:HG22	50:BP:52:ASP:O	2.17	0.44
51:BQ:85:THR:N	51:BQ:87:ARG:NH1	2.65	0.44
2:A:245:G:O2'	2:A:472:C:O2	2.23	0.44
2:A:2521:C:H42	2:A:2545:G:H1	1.66	0.44
4:C:97:TYR:HE2	4:C:103:ARG:HG3	1.82	0.44
17:P:120:ALA:O	17:P:125:LEU:HB2	2.17	0.44
22:U:34:HIS:HA	22:U:35:PRO:HD3	1.86	0.44
35:BA:456:C:H4'	35:BA:457:A:OP1	2.18	0.44
35:BA:714:G:N2	52:BR:73:GLU:OE2	2.50	0.44
35:BA:1324:C:H2'	35:BA:1325:G:C8	2.53	0.44
38:BD:167:GLN:HB2	38:BD:178:HIS:HE1	1.82	0.44
54:BT:27:SER:HB3	54:BT:57:LYS:NZ	2.31	0.44
55:BV:94:GLN:HG3	55:BV:146:ARG:O	2.16	0.44
2:A:206:A:H2'	2:A:207:C:O4'	2.17	0.44
2:A:291:C:H1'	2:A:338:C:OP2	2.17	0.44
2:A:700:U:H2'	2:A:701:A:H5'	1.99	0.44
2:A:782:U:H2'	2:A:783:G:O4'	2.17	0.44
2:A:821:A:H2'	2:A:822:G:O4'	2.18	0.44
2:A:869:U:P	31:d:2:ALA:HB2	2.56	0.44
2:A:998:G:H1	2:A:1009:U:H3	1.65	0.44
2:A:1430:C:H2'	2:A:1431:U:C6	2.52	0.44
2:A:2367:G:H1'	2:A:2371:G:H22	1.83	0.44
13:L:93:PRO:HG3	13:L:114:ILE:HG12	1.99	0.44
15:N:2:LEU:HB3	15:N:69:PHE:CE1	2.52	0.44
24:W:53:ASP:O	24:W:57:VAL:HG23	2.17	0.44
35:BA:445:C:H2'	35:BA:446:A:H8	1.82	0.44
35:BA:532:U:H4'	46:BL:84:GLY:O	2.18	0.44
35:BA:747:A:H2'	35:BA:748:A:O4'	2.17	0.44
35:BA:893:U:H2'	35:BA:894:C:C6	2.52	0.44
53:BS:36:ARG:NH1	53:BS:75:ALA:O	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:BV:111:LEU:HD12	55:BV:111:LEU:HA	1.79	0.44
2:A:1105:C:O2'	2:A:1118:A:N3	2.48	0.44
2:A:1188:A:N7	2:A:1214:A:O2'	2.49	0.44
2:A:1584:U:H2'	2:A:1586:C:H5	1.82	0.44
2:A:2740:G:C6	2:A:2741:C:N4	2.85	0.44
4:C:118:GLU:HG3	4:C:129:ASN:ND2	2.33	0.44
31:d:18:VAL:HG12	31:d:19:HIS:ND1	2.32	0.44
35:BA:1019:U:H2'	35:BA:1020:G:O4'	2.18	0.44
35:BA:1135:G:H2'	35:BA:1136:A:H8	1.83	0.44
35:BA:1168:G:O2'	43:BI:133:ARG:NH1	2.51	0.44
39:BE:182:ARG:NH2	39:BE:189:VAL:HA	2.33	0.44
41:BG:62:LEU:HD13	41:BG:124:ILE:HD13	1.97	0.44
42:BH:7:ILE:O	42:BH:10:PHE:HB3	2.17	0.44
51:BQ:38:VAL:HG21	51:BQ:76:LEU:HD11	1.99	0.44
55:BV:171:ILE:O	55:BV:175:GLU:HG3	2.18	0.44
2:A:580:G:H2'	2:A:581:G:O4'	2.18	0.44
2:A:3055:G:H2'	2:A:3100:A:N6	2.31	0.44
4:C:69:ARG:H	4:C:69:ARG:HG3	1.61	0.44
8:G:55:ARG:HD2	8:G:57:ASP:O	2.18	0.44
18:Q:111:GLU:OE1	18:Q:111:GLU:N	2.51	0.44
20:S:51:LYS:HB2	20:S:54:ASP:OD2	2.17	0.44
24:W:104:GLU:O	24:W:136:GLU:HA	2.18	0.44
24:W:134:GLU:HB2	24:W:171:ILE:HD11	1.99	0.44
35:BA:493:A:H2'	35:BA:494:C:C6	2.52	0.44
37:BC:120:ALA:HB1	37:BC:189:ALA:HB2	1.99	0.44
38:BD:140:VAL:HG21	38:BD:150:PHE:CZ	2.53	0.44
2:A:1256:G:N3	12:K:108:MET:HE2	2.32	0.44
2:A:1953:C:H2'	2:A:1954:C:O4'	2.18	0.44
2:A:2085:C:O2'	2:A:2086:U:P	2.76	0.44
2:A:2094:G:O2'	2:A:2095:G:H8	2.00	0.44
2:A:3044:A:OP1	5:D:123:PHE:HB2	2.17	0.44
7:F:59:GLY:HA3	7:F:157:ARG:HH12	1.82	0.44
18:Q:48:ARG:HD2	18:Q:50:GLN:NE2	2.33	0.44
18:Q:54:ILE:O	18:Q:54:ILE:HD13	2.18	0.44
35:BA:13:G:H5'	39:BE:133:GLY:HA3	2.00	0.44
35:BA:81:C:H3'	35:BA:82:U:H5''	2.00	0.44
46:BL:114:ARG:HG2	46:BL:119:ALA:HB3	1.99	0.44
49:BO:75:VAL:HB	49:BO:79:ARG:NH2	2.33	0.44
2:A:122:A:C5	31:d:13:ARG:HD3	2.53	0.44
2:A:1131:G:H21	19:R:122:ASN:ND2	2.16	0.44
2:A:1158:U:H3	2:A:1233:A:N6	2.13	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2027:A:H2'	2:A:2028:G:O4'	2.17	0.44
4:C:163:ILE:HG12	4:C:178:PRO:HD3	1.99	0.44
10:I:66:ILE:HG22	10:I:109:TYR:CG	2.53	0.44
14:M:49:MET:HB3	14:M:49:MET:HE2	1.86	0.44
18:Q:4:LEU:HD23	18:Q:4:LEU:HA	1.62	0.44
35:BA:427:U:OP1	38:BD:13:ARG:NH2	2.51	0.44
35:BA:452:A:H2	50:BP:47:SER:HB2	1.83	0.44
35:BA:504:G:H2'	35:BA:505:C:C6	2.53	0.44
35:BA:806:C:H5'	42:BH:13:ARG:HH21	1.83	0.44
35:BA:1098:U:H1'	35:BA:1160:A:C4	2.53	0.44
35:BA:1281:A:H2'	35:BA:1281:A:N3	2.32	0.44
37:BC:123:LEU:HB3	37:BC:196:ILE:HD11	1.99	0.44
43:BI:30:GLY:N	43:BI:102:ALA:HB2	2.33	0.44
55:BV:6:MET:HE2	55:BV:6:MET:HB3	1.90	0.44
55:BV:57:VAL:O	55:BV:61:VAL:HG23	2.18	0.44
2:A:159:A:H2'	2:A:160:A:C8	2.53	0.44
2:A:539:C:H4'	6:E:53:LYS:HZ1	1.82	0.44
2:A:747:A:N6	2:A:768:G:O2'	2.51	0.44
2:A:1665:U:H2'	2:A:1666:A:H8	1.82	0.44
5:D:96:GLU:O	5:D:99:GLN:HB3	2.17	0.44
7:F:45:MET:HE2	7:F:45:MET:HB3	1.80	0.44
8:G:152:LEU:HD23	8:G:152:LEU:HA	1.83	0.44
13:L:4:GLN:HE21	13:L:23:ARG:NH1	2.16	0.44
16:O:117:ARG:HA	16:O:117:ARG:HD3	1.78	0.44
21:T:7:PHE:HB2	21:T:115:GLU:OE1	2.18	0.44
35:BA:103:G:H2'	35:BA:104:A:O4'	2.17	0.44
35:BA:426:U:OP1	38:BD:31:TYR:OH	2.36	0.44
35:BA:1406:G:H2'	35:BA:1407:U:O4'	2.18	0.44
45:BK:37:ASN:HA	45:BK:67:SER:HB3	2.00	0.44
54:BT:81:LEU:HD12	54:BT:81:LEU:HA	1.84	0.44
2:A:1530:G:H2'	2:A:1531:C:O4'	2.18	0.43
4:C:120:GLY:O	4:C:131:LEU:HB3	2.18	0.43
5:D:113:ASP:OD1	5:D:178:GLN:HA	2.18	0.43
6:E:145:LEU:HD23	6:E:145:LEU:HA	1.76	0.43
10:I:94:LYS:HB2	10:I:94:LYS:HE3	1.56	0.43
11:J:57:PRO:HG2	11:J:73:LYS:HB2	2.00	0.43
16:O:9:ARG:HA	16:O:9:ARG:HD3	1.82	0.43
24:W:122:THR:HG23	24:W:181:VAL:HG13	2.00	0.43
35:BA:498:C:H4'	35:BA:499:C:O5'	2.17	0.43
35:BA:1152:C:H2'	35:BA:1153:U:C6	2.53	0.43
35:BA:1465:C:H2'	35:BA:1466:G:H5'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:BG:10:ARG:CG	41:BG:10:ARG:NH1	2.81	0.43
55:BV:4:VAL:HG11	55:BV:212:LEU:HD21	1.99	0.43
55:BV:87:VAL:HG21	55:BV:218:ALA:HB1	2.00	0.43
2:A:561:G:C2'	2:A:562:G:H5'	2.47	0.43
2:A:768:G:H2'	2:A:769:U:C6	2.53	0.43
2:A:1294:U:H2'	2:A:1295:U:C6	2.53	0.43
9:H:10:GLU:HB3	9:H:11:HIS:CD2	2.53	0.43
14:M:31:LYS:HE3	14:M:32:THR:HG23	1.99	0.43
15:N:2:LEU:O	15:N:3:ILE:HG23	2.17	0.43
23:V:8:THR:O	23:V:74:VAL:HG12	2.17	0.43
35:BA:427:U:H5''	35:BA:428:G:O5'	2.18	0.43
47:BM:106:ASN:O	47:BM:107:ALA:HB3	2.18	0.43
50:BP:55:ARG:HD3	50:BP:55:ARG:HA	1.61	0.43
56:BW:34:G:H1	57:BX:6:U:H3	1.65	0.43
2:A:1260:C:C6	12:K:27:ARG:NH1	2.85	0.43
2:A:1637:G:O2'	2:A:1805:G:O2'	2.36	0.43
4:C:25:THR:HG21	4:C:113:GLN:HE22	1.83	0.43
8:G:150:ARG:HG2	8:G:150:ARG:HH11	1.82	0.43
15:N:51:ARG:HH12	24:W:195:ALA:HB2	1.82	0.43
25:X:18:ALA:HB3	25:X:20:ARG:HH12	1.82	0.43
35:BA:527:A:OP2	38:BD:2:ALA:N	2.51	0.43
35:BA:1185:A:H2'	35:BA:1186:U:O4'	2.18	0.43
37:BC:19:LYS:O	37:BC:55:GLU:HA	2.18	0.43
41:BG:24:THR:O	41:BG:27:VAL:HG22	2.18	0.43
45:BK:63:GLY:O	45:BK:66:LYS:HG2	2.18	0.43
46:BL:25:LYS:HD3	46:BL:59:SER:HB3	2.00	0.43
2:A:2366:C:H2'	2:A:2367:G:O4'	2.19	0.43
5:D:189:ASN:O	5:D:191:VAL:HG23	2.18	0.43
14:M:61:LEU:HA	14:M:62:PRO:HD3	1.84	0.43
35:BA:185:G:H2'	35:BA:186:C:C6	2.53	0.43
35:BA:203:U:H2'	35:BA:204:A:H8	1.83	0.43
37:BC:6:ASN:HD22	48:BN:49:HIS:HB3	1.84	0.43
43:BI:53:ARG:NH1	43:BI:58:TYR:HD1	2.17	0.43
2:A:356:G:H4'	2:A:358:G:C2	2.53	0.43
2:A:2074:G:C6	2:A:2075:G:N1	2.86	0.43
2:A:2442:U:H2'	2:A:2443:U:O4'	2.19	0.43
7:F:90:MET:HB3	7:F:90:MET:HE2	1.74	0.43
8:G:46:ALA:HB3	8:G:50:ALA:HB3	2.00	0.43
29:b:37:ARG:HD2	29:b:54:LEU:HD13	2.01	0.43
31:d:26:ARG:HE	31:d:26:ARG:HB2	1.58	0.43
35:BA:1187:G:H2'	35:BA:1188:C:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:BE:137:ARG:NH1	39:BE:137:ARG:HB2	2.34	0.43
44:BJ:24:LYS:NZ	44:BJ:93:PRO:HD3	2.34	0.43
44:BJ:92:LEU:HD12	44:BJ:98:VAL:HG21	1.99	0.43
46:BL:38:TYR:N	46:BL:38:TYR:CD1	2.86	0.43
47:BM:67:GLU:HB3	47:BM:68:GLY:H	1.60	0.43
52:BR:48:ILE:HG12	52:BR:68:VAL:HG11	2.00	0.43
53:BS:18:LYS:HA	53:BS:18:LYS:HD3	1.88	0.43
54:BT:35:PHE:CE1	54:BT:51:LEU:HB2	2.53	0.43
2:A:1530:G:N2	2:A:1806:A:C6	2.86	0.43
2:A:2613:G:O5'	2:A:2614:U:H5'	2.19	0.43
4:C:16:ALA:HB2	4:C:207:GLY:HA3	2.01	0.43
7:F:50:ALA:HB1	7:F:57:ILE:HD11	2.00	0.43
35:BA:144:G:H2'	35:BA:145:G:C8	2.54	0.43
35:BA:1384:G:C6	35:BA:1385:C:C2	3.06	0.43
40:BF:15:ASP:OD1	40:BF:15:ASP:N	2.50	0.43
42:BH:53:ASP:OD1	42:BH:58:LYS:HG2	2.19	0.43
47:BM:49:THR:HG22	47:BM:50:ASP:H	1.83	0.43
51:BQ:35:THR:HG22	51:BQ:86:LYS:NZ	2.33	0.43
53:BS:12:ASP:OD1	53:BS:38:SER:HB3	2.18	0.43
55:BV:160:ALA:HB1	55:BV:184:ILE:HD11	2.01	0.43
2:A:156:C:H2'	2:A:157:U:H6	1.83	0.43
2:A:1048:A:C6	2:A:1050:A:C8	3.06	0.43
2:A:1165:G:O2'	2:A:1228:A:N1	2.46	0.43
2:A:2757:C:H2'	2:A:2758:A:O4'	2.19	0.43
6:E:20:LEU:HB3	6:E:25:PHE:CD1	2.54	0.43
14:M:49:MET:H	14:M:49:MET:HE3	1.83	0.43
14:M:49:MET:HB2	14:M:58:HIS:HE1	1.83	0.43
24:W:105:LYS:HA	24:W:105:LYS:HD3	1.70	0.43
24:W:117:ASP:H	24:W:149:GLU:HG3	1.83	0.43
34:g:58:VAL:HB	53:BS:64:GLU:OE2	2.17	0.43
39:BE:182:ARG:HH21	39:BE:189:VAL:HA	1.84	0.43
44:BJ:78:ASP:OD1	44:BJ:78:ASP:N	2.52	0.43
52:BR:24:SER:HB3	52:BR:26:LYS:HG2	2.00	0.43
2:A:686:A:H4'	32:e:63:ASN:O	2.18	0.43
2:A:1339:G:OP1	20:S:72:LYS:NZ	2.49	0.43
2:A:1379:G:OP1	29:b:16:ARG:NH2	2.35	0.43
2:A:1640:A:C3'	2:A:1641:U:H5''	2.47	0.43
5:D:83:GLU:O	5:D:84:LEU:HD23	2.19	0.43
7:F:66:LEU:HD23	7:F:66:LEU:HA	1.77	0.43
8:G:41:ILE:HD11	8:G:65:LEU:HB3	2.01	0.43
10:I:40:ARG:NH1	10:I:40:ARG:CG	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:73:LYS:HA	16:O:76:VAL:HG22	1.99	0.43
26:Y:39:VAL:HG21	26:Y:64:ALA:HB3	2.00	0.43
35:BA:53:U:H5''	35:BA:53:U:H6	1.84	0.43
35:BA:65:G:H2'	35:BA:66:U:O4'	2.19	0.43
35:BA:994:C:H2'	35:BA:995:A:H8	1.83	0.43
46:BL:54:ARG:NH1	46:BL:64:THR:HG23	2.30	0.43
50:BP:65:GLN:HA	50:BP:66:PRO:HD2	1.78	0.43
2:A:159:A:N3	2:A:2431:C:O2'	2.52	0.43
2:A:1400:G:N2	2:A:1443:G:H5''	2.34	0.43
2:A:1565:A:N6	2:A:1606:G:H1	2.17	0.43
2:A:1755:A:C2	2:A:1759:A:N6	2.87	0.43
2:A:2008:A:N6	2:A:2045:G:O2'	2.48	0.43
6:E:29:PRO:HD3	6:E:120:ARG:NH1	2.34	0.43
7:F:50:ALA:HA	7:F:53:ASP:O	2.19	0.43
25:X:54:GLY:N	25:X:58:THR:O	2.47	0.43
31:d:33:ILE:O	31:d:37:ARG:HG3	2.19	0.43
35:BA:196:G:H2'	35:BA:197:G:C8	2.54	0.43
35:BA:390:U:H2'	35:BA:391:G:H8	1.84	0.43
35:BA:614:C:H2'	35:BA:615:G:H8	1.83	0.43
35:BA:864:C:O2'	35:BA:865:C:H5'	2.19	0.43
42:BH:19:SER:HA	42:BH:72:ARG:NH1	2.33	0.43
46:BL:39:THR:HA	46:BL:50:ARG:O	2.19	0.43
50:BP:40:TYR:CZ	50:BP:42:PRO:HG3	2.54	0.43
2:A:601:A:H2'	2:A:602:A:O4'	2.19	0.43
2:A:1855:A:H2'	2:A:1856:C:C6	2.54	0.43
2:A:2585:U:H2'	2:A:2586:G:H5'	2.01	0.43
2:A:3082:U:H2'	2:A:3083:A:H8	1.83	0.43
6:E:94:LYS:HD3	6:E:94:LYS:HA	1.59	0.43
7:F:75:ARG:HD3	7:F:75:ARG:HA	1.86	0.43
8:G:110:TYR:CE1	8:G:153:ARG:NH1	2.87	0.43
9:H:98:ALA:HB2	9:H:114:LYS:HD2	2.01	0.43
10:I:82:VAL:HG21	10:I:86:ALA:O	2.18	0.43
14:M:24:ARG:HA	14:M:24:ARG:HD3	1.42	0.43
35:BA:595:C:H2'	35:BA:596:A:H8	1.84	0.43
45:BK:109:LEU:HD23	45:BK:109:LEU:HA	1.81	0.43
2:A:250:G:H2'	2:A:251:A:C8	2.54	0.42
4:C:26:ARG:NH1	4:C:30:GLU:OE1	2.49	0.42
6:E:28:GLU:HA	6:E:120:ARG:HH22	1.81	0.42
22:U:44:ILE:HA	22:U:47:GLU:OE2	2.18	0.42
24:W:77:LEU:HD12	24:W:77:LEU:HA	1.87	0.42
34:g:65:TYR:CD1	53:BS:9:PRO:HD3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BA:203:U:H2'	35:BA:204:A:C8	2.54	0.42
39:BE:99:VAL:HG12	39:BE:101:LEU:HG	2.01	0.42
47:BM:9:LEU:HA	47:BM:10:PRO:HD3	1.91	0.42
50:BP:48:LEU:HD11	50:BP:50:GLN:HG2	2.01	0.42
55:BV:52:LYS:O	55:BV:55:GLU:HG2	2.19	0.42
2:A:2425:U:O2'	2:A:2427:G:OP1	2.34	0.42
2:A:2548:U:H5'	2:A:2549:G:H5'	2.01	0.42
4:C:62:TYR:HA	4:C:87:ASN:HD21	1.84	0.42
4:C:70:HIS:CG	4:C:71:ASP:N	2.87	0.42
11:J:10:LEU:N	11:J:62:VAL:HG22	2.33	0.42
16:O:38:GLU:N	16:O:39:PRO:HD2	2.33	0.42
21:T:52:GLU:HB2	21:T:53:PRO:HD3	2.02	0.42
28:a:23:LEU:HD23	28:a:23:LEU:HA	1.78	0.42
29:b:10:ARG:HD3	29:b:14:ARG:HH12	1.84	0.42
35:BA:32:G:H2'	35:BA:33:A:O4'	2.19	0.42
35:BA:380:G:N2	35:BA:383:A:OP2	2.47	0.42
35:BA:728:A:OP2	35:BA:728:A:H8	2.01	0.42
35:BA:735:G:OP2	49:BO:65:ARG:HD3	2.19	0.42
35:BA:1271:A:H2'	35:BA:1272:G:H5'	2.01	0.42
36:BB:3:SER:OG	36:BB:5:ILE:HG13	2.19	0.42
44:BJ:90:ILE:HG22	44:BJ:92:LEU:HG	2.01	0.42
50:BP:82:LYS:HB2	50:BP:89:ALA:HB2	2.01	0.42
1:3:8:LYS:O	1:3:11:ARG:HG2	2.19	0.42
2:A:209:C:OP1	31:d:28:ARG:NH1	2.52	0.42
2:A:306:U:H2'	2:A:307:G:H8	1.84	0.42
2:A:684:G:H3'	2:A:685:G:C5'	2.49	0.42
4:C:68:ARG:HG3	4:C:68:ARG:O	2.18	0.42
8:G:88:MET:HE3	8:G:165:TYR:CD1	2.55	0.42
12:K:7:LYS:HD3	12:K:7:LYS:HA	1.67	0.42
14:M:80:VAL:HG23	14:M:113:LEU:O	2.18	0.42
22:U:44:ILE:O	22:U:47:GLU:HG2	2.18	0.42
35:BA:434:C:H2'	35:BA:435:U:C6	2.55	0.42
35:BA:642:C:H2'	35:BA:643:A:H8	1.83	0.42
35:BA:654:G:H2'	35:BA:655:A:C8	2.54	0.42
35:BA:669:C:H2'	35:BA:670:G:O4'	2.19	0.42
35:BA:884:G:H5'	36:BB:18:ARG:NH1	2.34	0.42
35:BA:965:A:H5'	35:BA:966:C:OP2	2.19	0.42
35:BA:1209:C:OP1	47:BM:108:ARG:NH1	2.43	0.42
41:BG:155:ARG:HA	41:BG:155:ARG:HD3	1.67	0.42
52:BR:45:ARG:HD3	52:BR:45:ARG:HA	1.88	0.42
2:A:289:A:N7	2:A:290:C:H5	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:326:A:H61	2:A:449:G:H1	1.67	0.42
2:A:1202:A:H62	10:I:36:LEU:HD11	1.84	0.42
2:A:1229:A:C8	2:A:1230:G:H1'	2.54	0.42
2:A:1795:C:H2'	2:A:1796:U:O4'	2.20	0.42
8:G:26:VAL:HG12	8:G:80:VAL:HG21	2.02	0.42
21:T:53:PRO:O	21:T:57:VAL:HG23	2.19	0.42
27:Z:45:ARG:HD3	27:Z:45:ARG:HA	1.76	0.42
29:b:10:ARG:CD	29:b:14:ARG:HH12	2.32	0.42
35:BA:390:U:H2'	35:BA:391:G:C8	2.55	0.42
35:BA:480:G:C6	35:BA:526:G:N2	2.86	0.42
35:BA:657:U:H3	35:BA:693:G:H22	1.67	0.42
38:BD:145:LEU:HG	38:BD:154:ARG:HH12	1.84	0.42
55:BV:100:MET:HA	55:BV:107:VAL:HG21	2.01	0.42
2:A:1805:G:H2'	2:A:1806:A:C8	2.54	0.42
2:A:2581:G:OP2	2:A:2581:G:H8	2.02	0.42
3:B:76:G:O2'	24:W:94:HIS:HE1	2.03	0.42
6:E:123:ARG:O	6:E:125:HIS:HD2	2.02	0.42
7:F:68:THR:HG21	7:F:96:VAL:HG11	2.01	0.42
7:F:159:MET:HE3	7:F:159:MET:HB3	1.87	0.42
9:H:77:ASP:HB3	9:H:147:ASN:ND2	2.35	0.42
18:Q:48:ARG:HG2	18:Q:59:THR:HB	2.01	0.42
27:Z:45:ARG:NH1	27:Z:48:ARG:NE	2.67	0.42
35:BA:70:A:H4'	35:BA:170:U:C5	2.54	0.42
35:BA:1461:U:H2'	35:BA:1462:C:C6	2.54	0.42
38:BD:182:GLU:O	38:BD:186:ILE:HG13	2.19	0.42
46:BL:90:LEU:HA	46:BL:91:PRO:HD3	1.81	0.42
50:BP:28:ARG:HG2	50:BP:28:ARG:HH11	1.84	0.42
55:BV:156:LYS:O	55:BV:157:VAL:HG22	2.20	0.42
2:A:300:G:N2	2:A:303:G:H5''	2.35	0.42
7:F:98:LEU:HD23	7:F:98:LEU:HA	1.81	0.42
15:N:76:LYS:HB3	15:N:91:GLU:HG3	2.01	0.42
23:V:64:ALA:HA	23:V:65:PRO:HD3	1.92	0.42
30:c:22:ASN:HD22	30:c:22:ASN:HA	1.62	0.42
34:g:12:THR:HA	34:g:31:GLY:O	2.19	0.42
35:BA:1110:A:H4'	43:BI:40:ARG:CZ	2.49	0.42
35:BA:1374:U:H2'	35:BA:1375:G:C8	2.55	0.42
38:BD:132:VAL:HG13	38:BD:136:ASP:OD2	2.20	0.42
39:BE:108:HIS:HE1	39:BE:173:GLN:H	1.66	0.42
41:BG:13:VAL:HG22	41:BG:14:ASN:H	1.83	0.42
45:BK:43:ILE:O	45:BK:51:ILE:HG13	2.20	0.42
55:BV:173:VAL:HG13	55:BV:183:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2035:U:OP2	4:C:157:ARG:NH1	2.53	0.42
2:A:2348:G:H21	2:A:2397:C:H42	1.68	0.42
13:L:2:ILE:HB	13:L:33:ALA:HB3	2.02	0.42
14:M:59:MET:HE2	14:M:59:MET:HB3	1.84	0.42
19:R:119:GLU:H	19:R:119:GLU:CD	2.26	0.42
21:T:95:ARG:HG3	21:T:101:PHE:CD2	2.55	0.42
24:W:109:GLU:HA	24:W:131:ILE:O	2.19	0.42
28:a:30:LYS:HD2	28:a:33:GLN:NE2	2.35	0.42
35:BA:159:A:C5	35:BA:160:C:H1'	2.55	0.42
35:BA:457:A:O2'	35:BA:458:A:O5'	2.27	0.42
35:BA:613:G:H2'	35:BA:614:C:C6	2.55	0.42
35:BA:693:G:H2'	35:BA:694:G:C8	2.55	0.42
2:A:326:A:H2'	2:A:326:A:N3	2.34	0.42
2:A:361:A:N1	2:A:440:U:O2'	2.49	0.42
2:A:443:C:H2'	2:A:444:U:O4'	2.18	0.42
2:A:834:C:O2'	2:A:835:C:H5'	2.19	0.42
2:A:1756:G:H1'	2:A:1758:G:C2	2.55	0.42
2:A:2925:C:O2'	16:O:73:LYS:HE3	2.20	0.42
2:A:3038:C:OP1	16:O:42:ARG:NH2	2.52	0.42
10:I:98:LYS:HB2	10:I:98:LYS:HE2	1.77	0.42
15:N:77:LYS:HB2	15:N:78:PRO:HD2	2.01	0.42
23:V:81:THR:HG21	23:V:100:THR:H	1.85	0.42
23:V:81:THR:HG23	23:V:100:THR:HG23	2.01	0.42
37:BC:126:ARG:HD3	37:BC:126:ARG:HA	1.76	0.42
37:BC:175:LEU:HD23	37:BC:182:ILE:HD12	2.02	0.42
53:BS:28:LYS:NZ	53:BS:46:GLY:HA3	2.34	0.42
2:A:720:C:H42	14:M:76:GLN:NE2	2.18	0.42
2:A:929:C:H1'	2:A:1339:G:N2	2.35	0.42
2:A:2350:G:H22	2:A:2384:C:H2'	1.85	0.42
2:A:2925:C:H3'	2:A:2926:A:C5'	2.50	0.42
2:A:2964:A:H2'	2:A:2965:A:C8	2.55	0.42
5:D:79:ARG:HG2	5:D:80:HIS:NE2	2.35	0.42
8:G:55:ARG:HG2	8:G:66:HIS:CE1	2.54	0.42
16:O:3:LYS:HA	16:O:4:PRO:HD3	1.81	0.42
32:e:44:LEU:HA	32:e:44:LEU:HD23	1.74	0.42
34:g:26:SER:OG	34:g:27:THR:N	2.53	0.42
35:BA:253:U:H2'	35:BA:254:G:H8	1.84	0.42
35:BA:485:G:C8	35:BA:515:A:C4	3.08	0.42
35:BA:493:A:H2'	35:BA:494:C:H6	1.85	0.42
35:BA:510:G:H2'	35:BA:510:G:N3	2.35	0.42
35:BA:1183:U:H2'	35:BA:1184:C:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BA:1208:A:C2	47:BM:117:ILE:HG21	2.54	0.42
35:BA:1258:C:H2'	35:BA:1260:A:H8	1.85	0.42
35:BA:1353:G:C2	35:BA:1354:G:C8	3.07	0.42
37:BC:190:LYS:HD3	37:BC:195:ARG:CZ	2.49	0.42
38:BD:41:ILE:HG21	38:BD:47:ARG:CZ	2.50	0.42
39:BE:106:ILE:HD13	39:BE:148:ILE:HD11	2.01	0.42
41:BG:21:GLN:HA	41:BG:24:THR:HG22	2.00	0.42
45:BK:121:ASP:OD1	45:BK:121:ASP:N	2.53	0.42
2:A:483:G:H2'	2:A:484:C:C6	2.55	0.42
2:A:1485:C:H2'	2:A:1486:G:O4'	2.20	0.42
2:A:1642:G:C2	2:A:1643:G:C8	3.08	0.42
9:H:85:ALA:HB2	9:H:92:PHE:CE1	2.55	0.42
13:L:44:LYS:HD3	13:L:44:LYS:HA	1.82	0.42
35:BA:1310:C:H2'	35:BA:1311:G:O4'	2.19	0.42
37:BC:23:TYR:C	37:BC:23:TYR:CD1	2.98	0.42
42:BH:128:LEU:HD23	42:BH:128:LEU:HA	1.77	0.42
51:BQ:36:ILE:HG13	51:BQ:61:ALA:HB3	2.02	0.42
55:BV:49:TYR:HB3	55:BV:199:PRO:O	2.20	0.42
2:A:1046:C:H4'	2:A:1047:A:OP2	2.20	0.41
2:A:1131:G:H21	19:R:122:ASN:HD22	1.68	0.41
2:A:2718:G:H4'	15:N:80:GLU:HG2	2.01	0.41
9:H:5:LEU:HD12	9:H:17:ASP:HB2	2.01	0.41
11:J:81:LEU:HD13	11:J:134:ALA:HB2	2.01	0.41
12:K:109:LEU:HD23	12:K:109:LEU:HA	1.85	0.41
33:f:30:PRO:O	33:f:33:LYS:HB3	2.20	0.41
35:BA:408:G:OP1	38:BD:107:ARG:HB2	2.20	0.41
35:BA:1261:A:O2'	35:BA:1262:U:H5'	2.20	0.41
35:BA:1315:A:H2'	35:BA:1316:G:O4'	2.20	0.41
43:BI:150:ARG:HD3	43:BI:150:ARG:HA	1.79	0.41
50:BP:5:ILE:HG13	50:BP:64:ALA:HB1	2.02	0.41
55:BV:83:GLU:OE2	55:BV:214:THR:HB	2.20	0.41
2:A:334:G:H1	2:A:347:U:H3	1.66	0.41
2:A:940:A:H2'	2:A:941:U:O4'	2.20	0.41
5:D:10:LYS:HB2	5:D:198:ILE:HD11	2.02	0.41
6:E:8:LYS:HD2	6:E:148:LEU:HD13	2.01	0.41
6:E:158:ILE:O	6:E:179:SER:HA	2.19	0.41
7:F:38:VAL:HA	7:F:165:THR:HG23	2.01	0.41
7:F:75:ARG:NH2	7:F:95:ARG:NH1	2.62	0.41
14:M:97:GLU:O	14:M:101:LYS:HG2	2.19	0.41
35:BA:715:G:H1'	52:BR:73:GLU:OE2	2.20	0.41
35:BA:777:C:H2'	35:BA:778:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BH:50:ARG:HG3	42:BH:52:GLU:OE2	2.20	0.41
43:BI:61:ASN:HD22	43:BI:64:HIS:HD2	1.62	0.41
46:BL:38:TYR:CE1	46:BL:52:VAL:HG12	2.55	0.41
49:BO:66:LEU:HD23	49:BO:66:LEU:HA	1.78	0.41
2:A:278:A:C2	2:A:279:U:H1'	2.55	0.41
2:A:543:U:C5	2:A:561:G:H5'	2.55	0.41
2:A:2084:A:H2'	2:A:2085:C:O4'	2.20	0.41
2:A:2952:U:O2'	5:D:25:PRO:HG2	2.20	0.41
4:C:25:THR:HG21	4:C:113:GLN:NE2	2.36	0.41
6:E:33:LEU:HD12	6:E:106:MET:HE3	2.02	0.41
7:F:126:PRO:O	7:F:174:ARG:NH1	2.53	0.41
11:J:40:PHE:CE1	11:J:58:VAL:HG21	2.45	0.41
15:N:37:LEU:HD21	15:N:130:ARG:HD3	2.02	0.41
24:W:119:THR:HG21	24:W:152:GLU:HG2	2.01	0.41
38:BD:13:ARG:HD2	38:BD:31:TYR:O	2.19	0.41
47:BM:108:ARG:NH2	47:BM:114:LYS:HA	2.36	0.41
55:BV:103:ASN:ND2	55:BV:106:THR:OG1	2.52	0.41
2:A:2074:G:O6	2:A:2075:G:N1	2.54	0.41
2:A:2691:C:H4'	15:N:123:HIS:CD2	2.55	0.41
4:C:17:SER:O	4:C:211:ARG:NH2	2.53	0.41
6:E:183:LEU:HA	6:E:183:LEU:HD12	1.80	0.41
7:F:11:LEU:HD23	7:F:11:LEU:HA	1.87	0.41
9:H:121:LYS:HA	9:H:121:LYS:HD3	1.91	0.41
10:I:17:PHE:CZ	10:I:66:ILE:HG12	2.55	0.41
11:J:59:GLU:O	11:J:70:PHE:HA	2.19	0.41
13:L:75:SER:CB	18:Q:71:ARG:HH21	2.33	0.41
15:N:8:LYS:HB3	15:N:9:HIS:ND1	2.36	0.41
18:Q:32:ILE:O	18:Q:32:ILE:HG13	2.19	0.41
19:R:109:LEU:HD23	19:R:109:LEU:HA	1.86	0.41
35:BA:210:A:OP2	35:BA:210:A:H8	2.02	0.41
35:BA:276:G:H4'	51:BQ:60:LYS:NZ	2.35	0.41
35:BA:988:C:H2'	35:BA:989:G:O4'	2.20	0.41
35:BA:1081:A:N7	55:BV:171:ILE:HG23	2.35	0.41
41:BG:78:ARG:HB2	41:BG:156:TRP:CZ3	2.56	0.41
46:BL:7:LEU:HD23	46:BL:7:LEU:HA	1.89	0.41
46:BL:67:ILE:HG12	46:BL:97:ILE:HD12	2.02	0.41
2:A:1185:A:H2'	2:A:1186:G:C8	2.54	0.41
2:A:1201:G:H21	2:A:1203:A:H3'	1.82	0.41
2:A:2532:G:N3	2:A:2532:G:H2'	2.36	0.41
4:C:123:ALA:HB3	4:C:131:LEU:HD22	2.02	0.41
7:F:137:PHE:CE1	7:F:161:ILE:HB	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:149:ILE:HG22	8:G:163:VAL:HG11	2.01	0.41
15:N:72:ARG:H	15:N:72:ARG:HG2	1.32	0.41
16:O:24:LEU:HD23	16:O:24:LEU:HA	1.83	0.41
18:Q:20:SER:OG	18:Q:21:PRO:HD2	2.21	0.41
20:S:68:THR:HG22	20:S:94:LEU:HB2	2.03	0.41
35:BA:134:C:H2'	35:BA:135:U:O4'	2.21	0.41
35:BA:286:G:H2'	35:BA:287:U:O4'	2.20	0.41
35:BA:716:U:H2'	35:BA:717:C:C6	2.56	0.41
35:BA:772:A:O2'	35:BA:774:A:C8	2.68	0.41
42:BH:101:LEU:HD23	42:BH:101:LEU:HA	1.80	0.41
43:BI:28:THR:HG21	43:BI:106:ALA:HB2	2.03	0.41
44:BJ:8:ILE:HD11	44:BJ:87:LEU:HD13	2.02	0.41
49:BO:7:GLN:H	49:BO:7:GLN:HG3	1.73	0.41
50:BP:81:GLN:O	50:BP:85:GLY:N	2.40	0.41
55:BV:83:GLU:O	55:BV:87:VAL:HG23	2.21	0.41
55:BV:138:THR:O	55:BV:142:ASN:HB2	2.20	0.41
57:BX:3:U:HO2'	57:BX:4:U:H5	1.68	0.41
2:A:693:G:OP1	6:E:30:ASN:ND2	2.54	0.41
2:A:2017:C:P	4:C:183:ARG:HH12	2.43	0.41
3:B:4:A:N1	3:B:23:G:O2'	2.49	0.41
20:S:69:LYS:HB2	20:S:69:LYS:HE3	1.78	0.41
35:BA:410:G:H21	35:BA:432:A:H62	1.67	0.41
35:BA:1125:G:H21	35:BA:1127:A:H62	1.67	0.41
35:BA:1177:A:HO2'	35:BA:1178:A:P	2.37	0.41
35:BA:1221:U:O4	41:BG:109:ARG:NH2	2.51	0.41
43:BI:47:GLN:HB2	43:BI:82:ASP:OD1	2.21	0.41
46:BL:101:SER:O	46:BL:104:THR:HG23	2.20	0.41
47:BM:25:ILE:HG23	47:BM:29:ARG:HB2	2.03	0.41
2:A:487:U:H2'	2:A:488:G:O4'	2.20	0.41
2:A:844:G:H5'	2:A:845:C:H5''	2.02	0.41
2:A:1078:G:N2	2:A:2254:A:OP1	2.47	0.41
2:A:2505:C:O2'	2:A:2506:G:H5'	2.20	0.41
3:B:12:C:H4'	3:B:13:C:OP2	2.20	0.41
6:E:158:ILE:HG22	6:E:159:GLY:O	2.21	0.41
7:F:165:THR:HG21	7:F:176:LEU:HD23	2.03	0.41
11:J:47:ALA:O	11:J:50:SER:HB2	2.21	0.41
23:V:13:SER:HB2	23:V:70:ASN:ND2	2.36	0.41
35:BA:1410:C:H2'	35:BA:1411:A:C8	2.56	0.41
37:BC:107:ASN:HA	37:BC:108:PRO:HD3	1.91	0.41
38:BD:191:THR:HG22	38:BD:193:GLN:HG2	2.03	0.41
41:BG:86:GLN:HB2	41:BG:148:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BH:14:LEU:HD23	42:BH:14:LEU:HA	1.86	0.41
44:BJ:42:LEU:HB2	44:BJ:71:LYS:HB2	2.01	0.41
50:BP:75:LYS:HA	50:BP:81:GLN:HE21	1.85	0.41
2:A:757:G:H2'	25:X:85:ARG:HD2	2.02	0.41
2:A:944:A:C8	2:A:2472:C:H5'	2.56	0.41
2:A:1199:U:H2'	2:A:1200:U:C6	2.56	0.41
2:A:1787:A:H2'	4:C:86:PRO:HG3	2.02	0.41
2:A:2070:A:H2'	2:A:2071:A:C8	2.55	0.41
2:A:3069:G:H3'	18:Q:92:ARG:O	2.21	0.41
2:A:3082:U:H2'	2:A:3083:A:C8	2.55	0.41
7:F:182:PHE:HA	7:F:183:PRO:HD3	1.69	0.41
15:N:71:ASP:OD1	15:N:71:ASP:N	2.37	0.41
29:b:10:ARG:NH1	29:b:10:ARG:HG3	2.36	0.41
35:BA:605:G:H2'	35:BA:606:U:H6	1.86	0.41
35:BA:1110:A:H61	35:BA:1125:G:H1'	1.85	0.41
40:BF:1:MET:HE3	40:BF:66:LYS:HB3	2.03	0.41
40:BF:41:ASP:C	40:BF:42:ILE:HG13	2.45	0.41
43:BI:53:ARG:HD3	43:BI:57:ASN:ND2	2.36	0.41
52:BR:29:THR:HG22	52:BR:30:ILE:H	1.85	0.41
53:BS:21:VAL:HG13	53:BS:25:LYS:HE3	2.02	0.41
55:BV:111:LEU:HD21	55:BV:152:ARG:HA	2.03	0.41
2:A:641:U:H6	2:A:641:U:H2'	1.69	0.41
2:A:981:U:O2'	2:A:982:A:O5'	2.38	0.41
2:A:1439:G:C2	2:A:1443:G:C6	3.08	0.41
2:A:1615:G:H2'	2:A:1616:A:O4'	2.21	0.41
2:A:1732:U:H2'	2:A:1733:C:C6	2.56	0.41
2:A:2358:A:N6	2:A:2379:G:HO2'	2.16	0.41
2:A:2367:G:H1'	2:A:2371:G:N2	2.36	0.41
2:A:2781:G:H2'	2:A:2782:C:C6	2.56	0.41
2:A:2926:A:OP1	16:O:73:LYS:NZ	2.48	0.41
4:C:182:ILE:HB	4:C:270:ARG:HH12	1.86	0.41
12:K:145:VAL:HG12	19:R:73:ASP:OD1	2.21	0.41
13:L:107:ARG:NH1	18:Q:33:GLU:OE2	2.54	0.41
14:M:22:VAL:HG23	14:M:29:LYS:HD2	2.02	0.41
14:M:137:ILE:HD13	14:M:137:ILE:HA	1.94	0.41
15:N:34:ILE:HD11	15:N:118:LEU:HD22	2.03	0.41
15:N:73:PRO:HB3	15:N:93:TRP:CZ3	2.56	0.41
19:R:38:GLN:O	19:R:42:SER:HB2	2.21	0.41
19:R:58:ARG:HA	19:R:61:TRP:CE3	2.55	0.41
23:V:1:MET:HE3	23:V:26:ALA:HB1	2.03	0.41
24:W:86:HIS:HA	24:W:87:PRO:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:14:THR:OG1	27:Z:15:ASP:N	2.54	0.41
27:Z:36:MET:HE2	27:Z:36:MET:HB3	1.95	0.41
35:BA:376:G:C4	35:BA:389:A:C2	3.09	0.41
35:BA:604:U:H2'	35:BA:605:G:H8	1.86	0.41
40:BF:29:VAL:O	40:BF:32:LYS:HG2	2.21	0.41
40:BF:46:ARG:HB3	40:BF:60:TYR:CE2	2.56	0.41
45:BK:31:HIS:CE1	45:BK:44:THR:HG21	2.55	0.41
45:BK:103:GLU:HB3	45:BK:107:ARG:HH21	1.83	0.41
46:BL:67:ILE:HA	46:BL:68:PRO:HD3	1.77	0.41
48:BN:36:LYS:HB3	48:BN:36:LYS:HE2	1.77	0.41
55:BV:137:LEU:HB3	55:BV:141:LYS:NZ	2.36	0.41
2:A:429:A:H2'	2:A:430:A:C8	2.56	0.41
2:A:844:G:H4'	2:A:878:G:H5'	2.03	0.41
2:A:1303:U:O2'	2:A:1304:A:H5'	2.21	0.41
2:A:1533:U:OP2	2:A:1535:C:N4	2.53	0.41
2:A:1602:U:H2'	2:A:1603:G:C8	2.56	0.41
2:A:1715:A:H2'	2:A:1716:A:C8	2.56	0.41
5:D:38:ARG:HD3	5:D:40:ARG:NH1	2.36	0.41
6:E:118:ARG:HA	6:E:118:ARG:HD3	1.93	0.41
6:E:150:GLU:H	6:E:150:GLU:HG2	1.68	0.41
8:G:176:LYS:HG3	8:G:177:THR:H	1.86	0.41
18:Q:88:ARG:HB2	18:Q:112:LYS:HB2	2.03	0.41
19:R:83:LEU:HD23	19:R:83:LEU:HA	1.63	0.41
33:f:24:MET:HE2	33:f:24:MET:HB3	1.83	0.41
35:BA:127:A:HI1'	35:BA:263:A:O2'	2.21	0.41
39:BE:54:ARG:HH11	39:BE:54:ARG:HG2	1.86	0.41
39:BE:199:ARG:HA	39:BE:202:GLU:OE1	2.21	0.41
41:BG:28:ASN:HD21	41:BG:36:LYS:HZ1	1.69	0.41
44:BJ:57:LYS:HB2	44:BJ:57:LYS:HE3	1.75	0.41
55:BV:43:LEU:O	55:BV:47:LEU:HG	2.20	0.41
2:A:700:U:OP1	6:E:103:PRO:HA	2.21	0.40
2:A:1078:G:H22	2:A:2254:A:P	2.45	0.40
2:A:1760:G:H2'	2:A:1761:G:H8	1.85	0.40
2:A:2217:U:H4'	5:D:138:ALA:HB3	2.03	0.40
6:E:54:THR:HG23	6:E:94:LYS:HZ1	1.85	0.40
29:b:14:ARG:HH11	29:b:14:ARG:CG	2.34	0.40
33:f:4:ASN:O	33:f:36:GLN:HA	2.21	0.40
35:BA:105:A:C6	35:BA:326:G:C6	3.09	0.40
35:BA:498:C:C5	35:BA:509:G:H3'	2.55	0.40
35:BA:1107:G:HI1'	35:BA:1261:A:C6	2.56	0.40
52:BR:74:VAL:HG23	52:BR:76:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:BT:68:HIS:HD2	54:BT:70:ASN:HB2	1.86	0.40
54:BT:71:GLN:HE21	54:BT:75:LYS:NZ	2.19	0.40
2:A:1204:A:H5''	2:A:1205:G:OP1	2.20	0.40
2:A:1688:G:N2	2:A:1748:A:H1'	2.36	0.40
5:D:127:MET:HB3	5:D:127:MET:HE2	1.62	0.40
6:E:29:PRO:CD	6:E:120:ARG:HH12	2.34	0.40
8:G:4:ILE:CG2	8:G:70:ARG:HD2	2.51	0.40
19:R:72:ASN:HD22	19:R:72:ASN:N	2.19	0.40
21:T:95:ARG:HG3	21:T:101:PHE:CE2	2.57	0.40
24:W:84:ASP:OD2	24:W:94:HIS:HB3	2.20	0.40
35:BA:355:C:H2'	35:BA:356:A:O4'	2.21	0.40
35:BA:595:C:H2'	35:BA:596:A:C8	2.56	0.40
35:BA:1486:A:H2'	35:BA:1488:G:C8	2.56	0.40
44:BJ:18:ILE:HA	44:BJ:18:ILE:HD12	1.73	0.40
45:BK:68:THR:OG1	45:BK:69:PRO:HD2	2.21	0.40
51:BQ:46:HIS:CG	51:BQ:47:PRO:HD2	2.56	0.40
55:BV:6:MET:HE1	55:BV:44:GLN:CD	2.47	0.40
2:A:159:A:C5	2:A:166:A:C2	3.10	0.40
2:A:322:A:OP2	2:A:322:A:H8	2.05	0.40
2:A:1541:G:N2	2:A:1631:A:H61	2.20	0.40
2:A:1640:A:H2'	2:A:1642:G:N7	2.36	0.40
2:A:1655:A:H2'	2:A:1656:A:O4'	2.21	0.40
2:A:2470:A:H2'	2:A:2471:A:C8	2.56	0.40
3:B:50:C:H2'	3:B:51:G:H8	1.86	0.40
4:C:127:PRO:HA	4:C:193:VAL:O	2.20	0.40
8:G:41:ILE:HD11	8:G:65:LEU:C	2.46	0.40
11:J:112:GLU:O	11:J:115:LYS:HB3	2.22	0.40
15:N:2:LEU:O	15:N:44:ASN:ND2	2.55	0.40
16:O:10:LEU:HB2	16:O:17:GLN:NE2	2.37	0.40
18:Q:43:LYS:NZ	18:Q:86:LEU:CD1	2.85	0.40
24:W:164:LEU:HD13	24:W:168:VAL:HG12	2.02	0.40
35:BA:671:G:O6	45:BK:66:LYS:HE2	2.22	0.40
35:BA:1007:U:H4'	35:BA:1008:C:H5'	2.04	0.40
37:BC:46:LEU:HD21	37:BC:86:ILE:HD11	2.04	0.40
45:BK:47:GLN:HB2	45:BK:49:ASN:ND2	2.36	0.40
2:A:135:G:H3'	2:A:136:U:H5''	2.04	0.40
2:A:1431:U:H1'	2:A:1507:G:H21	1.86	0.40
2:A:1612:U:O2	40:BF:17:ARG:NH1	2.54	0.40
2:A:2750:G:P	8:G:154:ARG:HH22	2.43	0.40
6:E:41:GLN:HE22	6:E:184:ASN:HB2	1.86	0.40
8:G:59:GLU:H	8:G:59:GLU:HG3	1.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:82:VAL:HG21	9:H:148:VAL:HG13	2.04	0.40
11:J:22:PRO:HB2	11:J:25:PRO:HD2	2.02	0.40
15:N:3:ILE:HG22	15:N:93:TRP:CD1	2.56	0.40
16:O:50:LYS:O	16:O:53:THR:HB	2.21	0.40
20:S:26:LYS:HA	20:S:95:THR:OG1	2.21	0.40
32:e:23:VAL:HG13	32:e:47:ARG:HB3	2.03	0.40
35:BA:1193:U:O2'	35:BA:1194:A:O4'	2.34	0.40
2:A:303:G:H2'	2:A:304:U:C6	2.56	0.40
2:A:401:C:H2'	2:A:402:G:O4'	2.21	0.40
2:A:815:G:H2'	2:A:816:G:O4'	2.21	0.40
2:A:1025:A:H62	15:N:12:GLN:HA	1.86	0.40
2:A:1553:C:C4	2:A:1618:C:H1'	2.57	0.40
2:A:2603:G:H2'	2:A:2604:U:C6	2.56	0.40
5:D:76:ASN:HA	5:D:77:PRO:HD3	1.81	0.40
6:E:154:VAL:HG23	6:E:193:ASP:HB2	2.04	0.40
7:F:132:THR:OG1	17:P:6:VAL:HG21	2.22	0.40
8:G:48:ASP:OD1	8:G:48:ASP:N	2.52	0.40
10:I:115:LEU:HB2	10:I:120:VAL:HG23	2.04	0.40
23:V:20:LYS:NZ	23:V:74:VAL:HG21	2.36	0.40
27:Z:62:ARG:HA	27:Z:62:ARG:HD2	1.89	0.40
35:BA:250:U:H4'	35:BA:251:G:O5'	2.21	0.40
35:BA:604:U:C2	35:BA:605:G:C8	3.08	0.40
35:BA:864:C:C2'	35:BA:865:C:H5'	2.52	0.40
37:BC:90:LEU:HB3	37:BC:98:VAL:HG21	2.03	0.40
50:BP:8:THR:O	50:BP:18:TYR:HA	2.22	0.40
53:BS:10:PHE:O	53:BS:39:THR:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	21/24 (88%)	21 (100%)	0	0	100	100
4	C	273/278 (98%)	261 (96%)	12 (4%)	0	100	100
5	D	212/217 (98%)	199 (94%)	12 (6%)	1 (0%)	24	56
6	E	207/215 (96%)	201 (97%)	5 (2%)	1 (0%)	24	56
7	F	180/187 (96%)	167 (93%)	12 (7%)	1 (1%)	21	52
8	G	174/179 (97%)	167 (96%)	7 (4%)	0	100	100
9	H	149/151 (99%)	139 (93%)	9 (6%)	1 (1%)	18	49
10	I	124/175 (71%)	115 (93%)	9 (7%)	0	100	100
11	J	131/142 (92%)	124 (95%)	6 (5%)	1 (1%)	16	45
12	K	144/147 (98%)	136 (94%)	8 (6%)	0	100	100
13	L	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
14	M	143/147 (97%)	135 (94%)	7 (5%)	1 (1%)	18	49
15	N	134/138 (97%)	123 (92%)	11 (8%)	0	100	100
16	O	116/199 (58%)	111 (96%)	5 (4%)	0	100	100
17	P	124/127 (98%)	122 (98%)	2 (2%)	0	100	100
18	Q	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
19	R	122/129 (95%)	117 (96%)	5 (4%)	0	100	100
20	S	98/103 (95%)	96 (98%)	2 (2%)	0	100	100
21	T	112/153 (73%)	109 (97%)	3 (3%)	0	100	100
22	U	95/100 (95%)	91 (96%)	4 (4%)	0	100	100
23	V	93/105 (89%)	89 (96%)	4 (4%)	0	100	100
24	W	190/215 (88%)	185 (97%)	5 (3%)	0	100	100
25	X	77/88 (88%)	73 (95%)	4 (5%)	0	100	100
26	Y	61/64 (95%)	61 (100%)	0	0	100	100
27	Z	62/77 (80%)	60 (97%)	2 (3%)	0	100	100
28	a	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
29	b	52/57 (91%)	51 (98%)	1 (2%)	0	100	100
30	c	47/55 (86%)	45 (96%)	1 (2%)	1 (2%)	5	27
31	d	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
32	e	61/64 (95%)	61 (100%)	0	0	100	100
33	f	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
34	g	55/75 (73%)	54 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BB	30/33 (91%)	28 (93%)	2 (7%)	0	100	100
37	BC	206/275 (75%)	190 (92%)	14 (7%)	2 (1%)	12	41
38	BD	198/201 (98%)	186 (94%)	12 (6%)	0	100	100
39	BE	178/214 (83%)	170 (96%)	8 (4%)	0	100	100
40	BF	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
41	BG	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
42	BH	129/132 (98%)	124 (96%)	5 (4%)	0	100	100
43	BI	124/150 (83%)	119 (96%)	5 (4%)	0	100	100
44	BJ	97/101 (96%)	90 (93%)	7 (7%)	0	100	100
45	BK	113/138 (82%)	106 (94%)	7 (6%)	0	100	100
46	BL	120/124 (97%)	112 (93%)	8 (7%)	0	100	100
47	BM	114/124 (92%)	106 (93%)	8 (7%)	0	100	100
48	BN	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
49	BO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
50	BP	111/156 (71%)	106 (96%)	5 (4%)	0	100	100
51	BQ	92/98 (94%)	88 (96%)	4 (4%)	0	100	100
52	BR	63/84 (75%)	62 (98%)	1 (2%)	0	100	100
53	BS	80/93 (86%)	76 (95%)	4 (5%)	0	100	100
54	BT	83/86 (96%)	81 (98%)	2 (2%)	0	100	100
55	BV	226/277 (82%)	207 (92%)	18 (8%)	1 (0%)	30	60
All	All	5979/6679 (90%)	5688 (95%)	281 (5%)	10 (0%)	44	72

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
30	c	7	VAL
37	BC	125	ASN
5	D	143	ALA
14	M	31	LYS
6	E	90	VAL
11	J	17	ALA
37	BC	162	MET
55	BV	156	LYS
9	H	124	ILE
7	F	131	GLY

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	3	18/19 (95%)	17 (94%)	1 (6%)	19	47
4	C	215/218 (99%)	191 (89%)	24 (11%)	6	22
5	D	160/163 (98%)	135 (84%)	25 (16%)	2	12
6	E	169/173 (98%)	149 (88%)	20 (12%)	5	21
7	F	151/156 (97%)	130 (86%)	21 (14%)	3	15
8	G	148/150 (99%)	134 (90%)	14 (10%)	8	30
9	H	90/116 (78%)	83 (92%)	7 (8%)	11	37
10	I	89/120 (74%)	79 (89%)	10 (11%)	6	22
11	J	102/108 (94%)	89 (87%)	13 (13%)	4	18
12	K	119/120 (99%)	109 (92%)	10 (8%)	10	35
13	L	100/100 (100%)	91 (91%)	9 (9%)	9	32
14	M	112/114 (98%)	102 (91%)	10 (9%)	9	32
15	N	114/116 (98%)	102 (90%)	12 (10%)	6	25
16	O	97/158 (61%)	87 (90%)	10 (10%)	7	26
17	P	93/94 (99%)	83 (89%)	10 (11%)	6	24
18	Q	100/100 (100%)	90 (90%)	10 (10%)	7	27
19	R	97/99 (98%)	92 (95%)	5 (5%)	21	49
20	S	81/83 (98%)	71 (88%)	10 (12%)	4	19
21	T	90/117 (77%)	82 (91%)	8 (9%)	9	32
22	U	83/85 (98%)	77 (93%)	6 (7%)	13	40
23	V	81/86 (94%)	74 (91%)	7 (9%)	10	34
24	W	155/168 (92%)	123 (79%)	32 (21%)	1	6
25	X	58/63 (92%)	53 (91%)	5 (9%)	10	34
26	Y	50/51 (98%)	45 (90%)	5 (10%)	7	27
27	Z	58/66 (88%)	55 (95%)	3 (5%)	21	49
28	a	52/54 (96%)	49 (94%)	3 (6%)	18	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	b	43/46 (94%)	36 (84%)	7 (16%)	2	11
30	c	47/52 (90%)	40 (85%)	7 (15%)	3	14
31	d	35/36 (97%)	32 (91%)	3 (9%)	10	34
32	e	53/54 (98%)	47 (89%)	6 (11%)	5	22
33	f	35/35 (100%)	33 (94%)	2 (6%)	18	47
34	g	51/63 (81%)	43 (84%)	8 (16%)	2	12
36	BB	30/31 (97%)	24 (80%)	6 (20%)	1	6
37	BC	170/212 (80%)	157 (92%)	13 (8%)	12	38
38	BD	175/176 (99%)	164 (94%)	11 (6%)	16	44
39	BE	127/147 (86%)	113 (89%)	14 (11%)	6	23
40	BF	85/85 (100%)	76 (89%)	9 (11%)	6	25
41	BG	131/132 (99%)	119 (91%)	12 (9%)	8	31
42	BH	107/108 (99%)	99 (92%)	8 (8%)	12	38
43	BI	102/125 (82%)	87 (85%)	15 (15%)	3	14
44	BJ	89/90 (99%)	81 (91%)	8 (9%)	9	32
45	BK	89/105 (85%)	80 (90%)	9 (10%)	7	27
46	BL	103/105 (98%)	86 (84%)	17 (16%)	2	11
47	BM	99/104 (95%)	85 (86%)	14 (14%)	3	15
48	BN	49/50 (98%)	45 (92%)	4 (8%)	10	36
49	BO	76/77 (99%)	71 (93%)	5 (7%)	15	43
50	BP	92/118 (78%)	80 (87%)	12 (13%)	4	17
51	BQ	80/83 (96%)	71 (89%)	9 (11%)	5	22
52	BR	55/72 (76%)	53 (96%)	2 (4%)	31	58
53	BS	73/84 (87%)	63 (86%)	10 (14%)	3	16
54	BT	69/70 (99%)	59 (86%)	10 (14%)	3	14
55	BV	191/218 (88%)	163 (85%)	28 (15%)	3	14
All	All	4938/5375 (92%)	4399 (89%)	539 (11%)	8	24

All (539) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	9	ARG
4	C	10	THR

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Mol	Chain	Res	Type
4	C	13	ARG
4	C	28	THR
4	C	54	LYS
4	C	60	ARG
4	C	63	ARG
4	C	69	ARG
4	C	78	LYS
4	C	89	THR
4	C	116	VAL
4	C	119	SER
4	C	126	LYS
4	C	127	PRO
4	C	131	LEU
4	C	148	ARG
4	C	157	ARG
4	C	161	VAL
4	C	177	MET
4	C	181	GLU
4	C	211	ARG
4	C	241	SER
4	C	247	VAL
4	C	265	ASP
4	C	272	ARG
5	D	11	LEU
5	D	19	GLU
5	D	23	VAL
5	D	58	SER
5	D	60	ARG
5	D	63	ILE
5	D	79	ARG
5	D	86	LEU
5	D	99	GLN
5	D	102	THR
5	D	127	MET
5	D	129	ARG
5	D	133	ARG
5	D	144	VAL
5	D	151	ILE
5	D	154	CYS
5	D	160	VAL
5	D	164	THR
5	D	169	ARG

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Mol	Chain	Res	Type
5	D	170	MET
5	D	176	THR
5	D	189	ASN
5	D	192	LEU
5	D	208	VAL
5	D	209	ARG
6	E	27	VAL
6	E	33	LEU
6	E	34	MET
6	E	36	GLN
6	E	39	THR
6	E	50	HIS
6	E	69	LYS
6	E	71	THR
6	E	78	SER
6	E	79	THR
6	E	97	ASP
6	E	112	ARG
6	E	128	THR
6	E	135	THR
6	E	137	SER
6	E	148	LEU
6	E	161	THR
6	E	169	VAL
6	E	181	ASP
6	E	201	LEU
7	F	10	ARG
7	F	11	LEU
7	F	20	ARG
7	F	31	ASN
7	F	38	VAL
7	F	44	ASN
7	F	49	ASP
7	F	83	GLN
7	F	87	ARG
7	F	96	VAL
7	F	102	ARG
7	F	136	THR
7	F	148	ILE
7	F	150	VAL
7	F	151	ASP
7	F	157	ARG

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Mol	Chain	Res	Type
7	F	159	MET
7	F	162	THR
7	F	163	VAL
7	F	164	VAL
7	F	165	THR
8	G	3	ARG
8	G	16	ASP
8	G	48	ASP
8	G	51	ILE
8	G	59	GLU
8	G	65	LEU
8	G	66	HIS
8	G	72	LEU
8	G	77	VAL
8	G	89	GLU
8	G	114	VAL
8	G	126	VAL
8	G	137	ILE
8	G	153	ARG
9	H	4	ILE
9	H	38	VAL
9	H	88	THR
9	H	124	ILE
9	H	134	VAL
9	H	137	HIS
9	H	146	LEU
10	I	23	THR
10	I	55	THR
10	I	79	ILE
10	I	82	VAL
10	I	85	GLU
10	I	87	VAL
10	I	93	ILE
10	I	104	VAL
10	I	115	LEU
10	I	117	VAL
11	J	15	ILE
11	J	30	LEU
11	J	35	VAL
11	J	37	ILE
11	J	42	LYS
11	J	48	THR

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Mol	Chain	Res	Type
11	J	52	ARG
11	J	55	VAL
11	J	56	ILE
11	J	58	VAL
11	J	87	VAL
11	J	113	THR
11	J	114	LYS
12	K	5	THR
12	K	17	VAL
12	K	70	THR
12	K	93	LEU
12	K	96	HIS
12	K	106	ILE
12	K	118	ILE
12	K	124	VAL
12	K	129	ASP
12	K	145	VAL
13	L	13	ASN
13	L	40	VAL
13	L	58	VAL
13	L	73	ASP
13	L	77	ILE
13	L	87	ILE
13	L	90	ASP
13	L	96	THR
13	L	112	MET
14	M	21	ARG
14	M	22	VAL
14	M	24	ARG
14	M	43	ARG
14	M	46	VAL
14	M	49	MET
14	M	92	THR
14	M	104	VAL
14	M	105	ARG
14	M	122	VAL
15	N	3	ILE
15	N	7	VAL
15	N	10	ARG
15	N	18	ARG
15	N	20	ILE
15	N	43	THR

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Mol	Chain	Res	Type
15	N	47	ILE
15	N	51	ARG
15	N	72	ARG
15	N	82	ARG
15	N	112	LYS
15	N	135	GLU
16	O	6	LYS
16	O	9	ARG
16	O	10	LEU
16	O	37	THR
16	O	53	THR
16	O	64	ARG
16	O	74	ASP
16	O	96	ARG
16	O	100	VAL
16	O	114	GLU
17	P	6	VAL
17	P	10	ILE
17	P	12	GLU
17	P	24	ARG
17	P	32	THR
17	P	40	VAL
17	P	51	LEU
17	P	69	ASP
17	P	74	ASP
17	P	87	LEU
18	Q	15	ASP
18	Q	25	VAL
18	Q	32	ILE
18	Q	38	ARG
18	Q	54	ILE
18	Q	57	THR
18	Q	79	ASN
18	Q	81	ASP
18	Q	91	VAL
18	Q	93	ARG
19	R	6	ARG
19	R	29	SER
19	R	33	ARG
19	R	44	THR
19	R	80	ILE
20	S	3	THR

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Mol	Chain	Res	Type
20	S	23	LYS
20	S	27	LEU
20	S	30	GLU
20	S	53	ASP
20	S	54	ASP
20	S	58	VAL
20	S	68	THR
20	S	72	LYS
20	S	94	LEU
21	T	19	VAL
21	T	22	THR
21	T	26	ARG
21	T	75	THR
21	T	81	VAL
21	T	84	ASP
21	T	104	ARG
21	T	107	THR
22	U	20	SER
22	U	27	ASN
22	U	46	ILE
22	U	53	LYS
22	U	62	ARG
22	U	81	ARG
23	V	12	ILE
23	V	30	ARG
23	V	38	VAL
23	V	42	LYS
23	V	69	SER
23	V	91	THR
23	V	97	ILE
24	W	12	THR
24	W	14	ASN
24	W	15	VAL
24	W	19	THR
24	W	33	VAL
24	W	36	VAL
24	W	42	THR
24	W	43	ASP
24	W	64	ASN
24	W	67	LEU
24	W	68	THR
24	W	79	LEU

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Mol	Chain	Res	Type
24	W	85	VAL
24	W	92	ILE
24	W	99	VAL
24	W	100	VAL
24	W	104	GLU
24	W	112	VAL
24	W	114	VAL
24	W	119	THR
24	W	130	THR
24	W	131	ILE
24	W	138	LEU
24	W	139	SER
24	W	140	ILE
24	W	146	VAL
24	W	148	VAL
24	W	151	VAL
24	W	158	THR
24	W	172	SER
24	W	177	LEU
24	W	181	VAL
25	X	11	ARG
25	X	38	VAL
25	X	41	ARG
25	X	78	VAL
25	X	80	ILE
26	Y	23	ARG
26	Y	24	ARG
26	Y	28	ARG
26	Y	45	ASN
26	Y	53	THR
27	Z	9	GLU
27	Z	36	MET
27	Z	44	ASN
28	a	20	ARG
28	a	36	VAL
28	a	48	ASN
29	b	3	VAL
29	b	6	ARG
29	b	8	MET
29	b	10	ARG
29	b	14	ARG
29	b	35	GLN

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Mol	Chain	Res	Type
29	b	39	VAL
30	c	6	ASP
30	c	11	ILE
30	c	12	THR
30	c	22	ASN
30	c	25	THR
30	c	38	ILE
30	c	47	THR
31	d	13	ARG
31	d	15	ARG
31	d	46	THR
32	e	11	SER
32	e	19	THR
32	e	23	VAL
32	e	47	ARG
32	e	56	SER
32	e	59	ASN
33	f	2	LYS
33	f	7	VAL
34	g	9	TYR
34	g	12	THR
34	g	22	PHE
34	g	24	THR
34	g	32	THR
34	g	37	VAL
34	g	46	THR
34	g	58	VAL
36	BB	4	VAL
36	BB	6	LYS
36	BB	10	LYS
36	BB	24	THR
36	BB	27	GLN
36	BB	30	LYS
37	BC	14	ILE
37	BC	21	ARG
37	BC	35	ASP
37	BC	46	LEU
37	BC	62	ARG
37	BC	75	VAL
37	BC	82	GLU
37	BC	103	LEU
37	BC	153	CYS

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Mol	Chain	Res	Type
37	BC	167	PHE
37	BC	169	ARG
37	BC	182	ILE
37	BC	204	LYS
38	BD	20	VAL
38	BD	86	LEU
38	BD	102	LEU
38	BD	110	ARG
38	BD	119	LEU
38	BD	123	VAL
38	BD	131	ARG
38	BD	145	LEU
38	BD	156	THR
38	BD	177	VAL
38	BD	188	VAL
39	BE	37	ILE
39	BE	39	ARG
39	BE	41	VAL
39	BE	59	THR
39	BE	70	MET
39	BE	71	VAL
39	BE	91	GLU
39	BE	95	ASN
39	BE	97	PHE
39	BE	110	VAL
39	BE	148	ILE
39	BE	156	ASP
39	BE	159	ILE
39	BE	176	GLU
40	BF	27	LEU
40	BF	30	ILE
40	BF	43	TRP
40	BF	57	GLU
40	BF	72	VAL
40	BF	77	ARG
40	BF	85	VAL
40	BF	87	ARG
40	BF	91	LEU
41	BG	3	ARG
41	BG	24	THR
41	BG	27	VAL
41	BG	38	LEU

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Mol	Chain	Res	Type
41	BG	70	LYS
41	BG	80	VAL
41	BG	98	THR
41	BG	99	LEU
41	BG	102	ARG
41	BG	129	ASN
41	BG	135	VAL
41	BG	144	MET
42	BH	14	LEU
42	BH	36	ILE
42	BH	55	ARG
42	BH	56	VAL
42	BH	79	ARG
42	BH	92	THR
42	BH	101	LEU
42	BH	115	ASP
43	BI	26	ILE
43	BI	29	VAL
43	BI	37	VAL
43	BI	38	ARG
43	BI	40	ARG
43	BI	42	VAL
43	BI	45	THR
43	BI	67	LEU
43	BI	78	VAL
43	BI	83	ILE
43	BI	87	LEU
43	BI	100	ARG
43	BI	105	ARG
43	BI	140	LYS
43	BI	147	TYR
44	BJ	15	HIS
44	BJ	18	ILE
44	BJ	32	THR
44	BJ	50	CYS
44	BJ	57	LYS
44	BJ	76	ILE
44	BJ	78	ASP
44	BJ	97	ASP
45	BK	25	VAL
45	BK	40	ILE
45	BK	49	ASN

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Mol	Chain	Res	Type
45	BK	51	ILE
45	BK	68	THR
45	BK	91	VAL
45	BK	95	VAL
45	BK	128	ASN
45	BK	131	ARG
46	BL	3	THR
46	BL	4	ILE
46	BL	19	VAL
46	BL	21	THR
46	BL	24	LEU
46	BL	27	SER
46	BL	29	GLN
46	BL	38	TYR
46	BL	39	THR
46	BL	41	THR
46	BL	49	LEU
46	BL	52	VAL
46	BL	63	VAL
46	BL	70	GLU
46	BL	73	ASN
46	BL	87	VAL
46	BL	104	THR
47	BM	5	VAL
47	BM	49	THR
47	BM	51	ASP
47	BM	56	LEU
47	BM	60	ILE
47	BM	63	ASN
47	BM	64	LEU
47	BM	70	LEU
47	BM	80	ARG
47	BM	82	ILE
47	BM	101	GLN
47	BM	109	THR
47	BM	110	ARG
47	BM	115	ARG
48	BN	22	THR
48	BN	24	CYS
48	BN	45	ARG
48	BN	56	VAL
49	BO	46	HIS

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Mol	Chain	Res	Type
49	BO	75	VAL
49	BO	82	ILE
49	BO	83	GLU
49	BO	89	ARG
50	BP	3	VAL
50	BP	9	ARG
50	BP	15	ASN
50	BP	21	ILE
50	BP	26	ARG
50	BP	36	VAL
50	BP	50	GLN
50	BP	67	THR
50	BP	70	VAL
50	BP	86	LEU
50	BP	90	GLU
50	BP	97	GLU
51	BQ	28	VAL
51	BQ	48	LEU
51	BQ	59	VAL
51	BQ	65	ASN
51	BQ	74	VAL
51	BQ	85	THR
51	BQ	89	ARG
51	BQ	92	GLU
51	BQ	93	ILE
52	BR	21	VAL
52	BR	31	ASP
53	BS	3	ARG
53	BS	11	VAL
53	BS	12	ASP
53	BS	15	LEU
53	BS	45	ILE
53	BS	51	VAL
53	BS	63	THR
53	BS	67	VAL
53	BS	78	ARG
53	BS	79	THR
54	BT	3	ASN
54	BT	6	SER
54	BT	26	SER
54	BT	28	LEU
54	BT	43	ASP

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Mol	Chain	Res	Type
54	BT	45	ASP
54	BT	50	LEU
54	BT	51	LEU
54	BT	59	ASP
54	BT	81	LEU
55	BV	4	VAL
55	BV	5	THR
55	BV	6	MET
55	BV	24	ASN
55	BV	32	PHE
55	BV	38	ILE
55	BV	50	ILE
55	BV	59	GLU
55	BV	66	THR
55	BV	73	LYS
55	BV	75	GLN
55	BV	79	SER
55	BV	83	GLU
55	BV	101	LEU
55	BV	102	THR
55	BV	113	ARG
55	BV	114	LEU
55	BV	134	ILE
55	BV	137	LEU
55	BV	146	ARG
55	BV	157	VAL
55	BV	167	ASN
55	BV	169	GLU
55	BV	184	ILE
55	BV	186	ILE
55	BV	189	THR
55	BV	195	VAL
55	BV	200	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	3	17	ASN
1	3	18	HIS
4	C	53	HIS
4	C	76	ASN
4	C	91	ASN

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Mol	Chain	Res	Type
4	C	129	ASN
4	C	130	ASN
4	C	143	HIS
4	C	205	ASN
5	D	34	ASN
5	D	130	HIS
5	D	179	ASN
6	E	91	HIS
6	E	100	GLN
6	E	121	ASN
6	E	151	ASN
6	E	176	HIS
6	E	202	ASN
7	F	62	ASN
7	F	146	HIS
8	G	66	HIS
9	H	118	GLN
9	H	147	ASN
10	I	16	GLN
10	I	54	ASN
11	J	33	HIS
11	J	54	ASN
12	K	77	HIS
12	K	103	ASN
13	L	51	ASN
14	M	54	GLN
14	M	58	HIS
14	M	76	GLN
14	M	107	ASN
14	M	127	ASN
15	N	123	HIS
16	O	17	GLN
16	O	61	HIS
17	P	22	HIS
17	P	53	ASN
18	Q	26	ASN
18	Q	79	ASN
19	R	41	HIS
19	R	72	ASN
19	R	122	ASN
20	S	67	HIS
20	S	76	HIS

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Mol	Chain	Res	Type
20	S	90	HIS
21	T	67	ASN
22	U	41	GLN
22	U	58	ASN
22	U	61	ASN
23	V	31	ASN
23	V	67	HIS
23	V	101	ASN
24	W	9	ASN
24	W	14	ASN
24	W	46	HIS
24	W	61	HIS
24	W	93	GLN
24	W	94	HIS
25	X	29	GLN
25	X	44	HIS
26	Y	22	HIS
26	Y	45	ASN
27	Z	43	ASN
29	b	19	GLN
30	c	22	ASN
30	c	48	HIS
31	d	36	ASN
32	e	25	GLN
32	e	31	HIS
32	e	59	ASN
32	e	63	ASN
37	BC	8	HIS
37	BC	122	GLN
38	BD	51	GLN
38	BD	77	GLN
38	BD	84	ASN
38	BD	95	ASN
38	BD	115	HIS
38	BD	151	GLN
39	BE	146	HIS
39	BE	160	ASN
40	BF	55	HIS
40	BF	80	ASN
41	BG	14	ASN
41	BG	28	ASN
41	BG	106	ASN

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Mol	Chain	Res	Type
42	BH	117	GLN
43	BI	57	ASN
43	BI	61	ASN
43	BI	146	GLN
44	BJ	15	HIS
44	BJ	56	HIS
44	BJ	64	HIS
44	BJ	101	GLN
45	BK	27	HIS
45	BK	49	ASN
45	BK	86	HIS
45	BK	128	ASN
46	BL	29	GLN
46	BL	73	ASN
47	BM	31	ASN
47	BM	42	ASN
47	BM	92	HIS
47	BM	101	GLN
48	BN	11	ASN
49	BO	18	HIS
49	BO	28	GLN
50	BP	41	HIS
50	BP	81	GLN
51	BQ	46	HIS
53	BS	14	HIS
53	BS	52	HIS
53	BS	57	HIS
54	BT	3	ASN
54	BT	7	GLN
54	BT	52	HIS
54	BT	68	HIS
54	BT	70	ASN
54	BT	71	GLN
55	BV	24	ASN
55	BV	45	GLN
55	BV	108	HIS
55	BV	167	ASN

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	3118/3120 (99%)	740 (23%)	29 (0%)
3	B	117/118 (99%)	23 (19%)	1 (0%)
35	BA	1510/1528 (98%)	363 (24%)	13 (0%)
56	BW	75/76 (98%)	20 (26%)	0
57	BX	5/6 (83%)	2 (40%)	0
All	All	4825/4848 (99%)	1148 (23%)	43 (0%)

All (1148) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	7	U
2	A	12	G
2	A	20	G
2	A	29	C
2	A	31	U
2	A	32	G
2	A	33	G
2	A	46	A
2	A	55	G
2	A	59	G
2	A	60	A
2	A	68	A
2	A	71	A
2	A	72	G
2	A	83	C
2	A	89	A
2	A	90	C
2	A	91	C
2	A	94	G
2	A	98	U
2	A	99	G
2	A	115	A
2	A	116	A
2	A	117	U
2	A	125	C
2	A	128	G
2	A	133	G
2	A	136	U
2	A	137	G
2	A	143	G
2	A	145	G

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Mol	Chain	Res	Type
2	A	148	A
2	A	161	U
2	A	164	A
2	A	171	U
2	A	172	C
2	A	175	G
2	A	177	G
2	A	195	A
2	A	198	A
2	A	203	A
2	A	212	A
2	A	214	G
2	A	215	A
2	A	221	A
2	A	222	A
2	A	227	A
2	A	228	A
2	A	229	U
2	A	230	G
2	A	231	U
2	A	237	C
2	A	248	G
2	A	264	G
2	A	270	U
2	A	271	A
2	A	272	A
2	A	274	C
2	A	275	C
2	A	279	U
2	A	282	A
2	A	283	U
2	A	285	U
2	A	286	G
2	A	287	A
2	A	288	U
2	A	290	C
2	A	291	C
2	A	292	G
2	A	293	G
2	A	294	G
2	A	297	G
2	A	299	G

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Mol	Chain	Res	Type
2	A	300	G
2	A	301	U
2	A	302	U
2	A	303	G
2	A	305	G
2	A	306	U
2	A	312	G
2	A	314	G
2	A	315	U
2	A	316	U
2	A	317	G
2	A	318	U
2	A	319	G
2	A	323	C
2	A	324	C
2	A	326	A
2	A	330	U
2	A	331	U
2	A	336	C
2	A	337	U
2	A	338	C
2	A	342	C
2	A	343	U
2	A	344	G
2	A	345	G
2	A	346	C
2	A	348	G
2	A	349	G
2	A	350	A
2	A	351	G
2	A	352	G
2	A	356	G
2	A	357	U
2	A	358	G
2	A	361	A
2	A	364	A
2	A	369	G
2	A	370	U
2	A	376	G
2	A	383	U
2	A	384	G
2	A	387	U

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Mol	Chain	Res	Type
2	A	388	U
2	A	393	U
2	A	399	G
2	A	404	A
2	A	406	A
2	A	412	A
2	A	413	G
2	A	417	C
2	A	424	G
2	A	426	G
2	A	434	G
2	A	438	U
2	A	445	U
2	A	446	G
2	A	450	G
2	A	452	G
2	A	454	U
2	A	459	A
2	A	460	G
2	A	472	C
2	A	474	G
2	A	489	A
2	A	490	A
2	A	491	U
2	A	493	U
2	A	494	G
2	A	498	G
2	A	499	G
2	A	500	A
2	A	505	C
2	A	509	U
2	A	512	G
2	A	542	A
2	A	543	U
2	A	544	U
2	A	562	G
2	A	567	A
2	A	569	G
2	A	570	U
2	A	581	G
2	A	589	A
2	A	591	G

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Mol	Chain	Res	Type
2	A	592	A
2	A	594	U
2	A	595	A
2	A	596	C
2	A	605	G
2	A	614	C
2	A	617	U
2	A	618	C
2	A	619	C
2	A	620	G
2	A	630	U
2	A	631	C
2	A	636	U
2	A	637	G
2	A	638	U
2	A	639	C
2	A	640	G
2	A	641	U
2	A	642	G
2	A	644	G
2	A	647	G
2	A	655	G
2	A	663	A
2	A	665	G
2	A	666	A
2	A	667	A
2	A	675	G
2	A	678	A
2	A	679	G
2	A	684	G
2	A	685	G
2	A	696	A
2	A	700	U
2	A	701	A
2	A	704	C
2	A	706	G
2	A	707	G
2	A	708	G
2	A	709	U
2	A	721	A
2	A	728	G
2	A	731	A

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Mol	Chain	Res	Type
2	A	738	A
2	A	740	A
2	A	742	G
2	A	747	A
2	A	753	A
2	A	757	G
2	A	758	A
2	A	759	G
2	A	760	U
2	A	764	U
2	A	765	G
2	A	766	G
2	A	767	U
2	A	768	G
2	A	774	G
2	A	783	G
2	A	784	G
2	A	785	A
2	A	793	C
2	A	801	U
2	A	816	G
2	A	827	G
2	A	829	U
2	A	832	G
2	A	839	U
2	A	845	C
2	A	862	U
2	A	863	G
2	A	864	A
2	A	868	C
2	A	872	G
2	A	878	G
2	A	879	A
2	A	880	G
2	A	890	G
2	A	891	G
2	A	892	G
2	A	897	A
2	A	899	G
2	A	900	G
2	A	917	A
2	A	919	A

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Mol	Chain	Res	Type
2	A	920	G
2	A	921	C
2	A	927	C
2	A	942	U
2	A	960	G
2	A	961	U
2	A	971	G
2	A	972	A
2	A	974	G
2	A	975	U
2	A	981	U
2	A	982	A
2	A	994	A
2	A	995	U
2	A	996	G
2	A	1000	C
2	A	1001	C
2	A	1002	C
2	A	1003	A
2	A	1005	A
2	A	1007	G
2	A	1009	U
2	A	1010	U
2	A	1011	A
2	A	1012	C
2	A	1013	U
2	A	1014	G
2	A	1022	C
2	A	1025	A
2	A	1030	C
2	A	1044	U
2	A	1046	C
2	A	1047	A
2	A	1049	G
2	A	1058	A
2	A	1063	G
2	A	1070	G
2	A	1075	U
2	A	1076	A
2	A	1078	G
2	A	1084	U
2	A	1085	G

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Mol	Chain	Res	Type
2	A	1091	A
2	A	1092	G
2	A	1099	A
2	A	1101	A
2	A	1114	G
2	A	1130	C
2	A	1131	G
2	A	1140	G
2	A	1143	G
2	A	1144	A
2	A	1148	G
2	A	1151	U
2	A	1163	A
2	A	1164	A
2	A	1165	G
2	A	1173	G
2	A	1174	G
2	A	1175	A
2	A	1176	G
2	A	1178	U
2	A	1184	U
2	A	1185	A
2	A	1186	G
2	A	1187	A
2	A	1188	A
2	A	1189	G
2	A	1190	C
2	A	1191	A
2	A	1192	G
2	A	1201	G
2	A	1202	A
2	A	1203	A
2	A	1204	A
2	A	1205	G
2	A	1206	A
2	A	1207	G
2	A	1208	U
2	A	1209	G
2	A	1212	U
2	A	1213	A
2	A	1214	A
2	A	1217	G

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Mol	Chain	Res	Type
2	A	1219	U
2	A	1227	C
2	A	1229	A
2	A	1230	G
2	A	1232	G
2	A	1233	A
2	A	1237	U
2	A	1238	G
2	A	1239	C
2	A	1240	G
2	A	1247	A
2	A	1250	U
2	A	1251	A
2	A	1253	C
2	A	1254	G
2	A	1260	C
2	A	1261	A
2	A	1275	A
2	A	1290	C
2	A	1292	U
2	A	1293	G
2	A	1294	U
2	A	1324	G
2	A	1325	U
2	A	1332	G
2	A	1335	G
2	A	1339	G
2	A	1344	A
2	A	1345	G
2	A	1353	G
2	A	1359	G
2	A	1362	A
2	A	1363	G
2	A	1368	A
2	A	1369	A
2	A	1371	G
2	A	1380	A
2	A	1386	G
2	A	1387	A
2	A	1389	U
2	A	1390	A
2	A	1404	C

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Mol	Chain	Res	Type
2	A	1415	A
2	A	1416	A
2	A	1417	A
2	A	1435	C
2	A	1437	A
2	A	1440	C
2	A	1448	C
2	A	1456	G
2	A	1457	A
2	A	1461	G
2	A	1462	G
2	A	1465	C
2	A	1467	U
2	A	1480	A
2	A	1494	U
2	A	1499	A
2	A	1502	G
2	A	1507	G
2	A	1510	A
2	A	1518	A
2	A	1521	C
2	A	1522	G
2	A	1531	C
2	A	1532	G
2	A	1533	U
2	A	1534	C
2	A	1540	U
2	A	1541	G
2	A	1543	A
2	A	1550	G
2	A	1551	U
2	A	1552	A
2	A	1553	C
2	A	1554	U
2	A	1563	A
2	A	1564	A
2	A	1565	A
2	A	1566	A
2	A	1574	G
2	A	1578	G
2	A	1579	C
2	A	1587	G

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Mol	Chain	Res	Type
2	A	1596	C
2	A	1599	U
2	A	1600	G
2	A	1625	G
2	A	1627	U
2	A	1628	A
2	A	1629	G
2	A	1631	A
2	A	1632	G
2	A	1633	U
2	A	1637	G
2	A	1638	C
2	A	1639	G
2	A	1640	A
2	A	1641	U
2	A	1648	A
2	A	1649	C
2	A	1659	U
2	A	1670	G
2	A	1673	A
2	A	1674	G
2	A	1679	A
2	A	1680	A
2	A	1681	U
2	A	1688	G
2	A	1703	G
2	A	1710	A
2	A	1711	G
2	A	1714	A
2	A	1715	A
2	A	1717	U
2	A	1723	U
2	A	1724	G
2	A	1728	U
2	A	1729	A
2	A	1730	U
2	A	1731	A
2	A	1737	A
2	A	1738	G
2	A	1745	U
2	A	1746	G
2	A	1754	G

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Mol	Chain	Res	Type
2	A	1755	A
2	A	1756	G
2	A	1757	U
2	A	1761	G
2	A	1767	U
2	A	1774	U
2	A	1785	C
2	A	1786	G
2	A	1789	A
2	A	1792	A
2	A	1796	U
2	A	1798	U
2	A	1802	G
2	A	1803	A
2	A	1806	A
2	A	1813	C
2	A	1826	A
2	A	1845	G
2	A	1857	U
2	A	1862	C
2	A	1864	U
2	A	1866	C
2	A	1867	G
2	A	1869	G
2	A	1870	U
2	A	1871	G
2	A	1872	A
2	A	1892	G
2	A	1893	C
2	A	1916	A
2	A	1932	U
2	A	1933	G
2	A	1945	U
2	A	1946	U
2	A	1947	U
2	A	1948	A
2	A	1950	G
2	A	1967	G
2	A	1973	C
2	A	1974	A
2	A	1975	A
2	A	1981	U

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Mol	Chain	Res	Type
2	A	1990	A
2	A	1999	U
2	A	2008	A
2	A	2017	C
2	A	2018	G
2	A	2026	A
2	A	2033	U
2	A	2046	A
2	A	2064	A
2	A	2065	A
2	A	2066	G
2	A	2073	A
2	A	2075	G
2	A	2084	A
2	A	2085	C
2	A	2086	U
2	A	2087	C
2	A	2088	C
2	A	2089	C
2	A	2091	U
2	A	2092	U
2	A	2093	G
2	A	2094	G
2	A	2095	G
2	A	2096	G
2	A	2106	A
2	A	2107	G
2	A	2108	A
2	A	2111	U
2	A	2112	U
2	A	2120	A
2	A	2129	C
2	A	2130	G
2	A	2131	G
2	A	2137	A
2	A	2138	C
2	A	2140	A
2	A	2141	U
2	A	2153	G
2	A	2154	G
2	A	2160	A
2	A	2162	A

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Mol	Chain	Res	Type
2	A	2163	U
2	A	2164	U
2	A	2179	U
2	A	2184	A
2	A	2190	A
2	A	2191	C
2	A	2194	A
2	A	2195	U
2	A	2196	G
2	A	2197	G
2	A	2215	U
2	A	2217	U
2	A	2221	A
2	A	2227	A
2	A	2235	C
2	A	2244	A
2	A	2247	A
2	A	2251	G
2	A	2254	A
2	A	2255	A
2	A	2256	G
2	A	2257	A
2	A	2263	G
2	A	2267	C
2	A	2274	C
2	A	2276	G
2	A	2279	C
2	A	2280	G
2	A	2284	A
2	A	2285	G
2	A	2286	A
2	A	2299	C
2	A	2316	G
2	A	2320	C
2	A	2324	A
2	A	2325	U
2	A	2328	G
2	A	2329	G
2	A	2333	G
2	A	2334	U
2	A	2335	G
2	A	2336	U

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Mol	Chain	Res	Type
2	A	2338	G
2	A	2339	G
2	A	2340	A
2	A	2341	U
2	A	2342	A
2	A	2343	G
2	A	2346	G
2	A	2349	A
2	A	2351	A
2	A	2354	G
2	A	2355	U
2	A	2356	G
2	A	2357	A
2	A	2362	C
2	A	2368	C
2	A	2371	G
2	A	2372	U
2	A	2380	G
2	A	2382	G
2	A	2383	U
2	A	2384	C
2	A	2386	U
2	A	2387	U
2	A	2388	G
2	A	2389	U
2	A	2390	U
2	A	2391	G
2	A	2392	A
2	A	2393	A
2	A	2394	A
2	A	2395	U
2	A	2396	A
2	A	2400	C
2	A	2401	U
2	A	2402	C
2	A	2407	C
2	A	2408	G
2	A	2409	U
2	A	2410	A
2	A	2413	G
2	A	2418	U
2	A	2421	A

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Mol	Chain	Res	Type
2	A	2422	A
2	A	2427	G
2	A	2434	A
2	A	2436	A
2	A	2447	G
2	A	2449	A
2	A	2462	G
2	A	2463	G
2	A	2467	U
2	A	2483	G
2	A	2502	A
2	A	2503	G
2	A	2504	G
2	A	2507	C
2	A	2508	C
2	A	2511	A
2	A	2529	A
2	A	2532	G
2	A	2545	G
2	A	2549	G
2	A	2551	A
2	A	2558	C
2	A	2559	A
2	A	2567	U
2	A	2571	C
2	A	2574	C
2	A	2585	U
2	A	2607	G
2	A	2609	A
2	A	2613	G
2	A	2626	U
2	A	2627	C
2	A	2643	U
2	A	2647	U
2	A	2649	A
2	A	2650	A
2	A	2653	G
2	A	2654	A
2	A	2655	U
2	A	2659	A
2	A	2665	C
2	A	2669	G

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Mol	Chain	Res	Type
2	A	2672	A
2	A	2673	U
2	A	2677	A
2	A	2688	C
2	A	2689	C
2	A	2693	A
2	A	2694	G
2	A	2698	C
2	A	2700	A
2	A	2702	A
2	A	2705	G
2	A	2715	U
2	A	2726	G
2	A	2729	G
2	A	2732	G
2	A	2742	A
2	A	2744	C
2	A	2753	G
2	A	2759	G
2	A	2778	U
2	A	2786	U
2	A	2790	A
2	A	2791	G
2	A	2796	A
2	A	2797	C
2	A	2802	G
2	A	2806	G
2	A	2826	A
2	A	2827	G
2	A	2833	U
2	A	2837	U
2	A	2839	U
2	A	2853	C
2	A	2856	A
2	A	2862	G
2	A	2885	G
2	A	2887	G
2	A	2913	U
2	A	2915	C
2	A	2926	A
2	A	2936	C
2	A	2938	G

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Mol	Chain	Res	Type
2	A	2948	C
2	A	2950	C
2	A	2956	G
2	A	2957	A
2	A	2968	G
2	A	2972	A
2	A	2982	A
2	A	2985	G
2	A	2989	A
2	A	3002	A
2	A	3004	C
2	A	3005	A
2	A	3009	U
2	A	3014	A
2	A	3015	C
2	A	3016	C
2	A	3020	U
2	A	3021	A
2	A	3022	G
2	A	3024	A
2	A	3027	G
2	A	3029	U
2	A	3042	A
2	A	3047	A
2	A	3056	A
2	A	3082	U
2	A	3088	C
2	A	3093	A
2	A	3095	C
2	A	3101	C
2	A	3105	C
2	A	3106	C
2	A	3107	G
2	A	3112	A
2	A	3113	A
2	A	3114	A
2	A	3115	A
3	B	4	A
3	B	7	G
3	B	11	U
3	B	12	C
3	B	13	C

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Mol	Chain	Res	Type
3	B	14	A
3	B	22	A
3	B	23	G
3	B	25	G
3	B	30	G
3	B	31	C
3	B	35	G
3	B	42	C
3	B	57	U
3	B	58	A
3	B	85	C
3	B	87	U
3	B	89	C
3	B	90	G
3	B	103	G
3	B	107	A
3	B	112	C
3	B	115	A
35	BA	8	U
35	BA	9	U
35	BA	11	G
35	BA	12	A
35	BA	13	G
35	BA	26	G
35	BA	36	A
35	BA	43	G
35	BA	45	G
35	BA	48	G
35	BA	51	C
35	BA	52	U
35	BA	53	U
35	BA	54	A
35	BA	55	A
35	BA	58	C
35	BA	59	A
35	BA	68	G
35	BA	77	G
35	BA	81	C
35	BA	82	U
35	BA	83	U
35	BA	85	C
35	BA	87	G

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Mol	Chain	Res	Type
35	BA	92	A
35	BA	93	C
35	BA	101	G
35	BA	116	A
35	BA	117	C
35	BA	118	A
35	BA	123	G
35	BA	128	U
35	BA	136	G
35	BA	139	C
35	BA	160	C
35	BA	174	G
35	BA	179	C
35	BA	180	A
35	BA	192	G
35	BA	194	A
35	BA	200	U
35	BA	201	G
35	BA	209	A
35	BA	210	A
35	BA	211	A
35	BA	214	U
35	BA	215	U
35	BA	216	U
35	BA	217	U
35	BA	218	G
35	BA	220	G
35	BA	226	G
35	BA	227	G
35	BA	242	U
35	BA	243	A
35	BA	245	C
35	BA	247	G
35	BA	251	G
35	BA	254	G
35	BA	266	G
35	BA	267	C
35	BA	279	A
35	BA	280	C
35	BA	281	G
35	BA	289	G
35	BA	301	G

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Mol	Chain	Res	Type
35	BA	316	C
35	BA	319	G
35	BA	321	A
35	BA	329	A
35	BA	332	G
35	BA	344	A
35	BA	345	C
35	BA	350	G
35	BA	351	G
35	BA	352	C
35	BA	353	A
35	BA	354	G
35	BA	356	A
35	BA	367	U
35	BA	372	C
35	BA	373	A
35	BA	382	A
35	BA	390	U
35	BA	392	C
35	BA	397	A
35	BA	398	C
35	BA	406	G
35	BA	411	A
35	BA	414	A
35	BA	421	U
35	BA	422	C
35	BA	423	G
35	BA	424	G
35	BA	426	U
35	BA	427	U
35	BA	428	G
35	BA	429	U
35	BA	430	A
35	BA	434	C
35	BA	438	U
35	BA	451	A
35	BA	452	A
35	BA	453	G
35	BA	454	C
35	BA	456	C
35	BA	457	A
35	BA	458	A

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Mol	Chain	Res	Type
35	BA	459	G
35	BA	461	G
35	BA	465	G
35	BA	466	U
35	BA	473	A
35	BA	477	G
35	BA	478	A
35	BA	479	A
35	BA	485	G
35	BA	486	G
35	BA	491	C
35	BA	496	U
35	BA	497	G
35	BA	498	C
35	BA	499	C
35	BA	505	C
35	BA	507	G
35	BA	509	G
35	BA	511	U
35	BA	512	A
35	BA	513	A
35	BA	515	A
35	BA	520	G
35	BA	525	C
35	BA	527	A
35	BA	539	A
35	BA	542	U
35	BA	544	C
35	BA	552	A
35	BA	553	A
35	BA	554	A
35	BA	556	A
35	BA	557	G
35	BA	602	A
35	BA	612	U
35	BA	613	G
35	BA	633	A
35	BA	641	G
35	BA	645	G
35	BA	666	U
35	BA	667	A
35	BA	668	G

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Mol	Chain	Res	Type
35	BA	680	G
35	BA	683	G
35	BA	700	C
35	BA	701	G
35	BA	702	G
35	BA	703	U
35	BA	711	G
35	BA	713	G
35	BA	729	A
35	BA	735	G
35	BA	757	A
35	BA	761	A
35	BA	764	A
35	BA	765	G
35	BA	772	A
35	BA	773	U
35	BA	774	A
35	BA	779	G
35	BA	782	A
35	BA	789	G
35	BA	794	A
35	BA	795	A
35	BA	797	C
35	BA	799	G
35	BA	808	A
35	BA	818	U
35	BA	821	C
35	BA	822	U
35	BA	823	U
35	BA	824	C
35	BA	825	C
35	BA	826	U
35	BA	827	U
35	BA	828	G
35	BA	840	G
35	BA	841	U
35	BA	865	C
35	BA	871	A
35	BA	884	G
35	BA	896	A
35	BA	901	A
35	BA	908	G

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Mol	Chain	Res	Type
35	BA	909	G
35	BA	913	C
35	BA	914	C
35	BA	915	G
35	BA	916	C
35	BA	917	A
35	BA	921	G
35	BA	924	G
35	BA	930	C
35	BA	932	U
35	BA	940	A
35	BA	942	U
35	BA	943	U
35	BA	947	U
35	BA	948	G
35	BA	950	A
35	BA	951	A
35	BA	953	G
35	BA	955	G
35	BA	956	A
35	BA	957	A
35	BA	959	A
35	BA	971	G
35	BA	973	U
35	BA	974	U
35	BA	975	G
35	BA	982	A
35	BA	984	A
35	BA	985	G
35	BA	986	G
35	BA	987	A
35	BA	988	C
35	BA	992	G
35	BA	999	A
35	BA	1000	U
35	BA	1007	U
35	BA	1008	C
35	BA	1010	C
35	BA	1013	G
35	BA	1014	U
35	BA	1020	G
35	BA	1021	U

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Mol	Chain	Res	Type
35	BA	1024	G
35	BA	1025	C
35	BA	1028	G
35	BA	1030	G
35	BA	1033	G
35	BA	1034	C
35	BA	1045	U
35	BA	1048	G
35	BA	1054	G
35	BA	1074	G
35	BA	1075	U
35	BA	1079	G
35	BA	1081	A
35	BA	1088	G
35	BA	1104	G
35	BA	1108	C
35	BA	1112	C
35	BA	1115	G
35	BA	1116	U
35	BA	1117	U
35	BA	1118	A
35	BA	1120	G
35	BA	1123	G
35	BA	1128	C
35	BA	1129	U
35	BA	1132	U
35	BA	1138	A
35	BA	1139	C
35	BA	1140	U
35	BA	1141	G
35	BA	1147	G
35	BA	1149	C
35	BA	1150	A
35	BA	1152	C
35	BA	1162	G
35	BA	1164	U
35	BA	1165	G
35	BA	1176	C
35	BA	1177	A
35	BA	1178	A
35	BA	1181	C
35	BA	1182	A

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Mol	Chain	Res	Type
35	BA	1183	U
35	BA	1193	U
35	BA	1194	A
35	BA	1206	U
35	BA	1207	C
35	BA	1217	A
35	BA	1219	A
35	BA	1231	A
35	BA	1233	A
35	BA	1238	U
35	BA	1239	G
35	BA	1241	G
35	BA	1248	U
35	BA	1251	G
35	BA	1260	A
35	BA	1261	A
35	BA	1266	U
35	BA	1267	U
35	BA	1268	C
35	BA	1269	A
35	BA	1271	A
35	BA	1272	G
35	BA	1281	A
35	BA	1282	G
35	BA	1283	U
35	BA	1284	U
35	BA	1285	C
35	BA	1287	G
35	BA	1299	C
35	BA	1301	A
35	BA	1302	C
35	BA	1304	C
35	BA	1305	G
35	BA	1313	G
35	BA	1320	G
35	BA	1322	G
35	BA	1327	U
35	BA	1328	A
35	BA	1329	G
35	BA	1335	G
35	BA	1343	G
35	BA	1344	C

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Mol	Chain	Res	Type
35	BA	1345	A
35	BA	1346	A
35	BA	1347	C
35	BA	1351	G
35	BA	1353	G
35	BA	1357	A
35	BA	1363	U
35	BA	1364	U
35	BA	1381	A
35	BA	1382	C
35	BA	1383	C
35	BA	1385	C
35	BA	1389	U
35	BA	1402	G
35	BA	1405	G
35	BA	1407	U
35	BA	1409	A
35	BA	1424	G
35	BA	1425	G
35	BA	1426	C
35	BA	1429	A
35	BA	1430	A
35	BA	1433	C
35	BA	1434	U
35	BA	1435	U
35	BA	1436	G
35	BA	1438	G
35	BA	1459	G
35	BA	1466	G
35	BA	1471	G
35	BA	1478	G
35	BA	1481	G
35	BA	1482	U
35	BA	1483	A
35	BA	1486	A
35	BA	1487	A
35	BA	1488	G
35	BA	1490	U
35	BA	1501	G
35	BA	1502	A
35	BA	1503	A
35	BA	1504	G

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Mol	Chain	Res	Type
35	BA	1513	G
35	BA	1514	G
35	BA	1516	U
56	BW	2	C
56	BW	6	G
56	BW	8	U
56	BW	16	U
56	BW	17	C
56	BW	18	G
56	BW	19	G
56	BW	20	U
56	BW	21	A
56	BW	22	G
56	BW	23	A
56	BW	32	U
56	BW	37	A
56	BW	42	C
56	BW	46	G
56	BW	47	U
56	BW	48	C
56	BW	52	G
56	BW	69	G
56	BW	76	A
57	BX	2	U
57	BX	3	U

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	89	A
2	A	97	U
2	A	284	G
2	A	287	A
2	A	316	U
2	A	357	U
2	A	445	U
2	A	759	G
2	A	919	A
2	A	974	G
2	A	980	C
2	A	981	U
2	A	1004	C

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Mol	Chain	Res	Type
2	A	1010	U
2	A	1046	C
2	A	1084	U
2	A	1186	G
2	A	1231	U
2	A	1368	A
2	A	1713	U
2	A	1730	U
2	A	1947	U
2	A	2085	C
2	A	2088	C
2	A	2094	G
2	A	2350	G
2	A	2381	A
2	A	2626	U
2	A	3113	A
3	B	10	G
35	BA	422	C
35	BA	429	U
35	BA	456	C
35	BA	485	G
35	BA	498	C
35	BA	895	A
35	BA	1007	U
35	BA	1116	U
35	BA	1117	U
35	BA	1149	C
35	BA	1266	U
35	BA	1477	A
35	BA	1482	U

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 632 ligands modelled in this entry, 631 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	PHE	BW	101	-	10,11,12	0.87	0	8,13,15	0.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PHE	BW	101	-	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

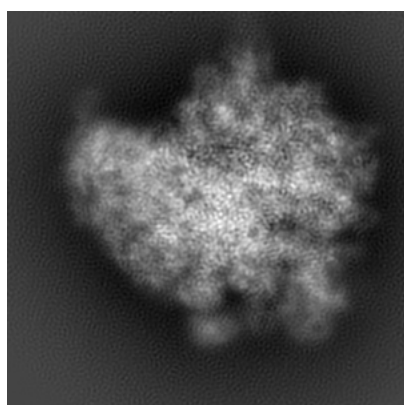
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3751. These allow visual inspection of the internal detail of the map and identification of artifacts.

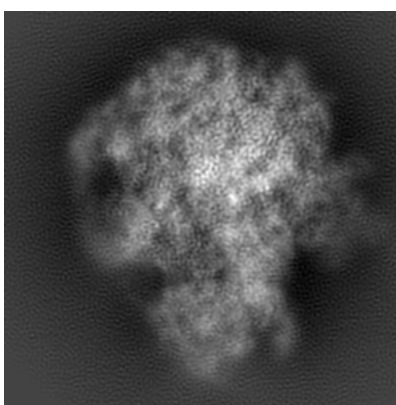
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

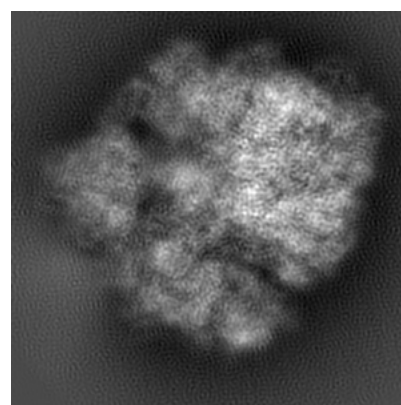
6.1.1 Primary map



X



Y

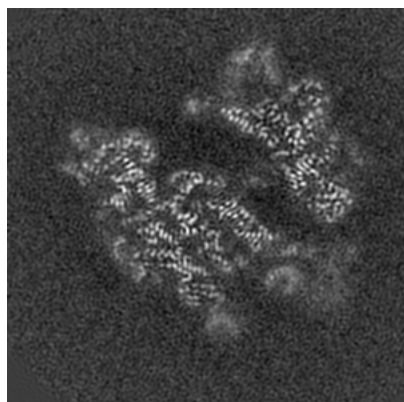


Z

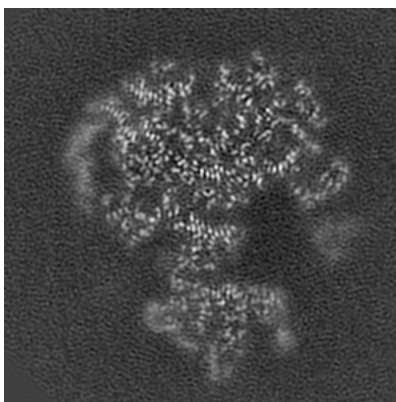
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

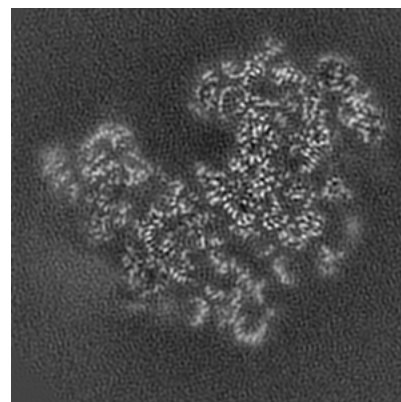
6.2.1 Primary map



X Index: 108



Y Index: 108

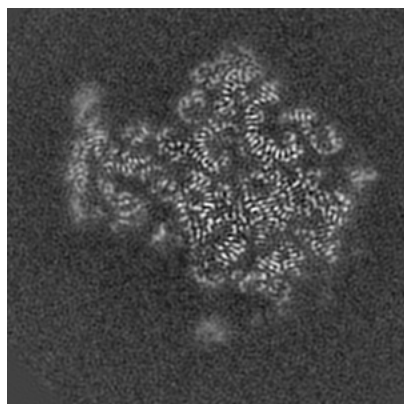


Z Index: 108

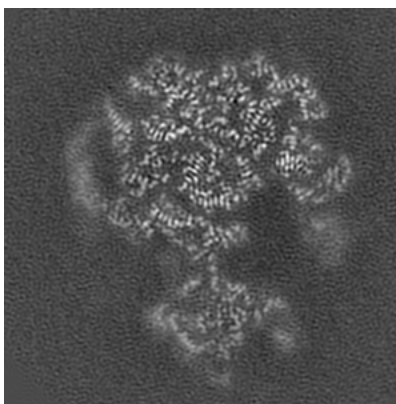
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

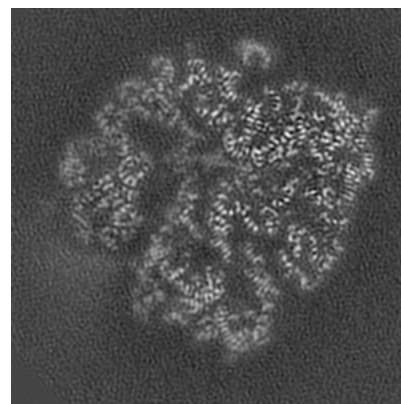
6.3.1 Primary map



X Index: 126



Y Index: 112

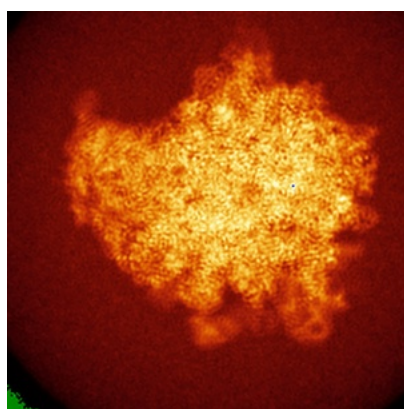


Z Index: 123

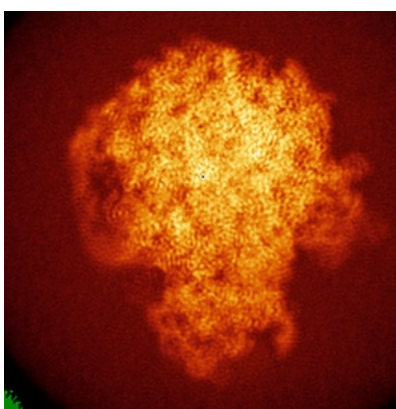
The images above show the largest variance slices of the map in three orthogonal directions.

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

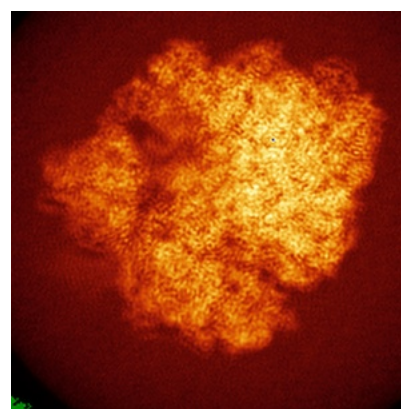
6.4.1 Primary map



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

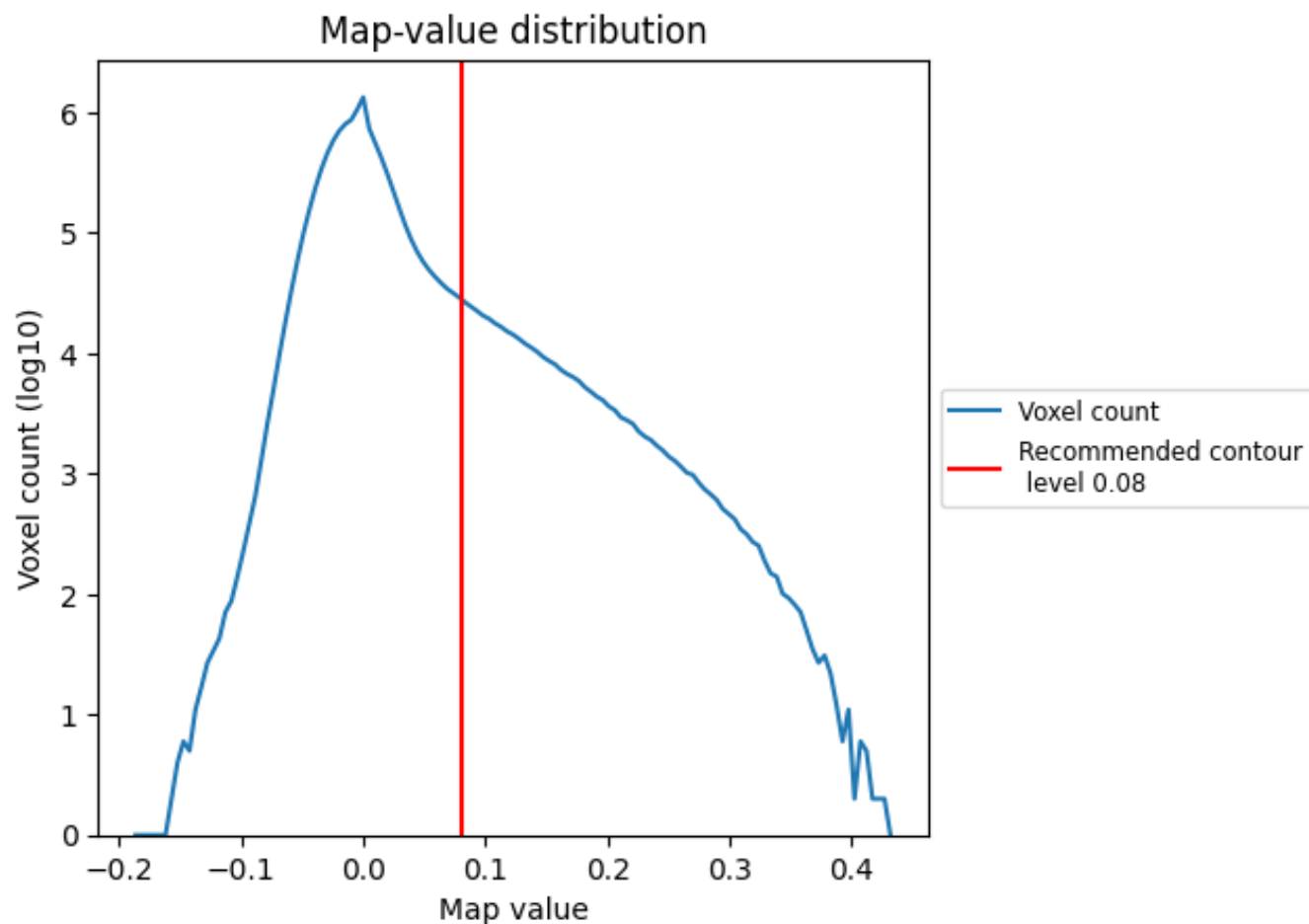
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

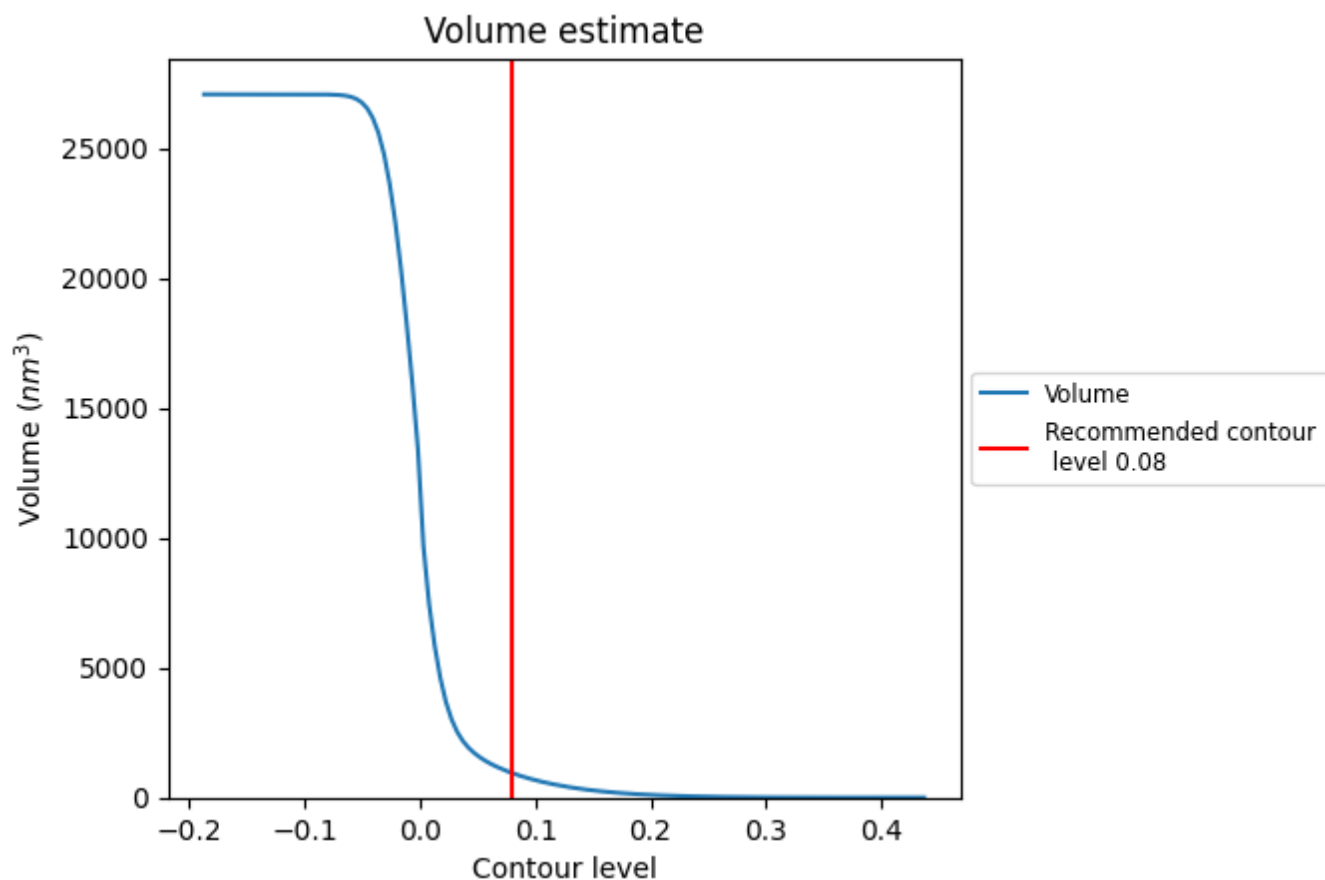
This section contains the results of statistical analysis of the map.

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.

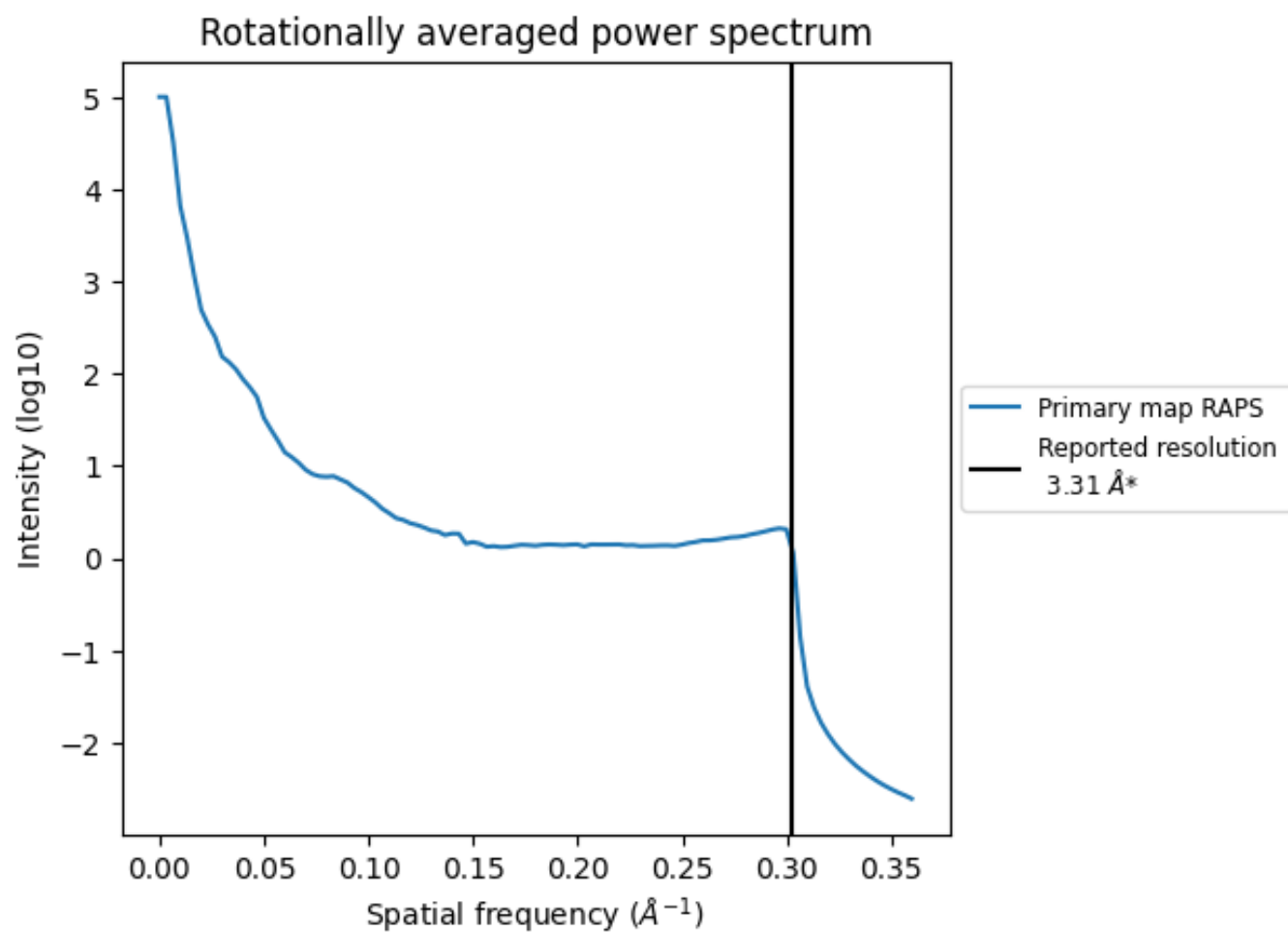
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 945 nm³; this corresponds to an approximate mass of 853 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 ⓘ

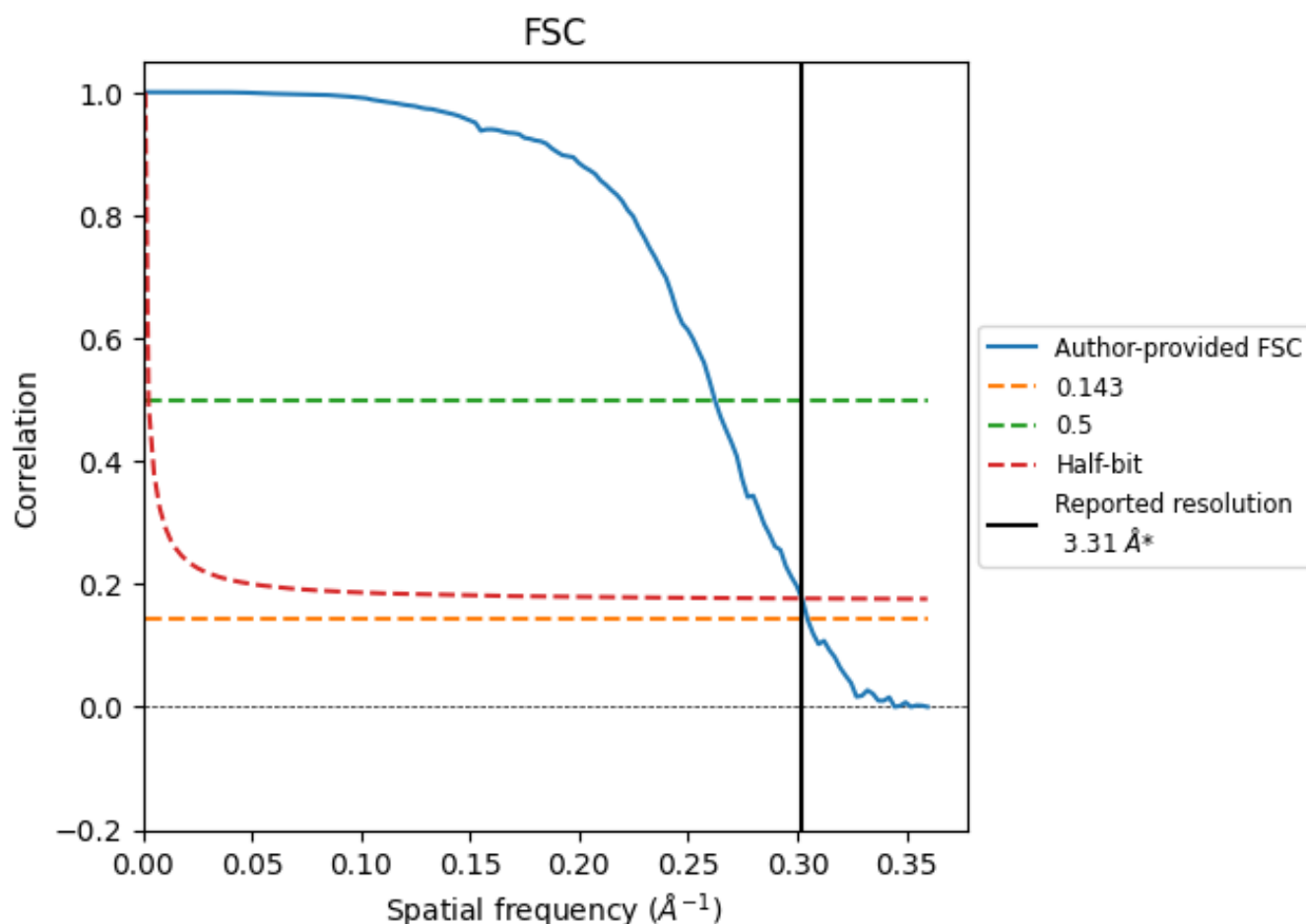


*Reported resolution corresponds to spatial frequency of 0.302 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.302 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

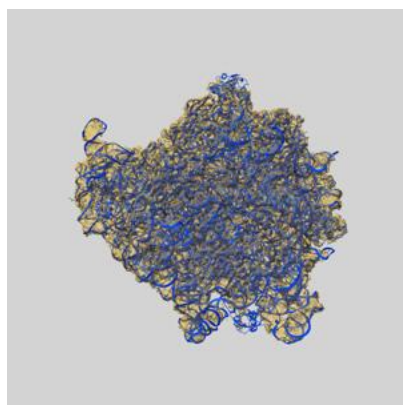
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.31	-	-
Author-provided FSC curve	3.28	3.81	3.31
Unmasked-calculated*	-	-	-

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

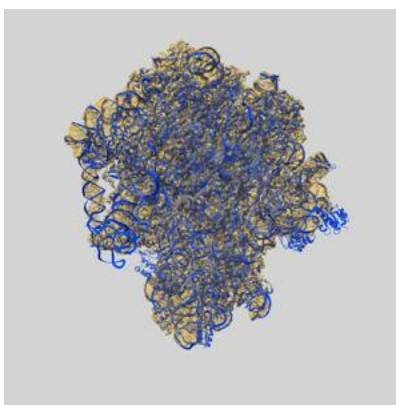
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3751 and PDB model 5O61. Per-residue inclusion information can be found in section [3](#) on page [16](#).

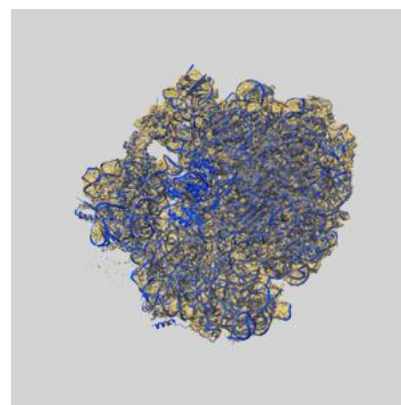
9.1 Map-model overlay [i](#)



X



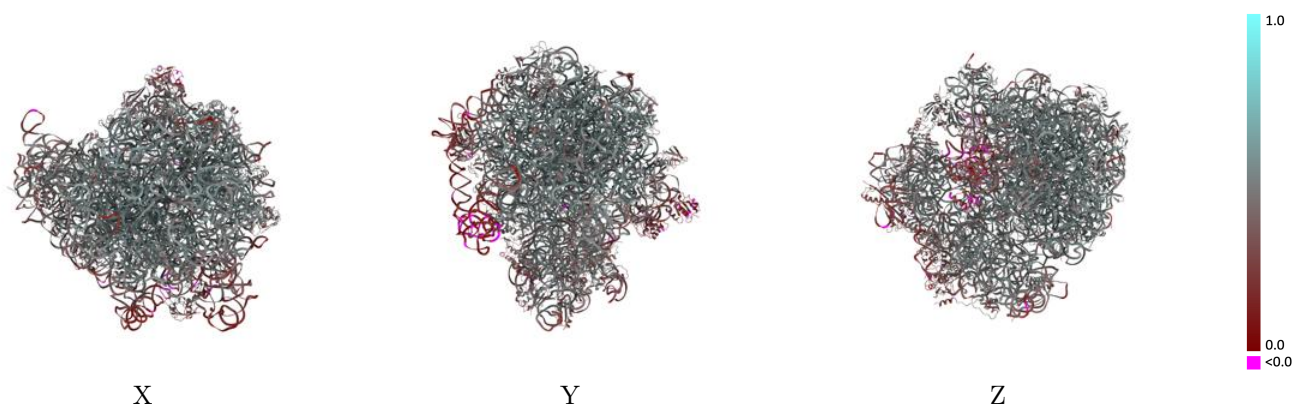
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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](#)



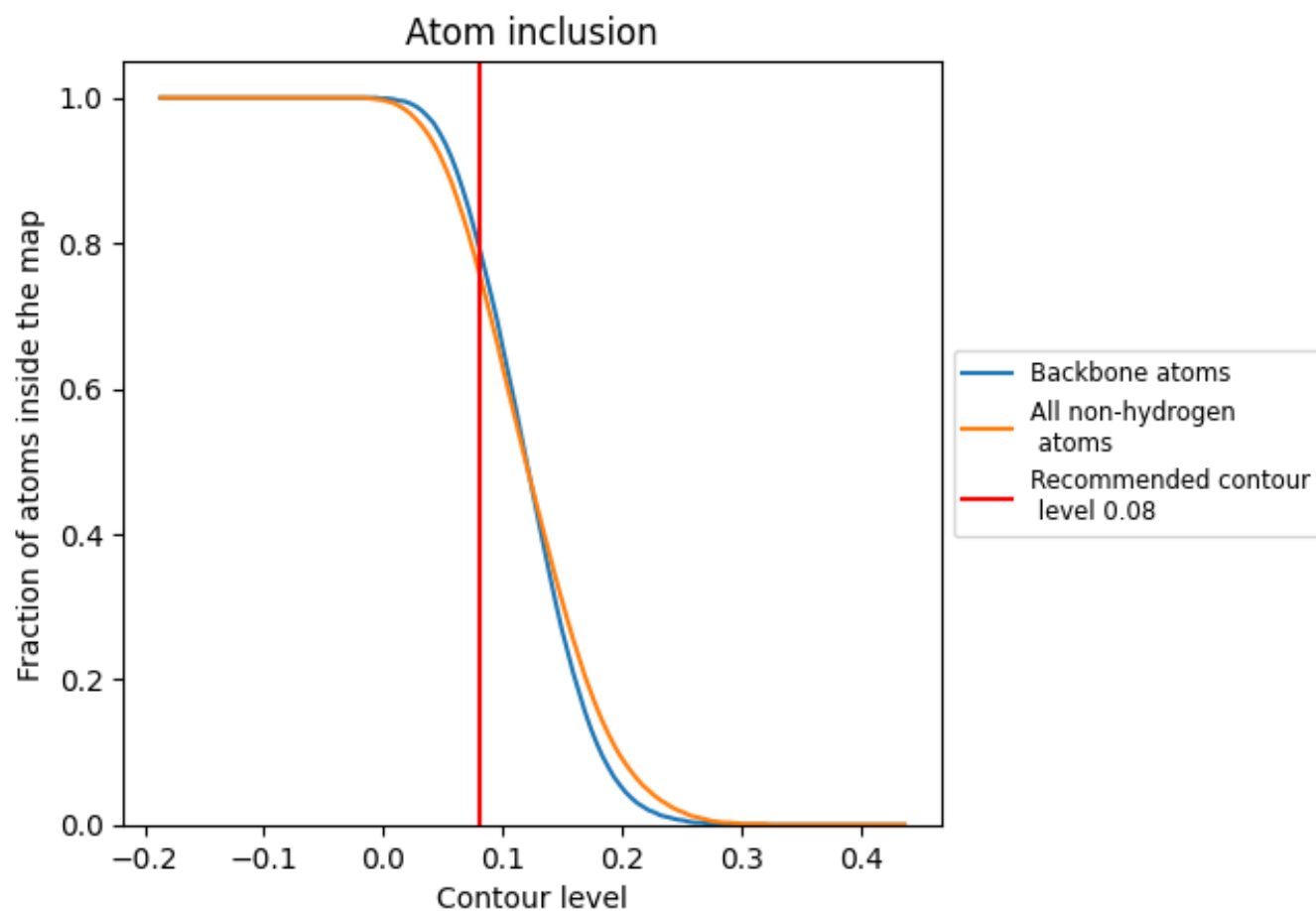
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 76% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7620	 0.4620
3	 0.7040	 0.5240
A	 0.8590	 0.4800
B	 0.9020	 0.4840
BA	 0.8550	 0.4660
BB	 0.3780	 0.4470
BC	 0.3910	 0.3980
BD	 0.3610	 0.3230
BE	 0.5240	 0.4420
BF	 0.5210	 0.4160
BG	 0.5020	 0.4050
BH	 0.6810	 0.4830
BI	 0.6010	 0.4290
BJ	 0.4170	 0.3740
BK	 0.6170	 0.4460
BL	 0.5590	 0.4300
BM	 0.5590	 0.4240
BN	 0.6410	 0.4820
BO	 0.6410	 0.4570
BP	 0.5360	 0.4050
BQ	 0.5220	 0.4060
BR	 0.6180	 0.4440
BS	 0.5380	 0.4370
BT	 0.6340	 0.4150
BV	 0.0260	 0.2650
BW	 0.2710	 0.3630
BX	 0.4620	 0.4330
C	 0.7050	 0.5220
D	 0.7460	 0.5190
E	 0.6900	 0.4870
F	 0.6260	 0.4240
G	 0.5840	 0.4130
H	 0.1910	 0.3450
I	 0.0490	 0.1790
J	 0.0730	 0.1860



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Chain	Atom inclusion	Q-score
K	 0.7330	 0.5090
L	 0.6170	 0.4860
M	 0.6860	 0.4880
N	 0.6710	 0.5050
O	 0.7430	 0.5120
P	 0.7310	 0.4750
Q	 0.6540	 0.4760
R	 0.7770	 0.5130
S	 0.6970	 0.5070
T	 0.7050	 0.5050
U	 0.6310	 0.4680
V	 0.5920	 0.4510
W	 0.5160	 0.4180
X	 0.7470	 0.5240
Y	 0.7050	 0.5150
Z	 0.6670	 0.4380
a	 0.7060	 0.4950
b	 0.6870	 0.5100
c	 0.7000	 0.4940
d	 0.7540	 0.5350
e	 0.7350	 0.5290
f	 0.7600	 0.5130
g	 0.6030	 0.3980