



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:36 PM UTC

PDB ID : 8T2Y / pdb_00008t2y
EMDB ID : EMD-40991
Title : Hypomethylated yeast 80S bound with cycloheximide, P-site tRNA, and A-site tRNA, messenger RNA, PRE
Authors : Zhao, Y.; Li, H.
Deposited on : 2023-06-07
Resolution : 2.20 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

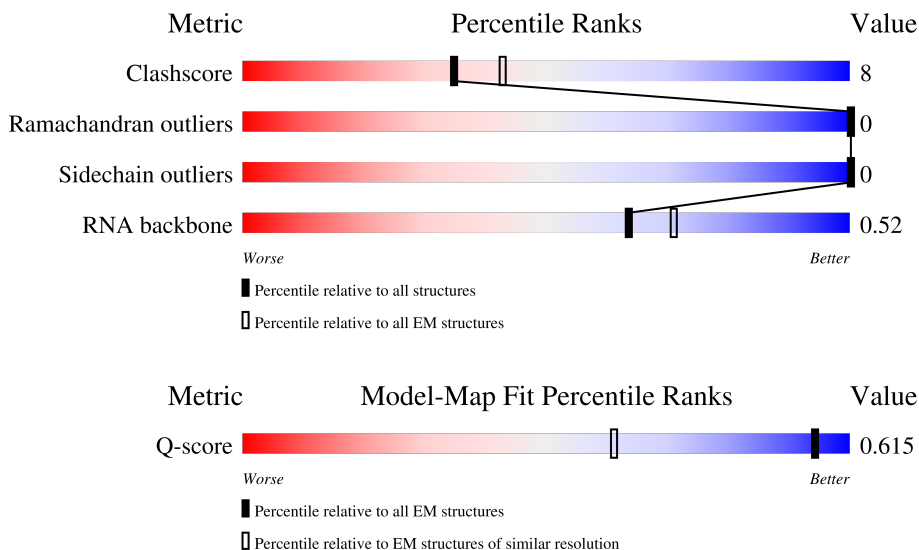
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 Å.

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



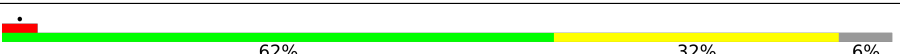
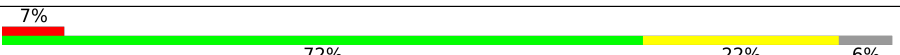
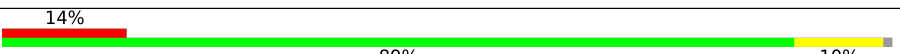
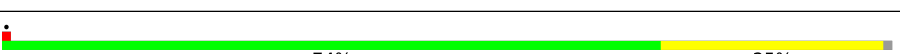
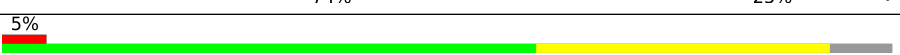
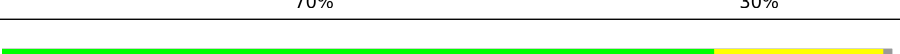
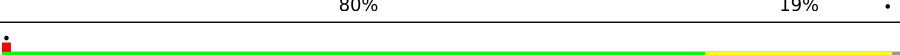
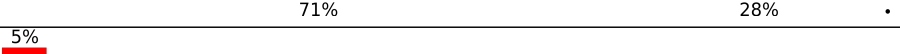
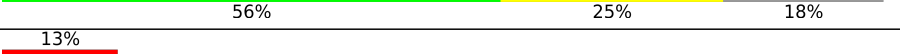
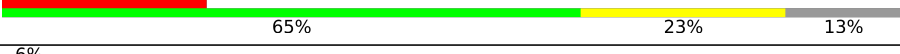
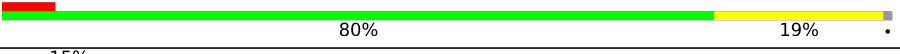
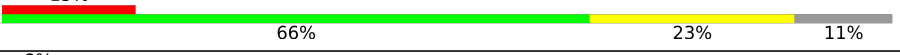
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3184 (1.71 - 2.70)

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	BA	252	5% 57% 25% 18%
2	BB	255	12% 49% 34% 16%
3	BC	254	71% 15% 15%

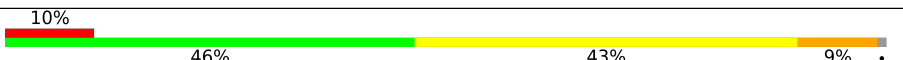
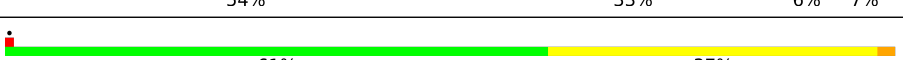
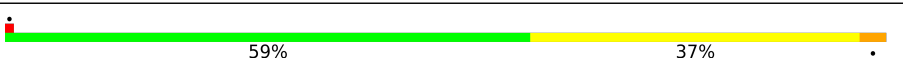
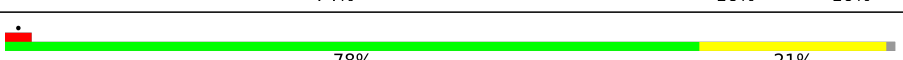
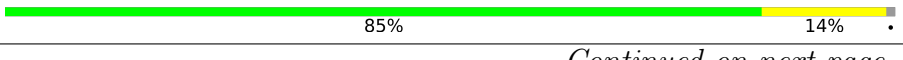
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Mol	Chain	Length	Quality of chain
4	BE	261	
5	BG	236	
6	BH	190	
7	BI	200	
8	BJ	197	
9	BL	156	
10	BN	151	
11	BO	137	
12	BV	87	
13	BW	130	
14	BX	145	
15	BY	135	
16	Ba	119	
17	Bb	82	
18	Be	63	
19	BD	240	
20	BF	225	
21	BK	105	
22	BP	142	
23	BQ	143	
24	BR	136	
25	BS	146	
26	BT	144	
27	BU	121	
28	BZ	108	

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Mol	Chain	Length	Quality of chain
29	Bc	67	
30	Bd	56	
31	Bg	319	
32	Bf	152	
33	BM	143	
34	B5	1798	
35	AA	254	
36	AB	387	
37	AC	362	
38	A1	3395	
39	A3	121	
40	A4	158	
41	AD	297	
42	AE	176	
43	AF	244	
44	AG	256	
45	AH	191	
46	AI	221	
47	AJ	174	
48	AL	199	
49	AM	138	
50	AN	204	
51	AO	199	
52	AP	184	
53	AQ	186	

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Mol	Chain	Length	Quality of chain
54	AR	189	
55	AS	178	
56	AT	160	
57	AU	121	
58	AV	137	
59	AW	155	
60	AX	142	
61	AY	127	
62	AZ	136	
63	Aa	149	
64	Ab	59	
65	Ac	105	
66	Ad	113	
67	Ae	130	
68	Af	107	
69	Ag	121	
70	Ah	120	
71	Ai	100	
72	Aj	88	
73	Ak	78	
74	Al	51	
75	Am	128	
76	An	25	
77	Ao	106	
78	Ap	92	

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Mol	Chain	Length	Quality of chain
79	tP	75	40% 28% 32%
80	tA	76	5% 41% 50% 9%
81	MR	12	8% 58% 42%

2 Entry composition

There are 85 unique types of molecules in this entry. The entry contains 202978 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 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BA	206	Total	C	N	O	S	0	0
			1612	1034	285	291	2		

- Molecule 2 is a protein called RPS1A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BB	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 3 is a protein called RPS2 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BC	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 4 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BE	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 5 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BG	226	Total	C	N	O	S	0	0
			1820	1142	350	325	3		

- Molecule 6 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	BH	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 7 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BI	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 8 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BJ	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 9 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BL	155	Total	C	N	O	S	0	0
			1244	798	235	208	3		

- Molecule 10 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BN	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 11 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BO	127	Total	C	N	O	S	0	0
			941	578	186	174	3		

- Molecule 12 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BV	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 13 is a protein called RPS22A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BW	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 14 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BX	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 15 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BY	134	Total	C	N	O	S	0	0
			1073	676	208	189			

- Molecule 16 is a protein called RPS26B isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ba	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 17 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Bb	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 18 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Be	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 19 is a protein called RPS3 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BD	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 20 is a protein called Rps5p.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BF	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 21 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BK	96	Total	C	N	O	S	0	0
			817	529	133	153	2		

- Molecule 22 is a protein called RPS15 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BP	124	Total	C	N	O	S	0	0
			991	631	187	166	7		

- Molecule 23 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BQ	141	Total	C	N	O	S	0	0
			1105	708	203	194			

- Molecule 24 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BR	121	Total	C	N	O	S	0	0
			948	596	179	171	2		

- Molecule 25 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BS	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 26 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BT	141	Total	C	N	O	S	0	0
			1095	685	206	202	2		

- Molecule 27 is a protein called RPS20 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BU	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 28 is a protein called RPS25A isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	BZ	70	Total	C	N	O	0	0
			563	360	104	99		

- Molecule 29 is a protein called RPS28A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Bc	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 30 is a protein called RPS29A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Bd	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 31 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bg	312	Total	C	N	O	S	0	0
			2401	1522	410	461	8		

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bf	75	Total	C	N	O	S	0	0
			605	386	116	99	4		

- Molecule 33 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BM	124	Total	C	N	O	S	0	0
			935	587	165	181	2		

- Molecule 34 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B5	1782	Total	C	N	O	P	1	0
			37987	16988	6718	12499	1782		

- Molecule 35 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AA	247	Total	C	N	O	S	0	0
			1878	1170	381	326	1		

- Molecule 36 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AB	386	Total	C	N	O	S	0	0
			3081	1956	584	533	8		

- Molecule 37 is a protein called RPL4A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AC	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 38 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A1	3159	Total	C	N	O	P	0	0
			67564	30183	12164	22058	3159		

- Molecule 39 is a RNA chain called 5s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	A3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 40 is a RNA chain called 5.8 S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A4	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 41 is a protein called RPL5 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AD	292	Total	C	N	O	S	0	0
			2341	1478	408	453	2		

- Molecule 42 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AE	167	Total	C	N	O	S	0	0
			1303	840	234	228	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	120	LYS	ASN	conflict	UNP Q02326

- Molecule 43 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AF	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 44 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AG	230	Total	C	N	O	S	0	0
			1798	1149	323	323	3		

- Molecule 45 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AH	190	Total	C	N	O	S	0	0
			1510	957	273	276	4		

- Molecule 46 is a protein called RPL10 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AI	217	Total	C	N	O	S	0	0
			1759	1114	333	305	7		

- Molecule 47 is a protein called RPL11A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AJ	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 48 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	AL	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 49 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AM	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 50 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AN	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 51 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AO	197	Total	C	N	O	S	197	0
			1555	1003	289	262	1		

- Molecule 52 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	AP	175	Total	C	N	O	0	0
			1388	862	277	249		

- Molecule 53 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AQ	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 54 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	AR	188	Total	C	N	O	0	0
			1521	935	326	260		

- Molecule 55 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AS	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 56 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AT	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 57 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AU	100	Total	C	N	O	S	0	0
			796	516	131	149			

- Molecule 58 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AV	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 59 is a protein called RPL24A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AW	63	Total	C	N	O	S	0	0
			521	336	102	82	1		

- Molecule 60 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AX	121	Total	C	N	O	S	0	0
			968	623	170	173	2		

- Molecule 61 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AY	126	Total	C	N	O	S	0	0
			993	625	192	176			

- Molecule 62 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	AZ	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 63 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Aa	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 64 is a protein called RPL29 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	Ab	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 65 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Ac	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 66 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Ad	109	Total	C	N	O	S	0	0
			890	565	168	156	1		

- Molecule 67 is a protein called RPL32 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Ae	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 68 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Af	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 69 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ag	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 70 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Ah	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 71 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Ai	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 72 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Aj	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 73 is a protein called RPL38 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
73	Ak	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 74 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Al	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 75 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Am	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 76 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	An	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 77 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ao	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 78 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Ap	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 79 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	tP	75	Total	C	N	O	P	0	0
			1606	716	297	518	75		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
tP	10	A	G	conflict	GB 176433

- Molecule 80 is a RNA chain called A site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	tA	76	Total	C	N	O	P	0	0
			1627	726	302	523	76		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
tA	10	A	G	conflict	GB 176433
tA	17	A	-	insertion	GB 176433

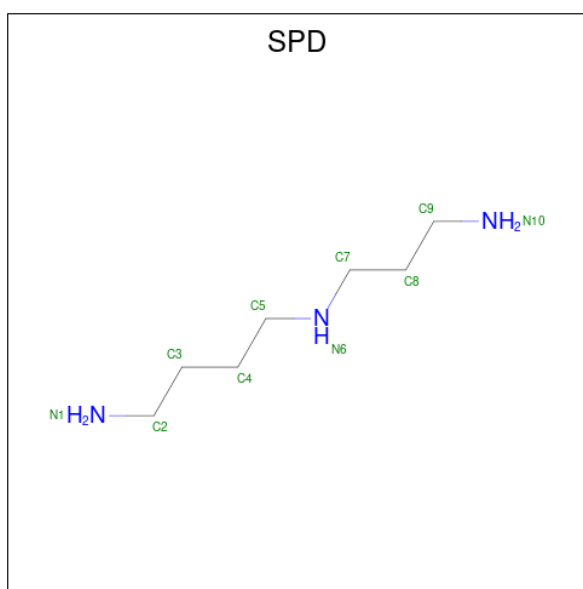
- Molecule 81 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	MR	12	Total	C	N	O	P	0	0
			259	117	51	79	12		

- Molecule 82 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

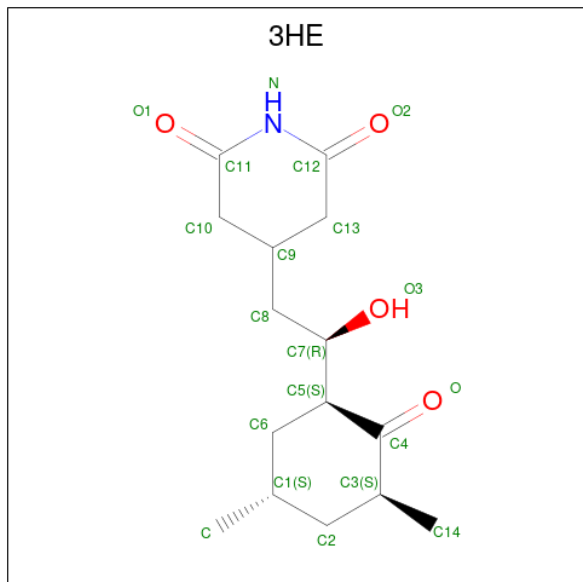
Mol	Chain	Residues	Atoms		AltConf
82	B5	46	Total	Mg	0
			46	46	
82	AA	1	Total	Mg	0
			1	1	
82	A1	145	Total	Mg	0
			145	145	
82	A4	1	Total	Mg	0
			1	1	
82	AP	1	Total	Mg	0
			1	1	
82	AV	1	Total	Mg	0
			1	1	
82	Ae	1	Total	Mg	0
			1	1	
82	MR	1	Total	Mg	0
			1	1	

- Molecule 83 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



Mol	Chain	Residues	Atoms			AltConf
83	A1	1	Total	C	N	0
			10	7	3	

- Molecule 84 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (CCD ID: 3HE) (formula: C₁₅H₂₃NO₄).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
84	A1	1	20	15	1	4	0

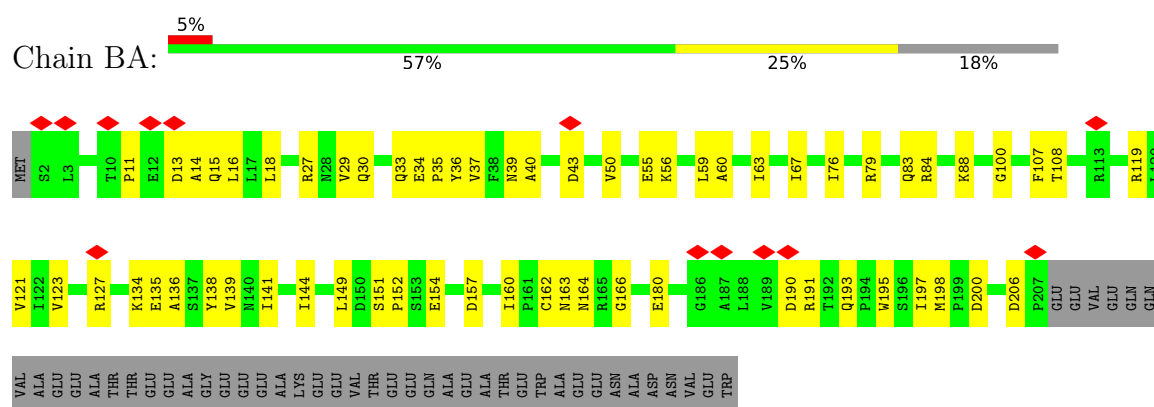
- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
85	Ao	1	1	1	0

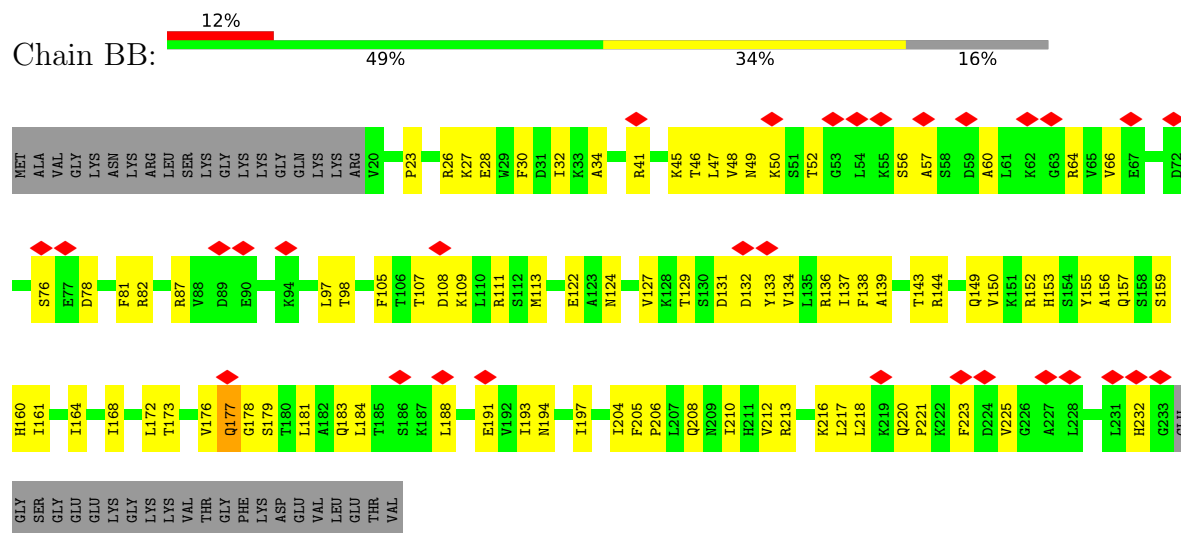
3 Residue-property plots

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.

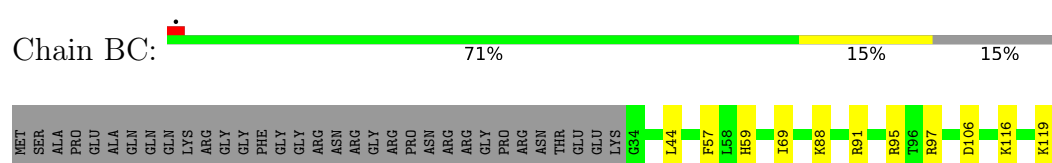
- Molecule 1: 40S ribosomal protein S0-A

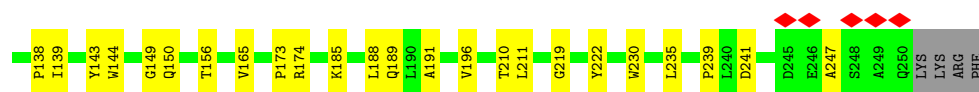


- Molecule 2: RPS1A isoform 1

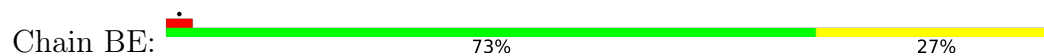


- Molecule 3: RPS2 isoform 1

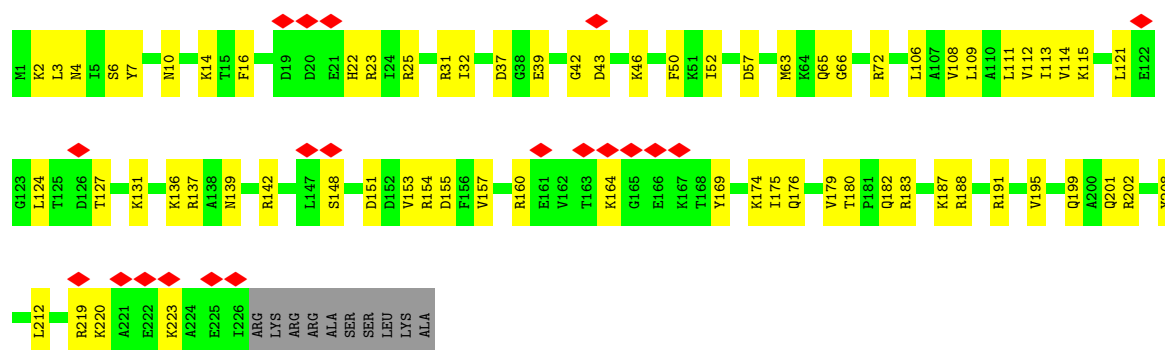




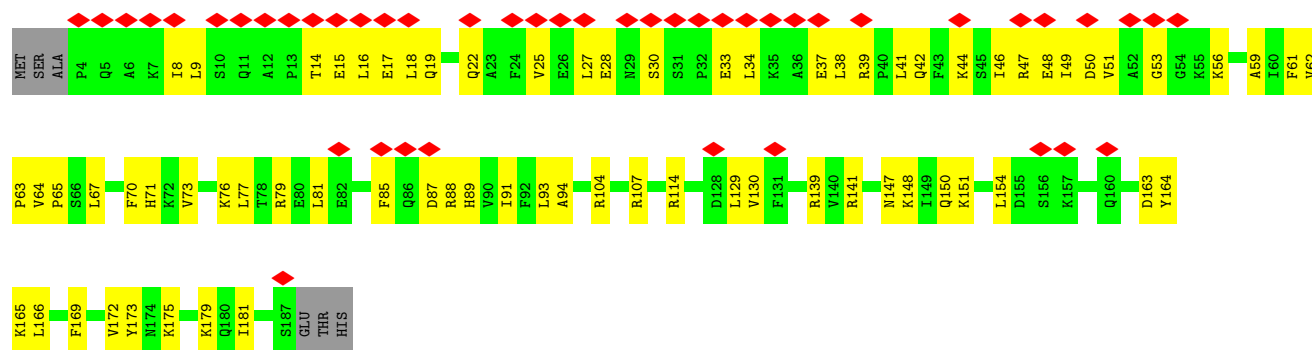
• Molecule 4: 40S ribosomal protein S4-A



• Molecule 5: 40S ribosomal protein S6-A

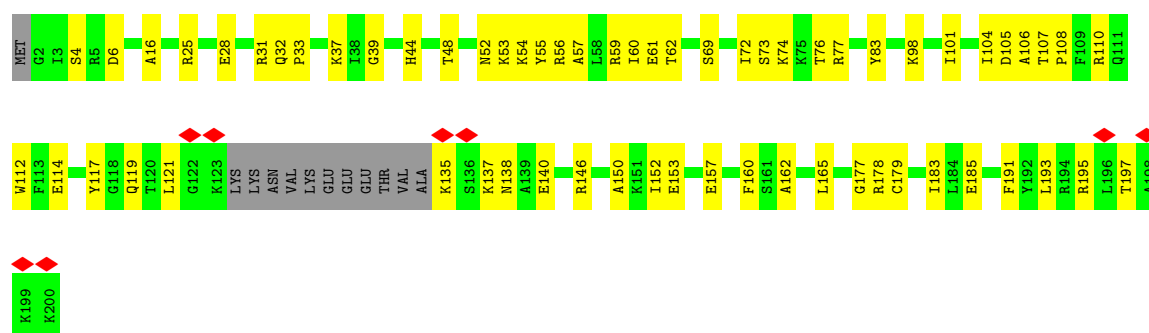


• Molecule 6: 40S ribosomal protein S7-A



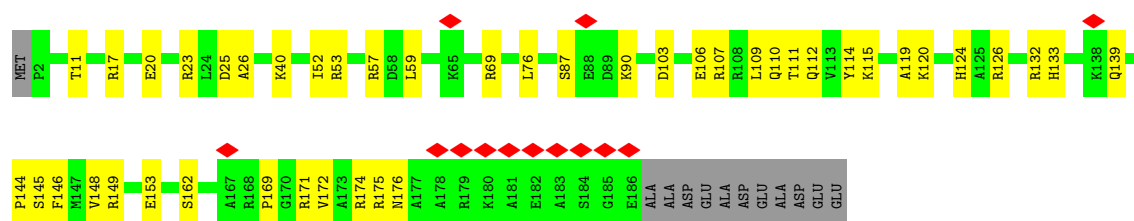
• Molecule 7: 40S ribosomal protein S8-A

Chain BI: 

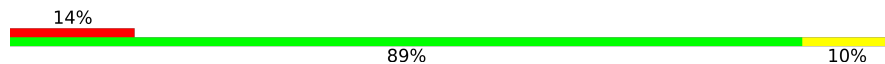


- Molecule 8: 40S ribosomal protein S9-A

Chain BJ: 



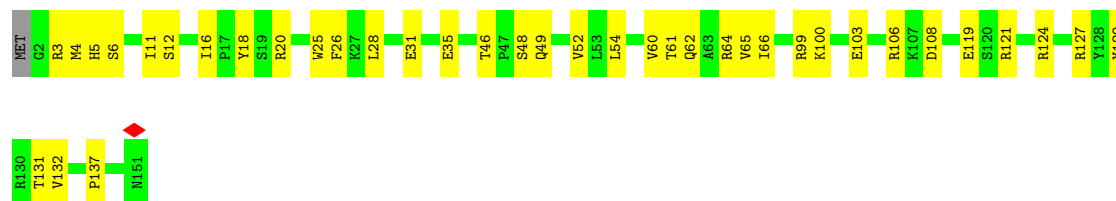
- Molecule 9: 40S ribosomal protein S11-A

Chain BL: 



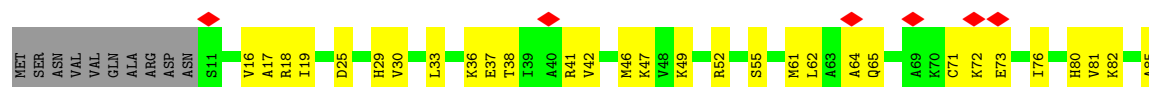
- Molecule 10: 40S ribosomal protein S13

Chain BN: 



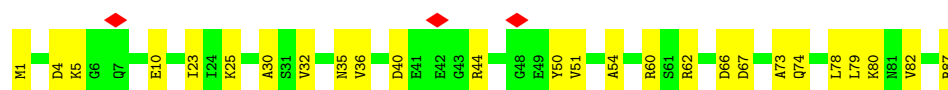
- Molecule 11: 40S ribosomal protein S14-A

Chain BO: 

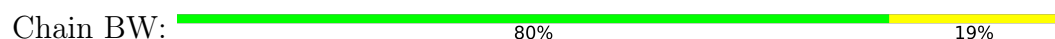




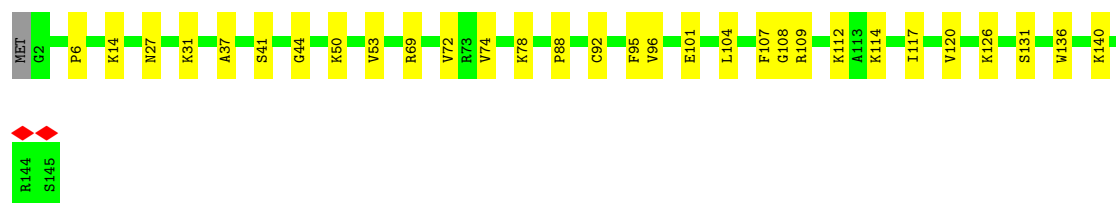
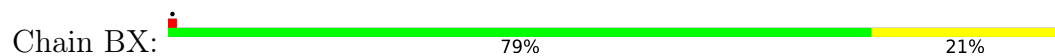
- Molecule 12: 40S ribosomal protein S21-A



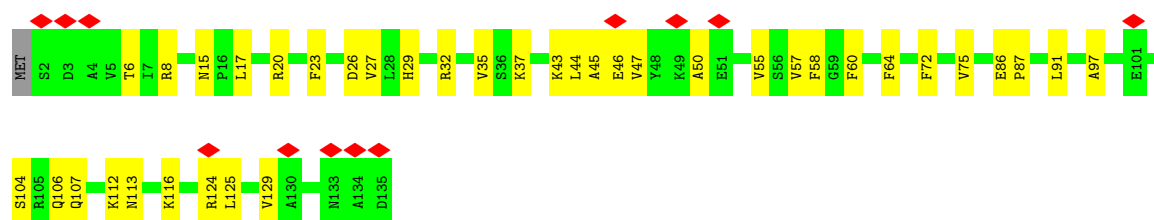
- Molecule 13: RPS22A isoform 1



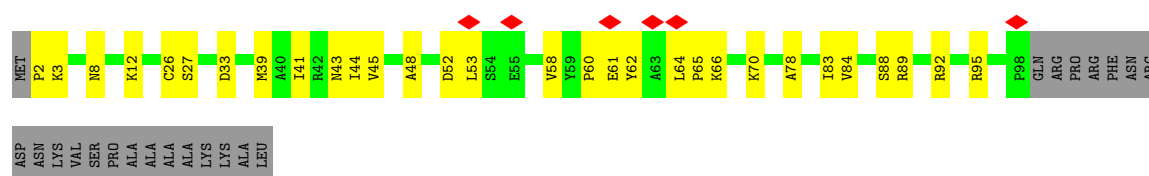
- Molecule 14: 40S ribosomal protein S23-A



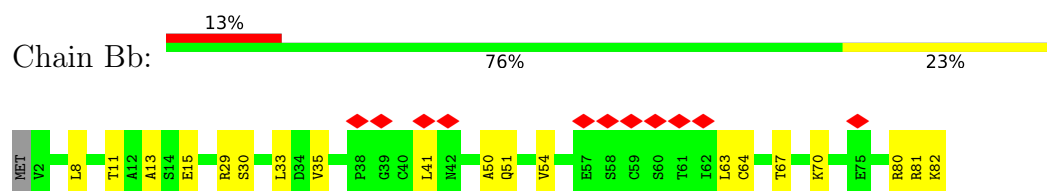
- Molecule 15: 40S ribosomal protein S24-A



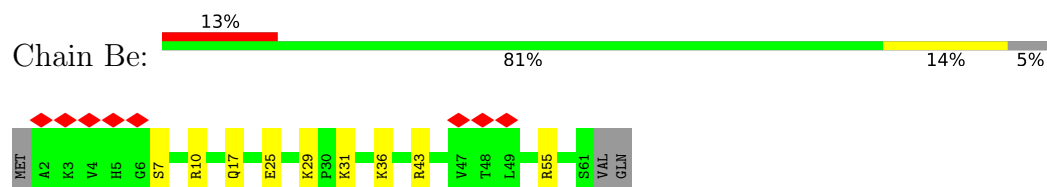
- Molecule 16: RPS26B isoform 1



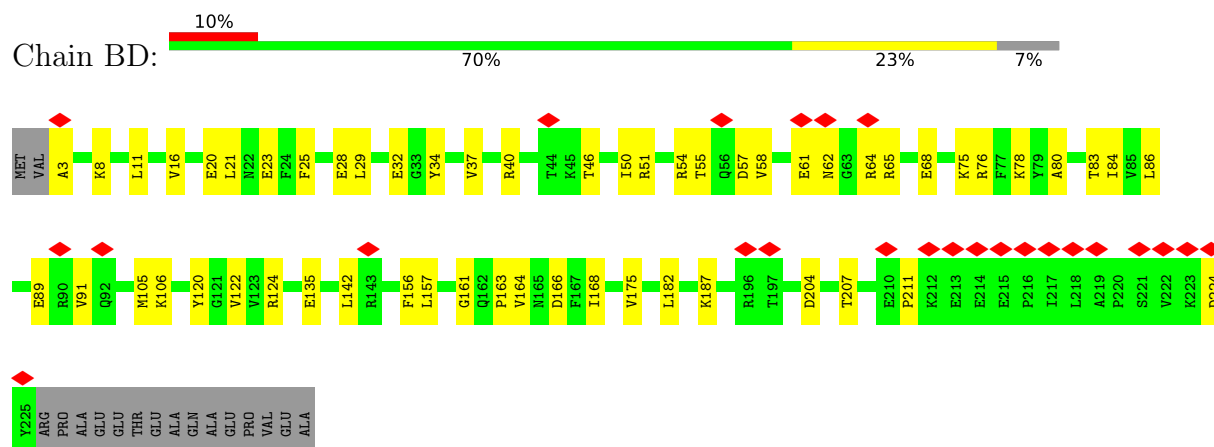
- Molecule 17: 40S ribosomal protein S27-A



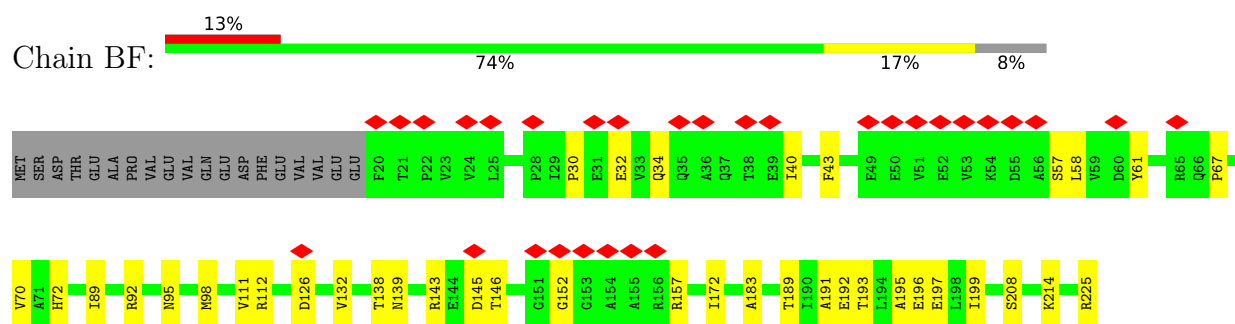
- Molecule 18: 40S ribosomal protein S30-A



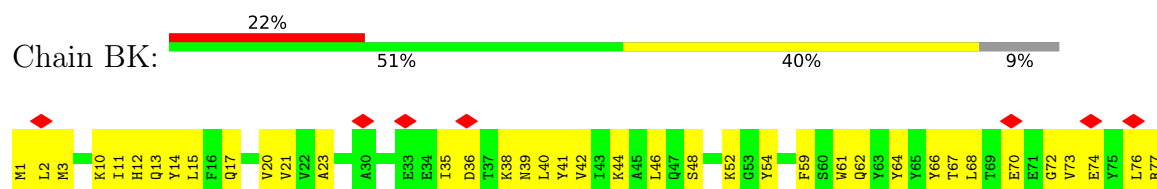
- Molecule 19: RPS3 isoform 1



- Molecule 20: Rps5p

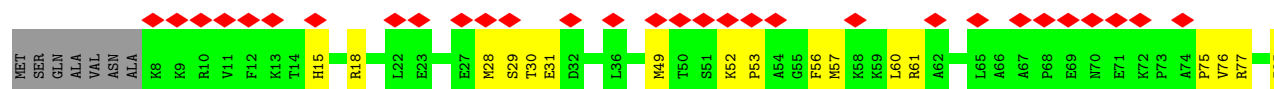


- Molecule 21: 40S ribosomal protein S10-A

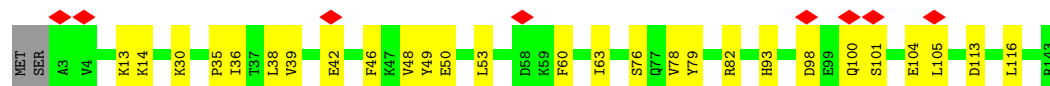
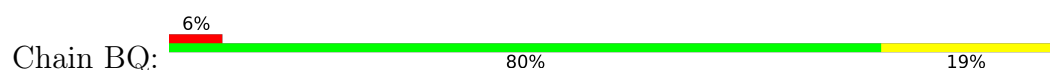




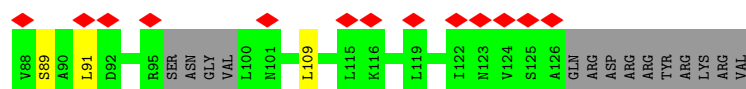
• Molecule 22: RPS15 isoform 1



• Molecule 23: 40S ribosomal protein S16-A



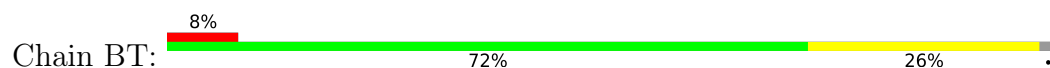
• Molecule 24: 40S ribosomal protein S17-A

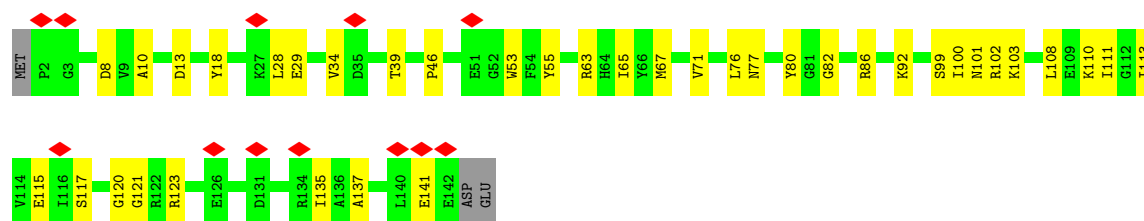


• Molecule 25: 40S ribosomal protein S18-A

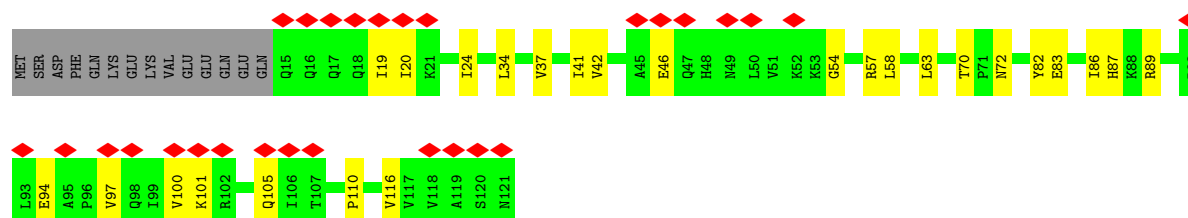


• Molecule 26: 40S ribosomal protein S19-A

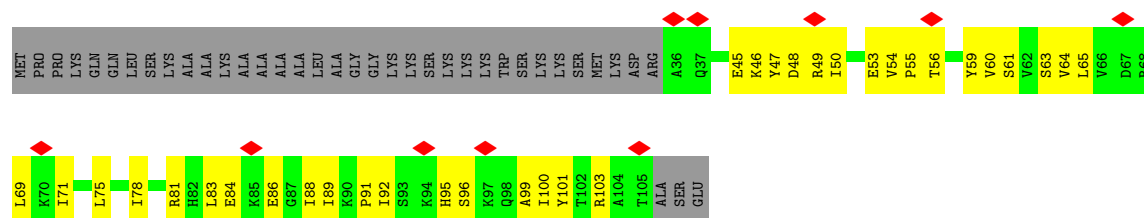




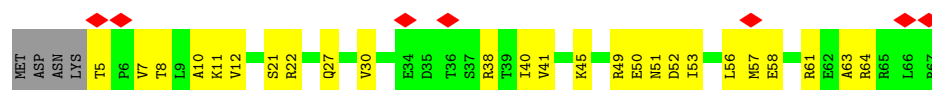
• Molecule 27: RPS20 isoform 1



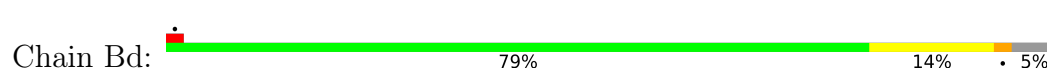
• Molecule 28: RPS25A isoform 1



• Molecule 29: RPS28A isoform 1

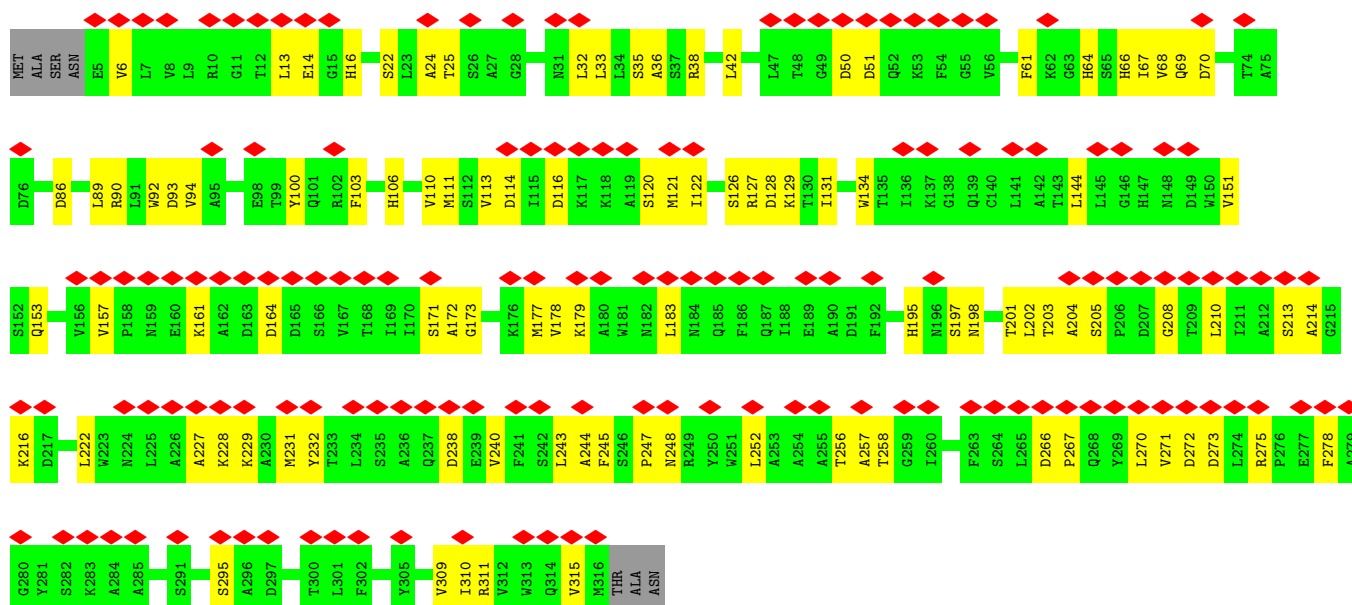


• Molecule 30: RPS29A isoform 1

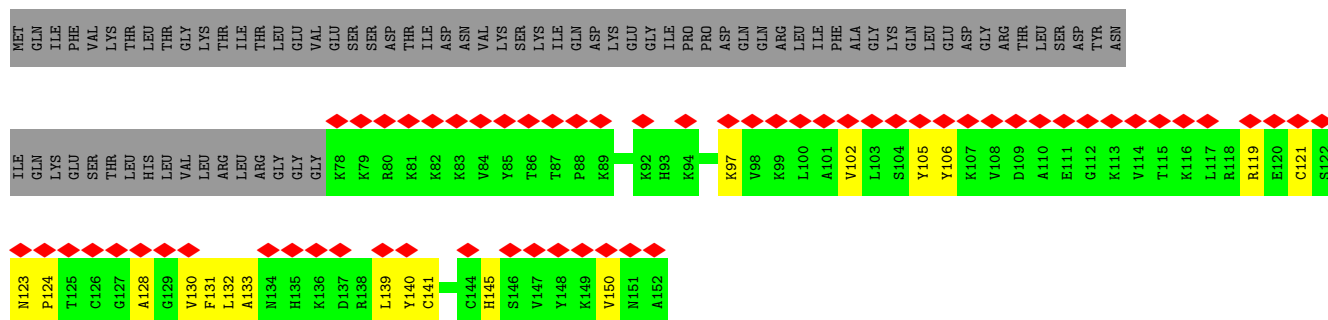
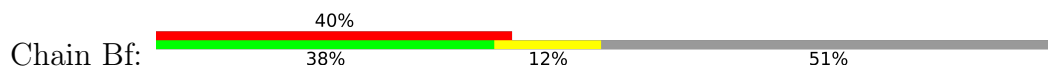


• Molecule 31: Guanine nucleotide-binding protein subunit beta-like protein

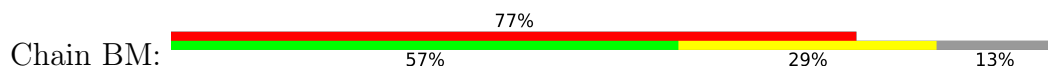




• Molecule 32: Ubiquitin-40S ribosomal protein S31



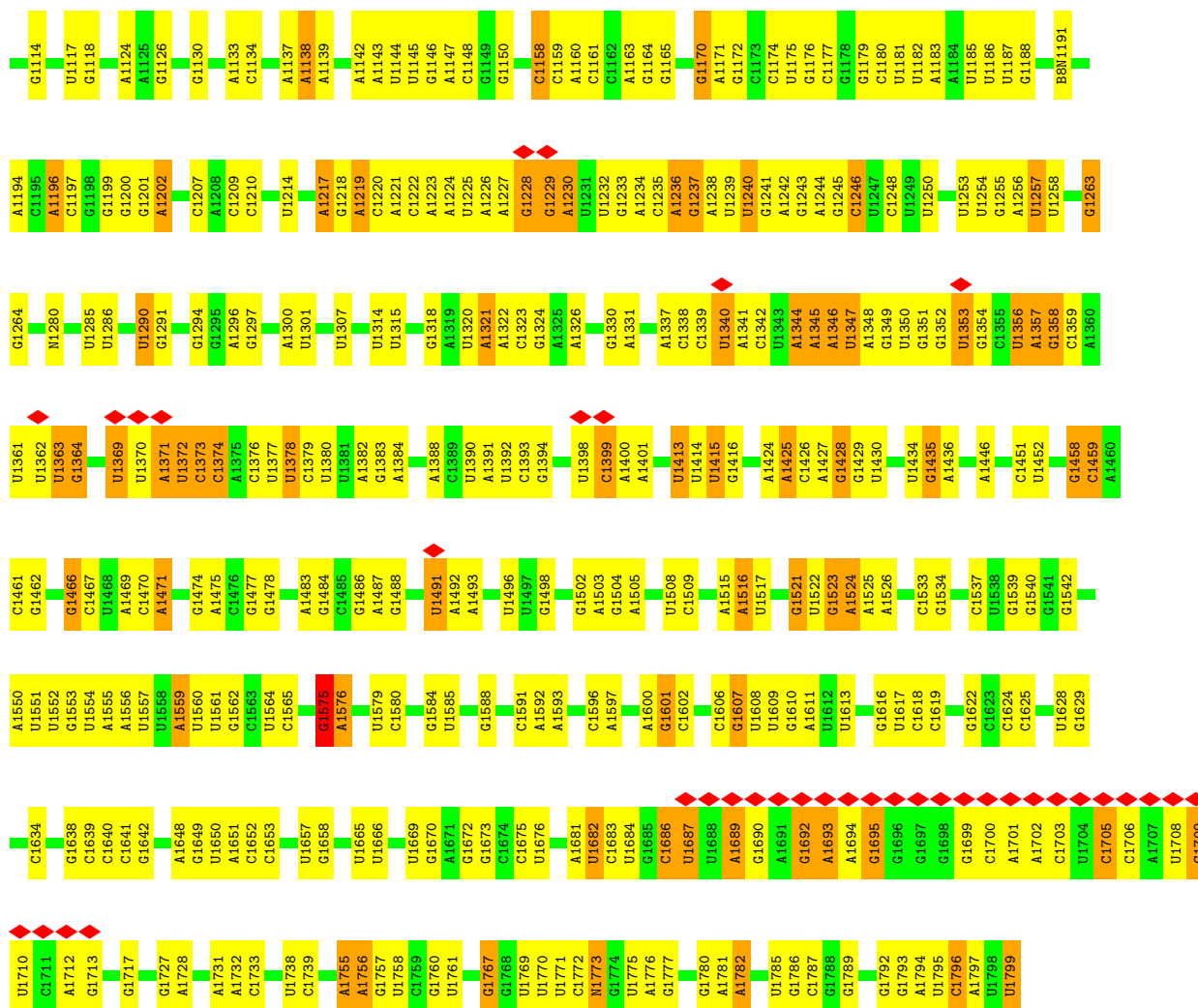
• Molecule 33: 40S ribosomal protein S12



• Molecule 34: 18S rRNA

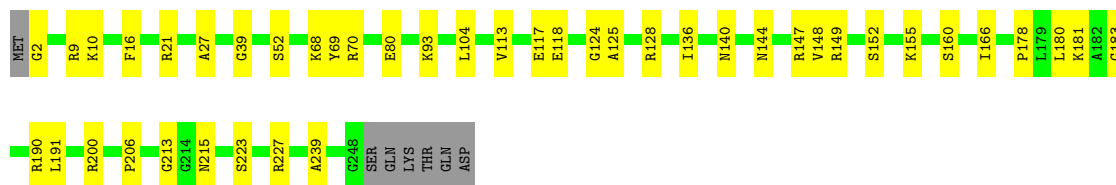






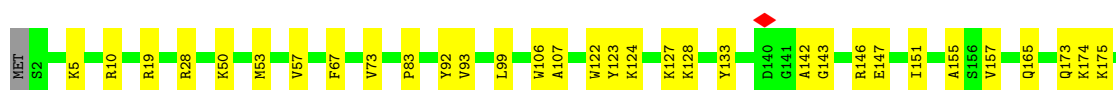
• Molecule 35: 60S ribosomal protein L2-A

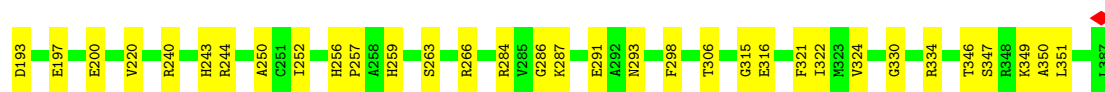
Chain AA: 80% 17%



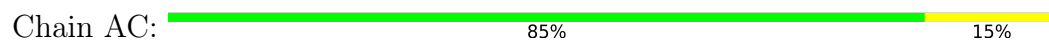
• Molecule 36: 60S ribosomal protein L3

Chain AB: 83% 17%

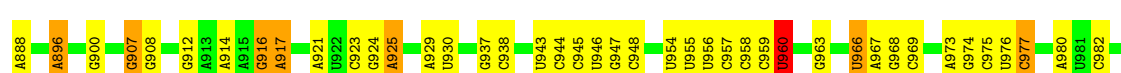
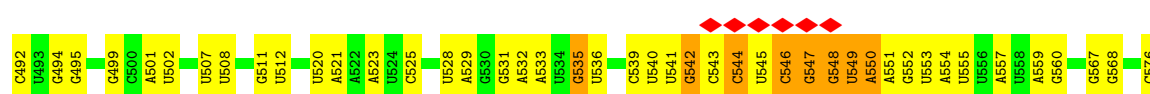
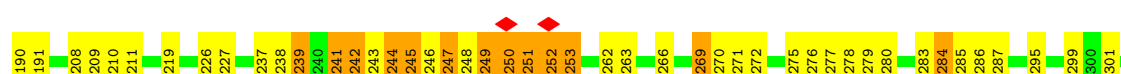
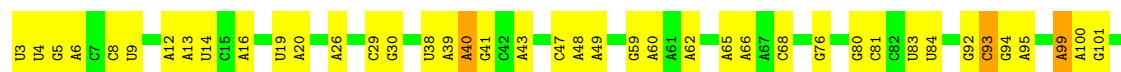




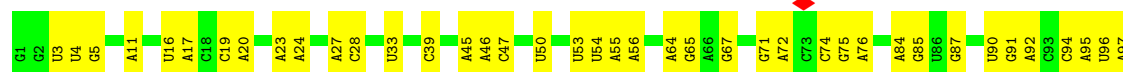
• Molecule 37: RPL4A isoform 1

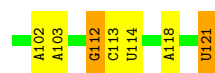


• Molecule 38: 25S rRNA

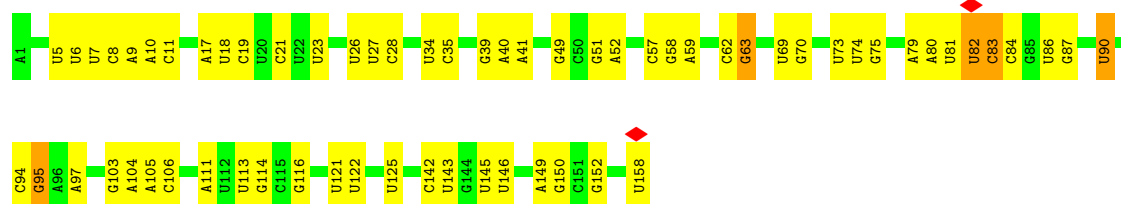




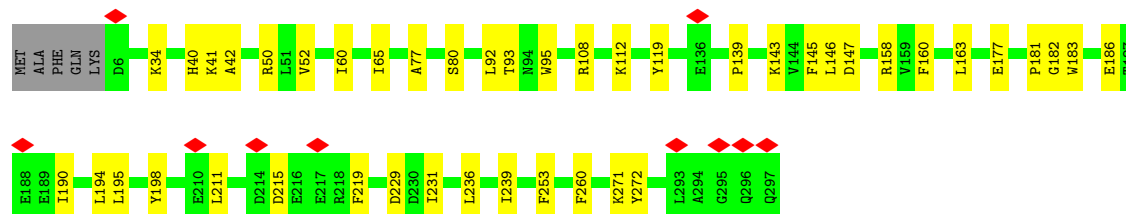
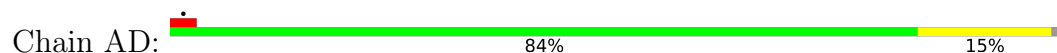




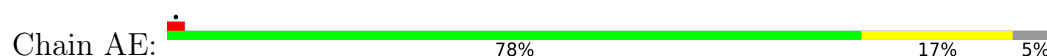
- Molecule 40: 5.8 S rRNA



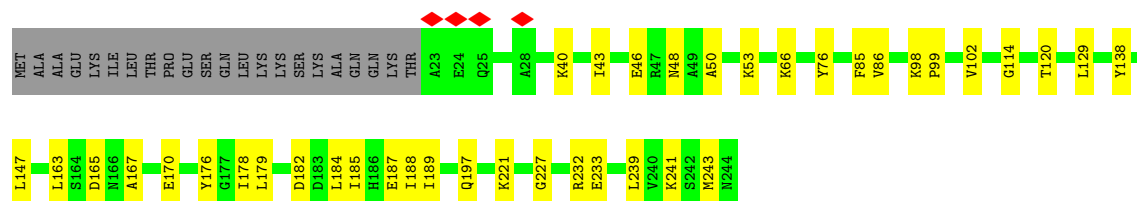
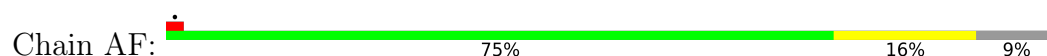
- Molecule 41: RPL5 isoform 1



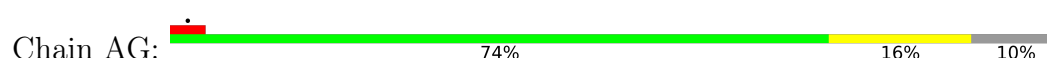
- Molecule 42: 60S ribosomal protein L6-A

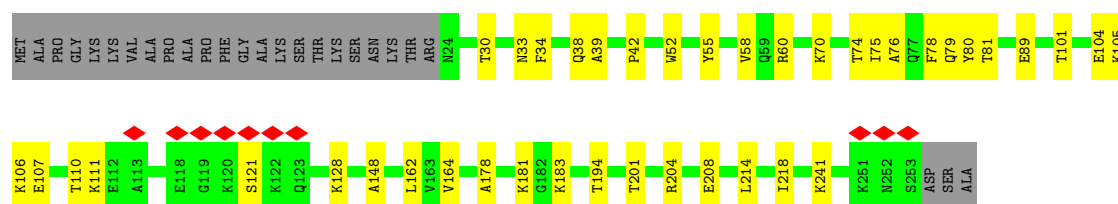


- Molecule 43: 60S ribosomal protein L7-A

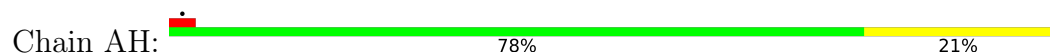


- Molecule 44: 60S ribosomal protein L8-A

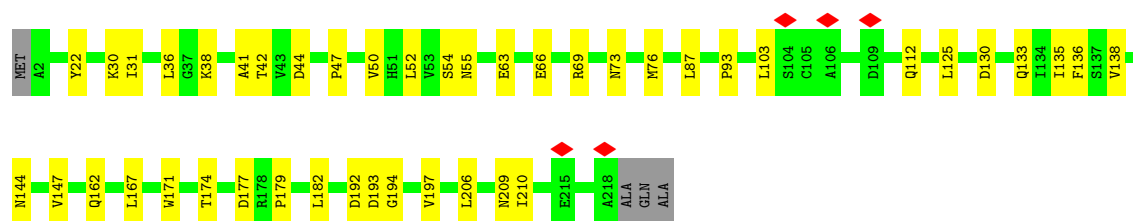
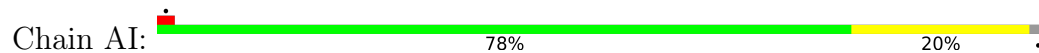




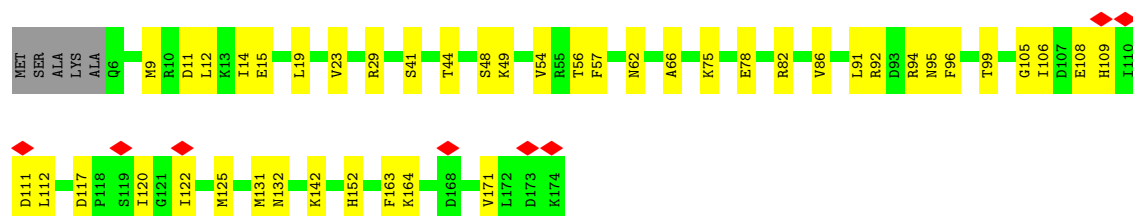
- Molecule 45: 60S ribosomal protein L9-A



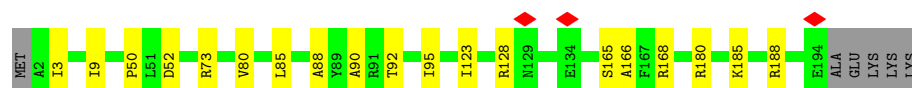
- Molecule 46: RPL10 isoform 1



- Molecule 47: RPL11A isoform 1

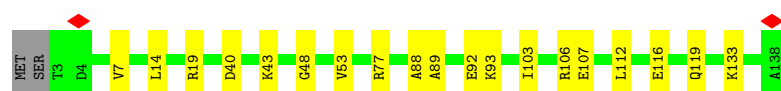


- Molecule 48: 60S ribosomal protein L13-A



- Molecule 49: 60S ribosomal protein L14-A

Chain AM:  85% 14%



- Molecule 50: 60S ribosomal protein L15-A

Chain AN:  87% 13%



- Molecule 51: 60S ribosomal protein L16-A

Chain AO:  84% 15%



- Molecule 52: 60S ribosomal protein L17-A

Chain AP:  86% 9% 5%



- Molecule 53: 60S ribosomal protein L18-A

Chain AQ:  85% 14%



- Molecule 54: 60S ribosomal protein L19-A

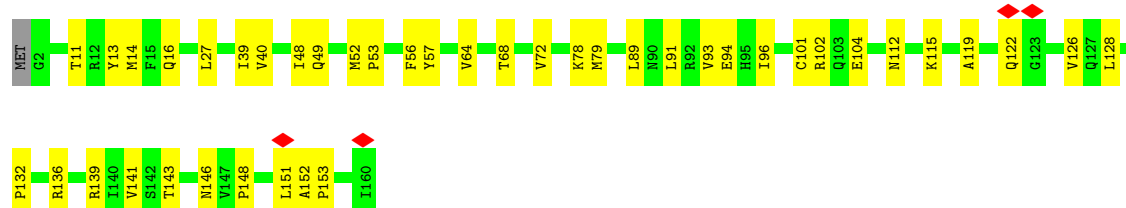
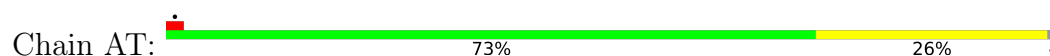
Chain AR:  11% 82% 17%



- Molecule 55: 60S ribosomal protein L20

Chain AS:  79% 18%

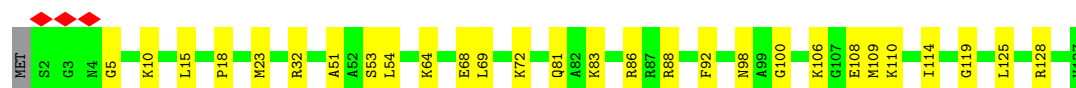
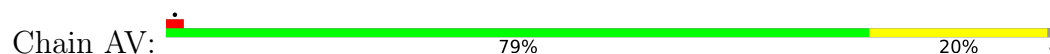
- Molecule 56: 60S ribosomal protein L21-A



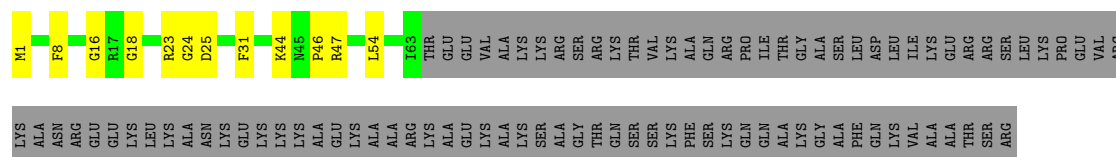
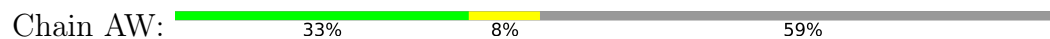
- Molecule 57: 60S ribosomal protein L22-A



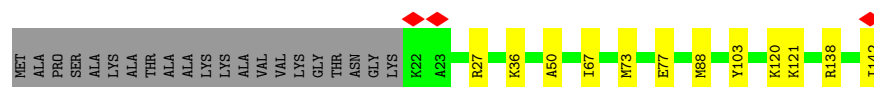
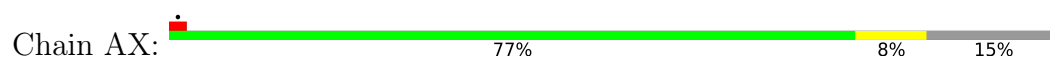
- Molecule 58: 60S ribosomal protein L23-A



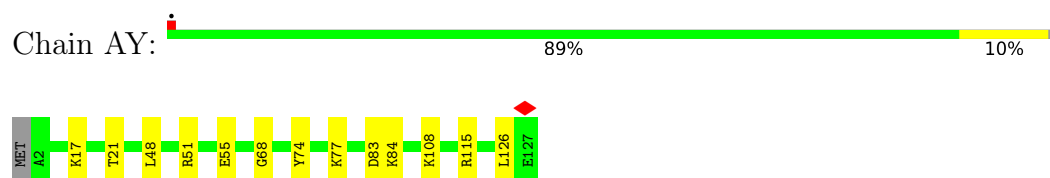
- Molecule 59: RPL24A isoform 1



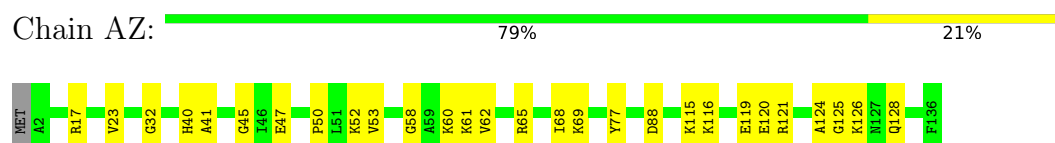
- Molecule 60: 60S ribosomal protein L25



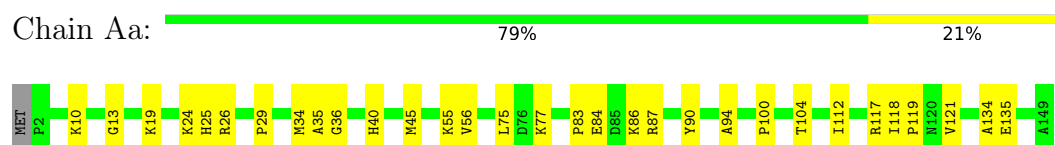
- Molecule 61: 60S ribosomal protein L26-A



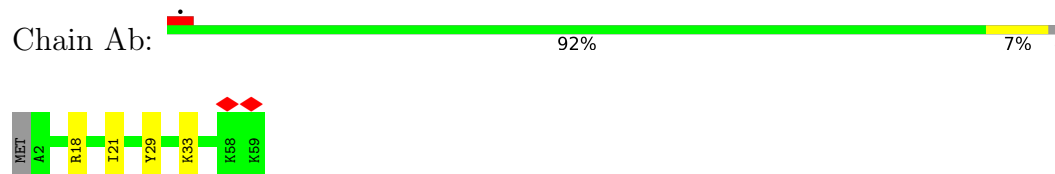
- Molecule 62: 60S ribosomal protein L27-A



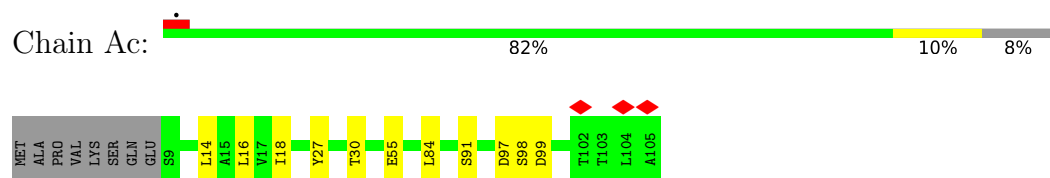
- Molecule 63: 60S ribosomal protein L28



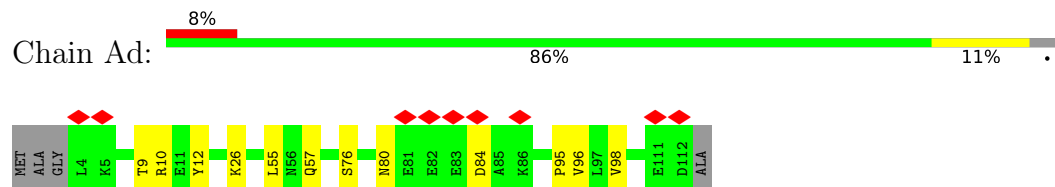
- Molecule 64: RPL29 isoform 1



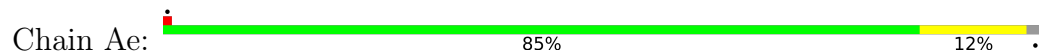
- Molecule 65: 60S ribosomal protein L30



- Molecule 66: 60S ribosomal protein L31-A



- Molecule 67: RPL32 isoform 1





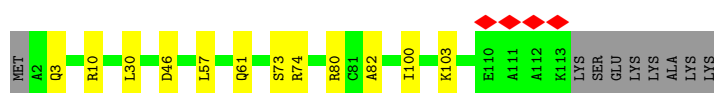
- Molecule 68: 60S ribosomal protein L33-A

Chain Af: 82% 17%



- Molecule 69: 60S ribosomal protein L34-A

Chain Ag: 83% 10% 7%



- Molecule 70: 60S ribosomal protein L35-A

Chain Ah: 86% 13%



- Molecule 71: 60S ribosomal protein L36-A

Chain Ai: 85% 14%



- Molecule 72: 60S ribosomal protein L37-A

Chain Aj: 81% 17%



- Molecule 73: RPL38 isoform 1

Chain Ak: 8% 79% 19%



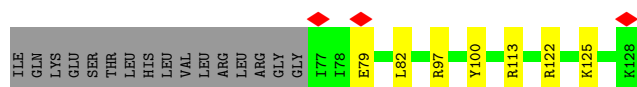
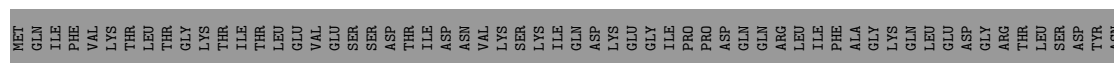
- Molecule 74: 60S ribosomal protein L39

Chain Al:  76% 22% .



- Molecule 75: Ubiquitin-60S ribosomal protein L40

Chain Am:  35% 5% 59%



- Molecule 76: 60S ribosomal protein L41-A

Chain An:  68% 32%



- Molecule 77: 60S ribosomal protein L42-A

Chain Ao:  86% 13% .

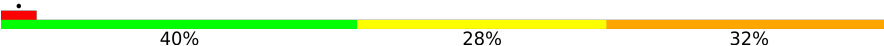


- Molecule 78: 60S ribosomal protein L43-A

Chain Ap:  84% 15% .



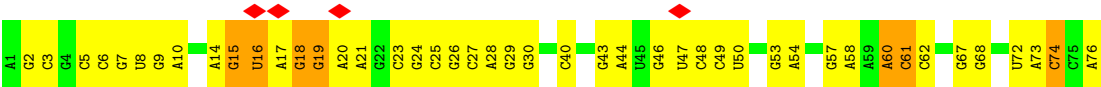
- Molecule 79: P site tRNA

Chain tP:  40% 28% 32%

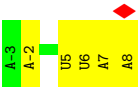


- Molecule 80: A site tRNA

Chain tA:  5% 41% 50% 9%



• Molecule 81: messenger RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	445683	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	9.938	Depositor
Minimum map value	-3.861	Depositor
Average map value	0.029	Depositor
Map value standard deviation	0.283	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, OMU, MG, 3HE, 5MC, B8N, PSU, G7M, OMG, 4AC, HIC, MA6, 1MA, UR3, SPD

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	BA	0.16	0/1653	0.38	0/2261
2	BB	0.17	0/1735	0.46	0/2335
3	BC	0.16	0/1665	0.32	0/2263
4	BE	0.15	0/2109	0.37	0/2839
5	BG	0.15	0/1844	0.37	0/2464
6	BH	0.19	0/1506	0.47	0/2028
7	BI	0.16	0/1514	0.41	0/2021
8	BJ	0.16	0/1519	0.37	0/2035
9	BL	0.15	0/1272	0.31	0/1712
10	BN	0.17	0/1215	0.41	0/1638
11	BO	0.19	0/952	0.51	0/1279
12	BV	0.17	0/693	0.40	0/935
13	BW	0.18	0/1038	0.38	0/1395
14	BX	0.17	0/1139	0.35	0/1518
15	BY	0.17	0/1087	0.39	0/1449
16	Ba	0.19	0/782	0.46	0/1047
17	Bb	0.14	0/620	0.35	0/838
18	Be	0.14	0/483	0.35	0/643
19	BD	0.16	0/1759	0.39	0/2368
20	BF	0.14	0/1629	0.35	0/2202
21	BK	0.19	0/837	0.57	2/1131 (0.2%)
22	BP	0.14	0/1012	0.38	0/1356
23	BQ	0.17	0/1125	0.41	0/1510
24	BR	0.14	0/957	0.35	0/1283
25	BS	0.14	0/1211	0.37	0/1628
26	BT	0.17	0/1113	0.44	0/1494
27	BU	0.16	0/865	0.42	0/1169
28	BZ	0.18	0/571	0.45	0/768
29	Bc	0.17	0/499	0.42	0/670
30	Bd	0.16	0/452	0.57	2/600 (0.3%)
31	Bg	0.14	0/2454	0.39	0/3340
32	Bf	0.10	0/616	0.29	0/817

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BM	0.14	0/943	0.41	0/1274
34	B5	0.16	1/42034 (0.0%)	0.30	0/65493
35	AA	0.19	0/1912	0.41	0/2569
36	AB	0.18	0/3139	0.38	0/4219
37	AC	0.18	0/2800	0.39	0/3790
38	A1	0.21	0/74791	0.32	0/116610
39	A3	0.17	0/2861	0.25	0/4457
40	A4	0.22	0/3724	0.33	0/5798
41	AD	0.15	0/2390	0.35	0/3225
42	AE	0.16	0/1324	0.37	0/1782
43	AF	0.19	0/1821	0.38	0/2451
44	AG	0.18	0/1830	0.39	0/2469
45	AH	0.17	0/1531	0.36	0/2062
46	AI	0.17	0/1796	0.38	0/2409
47	AJ	0.18	0/1374	0.45	0/1842
48	AL	0.17	0/1568	0.35	0/2106
49	AM	0.17	0/1068	0.34	0/1438
50	AN	0.20	0/1757	0.39	0/2354
51	AO	0.20	0/1585	0.42	0/2128
52	AP	0.19	0/1410	0.39	0/1893
53	AQ	0.17	0/1465	0.33	0/1965
54	AR	0.17	0/1538	0.34	0/2050
55	AS	0.19	0/1481	0.40	0/1990
56	AT	0.18	0/1300	0.37	0/1743
57	AU	0.14	0/812	0.30	0/1099
58	AV	0.18	0/1018	0.38	0/1369
59	AW	0.16	0/533	0.33	0/707
60	AX	0.17	0/983	0.36	0/1325
61	AY	0.19	0/1004	0.34	0/1341
62	AZ	0.17	0/1118	0.35	0/1497
63	Aa	0.18	0/1204	0.38	0/1612
64	Ab	0.17	0/473	0.35	0/629
65	Ac	0.17	0/751	0.34	0/1008
66	Ad	0.17	0/904	0.34	0/1213
67	Ae	0.17	0/1041	0.35	0/1394
68	Af	0.19	0/868	0.38	0/1168
69	Ag	0.17	0/890	0.36	0/1189
70	Ah	0.17	0/978	0.34	0/1301
71	Ai	0.17	0/778	0.36	0/1034
72	Aj	0.23	0/696	0.43	1/923 (0.1%)
73	Ak	0.17	0/618	0.38	0/826
74	Al	0.18	0/443	0.36	0/588
75	Am	0.16	0/423	0.35	0/562

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	An	0.20	0/234	0.47	0/300
77	Ao	0.17	0/860	0.36	0/1136
78	Ap	0.20	0/701	0.44	0/934
79	tP	0.23	0/1796	0.48	0/2799
80	tA	0.15	0/1820	0.32	0/2836
81	MR	0.17	0/291	0.24	0/451
All	All	0.19	1/216605 (0.0%)	0.34	5/318394 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	BB	0	1
14	BX	0	1
43	AF	0	1
44	AG	0	2
62	AZ	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1575	G7M	O3'-P	5.08	1.61	1.56

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Bd	4	GLU	CA-C-N	7.54	135.26	121.70
30	Bd	4	GLU	C-N-CA	7.54	135.26	121.70
21	BK	89	GLY	CA-C-N	5.80	132.14	121.70
21	BK	89	GLY	C-N-CA	5.80	132.14	121.70
72	Aj	25	ARG	CB-CG-CD	5.05	122.91	111.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
43	AF	232	ARG	Peptide
44	AG	121	SER	Peptide

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Mol	Chain	Res	Type	Group
44	AG	30	THR	Peptide
62	AZ	124	ALA	Peptide
2	BB	177	GLN	Peptide
14	BX	88	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BA	1612	0	1623	47	0
2	BB	1709	0	1784	66	0
3	BC	1635	0	1723	28	0
4	BE	2068	0	2154	52	0
5	BG	1820	0	1918	51	0
6	BH	1481	0	1572	54	0
7	BI	1489	0	1525	45	0
8	BJ	1494	0	1573	32	0
9	BL	1244	0	1314	12	0
10	BN	1192	0	1255	27	0
11	BO	941	0	979	37	0
12	BV	684	0	672	24	0
13	BW	1021	0	1060	24	0
14	BX	1121	0	1196	18	0
15	BY	1073	0	1132	27	0
16	Ba	769	0	818	28	0
17	Bb	610	0	633	16	0
18	Be	475	0	525	7	0
19	BD	1734	0	1817	40	0
20	BF	1609	0	1675	30	0
21	BK	817	0	804	36	0
22	BP	991	0	1035	23	0
23	BQ	1105	0	1166	21	0
24	BR	948	0	990	23	0
25	BS	1192	0	1222	41	0
26	BT	1095	0	1114	30	0
27	BU	855	0	917	22	0
28	BZ	563	0	603	22	0
29	Bc	497	0	535	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	Bd	442	0	432	6	0
31	Bg	2401	0	2356	70	0
32	Bf	605	0	654	14	0
33	BM	935	0	975	32	0
34	B5	37987	0	19106	572	0
35	AA	1878	0	1946	33	0
36	AB	3081	0	3162	47	0
37	AC	2748	0	2859	42	0
38	A1	67564	0	33963	755	0
39	A3	2579	0	1304	33	0
40	A4	3353	0	1695	38	0
41	AD	2341	0	2290	30	0
42	AE	1303	0	1376	20	0
43	AF	1784	0	1862	24	0
44	AG	1798	0	1894	25	0
45	AH	1510	0	1576	31	0
46	AI	1759	0	1799	28	0
47	AJ	1353	0	1383	36	0
48	AL	1543	0	1608	15	0
49	AM	1053	0	1149	13	0
50	AN	1720	0	1779	21	0
51	AO	1555	0	1659	19	0
52	AP	1388	0	1423	11	0
53	AQ	1441	0	1543	18	0
54	AR	1521	0	1617	28	0
55	AS	1445	0	1487	21	0
56	AT	1276	0	1323	30	0
57	AU	796	0	812	13	0
58	AV	1003	0	1048	19	0
59	AW	521	0	551	9	0
60	AX	968	0	1036	9	0
61	AY	993	0	1081	14	0
62	AZ	1092	0	1155	16	0
63	Aa	1173	0	1215	27	0
64	Ab	462	0	491	4	0
65	Ac	743	0	797	8	0
66	Ad	890	0	938	7	0
67	Ae	1020	0	1090	11	0
68	Af	850	0	880	16	0
69	Ag	880	0	945	9	0
70	Ah	969	0	1078	14	0
71	Ai	771	0	849	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	Aj	681	0	687	16	0
73	Ak	612	0	682	10	0
74	Al	436	0	475	7	0
75	Am	417	0	459	7	0
76	An	233	0	283	8	0
77	Ao	847	0	914	11	0
78	Ap	694	0	738	12	0
79	tP	1606	0	816	39	0
80	tA	1627	0	827	34	0
81	MR	259	0	130	3	0
82	A1	145	0	0	0	0
82	A4	1	0	0	0	0
82	AA	1	0	0	0	0
82	AP	1	0	0	0	0
82	AV	1	0	0	0	0
82	Ae	1	0	0	0	0
82	B5	46	0	0	0	0
82	MR	1	0	0	0	0
83	A1	10	0	19	1	0
84	A1	20	0	23	0	0
85	Ao	1	0	0	0	0
All	All	202978	0	149573	2807	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 (2807) 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)
79:tP:19:G:H4'	79:tP:20:A:H5''	1.44	0.98
34:B5:1291:G:H1	34:B5:1324:G:H22	1.15	0.95
58:AV:81:GLN:O	58:AV:98:ASN:ND2	2.04	0.91
38:A1:1953:G:H1	38:A1:2093:A:N6	1.68	0.91
38:A1:3348:G:H1	38:A1:3357:U:H3	1.20	0.89
40:A4:75:G:OP2	61:AY:74:TYR:OH	1.94	0.85
13:BW:2:THR:N	34:B5:1034:C:HO2'	1.73	0.85
56:AT:39:ILE:HD12	56:AT:102:ARG:HD3	1.59	0.83
34:B5:1426:C:O2'	34:B5:1428:G:OP2	1.96	0.83
11:BO:107:ARG:NH2	16:Ba:52:ASP:OD1	2.13	0.82
38:A1:845:G:H21	38:A1:848:A:H2	1.26	0.82
5:BG:160:ARG:NH2	34:B5:68:A:OP1	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:195:TRP:HE1	1:BA:197:ILE:HG12	1.44	0.81
6:BH:150:GLN:HB3	6:BH:181:ILE:HG22	1.60	0.81
11:BO:52:ARG:HG3	34:B5:905:A:H5''	1.63	0.81
75:Am:97:ARG:HH21	75:Am:122:ARG:HB3	1.45	0.81
80:tA:10:A:H61	80:tA:25:C:H42	1.27	0.81
62:AZ:125:GLY:O	62:AZ:128:GLN:NE2	2.14	0.80
34:B5:1339:C:O2'	34:B5:1341:A:N7	2.14	0.80
6:BH:41:LEU:HB3	6:BH:70:PHE:HE1	1.46	0.79
11:BO:61:MET:HG2	11:BO:104:ALA:HB2	1.62	0.79
25:BS:41:ARG:HH11	26:BT:46:PRO:HG3	1.46	0.79
31:Bg:153:GLN:HE21	31:Bg:201:THR:HA	1.47	0.79
34:B5:1588:G:H1	34:B5:1608:U:H3	1.28	0.78
14:BX:107:PHE:HB3	14:BX:114:LYS:HE3	1.66	0.78
31:Bg:93:ASP:HB2	31:Bg:100:TYR:HE2	1.47	0.78
34:B5:1363:U:O2'	34:B5:1364:G:OP2	2.01	0.78
34:B5:1585:U:H3	34:B5:1611:A:H2	1.28	0.78
79:tP:67:G:H3'	79:tP:68:G:H5''	1.64	0.78
48:AL:3:ILE:HG21	63:Aa:45:MET:HE3	1.66	0.77
45:AH:92:TYR:HB2	45:AH:142:ASP:HB3	1.65	0.77
4:BE:87:MET:HE2	4:BE:123:LEU:HB2	1.67	0.77
38:A1:2794:G:OP1	77:Ao:61:LYS:NZ	2.17	0.77
38:A1:1661:G:H2'	38:A1:1662:G:C8	2.19	0.76
60:AX:50:ALA:HB1	70:Ah:66:VAL:HG11	1.67	0.76
38:A1:1953:G:H1	38:A1:2093:A:H61	1.33	0.76
38:A1:1010:G:N2	46:AI:193:ASP:OD2	2.19	0.76
38:A1:1192:C:N4	38:A1:1300:G:OP2	2.19	0.76
61:AY:74:TYR:HD2	61:AY:77:LYS:HG2	1.51	0.76
80:tA:14:A:H2'	80:tA:15:G:H4'	1.68	0.75
10:BN:103:GLU:O	10:BN:106:ARG:NH1	2.19	0.75
34:B5:648:G:N1	34:B5:686:C:N3	2.33	0.75
38:A1:172:G:H1	38:A1:246:U:H3	1.32	0.75
2:BB:109:LYS:HG3	2:BB:113:MET:HE1	1.69	0.74
23:BQ:13:LYS:HG3	23:BQ:14:LYS:H	1.53	0.74
61:AY:74:TYR:CD2	61:AY:77:LYS:HG2	2.22	0.74
34:B5:992:A:O2'	34:B5:1785:U:O2	2.04	0.74
79:tP:53:G:H2'	79:tP:54:A:H8	1.50	0.74
17:Bb:35:VAL:HG11	17:Bb:63:LEU:HD21	1.70	0.73
38:A1:1221:A:H3'	38:A1:1222:G:H4'	1.69	0.73
1:BA:36:TYR:OH	1:BA:56:LYS:NZ	2.21	0.73
54:AR:171:ASP:OD1	54:AR:175:GLN:NE2	2.21	0.73
6:BH:48:GLU:OE2	6:BH:88:ARG:NH2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:868:G:H1	34:B5:960:U:H3	1.34	0.72
38:A1:1940:G:H21	38:A1:3362:A:H8	1.36	0.72
4:BE:100:ARG:HH21	4:BE:118:GLU:HG2	1.53	0.72
34:B5:1672:G:H2'	34:B5:1673:G:C8	2.24	0.72
8:BJ:132:ARG:NH2	34:B5:532:U:OP1	2.22	0.72
2:BB:64:ARG:HG2	11:BO:36:LYS:HE2	1.70	0.72
31:Bg:13:LEU:HB2	31:Bg:310:ILE:HB	1.72	0.72
34:B5:871:G:H2'	34:B5:872:G:C8	2.24	0.72
50:AN:159:ARG:HB2	50:AN:164:LEU:HB2	1.72	0.71
36:AB:19:ARG:NH2	38:A1:3045:G:OP1	2.23	0.71
38:A1:3343:G:H21	38:A1:3362:A:H2	1.38	0.71
35:AA:80:GLU:HG2	78:Ap:76:ALA:HB1	1.72	0.71
44:AG:75:ILE:HD11	50:AN:18:VAL:HG23	1.71	0.71
1:BA:35:PRO:HD3	12:BV:87:ARG:HH22	1.54	0.71
28:BZ:56:THR:HA	28:BZ:103:ARG:HE	1.55	0.71
38:A1:1553:U:H4'	38:A1:1554:U:H5'	1.72	0.71
80:tA:30:G:N1	80:tA:40:C:N3	2.32	0.71
73:Ak:31:LEU:HA	73:Ak:37:PRO:HA	1.73	0.71
38:A1:1923:C:H5''	76:An:25:LYS:HE2	1.72	0.71
38:A1:2213:A:H2'	38:A1:2214:A:C8	2.26	0.70
13:BW:30:SER:HB2	13:BW:61:ILE:HG12	1.73	0.70
27:BU:101:LYS:O	27:BU:105:GLN:NE2	2.24	0.70
37:AC:114:ASN:HB2	37:AC:117:GLU:HG3	1.72	0.70
38:A1:499:G:H5''	68:Af:48:ARG:HH12	1.56	0.70
15:BY:37:LYS:HG3	34:B5:522:U:H5''	1.73	0.70
40:A4:49:G:OP2	70:Ah:48:ARG:NH2	2.23	0.70
17:Bb:51:GLN:OE1	34:B5:957:G:N2	2.25	0.70
55:AS:14:LEU:HD12	55:AS:15:PRO:HD2	1.73	0.70
58:AV:10:LYS:HD3	58:AV:125:LEU:HD11	1.72	0.70
1:BA:30:GLN:HE21	1:BA:33:GLN:HG2	1.56	0.70
22:BP:98:ASN:ND2	22:BP:121:ILE:O	2.23	0.70
49:AM:48:GLY:HA3	49:AM:53:VAL:HB	1.72	0.70
38:A1:576:C:OP1	43:AF:241:LYS:NZ	2.24	0.70
38:A1:1831:U:O2'	40:A4:114:G:OP1	2.10	0.70
45:AH:21:LYS:HG3	45:AH:22:SER:H	1.56	0.69
34:B5:1003:A:O2'	34:B5:1005:A:N7	2.24	0.69
37:AC:20:LEU:HD11	37:AC:252:GLU:HG3	1.73	0.69
38:A1:176:G:C2	38:A1:177:U:H1'	2.26	0.69
34:B5:1474:G:H2'	34:B5:1475:A:H8	1.57	0.69
38:A1:1228:C:N4	38:A1:1282:G:O6	2.26	0.69
38:A1:3275:U:O2'	68:Af:99:ARG:NH1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BR:23:LYS:HA	31:Bg:198:ASN:HD21	1.57	0.69
2:BB:217:LEU:HD21	2:BB:220:GLN:HG3	1.75	0.69
4:BE:151:ASP:HB3	4:BE:154:ILE:HG13	1.75	0.69
6:BH:104:ARG:NH1	34:B5:803:A:N3	2.39	0.69
13:BW:81:VAL:O	13:BW:122:SER:OG	2.11	0.69
19:BD:204:ASP:HB2	24:BR:8:THR:HG21	1.75	0.69
21:BK:52:LYS:HE3	34:B5:1220:C:H5''	1.75	0.69
34:B5:1171:A:H2'	34:B5:1172:G:C8	2.27	0.69
36:AB:28:ARG:NH2	38:A1:3140:G:N7	2.40	0.69
34:B5:733:A:OP2	34:B5:735:C:N4	2.26	0.68
47:AJ:41:SER:O	47:AJ:75:LYS:NZ	2.22	0.68
69:Ag:46:ASP:OD1	69:Ag:80:ARG:NH1	2.25	0.68
56:AT:79:MET:HE1	64:Ab:21:ILE:HD12	1.74	0.68
1:BA:55:GLU:HG2	12:BV:79:LEU:HD22	1.74	0.68
21:BK:23:ALA:O	21:BK:64:TYR:HB2	1.94	0.68
19:BD:40:ARG:HG2	27:BU:110:PRO:HB3	1.76	0.68
28:BZ:99:ALA:HB1	28:BZ:101:TYR:HE1	1.59	0.68
38:A1:1717:U:H2'	38:A1:1718:G:C8	2.29	0.68
55:AS:77:VAL:HG11	55:AS:106:LEU:HD22	1.75	0.68
71:Ai:4:LYS:O	71:Ai:16:LYS:NZ	2.26	0.68
13:BW:57:ARG:HG2	34:B5:862:A:H4'	1.76	0.68
25:BS:75:ASN:HB3	25:BS:78:HIS:HD2	1.59	0.68
1:BA:195:TRP:NE1	1:BA:197:ILE:HG12	2.08	0.67
34:B5:1344:A:O2'	34:B5:1345:A:O4'	2.12	0.67
11:BO:80:HIS:HA	11:BO:113:GLY:O	1.95	0.67
31:Bg:172:ALA:HB2	31:Bg:202:LEU:HD23	1.75	0.67
35:AA:27:ALA:O	35:AA:128:ARG:NH2	2.21	0.67
38:A1:266:A:OP1	50:AN:5:LYS:NZ	2.26	0.67
2:BB:155:TYR:OH	34:B5:932:U:OP2	2.11	0.67
8:BJ:110:GLN:OE1	8:BJ:126:ARG:NH1	2.27	0.67
21:BK:10:LYS:NZ	21:BK:36:ASP:HB3	2.09	0.67
34:B5:511:A:N6	34:B5:539:G:O6	2.27	0.67
45:AH:90:MET:HE2	45:AH:179:ILE:HG22	1.77	0.67
50:AN:183:THR:HG22	50:AN:187:ARG:HB3	1.77	0.67
4:BE:191:ARG:HD3	4:BE:245:LYS:HE2	1.77	0.67
5:BG:180:THR:HG23	5:BG:183:ARG:H	1.58	0.67
37:AC:303:GLY:H	38:A1:1347:U:H5''	1.59	0.67
44:AG:101:THR:OG1	44:AG:104:GLU:OE1	2.13	0.67
33:BM:63:VAL:HG22	33:BM:65:SER:H	1.60	0.67
35:AA:80:GLU:HG2	78:Ap:76:ALA:CB	2.25	0.67
38:A1:664:U:H2'	38:A1:665:A:C8	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BS:139:LYS:NZ	34:B5:1179:G:O6	2.28	0.66
34:B5:65:A:H2	34:B5:84:A:H62	1.43	0.66
31:Bg:270:LEU:HD11	31:Bg:273:ASP:HB2	1.77	0.66
12:BV:79:LEU:HD13	12:BV:82:VAL:HG21	1.77	0.66
33:BM:133:LEU:HG	33:BM:137:MET:HE1	1.77	0.66
4:BE:108:ARG:NH2	34:B5:788:A:OP2	2.29	0.66
31:Bg:278:PHE:HE1	31:Bg:311:ARG:HH12	1.43	0.66
38:A1:1845:G:H5'	72:Aj:11:ARG:NH2	2.10	0.66
55:AS:22:PRO:O	56:AT:146:ASN:ND2	2.28	0.66
34:B5:1474:G:H2'	34:B5:1475:A:C8	2.30	0.66
38:A1:3016:A:H2'	38:A1:3017:A:C8	2.30	0.66
5:BG:72:ARG:NH2	34:B5:418:G:O2'	2.28	0.66
34:B5:1357:A:H2'	34:B5:1358:G:C8	2.30	0.66
1:BA:190:ASP:HB2	1:BA:193:GLN:HB2	1.77	0.65
25:BS:35:ILE:HG23	25:BS:102:ALA:HB2	1.78	0.65
23:BQ:35:PRO:HG2	23:BQ:38:LEU:HD23	1.78	0.65
33:BM:44:GLY:O	33:BM:48:SER:OG	2.07	0.65
38:A1:3092:C:O2'	38:A1:3094:A:OP2	2.13	0.65
2:BB:164:ILE:O	2:BB:168:ILE:HG12	1.97	0.65
7:BI:162:ALA:O	38:A1:3352:U:O2'	2.14	0.65
10:BN:46:THR:H	10:BN:49:GLN:HE21	1.42	0.65
10:BN:64:ARG:NH2	34:B5:861:U:OP1	2.28	0.65
34:B5:12:U:H2'	34:B5:13:C:C6	2.32	0.65
34:B5:1413:U:O2'	34:B5:1416:G:OP1	2.14	0.65
38:A1:1222:G:H2'	38:A1:1286:A:H61	1.60	0.65
5:BG:66:GLY:HA2	34:B5:1681:A:H1'	1.79	0.65
8:BJ:109:LEU:HB2	8:BJ:146:PHE:HB3	1.78	0.65
3:BC:88:LYS:HD3	3:BC:95:ARG:HH21	1.61	0.65
6:BH:30:SER:OG	6:BH:33:GLU:HB3	1.94	0.65
36:AB:244:ARG:NH1	38:A1:2948:C:OP1	2.29	0.65
38:A1:1560:G:H1	38:A1:1579:C:H42	1.43	0.65
3:BC:91:ARG:NH1	34:B5:1147:A:OP1	2.29	0.65
14:BX:72:VAL:HG11	14:BX:96:VAL:HG11	1.78	0.65
34:B5:1727:G:H2'	34:B5:1728:A:C8	2.31	0.65
2:BB:122:GLU:OE2	2:BB:213:ARG:NH2	2.29	0.65
25:BS:14:ILE:HD11	25:BS:21:ASN:HB3	1.79	0.65
34:B5:1692:G:H5''	34:B5:1693:A:N7	2.12	0.65
38:A1:446:U:O2	38:A1:488:U:N3	2.30	0.65
68:Af:31:LYS:NZ	68:Af:78:SER:O	2.30	0.65
6:BH:49:ILE:HD11	6:BH:172:VAL:HG12	1.78	0.65
44:AG:78:PHE:O	44:AG:79:GLN:HG3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BX:74:VAL:HG21	14:BX:104:LEU:HD11	1.79	0.65
47:AJ:19:LEU:HD23	47:AJ:125:MET:HE1	1.77	0.65
11:BO:81:VAL:HB	11:BO:115:ILE:HG22	1.78	0.65
34:B5:851:U:O2	34:B5:852:C:N4	2.30	0.64
38:A1:1724:U:H1'	38:A1:1725:C:C6	2.33	0.64
48:AL:123:ILE:HD11	70:Ah:116:TYR:HD2	1.63	0.64
20:BF:95:ASN:HA	20:BF:98:MET:HE2	1.79	0.64
57:AU:20:SER:OG	57:AU:61:THR:OG1	2.15	0.64
62:AZ:116:LYS:O	62:AZ:120:GLU:HG2	1.97	0.64
79:tP:66:C:H2'	79:tP:67:G:H8	1.63	0.64
2:BB:97:LEU:HB3	2:BB:232:HIS:CD2	2.33	0.64
7:BI:4:SER:OG	7:BI:6:ASP:OD1	2.13	0.64
12:BV:66:ASP:OD1	12:BV:67:ASP:N	2.29	0.64
31:Bg:238:ASP:HB2	31:Bg:257:ALA:HB3	1.79	0.64
16:Ba:3:LYS:NZ	16:Ba:8:ASN:OD1	2.29	0.64
38:A1:547:G:H4'	38:A1:548:G:H8	1.61	0.64
38:A1:2206:G:O2'	38:A1:2207:A:H5'	1.98	0.64
44:AG:178:ALA:HB2	44:AG:218:ILE:HD12	1.79	0.64
44:AG:183:LYS:HB2	44:AG:194:THR:HG23	1.79	0.64
38:A1:3233:C:H2'	38:A1:3234:A:C8	2.33	0.64
34:B5:908:U:O2	34:B5:1008:G:N2	2.30	0.64
31:Bg:243:LEU:HD22	31:Bg:252:LEU:HD21	1.78	0.64
7:BI:104:ILE:HG13	7:BI:105:ASP:H	1.63	0.64
80:tA:53:G:H2'	80:tA:54:A:C8	2.33	0.64
10:BN:99:ARG:NH2	10:BN:119:GLU:OE2	2.31	0.64
34:B5:512:A:N1	34:B5:538:A:N6	2.46	0.64
34:B5:818:C:H42	34:B5:853:G:H1	1.46	0.64
68:Af:58:GLU:HG3	68:Af:63:LYS:HZ2	1.63	0.64
1:BA:30:GLN:NE2	1:BA:151:SER:O	2.31	0.63
33:BM:119:SER:OG	34:B5:1227:A:O2'	2.14	0.63
80:tA:72:U:H2'	80:tA:73:A:H8	1.61	0.63
5:BG:136:LYS:NZ	34:B5:65:A:OP1	2.32	0.63
17:Bb:67:THR:OG1	17:Bb:70:LYS:O	2.16	0.63
29:Bc:12:VAL:HG12	29:Bc:52:ASP:H	1.63	0.63
11:BO:85:ALA:H	11:BO:119:THR:HG22	1.63	0.63
38:A1:237:G:H2'	38:A1:238:A:C8	2.33	0.63
31:Bg:205:SER:HB3	31:Bg:210:LEU:HB2	1.80	0.63
34:B5:1775:U:OP1	76:An:11:ARG:NH2	2.27	0.63
36:AB:240:ARG:NH2	38:A1:1907:C:O2	2.31	0.63
38:A1:655:C:H2'	38:A1:656:A:H8	1.64	0.63
47:AJ:49:LYS:HB3	47:AJ:62:ASN:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:AY:74:TYR:CE2	61:AY:77:LYS:HE3	2.34	0.63
22:BP:29:SER:OG	22:BP:31:GLU:OE1	2.16	0.63
38:A1:315:C:OP2	71:AI:28:TYR:OH	2.14	0.63
10:BN:3:ARG:HB3	10:BN:6:SER:HB3	1.80	0.63
13:BW:81:VAL:HG23	13:BW:85:ASP:HB2	1.80	0.63
2:BB:82:ARG:NH2	2:BB:188:LEU:O	2.28	0.63
6:BH:28:GLU:HA	6:BH:34:LEU:HD21	1.80	0.63
11:BO:103:ARG:NH1	16:BA:48:ALA:O	2.31	0.63
38:A1:1578:C:H2'	38:A1:1579:C:C6	2.33	0.63
38:A1:2767:U:O2'	77:Ao:30:ALA:O	2.15	0.63
38:A1:3348:G:O6	38:A1:3357:U:O4	2.17	0.63
69:Ag:10:ARG:HD2	74:AI:4:GLN:HE21	1.64	0.63
3:BC:139:ILE:HD13	3:BC:191:ALA:HB1	1.81	0.63
32:Bf:133:ALA:N	32:Bf:140:TYR:O	2.31	0.63
34:B5:1363:U:HO2'	34:B5:1364:G:P	2.20	0.63
51:AO:61[A]:ALA:HA	51:AO:70[A]:PRO:HD2	1.81	0.63
38:A1:1694:U:H5	38:A1:1752:A:N1	1.97	0.63
76:An:1:MET:HE2	76:An:6:ARG:HE	1.64	0.63
1:BA:107:PHE:HB3	1:BA:139:VAL:HG21	1.81	0.62
32:Bf:132:LEU:HD22	32:Bf:141:CYS:HA	1.81	0.62
38:A1:2282:U:OP1	38:A1:2973:G:O2'	2.15	0.62
38:A1:2534:G:O6	38:A1:2545:C:N4	2.32	0.62
11:BO:38:THR:HG21	34:B5:895:G:H21	1.64	0.62
34:B5:1382:A:HO2'	34:B5:1383:G:H8	1.47	0.62
40:A4:9:A:H2'	40:A4:10:A:C8	2.34	0.62
34:B5:1146:G:H2'	34:B5:1147:A:C8	2.34	0.62
4:BE:131:LEU:HD12	34:B5:251:A:H2	1.63	0.62
20:BF:58:LEU:HD12	20:BF:138:THR:HG22	1.82	0.62
36:AB:284:ARG:NH1	36:AB:293:ASN:O	2.32	0.62
38:A1:1230:G:N2	38:A1:1260:A:N3	2.46	0.62
80:tA:19:G:OP1	80:tA:60:A:N6	2.32	0.62
3:BC:185:LYS:O	3:BC:189:GLN:HG3	1.99	0.62
38:A1:1863:G:N1	38:A1:1866:C:OP2	2.26	0.62
2:BB:124:ASN:HD21	2:BB:136:ARG:HD3	1.63	0.62
6:BH:64:VAL:HB	6:BH:94:ALA:HB1	1.80	0.62
21:BK:64:TYR:OH	34:B5:1435:G:O6	2.15	0.62
31:Bg:231:MET:HG2	31:Bg:232:TYR:HD1	1.65	0.62
6:BH:22:GLN:HA	6:BH:25:VAL:HG12	1.80	0.62
34:B5:591:A:H2'	34:B5:592:A:C8	2.34	0.62
22:BP:61:ARG:NH1	22:BP:88:GLU:OE1	2.32	0.62
24:BR:59:LYS:NZ	34:B5:1392:U:OP1	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Bg:258:THR:O	31:Bg:275:ARG:NH1	2.33	0.62
36:AB:93:VAL:HG12	36:AB:155:ALA:H	1.63	0.62
41:AD:60:ILE:HB	41:AD:80:SER:HB2	1.82	0.62
46:AI:36:LEU:HD11	46:AI:69:ARG:HD3	1.80	0.62
55:AS:79:VAL:HG11	55:AS:106:LEU:HD21	1.81	0.62
6:BH:63:PRO:C	6:BH:65:PRO:HD3	2.24	0.62
12:BV:62:ARG:HH22	34:B5:1039:A:H4'	1.65	0.62
34:B5:163:G:N2	34:B5:163:G:OP2	2.29	0.62
37:AC:138:ARG:NH1	38:A1:1384:U:H5'	2.14	0.62
38:A1:2209:U:H3	38:A1:2236:G:H22	1.47	0.62
47:AJ:48:SER:HB2	47:AJ:66:ALA:HB3	1.81	0.62
80:tA:43:G:H2'	80:tA:44:A:C8	2.35	0.62
29:Bc:49:ARG:HG2	29:Bc:50:GLU:H	1.65	0.62
34:B5:1477:G:H2'	34:B5:1478:G:H8	1.65	0.62
55:AS:8:GLN:HB3	55:AS:64:ILE:HD11	1.82	0.62
62:AZ:23:VAL:HG12	62:AZ:45:GLY:HA3	1.82	0.62
27:BU:34:LEU:HD21	27:BU:89:ARG:HD3	1.82	0.61
34:B5:648:G:O6	34:B5:686:C:N4	2.32	0.61
34:B5:1354:G:H22	34:B5:1372:U:H3	1.46	0.61
38:A1:252:U:H4'	38:A1:253:A:O5'	2.00	0.61
38:A1:2509:U:H6	38:A1:2509:U:H5''	1.65	0.61
38:A1:266:A:H2'	71:AI:30:LYS:HE3	1.82	0.61
38:A1:3016:A:H2'	38:A1:3017:A:H8	1.65	0.61
1:BA:107:PHE:HB2	1:BA:135:GLU:HG2	1.81	0.61
34:B5:1776:A:H2'	34:B5:1777:G:C8	2.35	0.61
38:A1:874:U:OP2	38:A1:1907:C:O2'	2.18	0.61
38:A1:2200:U:H4'	38:A1:2418:G:H22	1.66	0.61
40:A4:94:C:OP1	72:Aj:75:LYS:NZ	2.31	0.61
5:BG:72:ARG:HH21	34:B5:419:G:H5'	1.65	0.61
34:B5:221:A:OP2	34:B5:832:U:O2'	2.16	0.61
38:A1:244:G:H3'	38:A1:245:U:H5''	1.82	0.61
38:A1:662:U:H2'	38:A1:663:C:C6	2.35	0.61
38:A1:1404:G:N2	38:A1:1407:A:OP2	2.30	0.61
38:A1:2356:A:H61	38:A1:2983:C:H5	1.49	0.61
1:BA:136:ALA:HB1	1:BA:141:ILE:HB	1.82	0.61
17:Bb:80:ARG:HD3	17:Bb:81:ARG:O	2.00	0.61
34:B5:1160:A:H2'	34:B5:1161:C:H6	1.66	0.61
1:BA:13:ASP:HA	1:BA:16:LEU:HD12	1.82	0.61
31:Bg:151:VAL:HA	31:Bg:173:GLY:HA2	1.81	0.61
41:AD:119:TYR:OH	41:AD:139:PRO:O	2.13	0.61
43:AF:48:ASN:ND2	43:AF:182:ASP:OD2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:AZ:88:ASP:HB3	62:AZ:121:ARG:HH12	1.63	0.61
10:BN:25:TRP:CD1	17:Bb:82:LYS:HZ2	2.19	0.61
11:BO:135:ARG:NH1	34:B5:1007:C:O3'	2.34	0.61
38:A1:1219:C:O2'	38:A1:1223:A:OP2	2.18	0.61
38:A1:3295:A:H2'	38:A1:3296:A:C8	2.35	0.61
40:A4:150:G:OP1	60:AX:27:ARG:NH2	2.34	0.61
44:AG:33:ASN:ND2	44:AG:38:GLN:OE1	2.32	0.61
5:BG:2:LYS:HB2	5:BG:108:VAL:HG22	1.81	0.61
7:BI:16:ALA:HB2	34:B5:354:C:H5''	1.82	0.61
25:BS:36:LYS:HB2	25:BS:102:ALA:HA	1.81	0.61
38:A1:394:G:N1	38:A1:397:A:OP2	2.34	0.61
38:A1:548:G:N2	38:A1:549:U:O4	2.32	0.61
38:A1:2573:G:OP2	62:AZ:58:GLY:N	2.26	0.61
1:BA:127:ARG:HE	1:BA:152:PRO:HD3	1.66	0.61
2:BB:149:GLN:HE21	34:B5:1066:C:H4'	1.66	0.61
37:AC:35:VAL:HG21	37:AC:244:LEU:HD21	1.83	0.61
38:A1:284:A:OP2	77:Ao:41:ARG:NH1	2.34	0.61
38:A1:945:C:H2'	38:A1:946:U:C6	2.35	0.61
38:A1:2160:G:H2'	38:A1:2161:G:H8	1.65	0.61
9:BL:148:LYS:O	9:BL:152:GLN:NE2	2.34	0.61
11:BO:72:LYS:O	11:BO:73:GLU:HG3	2.01	0.61
34:B5:648:G:N2	34:B5:686:C:O2	2.21	0.61
38:A1:567:G:H2'	38:A1:568:G:C8	2.36	0.61
15:BY:124:ARG:NH1	34:B5:151:G:O6	2.32	0.60
27:BU:24:ILE:HG22	27:BU:116:VAL:HG22	1.83	0.60
31:Bg:222:LEU:HB2	31:Bg:231:MET:SD	2.40	0.60
23:BQ:14:LYS:NZ	34:B5:1610:G:N7	2.49	0.60
31:Bg:271:VAL:HG23	31:Bg:272:ASP:H	1.66	0.60
34:B5:480:G:N1	34:B5:508:U:N3	2.49	0.60
25:BS:25:ASN:O	25:BS:57:ARG:NH2	2.34	0.60
34:B5:819:G:N7	34:B5:853:G:N2	2.49	0.60
34:B5:1776:A:H2'	34:B5:1777:G:H8	1.67	0.60
38:A1:2108:C:H1'	38:A1:3344:A:C8	2.36	0.60
38:A1:2364:G:H22	38:A1:2396:G:H1'	1.65	0.60
10:BN:5:HIS:HD2	10:BN:121:ARG:HE	1.49	0.60
20:BF:61:TYR:OH	29:Bc:52:ASP:OD2	2.15	0.60
22:BP:77:ARG:NH2	34:B5:1241:G:OP1	2.34	0.60
31:Bg:247:PRO:HD2	31:Bg:248:ASN:H	1.65	0.60
38:A1:446:U:H2'	38:A1:448:U:C4	2.35	0.60
38:A1:989:A:O2'	56:AT:104:GLU:OE1	2.18	0.60
38:A1:1667:A:H2'	38:A1:1668:G:C8	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A4:26:U:H2'	40:A4:27:U:C6	2.36	0.60
34:B5:800:U:H2'	34:B5:801:G:C8	2.36	0.60
34:B5:822:U:O4	34:B5:849:C:N4	2.34	0.60
38:A1:525:C:OP2	49:AM:77:ARG:NH2	2.34	0.60
38:A1:2426:U:H2'	38:A1:2427:U:C6	2.37	0.60
3:BC:116:LYS:HG2	3:BC:127:ALA:HB3	1.82	0.60
13:BW:114:GLU:OE1	13:BW:117:ARG:NH2	2.35	0.60
33:BM:135:MET:HA	33:BM:138:GLU:HG2	1.82	0.60
48:AL:123:ILE:HD11	70:Ah:116:TYR:CD2	2.37	0.60
38:A1:443:G:O6	38:A1:490:C:N4	2.34	0.60
38:A1:1228:C:H2'	38:A1:1229:G:C8	2.37	0.60
65:Ac:14:LEU:O	65:Ac:18:ILE:HG12	2.01	0.60
6:BH:17:GLU:HB3	6:BH:46:ILE:HG12	1.83	0.60
7:BI:76:THR:HG21	7:BI:104:ILE:HD12	1.84	0.60
31:Bg:89:LEU:HB2	31:Bg:103:PHE:HB2	1.84	0.60
35:AA:149:ARG:HG2	35:AA:155:LYS:HE3	1.84	0.60
37:AC:156:LEU:HD12	37:AC:159:ILE:HD12	1.83	0.60
38:A1:1203:A:H2'	38:A1:1204:A:C8	2.37	0.60
38:A1:3182:G:H4'	51:AO:161[A]:LYS:HG2	1.84	0.60
46:AI:206:LEU:O	46:AI:210:ILE:HG12	2.01	0.60
34:B5:800:U:H2'	34:B5:801:G:H8	1.66	0.60
34:B5:953:G:H2'	34:B5:954:G:H8	1.67	0.60
38:A1:1717:U:H2'	38:A1:1718:G:H8	1.67	0.60
38:A1:2697:A:H2'	38:A1:2698:G:C8	2.37	0.60
38:A1:2779:A:O2'	48:AL:180:ARG:NH2	2.35	0.60
50:AN:96:ARG:NH1	50:AN:104:GLU:OE1	2.35	0.60
76:An:8:LYS:HG2	76:An:12:ARG:NH1	2.17	0.60
15:BY:104:SER:H	15:BY:107:GLN:HE21	1.50	0.59
16:Ba:78:ALA:HA	16:Ba:83:ILE:HD12	1.84	0.59
7:BI:138:ASN:HD22	34:B5:187:G:H5''	1.66	0.59
18:Be:25:GLU:OE2	34:B5:540:G:N2	2.27	0.59
20:BF:145:ASP:OD2	29:Bc:45:LYS:NZ	2.34	0.59
25:BS:117:LYS:O	25:BS:120:ARG:NH1	2.34	0.59
34:B5:480:G:N2	34:B5:508:U:O2	2.35	0.59
34:B5:973:A:H4'	38:A1:848:A:H8	1.66	0.59
37:AC:150:LEU:HD23	37:AC:249:ILE:HG12	1.84	0.59
38:A1:775:A:O2'	38:A1:777:U:OP2	2.19	0.59
38:A1:2768:U:H2'	38:A1:2769:A:H8	1.67	0.59
14:BX:6:PRO:HG3	14:BX:14:LYS:HG2	1.84	0.59
38:A1:401:U:H5''	38:A1:402:A:H5''	1.82	0.59
38:A1:2631:U:OP1	38:A1:2757:U:O2'	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2767:U:H2'	38:A1:2768:U:C6	2.37	0.59
42:AE:108:LYS:O	42:AE:109:GLU:HG3	2.01	0.59
47:AJ:108:GLU:OE1	47:AJ:122:ILE:HG13	2.02	0.59
34:B5:1340:U:C2	34:B5:1378:U:H4'	2.37	0.59
38:A1:718:G:OP1	63:Aa:117:ARG:NH2	2.34	0.59
2:BB:134:VAL:HG13	2:BB:218:LEU:HB2	1.83	0.59
34:B5:816:G:OP2	54:AR:166:ASN:ND2	2.35	0.59
38:A1:3204:C:H2'	38:A1:3205:G:C8	2.37	0.59
4:BE:176:ASP:OD1	4:BE:177:ALA:N	2.35	0.59
27:BU:54:GLY:H	34:B5:1345:A:P	2.25	0.59
34:B5:1220:C:H2'	34:B5:1221:A:H8	1.68	0.59
34:B5:1591:C:H2'	34:B5:1592:A:C8	2.37	0.59
38:A1:123:A:OP1	44:AG:105:LYS:NZ	2.29	0.59
80:tA:60:A:N3	80:tA:60:A:H5''	2.17	0.59
6:BH:9:LEU:HD11	6:BH:17:GLU:HG3	1.84	0.59
6:BH:44:LYS:HE3	6:BH:63:PRO:HB3	1.83	0.59
11:BO:64:ALA:HB3	11:BO:104:ALA:HB3	1.84	0.59
79:tP:65:G:H2'	79:tP:66:C:H6	1.66	0.59
79:tP:66:C:H2'	79:tP:67:G:C8	2.37	0.59
34:B5:58:U:O2'	34:B5:451:A:N3	2.36	0.59
34:B5:909:U:H2'	34:B5:910:C:C6	2.38	0.59
34:B5:1477:G:H2'	34:B5:1478:G:C8	2.37	0.59
34:B5:1533:C:H4'	34:B5:1539:G:C6	2.37	0.59
34:B5:1591:C:H2'	34:B5:1592:A:H8	1.66	0.59
38:A1:307:A:H2'	38:A1:308:A:C8	2.38	0.59
54:AR:170:ARG:HH21	54:AR:173:ARG:HH21	1.51	0.59
6:BH:51:VAL:HG23	6:BH:53:GLY:H	1.67	0.59
20:BF:92:ARG:NH2	34:B5:1613:U:OP1	2.34	0.59
34:B5:138:A:H62	34:B5:266:A:H61	1.50	0.59
34:B5:1471:A:H2	34:B5:1474:G:N3	2.00	0.59
34:B5:1524:A:H2'	34:B5:1525:A:C8	2.37	0.59
38:A1:428:A:H2'	38:A1:429:U:C6	2.38	0.59
38:A1:2406:C:H2'	38:A1:2407:C:C6	2.38	0.59
65:Ac:30:THR:HG23	65:Ac:91:SER:HB2	1.85	0.59
1:BA:139:VAL:HG23	1:BA:141:ILE:HG12	1.84	0.59
26:BT:29:GLU:OE1	26:BT:29:GLU:N	2.36	0.59
36:AB:220:VAL:O	36:AB:334:ARG:NH1	2.35	0.59
38:A1:655:C:H2'	38:A1:656:A:C8	2.38	0.59
38:A1:2206:G:H1	38:A1:2237:C:H42	1.51	0.59
34:B5:1236:A:H2'	34:B5:1237:G:H8	1.68	0.58
38:A1:1555:U:H5'	38:A1:1556:C:OP2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AP:67:ILE:HD11	52:AP:80:LYS:HB3	1.85	0.58
80:tA:58:A:H2	80:tA:60:A:H2'	1.68	0.58
17:Bb:11:THR:HG22	17:Bb:13:ALA:H	1.69	0.58
19:BD:54:ARG:HB3	19:BD:57:ASP:HB2	1.85	0.58
20:BF:183:ALA:HB2	20:BF:193:THR:HG21	1.84	0.58
38:A1:2767:U:OP1	77:Ao:34:SER:HB3	2.03	0.58
38:A1:2433:U:H1'	50:AN:125:SER:HB3	1.85	0.58
40:A4:142:C:H2'	40:A4:143:U:C6	2.38	0.58
45:AH:57:VAL:HG23	45:AH:68:LEU:HD13	1.84	0.58
55:AS:90:MET:HE1	55:AS:114:HIS:CE1	2.38	0.58
61:AY:83:ASP:O	61:AY:84:LYS:HG2	2.03	0.58
42:AE:102:ASN:ND2	42:AE:104:GLU:OE2	2.36	0.58
35:AA:227:ARG:HG2	35:AA:239:ALA:HB2	1.83	0.58
38:A1:2720:G:OP1	53:AQ:180:ARG:NH2	2.36	0.58
38:A1:2960:C:H2'	38:A1:2961:G:C8	2.38	0.58
38:A1:3192:U:H2'	38:A1:3193:C:C6	2.39	0.58
27:BU:82:TYR:HB3	30:Bd:52:PHE:HB3	1.84	0.58
34:B5:1689:A:H2'	34:B5:1690:G:H8	1.69	0.58
37:AC:46:LYS:NZ	38:A1:691:A:OP1	2.36	0.58
43:AF:40:LYS:HZ3	43:AF:179:LEU:HB3	1.68	0.58
7:BI:178:ARG:NH1	34:B5:258:C:O2	2.37	0.58
34:B5:181:A:H2'	34:B5:182:A:C8	2.39	0.58
34:B5:1039:A:HO2'	34:B5:1040:G:H8	1.51	0.58
14:BX:53:VAL:HA	14:BX:74:VAL:HG12	1.86	0.58
31:Bg:240:VAL:HG12	31:Bg:256:THR:HA	1.84	0.58
5:BG:202:ARG:NH1	34:B5:127:G:N7	2.49	0.58
10:BN:11:ILE:HD11	34:B5:1072:C:H4'	1.86	0.58
10:BN:11:ILE:HG13	10:BN:12:SER:H	1.68	0.58
10:BN:127:ARG:O	10:BN:131:THR:HG23	2.04	0.58
50:AN:9:GLU:HG3	71:Ai:44:VAL:HG11	1.86	0.58
38:A1:129:U:H2'	38:A1:130:A:C8	2.39	0.58
15:BY:29:HIS:HB2	15:BY:32:ARG:HB3	1.86	0.57
34:B5:29:U:H2'	34:B5:30:G:H8	1.69	0.57
38:A1:1110:PSU:H2'	38:A1:1111:U:C6	2.39	0.57
54:AR:175:GLN:HG2	54:AR:176:ARG:HD2	1.84	0.57
80:tA:58:A:C2	80:tA:60:A:H2'	2.39	0.57
34:B5:647:G:H22	34:B5:687:G:H1	1.50	0.57
34:B5:884:A:H2'	34:B5:885:G:H8	1.69	0.57
34:B5:895:G:H1	34:B5:917:U:H3	1.52	0.57
34:B5:1160:A:H2'	34:B5:1161:C:C6	2.39	0.57
38:A1:651:G:O2'	38:A1:1435:A:OP1	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1579:C:H2'	38:A1:1580:A:O4'	2.03	0.57
38:A1:2684:C:H1'	47:AJ:99:THR:HG21	1.86	0.57
43:AF:167:ALA:HA	43:AF:170:GLU:HG2	1.85	0.57
54:AR:105:LEU:HD23	54:AR:138:LEU:HD23	1.86	0.57
68:Af:14:LEU:HD11	68:Af:31:LYS:HB2	1.85	0.57
79:tP:10:A:H61	79:tP:25:C:H42	1.51	0.57
7:BI:98:LYS:HB3	34:B5:329:G:H5''	1.86	0.57
17:Bb:15:GLU:O	17:Bb:29:ARG:NH2	2.37	0.57
33:BM:135:MET:O	33:BM:139:HIS:ND1	2.36	0.57
34:B5:1357:A:H2'	34:B5:1358:G:H8	1.69	0.57
34:B5:1641:C:H2'	34:B5:1642:G:C8	2.39	0.57
38:A1:649:A:OP2	38:A1:2868:U:O2'	2.23	0.57
38:A1:2228:A:H2'	38:A1:2229:A:C8	2.40	0.57
42:AE:154:LEU:HD12	49:AM:119:GLN:HG2	1.86	0.57
62:AZ:53:VAL:HG21	62:AZ:62:VAL:HG23	1.86	0.57
2:BB:176:VAL:O	2:BB:177:GLN:HG2	2.05	0.57
27:BU:97:VAL:HA	27:BU:100:VAL:HG22	1.87	0.57
34:B5:1290:PSU:H2'	34:B5:1291:G:C8	2.39	0.57
38:A1:110:G:OP2	48:AL:73:ARG:NH2	2.32	0.57
38:A1:1845:G:H5'	72:Aj:11:ARG:HH21	1.67	0.57
38:A1:2369:G:H2'	38:A1:2370:G:C8	2.39	0.57
26:BT:117:SER:OG	26:BT:123:ARG:N	2.38	0.57
27:BU:20:ILE:HD11	27:BU:97:VAL:HG22	1.86	0.57
35:AA:178:PRO:HG2	78:Ap:26:VAL:HG23	1.87	0.57
60:AX:103:TYR:O	60:AX:138:ARG:NH2	2.37	0.57
73:Ak:14:LEU:HD21	73:Ak:52:TYR:CG	2.39	0.57
11:BO:71:CYS:SG	11:BO:76:ILE:HB	2.45	0.57
33:BM:106:ILE:HG23	33:BM:110:GLY:HA2	1.86	0.57
38:A1:1873:U:OP1	54:AR:21:LYS:NZ	2.37	0.57
38:A1:3271:G:C2	42:AE:108:LYS:HG3	2.40	0.57
5:BG:174:LYS:HG3	34:B5:78:A:H2	1.70	0.57
35:AA:117:GLU:HG2	35:AA:124:GLY:H	1.69	0.57
38:A1:40:A:H5''	63:Aa:35:ALA:HB1	1.85	0.57
38:A1:309:U:H5	38:A1:2780:A:N1	2.03	0.57
78:Ap:46:THR:OG1	78:Ap:57:CYS:SG	2.60	0.57
20:BF:146:THR:OG1	20:BF:157:ARG:NH2	2.38	0.57
22:BP:28:MET:SD	22:BP:29:SER:N	2.78	0.57
27:BU:19:ILE:CG2	27:BU:94:GLU:HB2	2.34	0.57
34:B5:520:A:H2'	34:B5:521:A:C8	2.40	0.57
43:AF:50:ALA:HA	43:AF:53:LYS:HE3	1.87	0.57
79:tP:9:G:H5''	79:tP:46:G:H1'	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:95:ARG:HH12	3:BC:97:ARG:NE	2.02	0.57
4:BE:92:LEU:HD23	15:BY:17:LEU:HD21	1.87	0.57
5:BG:188:ARG:NH2	34:B5:284:G:O6	2.38	0.57
8:BJ:120:LYS:HD3	34:B5:479:C:H4'	1.87	0.57
21:BK:44:LYS:HE2	34:B5:1217:A:H5''	1.86	0.57
26:BT:76:LEU:HD12	26:BT:80:TYR:HE2	1.70	0.57
34:B5:924:A:H2'	34:B5:925:G:C8	2.39	0.57
38:A1:2961:G:H2'	38:A1:2962:U:C6	2.40	0.57
39:A3:112:G:H2'	39:A3:113:C:C6	2.40	0.57
69:Ag:74:ARG:NH2	69:Ag:82:ALA:HB2	2.20	0.57
23:BQ:113:ASP:HB3	23:BQ:116:LEU:HD23	1.85	0.57
31:Bg:201:THR:HB	31:Bg:214:ALA:HB3	1.85	0.57
34:B5:894:U:H2'	34:B5:895:G:C8	2.39	0.57
34:B5:895:G:H2'	34:B5:896:U:C6	2.40	0.57
38:A1:656:A:H2'	38:A1:657:A:C8	2.39	0.57
38:A1:1799:A:H2'	38:A1:1800:A:C8	2.40	0.57
4:BE:157:ASN:ND2	4:BE:222:LEU:HD21	2.20	0.56
19:BD:23:GLU:HG2	21:BK:61:TRP:NE1	2.20	0.56
38:A1:900:G:H1'	38:A1:1589:A:N6	2.20	0.56
39:A3:87:G:OP1	43:AF:221:LYS:NZ	2.38	0.56
46:AI:42:THR:OG1	46:AI:44:ASP:OD1	2.19	0.56
7:BI:178:ARG:NH1	34:B5:207:U:O2	2.37	0.56
16:Ba:89:ARG:NH2	34:B5:1088:A:O3'	2.38	0.56
34:B5:884:A:H2'	34:B5:885:G:C8	2.41	0.56
38:A1:3322:A:H2'	38:A1:3323:A:C8	2.39	0.56
2:BB:153:HIS:NE2	34:B5:1045:C:OP1	2.34	0.56
7:BI:152:ILE:HG13	7:BI:153:GLU:H	1.70	0.56
24:BR:27:ASP:OD1	24:BR:30:THR:HG22	2.05	0.56
26:BT:111:ILE:HG23	26:BT:113:ILE:HG12	1.87	0.56
31:Bg:14:GLU:HG3	31:Bg:309:VAL:HG12	1.86	0.56
31:Bg:22:SER:OG	31:Bg:69:GLN:O	2.21	0.56
38:A1:93:C:OP1	83:A1:3401:SPD:N1	2.33	0.56
38:A1:1696:A:H2'	38:A1:1697:A:C8	2.40	0.56
44:AG:107:GLU:O	44:AG:111:LYS:HG2	2.05	0.56
79:tP:67:G:C3'	79:tP:68:G:H5''	2.35	0.56
1:BA:108:THR:N	1:BA:135:GLU:OE2	2.29	0.56
7:BI:110:ARG:NH1	7:BI:121:LEU:O	2.39	0.56
33:BM:62:LEU:HD13	33:BM:120:VAL:HB	1.86	0.56
34:B5:393:C:H2'	34:B5:394:C:C6	2.40	0.56
38:A1:1389:G:OP1	67:Ae:104:ASN:ND2	2.32	0.56
45:AH:94:TYR:OH	45:AH:141:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BG:114:VAL:HG13	5:BG:115:LYS:HD2	1.87	0.56
5:BG:153:VAL:HG13	5:BG:175:ILE:HD13	1.85	0.56
11:BO:61:MET:SD	11:BO:65:GLN:NE2	2.79	0.56
24:BR:32:LYS:NZ	34:B5:1388:A:OP2	2.38	0.56
29:Bc:27:GLN:NE2	29:Bc:64:ARG:O	2.38	0.56
36:AB:250:ALA:HB3	38:A1:2880:PSU:H1'	1.88	0.56
49:AM:88:ALA:O	49:AM:93:LYS:NZ	2.39	0.56
73:Ak:8:ILE:HG23	73:Ak:65:LEU:HD11	1.87	0.56
4:BE:131:LEU:HD12	34:B5:251:A:C2	2.41	0.56
11:BO:41:ARG:NH1	34:B5:896:U:O2	2.37	0.56
19:BD:211:PRO:HG3	24:BR:19:ARG:HB3	1.86	0.56
29:Bc:11:LYS:NZ	29:Bc:51:ASN:OD1	2.32	0.56
37:AC:4:PRO:HG2	37:AC:22:LEU:HD22	1.87	0.56
34:B5:1223:A:H2'	34:B5:1224:A:H8	1.71	0.56
38:A1:2683:U:H2'	38:A1:2684:C:C6	2.41	0.56
19:BD:51:ARG:HG2	19:BD:89:GLU:OE2	2.06	0.56
20:BF:112:ARG:NH2	23:BQ:42:GLU:OE2	2.36	0.56
25:BS:38:VAL:HG23	25:BS:42:TYR:HD2	1.71	0.56
38:A1:993:G:N3	38:A1:2637:A:H2'	2.21	0.56
38:A1:1596:C:H2'	38:A1:1597:C:C6	2.41	0.56
38:A1:2160:G:H2'	38:A1:2161:G:C8	2.41	0.56
41:AD:34:LYS:HA	56:AT:27:LEU:HD11	1.88	0.56
41:AD:181:PRO:HG3	41:AD:198:TYR:CD2	2.41	0.56
45:AH:36:LYS:NZ	45:AH:152:GLU:OE2	2.35	0.56
80:tA:30:G:N2	80:tA:40:C:O2	2.26	0.56
2:BB:82:ARG:HG2	2:BB:105:PHE:CE1	2.41	0.56
5:BG:164:LYS:HD3	5:BG:169:TYR:HE2	1.71	0.56
38:A1:29:C:H4'	38:A1:62:A:H4'	1.89	0.56
47:AJ:86:VAL:HG23	47:AJ:112:LEU:HD12	1.87	0.56
5:BG:23:ARG:NH2	5:BG:42:GLY:HA2	2.22	0.55
25:BS:53:ASP:OD1	25:BS:54:LEU:N	2.38	0.55
26:BT:102:ARG:NH2	34:B5:1502:G:N7	2.53	0.55
34:B5:16:G:H2'	34:B5:17:C:C6	2.42	0.55
37:AC:317:PRO:C	37:AC:319:LYS:H	2.13	0.55
56:AT:151:LEU:HG	56:AT:152:ALA:H	1.71	0.55
12:BV:74:GLN:HE22	12:BV:80:LYS:C	2.14	0.55
34:B5:953:G:H2'	34:B5:954:G:C8	2.41	0.55
34:B5:1592:A:H2'	34:B5:1593:A:H8	1.72	0.55
37:AC:141:ARG:NH1	38:A1:1385:C:OP1	2.36	0.55
38:A1:1621:A:H2'	38:A1:1622:U:C6	2.41	0.55
38:A1:2568:C:O2'	38:A1:2569:A:O5'	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:AQ:125:ASP:OD1	53:AQ:126:GLN:N	2.39	0.55
72:Aj:2:GLY:O	72:Aj:7:SER:OG	2.15	0.55
34:B5:625:C:H2'	34:B5:626:U:C6	2.41	0.55
40:A4:63:G:H22	40:A4:97:A:H2	1.54	0.55
7:BI:56:ARG:NH2	34:B5:332:U:OP1	2.39	0.55
34:B5:368:U:H2'	34:B5:369:A:O4'	2.05	0.55
34:B5:472:U:H2'	34:B5:473:A:H8	1.72	0.55
34:B5:923:A:H2'	34:B5:924:A:C8	2.41	0.55
36:AB:315:GLY:HA2	38:A1:3379:C:H4'	1.88	0.55
38:A1:242:C:H2'	38:A1:243:G:C8	2.41	0.55
12:BV:36:VAL:HB	12:BV:51:VAL:HG23	1.87	0.55
21:BK:20:VAL:HG12	21:BK:67:THR:HA	1.87	0.55
23:BQ:48:VAL:HG23	23:BQ:78:VAL:HG13	1.88	0.55
32:Bf:102:VAL:HG22	33:BM:74:LEU:HD13	1.88	0.55
34:B5:809:A:H2'	34:B5:810:G:C8	2.41	0.55
34:B5:888:U:H2'	34:B5:889:U:C6	2.41	0.55
38:A1:1094:U:H4'	38:A1:1095:U:H5'	1.87	0.55
38:A1:2441:A:H5''	38:A1:2508:U:N3	2.21	0.55
53:AQ:94:PHE:CZ	63:Aa:119:PRO:HD3	2.42	0.55
56:AT:49:GLN:HA	56:AT:52:MET:HE2	1.88	0.55
5:BG:187:LYS:NZ	34:B5:140:A:OP2	2.39	0.55
31:Bg:116:ASP:CG	31:Bg:121:MET:H	2.15	0.55
35:AA:21:ARG:HD3	38:A1:824:C:H5''	1.89	0.55
36:AB:50:LYS:NZ	36:AB:330:GLY:O	2.36	0.55
38:A1:2572:C:H4'	62:AZ:61:LYS:HB2	1.88	0.55
47:AJ:106:ILE:HD11	47:AJ:109:HIS:HB2	1.89	0.55
58:AV:108:GLU:HG3	58:AV:128:ARG:HG3	1.89	0.55
2:BB:48:VAL:HG13	2:BB:49:ASN:H	1.72	0.55
7:BI:106:ALA:HB2	7:BI:165:LEU:HG	1.89	0.55
26:BT:86:ARG:NH1	34:B5:1601:G:OP1	2.27	0.55
31:Bg:131:ILE:HD11	31:Bg:151:VAL:HG21	1.89	0.55
34:B5:1356:U:H3'	34:B5:1357:A:H5''	1.89	0.55
35:AA:69:TYR:OH	38:A1:2557:A:OP1	2.22	0.55
38:A1:542:G:C5	38:A1:543:C:H1'	2.41	0.55
38:A1:2503:G:H2'	38:A1:2504:U:H6	1.71	0.55
40:A4:149:A:H2'	40:A4:150:G:C8	2.41	0.55
62:AZ:50:PRO:HD3	62:AZ:68:ILE:HG12	1.87	0.55
4:BE:139:VAL:HG13	4:BE:150:PRO:HG3	1.88	0.55
34:B5:891:A:H2'	34:B5:892:A:H8	1.72	0.55
34:B5:1237:G:H2'	34:B5:1238:A:H8	1.71	0.55
66:Ad:9:THR:HG23	66:Ad:76:SER:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:145:ARG:HH11	4:BE:162:ILE:HG21	1.72	0.55
7:BI:60:ILE:HD11	7:BI:179:CYS:HB2	1.89	0.55
15:BY:57:VAL:HB	15:BY:60:PHE:CE2	2.42	0.55
37:AC:159:ILE:HG23	37:AC:164:GLU:HG3	1.88	0.55
38:A1:1119:C:H2'	38:A1:1120:A:H8	1.70	0.55
38:A1:1534:A:H2'	38:A1:1535:A:C8	2.42	0.55
38:A1:1688:U:H2'	38:A1:1689:U:C6	2.41	0.55
38:A1:2762:A:H2'	38:A1:2763:U:H6	1.72	0.55
4:BE:129:VAL:HG22	4:BE:139:VAL:HG12	1.89	0.55
17:Bb:50:ALA:O	17:Bb:51:GLN:HG2	2.07	0.55
19:BD:61:GLU:OE1	19:BD:62:ASN:ND2	2.39	0.55
34:B5:181:A:H2'	34:B5:182:A:H8	1.72	0.55
34:B5:1346:A:N6	34:B5:1369:U:H3'	2.22	0.55
38:A1:674:G:O6	53:AQ:56:LYS:NZ	2.40	0.55
43:AF:40:LYS:HE3	43:AF:170:GLU:OE1	2.07	0.55
1:BA:135:GLU:O	1:BA:139:VAL:HG22	2.07	0.54
4:BE:48:LEU:HD21	4:BE:70:VAL:HG21	1.89	0.54
6:BH:8:ILE:HA	6:BH:42:GLN:HG3	1.87	0.54
6:BH:47:ARG:HB2	6:BH:59:ALA:HB3	1.87	0.54
21:BK:48:SER:OG	34:B5:1220:C:OP1	2.24	0.54
34:B5:1291:G:H22	34:B5:1324:G:N2	2.05	0.54
45:AH:135:GLU:HG2	45:AH:145:VAL:HB	1.89	0.54
46:AI:36:LEU:HD13	46:AI:73:ASN:HB2	1.87	0.54
5:BG:4:ASN:ND2	34:B5:152:U:O2	2.34	0.54
6:BH:89:HIS:CD2	6:BH:165:LYS:HG2	2.42	0.54
7:BI:72:ILE:HD13	7:BI:112:TRP:CD2	2.41	0.54
34:B5:947:U:H2'	34:B5:948:G:H8	1.71	0.54
38:A1:1659:U:H2'	38:A1:1660:C:C6	2.41	0.54
49:AM:89:ALA:HB1	49:AM:92:GLU:OE2	2.06	0.54
51:AO:74[A]:ARG:HD2	51:AO:145[A]:VAL:HG12	1.90	0.54
68:Af:58:GLU:HG3	68:Af:63:LYS:NZ	2.22	0.54
13:BW:53:ILE:HB	13:BW:60:LYS:HB2	1.88	0.54
34:B5:103:A:H4'	34:B5:105:A:C8	2.42	0.54
34:B5:119:A:H1'	34:B5:397:A:C4	2.42	0.54
38:A1:417:A:H2'	38:A1:418:A:C8	2.42	0.54
38:A1:817:A:O2'	72:Aj:11:ARG:HG2	2.07	0.54
80:tA:27:C:H2'	80:tA:28:A:H8	1.72	0.54
2:BB:144:ARG:HG3	2:BB:208:GLN:OE1	2.07	0.54
7:BI:39:GLY:HA2	7:BI:61:GLU:HB3	1.89	0.54
19:BD:28:GLU:OE2	19:BD:65:ARG:NH2	2.39	0.54
31:Bg:126:SER:OG	31:Bg:127:ARG:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:AB:67:PHE:CD1	58:AV:88:ARG:HD2	2.42	0.54
38:A1:2572:C:H5'	62:AZ:60:LYS:HB3	1.88	0.54
20:BF:192:GLU:OE1	28:BZ:63:SER:OG	2.24	0.54
20:BF:225:ARG:HD3	29:Bc:61:ARG:NH1	2.22	0.54
21:BK:54:TYR:HB3	21:BK:72:GLY:HA3	1.90	0.54
38:A1:446:U:H4'	38:A1:447:U:H5	1.72	0.54
38:A1:533:A:O2'	38:A1:535:G:OP2	2.24	0.54
38:A1:2895:G:O2'	75:Am:100:TYR:O	2.24	0.54
38:A1:2916:U:H5	38:A1:2935:U:HO2'	1.56	0.54
46:AI:30:LYS:HD2	46:AI:63:GLU:HG3	1.88	0.54
5:BG:65:GLN:HG3	34:B5:1681:A:H8	1.72	0.54
6:BH:14:THR:OG1	6:BH:15:GLU:OE1	2.26	0.54
34:B5:319:U:H4'	34:B5:323:A:C8	2.42	0.54
34:B5:885:G:H2'	34:B5:886:U:C6	2.43	0.54
38:A1:2882:U:H2'	38:A1:2883:U:C6	2.42	0.54
38:A1:2883:U:H2'	38:A1:2884:C:C6	2.43	0.54
7:BI:119:GLN:HG3	7:BI:150:ALA:HB1	1.90	0.54
11:BO:16:VAL:O	11:BO:30:VAL:HA	2.08	0.54
26:BT:63:ARG:O	26:BT:67:MET:HG2	2.07	0.54
34:B5:1164:G:H2'	34:B5:1165:G:C8	2.42	0.54
37:AC:120:TYR:CE2	37:AC:277:PRO:HB3	2.43	0.54
39:A3:39:C:H4'	47:AJ:44:THR:HG23	1.90	0.54
79:tP:65:G:H2'	79:tP:66:C:C6	2.42	0.54
2:BB:144:ARG:HB3	2:BB:206:PRO:HB2	1.89	0.54
27:BU:70:THR:OG1	27:BU:72:ASN:OD1	2.26	0.54
32:Bf:121:CYS:H	32:Bf:130:VAL:HG11	1.73	0.54
33:BM:114:LYS:HD3	34:B5:1226:A:N6	2.22	0.54
34:B5:861:U:O2'	34:B5:862:A:OP1	2.26	0.54
34:B5:1483:A:H2'	34:B5:1484:G:C8	2.43	0.54
34:B5:1488:G:H3'	34:B5:1515:A:H61	1.73	0.54
38:A1:1176:C:H2'	38:A1:1177:G:N2	2.23	0.54
38:A1:1188:U:OP1	38:A1:1210:U:O2'	2.20	0.54
38:A1:2367:A:H2'	38:A1:2368:A:C8	2.43	0.54
47:AJ:92:ARG:HH12	47:AJ:94:ARG:HH11	1.55	0.54
58:AV:23:MET:HE3	58:AV:100:GLY:HA3	1.89	0.54
69:Ag:57:LEU:HB3	69:Ag:61:GLN:HB2	1.89	0.54
19:BD:76:ARG:O	19:BD:78:LYS:HD3	2.07	0.54
24:BR:13:SER:O	24:BR:17:ILE:HG12	2.08	0.54
35:AA:2:GLY:O	38:A1:925:A:N6	2.33	0.54
36:AB:298:PHE:HE2	59:AW:1:MET:HG2	1.72	0.54
38:A1:675:C:O2'	38:A1:679:U:OP1	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2768:U:H2'	38:A1:2769:A:C8	2.43	0.54
72:Aj:14:LYS:HD3	74:A1:51:ILE:HD11	1.88	0.54
4:BE:157:ASN:HD21	4:BE:222:LEU:HD21	1.72	0.54
34:B5:30:G:H2'	34:B5:31:C:C6	2.43	0.54
38:A1:716:A:C5	63:Aa:117:ARG:HG3	2.43	0.54
38:A1:2782:U:OP1	48:AL:185:LYS:NZ	2.41	0.54
38:A1:2927:C:H2'	38:A1:2928:C:C6	2.43	0.54
38:A1:3294:A:H2'	38:A1:3295:A:O4'	2.08	0.54
19:BD:161:GLY:HA3	34:B5:1331:A:H61	1.73	0.53
21:BK:1:MET:HE2	21:BK:44:LYS:HB2	1.89	0.53
22:BP:18:ARG:NH1	25:BS:90:ASN:O	2.41	0.53
23:BQ:49:TYR:HB3	23:BQ:53:LEU:HD23	1.90	0.53
34:B5:447:U:H2'	34:B5:448:C:O4'	2.08	0.53
34:B5:1226:A:O2'	34:B5:1229:G:N3	2.40	0.53
38:A1:1474:A:O2'	66:Ad:57:GLN:NE2	2.41	0.53
73:Ak:32:ASN:OD1	73:Ak:36:LYS:N	2.41	0.53
4:BE:88:ASP:OD1	4:BE:122:LYS:NZ	2.41	0.53
24:BR:41:ILE:HG23	24:BR:46:LEU:HD23	1.90	0.53
31:Bg:231:MET:HG2	31:Bg:232:TYR:CD1	2.43	0.53
34:B5:1461:C:H2'	34:B5:1462:G:H8	1.74	0.53
38:A1:1264:G:H1'	38:A1:1265:U:H5	1.73	0.53
38:A1:3017:A:N1	38:A1:3037:U:H5	2.06	0.53
56:AT:13:TYR:HA	56:AT:16:GLN:HG2	1.89	0.53
56:AT:126:VAL:HG13	56:AT:128:LEU:HD22	1.89	0.53
2:BB:32:ILE:HD13	2:BB:66:VAL:HG21	1.91	0.53
5:BG:57:ASP:HA	5:BG:106:LEU:HA	1.90	0.53
16:Ba:70:LYS:HD3	34:B5:930:A:H5''	1.90	0.53
34:B5:1235:C:C2	34:B5:1236:A:C8	2.96	0.53
35:AA:104:LEU:HD22	35:AA:136:ILE:HD11	1.89	0.53
38:A1:1108:U:H2'	38:A1:1109:U:C6	2.43	0.53
38:A1:1676:A:OP1	57:AU:13:LYS:NZ	2.40	0.53
53:AQ:90:ASP:OD1	53:AQ:92:ARG:NE	2.27	0.53
2:BB:179:SER:HA	2:BB:183:GLN:HE21	1.73	0.53
2:BB:204:ILE:O	34:B5:1064:G:O2'	2.23	0.53
3:BC:156:THR:HG23	13:BW:95:PRO:HB2	1.90	0.53
21:BK:91:TYR:HD1	21:BK:92:ILE:HG13	1.73	0.53
24:BR:31:ASN:HD22	24:BR:55:THR:HB	1.73	0.53
28:BZ:75:LEU:HD12	28:BZ:78:ILE:HD11	1.90	0.53
37:AC:308:LYS:NZ	38:A1:609:G:N7	2.54	0.53
38:A1:943:U:H3'	63:Aa:13:GLY:HA2	1.90	0.53
38:A1:1751:G:H5'	73:Ak:26:LYS:HE2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:tP:25:C:H3'	79:tP:26:G:H8	1.73	0.53
25:BS:87:ASN:ND2	25:BS:100:THR:OG1	2.42	0.53
34:B5:29:U:H2'	34:B5:30:G:C8	2.43	0.53
34:B5:1147:A:H2'	34:B5:1148:C:C6	2.43	0.53
34:B5:1521:G:O2'	34:B5:1523:G:OP2	2.22	0.53
38:A1:723:U:O2'	64:Ab:29:TYR:OH	2.26	0.53
38:A1:1498:A:H2'	38:A1:1499:C:C6	2.44	0.53
38:A1:2676:A:H5'	38:A1:2677:G:C8	2.43	0.53
38:A1:3013:U:H2'	38:A1:3014:U:C6	2.44	0.53
42:AE:172:HIS:CE1	42:AE:173:MET:HE3	2.43	0.53
5:BG:43:ASP:HA	5:BG:46:LYS:HE3	1.90	0.53
13:BW:51:GLU:HG3	17:Bb:8:LEU:HD11	1.90	0.53
22:BP:30:THR:HG22	22:BP:87:PRO:HD2	1.91	0.53
38:A1:12:A:H2'	38:A1:13:A:C8	2.43	0.53
38:A1:1222:G:H2'	38:A1:1286:A:N6	2.23	0.53
38:A1:3164:C:O2'	38:A1:3165:A:H8	1.91	0.53
80:tA:23:C:H2'	80:tA:24:G:H8	1.74	0.53
34:B5:271:A:H2'	34:B5:272:U:O4'	2.08	0.53
34:B5:1592:A:H2'	34:B5:1593:A:C8	2.44	0.53
36:AB:142:ALA:O	36:AB:146:ARG:HG3	2.08	0.53
38:A1:242:C:H2'	38:A1:243:G:H8	1.73	0.53
38:A1:683:U:OP1	50:AN:204:LYS:NZ	2.41	0.53
38:A1:1083:G:H2'	38:A1:1084:A:C8	2.44	0.53
38:A1:1786:G:H2'	38:A1:1787:A:C8	2.44	0.53
38:A1:2696:A:H2'	38:A1:2697:A:C8	2.43	0.53
53:AQ:176:ARG:HA	53:AQ:182:LYS:O	2.08	0.53
55:AS:96:ASP:OD1	55:AS:97:VAL:N	2.38	0.53
80:tA:72:U:H2'	80:tA:73:A:C8	2.43	0.53
12:BV:73:ALA:HB1	12:BV:78:LEU:HB2	1.89	0.53
19:BD:55:THR:HA	19:BD:58:VAL:HG12	1.91	0.53
25:BS:123:ARG:HG3	25:BS:133:VAL:HB	1.90	0.53
31:Bg:22:SER:HB2	31:Bg:36:ALA:HB3	1.91	0.53
31:Bg:36:ALA:HB1	31:Bg:68:VAL:HG12	1.90	0.53
34:B5:107:C:H2'	34:B5:108:A:H8	1.74	0.53
38:A1:542:G:C2	38:A1:550:A:H1'	2.44	0.53
54:AR:105:LEU:HD22	54:AR:135:LYS:HG3	1.90	0.53
1:BA:198:MET:SD	1:BA:200:ASP:HB2	2.49	0.53
19:BD:68:GLU:HB2	21:BK:20:VAL:HG11	1.91	0.53
25:BS:62:THR:OG1	25:BS:65:GLU:OE1	2.18	0.53
31:Bg:25:THR:HG21	31:Bg:295:SER:HA	1.91	0.53
34:B5:513:U:H2'	34:B5:514:G:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:246:U:H2'	38:A1:247:C:O4'	2.09	0.53
38:A1:585:A:H2'	38:A1:586:C:C6	2.43	0.53
40:A4:58:G:O6	72:Aj:63:ARG:NH1	2.37	0.53
47:AJ:117:ASP:HB3	47:AJ:120:ILE:HD12	1.90	0.53
57:AU:27:VAL:HG21	57:AU:107:PHE:CE1	2.44	0.53
80:tA:27:C:H2'	80:tA:28:A:C8	2.44	0.53
26:BT:39:THR:HA	26:BT:100:ILE:HD12	1.91	0.53
34:B5:1628:U:H2'	34:B5:1629:G:C8	2.44	0.53
38:A1:1243:G:H22	38:A1:1269:U:H3	1.57	0.53
51:AO:121[A]:PRO:HA	51:AO:124[A]:LEU:HD12	1.91	0.53
59:AW:46:PRO:HB2	59:AW:54:LEU:HD23	1.91	0.53
70:Ah:83:LYS:O	72:Aj:73:ARG:NH2	2.41	0.53
1:BA:27:ARG:NH1	1:BA:43:ASP:O	2.42	0.52
15:BY:23:PHE:HE2	15:BY:75:VAL:HG22	1.72	0.52
16:Ba:92:ARG:HG2	34:B5:1796:C:O2	2.08	0.52
19:BD:135:GLU:HB3	19:BD:187:LYS:HB3	1.91	0.52
34:B5:205:U:H2'	34:B5:206:A:H8	1.74	0.52
34:B5:925:G:H2'	34:B5:926:A:C8	2.43	0.52
34:B5:1346:A:H61	34:B5:1369:U:H3'	1.74	0.52
35:AA:52:SER:HB3	35:AA:191:LEU:HD12	1.91	0.52
37:AC:317:PRO:O	37:AC:318:LEU:HB2	2.09	0.52
38:A1:1615:C:H2'	38:A1:1616:U:C6	2.45	0.52
47:AJ:12:LEU:HB3	47:AJ:131:MET:HE1	1.91	0.52
8:BJ:107:ARG:NH2	8:BJ:153:GLU:OE2	2.37	0.52
22:BP:49:MET:HA	22:BP:49:MET:HE3	1.91	0.52
28:BZ:55:PRO:O	28:BZ:56:THR:OG1	2.26	0.52
38:A1:120:G:N7	44:AG:128:LYS:HG3	2.24	0.52
38:A1:269:G:H5''	50:AN:14:LYS:HE2	1.91	0.52
38:A1:973:A:N1	38:A1:1108:U:H5	2.06	0.52
38:A1:2960:C:H2'	38:A1:2961:G:H8	1.74	0.52
20:BF:193:THR:HA	20:BF:196:GLU:HG2	1.91	0.52
21:BK:74:GLU:HA	21:BK:77:ARG:HG2	1.91	0.52
33:BM:98:GLY:HA3	33:BM:103:LEU:HD22	1.91	0.52
34:B5:52:U:H2'	34:B5:53:G:C8	2.44	0.52
34:B5:1089:U:O2'	34:B5:1093:A:N1	2.40	0.52
38:A1:907:G:H4'	38:A1:908:G:H5'	1.91	0.52
38:A1:2611:U:H2'	38:A1:2612:U:C6	2.44	0.52
38:A1:3047:U:O2'	38:A1:3048:A:H5'	2.09	0.52
41:AD:182:GLY:HA2	41:AD:194:LEU:HD23	1.91	0.52
2:BB:27:LYS:HD3	2:BB:47:LEU:HD13	1.90	0.52
2:BB:48:VAL:HG13	2:BB:49:ASN:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BF:72:HIS:HB2	20:BF:111:VAL:HG21	1.92	0.52
26:BT:77:ASN:OD1	26:BT:101:ASN:ND2	2.37	0.52
38:A1:2836:C:H5	38:A1:2852:C:H42	1.56	0.52
40:A4:57:C:H4'	40:A4:63:G:N7	2.24	0.52
40:A4:74:U:C4	61:AY:74:TYR:HD1	2.27	0.52
40:A4:82:U:OP2	40:A4:83:C:H2'	2.10	0.52
48:AL:9:ILE:HD12	63:Aa:34:MET:HE1	1.90	0.52
53:AQ:122:ILE:HG23	53:AQ:126:GLN:HB2	1.90	0.52
6:BH:163:ASP:OD1	6:BH:164:TYR:N	2.41	0.52
32:Bf:145:HIS:ND1	34:B5:1234:A:O2'	2.42	0.52
38:A1:2503:G:H2'	38:A1:2504:U:C6	2.44	0.52
38:A1:2745:G:N2	38:A1:2748:A:OP2	2.39	0.52
40:A4:103:G:OP2	40:A4:105:A:O2'	2.25	0.52
67:Ae:89:THR:HG22	67:Ae:117:ILE:HG13	1.92	0.52
1:BA:59:LEU:O	1:BA:63:ILE:HG12	2.10	0.52
2:BB:30:PHE:O	2:BB:45:LYS:HG2	2.10	0.52
6:BH:14:THR:HG23	6:BH:16:LEU:H	1.73	0.52
8:BJ:106:GLU:HA	8:BJ:111:THR:HG21	1.91	0.52
15:BY:27:VAL:HG11	15:BY:35:VAL:HG21	1.91	0.52
19:BD:142:LEU:HD21	19:BD:182:LEU:HD11	1.90	0.52
34:B5:108:A:H2'	34:B5:109:G:C8	2.45	0.52
34:B5:1525:A:H2'	34:B5:1526:A:C8	2.44	0.52
38:A1:47:C:OP2	38:A1:48:A:O2'	2.25	0.52
38:A1:407:A:C2	40:A4:17:A:H1'	2.45	0.52
38:A1:1290:A:H2'	38:A1:1291:A:C8	2.45	0.52
79:tP:69:C:H2'	79:tP:70:G:O4'	2.10	0.52
2:BB:108:ASP:OD1	2:BB:109:LYS:N	2.43	0.52
6:BH:49:ILE:HD11	6:BH:172:VAL:HA	1.91	0.52
20:BF:57:SER:HA	29:Bc:53:ILE:HB	1.91	0.52
30:Bd:36:LEU:HB3	30:Bd:38:ILE:HG22	1.92	0.52
32:Bf:106:TYR:HB2	33:BM:74:LEU:HD11	1.90	0.52
34:B5:407:A:H2'	34:B5:408:C:C6	2.45	0.52
34:B5:509:G:H2'	34:B5:510:G:C8	2.45	0.52
37:AC:10:SER:OG	37:AC:13:GLY:O	2.26	0.52
38:A1:633:C:O2'	68:Af:21:ARG:O	2.28	0.52
2:BB:34:ALA:O	2:BB:41:ARG:NE	2.41	0.52
23:BQ:30:LYS:HD2	23:BQ:35:PRO:HA	1.90	0.52
28:BZ:54:VAL:HG11	28:BZ:83:LEU:CD2	2.40	0.52
34:B5:1471:A:C8	34:B5:1540:G:H1'	2.45	0.52
34:B5:1738:U:H2'	34:B5:1739:C:C6	2.45	0.52
36:AB:53:MET:HE2	38:A1:3049:A:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1844:C:O2'	72:Aj:11:ARG:NH2	2.43	0.52
38:A1:2232:A:H2'	38:A1:2233:A:C8	2.44	0.52
41:AD:95:TRP:CD1	41:AD:158:ARG:HA	2.45	0.52
44:AG:74:THR:HG22	44:AG:164:VAL:HG22	1.90	0.52
5:BG:114:VAL:HG13	5:BG:115:LYS:CD	2.39	0.52
16:Ba:95:ARG:NE	34:B5:1797:A:H5'	2.24	0.52
34:B5:1503:A:H2'	34:B5:1504:G:O4'	2.10	0.52
38:A1:8:C:H2'	38:A1:9:U:C6	2.45	0.52
38:A1:245:U:H2'	38:A1:246:U:C6	2.45	0.52
38:A1:1194:G:H2'	38:A1:1195:A:C8	2.45	0.52
38:A1:1494:U:OP1	74:Al:42:ARG:NH1	2.39	0.52
38:A1:1621:A:H2'	38:A1:1622:U:H6	1.75	0.52
38:A1:2506:U:O2'	38:A1:2507:C:OP1	2.25	0.52
38:A1:3291:G:H2'	38:A1:3292:A:H8	1.75	0.52
38:A1:3359:A:H2'	38:A1:3360:C:C6	2.45	0.52
10:BN:129:TYR:HA	10:BN:132:VAL:HG12	1.91	0.52
11:BO:111:ARG:HG2	16:Ba:58:VAL:HG13	1.91	0.52
12:BV:32:VAL:HG22	12:BV:60:ARG:HD2	1.92	0.52
34:B5:891:A:H2'	34:B5:892:A:C8	2.45	0.52
38:A1:2419:A:H2'	38:A1:2420:C:C6	2.45	0.52
38:A1:2664:C:OP2	47:AJ:142:LYS:NZ	2.39	0.52
3:BC:95:ARG:HH12	3:BC:97:ARG:HE	1.57	0.51
31:Bg:157:VAL:HG23	31:Bg:204:ALA:HB1	1.92	0.51
34:B5:71:A:O2'	34:B5:72:A:OP1	2.24	0.51
34:B5:476:U:H5'	34:B5:477:A:O4'	2.10	0.51
34:B5:1373:C:H2'	34:B5:1374:C:C6	2.45	0.51
34:B5:1579:U:H2'	34:B5:1580:C:C6	2.45	0.51
40:A4:63:G:OP1	40:A4:90:U:H5''	2.10	0.51
6:BH:91:ILE:HG21	6:BH:129:LEU:HD12	1.92	0.51
8:BJ:59:LEU:HD11	8:BJ:69:ARG:HA	1.92	0.51
10:BN:16:ILE:HD11	34:B5:862:A:H5''	1.92	0.51
19:BD:224:ASP:OD1	31:Bg:228:LYS:NZ	2.43	0.51
34:B5:826:U:O4	34:B5:846:G:N1	2.32	0.51
38:A1:1279:C:H2'	38:A1:1280:C:H6	1.75	0.51
41:AD:80:SER:OG	41:AD:92:LEU:O	2.24	0.51
58:AV:15:LEU:HD23	58:AV:53:SER:HB3	1.92	0.51
2:BB:223:PHE:HD2	2:BB:225:VAL:HG22	1.76	0.51
15:BY:37:LYS:HD2	15:BY:57:VAL:HG23	1.92	0.51
31:Bg:197:SER:OG	31:Bg:216:LYS:N	2.44	0.51
34:B5:107:C:OP1	34:B5:383:G:O2'	2.26	0.51
34:B5:1087:A:H2'	34:B5:1088:A:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1170:G:C2	34:B5:1171:A:C8	2.98	0.51
36:AB:10:ARG:NH2	36:AB:263:SER:O	2.38	0.51
38:A1:1232:C:N4	38:A1:1233:G:O6	2.44	0.51
79:tP:54:A:H61	79:tP:58:A:H8	1.56	0.51
14:BX:140:LYS:NZ	34:B5:31:C:OP1	2.43	0.51
32:Bf:128:ALA:H	33:BM:54:ARG:HH12	1.57	0.51
35:AA:9:ARG:NH2	38:A1:912:G:OP2	2.39	0.51
38:A1:602:A:O2'	38:A1:603:A:OP1	2.27	0.51
38:A1:1597:C:H2'	38:A1:1598:G:C8	2.45	0.51
44:AG:75:ILE:CD1	50:AN:18:VAL:HG23	2.40	0.51
46:AI:171:TRP:CZ3	46:AI:182:LEU:HD21	2.45	0.51
55:AS:13:ARG:NH2	55:AS:50:LYS:O	2.42	0.51
4:BE:182:TYR:HD1	4:BE:192:ILE:HG12	1.75	0.51
10:BN:108:ASP:OD1	34:B5:878:G:O2'	2.29	0.51
25:BS:42:TYR:HA	25:BS:85:PHE:HE2	1.76	0.51
26:BT:28:LEU:HD23	26:BT:55:TYR:CD2	2.44	0.51
38:A1:1915:A:H2'	38:A1:1916:U:C6	2.45	0.51
46:AI:171:TRP:O	46:AI:174:THR:HG22	2.10	0.51
54:AR:180:LYS:HG2	54:AR:184:LEU:HD23	1.93	0.51
61:AY:17:LYS:O	61:AY:21:THR:OG1	2.24	0.51
2:BB:193:ILE:O	2:BB:197:ILE:HD12	2.11	0.51
4:BE:22:LYS:N	34:B5:773:C:OP1	2.43	0.51
19:BD:29:LEU:HB2	19:BD:34:TYR:HB2	1.92	0.51
27:BU:89:ARG:HH22	34:B5:1383:G:P	2.34	0.51
34:B5:138:A:N6	34:B5:266:A:H61	2.09	0.51
34:B5:1222:C:H2'	34:B5:1223:A:H8	1.75	0.51
38:A1:787:G:H2'	38:A1:788:C:C6	2.46	0.51
38:A1:1234:G:H3'	38:A1:1235:U:H5'	1.90	0.51
26:BT:137:ALA:O	26:BT:141:GLU:HG2	2.11	0.51
34:B5:1175:U:H2'	34:B5:1176:G:C8	2.46	0.51
34:B5:1294:G:O2'	34:B5:1321:A:N1	2.40	0.51
34:B5:1466:G:O2'	34:B5:1602:C:OP1	2.28	0.51
34:B5:1533:C:H4'	34:B5:1539:G:N1	2.26	0.51
35:AA:144:ASN:OD1	35:AA:160:SER:HB2	2.10	0.51
38:A1:314:U:H2'	38:A1:315:C:C6	2.45	0.51
38:A1:2945:G:O2'	38:A1:2948:C:OP2	2.20	0.51
53:AQ:95:GLU:N	53:AQ:95:GLU:OE2	2.43	0.51
6:BH:81:LEU:O	6:BH:85:PHE:HB2	2.10	0.51
6:BH:89:HIS:HD2	6:BH:165:LYS:HG2	1.76	0.51
34:B5:968:U:H2'	34:B5:969:C:O4'	2.11	0.51
38:A1:945:C:H2'	38:A1:946:U:H6	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1260:A:OP1	38:A1:1278:A:N6	2.44	0.51
38:A1:2357:A:H2'	38:A1:2358:A:C8	2.46	0.51
38:A1:2430:A:H2'	38:A1:2431:C:C6	2.46	0.51
38:A1:2544:U:H2'	38:A1:2545:C:C6	2.46	0.51
53:AQ:174:ARG:O	63:Aa:56:VAL:HG21	2.11	0.51
4:BE:62:LYS:HE3	34:B5:454:U:H4'	1.93	0.51
13:BW:107:SER:HB3	34:B5:802:G:H21	1.75	0.51
31:Bg:245:PHE:CE1	31:Bg:252:LEU:HD12	2.46	0.51
33:BM:43:ARG:HH12	33:BM:103:LEU:H	1.59	0.51
38:A1:156:G:OP2	71:Ai:25:LYS:HB3	2.11	0.51
38:A1:173:G:H1	38:A1:245:U:H3	1.58	0.51
38:A1:1495:U:H5	38:A1:1835:A:N1	2.08	0.51
38:A1:1560:G:H22	38:A1:1579:C:H42	1.59	0.51
38:A1:2801:A:O2'	38:A1:2802:A:H2'	2.10	0.51
80:tA:30:G:O6	80:tA:40:C:N4	2.24	0.51
1:BA:29:VAL:HG22	1:BA:149:LEU:HB3	1.92	0.51
2:BB:138:PHE:HE1	2:BB:216:LYS:HG2	1.75	0.51
4:BE:247:SER:O	4:BE:251:GLU:HG3	2.11	0.51
11:BO:111:ARG:CG	16:Ba:58:VAL:HG13	2.41	0.51
22:BP:124:THR:HB	34:B5:1182:U:H4'	1.93	0.51
38:A1:2138:A:C4	72:Aj:3:LYS:HB3	2.46	0.51
38:A1:3023:U:H2'	38:A1:3024:A:H8	1.75	0.51
71:Ai:66:GLU:OE2	71:Ai:91:ASN:ND2	2.40	0.51
1:BA:119:ARG:NH1	3:BC:241:ASP:OD1	2.44	0.50
3:BC:230:TRP:CD2	13:BW:68:ARG:HD2	2.46	0.50
5:BG:32:ILE:HD11	5:BG:63:MET:HE2	1.92	0.50
22:BP:52:LYS:HB2	22:BP:53:PRO:HD3	1.94	0.50
25:BS:38:VAL:HG21	25:BS:73:MET:HE2	1.93	0.50
31:Bg:161:LYS:HB3	31:Bg:164:ASP:OD1	2.10	0.50
34:B5:615:A:O2'	34:B5:621:A:N1	2.43	0.50
34:B5:973:A:H4'	38:A1:848:A:C8	2.44	0.50
34:B5:1229:G:N7	34:B5:1255:G:N2	2.60	0.50
38:A1:990:PSU:H1'	56:AT:101:CYS:HB2	1.92	0.50
39:A3:64:A:N7	46:AI:209:ASN:ND2	2.60	0.50
46:AI:38:LYS:HG2	46:AI:41:ALA:HB2	1.93	0.50
79:tP:19:G:H4'	79:tP:20:A:C5'	2.30	0.50
80:tA:8:U:O2	80:tA:15:G:N2	2.44	0.50
11:BO:42:VAL:HG23	11:BO:46:MET:SD	2.51	0.50
18:Be:17:GLN:NE2	34:B5:563:U:H4'	2.26	0.50
20:BF:189:THR:HG22	20:BF:191:ALA:H	1.77	0.50
21:BK:10:LYS:HZ3	21:BK:36:ASP:HB3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:BK:12:HIS:HB3	21:BK:80:LEU:HD21	1.93	0.50
31:Bg:177:MET:SD	31:Bg:179:LYS:HG3	2.52	0.50
32:Bf:139:LEU:HD21	32:Bf:150:VAL:HB	1.93	0.50
34:B5:5:U:H2'	34:B5:6:G:H8	1.77	0.50
34:B5:950:C:H2'	34:B5:951:A:C8	2.46	0.50
34:B5:1222:C:H2'	34:B5:1223:A:C8	2.46	0.50
35:AA:68:LYS:HD3	35:AA:70:ARG:HH11	1.77	0.50
39:A3:91:G:H2'	39:A3:92:A:C8	2.46	0.50
2:BB:81:PHE:CD2	2:BB:82:ARG:HG3	2.46	0.50
29:Bc:41:VAL:HG12	29:Bc:63:ALA:HB3	1.92	0.50
34:B5:1575:G7M:H2'	34:B5:1576:A:C8	2.46	0.50
37:AC:257:LYS:HA	37:AC:260:GLN:NE2	2.26	0.50
38:A1:501:A:H2'	38:A1:502:U:C6	2.47	0.50
38:A1:759:U:H2'	38:A1:760:G:O4'	2.11	0.50
38:A1:1119:C:H2'	38:A1:1120:A:C8	2.46	0.50
38:A1:2180:G:H2'	38:A1:2181:C:C6	2.46	0.50
38:A1:2376:G:H2'	38:A1:2377:G:C8	2.46	0.50
41:AD:52:VAL:HG21	41:AD:65:ILE:HD12	1.93	0.50
46:AI:144:ASN:OD1	46:AI:147:VAL:HB	2.12	0.50
28:BZ:45:GLU:O	28:BZ:48:ASP:OD1	2.28	0.50
43:AF:102:VAL:HG21	43:AF:129:LEU:HD23	1.92	0.50
8:BJ:172:VAL:HG23	8:BJ:175:ARG:NH2	2.26	0.50
13:BW:66:ASN:ND2	13:BW:68:ARG:HE	2.10	0.50
15:BY:43:LYS:HA	15:BY:46:GLU:HG2	1.93	0.50
23:BQ:93:HIS:CD2	23:BQ:105:LEU:HD11	2.46	0.50
34:B5:182:A:H2'	34:B5:183:U:C6	2.46	0.50
34:B5:472:U:O2'	34:B5:769:A:N3	2.37	0.50
36:AB:122:TRP:CE2	36:AB:127:LYS:HE3	2.47	0.50
37:AC:161:LYS:HB2	37:AC:164:GLU:HG2	1.93	0.50
38:A1:19:U:H2'	38:A1:20:A:C8	2.46	0.50
38:A1:2213:A:H2'	38:A1:2214:A:H8	1.74	0.50
41:AD:50:ARG:NH1	41:AD:147:ASP:OD2	2.42	0.50
41:AD:177:GLU:HB2	41:AD:190:ILE:HD12	1.94	0.50
58:AV:54:LEU:HD21	58:AV:119:GLY:HA3	1.94	0.50
80:tA:73:A:O2'	80:tA:74:C:OP1	2.27	0.50
4:BE:27:TYR:OH	34:B5:460:A:O2'	2.21	0.50
6:BH:28:GLU:OE2	6:BH:39:ARG:NH2	2.45	0.50
8:BJ:119:ALA:O	8:BJ:124:HIS:ND1	2.39	0.50
25:BS:44:ASN:OD1	25:BS:48:LYS:HE2	2.11	0.50
25:BS:75:ASN:HB3	25:BS:78:HIS:CD2	2.44	0.50
33:BM:59:LEU:O	33:BM:122:VAL:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BM:130:THR:HG23	33:BM:132:GLU:H	1.75	0.50
34:B5:1144:U:H2'	34:B5:1145:U:C6	2.46	0.50
80:tA:18:G:O2'	80:tA:57:G:N2	2.30	0.50
5:BG:10:ASN:ND2	5:BG:127:THR:O	2.45	0.50
7:BI:137:LYS:HA	7:BI:140:GLU:HB2	1.93	0.50
21:BK:2:LEU:HD22	34:B5:1258:U:H4'	1.94	0.50
31:Bg:70:ASP:OD2	31:Bg:113:VAL:N	2.40	0.50
34:B5:97:C:H2'	34:B5:98:U:C6	2.46	0.50
34:B5:390:G:O2'	34:B5:1731:A:H5''	2.12	0.50
34:B5:406:U:H2'	34:B5:407:A:C8	2.47	0.50
35:AA:206:PRO:HG3	35:AA:213:GLY:HA3	1.94	0.50
38:A1:1350:A:H1'	38:A1:1351:U:H5	1.77	0.50
38:A1:2204:C:H3'	38:A1:2205:U:O4'	2.12	0.50
42:AE:172:HIS:HE1	42:AE:173:MET:HE3	1.75	0.50
54:AR:181:ARG:HA	54:AR:186:LYS:HG3	1.93	0.50
55:AS:24:LEU:HD21	56:AT:141:VAL:HG11	1.94	0.50
63:Aa:24:LYS:O	63:Aa:26:ARG:HG2	2.11	0.50
2:BB:223:PHE:CD2	2:BB:225:VAL:HG22	2.46	0.50
8:BJ:111:THR:O	8:BJ:115:LYS:HG2	2.10	0.50
13:BW:31:SER:HB3	34:B5:636:A:H5''	1.93	0.50
18:Be:29:LYS:O	18:Be:31:LYS:NZ	2.45	0.50
24:BR:41:ILE:HG22	24:BR:43:SER:H	1.76	0.50
25:BS:127:HIS:CD2	25:BS:133:VAL:HG11	2.47	0.50
34:B5:1669:U:H3	34:B5:1732:A:H62	1.59	0.50
36:AB:173:GLN:HG2	36:AB:175:LYS:H	1.76	0.50
38:A1:1831:U:H2'	38:A1:1832:C:C6	2.47	0.50
38:A1:3259:U:H5''	38:A1:3261:C:H5	1.76	0.50
43:AF:185:ILE:O	43:AF:189:ILE:HG22	2.11	0.50
45:AH:141:LYS:NZ	45:AH:142:ASP:OD2	2.36	0.50
55:AS:10:ILE:HG12	55:AS:26:ARG:HB2	1.94	0.50
65:Ac:27:TYR:OH	65:Ac:55:GLU:OE1	2.28	0.50
74:Al:28:ARG:HA	74:Al:33:ASN:ND2	2.27	0.50
4:BE:212:ASP:OD1	4:BE:213:SER:N	2.41	0.50
5:BG:52:ILE:HD13	5:BG:111:LEU:HD21	1.94	0.50
9:BL:27:THR:HG23	9:BL:30:ARG:H	1.77	0.50
21:BK:46:LEU:HD13	21:BK:66:TYR:CD2	2.46	0.50
29:Bc:10:ALA:O	29:Bc:53:ILE:HA	2.11	0.50
34:B5:250:C:H2'	34:B5:251:A:H8	1.77	0.50
34:B5:406:U:H2'	34:B5:407:A:H8	1.76	0.50
34:B5:976:G:N1	34:B5:1023:A:O2'	2.41	0.50
34:B5:1174:C:O2'	34:B5:1196:A:N6	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1428:G:OP2	34:B5:1428:G:H8	1.95	0.50
35:AA:190:ARG:HG3	35:AA:191:LEU:HD22	1.94	0.50
38:A1:1239:C:H5	38:A1:1244:A:H2'	1.77	0.50
38:A1:2697:A:H2'	38:A1:2698:G:H8	1.74	0.50
39:A3:94:C:H2'	39:A3:95:A:C8	2.47	0.50
41:AD:211:LEU:HG	41:AD:219:PHE:HB2	1.94	0.50
42:AE:43:LEU:HD11	42:AE:85:ILE:HG13	1.94	0.50
69:Ag:100:ILE:HA	69:Ag:103:LYS:HZ3	1.76	0.50
4:BE:10:LYS:NZ	34:B5:96:G:OP1	2.35	0.49
7:BI:62:THR:HA	7:BI:77:ARG:HA	1.94	0.49
34:B5:107:C:H2'	34:B5:108:A:C8	2.46	0.49
34:B5:1164:G:H2'	34:B5:1165:G:H8	1.77	0.49
34:B5:1693:A:O2'	34:B5:1695:G:N7	2.43	0.49
38:A1:528:U:H2'	38:A1:529:A:C8	2.47	0.49
38:A1:1128:U:H2'	38:A1:1129:A:O4'	2.11	0.49
38:A1:2747:A:H2'	38:A1:2748:A:C8	2.46	0.49
46:AI:130:ASP:OD1	46:AI:133:GLN:HB2	2.12	0.49
57:AU:92:TRP:HD1	57:AU:108:TYR:HE1	1.60	0.49
1:BA:157:ASP:OD2	12:BV:32:VAL:HG21	2.11	0.49
4:BE:94:ALA:O	4:BE:95:THR:OG1	2.25	0.49
19:BD:156:PHE:CD1	34:B5:1326:A:H4'	2.47	0.49
23:BQ:46:PHE:O	23:BQ:50:GLU:HG3	2.11	0.49
25:BS:11:PHE:CE1	25:BS:59:GLY:HA3	2.47	0.49
29:Bc:38:ARG:O	29:Bc:40:ILE:HD12	2.11	0.49
34:B5:156:A:H2'	34:B5:157:A:O4'	2.11	0.49
38:A1:1658:G:H2'	38:A1:1659:U:C6	2.47	0.49
38:A1:2284:C:N4	38:A1:2308:C:OP2	2.43	0.49
2:BB:87:ARG:NH2	2:BB:220:GLN:OE1	2.45	0.49
7:BI:54:LYS:NZ	34:B5:333:A:OP2	2.43	0.49
10:BN:4:MET:HE2	10:BN:121:ARG:HG3	1.94	0.49
33:BM:103:LEU:HG	33:BM:116:VAL:HB	1.93	0.49
34:B5:393:C:H2'	34:B5:394:C:H6	1.78	0.49
38:A1:1223:A:H2'	38:A1:1224:C:H6	1.77	0.49
42:AE:97:ASN:ND2	42:AE:99:GLU:OE2	2.45	0.49
56:AT:56:PHE:CZ	56:AT:78:LYS:HG3	2.48	0.49
57:AU:30:PRO:HB2	57:AU:58:GLU:OE2	2.12	0.49
58:AV:18:PRO:HA	58:AV:51:ALA:HA	1.95	0.49
9:BL:2:SER:OG	9:BL:3:THR:N	2.43	0.49
18:Be:43:ARG:NH2	34:B5:590:C:OP1	2.42	0.49
21:BK:10:LYS:HZ1	21:BK:36:ASP:HB3	1.74	0.49
26:BT:10:ALA:HB3	26:BT:13:ASP:OD1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BZ:65:LEU:HB3	28:BZ:71:ILE:HD11	1.94	0.49
34:B5:828:U:H4'	34:B5:829:A:OP1	2.12	0.49
38:A1:2108:C:H1'	38:A1:3344:A:H8	1.74	0.49
80:tA:60:A:H5'	80:tA:61:C:H5	1.78	0.49
4:BE:49:ARG:NH1	34:B5:447:U:OP1	2.45	0.49
8:BJ:139:GLN:NE2	15:BY:64:PHE:O	2.34	0.49
12:BV:1:MET:HB2	12:BV:10:GLU:HB2	1.94	0.49
19:BD:80:ALA:O	19:BD:83:THR:HG22	2.13	0.49
30:Bd:4:GLU:HA	30:Bd:5:ASN:HB3	1.94	0.49
34:B5:980:G:H4'	34:B5:1776:A:H4'	1.94	0.49
37:AC:321:LYS:HA	37:AC:324:LEU:HB3	1.94	0.49
38:A1:1682:U:O4	57:AU:90:ARG:NH1	2.44	0.49
38:A1:1798:A:H2'	38:A1:1799:A:C8	2.48	0.49
38:A1:2520:A:H2'	38:A1:2521:U:C6	2.47	0.49
47:AJ:54:VAL:HG12	47:AJ:56:THR:H	1.77	0.49
61:AY:68:GLY:HA2	61:AY:84:LYS:HE3	1.95	0.49
63:Aa:75:LEU:HB3	63:Aa:118:ILE:HG23	1.94	0.49
74:Al:5:LYS:HE2	74:Al:13:MET:HE1	1.95	0.49
1:BA:63:ILE:HD13	12:BV:36:VAL:HG22	1.94	0.49
2:BB:76:SER:OG	2:BB:78:ASP:OD1	2.26	0.49
22:BP:102:PHE:CZ	34:B5:1241:G:H5'	2.48	0.49
27:BU:63:LEU:O	27:BU:83:GLU:HA	2.12	0.49
31:Bg:42:LEU:HB2	31:Bg:61:PHE:HB2	1.94	0.49
31:Bg:66:HIS:CE1	31:Bg:67:ILE:HG12	2.47	0.49
31:Bg:131:ILE:HB	31:Bg:144:LEU:HB2	1.95	0.49
34:B5:183:U:H2'	34:B5:184:C:H6	1.76	0.49
34:B5:754:A:H8	34:B5:754:A:O5'	1.95	0.49
38:A1:184:U:H2'	38:A1:185:C:C6	2.47	0.49
38:A1:531:G:H2'	38:A1:532:A:C8	2.47	0.49
38:A1:1497:C:H2'	38:A1:1498:A:H8	1.78	0.49
38:A1:3121:U:H1'	38:A1:3122:A:H5''	1.94	0.49
39:A3:4:U:H2'	39:A3:5:G:H8	1.77	0.49
39:A3:23:A:H2'	39:A3:24:A:C8	2.48	0.49
39:A3:72:A:O2'	39:A3:74:C:OP1	2.22	0.49
60:AX:88:MET:SD	60:AX:120:LYS:HB2	2.51	0.49
63:Aa:94:ALA:HB2	63:Aa:121:VAL:HG22	1.95	0.49
23:BQ:39:VAL:HG11	23:BQ:48:VAL:HG21	1.94	0.49
27:BU:37:VAL:O	27:BU:41:ILE:HG13	2.13	0.49
29:Bc:12:VAL:HA	29:Bc:30:VAL:HG12	1.94	0.49
34:B5:183:U:H2'	34:B5:184:C:C6	2.47	0.49
34:B5:920:U:H2'	34:B5:921:U:O4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:AA:183:GLY:HA2	38:A1:896:A:H5''	1.94	0.49
38:A1:2651:G:H5''	38:A1:2652:U:O4'	2.13	0.49
80:tA:6:C:H2'	80:tA:7:G:C8	2.48	0.49
81:MR:6:U:H2'	81:MR:7:A:O4'	2.13	0.49
11:BO:47:LYS:HZ1	11:BO:62:LEU:C	2.19	0.49
19:BD:207:THR:OG1	24:BR:40:THR:OG1	2.30	0.49
26:BT:65:ILE:HD13	26:BT:71:VAL:HB	1.95	0.49
34:B5:71:A:H2'	34:B5:72:A:C8	2.48	0.49
38:A1:2116:G:OP1	38:A1:2118:C:N4	2.42	0.49
38:A1:3193:C:H2'	38:A1:3194:C:C6	2.48	0.49
66:Ad:55:LEU:HB2	66:Ad:95:PRO:HD3	1.94	0.49
25:BS:70:VAL:O	25:BS:74:GLN:HG2	2.13	0.49
34:B5:501:U:H4'	34:B5:502:U:H5	1.78	0.49
34:B5:886:U:C2	34:B5:887:A:C8	3.00	0.49
34:B5:1027:A:OP1	34:B5:1789:G:O2'	2.28	0.49
37:AC:4:PRO:HD2	37:AC:22:LEU:HB2	1.94	0.49
38:A1:177:U:H3	38:A1:241:G:H1	1.58	0.49
38:A1:2357:A:H2'	38:A1:2358:A:H8	1.78	0.49
38:A1:2683:U:H2'	38:A1:2684:C:H6	1.76	0.49
63:Aa:19:LYS:HB3	63:Aa:25:HIS:HB2	1.94	0.49
4:BE:54:TYR:O	15:BY:15:ASN:ND2	2.44	0.49
7:BI:32:GLN:NE2	34:B5:1727:G:H21	2.11	0.49
7:BI:73:SER:OG	34:B5:257:A:H1'	2.13	0.49
9:BL:108:PRO:HB2	9:BL:135:VAL:HG22	1.95	0.49
10:BN:124:ARG:NH2	34:B5:967:A:OP2	2.42	0.49
15:BY:57:VAL:HB	15:BY:60:PHE:CZ	2.48	0.49
19:BD:75:LYS:HE3	21:BK:20:VAL:O	2.13	0.49
20:BF:89:ILE:HD11	20:BF:172:ILE:HD11	1.94	0.49
34:B5:15:U:H2'	34:B5:16:G:O4'	2.12	0.49
34:B5:231:U:O2'	34:B5:233:C:H5''	2.11	0.49
34:B5:1429:G:H2'	34:B5:1430:U:C6	2.48	0.49
38:A1:438:A:H2	38:A1:620:U:H5	1.61	0.49
38:A1:954:U:H5	38:A1:967:A:N1	2.10	0.49
38:A1:2200:U:H4'	38:A1:2418:G:N2	2.27	0.49
38:A1:2374:C:OP1	38:A1:2823:G:O2'	2.31	0.49
45:AH:94:TYR:HA	45:AH:177:ASP:OD1	2.12	0.49
2:BB:157:GLN:C	2:BB:159:SER:H	2.20	0.48
28:BZ:60:VAL:HB	28:BZ:101:TYR:HB2	1.95	0.48
31:Bg:203:THR:HG21	31:Bg:244:ALA:HA	1.94	0.48
34:B5:507:U:H5''	34:B5:508:U:C5	2.48	0.48
34:B5:1080:U:H2'	34:B5:1081:A:O4'	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1171:A:H2'	34:B5:1172:G:H8	1.76	0.48
34:B5:1236:A:O2'	34:B5:1237:G:OP1	2.30	0.48
34:B5:1550:A:H2'	34:B5:1551:U:H6	1.77	0.48
34:B5:1556:A:H1'	34:B5:1560:U:OP2	2.13	0.48
37:AC:138:ARG:NH2	37:AC:240:PRO:HB2	2.28	0.48
38:A1:1120:A:H2'	38:A1:1121:U:H6	1.77	0.48
38:A1:2816:G:N2	38:A1:2819:A:OP2	2.44	0.48
41:AD:236:LEU:HA	41:AD:239:ILE:HG22	1.95	0.48
52:AP:60:PHE:HB3	52:AP:64:ASN:HB3	1.95	0.48
68:Af:48:ARG:HG2	68:Af:104:PRO:HD3	1.94	0.48
76:An:2:ARG:HB3	76:An:5:TRP:CD1	2.48	0.48
2:BB:194:ASN:HA	2:BB:197:ILE:HD13	1.94	0.48
8:BJ:114:TYR:HA	8:BJ:119:ALA:HB3	1.95	0.48
15:BY:45:ALA:HA	15:BY:50:ALA:HB3	1.95	0.48
34:B5:182:A:H2'	34:B5:183:U:H6	1.78	0.48
34:B5:343:C:H2'	34:B5:344:A:H8	1.78	0.48
37:AC:23:PRO:HD2	37:AC:26:PHE:CD2	2.48	0.48
38:A1:968:G:H2'	38:A1:969:C:C6	2.48	0.48
38:A1:2407:C:H2'	38:A1:2408:U:C6	2.48	0.48
38:A1:2930:A:H2'	38:A1:2931:C:C6	2.47	0.48
69:Ag:74:ARG:CZ	69:Ag:82:ALA:HB2	2.43	0.48
80:tA:15:G:H2'	80:tA:16:U:C6	2.48	0.48
1:BA:79:ARG:NH1	1:BA:164:ASN:O	2.43	0.48
8:BJ:110:GLN:HG3	8:BJ:144:PRO:HB3	1.95	0.48
21:BK:59:PHE:CZ	21:BK:62:GLN:HA	2.48	0.48
31:Bg:38:ARG:HG2	31:Bg:67:ILE:HG23	1.95	0.48
34:B5:912:U:H3'	34:B5:913:G:H5'	1.95	0.48
34:B5:939:A:H2'	34:B5:940:A:C8	2.48	0.48
34:B5:1356:U:H5'	34:B5:1357:A:OP2	2.12	0.48
38:A1:1264:G:H1'	38:A1:1265:U:C5	2.48	0.48
44:AG:162:LEU:HD23	50:AN:7:LEU:HD11	1.94	0.48
72:Aj:54:LYS:O	72:Aj:58:THR:HB	2.13	0.48
34:B5:52:U:H2'	34:B5:53:G:H8	1.78	0.48
34:B5:1214:U:H5'	34:B5:1246:C:O2'	2.13	0.48
34:B5:1377:U:O2	34:B5:1379:C:N4	2.46	0.48
37:AC:138:ARG:HH12	38:A1:1384:U:H5'	1.78	0.48
38:A1:1576:G:H2'	38:A1:1577:G:C8	2.49	0.48
38:A1:1597:C:H5'	38:A1:1696:A:H1'	1.93	0.48
38:A1:3298:C:C2	38:A1:3299:A:C8	3.01	0.48
46:AI:66:GLU:OE2	46:AI:69:ARG:NH2	2.46	0.48
48:AL:165:SER:O	48:AL:168:ARG:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:AO:75[A]:ALA:HB3	51:AO:78[A]:ARG:HG2	1.95	0.48
63:Aa:90:TYR:CG	63:Aa:100:PRO:HG3	2.48	0.48
5:BG:50:PHE:HB3	5:BG:111:LEU:HD22	1.95	0.48
6:BH:15:GLU:HA	6:BH:18:LEU:HB3	1.94	0.48
6:BH:19:GLN:OE1	6:BH:85:PHE:HZ	1.97	0.48
6:BH:76:LYS:O	6:BH:79:ARG:HG2	2.13	0.48
7:BI:69:SER:OG	7:BI:185:GLU:OE1	2.32	0.48
14:BX:69:ARG:HG3	14:BX:117:ILE:HG12	1.94	0.48
31:Bg:93:ASP:HB2	31:Bg:100:TYR:CE2	2.36	0.48
34:B5:629:U:OP2	34:B5:969:C:N4	2.38	0.48
34:B5:751:G:H2'	34:B5:752:A:H8	1.78	0.48
34:B5:1372:U:C2'	34:B5:1373:C:H5'	2.43	0.48
34:B5:1617:U:H2'	34:B5:1618:C:C6	2.49	0.48
38:A1:929:A:H2'	38:A1:930:U:C6	2.48	0.48
38:A1:1157:G:H2'	38:A1:1158:A:O4'	2.14	0.48
43:AF:40:LYS:NZ	43:AF:179:LEU:HB3	2.27	0.48
53:AQ:67:ILE:HG12	53:AQ:81:VAL:HG11	1.95	0.48
60:AX:77:GLU:N	60:AX:77:GLU:OE1	2.46	0.48
4:BE:87:MET:HE1	4:BE:236:ILE:HG13	1.95	0.48
30:Bd:24:CYS:HB2	34:B5:1434:U:H4'	1.96	0.48
34:B5:855:A:C2	34:B5:857:U:H1'	2.49	0.48
34:B5:925:G:H2'	34:B5:926:A:H8	1.78	0.48
38:A1:370:U:H4'	38:A1:404:G:H5'	1.96	0.48
38:A1:796:U:H2'	38:A1:797:U:C6	2.49	0.48
38:A1:1497:C:H2'	38:A1:1498:A:C8	2.49	0.48
38:A1:2225:U:H2'	38:A1:2226:U:C6	2.49	0.48
38:A1:2406:C:H2'	38:A1:2407:C:H6	1.76	0.48
39:A3:95:A:N3	55:AS:119:ARG:HD2	2.28	0.48
44:AG:148:ALA:HA	44:AG:201:THR:HG22	1.94	0.48
54:AR:126:GLU:HG3	54:AR:132:PHE:CE2	2.48	0.48
9:BL:133:LYS:HB2	34:B5:337:G:H3'	1.96	0.48
25:BS:88:ARG:HD2	25:BS:108:LYS:HG2	1.95	0.48
25:BS:135:GLY:HA3	34:B5:1559:A:O5'	2.13	0.48
31:Bg:106:HIS:CE1	31:Bg:126:SER:HB2	2.49	0.48
33:BM:114:LYS:HD3	34:B5:1226:A:H62	1.78	0.48
38:A1:620:U:O5'	52:AP:167:ARG:NH2	2.47	0.48
38:A1:3089:C:H2'	38:A1:3090:U:O4'	2.13	0.48
38:A1:3164:C:HO2'	38:A1:3165:A:H8	1.61	0.48
38:A1:3236:U:N3	38:A1:3251:U:O4	2.39	0.48
42:AE:132:ALA:O	42:AE:135:VAL:HG22	2.12	0.48
47:AJ:15:GLU:HB2	47:AJ:132:ASN:CG	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Ag:3:GLN:NE2	69:Ag:30:LEU:H	2.11	0.48
1:BA:107:PHE:H	1:BA:135:GLU:CD	2.22	0.48
11:BO:80:HIS:ND1	11:BO:114:ARG:HB2	2.28	0.48
13:BW:30:SER:CB	13:BW:61:ILE:HG12	2.44	0.48
34:B5:1642:G:H5'	76:An:1:MET:HB2	1.96	0.48
38:A1:728:G:H5''	53:AQ:43:PRO:HB2	1.95	0.48
38:A1:741:U:H2'	38:A1:742:G:O4'	2.13	0.48
38:A1:3006:A:H2'	38:A1:3007:U:O4'	2.14	0.48
51:AO:85[A]:ARG:HH21	51:AO:90[A]:HIS:CE1	2.31	0.48
57:AU:22:PRO:HB2	57:AU:28:PHE:HB2	1.95	0.48
2:BB:127:VAL:HG11	2:BB:173:THR:HG22	1.95	0.48
2:BB:132:ASP:HB3	2:BB:221:PRO:HB3	1.95	0.48
5:BG:191:ARG:HG3	34:B5:178:U:H5	1.77	0.48
15:BY:6:THR:O	15:BY:8:ARG:HD3	2.13	0.48
17:Bb:41:LEU:HD23	17:Bb:41:LEU:H	1.78	0.48
21:BK:39:ASN:HA	21:BK:42:VAL:HG12	1.96	0.48
26:BT:34:VAL:HG13	26:BT:53:TRP:HE1	1.78	0.48
34:B5:1071:U:H2'	34:B5:1072:C:C6	2.49	0.48
34:B5:1114:G:O2'	34:B5:1130:G:O6	2.31	0.48
34:B5:1223:A:H2'	34:B5:1224:A:C8	2.49	0.48
34:B5:1770:U:H2'	34:B5:1771:U:C6	2.49	0.48
38:A1:275:U:H2'	38:A1:276:U:C6	2.49	0.48
38:A1:1084:A:H2'	38:A1:1085:A:C8	2.49	0.48
38:A1:2407:C:H2'	38:A1:2408:U:H6	1.79	0.48
38:A1:3334:U:H4'	38:A1:3335:A:H5'	1.94	0.48
43:AF:120:THR:HB	56:AT:132:PRO:HB2	1.94	0.48
69:Ag:100:ILE:HA	69:Ag:103:LYS:NZ	2.28	0.48
74:Al:44:TRP:CE2	74:Al:45:ARG:HG3	2.49	0.48
19:BD:157:LEU:HD21	19:BD:187:LYS:HD2	1.96	0.48
34:B5:300:A:H2'	34:B5:301:A:C8	2.49	0.48
34:B5:700:C:H2'	34:B5:701:U:C6	2.49	0.48
36:AB:123:TYR:CZ	36:AB:124:LYS:HG3	2.49	0.48
38:A1:673:U:H2'	38:A1:674:G:C8	2.49	0.48
38:A1:2427:U:H2'	38:A1:2428:U:C6	2.49	0.48
38:A1:2505:U:H2'	38:A1:2506:U:C6	2.49	0.48
41:AD:41:LYS:HD2	56:AT:93:VAL:HG11	1.94	0.48
44:AG:106:LYS:O	44:AG:110:THR:HG23	2.14	0.48
46:Al:52:LEU:HB3	46:Al:136:PHE:HB2	1.95	0.48
67:Ae:96:ILE:HG21	67:Ae:105:ARG:HG2	1.96	0.48
2:BB:136:ARG:HB3	2:BB:216:LYS:HG3	1.96	0.47
2:BB:176:VAL:HG22	2:BB:184:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BJ:103:ASP:HA	8:BJ:106:GLU:OE2	2.14	0.47
34:B5:826:U:H3	34:B5:846:G:N2	2.11	0.47
38:A1:1072:G:H2'	38:A1:1073:U:C6	2.49	0.47
38:A1:2441:A:H5''	38:A1:2508:U:H3	1.79	0.47
38:A1:2506:U:HO2'	38:A1:2507:C:P	2.36	0.47
40:A4:74:U:C4	61:AY:74:TYR:CD1	3.02	0.47
55:AS:71:LYS:O	55:AS:73:LYS:NZ	2.44	0.47
7:BI:32:GLN:HE22	34:B5:1727:G:H21	1.63	0.47
7:BI:37:LYS:C	7:BI:59:ARG:HA	2.40	0.47
12:BV:32:VAL:HG13	12:BV:60:ARG:NH1	2.28	0.47
19:BD:163:PRO:HA	19:BD:166:ASP:HB2	1.95	0.47
22:BP:56:PHE:O	22:BP:60:LEU:HD23	2.14	0.47
28:BZ:47:TYR:HA	28:BZ:50:ILE:HG22	1.96	0.47
36:AB:5:LYS:O	36:AB:5:LYS:HG2	2.15	0.47
38:A1:129:U:H2'	38:A1:130:A:H8	1.79	0.47
38:A1:1412:G:OP1	67:Ae:105:ARG:NH1	2.43	0.47
38:A1:2207:A:O2'	38:A1:2208:A:N3	2.47	0.47
38:A1:2268:U:H3	38:A1:2272:G:H22	1.62	0.47
38:A1:2848:G:OP1	75:Am:100:TYR:OH	2.18	0.47
38:A1:3291:G:H2'	38:A1:3292:A:C8	2.49	0.47
38:A1:3371:G:H2'	38:A1:3372:A:C8	2.48	0.47
44:AG:33:ASN:O	44:AG:39:ALA:HB3	2.13	0.47
49:AM:103:ILE:O	49:AM:107:GLU:OE1	2.31	0.47
54:AR:109:TYR:HB3	54:AR:115:ILE:HG12	1.96	0.47
63:Aa:84:GLU:HA	63:Aa:87:ARG:HB2	1.95	0.47
73:Ak:32:ASN:CG	73:Ak:36:LYS:H	2.22	0.47
15:BY:91:LEU:HB3	15:BY:97:ALA:HB3	1.96	0.47
31:Bg:114:ASP:O	31:Bg:122:ILE:HD12	2.14	0.47
34:B5:407:A:H2'	34:B5:408:C:H6	1.79	0.47
34:B5:648:G:H2'	34:B5:649:U:C6	2.49	0.47
34:B5:1383:G:H2'	34:B5:1384:A:C8	2.48	0.47
38:A1:168:U:H2'	38:A1:169:U:C6	2.49	0.47
38:A1:589:A:H8	38:A1:590:G:C8	2.32	0.47
38:A1:2585:G:H2'	38:A1:2585:G:N3	2.29	0.47
38:A1:2662:G:H2'	38:A1:2663:G:C8	2.48	0.47
38:A1:2769:A:O3'	77:Ao:80:ARG:HB2	2.14	0.47
52:AP:122:ALA:HB3	52:AP:143:PRO:HB2	1.95	0.47
5:BG:208:TYR:CZ	5:BG:212:LEU:HD21	2.49	0.47
8:BJ:20:GLU:HG3	8:BJ:23:ARG:HG3	1.96	0.47
21:BK:38:LYS:HG3	21:BK:41:TYR:H	1.78	0.47
26:BT:120:GLY:O	34:B5:1498:G:O2'	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BU:19:ILE:HG21	27:BU:94:GLU:HB2	1.95	0.47
33:BM:68:GLU:HG3	33:BM:70:ASN:H	1.79	0.47
34:B5:282:C:H2'	34:B5:283:U:O4'	2.15	0.47
34:B5:367:A:H2'	34:B5:368:U:O4'	2.13	0.47
38:A1:1073:U:H2'	38:A1:1074:U:C6	2.50	0.47
38:A1:2443:A:N7	38:A1:2444:C:O2'	2.45	0.47
38:A1:2680:A:C2	47:AJ:57:PHE:HB3	2.50	0.47
38:A1:2883:U:H2'	38:A1:2884:C:H6	1.78	0.47
40:A4:79:A:H2'	40:A4:80:A:C8	2.49	0.47
52:AP:116:HIS:HB3	52:AP:149:VAL:HB	1.95	0.47
1:BA:39:ASN:OD1	1:BA:40:ALA:N	2.47	0.47
34:B5:385:A:H2'	34:B5:386:G:C8	2.49	0.47
34:B5:1458:G:O2'	34:B5:1459:C:OP1	2.26	0.47
34:B5:1609:U:H2'	34:B5:1610:G:O4'	2.13	0.47
38:A1:577:C:O2'	38:A1:579:G:OP1	2.30	0.47
38:A1:792:G:H2'	38:A1:793:C:C6	2.50	0.47
38:A1:3107:U:H2'	38:A1:3108:G:C8	2.49	0.47
38:A1:3302:U:H3	38:A1:3312:U:H3	1.63	0.47
47:AJ:164:LYS:HE2	47:AJ:171:VAL:HG22	1.97	0.47
51:AO:54[A]:TYR:CE1	51:AO:145[A]:VAL:HG11	2.49	0.47
52:AP:13:LYS:HD2	52:AP:152:GLU:OE1	2.14	0.47
56:AT:143:THR:HG23	56:AT:148:PRO:HD3	1.96	0.47
76:An:1:MET:CE	76:An:6:ARG:HE	2.28	0.47
80:tA:14:A:C2'	80:tA:15:G:H4'	2.41	0.47
26:BT:86:ARG:HD2	26:BT:92:LYS:HG2	1.96	0.47
34:B5:1183:A:N3	34:B5:1210:C:O2'	2.43	0.47
34:B5:1297:G:N2	34:B5:1300:A:OP2	2.35	0.47
38:A1:1120:A:H2'	38:A1:1121:U:C6	2.49	0.47
38:A1:1482:A:H2'	38:A1:1482:A:N3	2.30	0.47
38:A1:2093:A:H2	38:A1:2094:C:C2	2.32	0.47
38:A1:2588:U:OP1	44:AG:241:LYS:NZ	2.47	0.47
45:AH:22:SER:O	45:AH:23:ARG:HD3	2.15	0.47
45:AH:90:MET:HG2	45:AH:181:VAL:HA	1.97	0.47
47:AJ:92:ARG:HH12	47:AJ:94:ARG:NH1	2.11	0.47
56:AT:115:LYS:HB3	56:AT:126:VAL:HG21	1.96	0.47
58:AV:81:GLN:HG2	58:AV:83:LYS:H	1.80	0.47
63:Aa:45:MET:HE2	63:Aa:45:MET:HA	1.96	0.47
1:BA:134:LYS:O	1:BA:138:TYR:HD1	1.98	0.47
4:BE:11:ARG:NH1	4:BE:20:LEU:HB3	2.29	0.47
5:BG:31:ARG:HH12	34:B5:1682:U:P	2.37	0.47
15:BY:112:LYS:NZ	34:B5:57:G:OP1	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BD:75:LYS:NZ	21:BK:20:VAL:HG23	2.28	0.47
20:BF:72:HIS:NE2	34:B5:1610:G:OP1	2.39	0.47
22:BP:75:PRO:HB3	22:BP:104:GLN:HE22	1.80	0.47
23:BQ:50:GLU:OE1	23:BQ:82:ARG:NH2	2.33	0.47
26:BT:18:TYR:CD1	26:BT:135:ILE:HG13	2.49	0.47
26:BT:71:VAL:HG12	26:BT:76:LEU:HD22	1.96	0.47
26:BT:82:GLY:HA2	34:B5:1525:A:OP1	2.15	0.47
28:BZ:91:PRO:HB3	28:BZ:101:TYR:CE2	2.50	0.47
28:BZ:92:ILE:HD13	28:BZ:100:ILE:HG22	1.97	0.47
33:BM:58:LEU:HA	33:BM:86:VAL:HG23	1.96	0.47
34:B5:604:A:H2'	34:B5:605:A:O4'	2.15	0.47
34:B5:852:C:H2'	34:B5:853:G:O4'	2.14	0.47
34:B5:1041:G:H2'	34:B5:1042:G:C8	2.50	0.47
34:B5:1330:G:H2'	34:B5:1331:A:O4'	2.15	0.47
34:B5:1466:G:H2'	34:B5:1467:C:C6	2.50	0.47
35:AA:10:LYS:HA	35:AA:16:PHE:CD2	2.50	0.47
36:AB:143:GLY:O	36:AB:147:GLU:HG2	2.15	0.47
38:A1:1048:A:H2'	46:AI:22:TYR:CZ	2.50	0.47
38:A1:1231:A:N6	38:A1:1276:U:OP2	2.47	0.47
38:A1:1667:A:H2'	38:A1:1668:G:H8	1.79	0.47
38:A1:1746:U:O2'	73:AK:4:GLU:OE1	2.24	0.47
38:A1:2265:C:H2'	38:A1:2266:PSU:C6	2.49	0.47
38:A1:2824:G:H2'	38:A1:2825:C:H6	1.80	0.47
39:A3:4:U:H2'	39:A3:5:G:C8	2.50	0.47
39:A3:71:G:H2'	39:A3:72:A:C8	2.50	0.47
40:A4:95:G:O2'	72:AJ:81:GLY:O	2.27	0.47
44:AG:81:THR:HG21	44:AG:181:LYS:HG3	1.96	0.47
46:AI:36:LEU:HD12	46:AI:87:LEU:HD23	1.96	0.47
54:AR:136:ARG:O	54:AR:140:GLU:HG3	2.15	0.47
55:AS:2:ALA:HB1	55:AS:104:GLU:HG2	1.95	0.47
6:BH:62:VAL:HG22	6:BH:70:PHE:HE2	1.79	0.47
7:BI:44:HIS:ND1	34:B5:1676:U:OP1	2.42	0.47
8:BJ:17:ARG:O	8:BJ:23:ARG:NH2	2.42	0.47
8:BJ:87:SER:H	8:BJ:90:LYS:NZ	2.12	0.47
20:BF:152:GLY:HA2	81:MR:-2:A:C8	2.50	0.47
22:BP:15:HIS:CE1	22:BP:110:GLU:HG3	2.50	0.47
34:B5:1321:A:H4'	34:B5:1322:A:O5'	2.15	0.47
35:AA:181:LYS:HB2	38:A1:860:G:C5	2.50	0.47
37:AC:138:ARG:HH21	37:AC:240:PRO:HG2	1.78	0.47
38:A1:209:A:H4'	38:A1:211:A:N7	2.30	0.47
38:A1:627:U:H2'	38:A1:628:A:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1267:U:H3	38:A1:1274:A:N6	2.13	0.47
38:A1:1616:U:H2'	38:A1:1617:G:C8	2.50	0.47
38:A1:2596:U:H2'	38:A1:2597:U:C6	2.50	0.47
39:A3:27:A:H2'	39:A3:28:C:C6	2.49	0.47
80:tA:58:A:H1'	80:tA:60:A:OP2	2.14	0.47
1:BA:180:GLU:OE2	1:BA:191:ARG:NH1	2.34	0.47
6:BH:114:ARG:HG3	34:B5:860:U:O4'	2.15	0.47
6:BH:130:VAL:HG21	6:BH:154:LEU:HD21	1.97	0.47
7:BI:83:TYR:HB3	7:BI:101:ILE:HB	1.97	0.47
10:BN:26:PHE:CZ	10:BN:28:LEU:HB2	2.50	0.47
16:Ba:26:CYS:O	16:Ba:27:SER:OG	2.31	0.47
25:BS:17:LEU:O	25:BS:20:THR:OG1	2.33	0.47
28:BZ:54:VAL:HG11	28:BZ:83:LEU:HD23	1.97	0.47
34:B5:751:G:H2'	34:B5:752:A:C8	2.50	0.47
34:B5:872:G:H2'	34:B5:873:U:O4'	2.15	0.47
38:A1:100:A:H2'	38:A1:101:G:N3	2.30	0.47
38:A1:385:A:H2'	38:A1:386:A:C8	2.50	0.47
38:A1:422:A:C2	38:A1:2363:A:H4'	2.49	0.47
38:A1:975:C:H2'	38:A1:976:U:C6	2.50	0.47
38:A1:1223:A:OP2	38:A1:1223:A:H8	1.98	0.47
38:A1:1666:G:H2'	38:A1:1667:A:H8	1.80	0.47
38:A1:2723:U:H2'	38:A1:2724:U:C6	2.49	0.47
41:AD:41:LYS:HB2	56:AT:68:THR:O	2.14	0.47
41:AD:160:PHE:HA	41:AD:163:LEU:HB3	1.97	0.47
62:AZ:47:GLU:OE1	62:AZ:69:LYS:NZ	2.46	0.47
2:BB:156:ALA:HB3	2:BB:161:ILE:HD11	1.97	0.47
4:BE:175:PHE:HE1	4:BE:198:LYS:HD2	1.80	0.47
6:BH:30:SER:O	6:BH:34:LEU:N	2.47	0.47
8:BJ:145:SER:OG	34:B5:474:A:OP1	2.25	0.47
19:BD:3:ALA:N	34:B5:1491:U:OP2	2.47	0.47
20:BF:126:ASP:OD1	20:BF:126:ASP:N	2.48	0.47
34:B5:424:C:O2'	34:B5:426:G:OP1	2.27	0.47
34:B5:565:C:H2'	34:B5:577:G:C4	2.50	0.47
34:B5:828:U:O2'	34:B5:829:A:O4'	2.33	0.47
34:B5:1078:C:H2'	34:B5:1079:U:C6	2.50	0.47
34:B5:1175:U:H2'	34:B5:1176:G:H8	1.80	0.47
36:AB:173:GLN:O	36:AB:174:LYS:HB2	2.15	0.47
38:A1:169:U:H4'	48:AL:128:ARG:CZ	2.45	0.47
38:A1:299:G:C4	71:AI:31:GLY:HA3	2.50	0.47
38:A1:664:U:H2'	38:A1:665:A:H8	1.78	0.47
38:A1:1597:C:H2'	38:A1:1598:G:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2615:G:H2'	38:A1:2616:C:H6	1.80	0.47
38:A1:3332:U:H2'	38:A1:3333:G:O4'	2.15	0.47
77:Ao:4:VAL:O	77:Ao:94:GLY:N	2.42	0.47
78:Ap:84:ARG:HG2	78:Ap:87:ARG:HH22	1.79	0.47
2:BB:149:GLN:HG3	34:B5:1066:C:H4'	1.97	0.46
3:BC:119:LYS:NZ	34:B5:1291:G:H5'	2.29	0.46
4:BE:246:LEU:HB3	4:BE:250:GLU:HG3	1.96	0.46
6:BH:141:ARG:HG2	13:BW:51:GLU:OE1	2.15	0.46
9:BL:40:LEU:HG	34:B5:246:G:N3	2.30	0.46
15:BY:27:VAL:HG21	15:BY:35:VAL:HG11	1.97	0.46
24:BR:34:LEU:O	24:BR:38:ILE:HG12	2.15	0.46
27:BU:87:HIS:HB3	27:BU:89:ARG:NH1	2.30	0.46
31:Bg:157:VAL:HG21	31:Bg:208:GLY:HA2	1.97	0.46
34:B5:58:U:OP1	34:B5:456:A:O2'	2.31	0.46
34:B5:218:A:N1	34:B5:843:U:C4	2.83	0.46
37:AC:60:THR:HG23	38:A1:364:G:OP1	2.15	0.46
38:A1:175:C:H2'	38:A1:176:G:C8	2.50	0.46
38:A1:1211:U:H2'	38:A1:1212:A:C8	2.51	0.46
38:A1:3209:A:C5	49:AM:106:ARG:HD3	2.49	0.46
40:A4:142:C:H2'	40:A4:143:U:H6	1.78	0.46
58:AV:109:MET:HE1	58:AV:114:ILE:HG13	1.97	0.46
8:BJ:169:PRO:HG2	8:BJ:174:ARG:HG3	1.98	0.46
29:Bc:8:THR:HG22	29:Bc:56:LEU:HB2	1.96	0.46
34:B5:1107:G:O2'	34:B5:1108:G:H5'	2.16	0.46
34:B5:1371:A:H4'	34:B5:1373:C:OP1	2.16	0.46
34:B5:1458:G:H2'	34:B5:1458:G:N3	2.30	0.46
38:A1:1460:A:H2'	38:A1:1461:A:C8	2.49	0.46
38:A1:1601:U:OP1	54:AR:42:ARG:NH2	2.43	0.46
38:A1:3050:U:O2'	59:AW:16:GLY:O	2.32	0.46
38:A1:3095:U:H2'	38:A1:3096:C:C6	2.50	0.46
51:AO:189[A]:ASP:O	51:AO:193[A]:GLN:HG3	2.16	0.46
56:AT:119:ALA:HA	56:AT:122:GLN:O	2.15	0.46
63:Aa:36:GLY:HA3	63:Aa:40:HIS:CE1	2.50	0.46
3:BC:219:GLY:O	12:BV:25:LYS:NZ	2.49	0.46
24:BR:60:ARG:HD2	34:B5:1400:A:H5'	1.96	0.46
31:Bg:111:MET:H	31:Bg:126:SER:HA	1.79	0.46
31:Bg:266:ASP:HB2	31:Bg:267:PRO:HD3	1.98	0.46
34:B5:947:U:H2'	34:B5:948:G:C8	2.50	0.46
38:A1:585:A:H5''	68:Af:70:LYS:HE3	1.97	0.46
38:A1:1799:A:H2'	38:A1:1800:A:H8	1.81	0.46
38:A1:2200:U:H2'	38:A1:2201:G:O4'	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:3198:U:O2	45:AH:21:LYS:N	2.48	0.46
20:BF:143:ARG:HH21	29:Bc:57:MET:HE1	1.80	0.46
34:B5:1353:U:O2'	34:B5:1354:G:N7	2.39	0.46
37:AC:181:VAL:O	37:AC:182:LEU:HG	2.16	0.46
38:A1:167:U:H2'	38:A1:168:U:H6	1.81	0.46
38:A1:2991:A:O2'	38:A1:3309:G:N7	2.48	0.46
38:A1:3150:A:H2'	38:A1:3151:U:O4'	2.15	0.46
43:AF:184:LEU:O	43:AF:188:ILE:HG12	2.15	0.46
43:AF:239:LEU:O	43:AF:243:MET:HG3	2.15	0.46
44:AG:55:TYR:HA	44:AG:58:VAL:HG12	1.96	0.46
58:AV:10:LYS:HB2	58:AV:125:LEU:HD11	1.97	0.46
62:AZ:41:ALA:HB2	62:AZ:77:TYR:HE1	1.80	0.46
4:BE:31:PRO:HG2	4:BE:38:LEU:HB2	1.97	0.46
5:BG:137:ARG:NH2	34:B5:144:U:O4	2.44	0.46
6:BH:50:ASP:HB3	6:BH:56:LYS:HG2	1.98	0.46
9:BL:152:GLN:HB3	10:BN:137:PRO:HD3	1.98	0.46
10:BN:60:VAL:HG23	10:BN:66:ILE:HD12	1.97	0.46
12:BV:30:ALA:O	12:BV:60:ARG:HD3	2.15	0.46
21:BK:1:MET:HE1	21:BK:40:LEU:HD23	1.98	0.46
34:B5:17:C:H2'	34:B5:18:C:C6	2.49	0.46
34:B5:499:U:O2'	34:B5:500:C:H5'	2.15	0.46
34:B5:607:G:H5'	34:B5:613:G:N2	2.31	0.46
34:B5:1502:G:N2	34:B5:1505:A:OP2	2.39	0.46
34:B5:1692:G:H5''	34:B5:1693:A:C8	2.50	0.46
38:A1:80:G:H2'	38:A1:81:C:H6	1.80	0.46
38:A1:602:A:HO2'	38:A1:603:A:P	2.37	0.46
38:A1:963:G:O2'	63:Aa:29:PRO:O	2.33	0.46
38:A1:992:A:O2'	38:A1:993:G:H5'	2.15	0.46
38:A1:1577:G:O2'	38:A1:1578:C:O5'	2.32	0.46
38:A1:1771:C:H2'	38:A1:1772:U:O4'	2.16	0.46
38:A1:2609:A:H2'	38:A1:2610:G:C8	2.50	0.46
38:A1:2674:A:H5''	47:AJ:105:GLY:HA3	1.97	0.46
41:AD:143:LYS:HD3	41:AD:145:PHE:CZ	2.50	0.46
80:tA:61:C:H2'	80:tA:62:C:C6	2.51	0.46
2:BB:150:VAL:H	34:B5:1067:C:H5''	1.81	0.46
4:BE:79:ASP:HB3	4:BE:82:TYR:HB2	1.98	0.46
8:BJ:119:ALA:O	8:BJ:120:LYS:HG2	2.16	0.46
11:BO:47:LYS:NZ	11:BO:62:LEU:O	2.48	0.46
34:B5:1382:A:O2'	34:B5:1383:G:H8	1.99	0.46
34:B5:1550:A:H2'	34:B5:1551:U:C6	2.50	0.46
38:A1:39:A:H5''	63:Aa:35:ALA:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:873:C:H5''	38:A1:874:U:O5'	2.16	0.46
38:A1:1003:A:N1	38:A1:1049:C:O2'	2.43	0.46
38:A1:1666:G:H2'	38:A1:1667:A:C8	2.50	0.46
38:A1:1770:G:H2'	38:A1:1771:C:C6	2.50	0.46
38:A1:2540:A:H4'	38:A1:2541:U:H5'	1.98	0.46
38:A1:2615:G:H2'	38:A1:2616:C:C6	2.51	0.46
38:A1:3252:G:H2'	38:A1:3253:G:C8	2.51	0.46
55:AS:1:MET:HA	55:AS:1:MET:HE3	1.96	0.46
80:tA:43:G:H2'	80:tA:44:A:H8	1.79	0.46
6:BH:163:ASP:HA	6:BH:166:LEU:HG	1.97	0.46
15:BY:106:GLN:NE2	34:B5:442:C:OP2	2.49	0.46
22:BP:109:PRO:O	22:BP:112:LEU:HD23	2.14	0.46
23:BQ:35:PRO:HD3	26:BT:8:ASP:OD2	2.16	0.46
29:Bc:21:SER:OG	29:Bc:22:ARG:HD2	2.16	0.46
32:Bf:105:TYR:HA	32:Bf:131:PHE:HZ	1.80	0.46
32:Bf:119:ARG:HB2	32:Bf:132:LEU:HD12	1.96	0.46
34:B5:69:G:H2'	34:B5:70:C:C6	2.51	0.46
34:B5:215:A:H2'	34:B5:216:U:O4'	2.14	0.46
34:B5:518:A:N3	34:B5:534:A:N6	2.63	0.46
34:B5:647:G:N2	34:B5:687:G:H1	2.13	0.46
34:B5:739:G:O2'	34:B5:740:A:H5'	2.16	0.46
34:B5:1236:A:H2'	34:B5:1237:G:C8	2.49	0.46
38:A1:93:C:C2	63:Aa:55:LYS:HE2	2.51	0.46
38:A1:1037:C:H2'	38:A1:1038:C:H6	1.81	0.46
38:A1:1054:A:H5''	38:A1:2637:A:H61	1.81	0.46
38:A1:1193:A:OP1	51:AO:49[A]:ARG:NH2	2.48	0.46
54:AR:180:LYS:HA	54:AR:184:LEU:HB3	1.97	0.46
62:AZ:32:GLY:HA2	62:AZ:40:HIS:CE1	2.50	0.46
79:tP:19:G:N2	79:tP:57:G:H1'	2.30	0.46
19:BD:11:LEU:HD12	27:BU:86:ILE:HD13	1.98	0.46
19:BD:29:LEU:HD22	19:BD:32:GLU:OE1	2.16	0.46
34:B5:187:G:N2	34:B5:198:A:N7	2.62	0.46
34:B5:1469:A:H2'	34:B5:1470:C:C6	2.51	0.46
34:B5:1606:C:H2'	34:B5:1607:G:C8	2.50	0.46
38:A1:421:G:O6	38:A1:2383:C:O2'	2.22	0.46
38:A1:544:C:H4'	38:A1:548:G:H22	1.80	0.46
38:A1:616:G:H2'	38:A1:617:G:C8	2.51	0.46
38:A1:630:A:H2'	38:A1:631:U:C6	2.51	0.46
38:A1:1279:C:H2'	38:A1:1280:C:C6	2.51	0.46
38:A1:1478:C:H2'	38:A1:1479:U:C6	2.51	0.46
38:A1:2148:U:H2'	38:A1:2149:A:C5	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2389:C:H2'	38:A1:2390:A:C8	2.51	0.46
38:A1:2426:U:H2'	38:A1:2427:U:H6	1.79	0.46
38:A1:2709:C:H2'	38:A1:2710:C:C6	2.51	0.46
38:A1:3322:A:H2'	38:A1:3323:A:H8	1.79	0.46
1:BA:76:ILE:HB	1:BA:123:VAL:HG12	1.98	0.46
2:BB:57:ALA:HA	2:BB:60:ALA:HB3	1.98	0.46
7:BI:107:THR:HB	7:BI:108:PRO:HD3	1.97	0.46
8:BJ:144:PRO:HD2	34:B5:474:A:H5''	1.98	0.46
10:BN:20:ARG:O	10:BN:65:VAL:HG13	2.16	0.46
15:BY:58:PHE:HB2	15:BY:72:PHE:HB3	1.98	0.46
31:Bg:116:ASP:OD2	31:Bg:120:SER:HB2	2.16	0.46
34:B5:472:U:H2'	34:B5:473:A:C8	2.51	0.46
34:B5:1291:G:H1	34:B5:1324:G:N2	1.97	0.46
34:B5:1767:G:OP1	34:B5:1770:U:H4'	2.16	0.46
36:AB:266:ARG:HD3	38:A1:2988:C:O2'	2.16	0.46
38:A1:270:U:H2'	38:A1:271:C:H6	1.80	0.46
38:A1:433:A:OP2	68:Af:57:LYS:NZ	2.40	0.46
38:A1:1791:C:H2'	38:A1:1792:C:C6	2.50	0.46
38:A1:1805:C:H2'	38:A1:1806:A:H8	1.80	0.46
38:A1:2204:C:H6	38:A1:2204:C:H5''	1.80	0.46
38:A1:2373:A:N3	38:A1:2824:G:O2'	2.39	0.46
38:A1:2714:G:H4'	38:A1:2715:A:H5''	1.98	0.46
38:A1:3072:C:H2'	38:A1:3073:A:O4'	2.15	0.46
38:A1:3170:A:H2'	38:A1:3171:U:C6	2.51	0.46
38:A1:3209:A:C4	49:AM:106:ARG:HD3	2.51	0.46
39:A3:90:U:H2'	39:A3:91:G:O4'	2.15	0.46
46:AI:93:PRO:HB2	46:AI:125:LEU:HB3	1.98	0.46
46:AI:177:ASP:HB3	46:AI:179:PRO:HD2	1.98	0.46
54:AR:134:HIS:CD2	54:AR:136:ARG:HG2	2.50	0.46
1:BA:88:LYS:NZ	24:BR:82:ASP:O	2.39	0.46
4:BE:45:ILE:HG13	4:BE:61:VAL:HG21	1.98	0.46
6:BH:56:LYS:HD3	6:BH:88:ARG:HH21	1.80	0.46
16:Ba:33:ASP:OD1	16:Ba:33:ASP:N	2.49	0.46
21:BK:48:SER:HA	34:B5:1219:A:O2'	2.15	0.46
23:BQ:36:ILE:HD11	23:BQ:48:VAL:HG12	1.98	0.46
23:BQ:60:PHE:HA	23:BQ:63:ILE:HG22	1.97	0.46
34:B5:12:U:H2'	34:B5:13:C:H6	1.79	0.46
34:B5:819:G:O6	34:B5:853:G:N2	2.49	0.46
38:A1:411:U:H2'	38:A1:412:G:H8	1.81	0.46
38:A1:663:C:H2'	38:A1:664:U:C6	2.51	0.46
38:A1:1635:G:N2	38:A1:1638:A:OP2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1740:U:H1'	38:A1:1741:A:H2	1.81	0.46
38:A1:2813:A:H2'	38:A1:2814:G:O4'	2.16	0.46
38:A1:3358:U:H2'	38:A1:3359:A:H8	1.81	0.46
43:AF:221:LYS:HB2	43:AF:227:GLY:HA3	1.98	0.46
45:AH:7:GLU:OE1	45:AH:9:GLN:NE2	2.49	0.46
53:AQ:106:PHE:CE2	53:AQ:121:CYS:HB3	2.51	0.46
61:AY:74:TYR:HE2	61:AY:77:LYS:HE3	1.78	0.46
79:tP:24:G:H2'	79:tP:25:C:C6	2.51	0.46
6:BH:67:LEU:O	6:BH:71:HIS:HD2	1.99	0.45
11:BO:19:ILE:HD11	11:BO:105:LEU:HD12	1.97	0.45
11:BO:82:LYS:NZ	11:BO:116:GLU:OE1	2.48	0.45
21:BK:11:ILE:HD13	21:BK:42:VAL:HA	1.98	0.45
31:Bg:197:SER:HB2	31:Bg:216:LYS:HB3	1.98	0.45
36:AB:128:LYS:NZ	38:A1:3151:U:OP1	2.48	0.45
38:A1:649:A:H2'	38:A1:650:C:C6	2.51	0.45
38:A1:1715:A:N7	65:Ac:84:LEU:HD12	2.30	0.45
38:A1:2441:A:H2'	38:A1:2442:G:O4'	2.15	0.45
38:A1:2655:U:H4'	38:A1:2656:A:O4'	2.16	0.45
39:A3:121:U:H5''	41:AD:260:PHE:HD2	1.81	0.45
41:AD:40:HIS:CE1	41:AD:42:ALA:HB3	2.51	0.45
44:AG:78:PHE:C	44:AG:80:TYR:H	2.24	0.45
67:Ae:3:SER:HB3	67:Ae:71:HIS:CE1	2.51	0.45
1:BA:34:GLU:O	1:BA:37:VAL:HG12	2.16	0.45
2:BB:66:VAL:HG13	11:BO:33:LEU:HG	1.98	0.45
5:BG:179:VAL:HG11	34:B5:140:A:H1'	1.98	0.45
16:Ba:44:ILE:HG23	16:Ba:45:VAL:HG13	1.98	0.45
19:BD:16:VAL:O	19:BD:20:GLU:HG2	2.16	0.45
23:BQ:101:SER:HA	23:BQ:104:GLU:OE1	2.16	0.45
24:BR:56:HIS:NE2	34:B5:1401:A:OP1	2.30	0.45
33:BM:45:LEU:HD23	33:BM:45:LEU:H	1.82	0.45
34:B5:71:A:HO2'	34:B5:72:A:P	2.39	0.45
34:B5:239:C:H2'	34:B5:241:U:H5''	1.98	0.45
34:B5:1320:U:O2	34:B5:1322:A:H5'	2.16	0.45
36:AB:287:LYS:HE2	36:AB:287:LYS:HA	1.98	0.45
37:AC:11:LEU:HD13	37:AC:159:ILE:HD11	1.98	0.45
37:AC:181:VAL:C	37:AC:183:LYS:H	2.24	0.45
38:A1:109:A:N1	38:A1:322:U:O2'	2.46	0.45
38:A1:2207:A:O2'	38:A1:2208:A:H5''	2.15	0.45
39:A3:76:A:N6	39:A3:103:A:N7	2.59	0.45
47:AJ:12:LEU:HB3	47:AJ:131:MET:CE	2.45	0.45
50:AN:147:ARG:HG3	70:Ah:101:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BI:53:LYS:HE3	7:BI:55:TYR:OH	2.16	0.45
15:BY:125:LEU:O	15:BY:129:VAL:HG22	2.16	0.45
28:BZ:81:ARG:O	28:BZ:84:GLU:HG3	2.16	0.45
31:Bg:32:LEU:HD21	31:Bg:94:VAL:HG11	1.98	0.45
34:B5:956:C:H2'	34:B5:957:G:H8	1.81	0.45
37:AC:11:LEU:HD21	37:AC:156:LEU:HB2	1.99	0.45
38:A1:632:G:H2'	38:A1:633:C:C6	2.51	0.45
38:A1:1470:U:H2'	38:A1:1471:U:C6	2.51	0.45
38:A1:1951:C:H2'	38:A1:1952:G:H8	1.80	0.45
38:A1:2344:U:H2'	38:A1:2345:A:C8	2.52	0.45
38:A1:3042:U:OP2	38:A1:3092:C:N4	2.39	0.45
38:A1:3295:A:H2'	38:A1:3296:A:H8	1.80	0.45
40:A4:97:A:OP1	70:Ah:63:ARG:NH2	2.37	0.45
45:AH:103:ILE:HG12	45:AH:136:PHE:CE2	2.51	0.45
56:AT:152:ALA:HB1	56:AT:153:PRO:HD2	1.99	0.45
58:AV:86:ARG:HB2	58:AV:92:PHE:CE2	2.50	0.45
79:tP:70:G:C8	79:tP:70:G:H5''	2.51	0.45
80:tA:67:G:H2'	80:tA:68:G:C8	2.52	0.45
1:BA:14:ALA:O	1:BA:18:LEU:HD23	2.16	0.45
16:Ba:39:MET:HG3	16:Ba:41:ILE:HG13	1.98	0.45
19:BD:25:PHE:CZ	19:BD:50:ILE:HD11	2.52	0.45
19:BD:25:PHE:HZ	19:BD:86:LEU:HD11	1.82	0.45
20:BF:132:VAL:HG11	20:BF:199:ILE:HD13	1.99	0.45
22:BP:57:MET:HE2	22:BP:57:MET:HA	1.97	0.45
22:BP:60:LEU:HD22	22:BP:76:VAL:HG11	1.99	0.45
25:BS:40:ARG:CZ	34:B5:1539:G:H4'	2.47	0.45
25:BS:139:LYS:HE3	34:B5:1177:C:N4	2.32	0.45
28:BZ:59:TYR:HE1	28:BZ:100:ILE:HG23	1.81	0.45
34:B5:1079:U:H2'	34:B5:1080:U:C6	2.52	0.45
36:AB:92:TYR:HB3	36:AB:99:LEU:HD11	1.98	0.45
38:A1:1221:A:H3'	38:A1:1222:G:C4'	2.41	0.45
38:A1:1460:A:H2'	38:A1:1461:A:H8	1.82	0.45
38:A1:1576:G:H2'	38:A1:1577:G:H8	1.82	0.45
38:A1:1595:U:C2	38:A1:1596:C:C5	3.05	0.45
38:A1:1744:G:H2'	38:A1:1745:C:C6	2.51	0.45
38:A1:2890:A:O2'	38:A1:2933:A:N3	2.46	0.45
43:AF:86:VAL:O	43:AF:114:GLY:HA2	2.17	0.45
43:AF:98:LYS:HB3	43:AF:99:PRO:HD3	1.98	0.45
45:AH:87:LYS:HD3	45:AH:89:LYS:HE2	1.99	0.45
48:AL:50:PRO:O	48:AL:52:ASP:N	2.50	0.45
51:AO:174[A]:PHE:HD1	51:AO:177[A]:LYS:HD3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:160:ILE:HG22	1:BA:162:CYS:SG	2.56	0.45
3:BC:143:TYR:OH	3:BC:149:GLY:O	2.33	0.45
4:BE:3:ARG:HG2	34:B5:399:A:H4'	1.98	0.45
6:BH:27:LEU:O	6:BH:27:LEU:HD23	2.17	0.45
11:BO:37:GLU:OE1	11:BO:37:GLU:N	2.49	0.45
38:A1:253:A:H5''	38:A1:253:A:C8	2.52	0.45
40:A4:145:U:H2'	40:A4:146:U:C6	2.51	0.45
45:AH:93:VAL:HG22	75:Am:82:LEU:HB3	1.98	0.45
22:BP:29:SER:OG	22:BP:30:THR:N	2.50	0.45
34:B5:304:U:H2'	34:B5:305:C:C6	2.51	0.45
35:AA:223:SER:HG	38:A1:2244:A:HO2'	1.64	0.45
38:A1:393:U:H2'	38:A1:394:G:O4'	2.17	0.45
38:A1:1334:U:H2'	38:A1:1335:C:C6	2.52	0.45
39:A3:45:A:H2'	39:A3:46:A:C8	2.52	0.45
45:AH:27:VAL:HG12	45:AH:82:VAL:HG21	1.98	0.45
45:AH:91:ARG:NH2	45:AH:141:LYS:O	2.50	0.45
48:AL:90:ALA:HB1	48:AL:95:ILE:HB	1.99	0.45
70:Ah:56:THR:O	70:Ah:60:GLU:HG3	2.17	0.45
8:BJ:52:ILE:HG23	8:BJ:76:LEU:HD11	1.98	0.45
14:BX:44:GLY:H	14:BX:78:LYS:NZ	2.15	0.45
22:BP:85:ILE:HD13	22:BP:111:MET:HB3	1.99	0.45
26:BT:117:SER:HB2	26:BT:121:GLY:O	2.17	0.45
33:BM:32:LEU:HG	33:BM:41:LEU:HD11	1.98	0.45
36:AB:57:VAL:HG22	36:AB:73:VAL:HG22	1.98	0.45
36:AB:350:ALA:O	36:AB:351:LEU:HD23	2.17	0.45
38:A1:245:U:OP1	38:A1:245:U:H4'	2.17	0.45
38:A1:616:G:H2'	38:A1:617:G:H8	1.81	0.45
38:A1:3156:U:OP1	38:A1:3158:G:O2'	2.26	0.45
48:AL:166:ALA:N	63:Aa:135:GLU:OE2	2.50	0.45
53:AQ:123:THR:OG1	53:AQ:125:ASP:OD1	2.35	0.45
74:Al:43:ASN:HB3	74:Al:46:ARG:HE	1.82	0.45
7:BI:33:PRO:HA	34:B5:331:A:H5'	1.99	0.45
31:Bg:231:MET:SD	31:Bg:231:MET:N	2.82	0.45
33:BM:131:ASP:OD1	33:BM:131:ASP:N	2.50	0.45
34:B5:138:A:C8	34:B5:142:G:H5'	2.52	0.45
34:B5:546:U:H2'	34:B5:547:U:C6	2.52	0.45
35:AA:39:GLY:HA2	35:AA:93:LYS:HG2	1.99	0.45
35:AA:152:SER:OG	38:A1:2157:G:N7	2.43	0.45
36:AB:266:ARG:NH2	38:A1:2392:C:H1'	2.31	0.45
38:A1:373:A:N1	38:A1:394:G:H4'	2.32	0.45
38:A1:947:G:H5''	67:Ae:55:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:996:A:H2'	38:A1:997:A:O4'	2.16	0.45
40:A4:69:U:H2'	40:A4:70:G:O4'	2.17	0.45
56:AT:91:LEU:HD12	56:AT:96:ILE:HD11	1.99	0.45
72:Aj:39:TYR:CD1	72:Aj:40:PRO:HA	2.52	0.45
79:tP:48:C:C4	79:tP:59:A:C8	3.04	0.45
2:BB:28:GLU:OE2	2:BB:50:LYS:HA	2.17	0.45
2:BB:138:PHE:C	2:BB:212:VAL:O	2.60	0.45
7:BI:32:GLN:NE2	34:B5:1675:C:H1'	2.32	0.45
10:BN:25:TRP:HD1	17:Bb:82:LYS:HZ2	1.62	0.45
12:BV:74:GLN:NE2	12:BV:80:LYS:O	2.48	0.45
19:BD:164:VAL:O	19:BD:168:ILE:HB	2.17	0.45
33:BM:43:ARG:NH1	33:BM:103:LEU:H	2.15	0.45
34:B5:236:A:H5''	34:B5:237:C:C5	2.51	0.45
34:B5:253:A:H2'	34:B5:254:A:H8	1.82	0.45
34:B5:485:A:N1	34:B5:503:G:N2	2.65	0.45
34:B5:835:U:O4	34:B5:837:G:N2	2.50	0.45
36:AB:83:PRO:O	36:AB:165:GLN:NE2	2.47	0.45
36:AB:286:GLY:HA3	36:AB:321:PHE:CZ	2.52	0.45
38:A1:132:C:H2'	38:A1:133:U:H5''	1.99	0.45
38:A1:138:U:H2'	38:A1:139:G:H8	1.82	0.45
38:A1:548:G:H1'	38:A1:549:U:C5	2.52	0.45
38:A1:716:A:C6	63:Aa:117:ARG:HG3	2.52	0.45
38:A1:3162:C:H2'	38:A1:3163:A:H8	1.81	0.45
77:Ao:46:LYS:HE2	77:Ao:54:THR:HB	1.99	0.45
5:BG:139:ASN:OD1	5:BG:142:ARG:NH1	2.50	0.45
6:BH:104:ARG:NH2	34:B5:805:U:O4	2.44	0.45
8:BJ:11:THR:HG23	34:B5:472:U:H5''	1.98	0.45
12:BV:40:ASP:OD1	12:BV:44:ARG:HB2	2.17	0.45
20:BF:30:PRO:O	20:BF:34:GLN:HG2	2.17	0.45
25:BS:145:ARG:NH1	34:B5:1172:G:H5''	2.32	0.45
26:BT:76:LEU:HD12	26:BT:80:TYR:CE2	2.51	0.45
34:B5:1018:U:H2'	34:B5:1019:A:C8	2.52	0.45
36:AB:92:TYR:HB2	36:AB:157:VAL:HB	1.99	0.45
38:A1:371:G:H4'	38:A1:396:A:N1	2.32	0.45
38:A1:2502:A:H2'	38:A1:2503:G:O4'	2.16	0.45
38:A1:3020:U:H2'	38:A1:3033:A:H61	1.82	0.45
40:A4:27:U:H2'	40:A4:28:C:C6	2.52	0.45
41:AD:186:GLU:OE1	41:AD:186:GLU:N	2.49	0.45
45:AH:8:GLN:HB3	45:AH:72:LYS:HD2	1.99	0.45
45:AH:9:GLN:O	45:AH:72:LYS:HE2	2.17	0.45
47:AJ:109:HIS:CD2	47:AJ:112:LEU:HD13	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:AN:64:VAL:CG1	50:AN:102:ALA:HB1	2.47	0.45
51:AO:108[A]:ILE:HD12	51:AO:160[A]:ARG:CZ	2.47	0.45
54:AR:123:LEU:HD23	54:AR:126:GLU:OE2	2.17	0.45
77:Ao:2:VAL:N	77:Ao:90:HIS:O	2.50	0.45
80:tA:72:U:O4	80:tA:73:A:N6	2.49	0.45
26:BT:117:SER:OG	26:BT:123:ARG:HG2	2.16	0.44
31:Bg:106:HIS:HD1	31:Bg:110:VAL:HG22	1.82	0.44
34:B5:790:U:H2'	34:B5:791:A:H8	1.81	0.44
34:B5:1451:C:H2'	34:B5:1452:U:H6	1.82	0.44
38:A1:142:C:H2'	38:A1:143:G:O4'	2.17	0.44
42:AE:13:GLU:HA	67:Ae:4:LEU:HD11	1.99	0.44
44:AG:34:PHE:CD1	44:AG:42:PRO:HD3	2.52	0.44
45:AH:41:ILE:HG21	45:AH:71:VAL:HG21	1.99	0.44
51:AO:162[A]:VAL:O	51:AO:166[A]:GLU:OE1	2.35	0.44
53:AQ:62:VAL:HG13	53:AQ:66:ARG:HD2	1.99	0.44
53:AQ:158:HIS:H	53:AQ:186:VAL:CG1	2.30	0.44
54:AR:134:HIS:HD2	54:AR:136:ARG:HG2	1.82	0.44
58:AV:69:LEU:HD21	58:AV:110:LYS:HE2	1.99	0.44
68:Af:49:ILE:HD11	68:Af:71:VAL:HG22	2.00	0.44
78:Ap:38:ASP:OD1	78:Ap:45:LYS:HD3	2.16	0.44
2:BB:132:ASP:O	2:BB:221:PRO:HD3	2.17	0.44
14:BX:126:LYS:HG2	14:BX:131:SER:HA	1.97	0.44
22:BP:130:ARG:NH1	22:BP:131:ALA:O	2.50	0.44
23:BQ:100:GLN:O	23:BQ:104:GLU:OE1	2.35	0.44
31:Bg:64:HIS:ND1	31:Bg:86:ASP:OD2	2.50	0.44
34:B5:205:U:C2	34:B5:206:A:C8	3.05	0.44
34:B5:381:C:O2'	34:B5:755:A:N1	2.43	0.44
34:B5:1296:A:N1	34:B5:1301:U:H5	2.16	0.44
38:A1:237:G:H2'	38:A1:238:A:H8	1.80	0.44
38:A1:753:C:H2'	38:A1:754:G:H8	1.81	0.44
38:A1:958:C:C4	38:A1:960:PSU:H1'	2.52	0.44
38:A1:1953:G:N2	38:A1:2093:A:N1	2.65	0.44
38:A1:3041:U:H2'	38:A1:3042:U:C6	2.53	0.44
44:AG:204:ARG:O	44:AG:208:GLU:HG2	2.17	0.44
46:AI:47:PRO:HB3	46:AI:171:TRP:CZ2	2.52	0.44
51:AO:186[A]:ALA:O	51:AO:187[A]:GLU:HG2	2.17	0.44
3:BC:150:GLN:O	3:BC:174:ARG:NH2	2.51	0.44
4:BE:77:ARG:NH2	34:B5:122:U:O3'	2.50	0.44
4:BE:105:VAL:HG21	4:BE:245:LYS:N	2.32	0.44
5:BG:148:SER:HG	5:BG:151:ASP:CG	2.25	0.44
5:BG:154:ARG:HB3	34:B5:78:A:H5'	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BY:55:VAL:HG22	15:BY:75:VAL:HG12	2.00	0.44
27:BU:101:LYS:HB3	27:BU:105:GLN:HE22	1.81	0.44
34:B5:778:G:N1	34:B5:780:A:N7	2.65	0.44
34:B5:1552:U:H2'	34:B5:1553:G:C8	2.52	0.44
35:AA:118:GLU:OE2	38:A1:2177:G:N2	2.50	0.44
38:A1:966:PSU:H2'	38:A1:967:A:C8	2.52	0.44
38:A1:1622:U:H2'	38:A1:1623:G:C8	2.52	0.44
38:A1:1867:A:H2'	38:A1:1868:G:C8	2.53	0.44
38:A1:1914:G:O2'	54:AR:82:LYS:O	2.33	0.44
61:AY:126:LEU:HD23	61:AY:126:LEU:O	2.17	0.44
4:BE:141:THR:OG1	4:BE:145:ARG:HB3	2.18	0.44
5:BG:37:ASP:HB3	5:BG:39:GLU:OE1	2.18	0.44
10:BN:100:LYS:O	10:BN:103:GLU:HG3	2.18	0.44
16:Ba:2:PRO:HG3	34:B5:1143:A:OP2	2.18	0.44
20:BF:197:GLU:OE2	20:BF:208:SER:HB2	2.18	0.44
21:BK:13:GLN:O	21:BK:17:GLN:HG2	2.17	0.44
34:B5:250:C:H2'	34:B5:251:A:C8	2.52	0.44
34:B5:522:U:H2'	34:B5:523:G:O4'	2.17	0.44
34:B5:888:U:H2'	34:B5:889:U:H6	1.80	0.44
34:B5:1424:A:H2'	34:B5:1425:A:O4'	2.17	0.44
34:B5:1461:C:H2'	34:B5:1462:G:C8	2.52	0.44
34:B5:1652:C:H2'	34:B5:1653:C:H6	1.82	0.44
36:AB:250:ALA:HB1	38:A1:2947:G:N3	2.33	0.44
37:AC:60:THR:HG22	37:AC:62:ALA:H	1.82	0.44
38:A1:76:G:H22	38:A1:315:C:H5'	1.82	0.44
38:A1:976:U:H2'	38:A1:977:C:O4'	2.18	0.44
38:A1:1446:A:H5''	52:AP:65:SER:OG	2.18	0.44
38:A1:1471:U:H2'	38:A1:1472:U:C6	2.53	0.44
38:A1:3160:U:H2'	38:A1:3161:C:C6	2.52	0.44
39:A3:3:U:H2'	39:A3:4:U:C6	2.53	0.44
39:A3:56:A:H4'	47:AJ:152:HIS:HB2	1.99	0.44
40:A4:8:C:H2'	40:A4:9:A:C8	2.52	0.44
43:AF:163:LEU:O	43:AF:165:ASP:N	2.50	0.44
50:AN:35:VAL:O	50:AN:64:VAL:HA	2.17	0.44
54:AR:169:ALA:HB1	54:AR:173:ARG:NH2	2.32	0.44
67:Ae:79:VAL:O	67:Ae:83:GLU:HG2	2.18	0.44
5:BG:136:LYS:NZ	5:BG:176:GLN:HG2	2.32	0.44
7:BI:193:LEU:HA	7:BI:197:THR:OG1	2.18	0.44
9:BL:53:TYR:CD1	9:BL:113:PRO:HG2	2.52	0.44
26:BT:108:LEU:HA	26:BT:111:ILE:HG22	1.98	0.44
34:B5:211:PSU:H5'	34:B5:211:PSU:H6	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1146:G:H2'	34:B5:1147:A:H8	1.81	0.44
38:A1:523:A:O2'	55:AS:69:PRO:HD2	2.18	0.44
38:A1:643:U:O2'	38:A1:1153:A:N1	2.42	0.44
38:A1:2352:A:H5''	52:AP:83:TRP:O	2.16	0.44
38:A1:2721:A:O3'	64:Ab:33:LYS:HD3	2.17	0.44
38:A1:2947:G:OP2	38:A1:2947:G:H4'	2.16	0.44
66:Ad:96:VAL:HG12	66:Ad:98:VAL:HG13	1.99	0.44
71:Ai:5:THR:HG23	71:Ai:12:ASN:HB2	1.98	0.44
73:Ak:27:ILE:HG21	73:Ak:39:ARG:CZ	2.47	0.44
1:BA:60:ALA:HB1	1:BA:144:ILE:HD13	1.99	0.44
10:BN:31:GLU:O	10:BN:35:GLU:OE1	2.35	0.44
11:BO:114:ARG:HH11	16:Ba:62:TYR:HE1	1.65	0.44
34:B5:1575:G7M:O5'	34:B5:1575:G7M:H8	2.18	0.44
35:AA:215:ASN:ND2	38:A1:2969:A:N7	2.64	0.44
36:AB:193:ASP:O	36:AB:197:GLU:OE1	2.35	0.44
36:AB:250:ALA:HB1	38:A1:2947:G:C2	2.53	0.44
38:A1:1190:A:H4'	75:Am:113:ARG:NH2	2.32	0.44
38:A1:1579:C:O5'	38:A1:1579:C:H6	2.01	0.44
38:A1:1719:G:N7	54:AR:121:HIS:HE1	2.16	0.44
38:A1:2347:U:H2'	38:A1:2348:A:O4'	2.17	0.44
53:AQ:89:ASP:OD1	53:AQ:90:ASP:N	2.50	0.44
80:tA:10:A:N6	80:tA:25:C:H42	2.06	0.44
5:BG:6:SER:OG	5:BG:112:VAL:HG12	2.17	0.44
5:BG:155:ASP:N	5:BG:155:ASP:OD1	2.48	0.44
12:BV:5:LYS:HB2	12:BV:5:LYS:HE2	1.59	0.44
14:BX:27:ASN:O	14:BX:31:LYS:HG3	2.18	0.44
14:BX:108:GLY:HA2	34:B5:600:U:OP2	2.18	0.44
25:BS:16:ARG:NH2	47:AJ:111:ASP:HB3	2.32	0.44
25:BS:64:GLU:OE1	25:BS:68:ARG:NH1	2.50	0.44
30:Bd:10:HIS:CG	30:Bd:11:PRO:HD2	2.53	0.44
31:Bg:195:HIS:NE2	31:Bg:213:SER:OG	2.41	0.44
32:Bf:145:HIS:HD1	34:B5:1234:A:HO2'	1.63	0.44
34:B5:889:U:H2'	34:B5:890:C:C6	2.53	0.44
34:B5:1345:A:N1	34:B5:1380:U:H5	2.16	0.44
34:B5:1373:C:H2'	34:B5:1374:C:H6	1.83	0.44
35:AA:136:ILE:HD13	35:AA:148:VAL:HG12	2.00	0.44
36:AB:252:ILE:HG12	38:A1:2393:G:H4'	1.98	0.44
38:A1:631:U:H2'	38:A1:632:G:C8	2.53	0.44
38:A1:2228:A:H2'	38:A1:2229:A:H8	1.81	0.44
38:A1:2443:A:N6	38:A1:2504:U:O4	2.51	0.44
38:A1:3131:U:H2'	38:A1:3132:C:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A4:6:U:H2'	40:A4:7:U:C6	2.52	0.44
40:A4:10:A:H2'	40:A4:11:C:C6	2.53	0.44
47:AJ:23:VAL:HG13	47:AJ:29:ARG:HH11	1.83	0.44
47:AJ:78:GLU:O	47:AJ:82:ARG:HG3	2.17	0.44
2:BB:108:ASP:OD2	16:Ba:65:PRO:HB3	2.17	0.44
2:BB:152:ARG:NH2	34:B5:1799:U:H3'	2.33	0.44
2:BB:176:VAL:C	2:BB:178:GLY:H	2.26	0.44
11:BO:115:ILE:HG12	16:Ba:62:TYR:HE2	1.82	0.44
25:BS:88:ARG:O	25:BS:98:TYR:N	2.50	0.44
33:BM:50:LYS:O	33:BM:54:ARG:HG2	2.18	0.44
34:B5:1649:G:H2'	34:B5:1650:U:C6	2.52	0.44
34:B5:1669:U:H2'	34:B5:1670:G:O4'	2.16	0.44
35:AA:180:LEU:HD11	78:Ap:26:VAL:HG21	2.00	0.44
37:AC:12:THR:OG1	37:AC:14:GLU:OE2	2.35	0.44
38:A1:434:U:H2'	38:A1:435:C:C6	2.53	0.44
45:AH:69:ARG:NH1	45:AH:72:LYS:HD3	2.32	0.44
75:Am:79:GLU:O	75:Am:82:LEU:N	2.51	0.44
79:tP:58:A:H4'	79:tP:59:A:OP1	2.17	0.44
2:BB:157:GLN:HB2	2:BB:160:HIS:CE1	2.52	0.44
16:Ba:43:ASN:HD22	16:Ba:66:LYS:HG2	1.83	0.44
16:Ba:95:ARG:HD3	34:B5:1796:C:O2'	2.17	0.44
20:BF:30:PRO:HB2	20:BF:32:GLU:CD	2.43	0.44
21:BK:70:GLU:O	21:BK:73:VAL:HG22	2.18	0.44
22:BP:86:VAL:HG23	22:BP:88:GLU:HG3	2.00	0.44
33:BM:27:ALA:O	33:BM:31:VAL:HG23	2.18	0.44
38:A1:544:C:HO2'	38:A1:548:G:H1	1.62	0.44
38:A1:1046:A:H2'	38:A1:1049:C:C5	2.53	0.44
38:A1:1813:A:H4'	38:A1:1817:G:H1'	1.99	0.44
38:A1:1927:G:C8	78:Ap:16:VAL:HG12	2.53	0.44
38:A1:2592:G:H4'	38:A1:2594:C:C2	2.53	0.44
39:A3:16:U:H2'	39:A3:17:A:C8	2.52	0.44
50:AN:65:ARG:HD2	50:AN:127:TYR:CG	2.53	0.44
50:AN:180:PHE:O	50:AN:184:LYS:HG3	2.18	0.44
51:AO:96[A]:LYS:O	51:AO:100[A]:GLU:OE1	2.35	0.44
63:Aa:83:PRO:HG2	63:Aa:86:LYS:HE2	2.00	0.44
4:BE:45:ILE:HA	4:BE:61:VAL:HG11	2.00	0.43
5:BG:14:LYS:HD3	5:BG:16:PHE:CE1	2.53	0.43
5:BG:22:HIS:CD2	5:BG:25:ARG:HH22	2.36	0.43
11:BO:127:ARG:NH2	34:B5:1787:C:OP1	2.51	0.43
20:BF:43:PHE:HE1	20:BF:70:VAL:HG23	1.83	0.43
21:BK:72:GLY:O	21:BK:76:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Bc:58:GLU:OE1	29:Bc:61:ARG:HG3	2.18	0.43
34:B5:226:A:N3	34:B5:226:A:H2'	2.31	0.43
34:B5:1202:A:H1'	34:B5:1207:C:N4	2.33	0.43
34:B5:1516:A:O2'	34:B5:1517:U:H5'	2.19	0.43
34:B5:1772:C:H2'	34:B5:1773:4AC:H6	2.00	0.43
36:AB:107:ALA:HB1	36:AB:200:GLU:HG3	2.00	0.43
38:A1:41:G:N2	38:A1:2803:A:H62	2.15	0.43
38:A1:99:A:H5'	50:AN:194:GLN:HG2	2.00	0.43
38:A1:307:A:H2'	38:A1:308:A:H8	1.79	0.43
38:A1:2094:C:H2'	38:A1:2095:G:C8	2.53	0.43
38:A1:2677:G:N3	38:A1:2677:G:H2'	2.32	0.43
38:A1:2699:G:H5''	56:AT:16:GLN:NE2	2.33	0.43
38:A1:3000:A:H2'	38:A1:3001:C:C6	2.53	0.43
42:AE:68:PRO:HB3	42:AE:142:ASP:OD1	2.18	0.43
59:AW:47:ARG:NH1	59:AW:54:LEU:HD21	2.33	0.43
4:BE:60:GLU:OE1	15:BY:20:ARG:NH2	2.43	0.43
6:BH:139:ARG:HB2	6:BH:151:LYS:HB3	2.00	0.43
14:BX:107:PHE:HE2	14:BX:120:VAL:HG12	1.83	0.43
18:Be:36:LYS:HA	18:Be:36:LYS:HD3	1.87	0.43
32:Bf:119:ARG:HE	32:Bf:119:ARG:HB3	1.56	0.43
33:BM:60:VAL:O	33:BM:60:VAL:HG12	2.18	0.43
34:B5:512:A:H2'	34:B5:513:U:H6	1.82	0.43
34:B5:1564:U:H2'	34:B5:1565:C:C6	2.53	0.43
38:A1:1340:G:H2'	38:A1:1341:U:C6	2.53	0.43
38:A1:1577:G:H1'	38:A1:1578:C:OP1	2.18	0.43
38:A1:1718:G:H2'	38:A1:1719:G:C8	2.53	0.43
38:A1:1925:U:O2'	38:A1:1927:G:N7	2.50	0.43
38:A1:2223:A:H2'	38:A1:2224:A:C8	2.54	0.43
38:A1:2767:U:H2'	38:A1:2768:U:H6	1.81	0.43
38:A1:3275:U:C2	68:Af:64:ILE:HG21	2.53	0.43
39:A3:74:C:H2'	39:A3:75:G:C8	2.53	0.43
41:AD:146:LEU:HD22	41:AD:163:LEU:HD22	2.00	0.43
57:AU:38:ILE:HD11	57:AU:56:VAL:HB	1.99	0.43
58:AV:10:LYS:HD3	58:AV:125:LEU:CD1	2.45	0.43
70:Ah:86:ARG:O	70:Ah:90:ARG:HG2	2.18	0.43
79:tP:52:G:C6	79:tP:53:G:N7	2.86	0.43
3:BC:88:LYS:HD3	3:BC:95:ARG:NH2	2.28	0.43
6:BH:41:LEU:HD22	6:BH:70:PHE:CD1	2.52	0.43
14:BX:92:CYS:HG	14:BX:136:TRP:CD1	2.36	0.43
22:BP:75:PRO:CB	22:BP:104:GLN:HE22	2.31	0.43
25:BS:16:ARG:CZ	47:AJ:111:ASP:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BS:53:ASP:HB3	25:BS:56:LYS:HE2	1.99	0.43
28:BZ:61:SER:H	28:BZ:64:VAL:HG22	1.83	0.43
31:Bg:203:THR:OG1	31:Bg:243:LEU:O	2.25	0.43
34:B5:17:C:O2'	34:B5:1137:A:N1	2.38	0.43
34:B5:301:A:H2'	34:B5:302:PSU:C6	2.54	0.43
34:B5:1561:U:H2'	34:B5:1562:G:H8	1.82	0.43
36:AB:10:ARG:HH22	36:AB:263:SER:C	2.26	0.43
36:AB:256:HIS:HA	36:AB:257:PRO:C	2.44	0.43
38:A1:250:U:H2'	38:A1:251:G:C4	2.53	0.43
38:A1:381:U:H2'	38:A1:382:U:C6	2.53	0.43
38:A1:1560:G:H22	38:A1:1579:C:N4	2.15	0.43
38:A1:1571:A:H2'	38:A1:1572:U:O4'	2.18	0.43
38:A1:3199:G:H2'	38:A1:3200:G:H8	1.83	0.43
39:A3:113:C:H2'	39:A3:114:U:O4'	2.18	0.43
41:AD:271:LYS:HG3	41:AD:272:TYR:CD1	2.53	0.43
46:AI:50:VAL:HG22	46:AI:167:LEU:HD23	1.99	0.43
56:AT:57:TYR:CG	56:AT:89:LEU:HD21	2.54	0.43
66:Ad:26:LYS:HD3	66:Ad:26:LYS:HA	1.74	0.43
68:Af:16:TYR:CZ	68:Af:91:ALA:HB2	2.53	0.43
1:BA:50:VAL:HG23	24:BR:109:LEU:HD21	1.99	0.43
8:BJ:133:HIS:HE2	34:B5:513:U:H5'	1.83	0.43
8:BJ:133:HIS:ND1	8:BJ:162:SER:HB2	2.34	0.43
8:BJ:149:ARG:HG2	34:B5:765:G:O6	2.18	0.43
10:BN:48:SER:O	10:BN:52:VAL:HG23	2.18	0.43
14:BX:107:PHE:CE2	14:BX:120:VAL:HG12	2.54	0.43
21:BK:15:LEU:HG	21:BK:68:LEU:HD13	2.00	0.43
32:Bf:123:ASN:OD1	32:Bf:124:PRO:HD2	2.18	0.43
34:B5:144:U:HO2'	34:B5:145:A:H8	1.65	0.43
34:B5:998:A:N1	34:B5:1006:C:N4	2.66	0.43
34:B5:1117:U:H2'	34:B5:1118:G:C8	2.53	0.43
35:AA:113:VAL:HG12	35:AA:166:ILE:HD13	2.00	0.43
38:A1:507:U:H2'	38:A1:508:U:C6	2.53	0.43
38:A1:947:G:H2'	38:A1:948:C:C6	2.53	0.43
38:A1:2152:A:H2'	38:A1:2153:U:H6	1.83	0.43
39:A3:94:C:H2'	39:A3:95:A:H8	1.82	0.43
63:Aa:75:LEU:HD11	63:Aa:134:ALA:HA	1.99	0.43
4:BE:156:VAL:O	4:BE:157:ASN:OD1	2.36	0.43
7:BI:25:ARG:O	7:BI:28:GLU:HG2	2.19	0.43
7:BI:56:ARG:HH22	34:B5:332:U:P	2.42	0.43
9:BL:36:LYS:HD3	34:B5:248:U:H4'	2.00	0.43
13:BW:52:TYR:HA	13:BW:61:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Bg:90:ARG:HD2	31:Bg:92:TRP:CZ2	2.54	0.43
33:BM:59:LEU:HB2	33:BM:123:VAL:HB	1.99	0.43
34:B5:1323:C:H2'	34:B5:1324:G:O4'	2.19	0.43
38:A1:691:A:N1	40:A4:28:C:O2'	2.48	0.43
39:A3:118:A:H5''	41:AD:253:PHE:CZ	2.54	0.43
6:BH:56:LYS:HD3	6:BH:88:ARG:NH2	2.33	0.43
6:BH:62:VAL:HG12	6:BH:64:VAL:H	1.84	0.43
11:BO:17:ALA:HA	11:BO:30:VAL:HG22	2.00	0.43
12:BV:36:VAL:HG11	12:BV:78:LEU:HD13	1.98	0.43
17:Bb:54:VAL:HG12	17:Bb:64:CYS:SG	2.58	0.43
34:B5:590:C:H2'	34:B5:591:A:C8	2.53	0.43
34:B5:602:U:H2'	34:B5:603:U:C6	2.54	0.43
34:B5:1346:A:H4'	34:B5:1347:U:OP1	2.19	0.43
34:B5:1600:A:H2'	34:B5:1600:A:N3	2.34	0.43
38:A1:156:G:OP2	71:Ai:27:SER:OG	2.27	0.43
38:A1:418:A:H2'	38:A1:419:G:C8	2.54	0.43
38:A1:708:G:N2	38:A1:711:A:OP2	2.44	0.43
38:A1:727:G:O6	38:A1:742:G:O2'	2.30	0.43
40:A4:27:U:H2'	40:A4:28:C:H6	1.83	0.43
41:AD:112:LYS:HE3	41:AD:112:LYS:HB2	1.87	0.43
44:AG:89:GLU:OE1	44:AG:214:LEU:HD21	2.19	0.43
59:AW:23:ARG:NH2	59:AW:25:ASP:OD2	2.38	0.43
66:Ad:10:ARG:HB2	66:Ad:12:TYR:CE1	2.54	0.43
16:Ba:60:PRO:O	16:Ba:61:GLU:HG3	2.18	0.43
16:Ba:84:VAL:O	34:B5:1797:A:N6	2.48	0.43
17:Bb:11:THR:HG22	17:Bb:13:ALA:N	2.34	0.43
25:BS:134:ARG:HB2	25:BS:136:GLN:HE22	1.83	0.43
31:Bg:66:HIS:CG	31:Bg:67:ILE:H	2.36	0.43
34:B5:5:U:H2'	34:B5:6:G:C8	2.53	0.43
38:A1:422:A:N1	38:A1:2362:C:O2'	2.43	0.43
38:A1:552:G:H2'	38:A1:553:U:C6	2.53	0.43
38:A1:1363:A:H2'	38:A1:1364:C:O4'	2.18	0.43
38:A1:1577:G:O2'	38:A1:1578:C:H6	2.01	0.43
38:A1:1616:U:H2'	38:A1:1617:G:H8	1.83	0.43
38:A1:2508:U:H2'	38:A1:2509:U:C6	2.54	0.43
39:A3:16:U:H2'	39:A3:17:A:H8	1.83	0.43
47:AJ:106:ILE:HD11	47:AJ:109:HIS:CD2	2.53	0.43
60:AX:36:LYS:HD3	60:AX:36:LYS:HA	1.87	0.43
80:tA:28:A:H2'	80:tA:29:G:C8	2.53	0.43
1:BA:206:ASP:OD1	1:BA:206:ASP:N	2.51	0.43
3:BC:69:ILE:HG13	3:BC:133:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:144:TRP:CE2	3:BC:173:PRO:HG3	2.53	0.43
4:BE:176:ASP:HB3	4:BE:179:LYS:HE2	2.01	0.43
12:BV:35:ASN:OD1	12:BV:50:TYR:HB3	2.18	0.43
20:BF:40:ILE:HB	20:BF:67:PRO:HB2	2.00	0.43
22:BP:121:ILE:HD11	22:BP:123:TYR:CZ	2.53	0.43
25:BS:134:ARG:HB2	25:BS:136:GLN:NE2	2.33	0.43
31:Bg:122:ILE:CG2	31:Bg:134:TRP:HB2	2.48	0.43
34:B5:158:U:O2'	34:B5:159:U:H3'	2.18	0.43
34:B5:1018:U:H2'	34:B5:1019:A:H8	1.84	0.43
34:B5:1055:U:O2'	34:B5:1056:U:OP1	2.33	0.43
34:B5:1233:G:H2'	34:B5:1234:A:O4'	2.19	0.43
34:B5:1358:G:H2'	34:B5:1359:C:C6	2.54	0.43
37:AC:64:SER:HA	37:AC:75:PRO:HA	2.01	0.43
38:A1:167:U:H2'	38:A1:168:U:C6	2.53	0.43
38:A1:1295:G:H2'	38:A1:1296:C:C6	2.53	0.43
38:A1:2836:C:H5	38:A1:2852:C:N4	2.16	0.43
38:A1:2989:U:H2'	38:A1:2990:G:O4'	2.19	0.43
38:A1:3045:G:H2'	38:A1:3046:A:O4'	2.18	0.43
39:A3:53:U:H1'	47:AJ:9:MET:HE1	2.01	0.43
48:AL:80:VAL:HG12	48:AL:85:LEU:O	2.19	0.43
49:AM:112:LEU:HD22	49:AM:116:GLU:HB3	2.01	0.43
60:AX:50:ALA:O	70:Ah:66:VAL:HG21	2.18	0.43
4:BE:105:VAL:HG21	4:BE:245:LYS:H	1.83	0.43
5:BG:219:ARG:CZ	5:BG:220:LYS:HE2	2.49	0.43
7:BI:110:ARG:O	7:BI:114:GLU:HG2	2.19	0.43
13:BW:51:GLU:HG3	17:Bb:8:LEU:CD1	2.49	0.43
15:BY:44:LEU:HA	15:BY:47:VAL:HG12	2.01	0.43
24:BR:76:GLU:OE1	24:BR:76:GLU:N	2.47	0.43
24:BR:89:SER:OG	24:BR:91:LEU:O	2.29	0.43
25:BS:36:LYS:HB3	25:BS:105:VAL:HG21	2.00	0.43
34:B5:825:U:H2'	34:B5:826:U:O4'	2.19	0.43
34:B5:989:U:H2'	34:B5:990:C:C6	2.53	0.43
34:B5:1133:A:H2'	34:B5:1134:C:O4'	2.18	0.43
34:B5:1202:A:H1'	34:B5:1207:C:H42	1.83	0.43
34:B5:1240:U:H2'	34:B5:1242:A:OP2	2.19	0.43
34:B5:1354:G:O6	34:B5:1369:U:O2	2.37	0.43
38:A1:172:G:O6	38:A1:247:C:N4	2.52	0.43
38:A1:396:A:O2'	38:A1:399:A:OP1	2.22	0.43
38:A1:528:U:H2'	38:A1:529:A:H8	1.83	0.43
38:A1:594:U:H2'	38:A1:609:G:O6	2.19	0.43
38:A1:2413:A:H2'	38:A1:2414:G:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2922:OMG:H1'	38:A1:2951:G:N3	2.34	0.43
38:A1:3162:C:H2'	38:A1:3163:A:C8	2.54	0.43
39:A3:84:A:H2'	39:A3:85:G:C8	2.54	0.43
46:AI:31:ILE:HA	46:AI:66:GLU:OE1	2.18	0.43
55:AS:46:GLN:HE22	55:AS:52:LYS:HB3	1.84	0.43
70:Ah:85:THR:HB	70:Ah:88:LEU:HD12	2.00	0.43
4:BE:117:GLU:CD	4:BE:117:GLU:H	2.27	0.43
20:BF:143:ARG:NH2	29:Bc:57:MET:HE1	2.34	0.43
24:BR:44:LYS:HG3	24:BR:47:ARG:NH2	2.34	0.43
31:Bg:106:HIS:ND1	31:Bg:126:SER:HB2	2.34	0.43
34:B5:585:A:H2'	34:B5:586:G:C8	2.54	0.43
36:AB:291:GLU:OE1	36:AB:291:GLU:N	2.39	0.43
38:A1:226:C:H2'	38:A1:227:G:O4'	2.18	0.43
45:AH:47:LYS:NZ	45:AH:50:ASN:OD1	2.52	0.43
46:AI:76:MET:HE1	46:AI:87:LEU:HD22	2.01	0.43
47:AJ:94:ARG:O	47:AJ:95:ASN:HB2	2.16	0.43
55:AS:139:TYR:CD1	55:AS:140:VAL:HG23	2.54	0.43
56:AT:64:VAL:HG13	56:AT:72:VAL:HG13	2.00	0.43
65:Ac:97:ASP:OD1	65:Ac:97:ASP:N	2.47	0.43
78:Ap:59:CYS:O	78:Ap:60:CYS:SG	2.75	0.43
4:BE:38:LEU:HD23	34:B5:298:C:H5''	2.00	0.42
6:BH:173:TYR:CE1	6:BH:179:LYS:HB2	2.54	0.42
19:BD:105:MET:HB2	19:BD:122:VAL:HG21	2.01	0.42
21:BK:21:VAL:HG21	21:BK:46:LEU:HD11	2.00	0.42
34:B5:190:C:O2'	34:B5:191:C:O4'	2.23	0.42
38:A1:123:A:C6	38:A1:150:A:C5	3.06	0.42
38:A1:987:U:H2'	38:A1:988:U:C6	2.53	0.42
38:A1:3021:A:N6	38:A1:3033:A:N7	2.56	0.42
38:A1:3232:G:C6	38:A1:3256:G:C6	3.07	0.42
54:AR:24:LEU:HB3	54:AR:32:ILE:HD13	2.01	0.42
76:An:8:LYS:HG2	76:An:12:ARG:HH12	1.83	0.42
79:tP:11:C:H2'	79:tP:12:G:C8	2.54	0.42
79:tP:21:A:N6	79:tP:46:G:H2'	2.34	0.42
2:BB:52:THR:O	2:BB:56:SER:HB3	2.19	0.42
2:BB:129:THR:OG1	2:BB:131:ASP:OD1	2.31	0.42
5:BG:201:GLN:HG3	34:B5:126:A:OP1	2.18	0.42
10:BN:18:TYR:O	13:BW:56:HIS:ND1	2.51	0.42
11:BO:112:ILE:HG21	16:Ba:53:LEU:HD12	2.01	0.42
23:BQ:101:SER:O	23:BQ:105:LEU:HG	2.19	0.42
25:BS:131:LEU:HD22	34:B5:1459:C:H5'	1.99	0.42
27:BU:42:VAL:O	27:BU:46:GLU:OE1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:17:C:H2'	34:B5:18:C:H6	1.83	0.42
34:B5:209:U:H2'	34:B5:210:A:C8	2.54	0.42
34:B5:828:U:O2'	34:B5:829:A:O5'	2.34	0.42
34:B5:1158:C:H5	34:B5:1163:A:H61	1.66	0.42
34:B5:1363:U:C2	34:B5:1364:G:C8	3.07	0.42
34:B5:1639:C:H2'	34:B5:1640:C:O4'	2.19	0.42
35:AA:140:ASN:OD1	35:AA:147:ARG:NH1	2.51	0.42
38:A1:549:U:O2'	38:A1:550:A:OP1	2.34	0.42
38:A1:938:C:OP1	38:A1:963:G:H5'	2.19	0.42
38:A1:1066:G:H2'	38:A1:1067:U:C6	2.54	0.42
38:A1:2911:A:H4'	38:A1:2912:G:C8	2.54	0.42
41:AD:183:TRP:HA	41:AD:190:ILE:HA	2.00	0.42
41:AD:215:ASP:OD1	41:AD:215:ASP:N	2.52	0.42
56:AT:136:ARG:HD2	56:AT:139:ARG:NH2	2.33	0.42
58:AV:32:ARG:CZ	58:AV:64:LYS:HB3	2.49	0.42
77:Ao:106:PHE:O	79:tP:19:G:O2'	2.31	0.42
79:tP:62:C:H2'	79:tP:63:G:O4'	2.18	0.42
1:BA:79:ARG:O	1:BA:83:GLN:HG2	2.19	0.42
13:BW:81:VAL:HG22	13:BW:82:LYS:O	2.19	0.42
20:BF:145:ASP:CG	20:BF:146:THR:H	2.27	0.42
26:BT:18:TYR:HD1	26:BT:135:ILE:HG13	1.84	0.42
26:BT:29:GLU:OE2	26:BT:110:LYS:HD2	2.19	0.42
34:B5:368:U:O2'	34:B5:603:U:O2'	2.30	0.42
34:B5:934:C:C4	34:B5:1077:C:H4'	2.55	0.42
34:B5:1220:C:H2'	34:B5:1221:A:C8	2.52	0.42
34:B5:1705:C:H2'	34:B5:1706:C:C6	2.54	0.42
36:AB:350:ALA:C	36:AB:351:LEU:HD23	2.44	0.42
37:AC:73:ARG:NH1	38:A1:2814:G:OP1	2.43	0.42
37:AC:179:LEU:O	37:AC:183:LYS:HB2	2.20	0.42
37:AC:300:ARG:NH1	38:A1:1347:U:OP1	2.50	0.42
38:A1:511:G:H2'	38:A1:512:U:O4'	2.19	0.42
38:A1:710:A:H2'	38:A1:711:A:C8	2.54	0.42
38:A1:1203:A:H2'	38:A1:1204:A:H8	1.82	0.42
38:A1:1622:U:H2'	38:A1:1623:G:H8	1.84	0.42
38:A1:2897:A:H5''	75:Am:125:LYS:HD2	2.01	0.42
55:AS:19:VAL:HG13	55:AS:19:VAL:O	2.19	0.42
1:BA:67:ILE:HD12	1:BA:67:ILE:H	1.84	0.42
2:BB:32:ILE:HD11	2:BB:46:THR:HG23	2.01	0.42
2:BB:139:ALA:HA	2:BB:212:VAL:HA	2.01	0.42
5:BG:157:VAL:HG11	34:B5:78:A:H4'	2.01	0.42
8:BJ:112:GLN:HG3	8:BJ:148:VAL:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Ba:12:LYS:HB2	16:Ba:33:ASP:OD2	2.19	0.42
19:BD:21:LEU:HD23	19:BD:21:LEU:HA	1.87	0.42
26:BT:115:GLU:N	26:BT:115:GLU:OE2	2.52	0.42
31:Bg:183:LEU:H	31:Bg:183:LEU:HD23	1.84	0.42
33:BM:42:ALA:HB3	33:BM:122:VAL:HB	2.02	0.42
34:B5:590:C:H2'	34:B5:591:A:H8	1.84	0.42
34:B5:961:U:H2'	34:B5:962:C:H6	1.84	0.42
34:B5:1624:C:H2'	34:B5:1625:C:C6	2.54	0.42
34:B5:1761:U:O4'	34:B5:1782:MA6:H2	2.19	0.42
38:A1:673:U:H2'	38:A1:674:G:H8	1.84	0.42
38:A1:1153:A:O2'	38:A1:1154:A:H5'	2.20	0.42
38:A1:2283:G:H1'	38:A1:2285:C:N4	2.34	0.42
38:A1:2545:C:H2'	38:A1:2546:C:C6	2.55	0.42
38:A1:3068:U:OP2	54:AR:62:ARG:NH2	2.38	0.42
38:A1:3174:A:C6	38:A1:3279:A:H1'	2.54	0.42
45:AH:89:LYS:HB3	45:AH:143:GLU:OE2	2.19	0.42
47:AJ:82:ARG:O	47:AJ:112:LEU:HD11	2.19	0.42
49:AM:40:ASP:OD1	49:AM:43:LYS:N	2.49	0.42
56:AT:40:VAL:HB	56:AT:96:ILE:HG23	2.01	0.42
57:AU:92:TRP:HD1	57:AU:108:TYR:CE1	2.37	0.42
58:AV:32:ARG:HH12	58:AV:64:LYS:HD3	1.84	0.42
58:AV:68:GLU:O	58:AV:72:LYS:NZ	2.42	0.42
59:AW:23:ARG:HG2	59:AW:24:GLY:H	1.83	0.42
70:Ah:15:GLU:H	70:Ah:15:GLU:CD	2.27	0.42
2:BB:197:ILE:HG22	2:BB:210:ILE:HD13	2.01	0.42
3:BC:211:LEU:HD23	3:BC:211:LEU:HA	1.82	0.42
5:BG:50:PHE:CE1	5:BG:113:ILE:HG13	2.55	0.42
7:BI:48:THR:OG1	7:BI:52:ASN:O	2.22	0.42
25:BS:38:VAL:HG23	25:BS:42:TYR:HB3	2.00	0.42
34:B5:490:C:H41	34:B5:492:A:H4'	1.84	0.42
34:B5:624:G:H2'	34:B5:625:C:C6	2.54	0.42
34:B5:777:C:H2'	34:B5:778:G:H5''	2.00	0.42
34:B5:1348:A:H2'	34:B5:1349:G:O4'	2.20	0.42
34:B5:1391:A:H2'	34:B5:1392:U:C6	2.54	0.42
36:AB:346:THR:HA	36:AB:351:LEU:HD22	2.01	0.42
38:A1:717:C:OP1	38:A1:751:A:O2'	2.35	0.42
38:A1:848:A:H3'	38:A1:849:C:O4'	2.19	0.42
38:A1:1169:A:H2'	38:A1:1170:A:C8	2.54	0.42
38:A1:1307:G:OP1	51:AO:60[A]:LYS:NZ	2.43	0.42
38:A1:1490:A:O2'	72:Aj:12:HIS:O	2.32	0.42
38:A1:3066:U:H2'	38:A1:3067:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:AO:138[A]:LEU:HD12	51:AO:138[A]:LEU:HA	1.78	0.42
53:AQ:83:VAL:O	53:AQ:103:ALA:HA	2.18	0.42
61:AY:55:GLU:HB2	61:AY:108:LYS:HB3	2.01	0.42
72:Aj:25:ARG:HD2	72:Aj:25:ARG:O	2.19	0.42
77:Ao:71:ARG:NH2	77:Ao:80:ARG:HE	2.17	0.42
1:BA:84:ARG:O	1:BA:88:LYS:HG2	2.19	0.42
6:BH:61:PHE:HA	6:BH:93:LEU:O	2.19	0.42
12:BV:4:ASP:OD1	12:BV:4:ASP:N	2.52	0.42
19:BD:25:PHE:HD2	19:BD:37:VAL:HG11	1.85	0.42
27:BU:57:ARG:HD3	27:BU:89:ARG:HH21	1.85	0.42
28:BZ:95:HIS:ND1	28:BZ:96:SER:O	2.53	0.42
31:Bg:128:ASP:O	31:Bg:129:LYS:HG2	2.19	0.42
31:Bg:231:MET:HG2	31:Bg:232:TYR:N	2.34	0.42
34:B5:30:G:H2'	34:B5:31:C:H6	1.84	0.42
34:B5:1451:C:H2'	34:B5:1452:U:C6	2.55	0.42
37:AC:48:GLN:NE2	38:A1:336:A:N3	2.66	0.42
38:A1:137:G:H2'	38:A1:138:U:C6	2.55	0.42
38:A1:144:A:H2'	38:A1:145:G:O4'	2.20	0.42
38:A1:956:U:H2'	38:A1:957:C:C6	2.55	0.42
38:A1:1449:A:H2'	38:A1:1450:G:O4'	2.20	0.42
38:A1:1915:A:H2'	38:A1:1916:U:H6	1.83	0.42
38:A1:2366:C:H2'	38:A1:2367:A:H8	1.85	0.42
38:A1:2662:G:H2'	38:A1:2663:G:H8	1.84	0.42
38:A1:2881:C:H2'	38:A1:2882:U:C6	2.55	0.42
38:A1:3020:U:O2	38:A1:3034:C:N4	2.40	0.42
38:A1:3083:G:H2'	38:A1:3084:C:O4'	2.20	0.42
38:A1:3232:G:H2'	38:A1:3233:C:C6	2.54	0.42
62:AZ:121:ARG:HH21	62:AZ:126:LYS:HD2	1.85	0.42
65:Ac:16:LEU:HD23	65:Ac:98:SER:HA	2.01	0.42
66:Ad:80:ASN:O	66:Ad:84:ASP:HB3	2.18	0.42
79:tP:8:U:O2'	79:tP:21:A:N1	2.39	0.42
79:tP:51:C:C2	79:tP:52:G:C8	3.08	0.42
6:BH:147:ASN:OD1	6:BH:148:LYS:N	2.53	0.42
7:BI:104:ILE:HD11	7:BI:183:ILE:HD11	2.01	0.42
17:Bb:30:SER:OG	34:B5:959:U:O2	2.38	0.42
19:BD:68:GLU:HB2	21:BK:20:VAL:CG1	2.50	0.42
21:BK:3:MET:O	34:B5:1257:U:H1'	2.20	0.42
21:BK:61:TRP:CZ3	30:Bd:23:VAL:HG22	2.54	0.42
25:BS:117:LYS:HE3	25:BS:128:PHE:HB2	2.02	0.42
31:Bg:6:VAL:O	31:Bg:315:VAL:HA	2.19	0.42
35:AA:68:LYS:HD3	35:AA:70:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:AB:151:ILE:O	36:AB:155:ALA:HB3	2.18	0.42
38:A1:138:U:H2'	38:A1:139:G:C8	2.55	0.42
38:A1:209:A:H4'	38:A1:211:A:C8	2.54	0.42
38:A1:1419:A:OP1	40:A4:21:C:H5'	2.20	0.42
38:A1:1657:C:O2'	38:A1:1797:A:OP2	2.16	0.42
38:A1:2507:C:H6	38:A1:2507:C:H5''	1.84	0.42
38:A1:2533:G:C6	38:A1:2547:A:C6	3.07	0.42
43:AF:66:LYS:HG3	43:AF:76:TYR:HD2	1.85	0.42
55:AS:43:TYR:CZ	55:AS:47:LYS:HD2	2.55	0.42
63:Aa:13:GLY:O	67:Ae:36:LYS:HD2	2.20	0.42
80:tA:61:C:H2'	80:tA:62:C:H6	1.85	0.42
7:BI:153:GLU:O	7:BI:157:GLU:HG2	2.20	0.42
10:BN:61:THR:OG1	10:BN:62:GLN:N	2.53	0.42
14:BX:92:CYS:HA	14:BX:95:PHE:CD2	2.55	0.42
15:BY:86:GLU:HA	15:BY:87:PRO:HD3	1.90	0.42
20:BF:195:ALA:O	20:BF:199:ILE:HG12	2.19	0.42
31:Bg:50:ASP:CG	31:Bg:51:ASP:H	2.28	0.42
31:Bg:106:HIS:ND1	31:Bg:110:VAL:HG22	2.34	0.42
34:B5:262:U:H2'	34:B5:263:C:C6	2.55	0.42
34:B5:972:G:O2'	38:A1:847:A:N6	2.53	0.42
34:B5:1001:A:H2'	34:B5:1002:G:C8	2.54	0.42
34:B5:1138:A:H2'	34:B5:1139:A:C8	2.54	0.42
34:B5:1254:U:H2'	34:B5:1255:G:C8	2.54	0.42
34:B5:1487:A:H2'	34:B5:1488:G:C8	2.54	0.42
34:B5:1553:G:N2	34:B5:1555:A:H3'	2.35	0.42
34:B5:1638:G:H2'	34:B5:1639:C:O4'	2.20	0.42
34:B5:1758:U:O2'	38:A1:2262:A:N1	2.43	0.42
38:A1:863:C:H2'	38:A1:864:G:O4'	2.20	0.42
38:A1:2093:A:C2	38:A1:2094:C:C2	3.08	0.42
38:A1:2265:C:H4'	38:A1:2266:PSU:OP1	2.19	0.42
38:A1:3387:U:H2'	38:A1:3388:C:C6	2.54	0.42
41:AD:229:ASP:O	41:AD:231:ILE:HG13	2.19	0.42
49:AM:14:LEU:H	49:AM:19:ARG:NH2	2.18	0.42
67:Ae:102:ALA:O	67:Ae:106:VAL:HG23	2.20	0.42
79:tP:24:G:H2'	79:tP:25:C:H6	1.84	0.42
5:BG:131:LYS:NZ	34:B5:166:C:OP1	2.31	0.42
9:BL:53:TYR:CG	9:BL:113:PRO:HG2	2.55	0.42
11:BO:99:GLN:NE2	16:Ba:44:ILE:O	2.44	0.42
21:BK:21:VAL:HG23	21:BK:66:TYR:HD2	1.85	0.42
24:BR:24:LEU:HB3	24:BR:58:MET:HE3	2.01	0.42
27:BU:58:LEU:HD11	34:B5:1347:U:C2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Bc:5:THR:HG22	29:Bc:7:VAL:HG13	2.01	0.42
34:B5:73:U:H2'	34:B5:76:A:H62	1.85	0.42
34:B5:486:G:O2'	34:B5:492:A:N6	2.47	0.42
34:B5:683:C:O2'	34:B5:684:A:H8	2.03	0.42
34:B5:869:A:H61	34:B5:958:U:H3	1.68	0.42
35:AA:117:GLU:HG2	35:AA:124:GLY:N	2.32	0.42
38:A1:38:U:H2'	38:A1:39:A:O4'	2.20	0.42
38:A1:547:G:H4'	38:A1:548:G:H2'	2.02	0.42
39:A3:3:U:H2'	39:A3:4:U:H6	1.84	0.42
44:AG:52:TRP:NE1	44:AG:60:ARG:HH12	2.17	0.42
46:AI:103:LEU:HB2	46:AI:112:GLN:HE22	1.84	0.42
50:AN:18:VAL:HG13	50:AN:19:LEU:HD12	2.02	0.42
52:AP:113:TYR:HB3	52:AP:153:LYS:HE3	2.01	0.42
1:BA:139:VAL:HG23	1:BA:141:ILE:CG1	2.50	0.42
1:BA:163:ASN:OD1	1:BA:166:GLY:N	2.53	0.42
3:BC:222:TYR:O	12:BV:23:ILE:HG21	2.20	0.42
7:BI:110:ARG:NH2	7:BI:160:PHE:O	2.52	0.42
9:BL:113:PRO:O	9:BL:116:ARG:NH1	2.51	0.42
10:BN:54:LEU:HB3	10:BN:60:VAL:CG1	2.50	0.42
32:Bf:97:LYS:HE2	34:B5:1230:A:OP2	2.20	0.42
34:B5:592:A:H2'	34:B5:593:U:O4'	2.19	0.42
34:B5:1188:G:O2'	34:B5:1430:U:OP1	2.31	0.42
36:AB:347:SER:C	36:AB:349:LYS:H	2.28	0.42
38:A1:249:U:O2	38:A1:250:U:N3	2.53	0.42
38:A1:1263:A:H2'	38:A1:1263:A:N3	2.35	0.42
38:A1:1546:A:H2'	38:A1:1547:G:O4'	2.20	0.42
38:A1:1682:U:O2	57:AU:82:LYS:HG2	2.20	0.42
38:A1:2282:U:O2	38:A1:2310:U:H4'	2.20	0.42
39:A3:47:C:OP2	41:AD:158:ARG:HD3	2.20	0.42
54:AR:170:ARG:HH21	54:AR:173:ARG:NH2	2.18	0.42
56:AT:48:ILE:HG13	56:AT:94:GLU:HG2	2.02	0.42
56:AT:112:ASN:CG	56:AT:128:LEU:HD12	2.45	0.42
1:BA:55:GLU:OE2	12:BV:80:LYS:N	2.42	0.41
1:BA:121:VAL:HG23	1:BA:141:ILE:HG21	2.02	0.41
3:BC:165:VAL:HG11	3:BC:210:THR:HA	2.02	0.41
4:BE:163:ASP:C	4:BE:165:ALA:H	2.28	0.41
6:BH:107:ARG:HG3	34:B5:698:U:C5	2.55	0.41
14:BX:109:ARG:O	14:BX:112:LYS:HB2	2.20	0.41
15:BY:113:ASN:HA	15:BY:116:LYS:HD3	2.01	0.41
34:B5:71:A:O2'	34:B5:72:A:P	2.78	0.41
34:B5:610:G:N3	34:B5:610:G:H2'	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:553:U:H2'	38:A1:554:A:O4'	2.19	0.41
38:A1:1037:C:H2'	38:A1:1038:C:C6	2.55	0.41
38:A1:1544:G:OP2	50:AN:35:VAL:HG21	2.19	0.41
38:A1:1620:U:H2'	38:A1:1621:A:C8	2.55	0.41
38:A1:1624:G:H2'	38:A1:1625:A:H8	1.85	0.41
38:A1:2251:G:O2'	79:tP:12:G:H5''	2.19	0.41
38:A1:2423:U:H2'	38:A1:2424:A:C8	2.55	0.41
38:A1:3163:A:H2'	38:A1:3164:C:C6	2.55	0.41
47:AJ:91:LEU:HD23	47:AJ:163:PHE:CZ	2.55	0.41
51:AO:81[A]:TYR:CE2	51:AO:85[A]:ARG:HD2	2.54	0.41
54:AR:70:LYS:HB3	54:AR:70:LYS:HE2	1.83	0.41
56:AT:52:MET:HG2	56:AT:53:PRO:HD2	2.02	0.41
59:AW:8:PHE:CD1	59:AW:46:PRO:HG3	2.55	0.41
62:AZ:52:LYS:O	62:AZ:65:ARG:NH2	2.47	0.41
70:Ah:101:THR:OG1	70:Ah:104:GLN:HG2	2.19	0.41
2:BB:82:ARG:NH1	2:BB:191:GLU:HG3	2.35	0.41
2:BB:107:THR:O	2:BB:111:ARG:HG2	2.20	0.41
3:BC:57:PHE:CG	3:BC:138:PRO:HG3	2.55	0.41
7:BI:31:ARG:O	34:B5:331:A:H4'	2.20	0.41
13:BW:11:LEU:HD12	13:BW:74:VAL:HG13	2.02	0.41
31:Bg:238:ASP:OD2	31:Bg:258:THR:N	2.54	0.41
34:B5:1467:C:O2	34:B5:1601:G:N2	2.45	0.41
34:B5:1624:C:H2'	34:B5:1625:C:H6	1.84	0.41
38:A1:68:C:OP2	38:A1:301:G:N2	2.53	0.41
38:A1:287:G:H5'	50:AN:179:LYS:O	2.19	0.41
38:A1:828:A:H2'	38:A1:829:U:C6	2.55	0.41
38:A1:1108:U:H2'	38:A1:1109:U:H6	1.84	0.41
38:A1:1375:G:O6	63:Aa:10:LYS:HE2	2.21	0.41
38:A1:1438:U:H2'	38:A1:1439:U:C6	2.55	0.41
38:A1:1694:U:O2'	38:A1:1695:U:H5'	2.20	0.41
38:A1:2218:G:H2'	38:A1:2219:A:H8	1.85	0.41
38:A1:2416:PSU:H2'	38:A1:2417:U:C6	2.55	0.41
38:A1:2428:U:H2'	38:A1:2429:G:C8	2.55	0.41
38:A1:2652:U:OP1	77:Ao:65:THR:OG1	2.30	0.41
38:A1:2909:U:H2'	38:A1:2910:A:O4'	2.20	0.41
52:AP:16:SER:HB3	52:AP:149:VAL:HG22	2.02	0.41
54:AR:126:GLU:HG3	54:AR:132:PHE:HE2	1.85	0.41
56:AT:119:ALA:HB2	56:AT:126:VAL:HB	2.03	0.41
57:AU:89:LEU:HB3	57:AU:93:ILE:HD12	2.02	0.41
58:AV:5:GLY:HA3	58:AV:106:LYS:O	2.20	0.41
59:AW:18:GLY:HA3	59:AW:31:PHE:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:173:ILE:HD11	4:BE:235:TYR:CD2	2.55	0.41
7:BI:117:TYR:HE1	7:BI:146:ARG:HB3	1.86	0.41
11:BO:49:LYS:HA	11:BO:49:LYS:HD3	1.84	0.41
28:BZ:83:LEU:HB3	28:BZ:89:ILE:HG12	2.02	0.41
31:Bg:16:HIS:NE2	31:Bg:35:SER:OG	2.38	0.41
34:B5:217:A:H8	34:B5:218:A:N1	2.17	0.41
34:B5:592:A:O2'	34:B5:596:C:OP1	2.36	0.41
34:B5:1109:G:O2'	34:B5:1138:A:N1	2.47	0.41
34:B5:1228:G:O2'	34:B5:1229:G:OP2	2.30	0.41
34:B5:1458:G:HO2'	34:B5:1459:C:P	2.42	0.41
38:A1:1047:A:H2'	38:A1:1048:A:C8	2.54	0.41
38:A1:1785:U:H2'	38:A1:1786:G:C8	2.55	0.41
38:A1:2812:C:H2'	38:A1:2813:A:C8	2.55	0.41
38:A1:2984:C:H2'	38:A1:2985:C:H6	1.85	0.41
42:AE:136:GLU:HA	42:AE:139:LYS:HZ3	1.86	0.41
2:BB:23:PRO:HA	2:BB:26:ARG:NH1	2.35	0.41
6:BH:77:LEU:O	6:BH:81:LEU:HD23	2.20	0.41
13:BW:36:LYS:O	13:BW:40:VAL:HG23	2.19	0.41
15:BY:8:ARG:HB2	15:BY:26:ASP:OD1	2.20	0.41
18:Be:55:ARG:HH11	18:Be:55:ARG:HG3	1.86	0.41
20:BF:189:THR:HB	20:BF:192:GLU:HG3	2.03	0.41
34:B5:585:A:H2'	34:B5:586:G:H8	1.84	0.41
34:B5:1732:A:H2'	34:B5:1733:C:O4'	2.20	0.41
36:AB:306:THR:HG21	36:AB:316:GLU:HG2	2.03	0.41
37:AC:22:LEU:HA	37:AC:23:PRO:HD3	1.86	0.41
37:AC:125:ALA:O	37:AC:129:THR:HG23	2.20	0.41
38:A1:969:C:O3'	64:Ab:18:ARG:HD2	2.20	0.41
38:A1:1709:C:H2'	38:A1:1710:C:H6	1.85	0.41
42:AE:40:LEU:HD11	42:AE:54:TYR:HB2	2.03	0.41
46:AI:54:SER:HB2	46:AI:135:ILE:HD11	2.02	0.41
50:AN:99:ARG:NH2	50:AN:167:THR:HB	2.34	0.41
79:tP:25:C:C2	79:tP:26:G:C8	3.09	0.41
80:tA:25:C:C2	80:tA:26:G:C8	3.08	0.41
2:BB:153:HIS:CD2	2:BB:155:TYR:CD2	3.09	0.41
2:BB:176:VAL:HG12	2:BB:177:GLN:N	2.34	0.41
2:BB:188:LEU:HD11	2:BB:212:VAL:HG21	2.01	0.41
2:BB:216:LYS:NZ	34:B5:885:G:OP1	2.38	0.41
3:BC:59:HIS:CE1	3:BC:239:PRO:HD3	2.56	0.41
11:BO:18:ARG:HB2	11:BO:29:HIS:O	2.20	0.41
14:BX:50:LYS:HD3	14:BX:101:GLU:OE2	2.21	0.41
16:Ba:88:SER:O	16:Ba:92:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Bb:33:LEU:HD23	17:Bb:81:ARG:HA	2.02	0.41
18:Be:7:SER:OG	18:Be:10:ARG:NH1	2.52	0.41
19:BD:120:TYR:HB3	19:BD:124:ARG:NH1	2.34	0.41
24:BR:10:LYS:HD3	24:BR:53:TYR:CE2	2.56	0.41
33:BM:107:ASP:OD2	33:BM:113:ARG:NH1	2.53	0.41
33:BM:133:LEU:HD23	33:BM:133:LEU:H	1.85	0.41
34:B5:236:A:H5''	34:B5:237:C:H5	1.85	0.41
34:B5:293:U:H2'	34:B5:294:C:C6	2.56	0.41
34:B5:889:U:H2'	34:B5:890:C:H6	1.85	0.41
34:B5:1665:U:H2'	34:B5:1666:U:O2	2.21	0.41
38:A1:855:U:H5''	54:AR:95:TRP:CG	2.56	0.41
38:A1:887:G:H2'	38:A1:888:A:C8	2.56	0.41
38:A1:1909:A:H2'	38:A1:1910:A:C8	2.56	0.41
38:A1:2129:PSU:H2'	38:A1:2130:G:C8	2.55	0.41
38:A1:2379:U:H2'	38:A1:2380:U:C6	2.56	0.41
38:A1:2536:A:H3'	38:A1:2537:U:H4'	2.02	0.41
38:A1:2899:C:O2'	38:A1:2901:G:OP2	2.32	0.41
38:A1:3065:G:H2'	38:A1:3066:U:C6	2.55	0.41
38:A1:3358:U:H2'	38:A1:3359:A:C8	2.55	0.41
40:A4:18:U:H2'	40:A4:19:C:C6	2.55	0.41
45:AH:91:ARG:HG2	45:AH:182:SER:HB3	2.01	0.41
65:Ac:14:LEU:HD23	65:Ac:14:LEU:HA	1.92	0.41
70:Ah:6:ALA:O	70:Ah:10:ARG:HG3	2.19	0.41
79:tP:43:G:H8	79:tP:43:G:H5''	1.86	0.41
79:tP:53:G:H2'	79:tP:54:A:C8	2.40	0.41
5:BG:220:LYS:HA	5:BG:223:LYS:HG3	2.02	0.41
6:BH:49:ILE:HG21	6:BH:175:LYS:HG2	2.02	0.41
8:BJ:40:LYS:HB3	8:BJ:40:LYS:HE2	1.97	0.41
21:BK:14:TYR:CD1	21:BK:35:ILE:HD11	2.55	0.41
31:Bg:24:ALA:O	31:Bg:33:LEU:HD12	2.20	0.41
34:B5:1393:C:H2'	34:B5:1394:G:H8	1.85	0.41
34:B5:1755:A:H4'	34:B5:1756[A]:A:OP1	2.20	0.41
36:AB:106:TRP:HB2	36:AB:133:TYR:CE1	2.55	0.41
38:A1:324:A:H2'	38:A1:325:A:C8	2.55	0.41
38:A1:656:A:H2'	38:A1:657:A:H8	1.82	0.41
38:A1:1214:U:H2'	38:A1:1215:U:C6	2.56	0.41
38:A1:1304:A:N6	38:A1:2860:U:H5''	2.36	0.41
38:A1:1306:G:C6	51:AO:62[A]:THR:HA	2.56	0.41
38:A1:1364:C:H5''	53:AQ:3:ILE:HD13	2.03	0.41
38:A1:1945:A:H2'	38:A1:1946:A:C8	2.56	0.41
38:A1:2726:C:O2'	38:A1:2727:A:H2'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:A3:19:C:H2'	39:A3:20:A:H8	1.86	0.41
43:AF:40:LYS:HE2	43:AF:179:LEU:HD13	2.03	0.41
45:AH:138:THR:O	45:AH:140:VAL:N	2.54	0.41
46:AI:87:LEU:HD13	46:AI:138:VAL:HG22	2.02	0.41
51:AO:186[A]:ALA:C	51:AO:188[A]:SER:H	2.28	0.41
62:AZ:17:ARG:HD3	69:Ag:73:SER:HB3	2.03	0.41
62:AZ:115:LYS:HE3	62:AZ:119:GLU:OE2	2.20	0.41
79:tP:55:U:H2'	79:tP:57:G:OP2	2.20	0.41
5:BG:121:LEU:HD22	5:BG:124:LEU:HD12	2.03	0.41
6:BH:37:GLU:HG3	6:BH:73:VAL:HG11	2.03	0.41
7:BI:135:LYS:HD2	7:BI:135:LYS:HA	1.90	0.41
9:BL:109:VAL:HG23	9:BL:137:PHE:C	2.46	0.41
14:BX:37:ALA:O	14:BX:41:SER:HB3	2.21	0.41
19:BD:46:THR:HG23	19:BD:84:ILE:HD12	2.03	0.41
26:BT:99:SER:O	26:BT:103:LYS:HG2	2.21	0.41
27:BU:19:ILE:HG23	27:BU:94:GLU:HB2	2.02	0.41
29:Bc:21:SER:HB2	34:B5:1619:C:O4'	2.20	0.41
34:B5:766:PSU:O4	34:B5:770:A:N6	2.53	0.41
38:A1:637:C:C2	38:A1:638:C:C5	3.09	0.41
38:A1:872:U:H2'	38:A1:873:C:C6	2.55	0.41
38:A1:1761:C:O2'	38:A1:1762:C:O3'	2.38	0.41
38:A1:1844:C:O2	72:Aj:9:GLY:HA2	2.21	0.41
38:A1:1953:G:N1	38:A1:1954:G:O6	2.54	0.41
38:A1:2201:G:H2'	38:A1:2202:C:H6	1.86	0.41
38:A1:2389:C:H2'	38:A1:2390:A:H8	1.86	0.41
38:A1:2428:U:H2'	38:A1:2429:G:H8	1.86	0.41
38:A1:3159:C:H2'	38:A1:3160:U:C6	2.56	0.41
38:A1:3215:A:H5''	68:Af:2:ALA:HB2	2.03	0.41
38:A1:3283:U:H2'	38:A1:3284:G:C8	2.56	0.41
1:BA:83:GLN:HE22	1:BA:100:GLY:HA2	1.86	0.41
4:BE:107:GLY:HA2	4:BE:189:LEU:HB3	2.02	0.41
8:BJ:25:ASP:OD1	8:BJ:26:ALA:N	2.53	0.41
11:BO:135:ARG:HE	11:BO:137:LEU:HD11	1.86	0.41
25:BS:18:LEU:HD21	25:BS:74:GLN:OE1	2.21	0.41
34:B5:1648:A:H2'	34:B5:1649:G:C8	2.55	0.41
35:AA:118:GLU:HG3	35:AA:125:ALA:HB3	2.02	0.41
37:AC:170:LYS:HG2	37:AC:175:HIS:HB2	2.03	0.41
38:A1:94:G:H2'	38:A1:95:A:C8	2.56	0.41
38:A1:208:C:H2'	38:A1:209:A:O4'	2.20	0.41
38:A1:283:G:OP2	38:A1:285:A:O2'	2.28	0.41
38:A1:810:A:H2'	38:A1:811:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:955:U:H2'	38:A1:956:U:C6	2.55	0.41
38:A1:1498:A:H2'	38:A1:1499:C:H6	1.84	0.41
38:A1:2094:C:H2'	38:A1:2095:G:H8	1.84	0.41
38:A1:2185:G:O2'	38:A1:2314:PSU:OP2	2.35	0.41
38:A1:3085:G:H5'	38:A1:3332:U:OP1	2.20	0.41
38:A1:3232:G:H1	38:A1:3255:U:H3	1.69	0.41
38:A1:3296:A:H2'	38:A1:3297:U:H6	1.85	0.41
38:A1:3320:A:H2'	38:A1:3321:C:C6	2.56	0.41
40:A4:7:U:H2'	40:A4:8:C:C6	2.56	0.41
40:A4:26:U:H2'	40:A4:27:U:H6	1.85	0.41
43:AF:85:PHE:CZ	43:AF:147:LEU:HD21	2.56	0.41
47:AJ:94:ARG:C	47:AJ:96:PHE:H	2.29	0.41
63:Aa:104:THR:HG21	63:Aa:112:ILE:HD11	2.02	0.41
79:tP:18:G:H5'	79:tP:60:A:N1	2.36	0.41
1:BA:152:PRO:HB2	1:BA:154:GLU:OE1	2.20	0.41
2:BB:98:THR:O	2:BB:232:HIS:NE2	2.53	0.41
2:BB:133:TYR:HD2	2:BB:181:LEU:HB2	1.86	0.41
3:BC:188:LEU:HD13	3:BC:196:VAL:HG11	2.03	0.41
4:BE:4:GLY:HA3	34:B5:93:A:O2'	2.21	0.41
5:BG:7:TYR:HB2	5:BG:113:ILE:HD13	2.01	0.41
6:BH:37:GLU:O	6:BH:38:LEU:HD22	2.21	0.41
6:BH:129:LEU:HD11	6:BH:172:VAL:HG21	2.03	0.41
7:BI:74:LYS:HE3	7:BI:112:TRP:HB2	2.02	0.41
11:BO:25:ASP:N	11:BO:55:SER:HB3	2.36	0.41
11:BO:135:ARG:NH2	34:B5:904:G:OP1	2.54	0.41
19:BD:64:ARG:HG3	19:BD:65:ARG:H	1.86	0.41
19:BD:106:LYS:HG3	19:BD:175:VAL:HG22	2.02	0.41
20:BF:139:ASN:O	20:BF:214:LYS:HE2	2.21	0.41
23:BQ:79:TYR:O	23:BQ:82:ARG:HG2	2.20	0.41
28:BZ:49:ARG:O	28:BZ:53:GLU:HG2	2.21	0.41
28:BZ:86:GLU:HG3	28:BZ:88:ILE:HG23	2.02	0.41
31:Bg:128:ASP:C	31:Bg:129:LYS:HG2	2.46	0.41
34:B5:82:U:H2'	34:B5:83:G:O4'	2.21	0.41
34:B5:153:G:H2'	34:B5:154:G:H8	1.86	0.41
34:B5:208:U:H2'	34:B5:209:U:C6	2.56	0.41
34:B5:281:G:H2'	34:B5:282:C:C6	2.56	0.41
34:B5:882:U:H2'	34:B5:883:C:C6	2.55	0.41
34:B5:898:A:H61	34:B5:912:U:H5''	1.86	0.41
34:B5:978:A:H2'	34:B5:979:A:O4'	2.21	0.41
34:B5:1237:G:N3	34:B5:1238:A:C8	2.88	0.41
34:B5:1350:U:H2'	34:B5:1351:G:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1508:U:H2'	34:B5:1509:C:C6	2.56	0.41
34:B5:1673:G:H22	34:B5:1728:A:H2	1.68	0.41
34:B5:1785:U:H2'	34:B5:1786:G:H8	1.86	0.41
36:AB:259:HIS:CE1	38:A1:2366:C:H5'	2.56	0.41
37:AC:230:VAL:HG21	37:AC:257:LYS:HD3	2.03	0.41
38:A1:80:G:H2'	38:A1:81:C:C6	2.55	0.41
38:A1:180:C:H2'	38:A1:181:U:H6	1.86	0.41
38:A1:239:G:N2	38:A1:241:G:O6	2.52	0.41
38:A1:448:U:O2	38:A1:488:U:O2'	2.25	0.41
38:A1:833:G:OP1	54:AR:86:GLU:HB3	2.21	0.41
38:A1:954:U:C5	38:A1:967:A:N1	2.89	0.41
38:A1:960:PSU:H4'	38:A1:963:G:N1	2.35	0.41
38:A1:1093:A:H1'	38:A1:1094:U:C6	2.55	0.41
38:A1:1109:U:H2'	38:A1:1110:PSU:O4'	2.21	0.41
38:A1:1141:C:O2'	38:A1:1153:A:N3	2.48	0.41
38:A1:1333:C:C2	38:A1:1334:U:C5	3.09	0.41
38:A1:1493:G:OP2	38:A1:1493:G:N2	2.47	0.41
38:A1:1495:U:C5	38:A1:1835:A:N1	2.88	0.41
38:A1:2111:G:H1'	59:AW:44:LYS:HD2	2.03	0.41
38:A1:2219:A:H2'	38:A1:2220:A:C8	2.56	0.41
38:A1:2417:U:H2'	38:A1:2419:A:OP2	2.21	0.41
38:A1:2424:A:H2'	38:A1:2425:G:O4'	2.20	0.41
38:A1:2535:A:H8	38:A1:2535:A:OP2	2.03	0.41
38:A1:2689:A:N3	38:A1:2689:A:H2'	2.36	0.41
38:A1:3113:A:O2'	45:AH:69:ARG:HB3	2.21	0.41
38:A1:3227:A:O2'	49:AM:133:LYS:HD2	2.21	0.41
38:A1:3284:G:H2'	38:A1:3285:C:C6	2.56	0.41
39:A3:53:U:O2'	47:AJ:9:MET:HE1	2.20	0.41
40:A4:83:C:O2	61:AY:51:ARG:NH2	2.52	0.41
40:A4:121:U:H2'	40:A4:122:U:C6	2.56	0.41
44:AG:70:LYS:HB3	44:AG:70:LYS:HE2	1.96	0.41
46:AI:193:ASP:CG	46:AI:194:GLY:H	2.28	0.41
47:AJ:9:MET:HE3	47:AJ:9:MET:HB2	1.88	0.41
48:AL:185:LYS:HG3	48:AL:188:ARG:HH21	1.86	0.41
58:AV:10:LYS:NZ	58:AV:53:SER:OG	2.53	0.41
65:Ac:99:ASP:OD1	65:Ac:99:ASP:N	2.52	0.41
73:Ak:3:ARG:HD2	73:Ak:52:TYR:CE2	2.56	0.41
80:tA:49:C:H2'	80:tA:50:U:C6	2.55	0.41
81:MR:5:U:H2'	81:MR:6:U:C6	2.56	0.41
3:BC:235:LEU:HD11	12:BV:54:ALA:HB2	2.02	0.41
4:BE:251:GLU:O	4:BE:255:ARG:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BG:3:LEU:HD22	5:BG:109:LEU:HB3	2.04	0.41
13:BW:51:GLU:O	13:BW:61:ILE:HA	2.21	0.41
19:BD:8:LYS:HD3	27:BU:63:LEU:HD11	2.03	0.41
34:B5:1351:G:H2'	34:B5:1352:G:C8	2.56	0.41
38:A1:83:U:H2'	38:A1:84:U:O4'	2.21	0.41
38:A1:279:U:H2'	38:A1:280:U:C6	2.56	0.41
38:A1:837:A:H5'	78:Ap:9:GLY:C	2.46	0.41
38:A1:916:G:H5'	38:A1:917:A:OP1	2.20	0.41
38:A1:1155:C:O2'	38:A1:1197:A:N1	2.43	0.41
38:A1:2544:U:O2'	38:A1:2545:C:OP1	2.26	0.41
38:A1:2799:A:H5''	38:A1:2800:G:O5'	2.21	0.41
38:A1:3020:U:H2'	38:A1:3033:A:N6	2.36	0.41
41:AD:77:ALA:O	41:AD:108:ARG:NH1	2.53	0.41
43:AF:176:TYR:CZ	43:AF:197:GLN:HG2	2.56	0.41
43:AF:178:ILE:HD11	43:AF:187:GLU:HG3	2.03	0.41
45:AH:53:ILE:HD12	49:AM:7:VAL:HG21	2.03	0.41
46:AI:55:ASN:ND2	46:AI:162:GLN:OE1	2.52	0.41
55:AS:77:VAL:HG12	55:AS:79:VAL:HG13	2.03	0.41
56:AT:11:THR:HA	56:AT:14:MET:HG2	2.03	0.41
60:AX:67:ILE:HD13	60:AX:121:LYS:HD3	2.03	0.41
79:tP:43:G:H2'	79:tP:44:A:O4'	2.21	0.41
2:BB:143:THR:HB	2:BB:205:PHE:HE2	1.86	0.40
4:BE:3:ARG:HB3	34:B5:93:A:H1'	2.03	0.40
4:BE:166:SER:O	4:BE:168:LYS:N	2.54	0.40
5:BG:195:VAL:HG13	5:BG:199:GLN:HE22	1.85	0.40
5:BG:219:ARG:NH1	5:BG:220:LYS:HE2	2.36	0.40
13:BW:83:ILE:HD13	13:BW:122:SER:HB2	2.02	0.40
13:BW:83:ILE:HG12	34:B5:749:U:H5''	2.03	0.40
28:BZ:46:LYS:HE3	28:BZ:69:LEU:HD23	2.03	0.40
28:BZ:47:TYR:O	28:BZ:50:ILE:HG22	2.20	0.40
34:B5:116:U:H2'	34:B5:117:U:C6	2.56	0.40
34:B5:296:U:H2'	34:B5:297:U:O2	2.21	0.40
34:B5:737:A:O2'	34:B5:738:G:H5''	2.21	0.40
34:B5:1399:C:H4'	34:B5:1400:A:C8	2.56	0.40
34:B5:1652:C:H2'	34:B5:1653:C:C6	2.57	0.40
37:AC:234:ASN:HB3	37:AC:237:GLN:HG3	2.03	0.40
37:AC:349:THR:HG22	38:A1:520:U:O4	2.21	0.40
38:A1:4:U:H2'	38:A1:5:G:C8	2.57	0.40
38:A1:277:G:H2'	38:A1:278:U:C6	2.56	0.40
38:A1:1182:A:H2'	38:A1:1183:C:C6	2.56	0.40
38:A1:2206:G:H2'	38:A1:2207:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2441:A:H3'	38:A1:2441:A:C8	2.56	0.40
42:AE:152:THR:HG23	42:AE:155:LEU:HG	2.02	0.40
45:AH:21:LYS:O	45:AH:22:SER:C	2.63	0.40
45:AH:90:MET:HB2	45:AH:144:ILE:HG23	2.03	0.40
73:AK:20:VAL:HG12	73:AK:47:GLY:HA2	2.01	0.40
79:tP:10:A:C2	79:tP:26:G:H1'	2.56	0.40
79:tP:16:U:H3'	79:tP:18:G:C5'	2.50	0.40
79:tP:23:C:H2'	79:tP:24:G:O4'	2.20	0.40
80:tA:15:G:H2'	80:tA:16:U:N1	2.36	0.40
3:BC:57:PHE:CE1	3:BC:138:PRO:HD3	2.57	0.40
3:BC:106:ASP:OD1	3:BC:106:ASP:N	2.53	0.40
8:BJ:172:VAL:HG22	8:BJ:176:ASN:OD1	2.21	0.40
10:BN:61:THR:HB	34:B5:959:U:C6	2.55	0.40
16:Ba:64:LEU:HD12	16:Ba:64:LEU:O	2.21	0.40
23:BQ:13:LYS:HG2	23:BQ:76:SER:HA	2.03	0.40
23:BQ:98:ASP:HB3	23:BQ:100:GLN:OE1	2.21	0.40
33:BM:35:ALA:CB	33:BM:123:VAL:HG13	2.51	0.40
34:B5:413:U:H5	34:B5:420:A:N1	2.19	0.40
34:B5:503:G:N3	34:B5:503:G:H2'	2.35	0.40
34:B5:706:A:H8	34:B5:733:A:N1	2.19	0.40
34:B5:795:U:C2	34:B5:796:A:C8	3.09	0.40
34:B5:961:U:H2'	34:B5:962:C:C6	2.56	0.40
34:B5:1576:A:H8	34:B5:1576:A:OP2	2.03	0.40
35:AA:200:ARG:NH2	38:A1:2147:A:OP2	2.42	0.40
38:A1:3:U:H2'	38:A1:4:U:C6	2.56	0.40
38:A1:411:U:H2'	38:A1:412:G:C8	2.56	0.40
38:A1:546:C:H4'	38:A1:548:G:O6	2.21	0.40
38:A1:634:C:H5'	68:Af:21:ARG:O	2.21	0.40
38:A1:789:A:H2'	38:A1:790:U:C6	2.56	0.40
38:A1:1072:G:H2'	38:A1:1073:U:H6	1.85	0.40
38:A1:1174:G:H1'	38:A1:1181:U:N3	2.35	0.40
38:A1:1267:U:H2'	38:A1:1268:G:H4'	2.03	0.40
38:A1:1354:G:H1'	42:AE:9:TRP:NE1	2.37	0.40
38:A1:1549:U:H2'	38:A1:1550:C:C6	2.56	0.40
38:A1:2419:A:H2'	38:A1:2420:C:H6	1.87	0.40
38:A1:3107:U:H2'	38:A1:3108:G:H8	1.86	0.40
38:A1:3268:A:OP1	42:AE:46:ARG:NH2	2.47	0.40
39:A3:11:A:N1	39:A3:67:G:O2'	2.52	0.40
40:A4:40:A:H2'	40:A4:41:A:C8	2.56	0.40
48:AL:88:ALA:O	48:AL:92:THR:HG23	2.21	0.40
52:AP:103:GLU:OE1	52:AP:103:GLU:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:AU:82:LYS:HB3	57:AU:82:LYS:HE3	1.90	0.40
67:Ae:11:LYS:O	67:Ae:12:LYS:HB2	2.20	0.40
79:tP:18:G:H1'	79:tP:57:G:N2	2.37	0.40
5:BG:182:GLN:HE22	34:B5:270:C:H41	1.68	0.40
8:BJ:53:ARG:HG2	8:BJ:57:ARG:HH21	1.86	0.40
19:BD:51:ARG:HB3	19:BD:91:VAL:HG22	2.03	0.40
24:BR:10:LYS:HD3	24:BR:53:TYR:CZ	2.55	0.40
24:BR:15:ALA:O	24:BR:19:ARG:HG2	2.20	0.40
31:Bg:171:SER:O	31:Bg:178:VAL:HG13	2.21	0.40
31:Bg:227:ALA:O	31:Bg:229:LYS:HG2	2.21	0.40
34:B5:1350:U:H2'	34:B5:1351:G:C8	2.56	0.40
34:B5:1392:U:H2'	34:B5:1393:C:C6	2.56	0.40
34:B5:1708:U:H2'	34:B5:1709:C:H2'	2.02	0.40
38:A1:271:C:H2'	38:A1:272:G:O4'	2.22	0.40
38:A1:598:A:H2'	38:A1:599:C:C6	2.57	0.40
38:A1:1675:G:H2'	38:A1:1676:A:C8	2.56	0.40
38:A1:1760:A:C2	38:A1:1766:G:C6	3.09	0.40
38:A1:2762:A:H2'	38:A1:2763:U:C6	2.53	0.40
38:A1:2855:U:H2'	38:A1:2856:G:O4'	2.21	0.40
40:A4:5:U:H2'	40:A4:6:U:C6	2.56	0.40
41:AD:190:ILE:HD11	41:AD:195:LEU:HD22	2.02	0.40
42:AE:60:ASP:OD1	42:AE:62:THR:OG1	2.27	0.40
47:AJ:14:ILE:HD13	47:AJ:131:MET:SD	2.62	0.40
54:AR:180:LYS:O	54:AR:185:LEU:HB3	2.22	0.40
60:AX:73:MET:HE2	60:AX:142:ILE:HB	2.04	0.40
61:AY:48:LEU:HD13	61:AY:115:ARG:HH21	1.85	0.40
78:Ap:37:TYR:C	78:Ap:45:LYS:HD2	2.46	0.40
79:tP:18:G:C5	79:tP:58:A:C6	3.09	0.40
1:BA:107:PHE:N	1:BA:135:GLU:OE2	2.53	0.40
3:BC:44:LEU:HD21	3:BC:247:ALA:HB2	2.03	0.40
5:BG:208:TYR:O	5:BG:212:LEU:HD23	2.22	0.40
7:BI:191:PHE:O	7:BI:195:ARG:HG2	2.21	0.40
25:BS:116:LEU:HB3	25:BS:124:GLY:HA3	2.04	0.40
34:B5:133:U:O2'	34:B5:134:U:H4'	2.21	0.40
34:B5:326:G:H2'	34:B5:327:U:C6	2.57	0.40
34:B5:609:U:H4'	34:B5:610:G:H5'	2.02	0.40
34:B5:645:C:H2'	34:B5:646:C:C6	2.56	0.40
34:B5:749:U:H2'	34:B5:750:U:C6	2.57	0.40
34:B5:900:A:H2'	34:B5:901:G:H8	1.86	0.40
34:B5:1017:U:H2'	34:B5:1018:U:C6	2.57	0.40
34:B5:1236:A:HO2'	34:B5:1237:G:P	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1650:U:H2'	34:B5:1651:A:C8	2.57	0.40
38:A1:591:G:C2	42:AE:18:LEU:HD22	2.56	0.40
38:A1:604:G:H2'	38:A1:605:U:C6	2.56	0.40
38:A1:629:U:H2'	38:A1:630:A:C8	2.57	0.40
38:A1:761:A:C2	38:A1:771:A:H1'	2.56	0.40
38:A1:1141:C:H2'	38:A1:1142:G:O4'	2.22	0.40
38:A1:1146:C:H4'	38:A1:1331:U:C4	2.56	0.40
38:A1:1326:A:H2'	38:A1:1327:C:O4'	2.22	0.40
38:A1:1688:U:H2'	38:A1:1689:U:H6	1.85	0.40
38:A1:2208:A:N3	38:A1:2208:A:H3'	2.37	0.40
38:A1:2578:U:H2'	38:A1:2579:G:O4'	2.21	0.40
38:A1:2770:G:H2'	38:A1:2771:U:C6	2.56	0.40
38:A1:2923:PSU:H2'	38:A1:2924:U:C6	2.56	0.40
41:AD:60:ILE:HD11	41:AD:93:THR:HA	2.02	0.40
43:AF:138:TYR:CD2	43:AF:233:GLU:HB3	2.56	0.40
46:AI:192:ASP:HA	46:AI:197:VAL:HG12	2.02	0.40
47:AJ:11:ASP:OD1	47:AJ:11:ASP:N	2.48	0.40
57:AU:92:TRP:CD1	57:AU:108:TYR:HE1	2.39	0.40
78:Ap:59:CYS:C	78:Ap:61:LYS:H	2.29	0.40
1:BA:11:PRO:O	1:BA:15:GLN:HG3	2.21	0.40
2:BB:137:ILE:HG21	2:BB:172:LEU:HD22	2.03	0.40
3:BC:95:ARG:NH1	3:BC:97:ARG:NE	2.69	0.40
4:BE:57:ASN:O	4:BE:61:VAL:HG23	2.21	0.40
6:BH:87:ASP:C	6:BH:88:ARG:HD2	2.46	0.40
6:BH:169:PHE:HA	6:BH:172:VAL:HG22	2.03	0.40
7:BI:57:ALA:HB2	7:BI:177:GLY:HA2	2.03	0.40
8:BJ:171:ARG:HD2	34:B5:537:G:N7	2.37	0.40
16:Ba:2:PRO:HB3	34:B5:1142:A:H5''	2.03	0.40
25:BS:41:ARG:NH1	26:BT:46:PRO:HG3	2.24	0.40
34:B5:160:C:H2'	34:B5:161:U:O4'	2.21	0.40
34:B5:1263:G:H2'	34:B5:1264:G:O4'	2.22	0.40
34:B5:1686:C:H2'	34:B5:1687:U:C5	2.57	0.40
36:AB:322:ILE:HG22	36:AB:324:VAL:HG13	2.04	0.40
38:A1:164:A:H2'	38:A1:165:A:C8	2.57	0.40
38:A1:785:G:N7	63:Aa:77:LYS:NZ	2.53	0.40
38:A1:873:C:H3'	38:A1:874:U:H4'	2.02	0.40
38:A1:1184:A:H2'	38:A1:1185:C:C6	2.57	0.40
38:A1:1781:C:H2'	38:A1:1782:U:C6	2.56	0.40
38:A1:2201:G:H2'	38:A1:2202:C:C6	2.56	0.40
39:A3:96:U:H2'	39:A3:97:A:H8	1.86	0.40
42:AE:80:ASN:HB3	42:AE:83:TYR:HD1	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:AE:145:LEU:HA	42:AE:145:LEU:HD23	1.89	0.40
43:AF:43:ILE:O	43:AF:46:GLU:HG3	2.22	0.40
44:AG:75:ILE:O	44:AG:76:ALA:HB3	2.21	0.40
45:AH:103:ILE:HD11	45:AH:134:ILE:HG21	2.03	0.40
55:AS:1:MET:HA	55:AS:32:SER:HB3	2.04	0.40
68:Af:16:TYR:OH	68:Af:89:LEU:O	2.38	0.40
71:Ai:80:PHE:CE2	71:Ai:84:LYS:HD3	2.56	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	BA	204/252 (81%)	186 (91%)	18 (9%)	0	100	100
2	BB	212/255 (83%)	178 (84%)	34 (16%)	0	100	100
3	BC	215/254 (85%)	209 (97%)	6 (3%)	0	100	100
4	BE	258/261 (99%)	236 (92%)	22 (8%)	0	100	100
5	BG	224/236 (95%)	216 (96%)	8 (4%)	0	100	100
6	BH	182/190 (96%)	167 (92%)	15 (8%)	0	100	100
7	BI	184/200 (92%)	168 (91%)	16 (9%)	0	100	100
8	BJ	183/197 (93%)	174 (95%)	9 (5%)	0	100	100
9	BL	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
10	BN	148/151 (98%)	140 (95%)	8 (5%)	0	100	100
11	BO	125/137 (91%)	111 (89%)	14 (11%)	0	100	100
12	BV	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
13	BW	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
14	BX	142/145 (98%)	133 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	BY	132/135 (98%)	125 (95%)	7 (5%)	0	100	100
16	Ba	95/119 (80%)	83 (87%)	12 (13%)	0	100	100
17	Bb	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
18	Be	58/63 (92%)	56 (97%)	2 (3%)	0	100	100
19	BD	221/240 (92%)	208 (94%)	13 (6%)	0	100	100
20	BF	204/225 (91%)	190 (93%)	14 (7%)	0	100	100
21	BK	94/105 (90%)	84 (89%)	10 (11%)	0	100	100
22	BP	122/142 (86%)	113 (93%)	9 (7%)	0	100	100
23	BQ	139/143 (97%)	135 (97%)	4 (3%)	0	100	100
24	BR	117/136 (86%)	114 (97%)	3 (3%)	0	100	100
25	BS	143/146 (98%)	130 (91%)	13 (9%)	0	100	100
26	BT	139/144 (96%)	121 (87%)	18 (13%)	0	100	100
27	BU	105/121 (87%)	97 (92%)	8 (8%)	0	100	100
28	BZ	68/108 (63%)	66 (97%)	2 (3%)	0	100	100
29	Bc	61/67 (91%)	58 (95%)	3 (5%)	0	100	100
30	Bd	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
31	Bg	310/319 (97%)	285 (92%)	25 (8%)	0	100	100
32	Bf	73/152 (48%)	68 (93%)	5 (7%)	0	100	100
33	BM	122/143 (85%)	107 (88%)	15 (12%)	0	100	100
35	AA	245/254 (96%)	235 (96%)	10 (4%)	0	100	100
36	AB	383/387 (99%)	366 (96%)	17 (4%)	0	100	100
37	AC	359/362 (99%)	339 (94%)	20 (6%)	0	100	100
41	AD	290/297 (98%)	276 (95%)	14 (5%)	0	100	100
42	AE	163/176 (93%)	152 (93%)	11 (7%)	0	100	100
43	AF	220/244 (90%)	210 (96%)	10 (4%)	0	100	100
44	AG	228/256 (89%)	211 (92%)	17 (8%)	0	100	100
45	AH	188/191 (98%)	172 (92%)	16 (8%)	0	100	100
46	AI	215/221 (97%)	205 (95%)	10 (5%)	0	100	100
47	AJ	167/174 (96%)	158 (95%)	9 (5%)	0	100	100
48	AL	191/199 (96%)	185 (97%)	6 (3%)	0	100	100
49	AM	134/138 (97%)	130 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	AN	201/204 (98%)	193 (96%)	8 (4%)	0	100	100
51	AO	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
52	AP	171/184 (93%)	167 (98%)	4 (2%)	0	100	100
53	AQ	183/186 (98%)	179 (98%)	4 (2%)	0	100	100
54	AR	186/189 (98%)	181 (97%)	5 (3%)	0	100	100
55	AS	170/178 (96%)	164 (96%)	6 (4%)	0	100	100
56	AT	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
57	AU	98/121 (81%)	95 (97%)	3 (3%)	0	100	100
58	AV	134/137 (98%)	131 (98%)	3 (2%)	0	100	100
59	AW	61/155 (39%)	60 (98%)	1 (2%)	0	100	100
60	AX	119/142 (84%)	116 (98%)	3 (2%)	0	100	100
61	AY	124/127 (98%)	119 (96%)	5 (4%)	0	100	100
62	AZ	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
63	Aa	146/149 (98%)	138 (94%)	8 (6%)	0	100	100
64	Ab	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
65	Ac	95/105 (90%)	95 (100%)	0	0	100	100
66	Ad	107/113 (95%)	102 (95%)	5 (5%)	0	100	100
67	Ae	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
68	Af	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
69	Ag	110/121 (91%)	107 (97%)	3 (3%)	0	100	100
70	Ah	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
71	Ai	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
72	Aj	85/88 (97%)	82 (96%)	3 (4%)	0	100	100
73	Ak	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
74	Al	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
75	Am	50/128 (39%)	47 (94%)	3 (6%)	0	100	100
76	An	23/25 (92%)	23 (100%)	0	0	100	100
77	Ao	103/106 (97%)	93 (90%)	10 (10%)	0	100	100
78	Ap	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
All	All	10920/11886 (92%)	10311 (94%)	609 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	BA	173/210 (82%)	173 (100%)	0	100	100
2	BB	191/224 (85%)	191 (100%)	0	100	100
3	BC	176/205 (86%)	176 (100%)	0	100	100
4	BE	221/222 (100%)	221 (100%)	0	100	100
5	BG	193/201 (96%)	193 (100%)	0	100	100
6	BH	165/170 (97%)	165 (100%)	0	100	100
7	BI	150/161 (93%)	150 (100%)	0	100	100
8	BJ	158/166 (95%)	158 (100%)	0	100	100
9	BL	136/137 (99%)	136 (100%)	0	100	100
10	BN	127/128 (99%)	127 (100%)	0	100	100
11	BO	96/105 (91%)	96 (100%)	0	100	100
12	BV	74/74 (100%)	74 (100%)	0	100	100
13	BW	110/111 (99%)	110 (100%)	0	100	100
14	BX	119/120 (99%)	119 (100%)	0	100	100
15	BY	112/113 (99%)	112 (100%)	0	100	100
16	Ba	83/100 (83%)	83 (100%)	0	100	100
17	Bb	70/71 (99%)	70 (100%)	0	100	100
18	Be	51/54 (94%)	51 (100%)	0	100	100
19	BD	182/195 (93%)	182 (100%)	0	100	100
20	BF	173/191 (91%)	173 (100%)	0	100	100
21	BK	89/98 (91%)	89 (100%)	0	100	100
22	BP	104/118 (88%)	104 (100%)	0	100	100
23	BQ	117/119 (98%)	117 (100%)	0	100	100
24	BR	101/124 (82%)	101 (100%)	0	100	100
25	BS	128/129 (99%)	128 (100%)	0	100	100
26	BT	113/116 (97%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	BU	100/114 (88%)	100 (100%)	0	100	100
28	BZ	61/89 (68%)	61 (100%)	0	100	100
29	Bc	56/60 (93%)	56 (100%)	0	100	100
30	Bd	47/49 (96%)	47 (100%)	0	100	100
31	Bg	256/262 (98%)	256 (100%)	0	100	100
32	Bf	66/135 (49%)	66 (100%)	0	100	100
33	BM	100/119 (84%)	100 (100%)	0	100	100
35	AA	189/196 (96%)	189 (100%)	0	100	100
36	AB	321/322 (100%)	321 (100%)	0	100	100
37	AC	288/289 (100%)	288 (100%)	0	100	100
41	AD	241/245 (98%)	241 (100%)	0	100	100
42	AE	137/153 (90%)	137 (100%)	0	100	100
43	AF	186/205 (91%)	186 (100%)	0	100	100
44	AG	189/208 (91%)	189 (100%)	0	100	100
45	AH	170/171 (99%)	170 (100%)	0	100	100
46	AI	185/187 (99%)	185 (100%)	0	100	100
47	AJ	147/150 (98%)	147 (100%)	0	100	100
48	AL	154/159 (97%)	154 (100%)	0	100	100
49	AM	107/109 (98%)	107 (100%)	0	100	100
50	AN	175/176 (99%)	175 (100%)	0	100	100
51	AO	160/162 (99%)	160 (100%)	0	100	100
52	AP	141/146 (97%)	141 (100%)	0	100	100
53	AQ	150/151 (99%)	150 (100%)	0	100	100
54	AR	153/154 (99%)	153 (100%)	0	100	100
55	AS	156/162 (96%)	156 (100%)	0	100	100
56	AT	136/137 (99%)	136 (100%)	0	100	100
57	AU	87/107 (81%)	87 (100%)	0	100	100
58	AV	104/105 (99%)	104 (100%)	0	100	100
59	AW	55/129 (43%)	55 (100%)	0	100	100
60	AX	105/118 (89%)	105 (100%)	0	100	100
61	AY	109/110 (99%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	AZ	115/116 (99%)	115 (100%)	0	100	100
63	Aa	118/119 (99%)	118 (100%)	0	100	100
64	Ab	46/47 (98%)	46 (100%)	0	100	100
65	Ac	81/88 (92%)	81 (100%)	0	100	100
66	Ad	96/97 (99%)	96 (100%)	0	100	100
67	Ae	109/111 (98%)	109 (100%)	0	100	100
68	Af	90/91 (99%)	90 (100%)	0	100	100
69	Ag	95/103 (92%)	95 (100%)	0	100	100
70	Ah	104/105 (99%)	104 (100%)	0	100	100
71	Ai	81/82 (99%)	81 (100%)	0	100	100
72	Aj	70/71 (99%)	70 (100%)	0	100	100
73	Ak	68/69 (99%)	68 (100%)	0	100	100
74	Al	45/46 (98%)	45 (100%)	0	100	100
75	Am	47/116 (40%)	47 (100%)	0	100	100
76	An	23/23 (100%)	23 (100%)	0	100	100
77	Ao	90/91 (99%)	90 (100%)	0	100	100
78	Ap	71/72 (99%)	71 (100%)	0	100	100
All	All	9292/9988 (93%)	9292 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	30	GLN
2	BB	79	HIS
3	BC	59	HIS
3	BC	82	ASN
3	BC	94	GLN
4	BE	50	ASN
4	BE	157	ASN
5	BG	56	ASN
5	BG	176	GLN
6	BH	174	ASN
7	BI	32	GLN
7	BI	35	ASN

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Mol	Chain	Res	Type
7	BI	88	ASN
7	BI	111	GLN
7	BI	138	ASN
7	BI	175	GLN
8	BJ	48	GLN
9	BL	92	HIS
9	BL	127	GLN
10	BN	21	ASN
10	BN	49	GLN
10	BN	62	GLN
10	BN	69	ASN
10	BN	105	ASN
10	BN	151	ASN
11	BO	65	GLN
12	BV	70	ASN
12	BV	75	ASN
13	BW	12	ASN
14	BX	89	ASN
15	BY	107	GLN
16	Ba	25	ASN
16	Ba	43	ASN
18	Be	17	GLN
19	BD	159	HIS
20	BF	127	GLN
20	BF	158	GLN
21	BK	39	ASN
21	BK	93	GLN
22	BP	15	HIS
22	BP	104	GLN
23	BQ	21	HIS
23	BQ	32	ASN
23	BQ	93	HIS
25	BS	78	HIS
25	BS	87	ASN
26	BT	12	GLN
26	BT	43	ASN
27	BU	15	GLN
27	BU	49	ASN
27	BU	105	GLN
28	BZ	82	HIS
31	Bg	159	ASN
35	AA	97	ASN

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Mol	Chain	Res	Type
36	AB	121	ASN
36	AB	224	HIS
37	AC	260	GLN
37	AC	361	HIS
41	AD	90	HIS
41	AD	296	GLN
42	AE	172	HIS
43	AF	64	GLN
43	AF	93	ASN
44	AG	28	HIS
44	AG	191	ASN
45	AH	51	GLN
45	AH	58	HIS
45	AH	96	HIS
46	AI	51	HIS
46	AI	92	HIS
47	AJ	20	ASN
47	AJ	90	GLN
48	AL	106	GLN
49	AM	56	GLN
49	AM	119	GLN
51	AO	31[A]	GLN
52	AP	45	GLN
52	AP	121	GLN
52	AP	133	HIS
53	AQ	136	ASN
54	AR	34	GLN
54	AR	68	GLN
56	AT	5	HIS
56	AT	131	GLN
56	AT	149	GLN
57	AU	40	HIS
57	AU	87	ASN
61	AY	42	GLN
62	AZ	122	HIS
63	Aa	120	ASN
66	Ad	21	HIS
66	Ad	57	GLN
67	Ae	20	HIS
69	Ag	98	GLN
70	Ah	99	GLN
72	Aj	20	ASN

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Mol	Chain	Res	Type
73	Ak	67	GLN
74	Al	4	GLN
75	Am	90	ASN
75	Am	120	GLN
77	Ao	59	HIS
77	Ao	90	HIS
77	Ao	105	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	B5	1780/1798 (98%)	438 (24%)	20 (1%)
38	A1	3154/3395 (92%)	532 (16%)	21 (0%)
39	A3	120/121 (99%)	7 (5%)	0
40	A4	157/158 (99%)	25 (15%)	2 (1%)
79	tP	74/75 (98%)	34 (45%)	0
80	tA	75/76 (98%)	18 (24%)	0
81	MR	11/12 (91%)	1 (9%)	0
All	All	5371/5635 (95%)	1055 (19%)	43 (0%)

All (1055) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	B5	2	A
34	B5	4	C
34	B5	25	C
34	B5	26	A
34	B5	34	G
34	B5	42	G
34	B5	45	U
34	B5	47	A
34	B5	57	G
34	B5	60	U
34	B5	63	G
34	B5	68	A
34	B5	70	C
34	B5	72	A
34	B5	73	U
34	B5	75	U
34	B5	76	A
34	B5	77	U

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Mol	Chain	Res	Type
34	B5	79	C
34	B5	94	U
34	B5	104	A
34	B5	114	C
34	B5	116	U
34	B5	126	A
34	B5	127	G
34	B5	128	U
34	B5	130	C
34	B5	131	C
34	B5	133	U
34	B5	134	U
34	B5	135	A
34	B5	136	C
34	B5	137	U
34	B5	138	A
34	B5	141	U
34	B5	144	U
34	B5	145	A
34	B5	149	C
34	B5	153	G
34	B5	159	U
34	B5	160	C
34	B5	166	C
34	B5	176	C
34	B5	178	U
34	B5	179	A
34	B5	188	A
34	B5	190	C
34	B5	191	C
34	B5	192	U
34	B5	193	U
34	B5	195	G
34	B5	196	G
34	B5	197	A
34	B5	199	G
34	B5	200	A
34	B5	212	U
34	B5	213	A
34	B5	217	A
34	B5	221	A
34	B5	224	C

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Mol	Chain	Res	Type
34	B5	225	A
34	B5	226	A
34	B5	229	U
34	B5	231	U
34	B5	233	C
34	B5	235	G
34	B5	238	U
34	B5	239	C
34	B5	240	U
34	B5	241	U
34	B5	253	A
34	B5	257	A
34	B5	260	U
34	B5	261	U
34	B5	276	C
34	B5	278	U
34	B5	280	U
34	B5	281	G
34	B5	287	G
34	B5	299	A
34	B5	302	PSU
34	B5	314	C
34	B5	316	A
34	B5	321	C
34	B5	322	G
34	B5	326	G
34	B5	337	G
34	B5	338	C
34	B5	352	A
34	B5	359	A
34	B5	360	A
34	B5	361	C
34	B5	365	G
34	B5	390	G
34	B5	400	A
34	B5	401	A
34	B5	402	C
34	B5	423	G
34	B5	424	C
34	B5	425	A
34	B5	426	G
34	B5	434	G

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Mol	Chain	Res	Type
34	B5	439	U
34	B5	444	C
34	B5	445	A
34	B5	448	C
34	B5	455	C
34	B5	460	A
34	B5	468	A
34	B5	475	A
34	B5	477	A
34	B5	482	U
34	B5	483	A
34	B5	484	C
34	B5	486	G
34	B5	487	G
34	B5	490	C
34	B5	491	C
34	B5	492	A
34	B5	494	U
34	B5	496	G
34	B5	497	G
34	B5	498	G
34	B5	499	U
34	B5	500	C
34	B5	501	U
34	B5	502	U
34	B5	504	U
34	B5	506	A
34	B5	508	U
34	B5	515	A
34	B5	518	A
34	B5	519	C
34	B5	524	U
34	B5	525	A
34	B5	526	A
34	B5	527	A
34	B5	534	A
34	B5	538	A
34	B5	539	G
34	B5	541	A
34	B5	542	A
34	B5	555	A
34	B5	558	U

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Mol	Chain	Res	Type
34	B5	559	C
34	B5	565	C
34	B5	576	G
34	B5	577	G
34	B5	578	U
34	B5	579	A
34	B5	582	U
34	B5	583	C
34	B5	594	A
34	B5	595	G
34	B5	606	A
34	B5	608	U
34	B5	610	G
34	B5	611	U
34	B5	619	A
34	B5	620	A
34	B5	621	A
34	B5	622	A
34	B5	623	A
34	B5	635	A
34	B5	638	U
34	B5	639	U
34	B5	648	G
34	B5	650	U
34	B5	651	G
34	B5	652	G
34	B5	654	C
34	B5	656	G
34	B5	658	C
34	B5	677	G
34	B5	679	U
34	B5	681	U
34	B5	683	C
34	B5	684	A
34	B5	688	G
34	B5	694	U
34	B5	696	C
34	B5	697	C
34	B5	698	U
34	B5	699	U
34	B5	702	G
34	B5	704	C

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Mol	Chain	Res	Type
34	B5	705	U
34	B5	706	A
34	B5	707	A
34	B5	708	C
34	B5	711	U
34	B5	712	G
34	B5	714	G
34	B5	715	U
34	B5	716	C
34	B5	717	C
34	B5	718	U
34	B5	719	U
34	B5	720	G
34	B5	722	G
34	B5	727	U
34	B5	728	U
34	B5	730	G
34	B5	732	G
34	B5	733	A
34	B5	735	C
34	B5	736	C
34	B5	739	G
34	B5	740	A
34	B5	741	C
34	B5	765	G
34	B5	766	PSU
34	B5	771	A
34	B5	774	A
34	B5	778	G
34	B5	782	U
34	B5	783	G
34	B5	784	C
34	B5	787	G
34	B5	789	A
34	B5	799	A
34	B5	804	A
34	B5	812	A
34	B5	819	G
34	B5	821	U
34	B5	822	U
34	B5	823	G
34	B5	824	G

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Mol	Chain	Res	Type
34	B5	825	U
34	B5	827	C
34	B5	829	A
34	B5	832	U
34	B5	833	U
34	B5	834	G
34	B5	837	G
34	B5	839	U
34	B5	840	U
34	B5	842	C
34	B5	843	U
34	B5	844	A
34	B5	845	G
34	B5	849	C
34	B5	851	U
34	B5	852	C
34	B5	853	G
34	B5	860	U
34	B5	862	A
34	B5	863	A
34	B5	864	U
34	B5	876	G
34	B5	890	C
34	B5	898	A
34	B5	901	G
34	B5	904	G
34	B5	912	U
34	B5	913	G
34	B5	914	G
34	B5	933	A
34	B5	935	U
34	B5	960	U
34	B5	966	A
34	B5	988	A
34	B5	991	G
34	B5	992	A
34	B5	993	A
34	B5	1003	A
34	B5	1004	U
34	B5	1005	A
34	B5	1014	G
34	B5	1020	A

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Mol	Chain	Res	Type
34	B5	1026	A
34	B5	1028	C
34	B5	1031	U
34	B5	1032	G
34	B5	1039	A
34	B5	1040	G
34	B5	1052	U
34	B5	1053	G
34	B5	1056	U
34	B5	1058	U
34	B5	1059	U
34	B5	1060	U
34	B5	1061	A
34	B5	1062	A
34	B5	1070	C
34	B5	1076	A
34	B5	1081	A
34	B5	1082	C
34	B5	1092	A
34	B5	1093	A
34	B5	1097	U
34	B5	1100	G
34	B5	1124	A
34	B5	1126	G
34	B5	1138	A
34	B5	1150	G
34	B5	1158	C
34	B5	1159	C
34	B5	1170	G
34	B5	1180	C
34	B5	1185	U
34	B5	1186	U
34	B5	1194	A
34	B5	1196	A
34	B5	1197	C
34	B5	1199	G
34	B5	1200	G
34	B5	1201	G
34	B5	1202	A
34	B5	1209	C
34	B5	1217	A
34	B5	1218	G

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Mol	Chain	Res	Type
34	B5	1219	A
34	B5	1225	U
34	B5	1228	G
34	B5	1229	G
34	B5	1230	A
34	B5	1232	U
34	B5	1237	G
34	B5	1239	U
34	B5	1240	U
34	B5	1243	G
34	B5	1244	A
34	B5	1245	G
34	B5	1246	C
34	B5	1248	C
34	B5	1250	U
34	B5	1253	U
34	B5	1256	A
34	B5	1257	U
34	B5	1263	G
34	B5	1286	U
34	B5	1307	U
34	B5	1314	U
34	B5	1315	U
34	B5	1318	G
34	B5	1321	A
34	B5	1337	A
34	B5	1338	C
34	B5	1340	U
34	B5	1342	C
34	B5	1344	A
34	B5	1345	A
34	B5	1346	A
34	B5	1347	U
34	B5	1353	U
34	B5	1356	U
34	B5	1357	A
34	B5	1358	G
34	B5	1361	U
34	B5	1362	U
34	B5	1363	U
34	B5	1364	G
34	B5	1369	U

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Mol	Chain	Res	Type
34	B5	1370	U
34	B5	1371	A
34	B5	1372	U
34	B5	1373	C
34	B5	1374	C
34	B5	1376	C
34	B5	1378	U
34	B5	1390	U
34	B5	1398	U
34	B5	1399	C
34	B5	1413	U
34	B5	1414	U
34	B5	1415	PSU
34	B5	1425	A
34	B5	1427	A
34	B5	1428	G
34	B5	1435	G
34	B5	1436	A
34	B5	1446	A
34	B5	1459	C
34	B5	1466	G
34	B5	1471	A
34	B5	1486	G
34	B5	1491	U
34	B5	1492	A
34	B5	1493	A
34	B5	1496	U
34	B5	1516	A
34	B5	1521	G
34	B5	1522	U
34	B5	1523	G
34	B5	1524	A
34	B5	1534	G
34	B5	1537	C
34	B5	1542	G
34	B5	1554	U
34	B5	1557	U
34	B5	1559	A
34	B5	1575	G7M
34	B5	1576	A
34	B5	1584	G
34	B5	1596	C

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Mol	Chain	Res	Type
34	B5	1597	A
34	B5	1601	G
34	B5	1607	G
34	B5	1616	G
34	B5	1622	G
34	B5	1634	C
34	B5	1657	U
34	B5	1658	G
34	B5	1682	U
34	B5	1683	C
34	B5	1684	U
34	B5	1686	C
34	B5	1687	U
34	B5	1689	A
34	B5	1692	G
34	B5	1693	A
34	B5	1694	A
34	B5	1695	G
34	B5	1699	G
34	B5	1700	C
34	B5	1701	A
34	B5	1702	A
34	B5	1703	C
34	B5	1705	C
34	B5	1709	C
34	B5	1710	U
34	B5	1712	A
34	B5	1713	G
34	B5	1717	G
34	B5	1755	A
34	B5	1756[A]	A
34	B5	1757	G
34	B5	1760	G
34	B5	1767	G
34	B5	1769	U
34	B5	1780	G
34	B5	1792	G
34	B5	1793	G
34	B5	1794	A
34	B5	1795	U
34	B5	1796	C
34	B5	1799	U

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Mol	Chain	Res	Type
38	A1	6	A
38	A1	14	U
38	A1	16	A
38	A1	26	A
38	A1	30	G
38	A1	40	A
38	A1	43	A
38	A1	49	A
38	A1	59	G
38	A1	60	A
38	A1	65	A
38	A1	66	A
38	A1	92	G
38	A1	93	C
38	A1	99	A
38	A1	110	G
38	A1	111	C
38	A1	116	A
38	A1	117	U
38	A1	122	A
38	A1	133	U
38	A1	135	C
38	A1	136	G
38	A1	156	G
38	A1	157	A
38	A1	160	G
38	A1	161	G
38	A1	162	G
38	A1	165	A
38	A1	166	C
38	A1	172	G
38	A1	173	G
38	A1	177	U
38	A1	187	A
38	A1	190	U
38	A1	191	U
38	A1	210	U
38	A1	219	A
38	A1	239	G
38	A1	241	G
38	A1	242	C
38	A1	244	G

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Mol	Chain	Res	Type
38	A1	245	U
38	A1	247	C
38	A1	248	U
38	A1	249	U
38	A1	250	U
38	A1	251	G
38	A1	252	U
38	A1	253	A
38	A1	262	U
38	A1	263	C
38	A1	269	G
38	A1	284	A
38	A1	286	U
38	A1	295	A
38	A1	305	U
38	A1	315	C
38	A1	329	U
38	A1	376	G
38	A1	398	A
38	A1	402	A
38	A1	403	C
38	A1	421	G
38	A1	422	A
38	A1	438	A
38	A1	440	A
38	A1	441	U
38	A1	442	G
38	A1	443	G
38	A1	444	U
38	A1	445	G
38	A1	446	U
38	A1	447	U
38	A1	448	U
38	A1	449	U
38	A1	450	G
38	A1	487	U
38	A1	488	U
38	A1	489	U
38	A1	491	A
38	A1	492	C
38	A1	494	G
38	A1	495	G

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Mol	Chain	Res	Type
38	A1	521	A
38	A1	535	G
38	A1	536	U
38	A1	539	C
38	A1	540	U
38	A1	541	U
38	A1	542	G
38	A1	544	C
38	A1	545	U
38	A1	546	C
38	A1	547	G
38	A1	548	G
38	A1	549	U
38	A1	550	A
38	A1	551	A
38	A1	555	U
38	A1	557	A
38	A1	559	A
38	A1	560	G
38	A1	579	G
38	A1	589	A
38	A1	592	A
38	A1	603	A
38	A1	611	A
38	A1	612	U
38	A1	620	U
38	A1	621	A
38	A1	622	A
38	A1	636	C
38	A1	649	A
38	A1	660	A
38	A1	677	A
38	A1	681	U
38	A1	690	A
38	A1	691	A
38	A1	705	A
38	A1	715	A
38	A1	735	A
38	A1	766	U
38	A1	767	U
38	A1	771	A
38	A1	772	U

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Mol	Chain	Res	Type
38	A1	776	PSU
38	A1	777	U
38	A1	780	A
38	A1	781	G
38	A1	785	G
38	A1	786	A
38	A1	799	G
38	A1	806	A
38	A1	817	A
38	A1	830	A
38	A1	844	G
38	A1	849	C
38	A1	861	C
38	A1	874	U
38	A1	879	U
38	A1	896	A
38	A1	907	G
38	A1	914	A
38	A1	916	G
38	A1	917	A
38	A1	921	A
38	A1	923	C
38	A1	924	G
38	A1	925	A
38	A1	937	G
38	A1	944	C
38	A1	959	C
38	A1	960	PSU
38	A1	974	G
38	A1	977	C
38	A1	980	A
38	A1	982	C
38	A1	991	G
38	A1	994	G
38	A1	1000	C
38	A1	1010	G
38	A1	1015	U
38	A1	1016	C
38	A1	1017	C
38	A1	1018	G
38	A1	1019	G
38	A1	1021	G

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Mol	Chain	Res	Type
38	A1	1031	C
38	A1	1032	C
38	A1	1034	U
38	A1	1047	A
38	A1	1064	A
38	A1	1072	G
38	A1	1081	U
38	A1	1082	U
38	A1	1093	A
38	A1	1094	U
38	A1	1095	U
38	A1	1096	U
38	A1	1097	G
38	A1	1098	A
38	A1	1103	A
38	A1	1104	G
38	A1	1117	G
38	A1	1131	G
38	A1	1144	U
38	A1	1153	A
38	A1	1159	A
38	A1	1160	C
38	A1	1180	A
38	A1	1181	U
38	A1	1182	A
38	A1	1192	C
38	A1	1193	A
38	A1	1196	C
38	A1	1201	C
38	A1	1208	U
38	A1	1219	C
38	A1	1221	A
38	A1	1222	G
38	A1	1223	A
38	A1	1226	G
38	A1	1227	C
38	A1	1231	A
38	A1	1232	C
38	A1	1235	U
38	A1	1236	G
38	A1	1237	G
38	A1	1238	C

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Mol	Chain	Res	Type
38	A1	1239	C
38	A1	1240	A
38	A1	1241	U
38	A1	1242	G
38	A1	1243	G
38	A1	1245	A
38	A1	1246	G
38	A1	1247	U
38	A1	1248	C
38	A1	1249	G
38	A1	1250	G
38	A1	1251	A
38	A1	1252	A
38	A1	1253	U
38	A1	1255	C
38	A1	1256	G
38	A1	1258	U
38	A1	1259	A
38	A1	1261	G
38	A1	1262	G
38	A1	1263	A
38	A1	1264	G
38	A1	1265	U
38	A1	1268	G
38	A1	1270	A
38	A1	1271	A
38	A1	1273	A
38	A1	1278	A
38	A1	1279	C
38	A1	1281	G
38	A1	1284	C
38	A1	1285	G
38	A1	1287	A
38	A1	1293	U
38	A1	1307	G
38	A1	1309	U
38	A1	1317	A
38	A1	1330	A
38	A1	1331	U
38	A1	1349	G
38	A1	1350	A
38	A1	1351	U

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Mol	Chain	Res	Type
38	A1	1353	U
38	A1	1356	U
38	A1	1357	G
38	A1	1386	A
38	A1	1392	G
38	A1	1399	A
38	A1	1400	G
38	A1	1418	A
38	A1	1419	A
38	A1	1434	G
38	A1	1437	C
38	A1	1446	A
38	A1	1469	C
38	A1	1481	A
38	A1	1482	A
38	A1	1483	G
38	A1	1487	G
38	A1	1527	C
38	A1	1539	A
38	A1	1555	U
38	A1	1556	C
38	A1	1560	G
38	A1	1562	C
38	A1	1567	U
38	A1	1568	U
38	A1	1569	U
38	A1	1570	U
38	A1	1572	U
38	A1	1574	C
38	A1	1576	G
38	A1	1578	C
38	A1	1579	C
38	A1	1580	A
38	A1	1582	C
38	A1	1583	A
38	A1	1587	A
38	A1	1589	A
38	A1	1628	C
38	A1	1629	U
38	A1	1630	U
38	A1	1642	A
38	A1	1643	A

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Mol	Chain	Res	Type
38	A1	1657	C
38	A1	1683	A
38	A1	1715	A
38	A1	1724	U
38	A1	1750	A
38	A1	1751	G
38	A1	1759	C
38	A1	1760	A
38	A1	1762	C
38	A1	1763	U
38	A1	1764	U
38	A1	1765	U
38	A1	1766	G
38	A1	1775	G
38	A1	1797	A
38	A1	1809	A
38	A1	1813	A
38	A1	1815	U
38	A1	1816	A
38	A1	1817	G
38	A1	1821	U
38	A1	1842	A
38	A1	1849	C
38	A1	1878	G
38	A1	1880	U
38	A1	1886	A
38	A1	1893	A
38	A1	1906	G
38	A1	1943	C
38	A1	1953	G
38	A1	1954	G
38	A1	2094	C
38	A1	2100	A
38	A1	2111	G
38	A1	2112	U
38	A1	2114	C
38	A1	2122	G
38	A1	2131	A
38	A1	2140	U
38	A1	2144	A
38	A1	2158	A
38	A1	2169	G

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Mol	Chain	Res	Type
38	A1	2188	A
38	A1	2204	C
38	A1	2205	U
38	A1	2206	G
38	A1	2207	A
38	A1	2208	A
38	A1	2210	G
38	A1	2249	G
38	A1	2256	A
38	A1	2258	PSU
38	A1	2260	PSU
38	A1	2266	PSU
38	A1	2270	A
38	A1	2272	G
38	A1	2273	G
38	A1	2279	A
38	A1	2280	A
38	A1	2307	G
38	A1	2310	U
38	A1	2313	A
38	A1	2315	G
38	A1	2318	U
38	A1	2334	U
38	A1	2335	G
38	A1	2336	U
38	A1	2366	C
38	A1	2373	A
38	A1	2374	C
38	A1	2375	G
38	A1	2383	C
38	A1	2385	G
38	A1	2391	G
38	A1	2393	G
38	A1	2394	G
38	A1	2397	A
38	A1	2402	A
38	A1	2403	G
38	A1	2404	A
38	A1	2411	U
38	A1	2435	G
38	A1	2438	A
38	A1	2439	A

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Mol	Chain	Res	Type
38	A1	2440	G
38	A1	2441	A
38	A1	2444	C
38	A1	2503	G
38	A1	2504	U
38	A1	2507	C
38	A1	2508	U
38	A1	2509	U
38	A1	2514	U
38	A1	2515	A
38	A1	2522	G
38	A1	2523	A
38	A1	2524	A
38	A1	2535	A
38	A1	2536	A
38	A1	2537	U
38	A1	2538	U
38	A1	2539	C
38	A1	2540	A
38	A1	2541	U
38	A1	2542	U
38	A1	2543	U
38	A1	2544	U
38	A1	2545	C
38	A1	2546	C
38	A1	2552	C
38	A1	2566	C
38	A1	2569	A
38	A1	2570	U
38	A1	2585	G
38	A1	2593	A
38	A1	2595	A
38	A1	2606	G
38	A1	2607	G
38	A1	2614	G
38	A1	2637	A
38	A1	2652	U
38	A1	2656	A
38	A1	2674	A
38	A1	2677	G
38	A1	2681	U
38	A1	2689	A

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Mol	Chain	Res	Type
38	A1	2691	A
38	A1	2704	A
38	A1	2708	C
38	A1	2714	G
38	A1	2719	U
38	A1	2728	G
38	A1	2729	U
38	A1	2752	U
38	A1	2753	G
38	A1	2772	C
38	A1	2773	C
38	A1	2777	G
38	A1	2778	G
38	A1	2780	A
38	A1	2796	G
38	A1	2800	G
38	A1	2801	A
38	A1	2803	A
38	A1	2810	C
38	A1	2814	G
38	A1	2817	A
38	A1	2842	U
38	A1	2845	A
38	A1	2856	G
38	A1	2867	C
38	A1	2871	G
38	A1	2875	U
38	A1	2887	A
38	A1	2898	G
38	A1	2923	PSU
38	A1	2935	U
38	A1	2936	A
38	A1	2938	G
38	A1	2942	C
38	A1	2947	G
38	A1	2971	A
38	A1	2972	G
38	A1	2983	C
38	A1	2990	G
38	A1	2997	G
38	A1	3012	A
38	A1	3022	G

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Mol	Chain	Res	Type
38	A1	3032	A
38	A1	3046	A
38	A1	3056	U
38	A1	3059	G
38	A1	3078	U
38	A1	3079	U
38	A1	3086	A
38	A1	3092	C
38	A1	3113	A
38	A1	3122	A
38	A1	3130	A
38	A1	3131	U
38	A1	3142	A
38	A1	3143	C
38	A1	3144	G
38	A1	3151	U
38	A1	3153	U
38	A1	3154	C
38	A1	3155	U
38	A1	3156	U
38	A1	3165	A
38	A1	3169	U
38	A1	3170	A
38	A1	3173	G
38	A1	3174	A
38	A1	3175	U
38	A1	3176	G
38	A1	3179	U
38	A1	3181	C
38	A1	3187	A
38	A1	3196	U
38	A1	3206	C
38	A1	3207	U
38	A1	3210	A
38	A1	3214	U
38	A1	3217	C
38	A1	3218	A
38	A1	3219	G
38	A1	3224	G
38	A1	3231	U
38	A1	3234	A
38	A1	3236	U

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Mol	Chain	Res	Type
38	A1	3243	A
38	A1	3247	G
38	A1	3250	U
38	A1	3256	G
38	A1	3259	U
38	A1	3275	U
38	A1	3276	G
38	A1	3279	A
38	A1	3281	U
38	A1	3289	G
38	A1	3294	A
38	A1	3304	U
38	A1	3307	A
38	A1	3313	U
38	A1	3316	A
38	A1	3317	U
38	A1	3318	G
38	A1	3319	U
38	A1	3320	A
38	A1	3341	U
38	A1	3345	G
38	A1	3353	G
38	A1	3354	U
38	A1	3355	U
38	A1	3356	G
38	A1	3369	G
38	A1	3378	C
38	A1	3386	G
39	A3	33	U
39	A3	54	U
39	A3	55	A
39	A3	65	G
39	A3	102	A
39	A3	112	G
39	A3	121	U
40	A4	23	U
40	A4	34	U
40	A4	35	C
40	A4	39	G
40	A4	51	G
40	A4	52	A
40	A4	59	A

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Mol	Chain	Res	Type
40	A4	62	C
40	A4	63	G
40	A4	81	U
40	A4	82	U
40	A4	83	C
40	A4	84	C
40	A4	86	U
40	A4	87	G
40	A4	90	U
40	A4	95	G
40	A4	104	A
40	A4	106	C
40	A4	111	A
40	A4	113	U
40	A4	116	G
40	A4	125	U
40	A4	152	G
40	A4	158	U
79	tP	9	G
79	tP	13	C
79	tP	18	G
79	tP	19	G
79	tP	20	A
79	tP	21	A
79	tP	22	G
79	tP	23	C
79	tP	24	G
79	tP	27	C
79	tP	43	G
79	tP	44	A
79	tP	45	U
79	tP	46	G
79	tP	47	U
79	tP	48	C
79	tP	51	C
79	tP	52	G
79	tP	53	G
79	tP	54	A
79	tP	55	U
79	tP	56	C
79	tP	57	G
79	tP	58	A

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Mol	Chain	Res	Type
79	tP	60	A
79	tP	61	C
79	tP	64	A
79	tP	65	G
79	tP	67	G
79	tP	68	G
79	tP	69	C
79	tP	70	G
79	tP	71	C
79	tP	76	A
80	tA	2	G
80	tA	3	C
80	tA	5	C
80	tA	9	G
80	tA	15	G
80	tA	16	U
80	tA	17	A
80	tA	18	G
80	tA	19	G
80	tA	20	A
80	tA	21	A
80	tA	46	G
80	tA	47	U
80	tA	48	C
80	tA	60	A
80	tA	61	C
80	tA	74	C
80	tA	76	A
81	MR	8	A

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	B5	71	A
34	B5	143	G
34	B5	695	U
34	B5	698	U
34	B5	828	U
34	B5	861	U
34	B5	862	A
34	B5	1055	U
34	B5	1228	G

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Mol	Chain	Res	Type
34	B5	1236	A
34	B5	1239	U
34	B5	1256	A
34	B5	1285	U
34	B5	1344	A
34	B5	1357	A
34	B5	1362	U
34	B5	1363	U
34	B5	1458	G
34	B5	1492	A
34	B5	1755	A
38	A1	250	U
38	A1	251	G
38	A1	252	U
38	A1	487	U
38	A1	541	U
38	A1	602	A
38	A1	843	A
38	A1	873	C
38	A1	916	G
38	A1	1094	U
38	A1	1225	A
38	A1	1292	C
38	A1	1577	G
38	A1	1580	A
38	A1	2204	C
38	A1	2207	A
38	A1	2506	U
38	A1	2508	U
38	A1	2544	U
38	A1	2772	C
38	A1	3121	U
40	A4	81	U
40	A4	83	C

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	HIC	AB	243	36	10,11,12	1.43	1 (10%)	9,14,16	1.40	2 (22%)
34	B8N	B5	1191	34	25,29,30	1.35	3 (12%)	28,42,45	3.77	6 (21%)
38	OMG	A1	2922	38	23,26,27	1.18	3 (13%)	32,38,41	2.03	6 (18%)
38	PSU	A1	2351	38	18,21,22	1.45	3 (16%)	21,30,33	2.06	4 (19%)
38	PSU	A1	990	38	18,21,22	1.39	3 (16%)	21,30,33	2.06	4 (19%)
38	PSU	A1	2416	38	18,21,22	1.43	3 (16%)	21,30,33	2.00	4 (19%)
38	PSU	A1	2264	38	18,21,22	1.39	3 (16%)	21,30,33	2.07	4 (19%)
34	PSU	B5	1181	34	18,21,22	1.36	2 (11%)	21,30,33	2.03	4 (19%)
34	PSU	B5	1290	34	18,21,22	1.39	2 (11%)	21,30,33	2.09	4 (19%)
39	PSU	A3	50	39	18,21,22	1.38	2 (11%)	21,30,33	2.02	3 (14%)
38	PSU	A1	1052	38	18,21,22	1.37	3 (16%)	21,30,33	2.00	4 (19%)
34	PSU	B5	999	34	18,21,22	1.37	2 (11%)	21,30,33	2.10	5 (23%)
38	PSU	A1	2129	38	18,21,22	1.42	3 (16%)	21,30,33	2.10	4 (19%)
38	PSU	A1	1110	38	18,21,22	1.37	3 (16%)	21,30,33	2.08	5 (23%)
34	PSU	B5	302	34	18,21,22	1.39	2 (11%)	21,30,33	2.07	3 (14%)
34	PSU	B5	632	34	18,21,22	1.41	3 (16%)	21,30,33	2.05	4 (19%)
38	PSU	A1	2258	38	18,21,22	1.39	2 (11%)	21,30,33	2.06	3 (14%)
38	PSU	A1	966	38	18,21,22	1.47	4 (22%)	21,30,33	2.12	4 (19%)
38	PSU	A1	2266	38	18,21,22	1.42	3 (16%)	21,30,33	2.03	3 (14%)
38	PSU	A1	2826	38	18,21,22	1.43	4 (22%)	21,30,33	2.15	5 (23%)
38	UR3	A1	2634	38	19,22,23	0.93	0	26,32,35	1.74	3 (11%)
38	PSU	A1	2975	38	18,21,22	1.39	3 (16%)	21,30,33	2.04	4 (19%)
34	PSU	B5	759	34	18,21,22	1.38	3 (16%)	21,30,33	2.11	4 (19%)
38	PSU	A1	2191	38	18,21,22	1.40	3 (16%)	21,30,33	2.08	5 (23%)
38	PSU	A1	776	38	18,21,22	1.45	3 (16%)	21,30,33	1.99	4 (19%)
34	PSU	B5	211	34	18,21,22	1.48	4 (22%)	21,30,33	2.01	4 (19%)
38	PSU	A1	2260	38	18,21,22	1.41	3 (16%)	21,30,33	2.07	3 (14%)
34	4AC	B5	1773	34	21,24,25	0.97	1 (4%)	28,34,37	2.11	5 (17%)
38	PSU	A1	2133	38	18,21,22	1.38	3 (16%)	21,30,33	2.16	4 (19%)
38	PSU	A1	986	38	18,21,22	1.41	3 (16%)	21,30,33	1.97	3 (14%)
38	PSU	A1	1056	38	18,21,22	1.39	3 (16%)	21,30,33	2.07	4 (19%)
38	OMU	A1	2921	82,38	19,22,23	1.23	3 (15%)	25,31,34	1.87	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	1MA	A1	645	82,38	21,25,26	1.33	3 (14%)	30,37,40	1.68	5 (16%)
38	PSU	A1	1124	38	18,21,22	1.37	2 (11%)	21,30,33	2.12	4 (19%)
34	MA6	B5	1782	34	23,26,27	1.48	5 (21%)	33,38,41	2.09	10 (30%)
38	PSU	A1	2735	38	18,21,22	1.40	3 (16%)	21,30,33	2.06	4 (19%)
38	5MC	A1	2870	38	19,22,23	1.51	3 (15%)	26,32,35	1.24	2 (7%)
34	PSU	B5	766	34	18,21,22	1.42	3 (16%)	21,30,33	2.08	5 (23%)
38	PSU	A1	2314	38	18,21,22	1.38	2 (11%)	21,30,33	2.11	4 (19%)
38	PSU	A1	2880	38	18,21,22	1.41	3 (16%)	21,30,33	2.06	5 (23%)
38	PSU	A1	2923	38	18,21,22	1.44	2 (11%)	21,30,33	2.12	3 (14%)
38	PSU	A1	960	38	18,21,22	1.41	3 (16%)	21,30,33	2.10	3 (14%)
38	PSU	A1	2349	82,38	18,21,22	1.38	2 (11%)	21,30,33	2.04	3 (14%)
38	PSU	A1	2865	38	18,21,22	1.37	2 (11%)	21,30,33	2.10	4 (19%)
38	PSU	A1	1004	38	18,21,22	1.38	2 (11%)	21,30,33	2.17	5 (23%)
34	PSU	B5	106	34	18,21,22	1.38	3 (16%)	21,30,33	2.10	4 (19%)
34	MA6	B5	1781	34	23,26,27	1.51	5 (21%)	33,38,41	2.07	10 (30%)
38	PSU	A1	2944	82,38	18,21,22	1.39	3 (16%)	21,30,33	2.10	4 (19%)
34	PSU	B5	466	34	18,21,22	1.37	2 (11%)	21,30,33	2.07	4 (19%)
34	PSU	B5	1415	34	18,21,22	1.38	3 (16%)	21,30,33	2.00	3 (14%)
34	G7M	B5	1575	34	23,26,27	2.45	6 (26%)	34,39,42	1.77	7 (20%)
34	PSU	B5	1187	34	18,21,22	1.36	2 (11%)	21,30,33	2.08	4 (19%)
38	PSU	A1	1042	38	18,21,22	1.41	3 (16%)	21,30,33	2.08	4 (19%)
34	4AC	B5	1280	34	21,24,25	0.98	1 (4%)	28,34,37	1.10	3 (10%)
38	1MA	A1	2142	82,38	21,25,26	1.35	4 (19%)	30,37,40	1.73	4 (13%)
38	PSU	A1	2340	38	18,21,22	1.44	3 (16%)	21,30,33	2.07	3 (14%)
40	PSU	A4	73	40	18,21,22	1.40	2 (11%)	21,30,33	2.02	4 (19%)
34	PSU	B5	120	34	18,21,22	1.40	3 (16%)	21,30,33	2.04	3 (14%)
38	5MC	A1	2278	82,38	19,22,23	1.60	3 (15%)	26,32,35	1.15	3 (11%)

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
36	HIC	AB	243	36	-	0/5/6/8	0/1/1/1
34	B8N	B5	1191	34	-	7/16/34/35	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	OMG	A1	2922	38	-	1/9/27/28	0/3/3/3
38	PSU	A1	2351	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	990	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2416	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2264	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	1181	34	-	0/7/25/26	0/2/2/2
34	PSU	B5	1290	34	-	0/7/25/26	0/2/2/2
39	PSU	A3	50	39	-	0/7/25/26	0/2/2/2
38	PSU	A1	1052	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	999	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	2129	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	1110	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	302	34	-	2/7/25/26	0/2/2/2
34	PSU	B5	632	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	2258	38	-	2/7/25/26	0/2/2/2
38	PSU	A1	966	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2266	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2826	38	-	0/7/25/26	0/2/2/2
38	UR3	A1	2634	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2975	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	759	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	2191	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	776	38	-	3/7/25/26	0/2/2/2
34	PSU	B5	211	34	-	2/7/25/26	0/2/2/2
38	PSU	A1	2260	38	-	2/7/25/26	0/2/2/2
34	4AC	B5	1773	34	-	3/11/29/30	0/2/2/2
38	PSU	A1	2133	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	986	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	1056	38	-	0/7/25/26	0/2/2/2
38	OMU	A1	2921	82,38	-	0/9/27/28	0/2/2/2
38	1MA	A1	645	82,38	-	2/7/25/26	0/3/3/3
38	PSU	A1	1124	38	-	0/7/25/26	0/2/2/2
34	MA6	B5	1782	34	-	2/11/29/30	0/3/3/3
38	PSU	A1	2735	38	-	0/7/25/26	0/2/2/2
38	5MC	A1	2870	38	-	4/7/25/26	0/2/2/2
34	PSU	B5	766	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	2314	38	-	1/7/25/26	0/2/2/2
38	PSU	A1	2880	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2923	38	-	4/7/25/26	0/2/2/2
38	PSU	A1	960	38	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	PSU	A1	2349	82,38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2865	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	1004	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	106	34	-	0/7/25/26	0/2/2/2
34	MA6	B5	1781	34	-	0/11/29/30	0/3/3/3
38	PSU	A1	2944	82,38	-	0/7/25/26	0/2/2/2
34	PSU	B5	466	34	-	0/7/25/26	0/2/2/2
34	PSU	B5	1415	34	-	2/7/25/26	0/2/2/2
34	G7M	B5	1575	34	-	1/7/25/26	0/3/3/3
34	PSU	B5	1187	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	1042	38	-	0/7/25/26	0/2/2/2
34	4AC	B5	1280	34	-	4/11/29/30	0/2/2/2
38	1MA	A1	2142	82,38	-	0/7/25/26	0/3/3/3
38	PSU	A1	2340	38	-	1/7/25/26	0/2/2/2
40	PSU	A4	73	40	-	0/7/25/26	0/2/2/2
34	PSU	B5	120	34	-	0/7/25/26	0/2/2/2
38	5MC	A1	2278	82,38	-	0/7/25/26	0/2/2/2

All (164) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1575	G7M	O6-C6	7.05	1.36	1.23
38	A1	2278	5MC	C5-C4	5.86	1.48	1.44
34	B5	1575	G7M	C2-N2	5.66	1.47	1.34
38	A1	2870	5MC	C5-C4	5.06	1.47	1.44
34	B5	1575	G7M	C5-N7	-4.85	1.33	1.39
34	B5	1781	MA6	C5-C4	4.64	1.47	1.39
34	B5	1782	MA6	C5-C4	4.49	1.47	1.39
34	B5	1191	B8N	C4-C5	-3.81	1.38	1.47
34	B5	211	PSU	C6-C5	3.55	1.39	1.35
38	A1	776	PSU	C6-C5	3.47	1.39	1.35
38	A1	2416	PSU	C6-C5	3.46	1.39	1.35
38	A1	2923	PSU	C6-C5	3.44	1.39	1.35
39	A3	50	PSU	C6-C5	3.42	1.39	1.35
38	A1	2340	PSU	C6-C5	3.40	1.39	1.35
38	A1	2351	PSU	C6-C5	3.39	1.39	1.35
38	A1	2191	PSU	C6-C5	3.36	1.39	1.35
34	B5	1575	G7M	CN7-N7	3.36	1.52	1.46
38	A1	2129	PSU	C6-C5	3.35	1.39	1.35
34	B5	759	PSU	C6-C5	3.32	1.39	1.35
40	A4	73	PSU	C6-C5	3.30	1.38	1.35
38	A1	1042	PSU	C6-C5	3.27	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	2266	PSU	C6-C5	3.27	1.38	1.35
38	A1	2264	PSU	C6-C5	3.25	1.38	1.35
34	B5	1181	PSU	C6-C5	3.25	1.38	1.35
34	B5	632	PSU	C6-C5	3.23	1.38	1.35
34	B5	1290	PSU	C6-C5	3.23	1.38	1.35
38	A1	2975	PSU	C6-C5	3.23	1.38	1.35
38	A1	2258	PSU	C6-C5	3.22	1.38	1.35
38	A1	2944	PSU	C6-C5	3.20	1.38	1.35
38	A1	1056	PSU	C6-C5	3.19	1.38	1.35
38	A1	1110	PSU	C6-C5	3.19	1.38	1.35
34	B5	1415	PSU	C6-C5	3.17	1.38	1.35
38	A1	2880	PSU	C6-C5	3.16	1.38	1.35
38	A1	966	PSU	C6-C5	3.14	1.38	1.35
38	A1	990	PSU	C6-C5	3.14	1.38	1.35
38	A1	2260	PSU	C6-C5	3.13	1.38	1.35
38	A1	986	PSU	C6-C5	3.13	1.38	1.35
34	B5	302	PSU	C6-C5	3.13	1.38	1.35
38	A1	1004	PSU	C6-C5	3.12	1.38	1.35
34	B5	106	PSU	C6-C5	3.12	1.38	1.35
34	B5	766	PSU	C6-C5	3.12	1.38	1.35
38	A1	2865	PSU	C6-C5	3.11	1.38	1.35
34	B5	999	PSU	C6-C5	3.10	1.38	1.35
34	B5	1187	PSU	C6-C5	3.10	1.38	1.35
38	A1	2133	PSU	C6-C5	3.10	1.38	1.35
34	B5	120	PSU	C6-C5	3.09	1.38	1.35
38	A1	1052	PSU	C6-C5	3.09	1.38	1.35
38	A1	2314	PSU	C6-C5	3.09	1.38	1.35
38	A1	2735	PSU	C6-C5	3.08	1.38	1.35
38	A1	2870	5MC	C6-C5	3.06	1.39	1.34
34	B5	466	PSU	C6-C5	3.06	1.38	1.35
38	A1	645	1MA	C5-C4	3.06	1.47	1.38
38	A1	2142	1MA	C5-C4	3.06	1.47	1.38
38	A1	2349	PSU	C6-C5	3.02	1.38	1.35
38	A1	966	PSU	C4-N3	-3.01	1.33	1.38
38	A1	1124	PSU	C6-C5	3.01	1.38	1.35
38	A1	2142	1MA	C6-N6	3.00	1.35	1.28
34	B5	1782	MA6	C5-C6	3.00	1.49	1.41
34	B5	1781	MA6	C5-C6	2.97	1.49	1.41
38	A1	2922	OMG	C5-C4	2.96	1.46	1.38
38	A1	2351	PSU	C4-N3	-2.94	1.33	1.38
38	A1	2416	PSU	C4-N3	-2.93	1.33	1.38
34	B5	632	PSU	C4-N3	-2.90	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	990	PSU	C4-N3	-2.90	1.33	1.38
38	A1	2826	PSU	C6-C5	2.89	1.38	1.35
38	A1	2133	PSU	C4-N3	-2.89	1.33	1.38
38	A1	1124	PSU	C4-N3	-2.89	1.33	1.38
38	A1	2735	PSU	C4-N3	-2.88	1.33	1.38
38	A1	2944	PSU	C4-N3	-2.88	1.33	1.38
38	A1	645	1MA	C6-N6	2.88	1.34	1.28
38	A1	2340	PSU	C4-N3	-2.88	1.33	1.38
38	A1	2260	PSU	C4-N3	-2.87	1.33	1.38
34	B5	1187	PSU	C4-N3	-2.86	1.33	1.38
38	A1	2826	PSU	C4-N3	-2.85	1.33	1.38
38	A1	2129	PSU	C4-N3	-2.85	1.33	1.38
38	A1	986	PSU	C4-N3	-2.85	1.33	1.38
36	AB	243	HIC	CD2-CG	2.85	1.41	1.36
38	A1	2314	PSU	C4-N3	-2.85	1.33	1.38
38	A1	1042	PSU	C4-N3	-2.83	1.33	1.38
34	B5	1191	B8N	C6-C5	2.83	1.39	1.35
34	B5	1290	PSU	C4-N3	-2.83	1.33	1.38
34	B5	999	PSU	C4-N3	-2.82	1.33	1.38
38	A1	2880	PSU	C4-N3	-2.82	1.33	1.38
38	A1	2923	PSU	C4-N3	-2.81	1.33	1.38
34	B5	1575	G7M	C6-N1	-2.80	1.33	1.38
38	A1	2975	PSU	C4-N3	-2.80	1.33	1.38
38	A1	2264	PSU	C4-N3	-2.79	1.33	1.38
38	A1	2191	PSU	C4-N3	-2.78	1.33	1.38
38	A1	1056	PSU	C4-N3	-2.78	1.33	1.38
38	A1	776	PSU	C4-N3	-2.77	1.33	1.38
34	B5	759	PSU	C4-N3	-2.77	1.33	1.38
40	A4	73	PSU	C4-N3	-2.77	1.33	1.38
38	A1	2921	OMU	C4-N3	-2.75	1.33	1.38
38	A1	960	PSU	C6-C5	2.75	1.38	1.35
34	B5	106	PSU	C4-N3	-2.75	1.33	1.38
38	A1	1052	PSU	C4-N3	-2.75	1.33	1.38
34	B5	120	PSU	C4-N3	-2.73	1.33	1.38
34	B5	1415	PSU	C4-N3	-2.73	1.33	1.38
34	B5	466	PSU	C4-N3	-2.72	1.33	1.38
38	A1	1110	PSU	C4-N3	-2.72	1.33	1.38
38	A1	2865	PSU	C4-N3	-2.72	1.33	1.38
38	A1	2258	PSU	C4-N3	-2.71	1.33	1.38
34	B5	1181	PSU	C4-N3	-2.71	1.33	1.38
34	B5	766	PSU	C4-N3	-2.68	1.33	1.38
39	A3	50	PSU	C4-N3	-2.68	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1280	4AC	C4-N4	-2.68	1.35	1.39
38	A1	2349	PSU	C4-N3	-2.67	1.33	1.38
34	B5	302	PSU	C4-N3	-2.67	1.33	1.38
38	A1	2922	OMG	C6-N1	-2.66	1.33	1.38
34	B5	211	PSU	C4-N3	-2.65	1.33	1.38
38	A1	1004	PSU	C4-N3	-2.65	1.33	1.38
38	A1	960	PSU	C4-N3	-2.64	1.33	1.38
38	A1	2278	5MC	C6-C5	2.64	1.38	1.34
38	A1	2266	PSU	C4-N3	-2.63	1.33	1.38
38	A1	960	PSU	O4'-C1'	-2.62	1.40	1.43
38	A1	2921	OMU	C2-N3	-2.45	1.33	1.38
38	A1	2351	PSU	C2-N3	-2.34	1.33	1.37
38	A1	2142	1MA	C5-N7	-2.34	1.34	1.39
38	A1	645	1MA	C5-N7	-2.33	1.34	1.39
34	B5	1773	4AC	C4-N4	-2.33	1.36	1.39
38	A1	2278	5MC	C6-N1	-2.32	1.34	1.38
34	B5	766	PSU	O4'-C1'	-2.31	1.40	1.43
34	B5	1781	MA6	C5-N7	-2.31	1.34	1.39
34	B5	1782	MA6	C5-N7	-2.29	1.34	1.39
38	A1	2921	OMU	C5-C4	-2.28	1.38	1.43
38	A1	966	PSU	C2-N3	-2.27	1.33	1.37
34	B5	1782	MA6	C4-N9	-2.24	1.33	1.37
38	A1	2975	PSU	C2-N3	-2.21	1.33	1.37
38	A1	2142	1MA	C2-N3	2.21	1.34	1.30
38	A1	2870	5MC	C6-N1	-2.21	1.34	1.38
38	A1	966	PSU	C2-N1	-2.21	1.33	1.36
38	A1	2944	PSU	C2-N3	-2.20	1.33	1.37
34	B5	1781	MA6	C4-N9	-2.19	1.33	1.37
38	A1	2826	PSU	C2-N1	-2.18	1.33	1.36
38	A1	2416	PSU	C2-N3	-2.17	1.33	1.37
38	A1	2922	OMG	C5-N7	-2.17	1.34	1.39
38	A1	2340	PSU	C2-N3	-2.17	1.33	1.37
38	A1	1052	PSU	C2-N3	-2.15	1.33	1.37
38	A1	1056	PSU	C2-N3	-2.15	1.33	1.37
34	B5	1575	G7M	C2-N1	-2.15	1.32	1.37
38	A1	2880	PSU	C2-N3	-2.14	1.33	1.37
38	A1	776	PSU	C2-N3	-2.14	1.33	1.37
34	B5	211	PSU	O4'-C1'	-2.13	1.40	1.43
38	A1	2826	PSU	C2-N3	-2.13	1.34	1.37
38	A1	1042	PSU	C2-N3	-2.11	1.34	1.37
38	A1	2133	PSU	C2-N3	-2.11	1.34	1.37
34	B5	1782	MA6	C8-N7	2.09	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	2129	PSU	C2-N3	-2.09	1.34	1.37
34	B5	632	PSU	C2-N3	-2.08	1.34	1.37
34	B5	1191	B8N	CN1-N1	2.08	1.50	1.46
38	A1	2266	PSU	C2-N1	-2.07	1.34	1.36
38	A1	2191	PSU	C2-N3	-2.07	1.34	1.37
38	A1	986	PSU	C2-N3	-2.07	1.34	1.37
38	A1	2260	PSU	C2-N3	-2.06	1.34	1.37
34	B5	120	PSU	C2-N3	-2.05	1.34	1.37
34	B5	1415	PSU	C2-N3	-2.04	1.34	1.37
34	B5	1781	MA6	C8-N7	2.04	1.35	1.31
34	B5	759	PSU	C2-N3	-2.04	1.34	1.37
38	A1	2735	PSU	C2-N3	-2.04	1.34	1.37
38	A1	2264	PSU	C2-N3	-2.03	1.34	1.37
38	A1	1110	PSU	C2-N3	-2.03	1.34	1.37
38	A1	990	PSU	C2-N3	-2.01	1.34	1.37
34	B5	106	PSU	C2-N3	-2.01	1.34	1.37
34	B5	211	PSU	C2-N3	-2.01	1.34	1.37

All (246) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1191	B8N	C32-C31-N3	17.94	143.51	112.16
34	B5	1773	4AC	N4-C4-N3	7.73	126.42	113.87
38	A1	2634	UR3	C4-N3-C2	-6.96	118.98	124.58
38	A1	966	PSU	N1-C2-N3	6.78	122.32	115.17
38	A1	2133	PSU	N1-C2-N3	6.74	122.28	115.17
38	A1	2923	PSU	N1-C2-N3	6.71	122.24	115.17
38	A1	2260	PSU	N1-C2-N3	6.65	122.18	115.17
38	A1	2314	PSU	N1-C2-N3	6.63	122.16	115.17
38	A1	2944	PSU	N1-C2-N3	6.62	122.15	115.17
38	A1	1124	PSU	N1-C2-N3	6.61	122.14	115.17
38	A1	2351	PSU	N1-C2-N3	6.60	122.13	115.17
38	A1	1004	PSU	N1-C2-N3	6.60	122.13	115.17
38	A1	2129	PSU	N1-C2-N3	6.57	122.10	115.17
34	B5	999	PSU	N1-C2-N3	6.56	122.09	115.17
38	A1	1042	PSU	N1-C2-N3	6.56	122.09	115.17
38	A1	2340	PSU	N1-C2-N3	6.55	122.07	115.17
34	B5	106	PSU	N1-C2-N3	6.54	122.07	115.17
38	A1	2191	PSU	N1-C2-N3	6.54	122.06	115.17
34	B5	759	PSU	N1-C2-N3	6.54	122.06	115.17
34	B5	1187	PSU	N1-C2-N3	6.53	122.06	115.17
38	A1	2735	PSU	N1-C2-N3	6.51	122.03	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2865	PSU	N1-C2-N3	6.50	122.03	115.17
38	A1	2826	PSU	N1-C2-N3	6.50	122.03	115.17
34	B5	1290	PSU	N1-C2-N3	6.49	122.02	115.17
34	B5	632	PSU	N1-C2-N3	6.49	122.02	115.17
38	A1	990	PSU	N1-C2-N3	6.49	122.01	115.17
38	A1	2258	PSU	N1-C2-N3	6.48	122.01	115.17
34	B5	120	PSU	N1-C2-N3	6.48	122.00	115.17
38	A1	960	PSU	N1-C2-N3	6.45	121.97	115.17
34	B5	466	PSU	N1-C2-N3	6.43	121.95	115.17
38	A1	2264	PSU	N1-C2-N3	6.43	121.95	115.17
38	A1	1056	PSU	N1-C2-N3	6.42	121.94	115.17
34	B5	766	PSU	N1-C2-N3	6.42	121.94	115.17
34	B5	302	PSU	N1-C2-N3	6.41	121.92	115.17
40	A4	73	PSU	N1-C2-N3	6.37	121.89	115.17
38	A1	2349	PSU	N1-C2-N3	6.36	121.87	115.17
38	A1	2975	PSU	N1-C2-N3	6.35	121.87	115.17
38	A1	2266	PSU	N1-C2-N3	6.35	121.87	115.17
39	A3	50	PSU	N1-C2-N3	6.33	121.85	115.17
38	A1	986	PSU	N1-C2-N3	6.32	121.83	115.17
38	A1	2880	PSU	N1-C2-N3	6.32	121.83	115.17
34	B5	1181	PSU	N1-C2-N3	6.31	121.83	115.17
38	A1	776	PSU	N1-C2-N3	6.30	121.81	115.17
38	A1	2922	OMG	C5-C4-N3	-6.28	118.40	128.39
34	B5	1415	PSU	N1-C2-N3	6.26	121.77	115.17
38	A1	1110	PSU	N1-C2-N3	6.26	121.77	115.17
38	A1	2416	PSU	N1-C2-N3	6.22	121.72	115.17
34	B5	211	PSU	N1-C2-N3	6.15	121.66	115.17
38	A1	1052	PSU	N1-C2-N3	6.12	121.62	115.17
34	B5	1191	B8N	C4-N3-C2	-5.65	118.67	125.62
38	A1	2142	1MA	C5-C4-N3	-5.41	119.30	127.27
34	B5	1782	MA6	C5-C4-N3	-5.27	119.46	126.72
38	A1	2922	OMG	C2-N3-C4	5.16	121.19	112.30
38	A1	645	1MA	C5-C4-N3	-5.15	119.69	127.27
38	A1	2921	OMU	C4-N3-C2	-5.03	120.37	126.61
34	B5	1781	MA6	C5-C4-N3	-5.01	119.81	126.72
34	B5	1575	G7M	C2-N3-C4	4.91	120.76	112.30
38	A1	2922	OMG	N9-C4-N3	4.84	135.63	125.95
34	B5	1773	4AC	C5-C4-N4	-4.66	115.10	122.94
38	A1	2133	PSU	C4-N3-C2	-4.57	120.08	126.37
38	A1	645	1MA	C2-N3-C4	4.50	121.36	112.53
34	B5	1781	MA6	C2-N1-C6	4.50	122.82	111.83
38	A1	2142	1MA	C2-N3-C4	4.48	121.31	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	1004	PSU	C4-N3-C2	-4.43	120.27	126.37
34	B5	106	PSU	C4-N3-C2	-4.36	120.37	126.37
38	A1	2921	OMU	N3-C2-N1	4.36	120.56	114.89
38	A1	1110	PSU	C4-N3-C2	-4.32	120.42	126.37
34	B5	759	PSU	C4-N3-C2	-4.30	120.45	126.37
34	B5	1782	MA6	C2-N1-C6	4.30	122.32	111.83
38	A1	2944	PSU	C4-N3-C2	-4.29	120.46	126.37
38	A1	1124	PSU	C4-N3-C2	-4.29	120.47	126.37
38	A1	2826	PSU	C4-N3-C2	-4.27	120.49	126.37
38	A1	960	PSU	C4-N3-C2	-4.26	120.50	126.37
38	A1	2129	PSU	C4-N3-C2	-4.26	120.50	126.37
38	A1	1056	PSU	C4-N3-C2	-4.26	120.51	126.37
34	B5	466	PSU	C4-N3-C2	-4.24	120.53	126.37
34	B5	999	PSU	C4-N3-C2	-4.23	120.54	126.37
38	A1	2314	PSU	C4-N3-C2	-4.23	120.54	126.37
38	A1	1004	PSU	O2-C2-N1	-4.22	118.43	122.79
38	A1	2865	PSU	C4-N3-C2	-4.22	120.56	126.37
38	A1	2826	PSU	O2-C2-N1	-4.19	118.47	122.79
38	A1	2880	PSU	C4-N3-C2	-4.19	120.60	126.37
34	B5	1187	PSU	C4-N3-C2	-4.18	120.61	126.37
34	B5	766	PSU	C4-N3-C2	-4.18	120.61	126.37
38	A1	2264	PSU	C4-N3-C2	-4.16	120.64	126.37
34	B5	302	PSU	C4-N3-C2	-4.16	120.65	126.37
38	A1	1042	PSU	C4-N3-C2	-4.15	120.65	126.37
38	A1	966	PSU	C4-N3-C2	-4.15	120.65	126.37
38	A1	2975	PSU	C4-N3-C2	-4.14	120.66	126.37
38	A1	2340	PSU	C4-N3-C2	-4.13	120.68	126.37
34	B5	1290	PSU	C4-N3-C2	-4.13	120.68	126.37
38	A1	990	PSU	C4-N3-C2	-4.13	120.68	126.37
34	B5	1781	MA6	C4-C5-N7	-4.13	105.86	110.58
34	B5	1782	MA6	C4-C5-N7	-4.13	105.86	110.58
34	B5	1181	PSU	C4-N3-C2	-4.11	120.70	126.37
39	A3	50	PSU	C4-N3-C2	-4.10	120.72	126.37
38	A1	2735	PSU	C4-N3-C2	-4.09	120.73	126.37
38	A1	2921	OMU	C5-C4-N3	4.09	120.53	114.80
38	A1	2191	PSU	C4-N3-C2	-4.08	120.75	126.37
38	A1	2260	PSU	C4-N3-C2	-4.08	120.76	126.37
38	A1	2923	PSU	C4-N3-C2	-4.08	120.76	126.37
38	A1	2258	PSU	C4-N3-C2	-4.07	120.76	126.37
34	B5	632	PSU	C4-N3-C2	-4.06	120.78	126.37
38	A1	1052	PSU	C4-N3-C2	-4.05	120.80	126.37
38	A1	2923	PSU	O2-C2-N1	-4.04	118.62	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	A4	73	PSU	C4-N3-C2	-4.03	120.82	126.37
34	B5	1575	G7M	C5-C4-N3	-4.03	120.53	128.15
34	B5	120	PSU	C4-N3-C2	-4.01	120.85	126.37
38	A1	2349	PSU	C4-N3-C2	-3.99	120.87	126.37
38	A1	2351	PSU	C4-N3-C2	-3.99	120.87	126.37
38	A1	2416	PSU	C4-N3-C2	-3.99	120.88	126.37
38	A1	2870	5MC	C5-C6-N1	-3.98	118.99	123.31
38	A1	2349	PSU	O2-C2-N1	-3.96	118.70	122.79
34	B5	1415	PSU	C4-N3-C2	-3.95	120.93	126.37
34	B5	302	PSU	O2-C2-N1	-3.94	118.73	122.79
38	A1	960	PSU	O2-C2-N1	-3.94	118.73	122.79
34	B5	1782	MA6	N3-C4-N9	3.93	133.85	127.17
34	B5	1290	PSU	O2-C2-N1	-3.92	118.75	122.79
38	A1	2258	PSU	O2-C2-N1	-3.92	118.75	122.79
38	A1	2266	PSU	C4-N3-C2	-3.90	121.00	126.37
34	B5	211	PSU	C4-N3-C2	-3.89	121.01	126.37
38	A1	2865	PSU	O2-C2-N1	-3.88	118.79	122.79
38	A1	2266	PSU	O2-C2-N1	-3.87	118.80	122.79
34	B5	1781	MA6	N3-C4-N9	3.84	133.70	127.17
34	B5	1575	G7M	C5-C6-N1	3.82	119.73	111.84
38	A1	2142	1MA	N9-C4-N3	3.81	135.57	126.90
38	A1	1124	PSU	O2-C2-N1	-3.78	118.89	122.79
34	B5	120	PSU	O2-C2-N1	-3.76	118.91	122.79
34	B5	766	PSU	O2-C2-N1	-3.73	118.94	122.79
38	A1	986	PSU	C4-N3-C2	-3.73	121.23	126.37
38	A1	776	PSU	C4-N3-C2	-3.73	121.24	126.37
38	A1	2278	5MC	C5-C6-N1	-3.72	119.28	123.31
38	A1	966	PSU	O2-C2-N1	-3.71	118.97	122.79
38	A1	2735	PSU	O2-C2-N1	-3.69	118.99	122.79
38	A1	2129	PSU	O2-C2-N1	-3.68	119.00	122.79
38	A1	2264	PSU	O2-C2-N1	-3.67	119.00	122.79
34	B5	466	PSU	O2-C2-N1	-3.67	119.00	122.79
34	B5	1782	MA6	C2-N3-C4	3.63	120.70	111.83
34	B5	106	PSU	O2-C2-N1	-3.63	119.05	122.79
34	B5	999	PSU	O2-C2-N1	-3.63	119.05	122.79
38	A1	1042	PSU	O2-C2-N1	-3.58	119.09	122.79
38	A1	1056	PSU	O2-C2-N1	-3.56	119.12	122.79
34	B5	759	PSU	O2-C2-N1	-3.55	119.13	122.79
34	B5	1187	PSU	O2-C2-N1	-3.55	119.13	122.79
34	B5	1575	G7M	O6-C6-C5	-3.55	120.09	128.01
38	A1	2314	PSU	O2-C2-N1	-3.54	119.13	122.79
38	A1	2340	PSU	O2-C2-N1	-3.53	119.15	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2133	PSU	O2-C2-N1	-3.52	119.16	122.79
38	A1	2191	PSU	O2-C2-N1	-3.51	119.17	122.79
38	A1	986	PSU	O2-C2-N1	-3.50	119.17	122.79
34	B5	211	PSU	O2-C2-N1	-3.48	119.20	122.79
39	A3	50	PSU	O2-C2-N1	-3.47	119.20	122.79
38	A1	2351	PSU	O2-C2-N1	-3.46	119.22	122.79
34	B5	1781	MA6	C2-N3-C4	3.46	120.28	111.83
34	B5	1415	PSU	O2-C2-N1	-3.45	119.23	122.79
34	B5	1181	PSU	O2-C2-N1	-3.44	119.24	122.79
38	A1	2260	PSU	O2-C2-N1	-3.42	119.26	122.79
38	A1	990	PSU	O2-C2-N1	-3.41	119.27	122.79
34	B5	1781	MA6	N1-C2-N3	-3.39	123.45	128.58
40	A4	73	PSU	O2-C2-N1	-3.39	119.30	122.79
34	B5	1773	4AC	CM7-C7-N4	3.37	120.70	115.27
38	A1	2880	PSU	O2-C2-N1	-3.36	119.33	122.79
34	B5	1575	G7M	C6-C5-N7	3.35	136.38	132.17
38	A1	1052	PSU	O2-C2-N1	-3.35	119.34	122.79
38	A1	1110	PSU	O2-C2-N1	-3.34	119.34	122.79
34	B5	1782	MA6	N1-C2-N3	-3.33	123.54	128.58
34	B5	1575	G7M	N9-C4-N3	3.33	132.61	125.95
38	A1	2634	UR3	C5-C4-N3	3.32	119.41	115.04
38	A1	2416	PSU	O2-C2-N1	-3.29	119.40	122.79
38	A1	2975	PSU	O2-C2-N1	-3.28	119.41	122.79
34	B5	632	PSU	O2-C2-N1	-3.28	119.41	122.79
38	A1	645	1MA	N9-C4-N3	3.26	134.33	126.90
34	B5	1191	B8N	N3-C2-N1	3.26	120.70	116.72
38	A1	2944	PSU	O2-C2-N1	-3.25	119.44	122.79
34	B5	1773	4AC	C6-C5-C4	3.19	120.85	117.00
34	B5	1280	4AC	N4-C4-N3	3.18	119.03	113.87
38	A1	2922	OMG	C6-C5-N7	3.17	136.06	130.29
38	A1	2921	OMU	O4-C4-C5	-3.17	119.69	125.16
38	A1	776	PSU	O2-C2-N1	-3.09	119.61	122.79
36	AB	243	HIC	NE2-CE1-ND1	-3.05	111.50	112.66
34	B5	1781	MA6	C4-N9-C8	3.02	108.91	105.74
34	B5	1781	MA6	C5-N7-C8	2.99	108.14	103.45
34	B5	1782	MA6	C5-N7-C8	2.94	108.07	103.45
34	B5	1782	MA6	C4-N9-C8	2.89	108.78	105.74
38	A1	2870	5MC	C5-C4-N3	-2.77	118.92	121.75
34	B5	1773	4AC	C5-C4-N3	-2.64	118.47	122.60
34	B5	1280	4AC	C6-C5-C4	2.63	120.17	117.00
34	B5	1782	MA6	C6-C5-N7	2.57	137.53	133.43
34	B5	1781	MA6	C6-C5-N7	2.54	137.50	133.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1191	B8N	C31-N3-C2	2.53	121.38	117.64
38	A1	2278	5MC	C5-C4-N3	-2.53	119.16	121.75
38	A1	2133	PSU	C5-C6-N1	-2.50	118.67	122.14
38	A1	2921	OMU	O2-C2-N1	-2.50	119.55	122.80
38	A1	645	1MA	C4-C5-N7	-2.49	106.72	110.67
38	A1	2922	OMG	C4-C5-N7	-2.48	106.75	110.67
34	B5	999	PSU	C5-C6-N1	-2.41	118.79	122.14
34	B5	211	PSU	C6-C5-C4	-2.37	116.57	118.17
34	B5	1191	B8N	C1'-C5-C4	2.35	121.18	117.61
34	B5	1781	MA6	N9-C8-N7	-2.35	110.60	113.94
34	B5	1782	MA6	N9-C8-N7	-2.35	110.60	113.94
38	A1	2634	UR3	C3U-N3-C4	2.33	121.10	117.87
34	B5	1575	G7M	C2-N1-C6	-2.32	120.91	125.11
38	A1	2826	PSU	O4'-C1'-C2'	2.30	108.33	105.15
38	A1	645	1MA	C6-C5-N7	2.30	136.22	132.16
34	B5	759	PSU	C5-C6-N1	-2.30	118.95	122.14
38	A1	2314	PSU	C5-C6-N1	-2.29	118.96	122.14
38	A1	2278	5MC	O2-C2-N3	-2.28	118.74	122.33
38	A1	2880	PSU	C5-C6-N1	-2.26	119.00	122.14
38	A1	776	PSU	C6-C5-C4	-2.25	116.66	118.17
38	A1	1004	PSU	C5-C6-N1	-2.25	119.02	122.14
38	A1	2826	PSU	C5-C6-N1	-2.24	119.03	122.14
38	A1	1124	PSU	C5-C6-N1	-2.23	119.04	122.14
38	A1	2142	1MA	C4-C5-N7	-2.22	107.16	110.67
38	A1	2922	OMG	O6-C6-C5	-2.19	120.74	126.53
34	B5	1187	PSU	C5-C6-N1	-2.19	119.11	122.14
34	B5	1191	B8N	O4'-C1'-C2'	2.18	108.17	105.15
38	A1	2351	PSU	C5-C6-N1	-2.16	119.14	122.14
34	B5	106	PSU	C5-C6-N1	-2.15	119.15	122.14
38	A1	1056	PSU	C5-C6-N1	-2.14	119.16	122.14
36	AB	243	HIC	CB-CG-CD2	-2.14	124.79	129.96
34	B5	1290	PSU	C5-C6-N1	-2.13	119.18	122.14
38	A1	2865	PSU	O4'-C1'-C2'	2.13	108.09	105.15
38	A1	2880	PSU	O4'-C1'-C2'	2.12	108.09	105.15
38	A1	2944	PSU	C5-C6-N1	-2.12	119.19	122.14
38	A1	1042	PSU	C5-C6-N1	-2.12	119.19	122.14
38	A1	2129	PSU	C5-C6-N1	-2.12	119.20	122.14
38	A1	990	PSU	C5-C6-N1	-2.12	119.20	122.14
38	A1	1110	PSU	C6-C5-C4	-2.09	116.76	118.17
34	B5	999	PSU	O4'-C1'-C2'	2.09	108.04	105.15
38	A1	1110	PSU	O4'-C1'-C2'	2.08	108.03	105.15
38	A1	2264	PSU	C5-C6-N1	-2.08	119.26	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	766	PSU	O4'-C1'-C2'	2.07	108.02	105.15
38	A1	1004	PSU	O4'-C1'-C2'	2.07	108.02	105.15
34	B5	1181	PSU	C5-C6-N1	-2.07	119.27	122.14
38	A1	2735	PSU	C5-C6-N1	-2.07	119.27	122.14
38	A1	2191	PSU	C5-C6-N1	-2.07	119.27	122.14
34	B5	466	PSU	C5-C6-N1	-2.06	119.28	122.14
34	B5	766	PSU	C5-C6-N1	-2.06	119.29	122.14
38	A1	2416	PSU	C5-C6-N1	-2.04	119.30	122.14
38	A1	2975	PSU	C5-C6-N1	-2.04	119.30	122.14
38	A1	2191	PSU	O4'-C1'-C2'	2.04	107.97	105.15
34	B5	632	PSU	C5-C6-N1	-2.02	119.33	122.14
38	A1	1052	PSU	C5-C6-N1	-2.02	119.34	122.14
38	A1	966	PSU	C5-C6-N1	-2.01	119.35	122.14
40	A4	73	PSU	C5-C6-N1	-2.00	119.36	122.14
34	B5	1280	4AC	C5-C4-N3	-2.00	119.47	122.60

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	B5	1191	B8N	C32-C31-N3-C2
34	B5	1191	B8N	C32-C31-N3-C4
34	B5	1280	4AC	N3-C4-N4-C7
34	B5	1280	4AC	C5-C4-N4-C7
34	B5	1280	4AC	O7-C7-N4-C4
34	B5	1280	4AC	CM7-C7-N4-C4
34	B5	1773	4AC	N3-C4-N4-C7
38	A1	776	PSU	C2'-C1'-C5-C4
38	A1	2258	PSU	O4'-C4'-C5'-O5'
34	B5	302	PSU	C3'-C4'-C5'-O5'
34	B5	302	PSU	O4'-C4'-C5'-O5'
34	B5	1782	MA6	O4'-C4'-C5'-O5'
38	A1	776	PSU	O4'-C4'-C5'-O5'
38	A1	2258	PSU	C3'-C4'-C5'-O5'
38	A1	2260	PSU	C3'-C4'-C5'-O5'
38	A1	2260	PSU	O4'-C4'-C5'-O5'
38	A1	2923	PSU	C3'-C4'-C5'-O5'
38	A1	2923	PSU	O4'-C4'-C5'-O5'
34	B5	1191	B8N	N34-C33-C34-O36
34	B5	211	PSU	C3'-C4'-C5'-O5'
34	B5	1782	MA6	C3'-C4'-C5'-O5'
38	A1	776	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
34	B5	1191	B8N	N34-C33-C34-O35
38	A1	2870	5MC	C2'-C1'-N1-C6
34	B5	1773	4AC	O7-C7-N4-C4
34	B5	1773	4AC	CM7-C7-N4-C4
38	A1	2870	5MC	O4'-C1'-N1-C6
38	A1	2314	PSU	C4'-C5'-O5'-P
34	B5	1191	B8N	O4'-C1'-C5-C4
38	A1	960	PSU	O4'-C1'-C5-C4
38	A1	2923	PSU	O4'-C1'-C5-C4
34	B5	1415	PSU	C3'-C4'-C5'-O5'
38	A1	2922	OMG	C3'-C2'-O2'-CM2
38	A1	2340	PSU	C4'-C5'-O5'-P
38	A1	2870	5MC	O4'-C1'-N1-C2
38	A1	645	1MA	C2'-C1'-N9-C8
38	A1	2923	PSU	C4'-C5'-O5'-P
34	B5	1415	PSU	O4'-C4'-C5'-O5'
34	B5	1191	B8N	O4'-C1'-C5-C6
38	A1	960	PSU	O4'-C1'-C5-C6
34	B5	1575	G7M	C3'-C4'-C5'-O5'
34	B5	1191	B8N	C32-C33-C34-O35
34	B5	211	PSU	O4'-C4'-C5'-O5'
38	A1	2870	5MC	C2'-C1'-N1-C2
38	A1	645	1MA	C2'-C1'-N9-C4

There are no ring outliers.

18 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	A1	2922	OMG	1	0
38	A1	990	PSU	1	0
38	A1	2416	PSU	1	0
34	B5	1290	PSU	1	0
38	A1	2129	PSU	1	0
38	A1	1110	PSU	2	0
34	B5	302	PSU	1	0
38	A1	966	PSU	1	0
38	A1	2266	PSU	2	0
34	B5	211	PSU	1	0
34	B5	1773	4AC	1	0
34	B5	1782	MA6	1	0
34	B5	766	PSU	1	0
38	A1	2314	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	A1	2880	PSU	1	0
38	A1	2923	PSU	1	0
38	A1	960	PSU	2	0
34	B5	1575	G7M	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 200 ligands modelled in this entry, 198 are monoatomic - leaving 2 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	$\# Z > 2$
83	SPD	A1	3401	-	9,9,9	0.34	0	8,8,8	0.84	0
84	3HE	A1	3402	-	21,21,21	0.40	0	23,30,30	0.70	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	SPD	A1	3401	-	-	6/7/7/7	-
84	3HE	A1	3402	-	-	2/8/36/36	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	A1	3402	3HE	C9-C13-C12	-2.05	111.01	114.46

There are no chirality outliers.

All (8) torsion outliers are listed below:

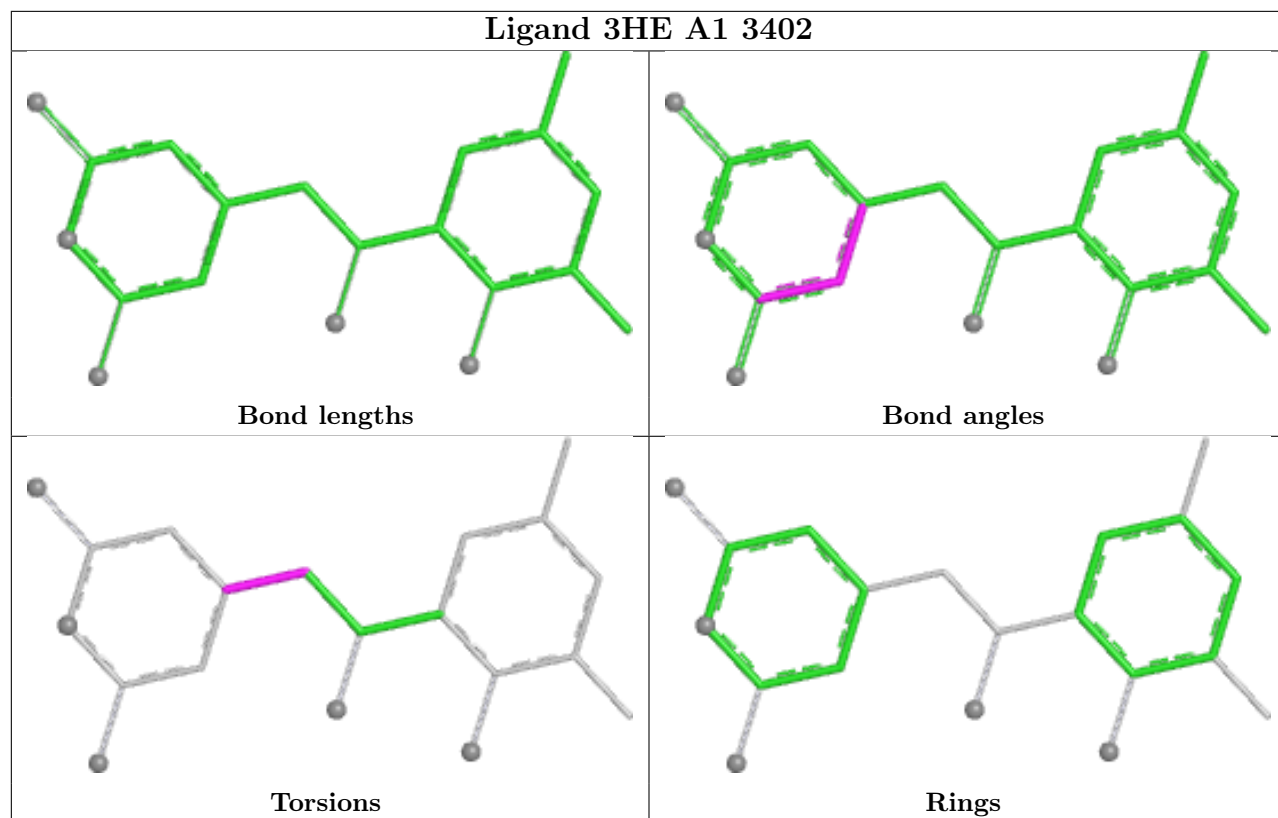
Mol	Chain	Res	Type	Atoms
84	A1	3402	3HE	C7-C8-C9-C10
83	A1	3401	SPD	C3-C4-C5-N6
83	A1	3401	SPD	N6-C7-C8-C9
84	A1	3402	3HE	C7-C8-C9-C13
83	A1	3401	SPD	C2-C3-C4-C5
83	A1	3401	SPD	C4-C5-N6-C7
83	A1	3401	SPD	C8-C7-N6-C5
83	A1	3401	SPD	N1-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	A1	3401	SPD	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

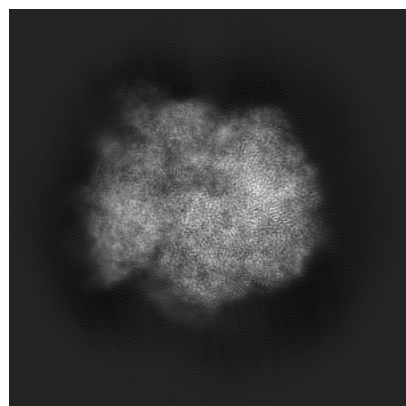
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40991. These allow visual inspection of the internal detail of the map and identification of artifacts.

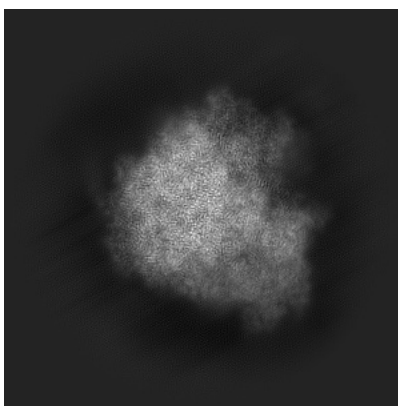
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

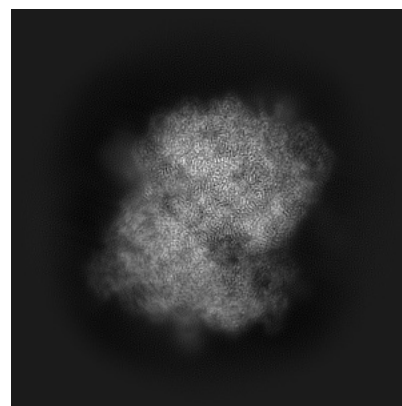
6.1.1 Primary map



X

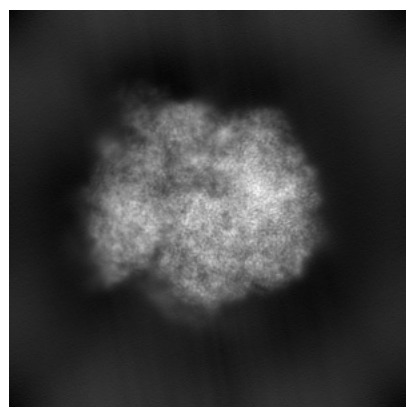


Y

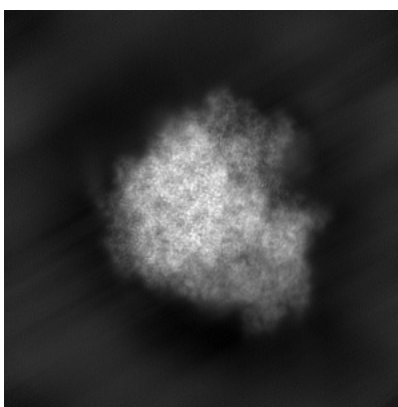


Z

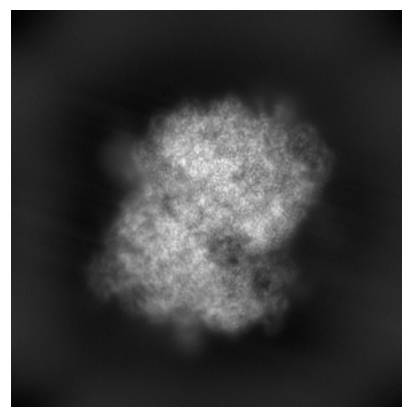
6.1.2 Raw map



X



Y

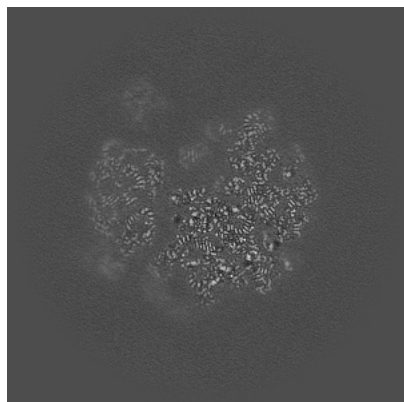


Z

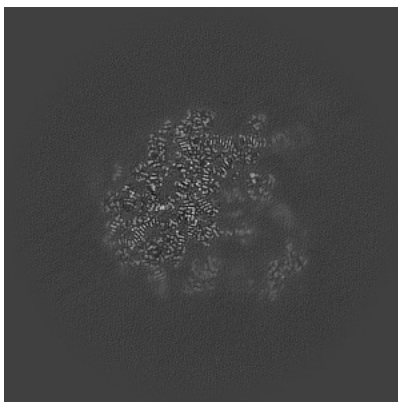
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

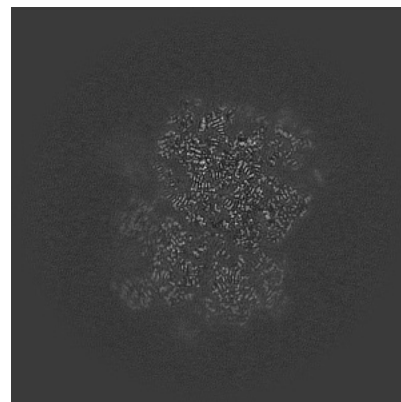
6.2.1 Primary map



X Index: 200

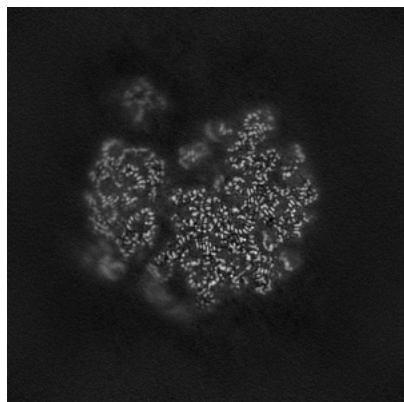


Y Index: 200

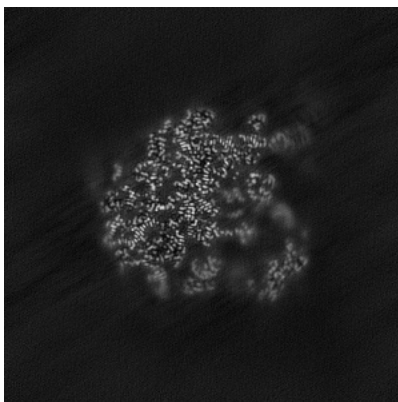


Z Index: 200

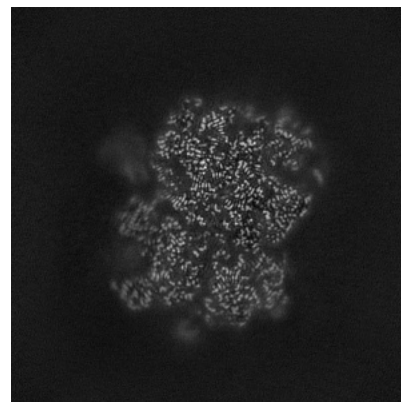
6.2.2 Raw map



X Index: 200



Y Index: 200

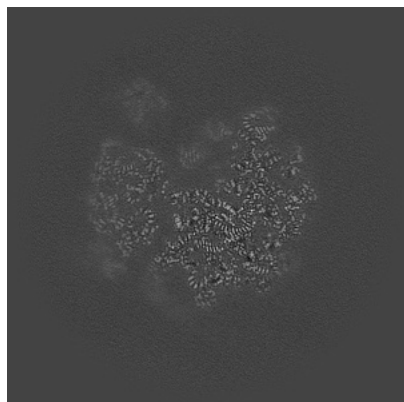


Z Index: 200

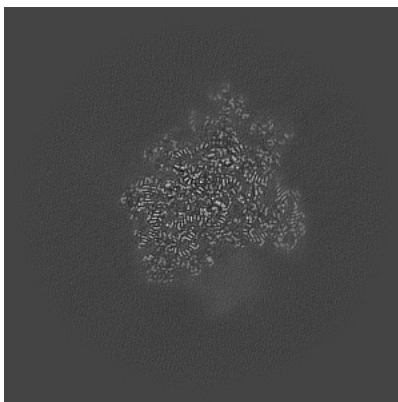
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

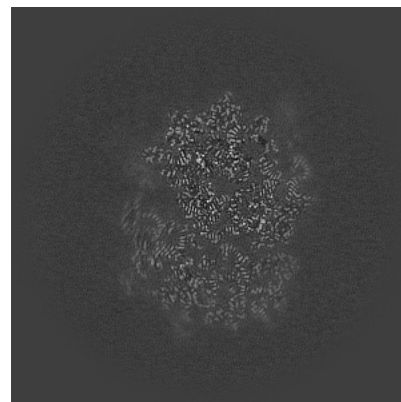
6.3.1 Primary map



X Index: 198

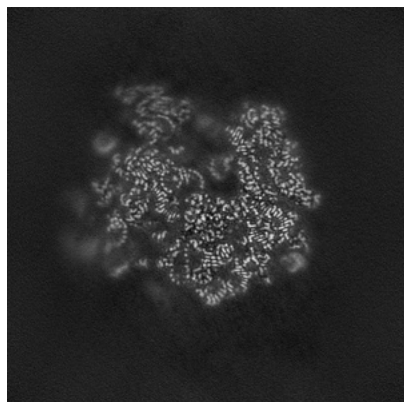


Y Index: 247

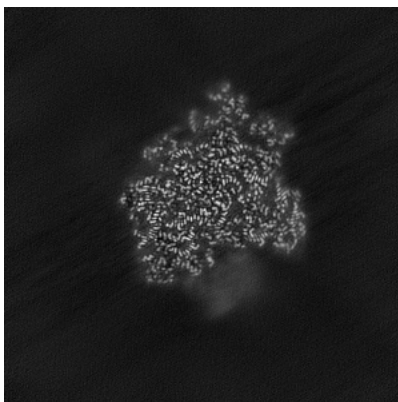


Z Index: 187

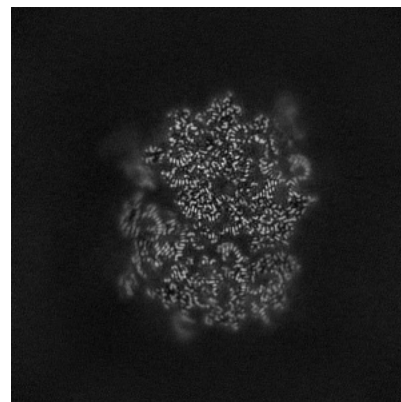
6.3.2 Raw map



X Index: 184



Y Index: 247

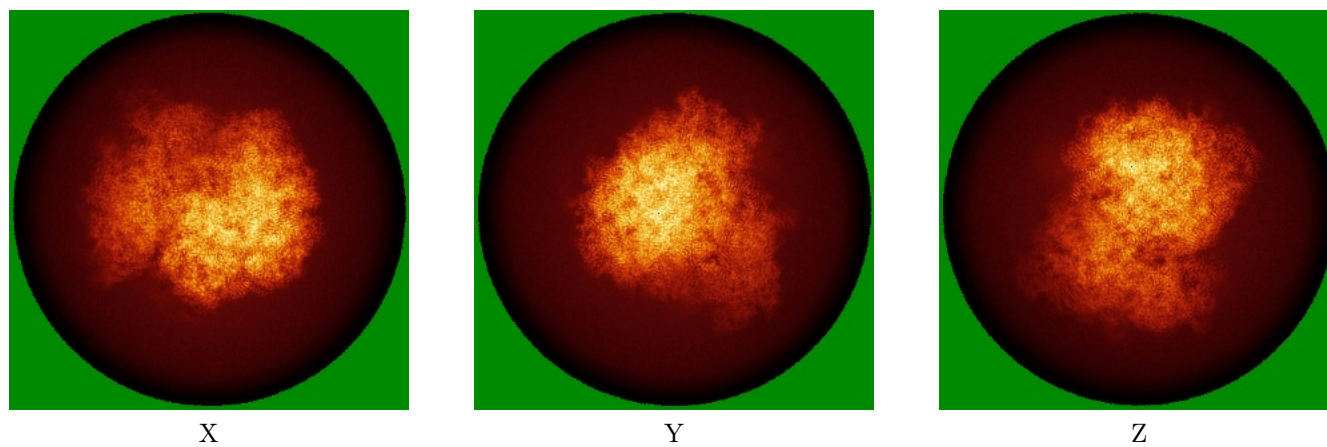


Z Index: 188

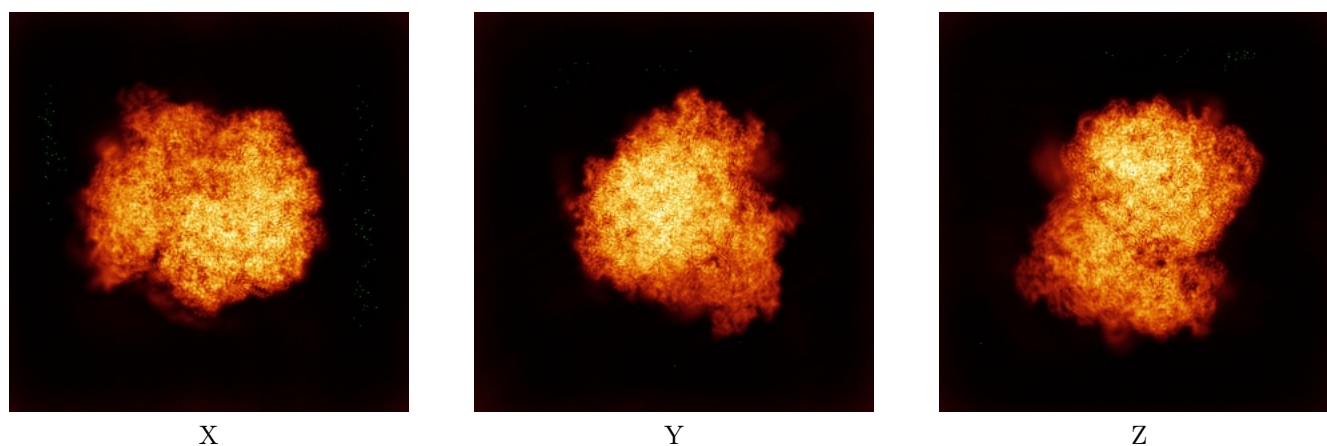
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

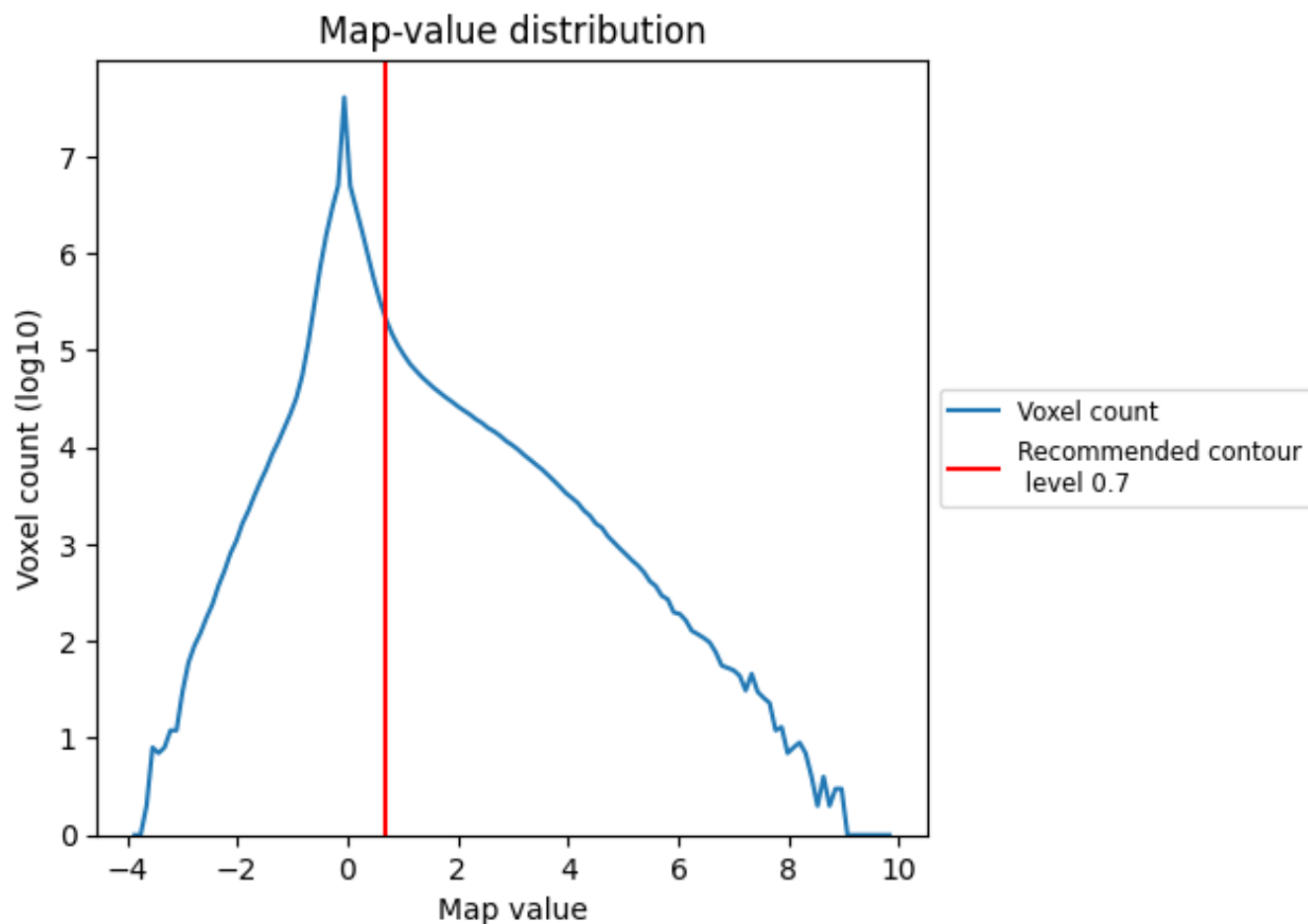
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

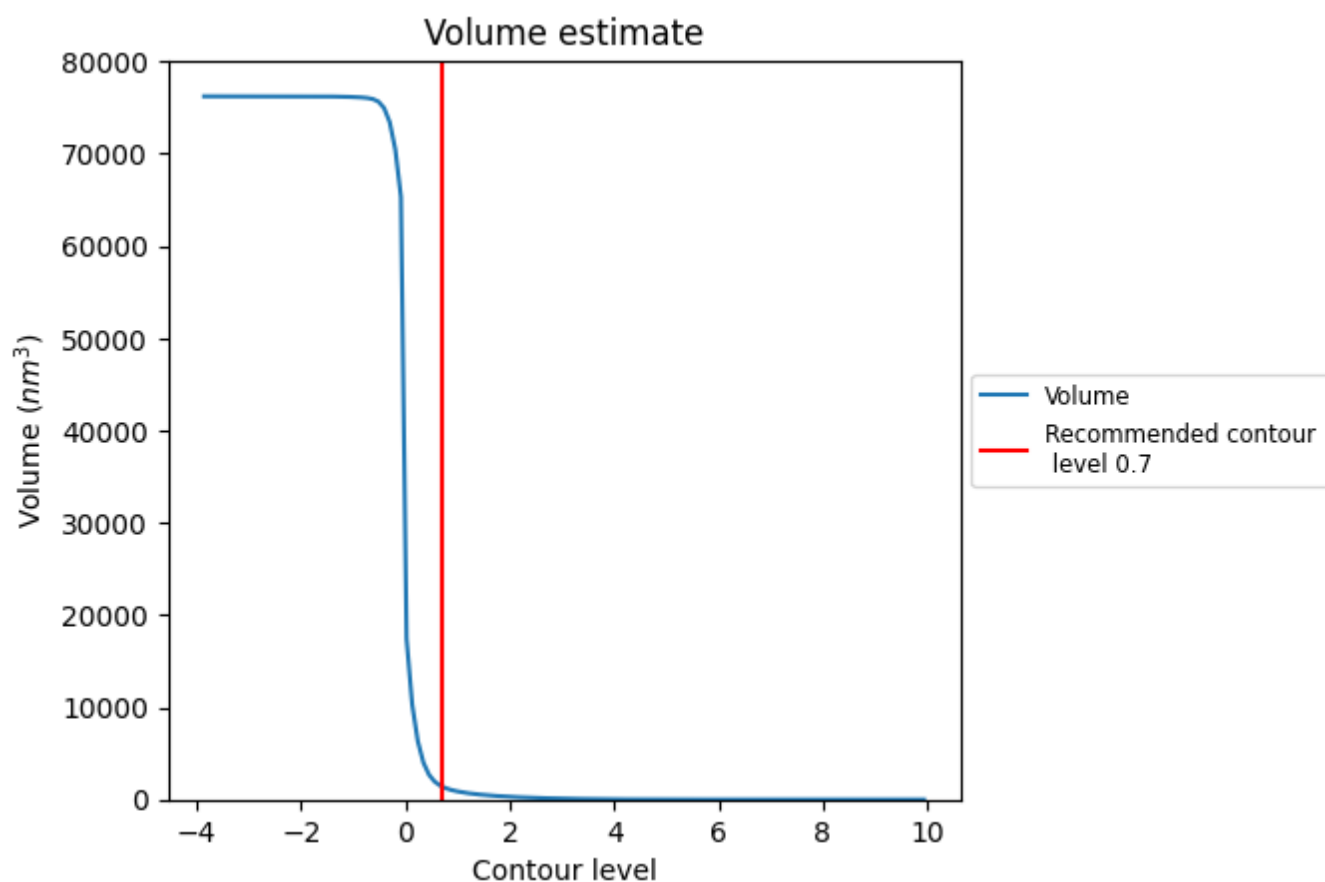
This section contains the results of statistical analysis of the map.

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.

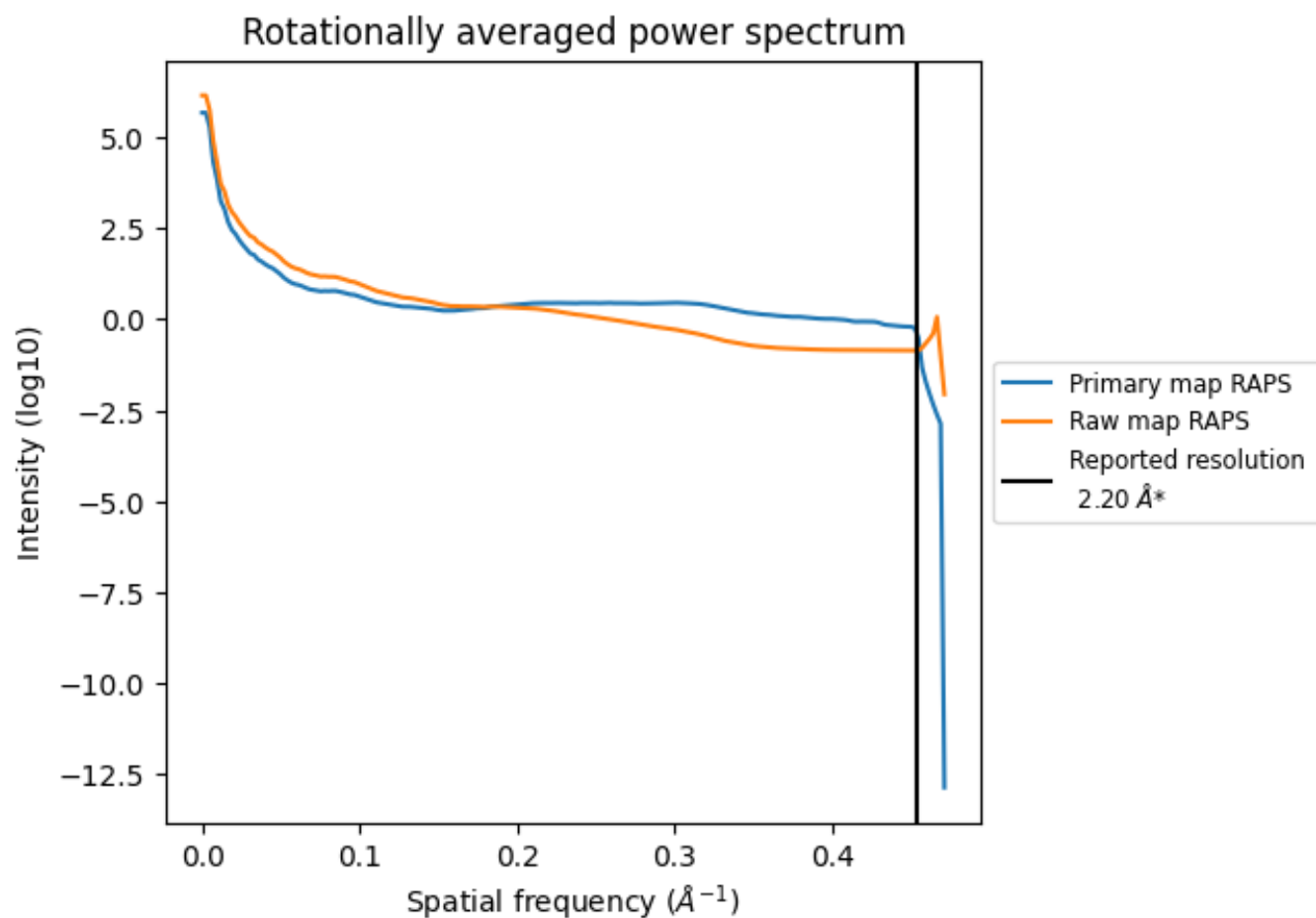
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1419 nm³; this corresponds to an approximate mass of 1282 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 ⓘ

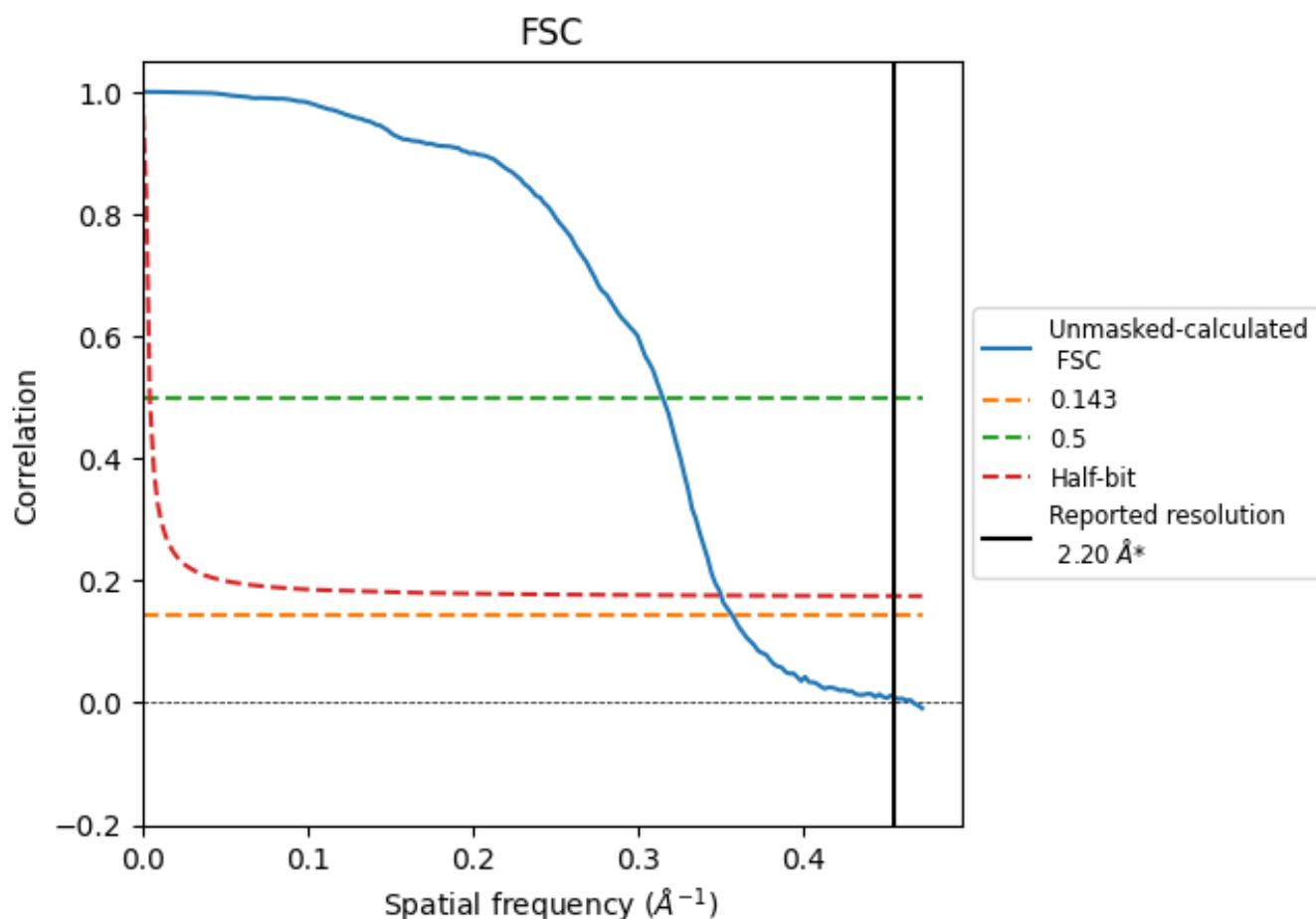


*Reported resolution corresponds to spatial frequency of 0.455 $\text{\AA}^{-1}$

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 0.455 Å⁻¹

8.2 Resolution estimates [i](#)

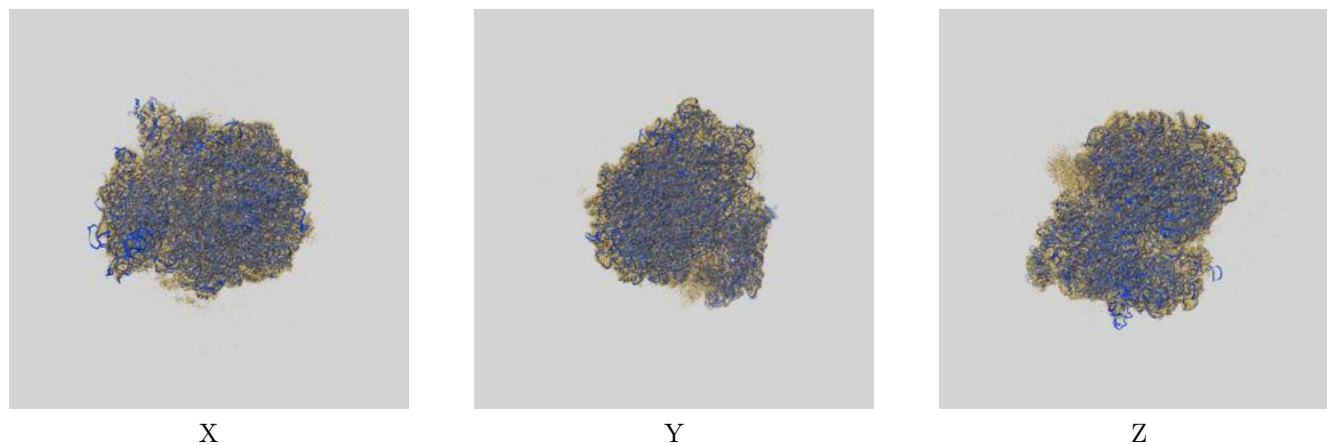
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.80	3.18	2.86

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.80 differs from the reported value 2.2 by more than 10 %

9 Map-model fit [i](#)

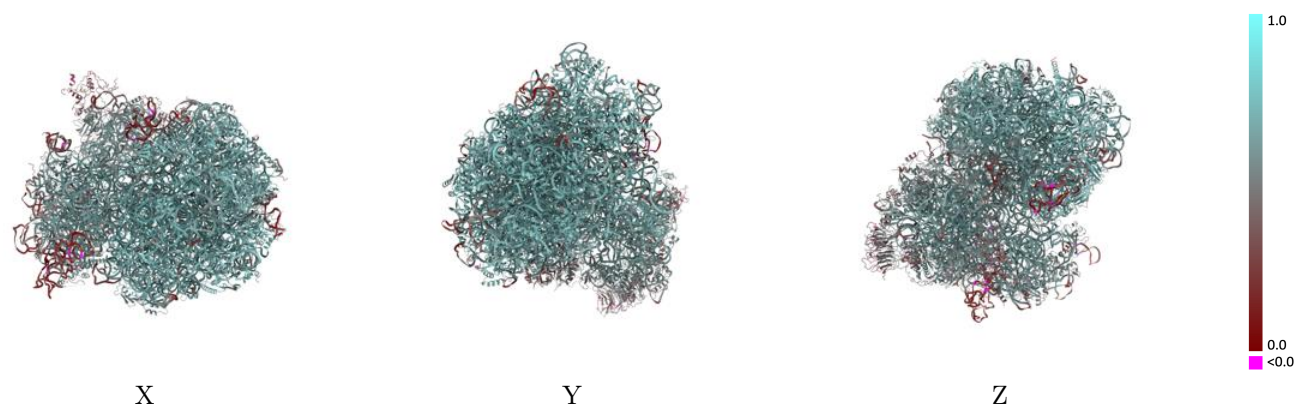
This section contains information regarding the fit between EMDB map EMD-40991 and PDB model 8T2Y. Per-residue inclusion information can be found in [section 3](#) on [page 21](#).

9.1 Map-model overlay [i](#)



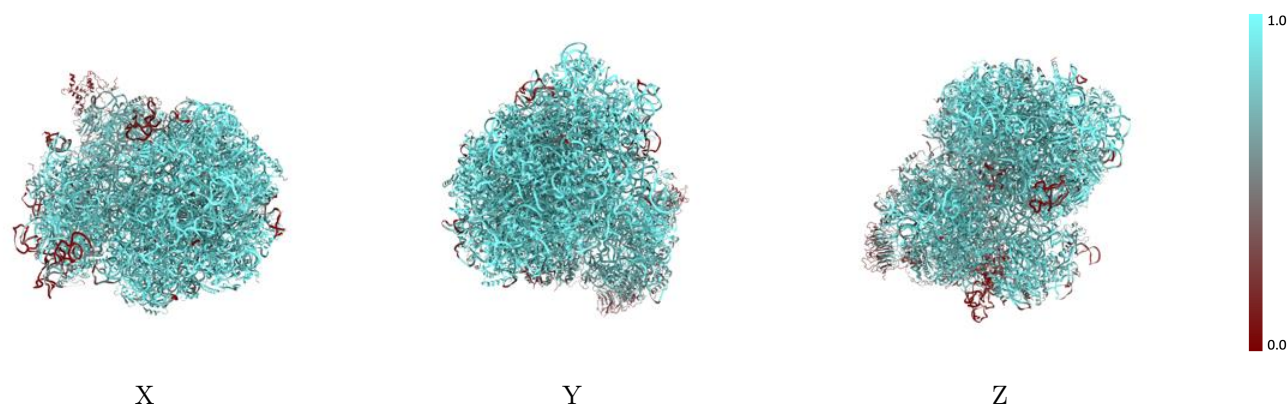
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



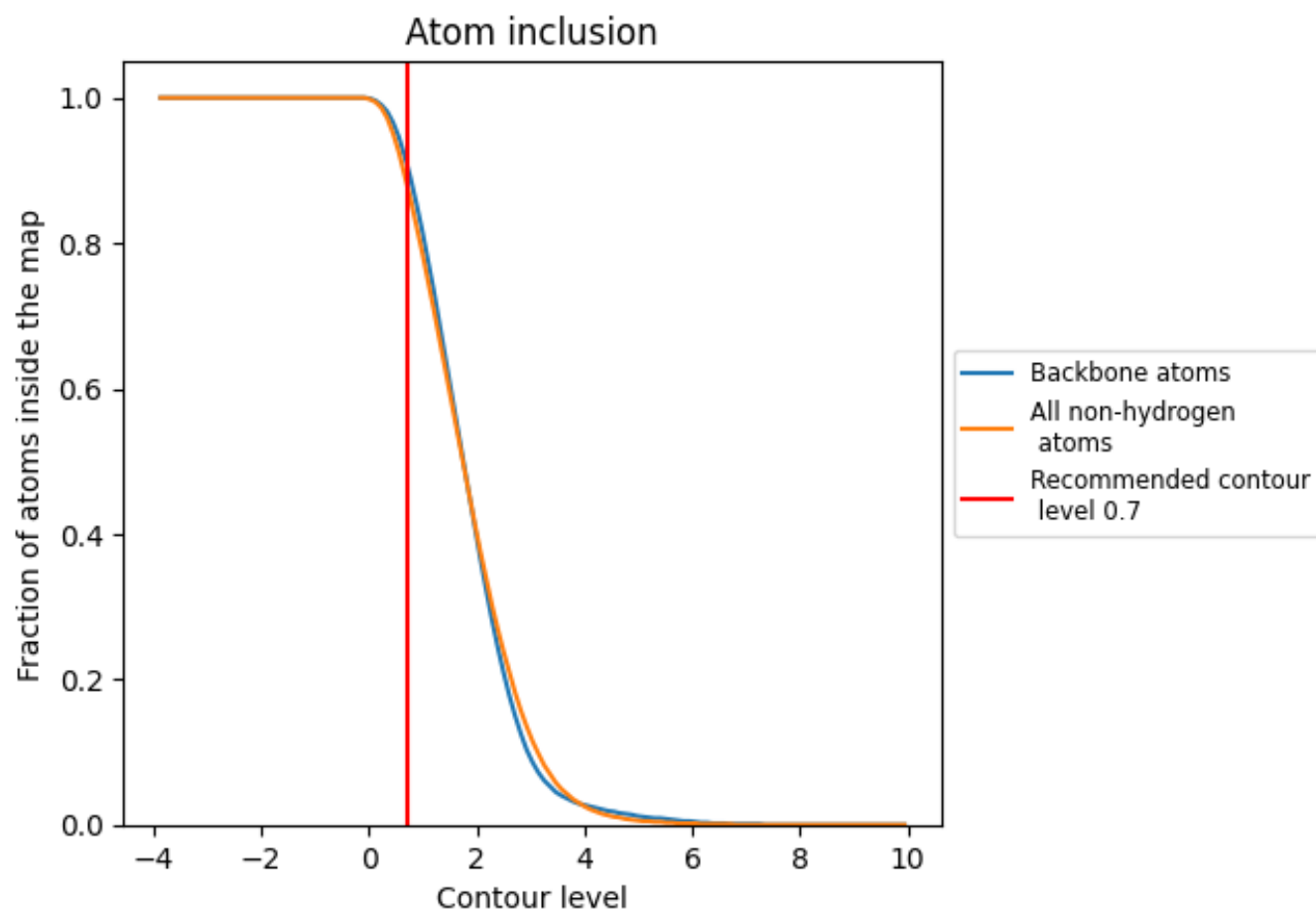
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 88% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8840	 0.6150
A1	 0.9420	 0.6520
A3	 0.9850	 0.6530
A4	 0.9820	 0.6820
AA	 0.9820	 0.7120
AB	 0.9680	 0.6930
AC	 0.9640	 0.6880
AD	 0.8710	 0.6070
AE	 0.8810	 0.6180
AF	 0.9430	 0.6790
AG	 0.9070	 0.6410
AH	 0.9170	 0.6520
AI	 0.9000	 0.6210
AJ	 0.8090	 0.5600
AL	 0.9360	 0.6750
AM	 0.9390	 0.6590
AN	 0.9920	 0.7210
AO	 0.9680	 0.6930
AP	 0.9500	 0.6960
AQ	 0.9770	 0.7060
AR	 0.8510	 0.6270
AS	 0.9460	 0.6720
AT	 0.9310	 0.6690
AU	 0.8670	 0.6080
AV	 0.9420	 0.6900
AW	 0.9600	 0.6930
AX	 0.9510	 0.6830
AY	 0.9490	 0.6710
AZ	 0.9110	 0.6550
Aa	 0.9690	 0.6960
Ab	 0.9340	 0.6430
Ac	 0.9070	 0.6510
Ad	 0.8970	 0.6610
Ae	 0.9600	 0.7000
Af	 0.9810	 0.7060



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Chain	Atom inclusion	Q-score
Ag	 0.9290	 0.6790
Ah	 0.9530	 0.6800
Ai	 0.9180	 0.6460
Aj	 0.9760	 0.7100
Ak	 0.8050	 0.5960
Al	 0.9760	 0.6930
Am	 0.9180	 0.6660
An	 0.8960	 0.6440
Ao	 0.9200	 0.6640
Ap	 0.9450	 0.6830
B5	 0.8570	 0.5640
BA	 0.7840	 0.5440
BB	 0.6690	 0.4860
BC	 0.9110	 0.6290
BD	 0.7370	 0.5330
BE	 0.8720	 0.5950
BF	 0.7140	 0.5300
BG	 0.7710	 0.5400
BH	 0.5950	 0.4550
BI	 0.8750	 0.6140
BJ	 0.8160	 0.5590
BK	 0.6110	 0.4350
BL	 0.8240	 0.6000
BM	 0.1420	 0.2730
BN	 0.8760	 0.6050
BO	 0.7760	 0.5250
BP	 0.6330	 0.4930
BQ	 0.7750	 0.5560
BR	 0.6920	 0.5210
BS	 0.7520	 0.5210
BT	 0.7790	 0.5510
BU	 0.6330	 0.4850
BV	 0.8310	 0.5700
BW	 0.9470	 0.6460
BX	 0.9300	 0.6590
BY	 0.7610	 0.5260
BZ	 0.6380	 0.4700
Ba	 0.8440	 0.5880
Bb	 0.7300	 0.5220
Bc	 0.6790	 0.5100
Bd	 0.9310	 0.6290
Be	 0.7580	 0.5360

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Chain	Atom inclusion	Q-score
Bf	 0.2300	 0.3140
Bg	 0.4390	 0.3930
MR	 0.9150	 0.6130
tA	 0.8430	 0.5230
tP	 0.8840	 0.5620