



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 11:38 AM UTC

PDB ID : 8EVQ / pdb_00008evq
EMDB ID : EMD-28633
Title : Hypopseudouridylated Ribosome bound with TSV IRES, eEF2, GDP, and sordarin, Structure I
Authors : Zhao, Y.; Rai, J.; Li, H.
Deposited on : 2022-10-20
Resolution : 2.72 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:

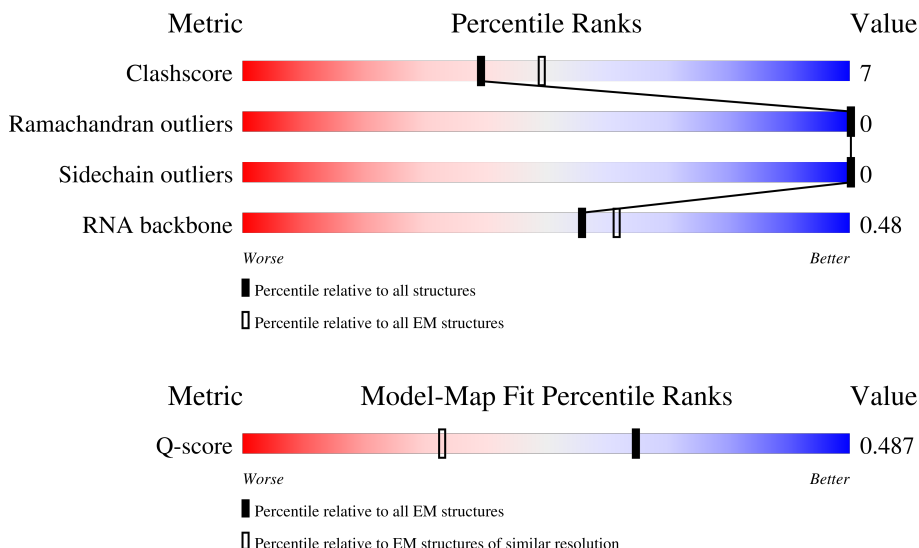
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.72 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.



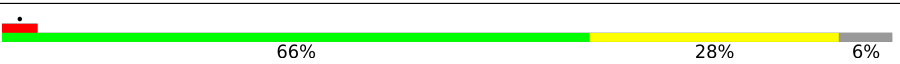
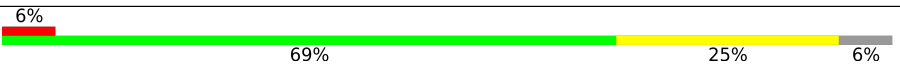
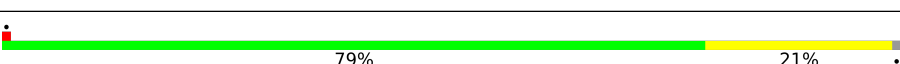
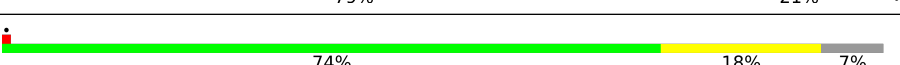
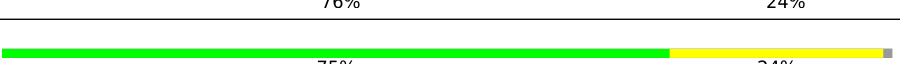
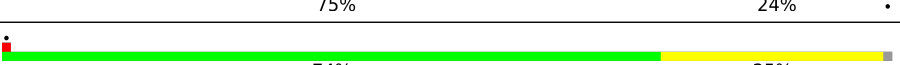
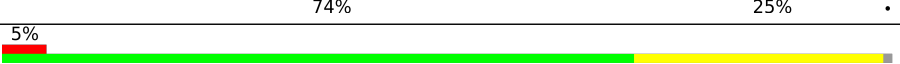
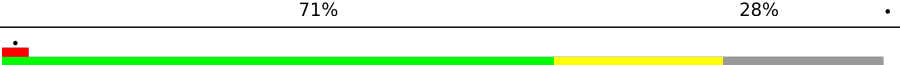
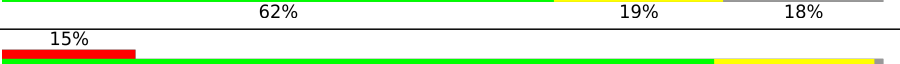
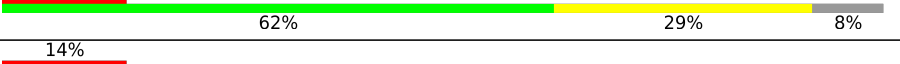
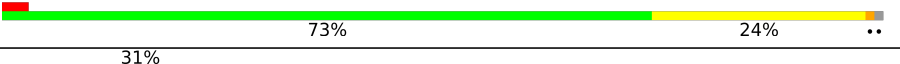
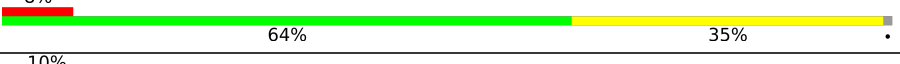
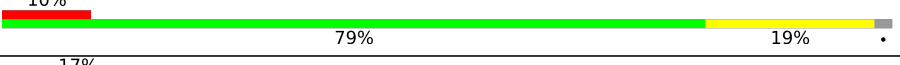
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10355 (2.22 - 3.22)

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	
2	BB	255	
3	BC	254	

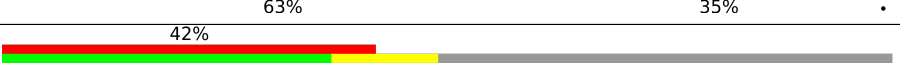
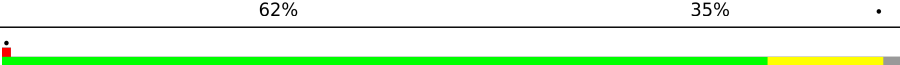
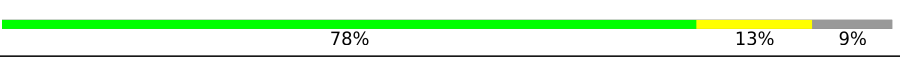
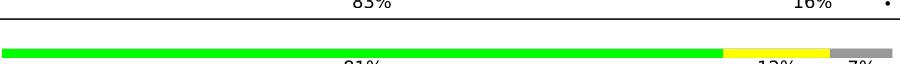
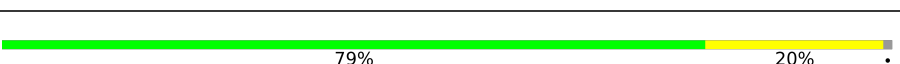
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Mol	Chain	Length	Quality of chain
4	BE	261	
5	BG	236	
6	BH	190	
7	BI	200	
8	BJ	197	
9	BL	156	
10	BN	151	
11	BO	137	
12	BV	87	
13	BW	130	
14	BX	145	
15	BY	135	
16	Ba	119	
17	Bb	82	
18	Be	63	
19	BD	240	
20	BF	225	
21	BK	105	
22	BP	142	
23	BQ	143	
24	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	3360	
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	E	217	
80	DC	842	
81	V	312	
82	EC	202	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	SO1	DC	903	X	-	-	-

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 214176 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
			975	611	183	179	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	69	Total	C	N	O	0	0
			558	357	103	98		

- 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
			38004	17005	6718	12499	1782		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	1280	4AC	C	conflict	GB 1329886537
B5	1773	4AC	C	conflict	GB 1329886537

- 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
			3080	1955	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	3198	Total	C	N	O	P	0	0
			68445	30596	12331	22320	3198		

- 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	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- 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	205	Total	C	N	O	S	0	0
			1672	1063	316	288	5		

- 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 protein called RPL1A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	E	217	Total	C	N	O	S	0	0
			1718	1097	299	312	10		

- Molecule 80 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	DC	824	Total	C	N	O	S	0	0
			6419	4085	1096	1208	30		

- Molecule 81 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	V	189	Total	C	N	O	S	0	0
			1473	942	257	270	4		

- Molecule 82 is a RNA chain called Taura syndrome virus (TSV) internal ribosome entry site (IRES) RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	EC	200	Total	C	N	O	P	0	0
			4235	1891	751	1393	200		

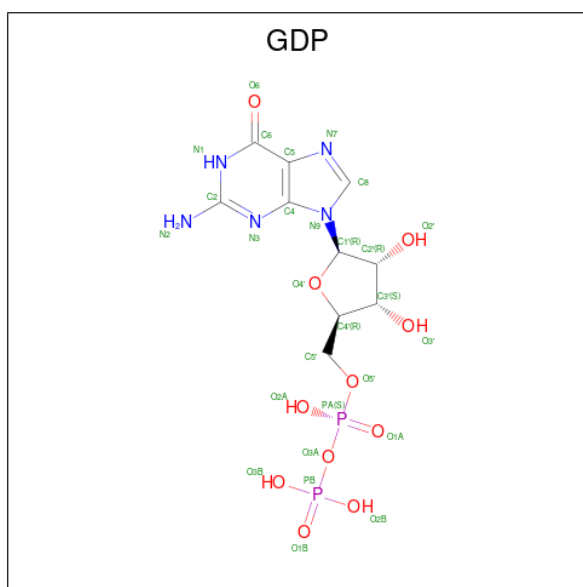
- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
83	BN	1	Total 1	Mg 1	0
83	Ba	1	Total 1	Mg 1	0
83	B5	53	Total 53	Mg 53	0
83	AB	1	Total 1	Mg 1	0
83	AC	1	Total 1	Mg 1	0
83	A1	172	Total 172	Mg 172	0
83	A3	2	Total 2	Mg 2	0
83	A4	3	Total 3	Mg 3	0
83	AI	1	Total 1	Mg 1	0
83	AL	1	Total 1	Mg 1	0
83	AP	1	Total 1	Mg 1	0
83	Ae	2	Total 2	Mg 2	0
83	Ah	1	Total 1	Mg 1	0
83	DC	1	Total 1	Mg 1	0

- Molecule 84 is ZINC ION (CCD ID: ZN) (formula: Zn).

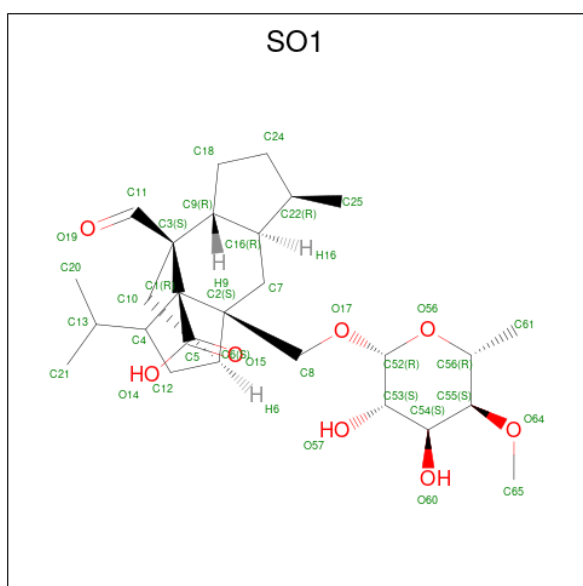
Mol	Chain	Residues	Atoms		AltConf
84	Ao	1	Total 1	Zn 1	0

- Molecule 85 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
85	DC	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 86 is [1R-(1.ALPHA.,3A.BETA.,4.BETA.,4A.BETA.,7.BETA.,7A.ALPHA.,8A.BETA.)]8A-[(6-DEOXY-4-O-METHYL-BETA-D-ALTROPYRANOSYLOXY)METHYL]-4-FORMYL-4,4A,5,6,7,7A,8,8A-OCTAHYDRO-7-METHYL-3-(1-METHYLETHYL)-1,4-METHANO-S-INDACENE-3A(1H)-CARBOXYLIC ACID (CCD ID: SO1) (formula: C₂₇H₄₂O₈).

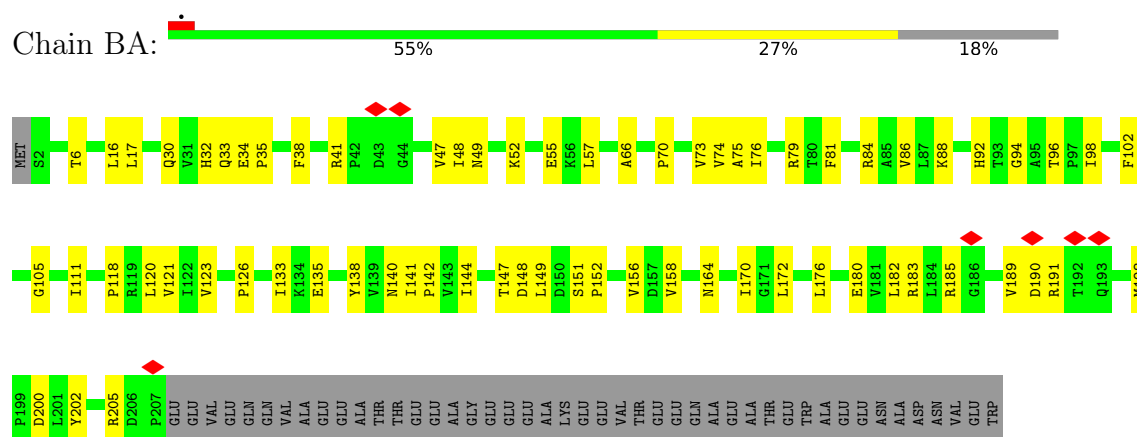


Mol	Chain	Residues	Atoms			AltConf
86	DC	1	Total	C	O	0
			35	27	8	

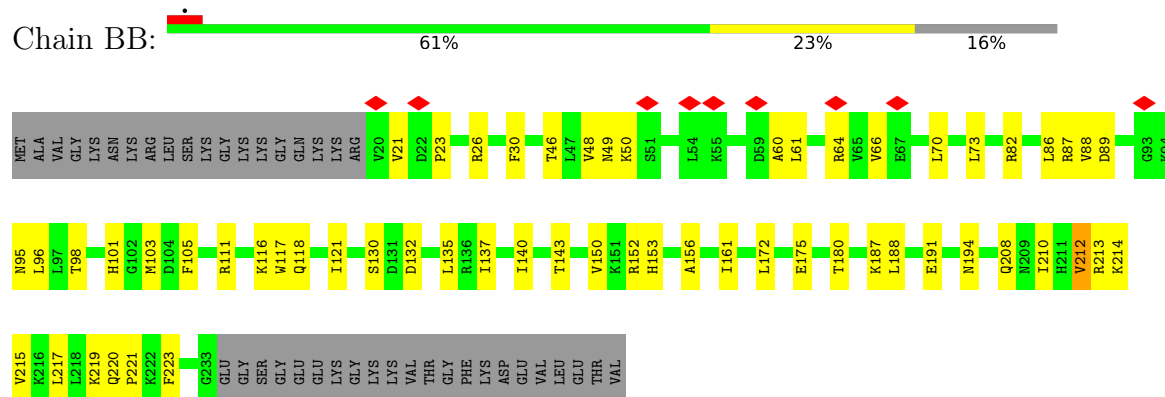
3 Residue-property plots

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.

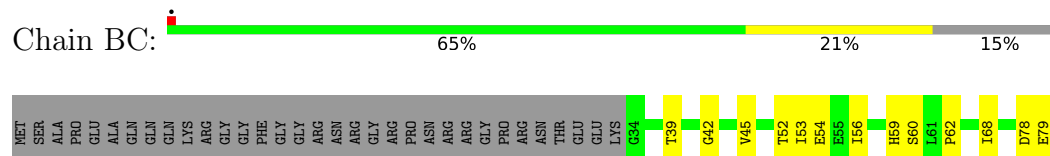
• Molecule 1: 40S ribosomal protein S0-A

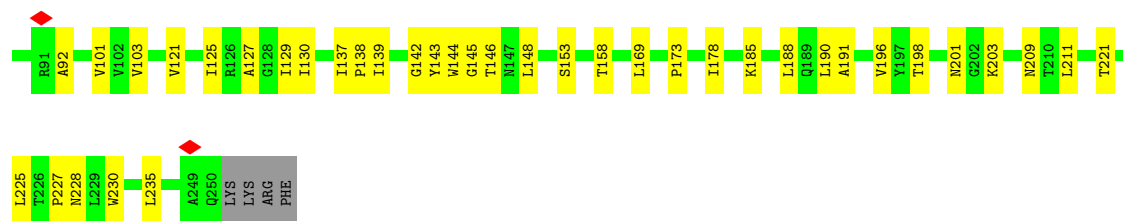


• Molecule 2: RPS1A isoform 1

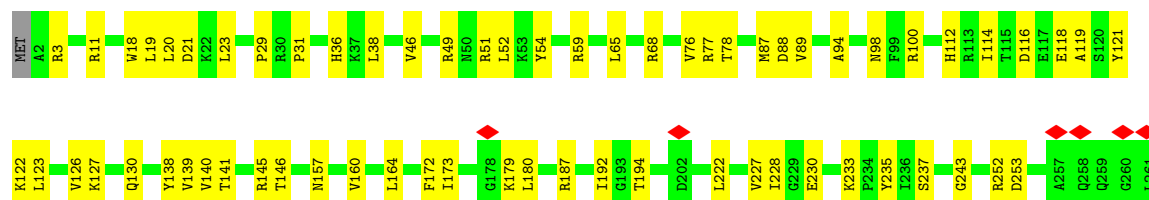
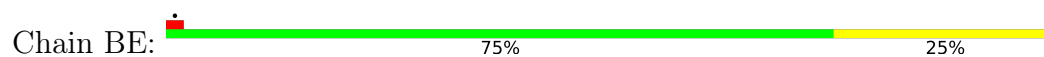


• Molecule 3: RPS2 isoform 1

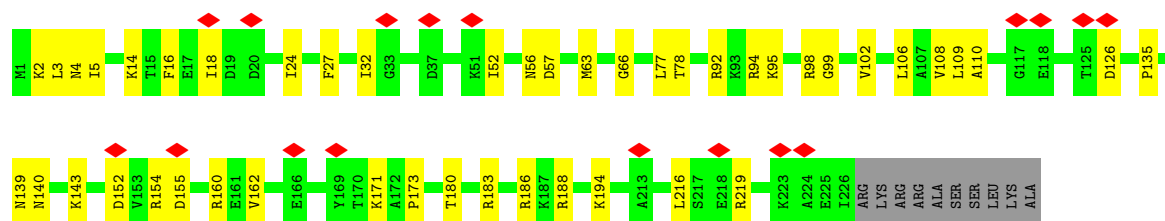
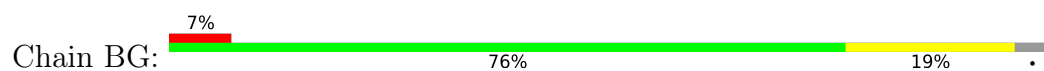




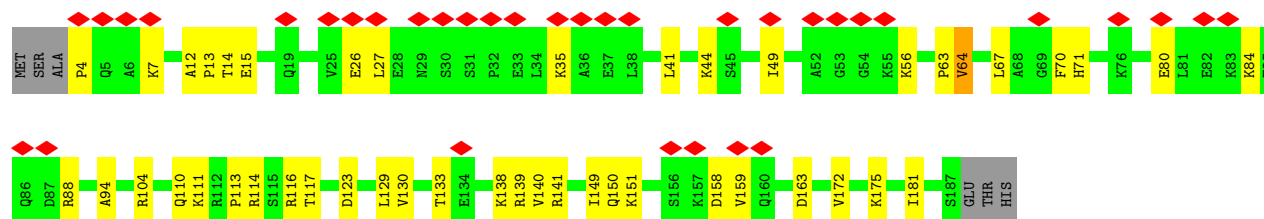
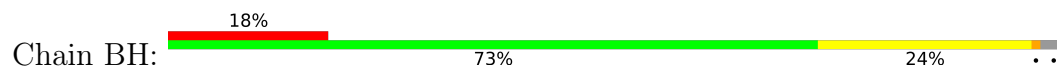
- Molecule 4: 40S ribosomal protein S4-A



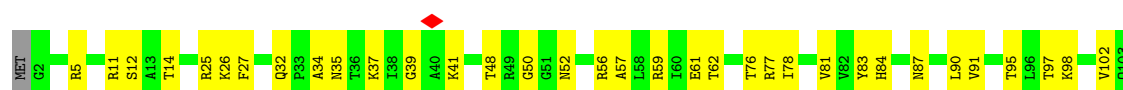
- Molecule 5: 40S ribosomal protein S6-A



- Molecule 6: 40S ribosomal protein S7-A



- Molecule 7: 40S ribosomal protein S8-A

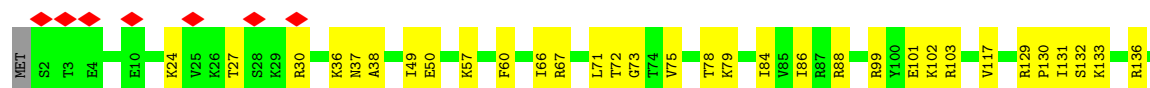
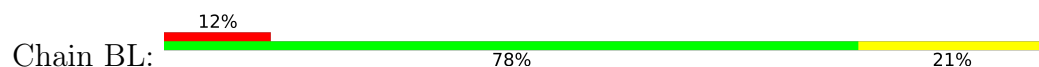




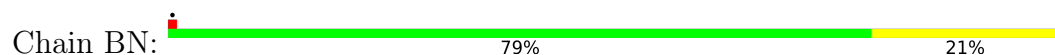
- Molecule 8: 40S ribosomal protein S9-A



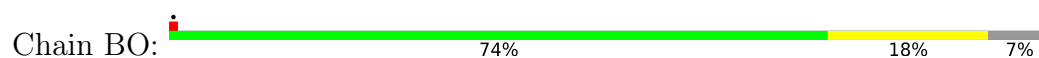
- Molecule 9: 40S ribosomal protein S11-A



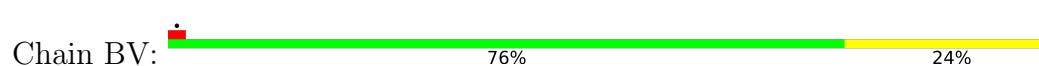
- Molecule 10: 40S ribosomal protein S13



- Molecule 11: 40S ribosomal protein S14-A



- Molecule 12: 40S ribosomal protein S21-A





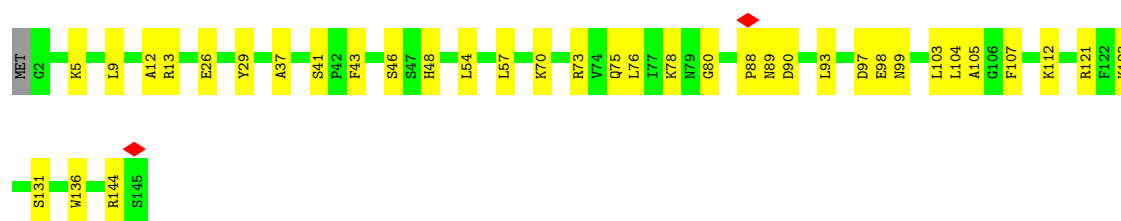
- Molecule 13: RPS22A isoform 1

Chain BW: 75% 24%



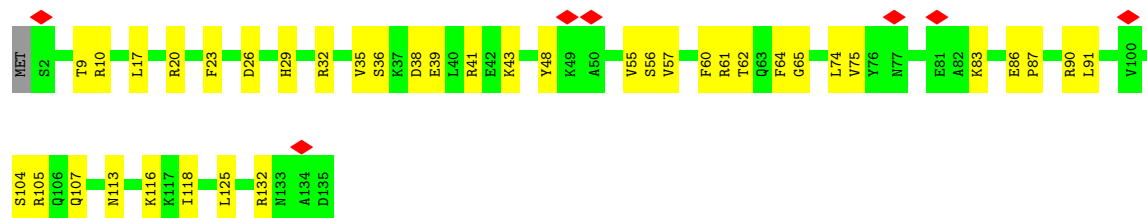
- Molecule 14: 40S ribosomal protein S23-A

Chain BX: 74% 25%



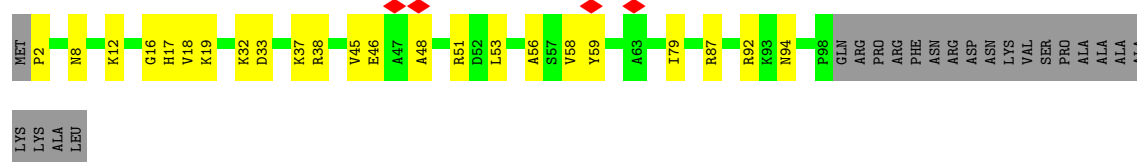
- Molecule 15: 40S ribosomal protein S24-A

Chain BY: 5% 71% 28%



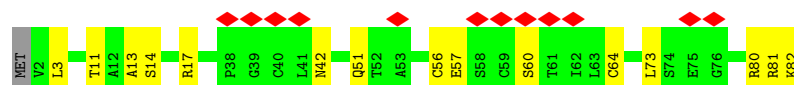
- Molecule 16: RPS26B isoform 1

Chain Ba: 62% 19% 18%

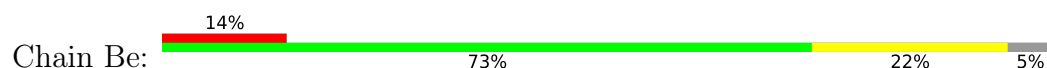


- Molecule 17: 40S ribosomal protein S27-A

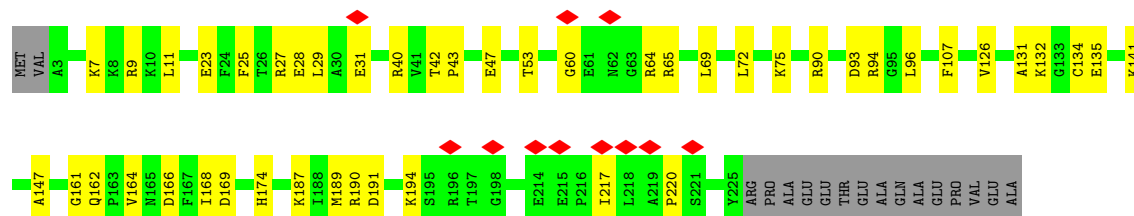
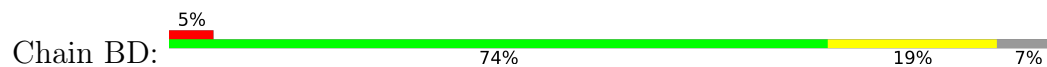
Chain Bb: 15% 80% 18%



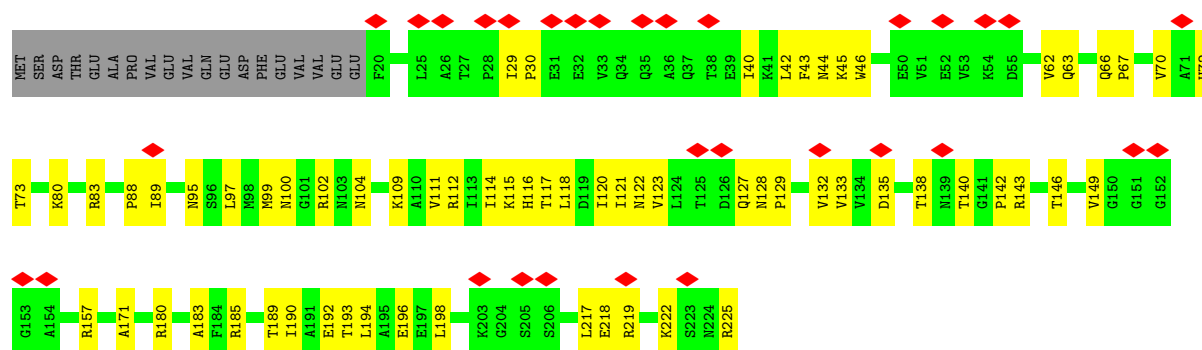
- Molecule 18: 40S ribosomal protein S30-A



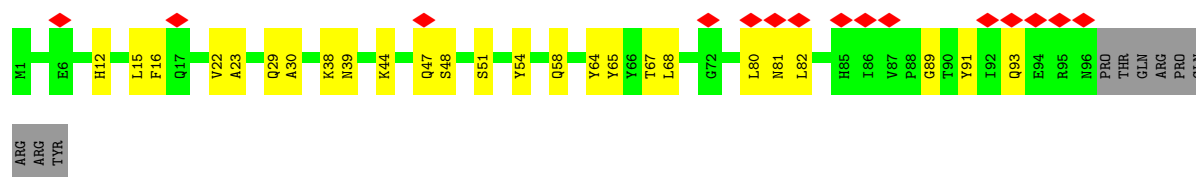
- Molecule 19: RPS3 isoform 1



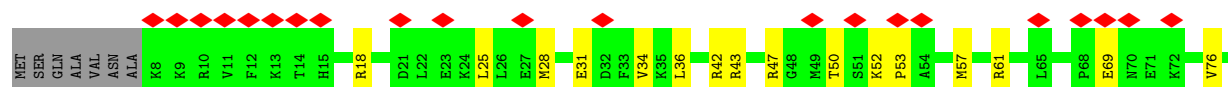
- Molecule 20: Rps5p



- Molecule 21: 40S ribosomal protein S10-A

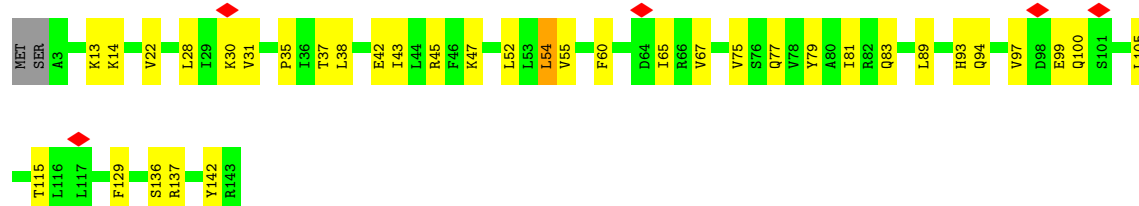
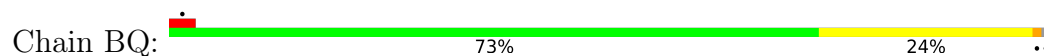


- Molecule 22: RPS15 isoform 1

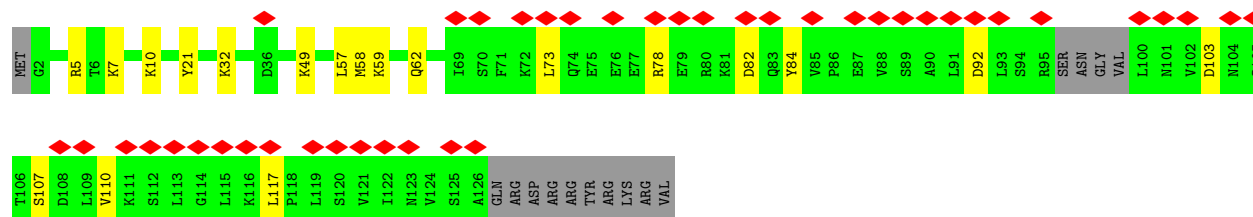
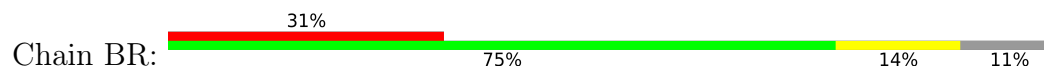




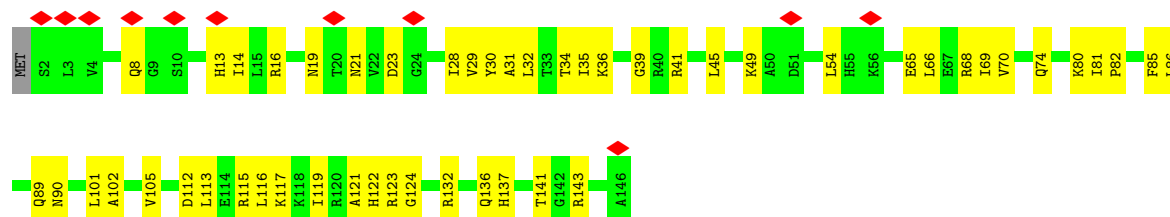
- Molecule 23: 40S ribosomal protein S16-A



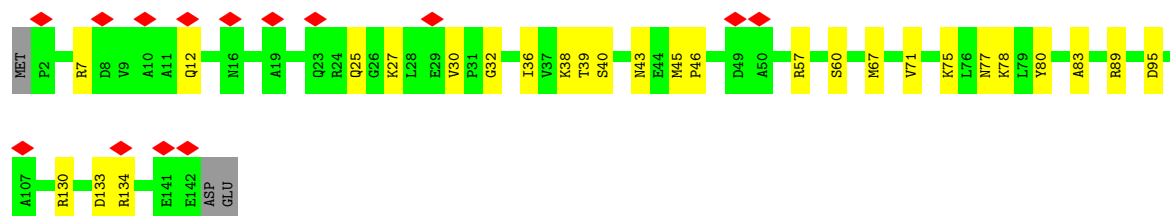
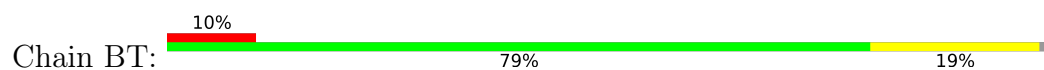
- Molecule 24: 40S ribosomal protein S17-A



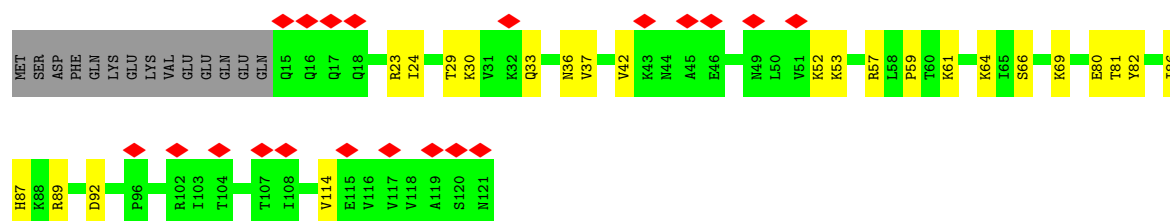
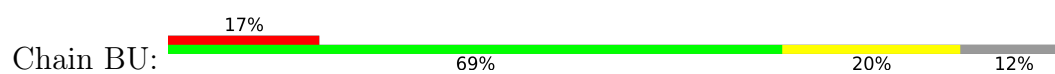
- Molecule 25: 40S ribosomal protein S18-A



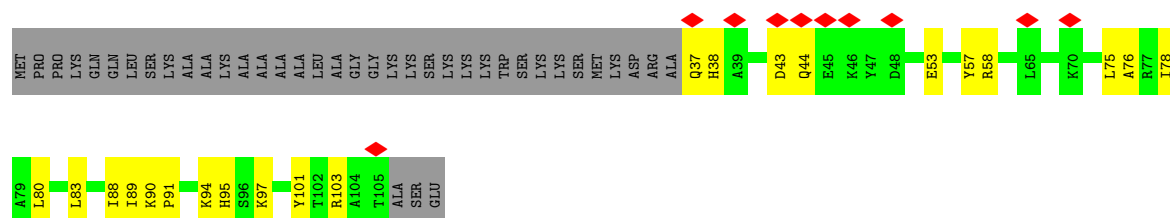
- Molecule 26: 40S ribosomal protein S19-A



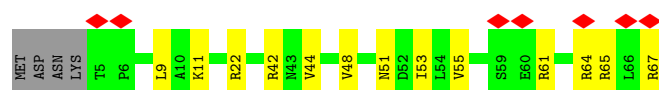
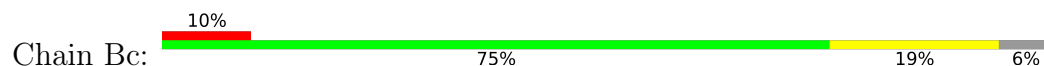
- Molecule 27: RPS20 isoform 1



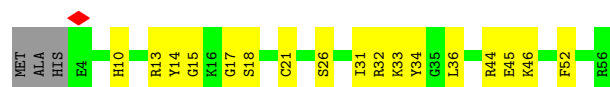
• Molecule 28: RPS25A isoform 1



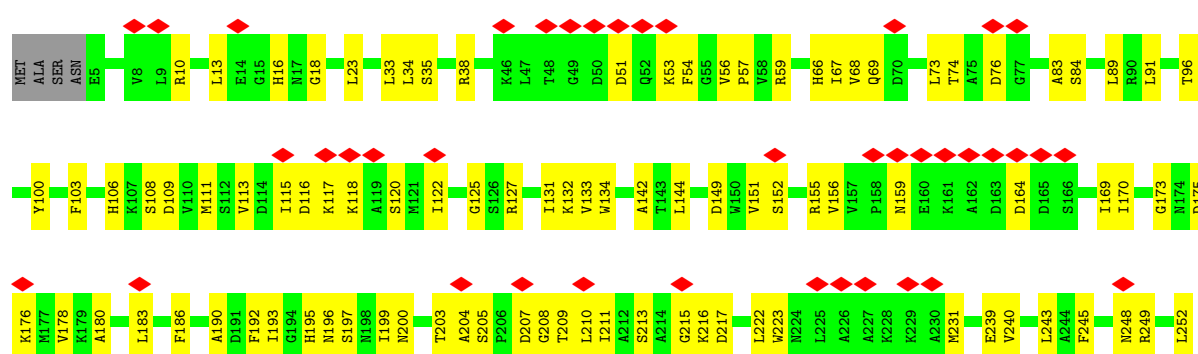
• Molecule 29: RPS28A isoform 1

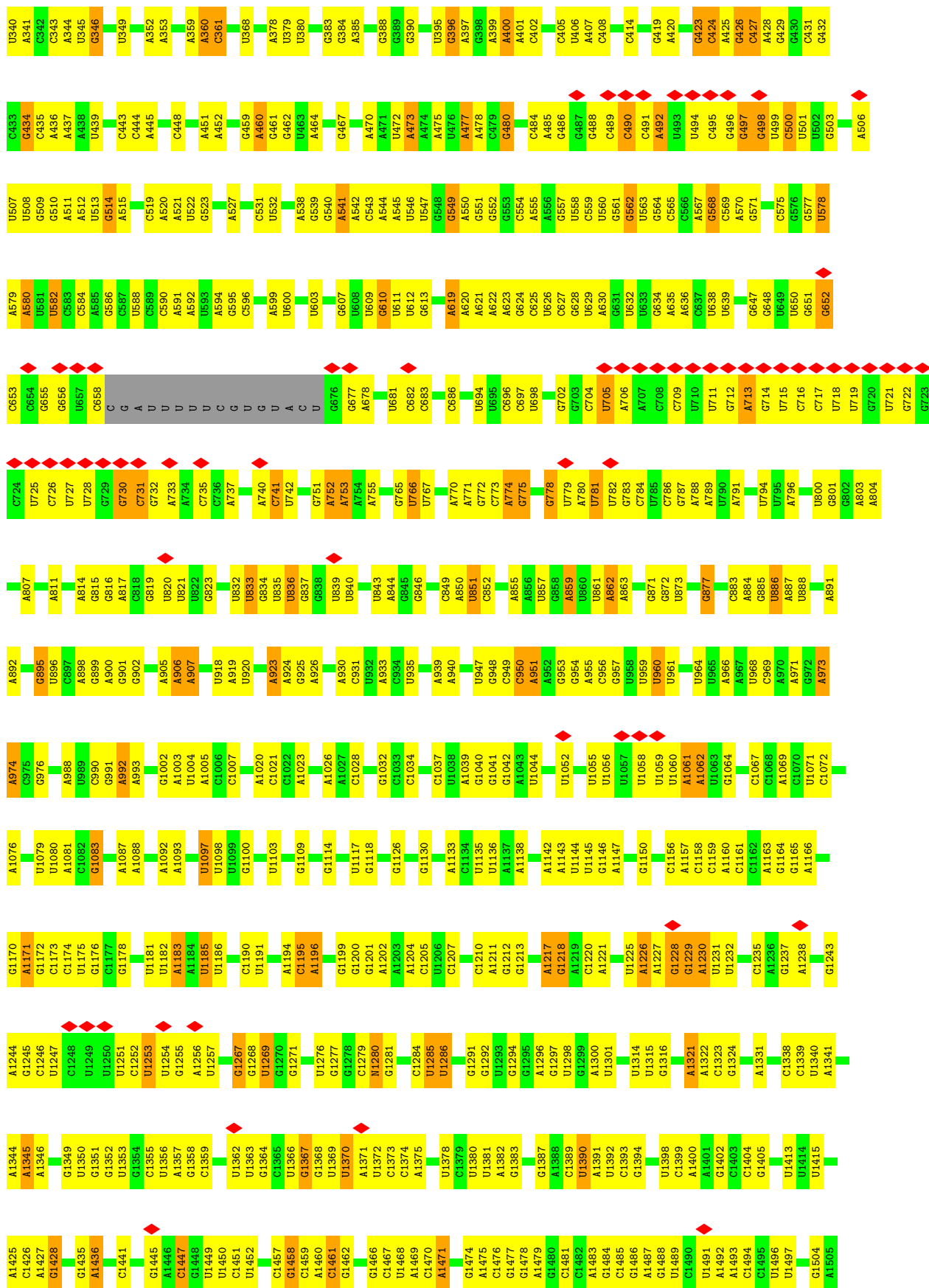


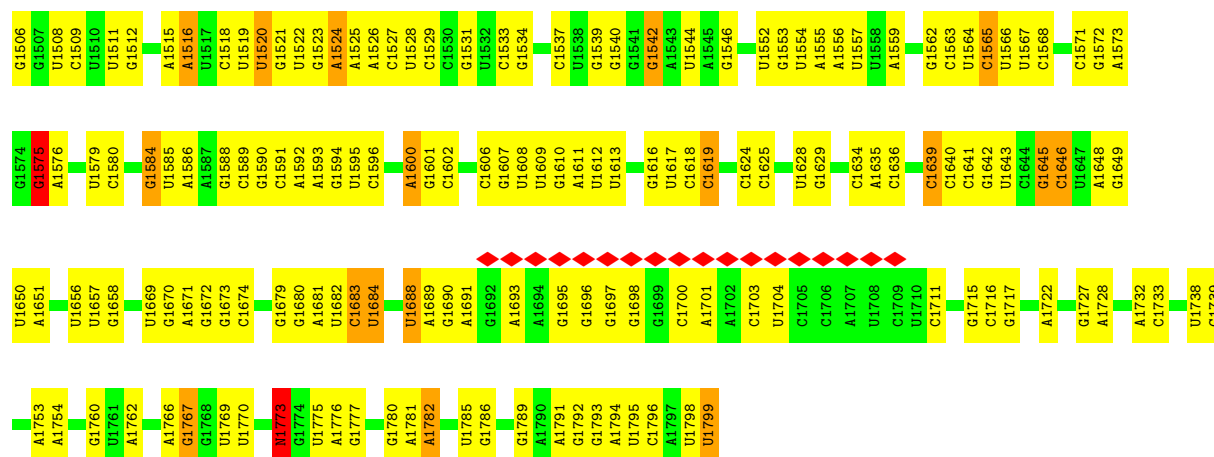
• Molecule 30: RPS29A isoform 1



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







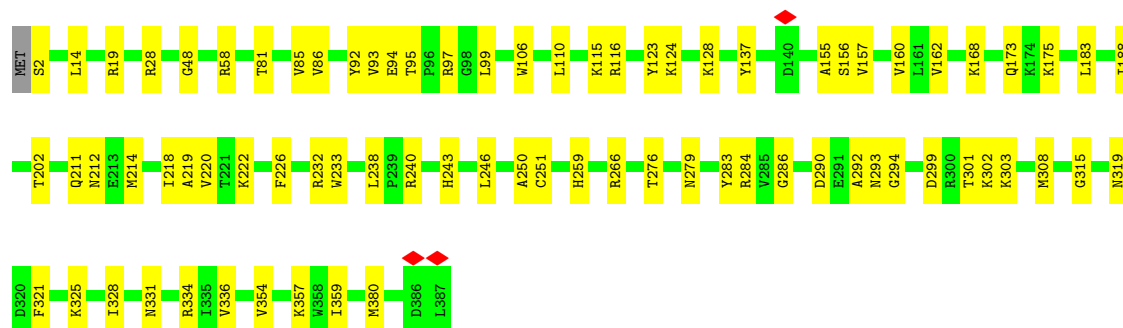
• Molecule 35: 60S ribosomal protein L2-A

Chain AA: 81% 16%



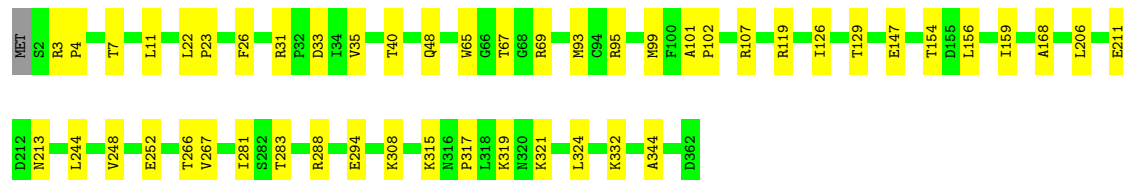
• Molecule 36: 60S ribosomal protein L3

Chain AB: 80% 20%



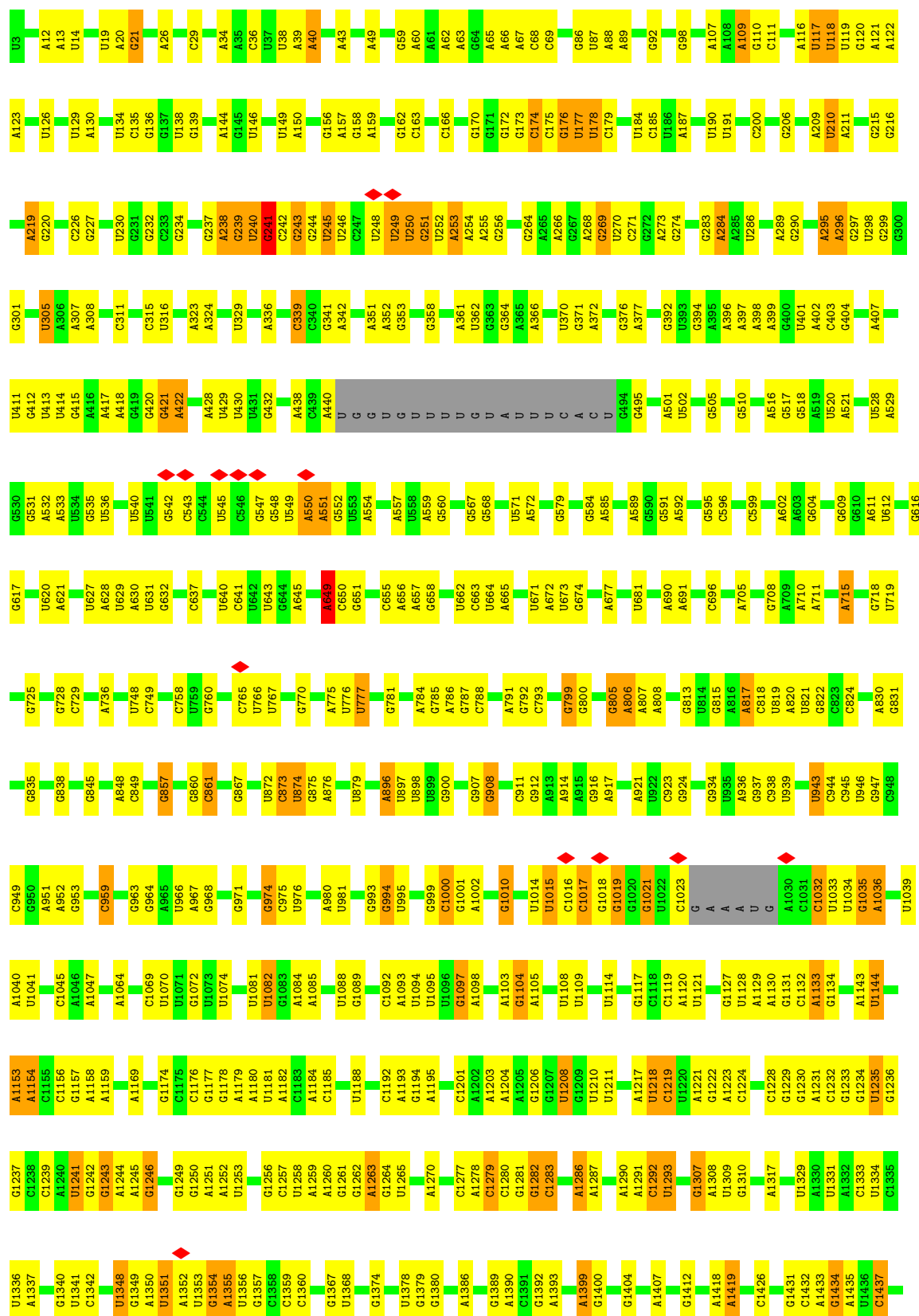
• Molecule 37: RPL4A isoform 1

Chain AC: 86% 14%

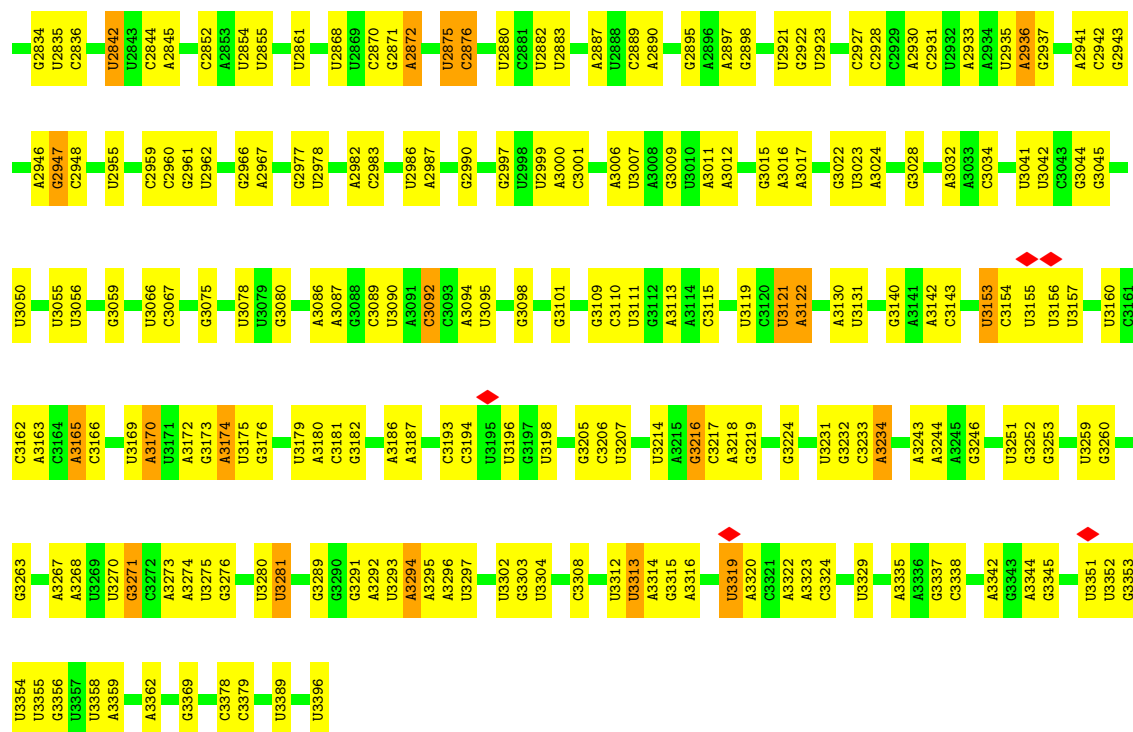


• Molecule 38: 25S rRNA

Chain A1: 



A2727	A2635	G2530	G2393	C2284	G2194	C	C	G1758	C1644	A1566	A1446
G2728	A2636	G2534	A2397	G2288	C2197	A	A	C1759	U1645	U1567	G1447
U2729	A2637	G2535	G2402	G2289	C2198	U	U	G1760	G1646	U1568	U1448
A2737	A2640	A2536	A2403	G2292	G2201	U	C	C1761		U1569	A1449
C2738	A2641	A2537	A2404	G2293	G2202	U	A	U1762	A1656	U1570	G1450
A2744	A2642	U2537	G2405	G2307	U2203	G	A	U1763	C1657	A1571	U1455
G2745	G2648	U2538	C2406	C2308	C2204	G	A	U1764	G1658	U1572	A1460
G2746	G2651	C2538	C2407	C2309	C2205	G	C	U1765	U1659	U1573	A1461
U2747	U2652	U2539	U2408	G2310	G2206	G	C	G1766	C1660	A1574	
A2748	G2653	A2540	U2409	G2311	A2207	U	G		G1661	A1575	
U2749	A2656	U2541	U2410	A2312	A2208	U	C	G1775	G1662	G1576	A1477
U2750	G2660	U2542	U2411	A2313	A2209	C	A		G1666		
G2751	G2661	U2543	G2412	U2314	A2210	U	C	U1783	A1667	C1579	A1481
U2752	G2662	U2544	G2413	U2315	A2211	U	C	U1784	U1668	A1580	
G2753	G2663	G2549	G2414	G2323	G2212	G	G	U1785	C1669	C1581	G1492
G2754		C2552	U2417	A2324	G2213	U	C	U1786	A1676	C1582	G1493
C2755		U2553	G2418	G2325	A2214	U	C	U1787	G1677	A1583	
A2758		A2554	A2419	G2326	A2215	U	C		G1678	A1589	C1496
U2767	A2667	A2557	U2420	U2334	G2221	G	U	G1796	A1683	G1592	C1497
U2768	A2674	U2558	U2421	U2335	A2222	A	G	A1797		A1593	C1498
A2769	G2677	U2559	U2422	U2336	A2223	G	C	U1798	U1687	U1594	
G2773	A2678	U2560	U2423	U2337	A2224	U	C	A1799		U1595	G1506
U2774	U2681	A2561	A2424	C2338	A2225	G	U	A1800	U1689	G1507	G1508
U2775	C2682	C2562	U2425	C2339	A2226	G	U		U1695	C1509	
C2776	C2683	U2563	U2426	U2340	A2227	C	G	A1804	A1696	C1597	C1516
U2777	A2684	A2564	U2427	U2341	A2228	U	C	A1805	A1697	G1598	G1517
C2778	U2685	A2565	U2428	U2342	A2229	U	C	A1806	C1708	G1602	
G2784	U2686	C2572	U2429	U2343	A2230	G	U	G1807	C1709	U1522	U1523
U2785	C2687	G2573	A2430	C2344	A2231	U	C	A1808		U1524	U1524
G2786	A2691	U2584	U2431	U2345	A2232	A	G	U1809	U1717	G1526	
C2791	A2696	C2585	U2432	U2346	A2233	G	U	A1810	G1718	A1612	A1534
A2792	G2697	U2588	U2433	U2347	A2234	U	C	G1811	U1719	A1613	A1535
G2793	G2698	A2593	G2434	U2348	A2235	U	C	A1812	U1720	C1614	G1536
G2796	G2700	C2594	A2445	U2349	A2236	G	U	A1813		C1615	
U2799	U2701	G2606	U2446	C2350	A2237	U	C	A1814	U1724	U1616	A1539
A2800	A2702	G2607	U2447	U2351	A2238	U	C	U1815	A1729	G1617	
A2801	A2703	G2608	G2448	U2352	U2258	U	C	A1816	U1734	G1618	G1542
A2802	A2704	U2505	A2449	U2353	U2259	G	C	A1817		A1619	G1543
A2803	A2705	U2506	U2450	C2354	U2260	U	C	U1820	G1738	A1621	
C2810	C2709	G2610	G2451	U2355	G2261	U	C	U1821	U1739	G1622	C1651
A2811	C2710	U2611	U2452	A2356	A2262	C	U	A1822	U1740	G1623	U1552
C2812	G2714	U2612	U2453	U2357	A2263	G	U	G1823	U1741	U1553	U1554
A2813	G2715	G2613	G2454	C2358	C2264	U	C	U1831	U1742	U1555	
G2814	G2716	U2614	U2455	U2359	A2265	U	C	U1832	G1743	C1628	U1556
G2815	U2719	U2615	U2456	U2360	G2272	C	C	G1833	G1744	U1629	C1557
G2816	G2720	C2616	G2457	C2361	G2273	U	C	U1834	U1745	U1630	A1558
A2817		G2619	U2458	C2362	C2274	U	C	G1840	G1746	A1559	
U2723	U2724	U2620	A2459	U2363	C2275	A	A	U1841	A1750	G1634	G1560
U2725	U2726	U2621	A2460	U2364	C2276	G	G	A1842	G1751	G1635	C1561
U2727	C2726	U2622	A2461	G2391	U2282	C	C	A1843	A1752	A1638	C1562
G2828		U2623	A2462	C2392	G2283	U	A	C1846	A1757	U1642	U1564
		C2526	G2527			C	U	G1848		A1643	G1565



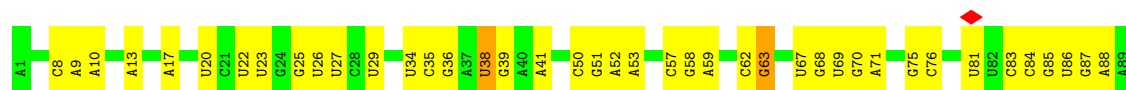
• Molecule 39: 5s rRNA

Chain A3: 69% 28% .



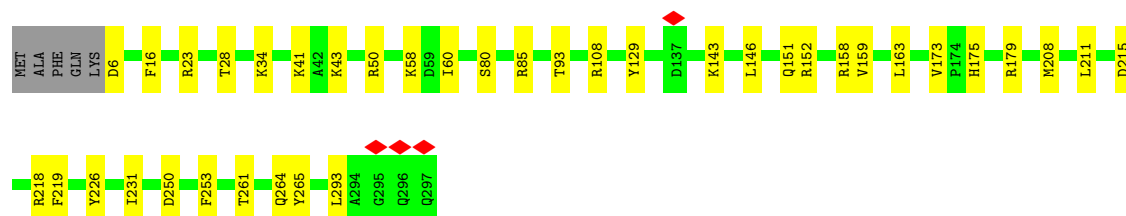
• Molecule 40: 5.8 S rRNA

Chain A4: 62% 35% .



• Molecule 41: RPL5 isoform 1

Chain AD: 86% 13% .



- Molecule 42: 60S ribosomal protein L6-A

Chain AE:  73% 15% 11%



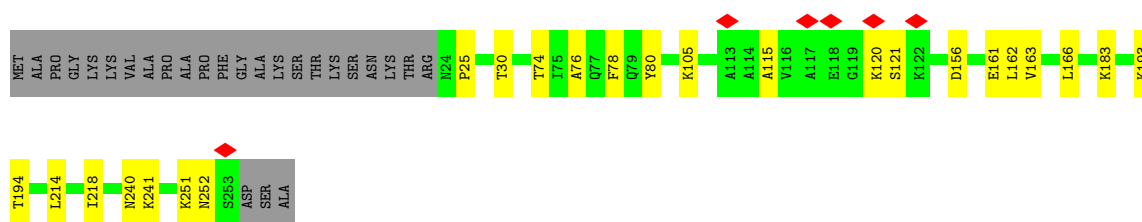
- Molecule 43: 60S ribosomal protein L7-A

Chain AF:  78% 13% 9%



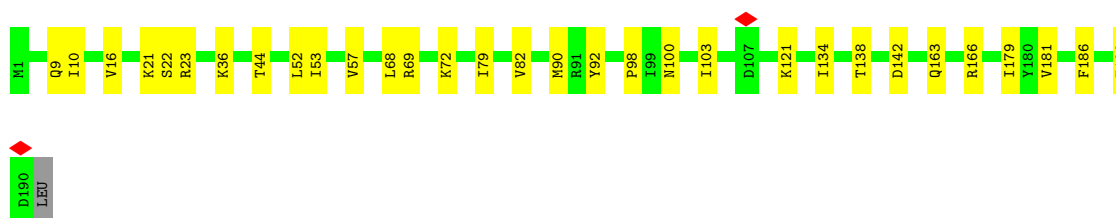
- Molecule 44: 60S ribosomal protein L8-A

Chain AG:  80% 9% 10%



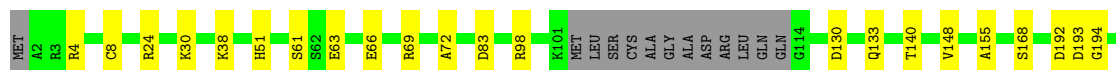
- Molecule 45: 60S ribosomal protein L9-A

Chain AH:  83% 16% 1%



- Molecule 46: RPL10 isoform 1

Chain AI:  81% 12% 7%





- Molecule 47: RPL11A isoform 1

Chain AJ: 6% 78% 19% ..



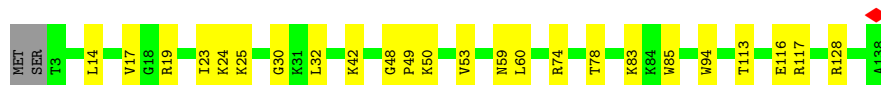
- Molecule 48: 60S ribosomal protein L13-A

Chain AL: 89% 8% .



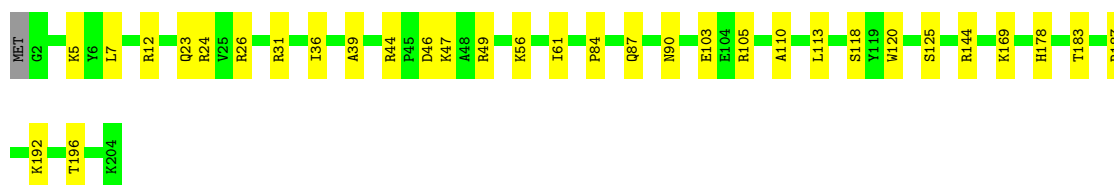
- Molecule 49: 60S ribosomal protein L14-A

Chain AM: 81% 17% .



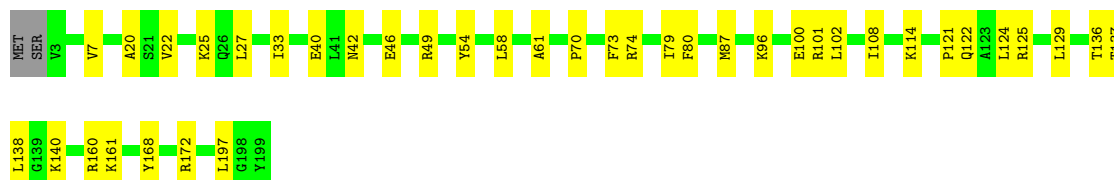
- Molecule 50: 60S ribosomal protein L15-A

Chain AN: 84% 16%

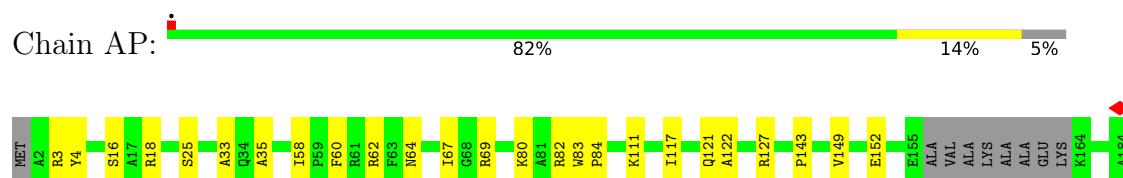


- Molecule 51: 60S ribosomal protein L16-A

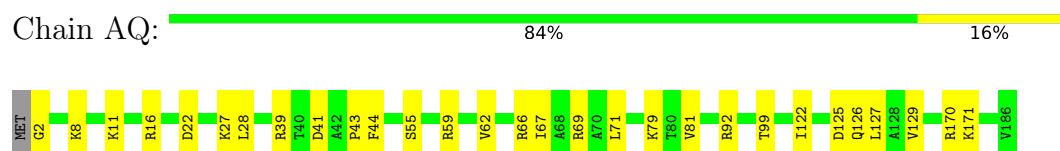
Chain AO: 79% 20% .



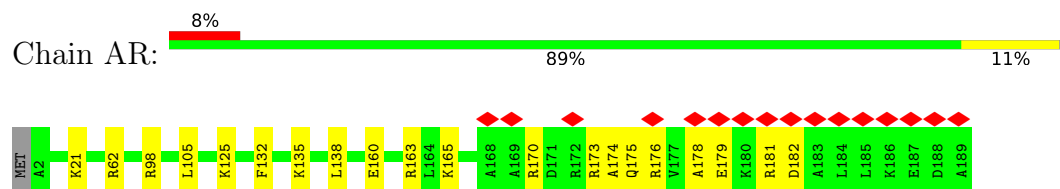
• Molecule 52: 60S ribosomal protein L17-A



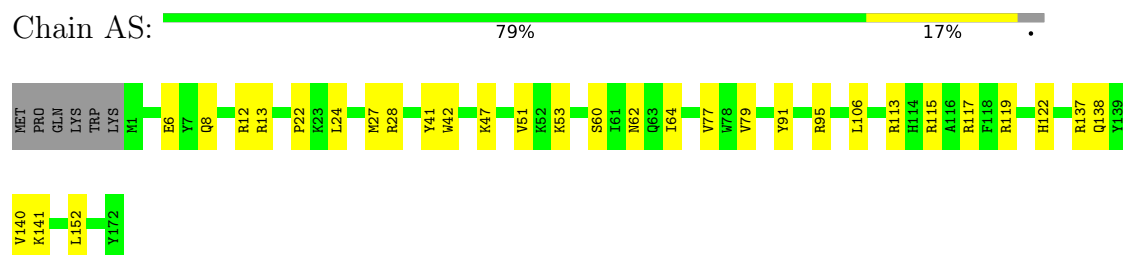
• Molecule 53: 60S ribosomal protein L18-A



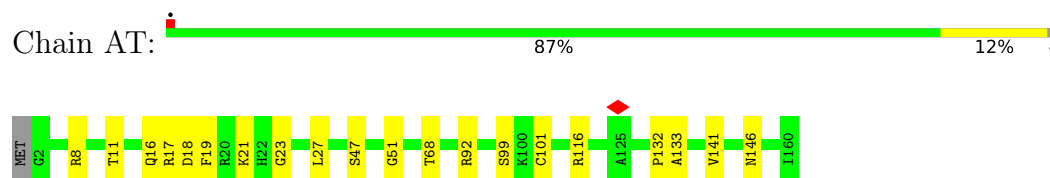
• Molecule 54: 60S ribosomal protein L19-A



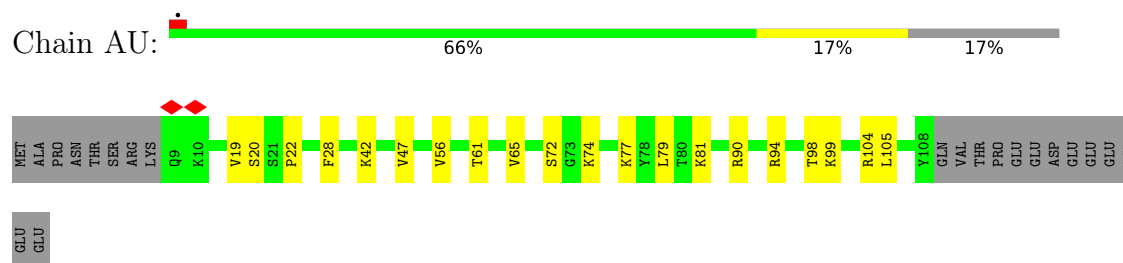
• Molecule 55: 60S ribosomal protein L20



• Molecule 56: 60S ribosomal protein L21-A



• Molecule 57: 60S ribosomal protein L22-A



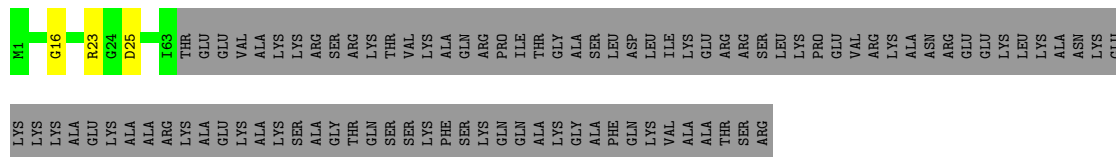
- Molecule 58: 60S ribosomal protein L23-A

Chain AV:  85% 15%



- Molecule 59: RPL24A isoform 1

Chain AW:  39% 59%



- Molecule 60: 60S ribosomal protein L25

Chain AX:  75% 10% 15%



- Molecule 61: 60S ribosomal protein L26-A

Chain AY:  82% 17%



- Molecule 62: 60S ribosomal protein L27-A

Chain AZ:  83% 16%



- Molecule 63: 60S ribosomal protein L28

Chain Aa:  78% 21%

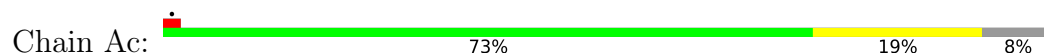


- Molecule 64: RPL29 isoform 1

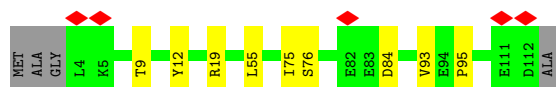
Chain Ab:  85% 14%



- Molecule 65: 60S ribosomal protein L30



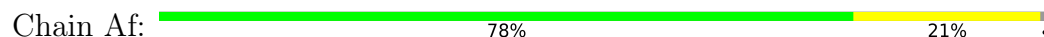
- Molecule 66: 60S ribosomal protein L31-A



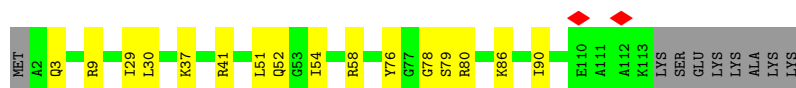
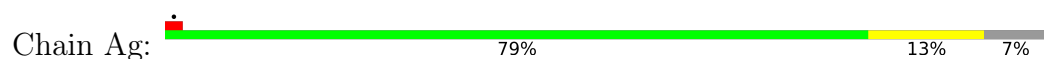
- Molecule 67: RPL32 isoform 1



- Molecule 68: 60S ribosomal protein L33-A



- Molecule 69: 60S ribosomal protein L34-A



- Molecule 70: 60S ribosomal protein L35-A



- Molecule 71: 60S ribosomal protein L36-A

Chain Ai:  85% 14%



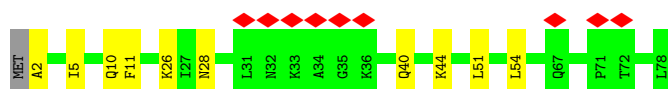
- Molecule 72: 60S ribosomal protein L37-A

Chain Aj:  84% 15%



- Molecule 73: RPL38 isoform 1

Chain Ak:  12% 86% 13%



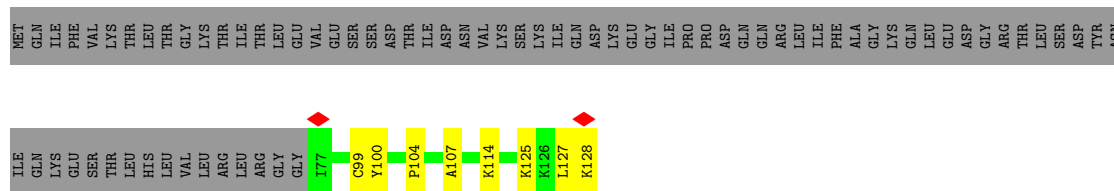
- Molecule 74: 60S ribosomal protein L39

Chain Al:  84% 14%



- Molecule 75: Ubiquitin-60S ribosomal protein L40

Chain Am:  34% 6% 59%



- Molecule 76: 60S ribosomal protein L41-A

Chain An:  80% 20%

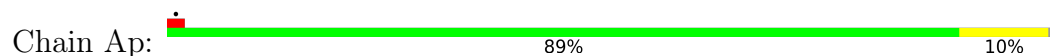


- Molecule 77: 60S ribosomal protein L42-A

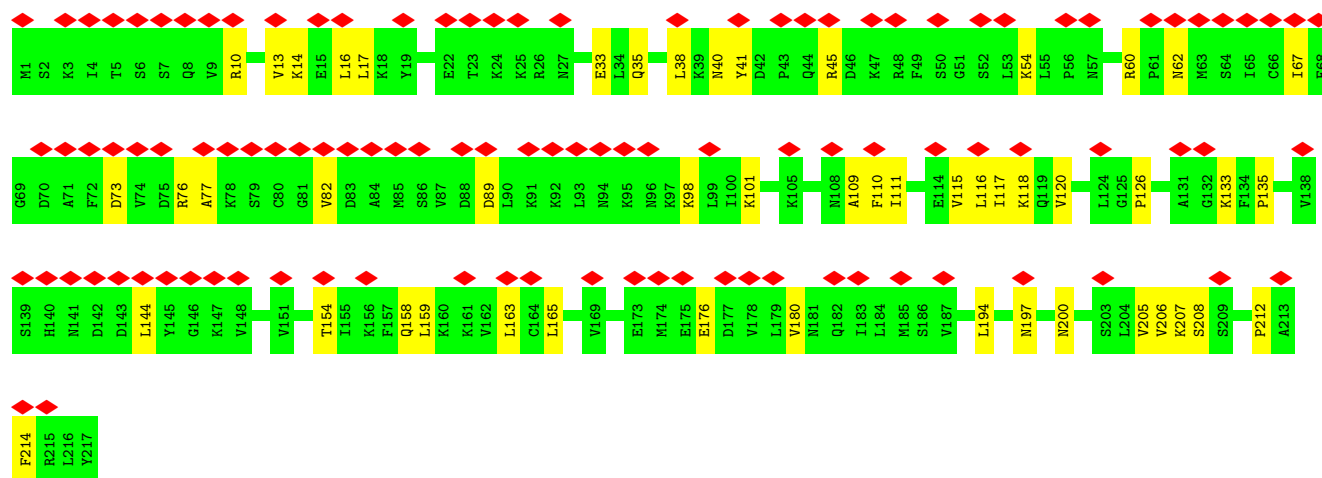
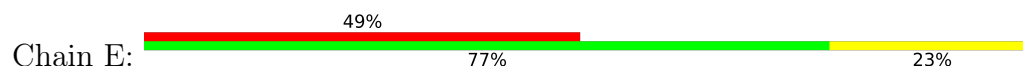
Chain Ao:  84% 14%



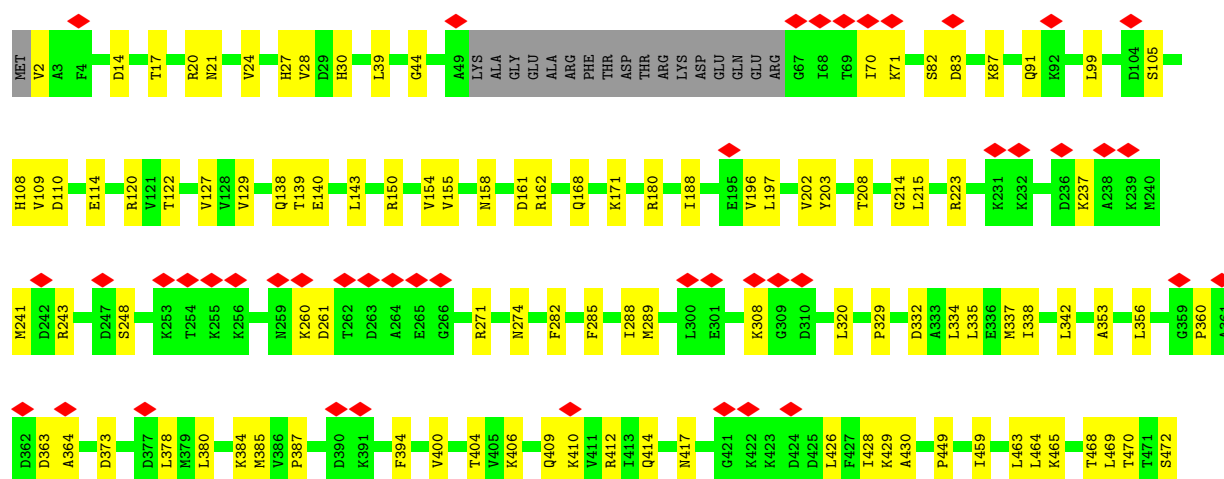
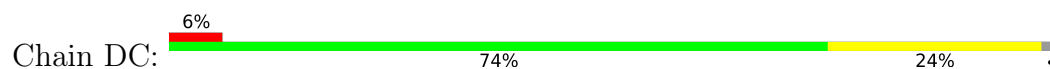
- Molecule 78: 60S ribosomal protein L43-A

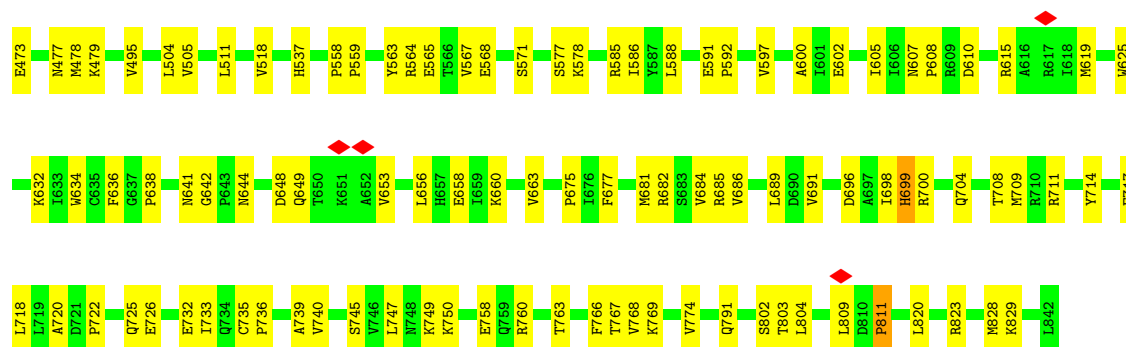


- Molecule 79: RPL1A isoform 1

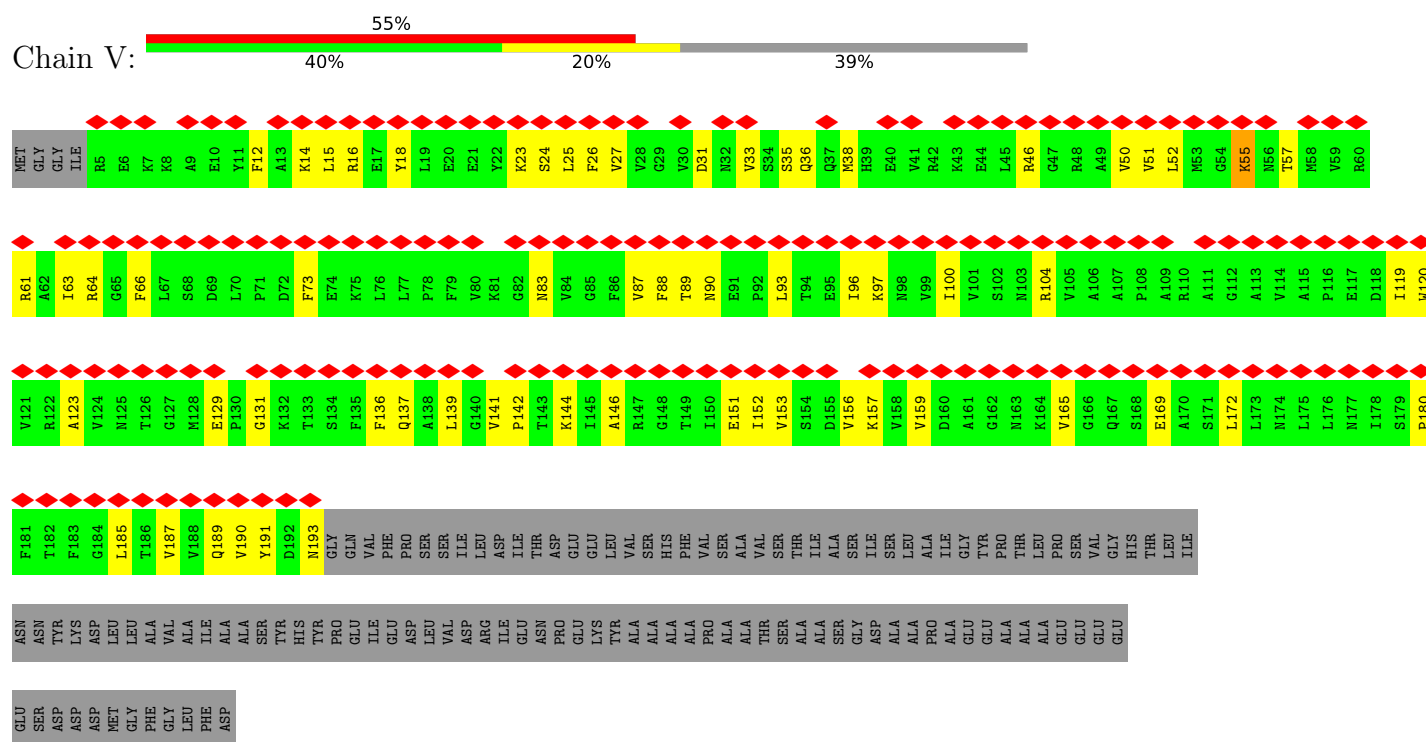


- Molecule 80: Elongation factor 2

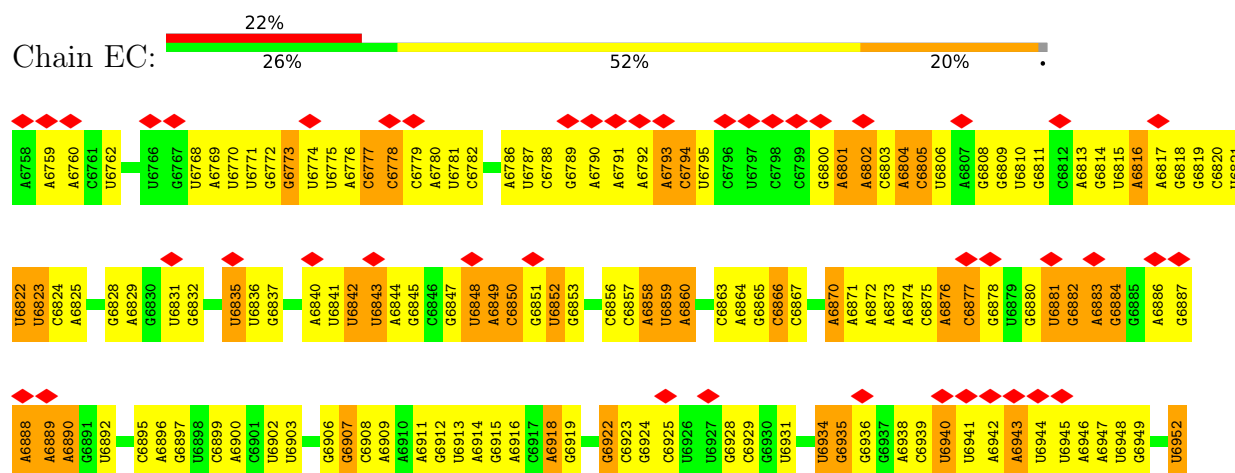




• Molecule 81: 60S acidic ribosomal protein P0



• Molecule 82: Taura syndrome virus (TSV) internal ribosome entry site (IRES) RNA



06953	06954	06955	06956	06957	C	C
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82327	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	6.565	Depositor
Minimum map value	-2.598	Depositor
Average map value	0.049	Depositor
Map value standard deviation	0.250	Depositor
Recommended contour level	0.6	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: A2M, XSX, HIC, MG, UR3, MA6, OMG, OMU, 5MC, SO1, DDE, GDP, OMC, ZN, G7M, 4AC, 1MA

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	0.19	0/1653	0.53	0/2261
2	BB	0.20	0/1735	0.55	2/2335 (0.1%)
3	BC	0.17	0/1665	0.43	0/2263
4	BE	0.18	0/2109	0.53	0/2839
5	BG	0.13	0/1844	0.36	0/2464
6	BH	0.19	0/1506	0.53	0/2028
7	BI	0.17	0/1514	0.49	0/2021
8	BJ	0.17	0/1519	0.46	0/2035
9	BL	0.16	0/1272	0.41	0/1712
10	BN	0.17	0/1215	0.49	0/1638
11	BO	0.21	0/952	0.55	0/1279
12	BV	0.22	0/693	0.61	0/935
13	BW	0.15	0/1038	0.43	0/1395
14	BX	0.16	0/1139	0.50	0/1518
15	BY	0.17	0/1087	0.46	0/1449
16	Ba	0.20	0/782	0.60	0/1047
17	Bb	0.20	0/620	0.55	0/838
18	Be	0.14	0/483	0.46	0/643
19	BD	0.18	0/1759	0.50	0/2368
20	BF	0.20	0/1629	0.58	2/2202 (0.1%)
21	BK	0.19	0/837	0.61	2/1131 (0.2%)
22	BP	0.19	0/1012	0.61	2/1356 (0.1%)
23	BQ	0.17	0/1125	0.46	1/1510 (0.1%)
24	BR	0.19	0/984	0.47	0/1318
25	BS	0.18	0/1211	0.51	0/1628
26	BT	0.20	0/1113	0.53	0/1494
27	BU	0.17	0/865	0.46	0/1169
28	BZ	0.15	0/566	0.43	0/761
29	Bc	0.16	0/499	0.48	0/670
30	Bd	0.17	0/452	0.46	0/600
31	Bg	0.17	0/2454	0.50	0/3340

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Bf	0.17	0/616	0.55	1/817 (0.1%)
33	BM	0.17	0/943	0.51	0/1274
34	B5	0.16	4/41880 (0.0%)	0.33	0/65248
35	AA	0.16	0/1912	0.39	0/2569
36	AB	0.17	0/3138	0.41	0/4217
37	AC	0.17	0/2800	0.41	0/3790
38	A1	0.18	1/75561 (0.0%)	0.33	1/117806 (0.0%)
39	A3	0.15	0/2883	0.28	0/4491
40	A4	0.16	0/3746	0.31	0/5832
41	AD	0.15	0/2390	0.41	1/3225 (0.0%)
42	AE	0.17	0/1260	0.44	0/1694
43	AF	0.16	0/1821	0.38	0/2451
44	AG	0.16	0/1830	0.43	0/2469
45	AH	0.18	0/1531	0.46	2/2062 (0.1%)
46	AI	0.16	0/1708	0.33	0/2290
47	AJ	0.19	0/1374	0.57	2/1842 (0.1%)
48	AL	0.14	0/1568	0.36	0/2106
49	AM	0.13	0/1068	0.32	0/1438
50	AN	0.16	0/1757	0.36	0/2354
51	AO	0.18	0/1585	0.42	0/2128
52	AP	0.16	0/1410	0.38	0/1893
53	AQ	0.15	0/1465	0.38	0/1965
54	AR	0.15	0/1538	0.38	0/2050
55	AS	0.18	0/1481	0.39	0/1990
56	AT	0.15	0/1300	0.34	0/1743
57	AU	0.18	0/812	0.51	0/1099
58	AV	0.17	0/1018	0.41	0/1369
59	AW	0.16	0/533	0.41	0/707
60	AX	0.17	0/983	0.39	0/1325
61	AY	0.18	0/1004	0.42	0/1341
62	AZ	0.15	0/1118	0.37	0/1497
63	Aa	0.19	0/1204	0.44	0/1612
64	Ab	0.15	0/473	0.39	0/629
65	Ac	0.14	0/751	0.34	0/1008
66	Ad	0.15	0/904	0.39	0/1213
67	Ae	0.16	0/1041	0.39	0/1394
68	Af	0.18	0/868	0.37	0/1168
69	Ag	0.19	0/890	0.41	0/1189
70	Ah	0.15	0/978	0.41	0/1301
71	Ai	0.16	0/778	0.41	0/1034
72	Aj	0.17	0/696	0.43	0/923
73	Ak	0.17	0/618	0.45	0/826
74	Al	0.16	0/443	0.42	0/588

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Am	0.21	0/423	0.41	0/562
76	An	0.23	0/234	0.76	0/300
77	Ao	0.17	0/860	0.46	0/1136
78	Ap	0.15	0/701	0.42	0/934
79	E	0.16	0/1745	0.43	0/2342
80	DC	0.18	0/6521	0.50	2/8830 (0.0%)
81	V	0.23	0/1498	0.61	2/2025 (0.1%)
82	EC	0.15	0/4733	0.40	0/7369
All	All	0.17	5/227724 (0.0%)	0.39	20/333712 (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
3	BC	0	1
6	BH	0	1
11	BO	0	1
41	AD	0	1
43	AF	0	1
44	AG	0	3
47	AJ	0	1
77	Ao	0	1
All	All	0	10

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	796	A2M	O3'-P	5.32	1.61	1.56
38	A1	2946	A2M	O3'-P	5.13	1.61	1.56
34	B5	436	A2M	O3'-P	5.10	1.61	1.56
34	B5	541	A2M	O3'-P	5.06	1.61	1.56
34	B5	1269	OMU	O3'-P	5.03	1.61	1.56

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	BF	43	PHE	CA-C-N	7.97	136.77	121.54
20	BF	43	PHE	C-N-CA	7.97	136.77	121.54
81	V	55	LYS	CA-C-N	6.70	133.76	121.70
81	V	55	LYS	C-N-CA	6.70	133.76	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	DC	811	PRO	N-CD-CG	-5.99	94.21	103.20
32	Bf	144	CYS	CA-CB-SG	5.94	128.07	114.40
45	AH	138	THR	CA-C-N	5.56	135.94	125.66
45	AH	138	THR	C-N-CA	5.56	135.94	125.66
47	AJ	54	VAL	CA-C-N	5.56	132.15	121.54
47	AJ	54	VAL	C-N-CA	5.56	132.15	121.54
2	BB	212	VAL	CA-C-N	5.54	132.13	121.54
2	BB	212	VAL	C-N-CA	5.54	132.13	121.54
80	DC	811	PRO	CA-N-CD	-5.43	104.39	112.00
38	A1	241	G	P-O3'-C3'	5.33	128.20	120.20
21	BK	89	GLY	CA-C-N	5.20	131.07	121.70
21	BK	89	GLY	C-N-CA	5.20	131.07	121.70
22	BP	69	GLU	CA-C-N	5.08	129.36	122.19
22	BP	69	GLU	C-N-CA	5.08	129.36	122.19
41	AD	208	MET	CA-CB-CG	5.08	124.25	114.10
23	BQ	54	LEU	CA-CB-CG	5.02	133.88	116.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
41	AD	43	LYS	Peptide
43	AF	232	ARG	Peptide
44	AG	121	SER	Peptide
44	AG	30	THR	Peptide
44	AG	76	ALA	Peptide
47	AJ	166	LYS	Peptide
77	Ao	103	ALA	Peptide
3	BC	144	TRP	Peptide
6	BH	64	VAL	Peptide
11	BO	123	SER	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	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BB	1709	0	1784	41	0
3	BC	1635	0	1723	35	0
4	BE	2068	0	2154	44	0
5	BG	1820	0	1918	38	0
6	BH	1481	0	1572	30	0
7	BI	1489	0	1525	40	0
8	BJ	1494	0	1573	40	0
9	BL	1244	0	1314	27	0
10	BN	1192	0	1255	26	0
11	BO	941	0	979	17	0
12	BV	684	0	672	22	0
13	BW	1021	0	1060	23	0
14	BX	1121	0	1196	32	0
15	BY	1073	0	1132	27	0
16	Ba	769	0	818	18	0
17	Bb	610	0	633	13	0
18	Be	475	0	525	13	0
19	BD	1734	0	1817	37	0
20	BF	1609	0	1675	55	0
21	BK	817	0	804	18	0
22	BP	991	0	1035	25	0
23	BQ	1105	0	1166	26	0
24	BR	975	0	1039	16	0
25	BS	1192	0	1222	46	0
26	BT	1095	0	1114	24	0
27	BU	855	0	917	17	0
28	BZ	558	0	598	16	0
29	Bc	497	0	535	11	0
30	Bd	442	0	432	15	0
31	Bg	2401	0	2356	71	0
32	Bf	605	0	654	15	0
33	BM	935	0	975	22	0
34	B5	38004	0	19142	542	0
35	AA	1878	0	1946	30	0
36	AB	3080	0	3158	59	0
37	AC	2748	0	2859	33	0
38	A1	68445	0	34458	692	0
39	A3	2579	0	1304	26	0
40	A4	3353	0	1695	29	0
41	AD	2341	0	2290	28	0
42	AE	1239	0	1326	21	0
43	AF	1784	0	1862	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	AG	1798	0	1894	15	0
45	AH	1510	0	1576	22	0
46	AI	1672	0	1711	20	0
47	AJ	1353	0	1383	22	0
48	AL	1543	0	1608	10	0
49	AM	1053	0	1149	15	0
50	AN	1720	0	1779	23	0
51	AO	1555	0	1659	24	0
52	AP	1388	0	1423	18	0
53	AQ	1441	0	1543	23	0
54	AR	1521	0	1617	18	0
55	AS	1445	0	1487	20	0
56	AT	1276	0	1323	17	0
57	AU	796	0	812	13	0
58	AV	1003	0	1048	12	0
59	AW	521	0	551	3	0
60	AX	968	0	1036	10	0
61	AY	993	0	1081	20	0
62	AZ	1092	0	1155	16	0
63	Aa	1173	0	1215	29	0
64	Ab	462	0	491	6	0
65	Ac	743	0	797	12	0
66	Ad	890	0	938	6	0
67	Ae	1020	0	1090	6	0
68	Af	850	0	880	16	0
69	Ag	880	0	945	13	0
70	Ah	969	0	1078	7	0
71	Ai	771	0	849	13	0
72	Aj	681	0	687	12	0
73	Ak	612	0	682	10	0
74	Al	436	0	475	7	0
75	Am	417	0	459	6	0
76	An	233	0	279	4	0
77	Ao	847	0	914	12	0
78	Ap	694	0	738	7	0
79	E	1718	0	1811	36	0
80	DC	6419	0	6493	138	0
81	V	1473	0	1514	47	0
82	EC	4235	0	2136	49	0
83	A1	172	0	0	0	0
83	A3	2	0	0	0	0
83	A4	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	AB	1	0	0	0	0
83	AC	1	0	0	0	0
83	AI	1	0	0	0	0
83	AL	1	0	0	0	0
83	AP	1	0	0	0	0
83	Ae	2	0	0	0	0
83	Ah	1	0	0	0	0
83	B5	53	0	0	0	0
83	BN	1	0	0	0	0
83	Ba	1	0	0	0	0
83	DC	1	0	0	0	0
84	Ao	1	0	0	0	0
85	DC	28	0	11	1	0
86	DC	35	0	41	1	0
All	All	214176	0	160193	2623	0

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

All (2623) 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)
34:B5:126:A:H62	34:B5:291:G:N2	1.46	1.13
34:B5:976:G:H1	34:B5:1023:A:HO2'	1.08	1.02
34:B5:766:U:H3	34:B5:770:A:H62	1.04	1.01
34:B5:1679:G:H21	34:B5:1722:A:H62	1.10	0.98
34:B5:126:A:N6	34:B5:291:G:H21	1.60	0.97
38:A1:2138:A:HO2'	72:Aj:2:GLY:N	1.66	0.92
34:B5:1213:G:H1	34:B5:1450:U:H3	1.07	0.91
38:A1:172:G:H1	38:A1:245:U:H3	1.20	0.88
13:BW:2:THR:N	34:B5:1034:C:HO2'	1.76	0.84
34:B5:1542:G:H1	34:B5:1568:C:HO2'	1.27	0.82
34:B5:1679:G:N2	34:B5:1722:A:H62	1.77	0.82
20:BF:97:LEU:O	20:BF:180:ARG:NH2	2.14	0.81
1:BA:16:LEU:HD13	1:BA:172:LEU:HD11	1.65	0.79
34:B5:126:A:H62	34:B5:291:G:H21	0.81	0.76
79:E:54:LYS:HD3	79:E:154:THR:HB	1.67	0.76
34:B5:40:A:H62	34:B5:467:G:H21	1.34	0.76
38:A1:2465:G:N1	38:A1:2491:A:C6	2.55	0.75
34:B5:1679:G:H21	34:B5:1722:A:N6	1.84	0.74
37:AC:3:ARG:HH21	37:AC:22:LEU:HB3	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1237:G:H1	38:A1:1251:A:H61	1.36	0.73
34:B5:900:A:H3'	34:B5:901:G:H21	1.54	0.73
80:DC:385:MET:HE1	80:DC:465:LYS:HA	1.70	0.73
79:E:14:LYS:HD3	79:E:17:LEU:HD21	1.71	0.72
81:V:129:GLU:HG3	81:V:131:GLY:H	1.55	0.72
23:BQ:54:LEU:HD12	23:BQ:55:VAL:HG13	1.71	0.72
80:DC:568:GLU:HA	80:DC:592:PRO:HG3	1.70	0.72
15:BY:20:ARG:HD3	15:BY:74:LEU:HD11	1.70	0.72
80:DC:110:ASP:HB3	80:DC:537:HIS:HB2	1.72	0.72
31:Bg:239:GLU:HB3	31:Bg:257:ALA:HB2	1.71	0.71
2:BB:60:ALA:O	2:BB:64:ARG:NH1	2.23	0.71
7:BI:87:ASN:HB3	7:BI:90:LEU:HD23	1.73	0.71
55:AS:13:ARG:HE	55:AS:51:VAL:HG12	1.55	0.71
4:BE:179:LYS:HG2	4:BE:230:GLU:HA	1.72	0.71
25:BS:14:ILE:HD11	25:BS:21:ASN:HB2	1.72	0.71
29:Bc:11:LYS:HE2	29:Bc:51:ASN:HA	1.73	0.71
19:BD:28:GLU:OE1	21:BK:58:GLN:NE2	2.24	0.71
26:BT:7:ARG:NH1	26:BT:67:MET:SD	2.65	0.70
79:E:45:ARG:NH2	82:EC:6815:U:O2'	2.24	0.70
18:Be:14:VAL:HA	18:Be:17:GLN:HE21	1.55	0.70
31:Bg:176:LYS:HE3	31:Bg:196:ASN:HA	1.72	0.70
38:A1:2219:A:H2'	38:A1:2220:A2M:H8	1.74	0.70
38:A1:2700:G:H5''	56:AT:17:ARG:HG2	1.74	0.70
81:V:24:SER:HB2	81:V:89:THR:O	1.91	0.70
3:BC:225:LEU:HB2	12:BV:23:ILE:HD11	1.74	0.69
34:B5:1291:G:H1	34:B5:1324:G:H22	1.39	0.69
38:A1:1260:A:N6	81:V:38:MET:SD	2.64	0.69
50:AN:183:THR:HG22	50:AN:187:ARG:HB3	1.74	0.69
7:BI:153:GLU:HB2	7:BI:156:VAL:HG12	1.73	0.69
8:BJ:126:ARG:HD3	18:Be:33:ARG:HE	1.56	0.69
25:BS:41:ARG:HG2	25:BS:85:PHE:HZ	1.58	0.69
38:A1:1243:G:N2	38:A1:1270:A:O2'	2.25	0.69
31:Bg:18:GLY:HA3	31:Bg:38:ARG:HB2	1.74	0.69
38:A1:2465:G:N1	38:A1:2491:A:N6	2.41	0.69
2:BB:150:VAL:HG22	34:B5:1067:C:H5''	1.74	0.69
10:BN:104:ARG:NH2	34:B5:951:A:OP1	2.26	0.69
13:BW:15:ASN:ND2	13:BW:72:CYS:O	2.26	0.68
4:BE:65:LEU:HD12	4:BE:78:THR:HA	1.74	0.68
38:A1:2738:A:O2'	64:Ab:41:ARG:NH2	2.26	0.68
58:AV:81:GLN:O	58:AV:98:ASN:ND2	2.26	0.68
35:AA:21:ARG:HD3	38:A1:824:C:H5''	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:DC:360:PRO:HB2	80:DC:363:ASP:HB2	1.75	0.68
34:B5:1339:C:O2'	34:B5:1341:A:N7	2.25	0.68
20:BF:80:LYS:HB2	20:BF:83:ARG:HG3	1.75	0.68
21:BK:22:VAL:HG12	21:BK:65:TYR:HA	1.76	0.68
31:Bg:211:ILE:HB	31:Bg:223:TRP:HB2	1.74	0.68
33:BM:42:ALA:HB1	33:BM:47:GLU:HG3	1.75	0.68
34:B5:992:A:O2'	34:B5:1785:U:O2	2.12	0.68
4:BE:145:ARG:NH1	4:BE:146:THR:O	2.27	0.68
38:A1:266:A:H2'	71:Ai:30:LYS:HE3	1.73	0.68
4:BE:18:TRP:O	4:BE:51:ARG:NH1	2.26	0.68
52:AP:58:ILE:HD12	52:AP:84:PRO:HD2	1.76	0.68
15:BY:118:ILE:HG23	15:BY:125:LEU:HD21	1.76	0.67
40:A4:71:A:OP2	61:AY:51:ARG:NH1	2.26	0.67
34:B5:126:A:N6	34:B5:291:G:N2	2.30	0.67
2:BB:132:ASP:HB2	2:BB:221:PRO:HB3	1.75	0.67
4:BE:130:GLN:NE2	34:B5:251:A:O2'	2.28	0.67
62:AZ:88:ASP:HB3	62:AZ:121:ARG:HH22	1.59	0.67
23:BQ:35:PRO:HG2	23:BQ:38:LEU:HD13	1.74	0.67
38:A1:2261:G:O2'	38:A1:2263:C:N4	2.28	0.67
6:BH:139:ARG:HB2	6:BH:151:LYS:HB3	1.75	0.67
12:BV:74:GLN:HE21	12:BV:83:TRP:H	1.41	0.67
26:BT:133:ASP:OD2	34:B5:1359:C:O2'	2.13	0.67
81:V:100:ILE:HB	81:V:185:LEU:HD23	1.75	0.67
23:BQ:136:SER:HB3	34:B5:1586:A:H5''	1.77	0.67
7:BI:104:ILE:HG13	7:BI:105:ASP:H	1.60	0.66
34:B5:871:G:H2'	34:B5:872:G:C8	2.30	0.66
38:A1:2786:G:N2	63:Aa:58:MET:SD	2.66	0.66
2:BB:111:ARG:NH2	34:B5:930:A:N3	2.43	0.66
55:AS:22:PRO:O	56:AT:146:ASN:ND2	2.27	0.66
4:BE:112:HIS:NE2	4:BE:237:SER:O	2.28	0.66
37:AC:211:GLU:OE1	37:AC:213:ASN:ND2	2.29	0.66
82:EC:6922:G:H1	82:EC:6931:U:H3	1.44	0.66
38:A1:1448:U:H2'	38:A1:1449:A2M:H8	1.78	0.66
38:A1:3268:A:OP1	42:AE:46:ARG:NH2	2.28	0.66
56:AT:17:ARG:NH1	56:AT:47:SER:OG	2.28	0.66
65:Ac:17:VAL:HG11	65:Ac:92:ILE:HD12	1.77	0.66
3:BC:201:ASN:OD1	34:B5:607:G:O2'	2.14	0.66
23:BQ:142:TYR:O	34:B5:1195:C:N4	2.28	0.66
34:B5:1213:G:N2	34:B5:1450:U:O2	2.24	0.66
55:AS:60:SER:OG	55:AS:62:ASN:ND2	2.29	0.66
80:DC:71:LYS:HD2	80:DC:387:PRO:HD2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1656:U:HO2'	38:A1:2292:U:HO2'	1.43	0.65
34:B5:1588:G:H1	34:B5:1608:U:H3	1.42	0.65
38:A1:1656:A:OP2	69:Ag:37:LYS:NZ	2.29	0.65
80:DC:649:GLN:HB2	80:DC:689:LEU:HA	1.77	0.65
5:BG:180:THR:HG23	5:BG:183:ARG:H	1.61	0.65
34:B5:1585:U:H3	34:B5:1611:A:H2	1.42	0.65
34:B5:1640:C:N4	82:EC:6952:U:OP1	2.26	0.65
35:AA:37:ARG:NH1	38:A1:2526:C:OP1	2.29	0.65
42:AE:76:LEU:HD21	42:AE:141:VAL:HG11	1.78	0.65
45:AH:186:PHE:HB2	45:AH:189:GLU:HB2	1.77	0.65
8:BJ:108:ARG:NH2	8:BJ:110:GLN:OE1	2.30	0.65
36:AB:290:ASP:O	36:AB:293:ASN:ND2	2.29	0.65
2:BB:214:LYS:NZ	34:B5:886:U:OP1	2.30	0.65
73:Ak:5:ILE:HD12	73:Ak:10:GLN:HE22	1.62	0.65
36:AB:240:ARG:NH2	38:A1:1907:C:O2	2.27	0.65
38:A1:845:G:H21	38:A1:848:A:H2	1.45	0.65
14:BX:75:GLN:HE21	14:BX:80:GLY:HA2	1.62	0.65
34:B5:361:C:N4	34:B5:379:U:OP1	2.30	0.65
36:AB:110:LEU:HB2	36:AB:115:LYS:HE3	1.78	0.65
38:A1:283:G:OP2	77:Ao:45:ARG:NH1	2.30	0.65
38:A1:2467:G:OP1	79:E:60:ARG:NH2	2.30	0.65
39:A3:64:A:N7	46:AI:209:ASN:ND2	2.44	0.65
79:E:73:ASP:HA	79:E:76:ARG:HG2	1.79	0.65
38:A1:249:U:H1'	38:A1:251:G:H2'	1.79	0.64
26:BT:25:GLN:HE22	26:BT:27:LYS:HD3	1.63	0.64
31:Bg:59:ARG:HD3	31:Bg:96:THR:HA	1.79	0.64
38:A1:68:C:OP2	38:A1:301:G:N2	2.30	0.64
61:AY:81:GLN:OE1	61:AY:98:ASN:ND2	2.30	0.64
79:E:67:ILE:HG12	79:E:111:ILE:HD11	1.78	0.64
3:BC:39:THR:HG23	3:BC:42:GLY:H	1.61	0.64
20:BF:63:GLN:HB3	20:BF:88:PRO:HA	1.78	0.64
26:BT:130:ARG:NH1	34:B5:1359:C:OP1	2.31	0.64
34:B5:162:A:H3'	34:B5:163:G:H21	1.62	0.64
19:BD:161:GLY:HA3	34:B5:1331:A:H61	1.61	0.64
31:Bg:89:LEU:HB2	31:Bg:103:PHE:HB2	1.80	0.64
38:A1:655:C:H2'	38:A1:656:A:H8	1.61	0.64
80:DC:28:VAL:HG22	80:DC:108:HIS:HA	1.78	0.64
3:BC:143:TYR:HB3	3:BC:145:GLY:HA3	1.78	0.64
22:BP:18:ARG:NH1	25:BS:90:ASN:O	2.31	0.64
80:DC:658:GLU:OE2	80:DC:700:ARG:NH1	2.28	0.64
34:B5:480:G:O6	34:B5:508:U:O2	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2767:U:OP1	77:Ao:34:SER:OG	2.15	0.64
26:BT:89:ARG:NH1	34:B5:1562:G:OP1	2.31	0.64
27:BU:82:TYR:HB3	30:Bd:52:PHE:HB3	1.79	0.64
28:BZ:57:TYR:OH	82:EC:6866:C:N4	2.31	0.64
13:BW:118:ARG:NH1	34:B5:686:C:O3'	2.31	0.64
18:Be:26:LYS:NZ	34:B5:588:U:OP2	2.31	0.64
34:B5:702:G:O6	34:B5:737:A:N6	2.31	0.64
61:AY:54:ASP:HB2	61:AY:70:ILE:HD12	1.80	0.64
82:EC:6934:U:H5''	82:EC:6935:G:H4'	1.80	0.64
4:BE:187:ARG:NH2	34:B5:791:A:OP2	2.30	0.63
19:BD:72:LEU:HD12	21:BK:65:TYR:HD2	1.63	0.63
33:BM:76:GLU:O	33:BM:80:ASN:ND2	2.31	0.63
34:B5:65:A:H2	34:B5:84:A:H62	1.46	0.63
34:B5:1280:4AC:H2'	34:B5:1281:G:H8	1.62	0.63
34:B5:1594:G:OP2	34:B5:1596:C:N4	2.30	0.63
8:BJ:30:LEU:HD13	8:BJ:105:LEU:HD11	1.80	0.63
34:B5:95:G:HO2'	34:B5:460:A:HO2'	1.43	0.63
38:A1:1132:C:H2'	38:A1:1133:A2M:H8	1.80	0.63
47:AJ:49:LYS:HG2	47:AJ:64:LYS:HG2	1.80	0.63
21:BK:81:ASN:ND2	33:BM:37:VAL:O	2.30	0.63
38:A1:2836:C:H5	38:A1:2852:C:H42	1.44	0.63
38:A1:831:G:O2'	38:A1:1864:A:N3	2.29	0.63
38:A1:1805:C:H2'	38:A1:1806:A:H8	1.64	0.63
38:A1:3042:U:OP2	38:A1:3092:C:N4	2.30	0.63
80:DC:470:THR:HG22	80:DC:472:SER:H	1.63	0.63
6:BH:44:LYS:HE2	6:BH:63:PRO:HB3	1.81	0.63
26:BT:60:SER:HG	26:BT:80:TYR:HH	1.41	0.63
58:AV:14:SER:O	58:AV:81:GLN:NE2	2.32	0.63
81:V:25:LEU:HB3	81:V:191:TYR:HB3	1.80	0.63
8:BJ:59:LEU:HD12	8:BJ:69:ARG:HA	1.79	0.63
23:BQ:94:GLN:O	31:Bg:59:ARG:NH2	2.31	0.63
42:AE:51:ARG:O	42:AE:72:ASN:ND2	2.32	0.63
51:AO:61[A]:ALA:HA	51:AO:70[A]:PRO:HD2	1.81	0.63
38:A1:1237:G:H1	38:A1:1251:A:N6	1.96	0.63
71:Ai:70:ARG:HD2	71:Ai:84:LYS:HG2	1.81	0.63
80:DC:243:ARG:O	80:DC:248:SER:OG	2.16	0.63
82:EC:6794:C:N4	82:EC:6940:U:O2'	2.32	0.63
38:A1:1351:U:H1'	38:A1:1355:A:H62	1.64	0.62
38:A1:2485:A:OP1	79:E:101:LYS:NZ	2.32	0.62
19:BD:135:GLU:HB3	19:BD:187:LYS:HB3	1.81	0.62
37:AC:308:LYS:NZ	38:A1:609:G:N7	2.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BD:168:ILE:HD13	19:BD:189:MET:HB3	1.80	0.62
36:AB:292:ALA:HB2	36:AB:302:LYS:HD2	1.81	0.62
38:A1:1627:U:N3	38:A1:1817:G:O6	2.33	0.62
15:BY:32:ARG:HH11	15:BY:35:VAL:HG21	1.64	0.62
19:BD:126:VAL:HG21	19:BD:134:CYS:HB2	1.81	0.62
27:BU:53:LYS:HD2	34:B5:1345:A:H5'	1.81	0.62
54:AR:175:GLN:HA	54:AR:179:GLU:HB2	1.81	0.62
55:AS:6:GLU:OE2	55:AS:28:ARG:NH1	2.33	0.62
62:AZ:81:LEU:HD11	69:Ag:90:ILE:HD13	1.82	0.62
29:Bc:64:ARG:HG3	29:Bc:65:ARG:H	1.64	0.62
38:A1:1677:G:N7	57:AU:74:LYS:NZ	2.46	0.62
42:AE:171:PRO:HA	42:AE:174:LEU:HB2	1.80	0.62
5:BG:186:ARG:NH2	34:B5:269:G:OP2	2.31	0.62
34:B5:1226:A:N6	34:B5:1230:A:N3	2.46	0.62
38:A1:184:U:H3	38:A1:232:G:H1	1.48	0.62
38:A1:799:G:O2'	48:AL:18:TRP:NE1	2.31	0.62
80:DC:14:ASP:HA	80:DC:449:PRO:HG3	1.81	0.62
6:BH:150:GLN:HB3	6:BH:181:ILE:HG22	1.81	0.62
15:BY:83:LYS:HZ2	15:BY:91:LEU:HD22	1.64	0.62
20:BF:100:ASN:ND2	20:BF:180:ARG:HH11	1.98	0.62
20:BF:219:ARG:HA	20:BF:222:LYS:HE2	1.82	0.62
34:B5:647:G:N2	34:B5:648:G:O6	2.33	0.62
38:A1:1592:G:OP1	69:Ag:58:ARG:NH2	2.33	0.62
82:EC:6892:U:O2'	82:EC:6943:A:N6	2.32	0.62
13:BW:22:LYS:HA	17:Bb:3:LEU:HG	1.82	0.62
19:BD:40:ARG:HB2	19:BD:47:GLU:HG3	1.82	0.62
28:BZ:97:LYS:NZ	34:B5:1474:G:N7	2.48	0.62
34:B5:1697:G:H1	34:B5:1704:U:H3	1.48	0.62
38:A1:1757:A:OP1	57:AU:94:ARG:NH2	2.33	0.62
38:A1:2466:G:H4'	79:E:60:ARG:HH12	1.63	0.62
77:Ao:103:ALA:HB1	77:Ao:104:LEU:HD22	1.82	0.62
9:BL:72:THR:O	9:BL:88:ARG:NH1	2.33	0.61
19:BD:60:GLY:HA3	19:BD:64:ARG:HB2	1.81	0.61
38:A1:2467:G:OP1	79:E:62:ASN:ND2	2.27	0.61
77:Ao:2:VAL:N	77:Ao:90:HIS:O	2.33	0.61
81:V:63:ILE:HD11	81:V:73:PHE:HB3	1.81	0.61
4:BE:23:LEU:HD11	8:BJ:3:ARG:HH21	1.65	0.61
8:BJ:139:GLN:NE2	15:BY:64:PHE:O	2.30	0.61
8:BJ:90:LYS:HB2	8:BJ:95:TYR:HD2	1.66	0.61
11:BO:114:ARG:HH22	16:Ba:59:TYR:HB2	1.64	0.61
20:BF:225:ARG:HD2	29:Bc:61:ARG:HH21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:A3:31:U:O2'	41:AD:218:ARG:NH2	2.32	0.61
62:AZ:5:LEU:HD11	65:Ac:35:ARG:HD2	1.82	0.61
81:V:55:LYS:HE3	81:V:83:ASN:HA	1.82	0.61
13:BW:115:GLU:OE1	13:BW:118:ARG:NH2	2.34	0.61
34:B5:1591:C:H2'	34:B5:1592:A:H8	1.64	0.61
8:BJ:132:ARG:NH2	34:B5:532:U:OP1	2.34	0.61
80:DC:271:ARG:HG3	80:DC:274:ASN:H	1.66	0.61
1:BA:79:ARG:HH12	1:BA:164:ASN:HB3	1.65	0.61
7:BI:37:LYS:HB2	7:BI:59:ARG:HG3	1.81	0.61
31:Bg:243:LEU:HD22	31:Bg:252:LEU:HD11	1.83	0.61
80:DC:120:ARG:NH1	80:DC:479:LYS:O	2.34	0.61
3:BC:81:MET:HB2	3:BC:101:VAL:HG13	1.83	0.61
36:AB:19:ARG:NH2	38:A1:3045:G:OP1	2.34	0.61
7:BI:159:GLN:HE22	7:BI:189:LEU:HD11	1.65	0.61
20:BF:63:GLN:HE22	20:BF:66:GLN:H	1.49	0.61
34:B5:1370:U:H3	34:B5:1374:C:H41	1.49	0.61
80:DC:698:ILE:HG12	80:DC:699:DDE:HAB3	1.81	0.61
8:BJ:41:GLU:OE1	8:BJ:44:ARG:NH2	2.34	0.61
14:BX:144:ARG:HH12	80:DC:417:ASN:HD21	1.49	0.61
19:BD:9:ARG:NH2	34:B5:1489:U:OP2	2.34	0.60
34:B5:472:U:H2'	34:B5:473:A:H8	1.65	0.60
2:BB:194:ASN:HD22	2:BB:210:ILE:HG22	1.66	0.60
7:BI:25:ARG:HH21	34:B5:400:A:H5'	1.66	0.60
38:A1:2842:U:OP1	38:A1:2844:C:N4	2.35	0.60
45:AH:90:MET:HE2	45:AH:179:ILE:HG22	1.83	0.60
80:DC:409:GLN:NE2	80:DC:410:LYS:O	2.35	0.60
27:BU:24:ILE:HD11	27:BU:114:VAL:HB	1.82	0.60
34:B5:766:U:H3	34:B5:770:A:N6	1.88	0.60
36:AB:173:GLN:NE2	38:A1:3313:U:O5'	2.28	0.60
20:BF:122:ASN:OD1	20:BF:123:VAL:N	2.34	0.60
20:BF:142:PRO:HB3	20:BF:217:LEU:HD11	1.82	0.60
38:A1:2438:A:H2'	38:A1:2439:A:H8	1.65	0.60
38:A1:2768:U:H2'	38:A1:2769:A:H8	1.66	0.60
50:AN:44:ARG:NH1	50:AN:120:TRP:O	2.34	0.60
1:BA:55:GLU:HG2	12:BV:79:LEU:HD12	1.81	0.60
35:AA:9:ARG:NH2	38:A1:912:G:OP2	2.34	0.60
38:A1:2568:C:O2'	38:A1:2569:A:O4'	2.18	0.60
43:AF:48:ASN:ND2	43:AF:182:ASP:OD2	2.34	0.60
45:AH:98:PRO:HG2	80:DC:168:GLN:HB2	1.83	0.60
53:AQ:122:ILE:HG23	53:AQ:126:GLN:HB2	1.84	0.60
60:AX:96:LYS:NZ	60:AX:107:VAL:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:209:ASN:HD21	34:B5:1298:U:H1'	1.64	0.60
5:BG:152:ASP:OD1	5:BG:154:ARG:NH1	2.35	0.60
14:BX:88:PRO:O	14:BX:89:ASN:ND2	2.34	0.60
36:AB:85:VAL:HG22	36:AB:202:THR:HG22	1.82	0.60
38:A1:1348:U:OP1	53:AQ:39:ARG:NH1	2.34	0.60
38:A1:1389:G:OP1	67:Ae:104:ASN:ND2	2.30	0.60
51:AO:121[A]:PRO:HA	51:AO:124[A]:LEU:HD12	1.83	0.60
3:BC:53:ILE:HD12	3:BC:56:ILE:HD13	1.84	0.60
32:Bf:123:ASN:HB3	32:Bf:126:CYS:HB2	1.84	0.60
38:A1:1808:G:OP1	62:AZ:135:ARG:NH2	2.34	0.60
40:A4:103:G:OP2	40:A4:105:A:O2'	2.19	0.60
31:Bg:74:THR:HA	31:Bg:115:ILE:HD11	1.83	0.60
38:A1:1661:G:H2'	38:A1:1662:G:C8	2.37	0.60
9:BL:101:GLU:HG3	14:BX:13:ARG:HB2	1.83	0.60
32:Bf:87:THR:O	34:B5:1445:G:N2	2.34	0.60
34:B5:71:A:N6	34:B5:72:A:N3	2.50	0.60
34:B5:973:A:H2'	34:B5:974:A2M:H8	1.84	0.60
34:B5:1229:G:N2	34:B5:1255:G:N3	2.50	0.60
45:AH:57:VAL:HG23	45:AH:68:LEU:HD13	1.82	0.60
46:AI:30:LYS:HG3	46:AI:63:GLU:HG3	1.83	0.60
68:Af:14:LEU:HD11	68:Af:31:LYS:HB2	1.84	0.60
7:BI:5:ARG:NH2	34:B5:334:G:O6	2.35	0.59
20:BF:112:ARG:HH22	23:BQ:42:GLU:HB2	1.66	0.59
30:Bd:10:HIS:NE2	34:B5:1554:U:O4	2.34	0.59
37:AC:156:LEU:HD12	37:AC:159:ILE:HD12	1.84	0.59
38:A1:2516:U:OP1	50:AN:31:ARG:NH1	2.35	0.59
70:Ah:83:LYS:O	72:Aj:73:ARG:NH2	2.35	0.59
31:Bg:222:LEU:HB3	31:Bg:231:MET:HE2	1.84	0.59
32:Bf:132:LEU:HD22	32:Bf:141:CYS:HA	1.84	0.59
38:A1:3153:U:H5	38:A1:3293:U:H3	1.50	0.59
8:BJ:17:ARG:NH2	34:B5:4:C:O2'	2.35	0.59
28:BZ:90:LYS:NZ	28:BZ:103:ARG:O	2.34	0.59
31:Bg:122:ILE:HB	31:Bg:134:TRP:HB2	1.84	0.59
34:B5:187:G:H21	34:B5:198:A:H62	1.49	0.59
34:B5:947:U:H2'	34:B5:948:G:H8	1.67	0.59
48:AL:76:THR:OG1	48:AL:103:ASN:ND2	2.35	0.59
80:DC:653:VAL:HG13	80:DC:656:LEU:HB2	1.83	0.59
2:BB:121:ILE:HD11	2:BB:161:ILE:HD12	1.85	0.59
6:BH:26:GLU:OE2	6:BH:84:LYS:NZ	2.35	0.59
16:Ba:46:GLU:HG3	16:Ba:48:ALA:H	1.66	0.59
70:Ah:38:ARG:HD2	70:Ah:41:LEU:HD21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Bb:17:ARG:NH2	34:B5:1069:A:O2'	2.35	0.59
23:BQ:83:GLN:NE2	23:BQ:115:THR:O	2.36	0.59
34:B5:653:C:OP2	34:B5:682:C:N4	2.33	0.59
35:AA:60:LYS:HZ3	35:AA:75:ILE:HG12	1.67	0.59
38:A1:215:G:OP1	61:AY:12:ARG:NH1	2.32	0.59
38:A1:952:A:OP1	64:Ab:18:ARG:NH2	2.36	0.59
4:BE:100:ARG:HB2	4:BE:114:ILE:HD13	1.85	0.59
7:BI:62:THR:HG22	7:BI:77:ARG:HG2	1.84	0.59
20:BF:218:GLU:HG3	20:BF:222:LYS:HZ3	1.68	0.59
38:A1:1021:G:N2	38:A1:1032:C:OP2	2.35	0.59
40:A4:29:U:H5''	48:AL:27:ASP:HB3	1.85	0.59
2:BB:175:GLU:OE1	2:BB:187:LYS:NZ	2.31	0.59
9:BL:66:ILE:O	34:B5:246:G:N2	2.32	0.59
34:B5:1470:C:H3'	34:B5:1573:A:H62	1.68	0.59
63:Aa:104:THR:HG21	63:Aa:112:ILE:HD11	1.83	0.59
7:BI:152:ILE:HG13	7:BI:153:GLU:H	1.67	0.59
13:BW:56:HIS:O	34:B5:861:U:O2'	2.19	0.59
34:B5:628:G:H21	34:B5:971:A:H62	1.49	0.59
34:B5:1284:C:H4'	34:B5:1285:U:H5'	1.85	0.59
38:A1:411:U:H2'	38:A1:412:G:H8	1.66	0.59
38:A1:2185:G:O2'	38:A1:2314:U:OP2	2.16	0.59
9:BL:129:ARG:HD3	34:B5:115:G:H5'	1.84	0.59
38:A1:316:U:O2'	71:Ai:30:LYS:NZ	2.31	0.59
39:A3:6:C:O2'	41:AD:50:ARG:NH2	2.36	0.59
51:AO:27[A]:LEU:HD21	51:AO:102[A]:LEU:HB2	1.84	0.59
4:BE:77:ARG:NH1	34:B5:122:U:OP1	2.36	0.58
21:BK:54:TYR:OH	33:BM:108:ARG:NH1	2.35	0.58
34:B5:1202:A:H1'	34:B5:1207:C:H42	1.68	0.58
36:AB:218:ILE:HG12	36:AB:276:THR:HG22	1.84	0.58
38:A1:1729:A:O4'	65:Ac:52:ARG:NH1	2.35	0.58
38:A1:2207:A:H4'	38:A1:2208:A:H5'	1.84	0.58
38:A1:2464:U:OP1	38:A1:2485:A:O2'	2.18	0.58
38:A1:2895:G:O2'	75:Am:100:TYR:O	2.20	0.58
5:BG:216:LEU:HD13	5:BG:219:ARG:HH21	1.67	0.58
34:B5:852:C:OP2	54:AR:170:ARG:NH2	2.36	0.58
38:A1:718:G:OP1	63:Aa:117:ARG:NH2	2.36	0.58
81:V:139:LEU:HD11	81:V:169:GLU:HA	1.86	0.58
16:Ba:18:VAL:HG23	16:Ba:19:LYS:H	1.67	0.58
17:Bb:64:CYS:HB3	17:Bb:73:LEU:HD23	1.85	0.58
26:BT:38:LYS:NZ	34:B5:1564:U:OP1	2.35	0.58
38:A1:664:U:H2'	38:A1:665:A:C8	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AH:90:MET:HG2	45:AH:181:VAL:HA	1.86	0.58
46:AI:72:ALA:HB2	46:AI:155:ALA:HB2	1.84	0.58
80:DC:108:HIS:O	80:DC:138:GLN:NE2	2.35	0.58
1:BA:140:ASN:HD22	3:BC:62:PRO:HD3	1.68	0.58
38:A1:1477:A:OP1	38:A1:3075:G:O2'	2.19	0.58
38:A1:2193:U:H5''	38:A1:2194:G:H5'	1.84	0.58
42:AE:96:VAL:HG21	42:AE:141:VAL:HG23	1.86	0.58
80:DC:196:VAL:HG23	80:DC:197:LEU:HD12	1.86	0.58
81:V:26:PHE:HZ	81:V:187:VAL:HG22	1.69	0.58
8:BJ:168:ARG:NH1	34:B5:513:U:OP1	2.37	0.58
15:BY:36:SER:OG	15:BY:39:GLU:OE1	2.20	0.58
34:B5:161:U:H2'	34:B5:162:A:H8	1.69	0.58
37:AC:48:GLN:NE2	38:A1:336:A:O2'	2.36	0.58
37:AC:344:ALA:HB2	38:A1:516:A:H5''	1.85	0.58
60:AX:50:ALA:HB1	70:Ah:66:VAL:HG11	1.84	0.58
10:BN:11:ILE:HG13	10:BN:12:SER:H	1.69	0.58
31:Bg:131:ILE:HD12	31:Bg:144:LEU:HD22	1.85	0.58
34:B5:1575:G7M:H2'	34:B5:1576:A:C8	2.39	0.58
52:AP:33:ALA:HB1	52:AP:117:ILE:HG12	1.86	0.58
55:AS:77:VAL:HG11	55:AS:106:LEU:HD22	1.84	0.58
82:EC:6777:C:H5'	82:EC:6778:C:H2'	1.84	0.58
4:BE:157:ASN:HD22	4:BE:222:LEU:HD21	1.69	0.58
5:BG:92:ARG:O	34:B5:405:C:O2'	2.20	0.58
19:BD:53:THR:O	19:BD:90:ARG:NH1	2.37	0.58
19:BD:75:LYS:HZ2	21:BK:22:VAL:HG13	1.68	0.58
38:A1:417:A:H2'	38:A1:418:A:C8	2.39	0.58
80:DC:653:VAL:HG21	80:DC:691:VAL:HG23	1.85	0.58
34:B5:591:A:H2'	34:B5:592:A:C8	2.39	0.58
38:A1:2160:G:H2'	38:A1:2161:G:H8	1.69	0.58
58:AV:21:ALA:HB3	58:AV:36:ILE:HD12	1.86	0.58
14:BX:48:HIS:HB3	14:BX:103:LEU:HD11	1.84	0.58
38:A1:353:G:O6	72:Aj:55:ARG:NH2	2.36	0.58
43:AF:163:LEU:HD13	43:AF:169:ILE:HD11	1.84	0.58
80:DC:353:ALA:HA	80:DC:356:LEU:HG	1.86	0.58
7:BI:149:SER:O	9:BL:24:LYS:NZ	2.31	0.57
34:B5:129:U:O4'	34:B5:264:G:N1	2.37	0.57
38:A1:3092:C:O2'	38:A1:3094:A:OP2	2.18	0.57
65:Ac:30:THR:HG23	65:Ac:91:SER:HB3	1.86	0.57
80:DC:161:ASP:OD1	80:DC:162:ARG:N	2.37	0.57
1:BA:126:PRO:HG3	1:BA:147:THR:HG22	1.86	0.57
8:BJ:44:ARG:HG2	8:BJ:48:GLN:HE22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BX:121:ARG:NH2	34:B5:1135:U:OP2	2.38	0.57
38:A1:1390:A:N6	38:A1:1418:A:O2'	2.36	0.57
38:A1:3302:U:H3	38:A1:3312:U:H3	1.52	0.57
49:AM:60:LEU:HD13	55:AS:152:LEU:HD11	1.86	0.57
58:AV:104:ASN:OD1	58:AV:108:GLU:N	2.32	0.57
8:BJ:85:VAL:HG12	8:BJ:107:ARG:HG3	1.86	0.57
31:Bg:195:HIS:NE2	31:Bg:213:SER:OG	2.23	0.57
38:A1:126:U:OP1	50:AN:144:ARG:NH1	2.34	0.57
38:A1:1497:C:H2'	38:A1:1498:A:H8	1.69	0.57
34:B5:751:G:H2'	34:B5:752:A:H8	1.69	0.57
38:A1:1259:A:N3	38:A1:1280:C:O2'	2.33	0.57
38:A1:1277:C:H2'	38:A1:1278:A:H8	1.67	0.57
38:A1:1606:U:O4	69:Ag:9:ARG:NE	2.33	0.57
38:A1:2890:A:O2'	38:A1:2933:A:N3	2.34	0.57
19:BD:174:HIS:HE1	34:B5:1277:G:H21	1.51	0.57
35:AA:117:GLU:HG2	35:AA:124:GLY:H	1.70	0.57
38:A1:394:G:N1	38:A1:397:A:OP2	2.37	0.57
38:A1:3291:G:H2'	38:A1:3292:A:H8	1.70	0.57
47:AJ:77:GLU:OE2	47:AJ:166:LYS:NZ	2.38	0.57
11:BO:20:TYR:HB3	11:BO:27:PHE:HB2	1.87	0.57
31:Bg:68:VAL:HG12	31:Bg:84:SER:HB2	1.87	0.57
34:B5:509:G:H2'	34:B5:510:G:C8	2.39	0.57
38:A1:959:C:O2'	38:A1:2410:U:N3	2.38	0.57
38:A1:3234:A:H61	38:A1:3253:G:H1	1.52	0.57
46:AI:38:LYS:HD3	46:AI:83:ASP:HB2	1.86	0.57
47:AJ:101:ASN:HD22	47:AJ:131:MET:H	1.53	0.57
52:AP:111:LYS:HE2	52:AP:152:GLU:HB3	1.87	0.57
80:DC:2:VAL:N	80:DC:44:GLY:O	2.37	0.57
34:B5:1229:G:N2	34:B5:1255:G:O2'	2.30	0.57
38:A1:655:C:H2'	38:A1:656:A:C8	2.38	0.57
38:A1:3162:C:H2'	38:A1:3163:A:H8	1.70	0.57
41:AD:293:LEU:HD13	46:AI:210:ILE:HD13	1.87	0.57
49:AM:42:LYS:O	49:AM:59:ASN:ND2	2.38	0.57
11:BO:88:GLY:O	11:BO:92:LYS:NZ	2.37	0.57
34:B5:434:G:N2	34:B5:437:A:OP2	2.37	0.57
38:A1:3016:A:H2'	38:A1:3017:A:C8	2.40	0.57
38:A1:3280:U:O2'	38:A1:3281:U:O5'	2.22	0.57
8:BJ:176:ASN:ND2	34:B5:511:A:OP2	2.38	0.57
12:BV:38:LYS:HD2	12:BV:49:GLU:HB3	1.87	0.57
19:BD:217:ILE:O	31:Bg:196:ASN:ND2	2.37	0.57
25:BS:132:ARG:HE	25:BS:136:GLN:HB2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:396:G:N1	34:B5:399:A:OP2	2.37	0.57
34:B5:1171:A:H2'	34:B5:1172:G:C8	2.39	0.57
38:A1:1208:U:O2'	38:A1:3115:C:N4	2.37	0.57
38:A1:1221:A:OP2	81:V:64:ARG:NH2	2.37	0.57
40:A4:38:U:O2'	70:Ah:83:LYS:NZ	2.38	0.57
2:BB:21:VAL:HG13	2:BB:23:PRO:HD3	1.87	0.57
4:BE:127:LYS:HB2	4:BE:140:VAL:HG13	1.86	0.57
6:BH:140:VAL:HB	13:BW:52:TYR:HB3	1.87	0.57
9:BL:57:LYS:HG2	9:BL:131:ILE:HG23	1.86	0.57
15:BY:113:ASN:OD1	15:BY:116:LYS:NZ	2.36	0.57
34:B5:1380:U:O2'	34:B5:1516:A:N1	2.38	0.57
36:AB:160:VAL:HB	36:AB:183:LEU:HD21	1.87	0.57
39:A3:23:A:O2'	39:A3:121:U:O3'	2.23	0.57
69:Ag:41:ARG:NH2	69:Ag:51:LEU:O	2.38	0.57
11:BO:87:GLY:HA3	11:BO:120:PRO:HG2	1.87	0.56
12:BV:58:TYR:OH	12:BV:62:ARG:NH1	2.37	0.56
20:BF:189:THR:OG1	20:BF:192:GLU:OE1	2.22	0.56
24:BR:49:LYS:NZ	34:B5:1390:U:OP2	2.37	0.56
25:BS:16:ARG:HD2	25:BS:19:ASN:HA	1.87	0.56
34:B5:162:A:H2'	34:B5:163:G:H5'	1.87	0.56
80:DC:412:ARG:HG2	80:DC:428:ILE:HG22	1.88	0.56
80:DC:610:ASP:O	80:DC:615:ARG:NH2	2.38	0.56
6:BH:123:ASP:OD1	6:BH:138:LYS:NZ	2.38	0.56
38:A1:3322:A:H2'	38:A1:3323:A:C8	2.40	0.56
42:AE:175:LYS:O	49:AM:117:ARG:NH2	2.38	0.56
82:EC:6787:U:OP2	82:EC:6804:A:N6	2.38	0.56
7:BI:57:ALA:HB2	7:BI:177:GLY:HA2	1.87	0.56
10:BN:3:ARG:HB3	10:BN:6:SER:HB3	1.87	0.56
17:Bb:42:ASN:ND2	17:Bb:57:GLU:OE2	2.38	0.56
22:BP:43:ARG:NH2	34:B5:1553:G:N7	2.53	0.56
23:BQ:13:LYS:HG3	23:BQ:14:LYS:H	1.68	0.56
23:BQ:100:GLN:NE2	31:Bg:57:PRO:O	2.35	0.56
34:B5:850:A:H4'	54:AR:165:LYS:HG2	1.86	0.56
34:B5:1171:A:H2'	34:B5:1172:G:H8	1.70	0.56
35:AA:69:TYR:OH	38:A1:2557:A:OP1	2.19	0.56
38:A1:358:G:N2	38:A1:361:A:OP2	2.32	0.56
38:A1:1282:G:O2'	38:A1:1283:C:O4'	2.24	0.56
38:A1:2960:C:H2'	38:A1:2961:G:C8	2.41	0.56
40:A4:75:G:OP2	61:AY:74:TYR:OH	2.23	0.56
66:Ad:75:ILE:HG12	66:Ad:93:VAL:HG22	1.87	0.56
80:DC:39:LEU:HD11	80:DC:334:LEU:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BJ:119:ALA:O	8:BJ:124:HIS:ND1	2.29	0.56
2:BB:135:LEU:HB3	2:BB:217:LEU:HD13	1.87	0.56
3:BC:158:THR:HG21	3:BC:221:THR:HG22	1.88	0.56
10:BN:16:ILE:O	13:BW:57:ARG:NH2	2.33	0.56
26:BT:83:ALA:HB2	34:B5:1525:A:H4'	1.87	0.56
31:Bg:199:ILE:HA	31:Bg:215:GLY:HA2	1.88	0.56
32:Bf:93:HIS:N	34:B5:1247:U:OP1	2.32	0.56
34:B5:129:U:H5'	34:B5:264:G:H22	1.70	0.56
34:B5:1081:A:O2'	34:B5:1083:G:N7	2.39	0.56
80:DC:17:THR:O	80:DC:91:GLN:NE2	2.38	0.56
80:DC:335:LEU:HA	80:DC:338:ILE:HD12	1.87	0.56
1:BA:180:GLU:HA	1:BA:183:ARG:HB3	1.87	0.56
32:Bf:120:GLU:HG3	32:Bf:128:ALA:HA	1.87	0.56
34:B5:766:U:O4	34:B5:770:A:N7	2.38	0.56
35:AA:111:THR:HB	35:AA:136:ILE:HD13	1.88	0.56
35:AA:244:GLY:HA3	38:A1:2242:A:H5''	1.87	0.56
38:A1:2213:A:H2'	38:A1:2214:A:C8	2.40	0.56
52:AP:122:ALA:HB3	52:AP:143:PRO:HB2	1.88	0.56
79:E:194:LEU:O	79:E:197:ASN:ND2	2.38	0.56
2:BB:82:ARG:NH1	2:BB:191:GLU:OE2	2.39	0.56
36:AB:211:GLN:NE2	36:AB:283:TYR:O	2.38	0.56
38:A1:1114:U:OP1	63:Aa:23:GLY:N	2.35	0.56
10:BN:124:ARG:NH1	34:B5:628:G:OP1	2.34	0.56
25:BS:28:ILE:HD11	25:BS:54:LEU:HD13	1.88	0.56
25:BS:36:LYS:HB3	25:BS:102:ALA:HA	1.88	0.56
38:A1:2947:G:OP1	38:A1:2982:A:N6	2.37	0.56
10:BN:25:TRP:CD1	17:Bb:82:LYS:HZ2	2.24	0.56
31:Bg:16:HIS:NE2	31:Bg:35:SER:OG	2.26	0.56
31:Bg:69:GLN:NE2	31:Bg:111:MET:HB2	2.20	0.56
38:A1:3231:U:H2'	38:A1:3232:G:H8	1.71	0.56
78:Ap:46:THR:OG1	78:Ap:57:CYS:SG	2.62	0.56
11:BO:17:ALA:HB3	11:BO:81:VAL:HA	1.87	0.56
13:BW:57:ARG:HG2	34:B5:862:A:H4'	1.87	0.56
34:B5:395:U:H3	34:B5:399:A:H62	1.54	0.56
38:A1:966:U:OP1	63:Aa:44:ASN:ND2	2.39	0.56
48:AL:179:PHE:HD1	48:AL:182:ILE:HD11	1.71	0.56
63:Aa:56:VAL:HG12	63:Aa:57:GLY:H	1.70	0.56
31:Bg:10:ARG:HG3	31:Bg:314:GLN:HB2	1.88	0.55
33:BM:102:GLY:O	33:BM:104:GLY:N	2.38	0.55
34:B5:40:A:H62	34:B5:467:G:N2	2.01	0.55
34:B5:1280:4AC:H2'	34:B5:1281:G:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:A3:5:G:OP1	47:AJ:143:ARG:NH2	2.39	0.55
57:AU:42:LYS:HG2	57:AU:47:VAL:HG22	1.87	0.55
11:BO:47:LYS:NZ	11:BO:66:ASP:OD2	2.24	0.55
38:A1:1015:U:O2	38:A1:1035:G:O6	2.24	0.55
38:A1:1203:A:N3	38:A1:2855:U:O2'	2.37	0.55
38:A1:2213:A:H2'	38:A1:2214:A:H8	1.71	0.55
38:A1:2474:G:N2	38:A1:2475:G:O6	2.40	0.55
38:A1:2494:A:H5''	38:A1:2495:C:H6	1.69	0.55
41:AD:60:ILE:HB	41:AD:80:SER:HB2	1.89	0.55
50:AN:39:ALA:HB3	50:AN:61:ILE:HG22	1.89	0.55
53:AQ:92:ARG:HG2	63:Aa:76:ASP:HB2	1.88	0.55
80:DC:636:PHE:O	80:DC:642:GLY:N	2.35	0.55
2:BB:95:ASN:OD1	2:BB:96:LEU:N	2.40	0.55
4:BE:52:LEU:HD12	4:BE:54:TYR:H	1.71	0.55
20:BF:133:VAL:HG22	20:BF:198:LEU:HD13	1.88	0.55
24:BR:59:LYS:NZ	34:B5:1393:C:OP2	2.33	0.55
30:Bd:44:ARG:NH2	34:B5:1279:C:O3'	2.39	0.55
36:AB:212:ASN:HD21	36:AB:354:VAL:H	1.54	0.55
38:A1:1786:G:H2'	38:A1:1787:A:C8	2.41	0.55
47:AJ:26:SER:HA	47:AJ:30:LEU:HB2	1.87	0.55
52:AP:16:SER:HB3	52:AP:149:VAL:HG22	1.87	0.55
80:DC:338:ILE:HG23	80:DC:342:LEU:HD12	1.89	0.55
19:BD:23:GLU:OE2	19:BD:27:ARG:NE	2.36	0.55
20:BF:40:ILE:HG22	20:BF:67:PRO:HB2	1.87	0.55
38:A1:1310:G:HO2'	38:A1:2380:U:HO2'	1.54	0.55
38:A1:2116:G:OP1	38:A1:2118:C:N4	2.39	0.55
40:A4:58:G:O6	72:Aj:63:ARG:NH1	2.39	0.55
15:BY:61:ARG:NH2	34:B5:531:C:O2	2.39	0.55
20:BF:129:PRO:HA	20:BF:132:VAL:HG12	1.89	0.55
22:BP:122:THR:O	34:B5:1183:A:N6	2.39	0.55
32:Bf:83:LYS:NZ	34:B5:1211:A:OP2	2.37	0.55
38:A1:3291:G:H2'	38:A1:3292:A:C8	2.41	0.55
54:AR:178:ALA:HA	54:AR:181:ARG:HB3	1.89	0.55
10:BN:19:SER:OG	10:BN:21:ASN:O	2.24	0.55
14:BX:90:ASP:O	14:BX:136:TRP:NE1	2.38	0.55
34:B5:107:C:OP1	34:B5:383:G:O2'	2.23	0.55
38:A1:98:G:N7	48:AL:13:HIS:NE2	2.53	0.55
39:A3:44:C:H4'	41:AD:152:ARG:HE	1.70	0.55
50:AN:110:ALA:HB1	50:AN:113:LEU:HD12	1.88	0.55
53:AQ:62:VAL:HG13	53:AQ:66:ARG:HD2	1.87	0.55
14:BX:78:LYS:HB3	34:B5:434:G:H5'	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BP:47:ARG:NH2	34:B5:1555:A:OP2	2.39	0.55
27:BU:42:VAL:HG13	27:BU:52:LYS:HZ1	1.70	0.55
32:Bf:108:VAL:HA	33:BM:73:LYS:HZ3	1.70	0.55
34:B5:264:G:H5''	34:B5:265:A:H5'	1.88	0.55
43:AF:120:THR:HB	56:AT:132:PRO:HB2	1.89	0.55
45:AH:163:GLN:O	45:AH:166:ARG:NE	2.35	0.55
14:BX:144:ARG:HD2	80:DC:464:LEU:HD11	1.89	0.55
25:BS:143:ARG:NH1	34:B5:1462:G:OP2	2.39	0.55
34:B5:956:C:H2'	34:B5:957:G:H8	1.72	0.55
62:AZ:23:VAL:HG12	62:AZ:45:GLY:HA3	1.89	0.55
82:EC:6877:C:H1'	82:EC:6878:G:H21	1.72	0.55
5:BG:98:ARG:NH1	5:BG:99:GLY:O	2.40	0.55
6:BH:27:LEU:HD11	6:BH:80:GLU:HG3	1.88	0.55
20:BF:70:VAL:HG13	20:BF:72:HIS:H	1.72	0.55
20:BF:72:HIS:O	23:BQ:79:TYR:OH	2.24	0.55
38:A1:1717:U:H2'	38:A1:1718:G:C8	2.42	0.55
79:E:98:LYS:HD3	79:E:101:LYS:HD3	1.89	0.55
80:DC:155:VAL:HG23	80:DC:202:VAL:HG21	1.88	0.55
82:EC:6804:A:H4'	82:EC:6805:C:H5'	1.88	0.55
17:Bb:80:ARG:HD2	17:Bb:81:ARG:O	2.07	0.55
36:AB:128:LYS:NZ	38:A1:3294:A:OP1	2.40	0.55
38:A1:173:G:H3'	38:A1:174:C:H6	1.72	0.55
66:Ad:55:LEU:HB2	66:Ad:95:PRO:HD3	1.89	0.55
80:DC:722:PRO:HG2	80:DC:809:LEU:HD21	1.89	0.55
81:V:159:VAL:HG21	81:V:165:VAL:HG12	1.87	0.55
1:BA:52:LYS:HG2	12:BV:82:VAL:HA	1.89	0.54
8:BJ:24:LEU:HD22	34:B5:591:A:H5''	1.88	0.54
10:BN:47:PRO:HD2	10:BN:86:GLU:HG3	1.88	0.54
10:BN:132:VAL:HG13	10:BN:134:VAL:HG23	1.88	0.54
25:BS:65:GLU:HG2	25:BS:68:ARG:HH22	1.72	0.54
34:B5:554:C:N4	34:B5:571:G:O6	2.40	0.54
34:B5:833:U:H5'	34:B5:834:G:H5''	1.87	0.54
38:A1:1596:C:H2'	38:A1:1597:C:C6	2.43	0.54
38:A1:1618:G:O2'	40:A4:126:A:N1	2.40	0.54
38:A1:1799:A:H2'	38:A1:1800:A:C8	2.41	0.54
38:A1:3016:A:H2'	38:A1:3017:A:H8	1.72	0.54
62:AZ:41:ALA:HB2	62:AZ:77:TYR:HE1	1.72	0.54
80:DC:127:VAL:HG11	80:DC:143:LEU:HD13	1.89	0.54
30:Bd:13:ARG:HG3	30:Bd:14:TYR:HD1	1.72	0.54
38:A1:364:G:OP2	72:Aj:52:LYS:NZ	2.32	0.54
38:A1:412:G:OP1	52:AP:62:ARG:NH1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:595:G:OP1	43:AF:33:ARG:NH2	2.40	0.54
38:A1:2438:A:H2'	38:A1:2439:A:C8	2.42	0.54
1:BA:88:LYS:NZ	24:BR:82:ASP:OD1	2.35	0.54
4:BE:180:LEU:HA	4:BE:194:THR:HA	1.90	0.54
11:BO:18:ARG:NH1	11:BO:31:THR:OG1	2.40	0.54
12:BV:70:ASN:HB3	12:BV:83:TRP:HB2	1.87	0.54
16:Ba:45:VAL:HG23	16:Ba:46:GLU:H	1.71	0.54
20:BF:95:ASN:ND2	34:B5:1611:A:O3'	2.38	0.54
34:B5:51:A:H62	34:B5:429:G:H21	1.53	0.54
36:AB:28:ARG:NH2	38:A1:3140:G:N7	2.46	0.54
38:A1:760:G:O2'	38:A1:770:G:N2	2.36	0.54
51:AO:22[A]:VAL:HG11	51:AO:122[A]:GLN:NE2	2.22	0.54
11:BO:126:THR:HG21	34:B5:888:U:H1'	1.90	0.54
31:Bg:53:LYS:HE3	31:Bg:56:VAL:HG22	1.89	0.54
34:B5:843:U:H2'	34:B5:844:A:H8	1.71	0.54
34:B5:1182:U:H3	34:B5:1185:U:H5''	1.72	0.54
38:A1:2660:G:OP1	38:A1:2750:U:O2'	2.25	0.54
41:AD:211:LEU:HB3	41:AD:219:PHE:HB2	1.88	0.54
19:BD:72:LEU:HA	19:BD:75:LYS:HE2	1.88	0.54
29:Bc:44:VAL:HG11	29:Bc:48:VAL:HG21	1.88	0.54
34:B5:1466:G:O2'	34:B5:1602:C:OP1	2.25	0.54
34:B5:1593:A:H2'	34:B5:1594:G:H8	1.71	0.54
38:A1:627:U:H2'	38:A1:628:A:C8	2.43	0.54
38:A1:900:G:H1'	38:A1:1589:A:N6	2.22	0.54
1:BA:126:PRO:HG2	1:BA:151:SER:HB3	1.90	0.54
5:BG:66:GLY:HA2	34:B5:1681:A:H1'	1.90	0.54
21:BK:15:LEU:HD21	21:BK:68:LEU:HD21	1.90	0.54
38:A1:2404:A:N7	38:A1:2872:A:N6	2.55	0.54
38:A1:2507:C:H2'	38:A1:2508:U:C6	2.43	0.54
51:AO:125[A]:ARG:HG3	51:AO:129[A]:LEU:HD12	1.88	0.54
58:AV:23:MET:HE1	58:AV:78:VAL:HG22	1.90	0.54
82:EC:6852:U:H2'	82:EC:6853:G:C8	2.43	0.54
3:BC:45:VAL:HG21	3:BC:68:ILE:HG23	1.90	0.54
30:Bd:10:HIS:ND1	34:B5:1452:U:OP1	2.38	0.54
34:B5:705:U:H2'	34:B5:730:G:H1	1.72	0.54
55:AS:47:LYS:HE2	55:AS:122:HIS:HE1	1.73	0.54
1:BA:41:ARG:NH2	24:BR:103:ASP:OD2	2.40	0.54
2:BB:118:GLN:OE1	2:BB:208:GLN:NE2	2.40	0.54
9:BL:71:LEU:HD12	9:BL:88:ARG:CZ	2.37	0.54
9:BL:133:LYS:O	9:BL:136:ARG:NH1	2.40	0.54
20:BF:62:VAL:HB	20:BF:89:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BR:58:MET:O	24:BR:62:GLN:NE2	2.40	0.54
31:Bg:178:VAL:HB	31:Bg:192:PHE:HB2	1.89	0.54
34:B5:800:U:H2'	34:B5:801:G:H8	1.70	0.54
38:A1:728:G:H5''	53:AQ:43:PRO:HB2	1.90	0.54
38:A1:1156:C:OP2	43:AF:94:LYS:NZ	2.36	0.54
38:A1:1282:G:O2'	38:A1:1283:C:O5'	2.19	0.54
40:A4:8:C:H2'	40:A4:9:A:C8	2.42	0.54
47:AJ:83:GLY:HA3	47:AJ:127:PHE:HE2	1.72	0.54
1:BA:92:HIS:HB3	1:BA:182:LEU:HD21	1.89	0.54
5:BG:94:ARG:NH2	34:B5:406:U:O2'	2.34	0.54
9:BL:72:THR:H	9:BL:88:ARG:HH12	1.56	0.54
34:B5:956:C:OP1	34:B5:1072:C:O2'	2.25	0.54
34:B5:1504:G:N3	34:B5:1563:C:O2'	2.39	0.54
38:A1:1119:C:H2'	38:A1:1120:A:H8	1.72	0.54
54:AR:175:GLN:HG2	54:AR:176:ARG:HD2	1.89	0.54
2:BB:70:LEU:HD12	2:BB:73:LEU:HD11	1.89	0.54
8:BJ:163:PRO:HD3	8:BJ:168:ARG:HH11	1.73	0.54
34:B5:953:G:H2'	34:B5:954:G:C8	2.43	0.54
34:B5:1356:U:H3	34:B5:1367:G:H1	1.56	0.54
38:A1:1222:G:OP2	81:V:57:THR:OG1	2.21	0.54
38:A1:2552:C:H2'	65:Ac:50:VAL:HG11	1.90	0.54
79:E:212:PRO:HG2	79:E:214:PHE:HE1	1.73	0.54
1:BA:81:PHE:HB3	1:BA:170:ILE:HG21	1.90	0.53
14:BX:88:PRO:HG3	14:BX:123:LYS:HB2	1.89	0.53
20:BF:42:LEU:HB3	20:BF:46:TRP:HB2	1.90	0.53
22:BP:98:ASN:ND2	22:BP:121:ILE:O	2.40	0.53
30:Bd:15:GLY:HA3	34:B5:1204:A:H61	1.72	0.53
36:AB:116:ARG:NH2	38:A1:3315:G:OP1	2.34	0.53
38:A1:1646:G:O2'	38:A1:1808:G:N2	2.34	0.53
45:AH:16:VAL:HG21	45:AH:79:ILE:HG23	1.90	0.53
2:BB:143:THR:O	2:BB:208:GLN:NE2	2.41	0.53
34:B5:884:A:H2'	34:B5:885:G:C8	2.43	0.53
35:AA:36:GLU:OE1	35:AA:163:ARG:NH1	2.40	0.53
37:AC:7:THR:OG1	37:AC:147:GLU:OE2	2.26	0.53
38:A1:806:A:N3	38:A1:2812:C:O2'	2.39	0.53
38:A1:1863:G:N1	38:A1:1866:C:OP2	2.31	0.53
38:A1:2541:U:H4'	38:A1:2542:U:H5'	1.90	0.53
61:AY:81:GLN:NE2	61:AY:96:PRO:HB2	2.24	0.53
80:DC:725:GLN:HA	80:DC:803:THR:HB	1.90	0.53
9:BL:103:ARG:NH1	34:B5:307:G:OP1	2.40	0.53
10:BN:3:ARG:NH1	34:B5:955:A:OP1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Bg:197:SER:HB2	31:Bg:216:LYS:HG2	1.90	0.53
38:A1:651:G:O2'	38:A1:1435:A:OP1	2.26	0.53
39:A3:56:A:H4'	47:AJ:152:HIS:HB2	1.89	0.53
42:AE:39:VAL:HB	42:AE:89:THR:HG23	1.89	0.53
59:AW:23:ARG:NH2	59:AW:25:ASP:OD2	2.40	0.53
63:Aa:24:LYS:O	63:Aa:26:ARG:HG2	2.08	0.53
80:DC:24:VAL:O	80:DC:105:SER:OG	2.26	0.53
80:DC:329:PRO:HG2	80:DC:332:ASP:HB2	1.90	0.53
80:DC:565:GLU:HB3	80:DC:717:PHE:CZ	2.44	0.53
2:BB:103:MET:HE3	2:BB:215:VAL:HG23	1.91	0.53
8:BJ:34:PHE:HZ	8:BJ:106:GLU:HG3	1.73	0.53
37:AC:126:ILE:O	37:AC:129:THR:OG1	2.26	0.53
37:AC:317:PRO:C	37:AC:319:LYS:H	2.17	0.53
38:A1:1846:C:OP1	38:A1:1849:C:N4	2.35	0.53
38:A1:3216:G:OP2	68:Af:2:ALA:N	2.40	0.53
49:AM:24:LYS:HE2	49:AM:25:LYS:HD2	1.90	0.53
80:DC:114:GLU:OE2	80:DC:384:LYS:NZ	2.37	0.53
82:EC:6794:C:H1'	82:EC:6890:A:H2	1.73	0.53
5:BG:160:ARG:NH1	34:B5:66:U:O2	2.39	0.53
20:BF:63:GLN:NE2	20:BF:66:GLN:OE1	2.41	0.53
38:A1:2767:U:O2'	77:Ao:30:ALA:O	2.24	0.53
40:A4:9:A:H2'	40:A4:10:A:C8	2.44	0.53
80:DC:387:PRO:HA	80:DC:394:PHE:CD1	2.44	0.53
81:V:142:PRO:HB2	81:V:153:VAL:HB	1.89	0.53
22:BP:118:GLU:HG2	25:BS:122:HIS:H	1.72	0.53
38:A1:40:A:H5''	63:Aa:35:ALA:HB1	1.89	0.53
38:A1:421:G:O6	38:A1:2383:C:O2'	2.23	0.53
38:A1:3121:U:H1'	38:A1:3122:A:H5''	1.90	0.53
55:AS:138:GLN:HA	55:AS:141:LYS:HB2	1.91	0.53
80:DC:563:TYR:HB2	80:DC:677:PHE:HZ	1.74	0.53
23:BQ:37:THR:O	23:BQ:45:ARG:NE	2.42	0.53
34:B5:1476:C:H2'	34:B5:1477:G:H8	1.74	0.53
38:A1:2648:G:OP1	46:AI:24:ARG:NH2	2.38	0.53
41:AD:226:TYR:HD1	41:AD:231:ILE:HB	1.74	0.53
80:DC:143:LEU:HD23	80:DC:188:ILE:HD11	1.89	0.53
80:DC:811:PRO:HB3	80:DC:820:LEU:HD12	1.90	0.53
16:Ba:32:LYS:O	16:Ba:37:LYS:NZ	2.41	0.53
31:Bg:248:ASN:HD21	31:Bg:249:ARG:HH11	1.55	0.53
34:B5:102:U:H3'	34:B5:360:A:H61	1.73	0.53
34:B5:1592:A:H2'	34:B5:1593:A:H8	1.73	0.53
42:AE:3:ALA:HB2	67:Ae:77:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:AE:39:VAL:O	42:AE:87:THR:OG1	2.21	0.53
73:Ak:5:ILE:HG21	73:Ak:11:PHE:HB2	1.88	0.53
2:BB:48:VAL:HG23	2:BB:49:ASN:H	1.72	0.53
16:Ba:45:VAL:HG11	16:Ba:53:LEU:HG	1.91	0.53
19:BD:93:ASP:HB3	19:BD:96:LEU:HB2	1.90	0.53
34:B5:497:G:OP1	34:B5:498:G:N2	2.41	0.53
34:B5:1477:G:H2'	34:B5:1478:G:C8	2.44	0.53
36:AB:220:VAL:O	36:AB:334:ARG:NH1	2.42	0.53
38:A1:1229:G:O2'	81:V:31:ASP:O	2.26	0.53
40:A4:41:A:H4'	72:Aj:59:THR:HG23	1.90	0.53
48:AL:59:ARG:HD2	48:AL:69:VAL:HG12	1.90	0.53
79:E:126:PRO:HA	82:EC:6773:G:H4'	1.90	0.53
81:V:61:ARG:HA	81:V:64:ARG:HG2	1.90	0.53
81:V:97:LYS:HE2	81:V:187:VAL:HG11	1.91	0.53
7:BI:11:ARG:NH2	34:B5:319:U:OP1	2.42	0.53
7:BI:78:ILE:HD11	7:BI:102:VAL:HG11	1.91	0.53
34:B5:477:A:H2'	34:B5:478:A:H8	1.74	0.53
35:AA:188:LYS:NZ	38:A1:1793:C:O2	2.42	0.53
38:A1:520:U:OP2	43:AF:70:LYS:NZ	2.38	0.53
38:A1:1241:U:N3	38:A1:1244:A:OP2	2.31	0.53
2:BB:88:VAL:HG21	2:BB:96:LEU:HD23	1.90	0.52
4:BE:87:MET:HE1	4:BE:123:LEU:H	1.74	0.52
23:BQ:99:GLU:OE2	31:Bg:59:ARG:NH2	2.42	0.52
34:B5:273:G:O6	34:B5:283:U:O2	2.28	0.52
38:A1:216:G:OP1	61:AY:16:ARG:NH1	2.42	0.52
80:DC:740:VAL:HG21	80:DC:766:PHE:CD2	2.43	0.52
1:BA:111:ILE:HD11	34:B5:1292:G:H21	1.72	0.52
31:Bg:259:GLY:HA3	31:Bg:275:ARG:HD3	1.91	0.52
34:B5:1477:G:H2'	34:B5:1478:G:H8	1.74	0.52
38:A1:2828:G:HO2'	46:AI:4:ARG:HH21	1.56	0.52
80:DC:27:HIS:HB3	80:DC:30:HIS:CD2	2.44	0.52
6:BH:49:ILE:HG13	6:BH:172:VAL:HG23	1.90	0.52
6:BH:113:PRO:HG2	6:BH:116:ARG:HD3	1.91	0.52
10:BN:35:GLU:HA	10:BN:38:VAL:HG22	1.91	0.52
34:B5:741:C:H4'	34:B5:742:U:H5'	1.91	0.52
36:AB:219:ALA:HB2	36:AB:336:VAL:HG23	1.89	0.52
41:AD:146:LEU:HD22	41:AD:163:LEU:HD13	1.90	0.52
54:AR:105:LEU:HD13	54:AR:135:LYS:HE3	1.90	0.52
82:EC:6842:U:H4'	82:EC:6843:U:H5''	1.91	0.52
1:BA:156:VAL:O	12:BV:65:SER:OG	2.27	0.52
9:BL:38:ALA:HB1	9:BL:66:ILE:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:488:G:N2	34:B5:500:C:OP1	2.41	0.52
34:B5:1553:G:N1	34:B5:1556:A:OP2	2.42	0.52
36:AB:259:HIS:NE2	38:A1:2366:C:OP1	2.38	0.52
38:A1:528:U:H2'	38:A1:529:A:C8	2.44	0.52
38:A1:1157:G:O2'	38:A1:1169:A:N3	2.38	0.52
38:A1:1634:G:N7	62:AZ:17:ARG:NH1	2.58	0.52
38:A1:2446:U:H3	38:A1:2500:A:H61	1.58	0.52
42:AE:51:ARG:HB3	42:AE:159:LEU:HD23	1.90	0.52
68:Af:67:MET:HE1	68:Af:90:PRO:HD3	1.91	0.52
80:DC:591:GLU:HG2	80:DC:685:ARG:HB3	1.91	0.52
82:EC:6804:A:O2'	82:EC:6808:G:N2	2.37	0.52
34:B5:343:C:H2'	34:B5:344:A:H8	1.75	0.52
34:B5:1220:C:H2'	34:B5:1221:A:H8	1.73	0.52
38:A1:1127:G:OP2	46:AI:98:ARG:NH2	2.38	0.52
1:BA:35:PRO:O	1:BA:52:LYS:NZ	2.35	0.52
13:BW:102:VAL:HB	13:BW:113:HIS:HB3	1.92	0.52
24:BR:5:ARG:HB2	24:BR:10:LYS:HE3	1.92	0.52
31:Bg:116:ASP:HB3	31:Bg:120:SER:HB3	1.91	0.52
34:B5:424:C:O2'	34:B5:426:G:OP1	2.22	0.52
38:A1:362:U:O4	72:Aj:24:ARG:NH2	2.42	0.52
38:A1:1669:C:H5'	69:Ag:30:LEU:HD21	1.90	0.52
38:A1:1751:G:H5'	73:Ak:26:LYS:HE2	1.92	0.52
38:A1:2219:A:H2'	38:A1:2220:A2M:C8	2.40	0.52
65:Ac:43:ILE:HG13	65:Ac:68:TYR:HB3	1.92	0.52
7:BI:146:ARG:NH2	34:B5:186:C:OP1	2.43	0.52
30:Bd:33:LYS:HD3	34:B5:1594:G:H5'	1.91	0.52
34:B5:976:G:N1	34:B5:1023:A:O2'	2.25	0.52
38:A1:121:A:O2'	44:AG:105:LYS:NZ	2.42	0.52
80:DC:718:LEU:HD23	80:DC:722:PRO:HG3	1.92	0.52
12:BV:62:ARG:HH12	13:BW:20:THR:HG23	1.74	0.52
38:A1:117:U:O2'	38:A1:119:U:OP2	2.22	0.52
39:A3:121:U:OP2	41:AD:265:TYR:OH	2.24	0.52
51:AO:54[A]:TYR:OH	51:AO:73[A]:PHE:O	2.26	0.52
10:BN:128:TYR:OH	34:B5:964:U:OP1	2.27	0.52
20:BF:100:ASN:HD22	20:BF:180:ARG:HH11	1.58	0.52
22:BP:50:THR:OG1	22:BP:52:LYS:NZ	2.43	0.52
27:BU:59:PRO:HG3	34:B5:1381:U:H4'	1.92	0.52
34:B5:12:U:H2'	34:B5:13:C:C6	2.45	0.52
34:B5:64:U:O2'	34:B5:168:A:N3	2.37	0.52
34:B5:1220:C:H2'	34:B5:1221:A:C8	2.44	0.52
34:B5:1357:A:H2'	34:B5:1358:G:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1336:U:H2'	38:A1:1337:A:H8	1.75	0.52
14:BX:5:LYS:NZ	34:B5:612:U:OP2	2.43	0.52
16:Ba:12:LYS:HZ2	16:Ba:16:GLY:H	1.56	0.52
32:Bf:118:ARG:NH2	32:Bf:132:LEU:O	2.43	0.52
38:A1:591:G:O2'	42:AE:17:ALA:O	2.25	0.52
38:A1:650:OMC:H2'	38:A1:651:G:C8	2.45	0.52
38:A1:1188:U:OP1	38:A1:1210:U:O2'	2.18	0.52
38:A1:1493:G:O6	74:A1:2:ALA:N	2.43	0.52
1:BA:190:ASP:N	1:BA:190:ASP:OD1	2.43	0.51
7:BI:37:LYS:HE2	7:BI:95:THR:HG22	1.93	0.51
7:BI:138:ASN:HD22	34:B5:187:G:H2'	1.73	0.51
9:BL:67:ARG:NH2	34:B5:115:G:N7	2.58	0.51
38:A1:21:G:OP2	40:A4:36:G:N2	2.41	0.51
38:A1:2703:A:N6	41:AD:28:THR:O	2.40	0.51
63:Aa:36:GLY:HA3	63:Aa:40:HIS:CE1	2.46	0.51
77:Ao:32:LYS:HD2	77:Ao:34:SER:H	1.74	0.51
80:DC:260:LYS:HG3	80:DC:261:ASP:H	1.75	0.51
80:DC:600:ALA:HB1	80:DC:605:ILE:HB	1.93	0.51
8:BJ:44:ARG:O	8:BJ:48:GLN:NE2	2.43	0.51
15:BY:39:GLU:HB2	15:BY:43:LYS:HZ3	1.75	0.51
20:BF:42:LEU:O	20:BF:44:ASN:N	2.43	0.51
34:B5:1488:G:O2'	34:B5:1494:C:O2	2.22	0.51
38:A1:172:G:H2'	38:A1:173:G:H8	1.73	0.51
38:A1:966:U:H2'	38:A1:967:A:C8	2.44	0.51
38:A1:3182:G:H4'	51:AO:161[A]:LYS:HD2	1.93	0.51
57:AU:56:VAL:HG22	57:AU:65:VAL:HG12	1.92	0.51
79:E:38:LEU:HB2	79:E:163:LEU:HB2	1.92	0.51
3:BC:227:PRO:HA	3:BC:230:TRP:CE2	2.45	0.51
5:BG:92:ARG:NH1	34:B5:1674:C:OP1	2.39	0.51
31:Bg:13:LEU:HB2	31:Bg:310:ILE:HB	1.92	0.51
34:B5:424:C:O2	34:B5:427:C:N4	2.43	0.51
34:B5:1525:A:H2'	34:B5:1526:A:C8	2.45	0.51
36:AB:279:ASN:ND2	38:A1:3098:G:OP1	2.41	0.51
37:AC:35:VAL:HG21	37:AC:244:LEU:HD21	1.92	0.51
38:A1:1759:C:H2'	38:A1:1760:A:H8	1.76	0.51
38:A1:3319:U:H5'	38:A1:3320:A:H5'	1.92	0.51
39:A3:84:A:H2'	39:A3:85:G:C8	2.45	0.51
80:DC:681:MET:HE3	80:DC:684:VAL:HG21	1.93	0.51
20:BF:46:TRP:HH2	20:BF:122:ASN:HD22	1.57	0.51
26:BT:43:ASN:ND2	34:B5:1477:G:OP1	2.42	0.51
31:Bg:159:ASN:HD21	31:Bg:164:ASP:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1276:U:H2'	34:B5:1277:G:H8	1.76	0.51
34:B5:1683:C:O2'	34:B5:1684:U:O5'	2.25	0.51
38:A1:29:C:H4'	38:A1:62:A:H4'	1.92	0.51
38:A1:1873:U:OP1	54:AR:21:LYS:NZ	2.43	0.51
38:A1:2218:G:H2'	38:A1:2219:A:H8	1.73	0.51
58:AV:18:PRO:HA	58:AV:51:ALA:HA	1.92	0.51
6:BH:133:THR:HG22	6:BH:158:ASP:HB3	1.93	0.51
14:BX:75:GLN:NE2	14:BX:76:LEU:O	2.43	0.51
16:Ba:2:PRO:HB3	34:B5:1142:A:H5''	1.93	0.51
33:BM:59:LEU:HD12	33:BM:123:VAL:HG21	1.91	0.51
34:B5:1175:U:H2'	34:B5:1176:G:H8	1.76	0.51
36:AB:106:TRP:O	36:AB:137:TYR:OH	2.23	0.51
38:A1:411:U:H2'	38:A1:412:G:C8	2.46	0.51
38:A1:627:U:H4'	38:A1:1399:A:H1'	1.92	0.51
38:A1:2468:A:N6	38:A1:2477:G:O2'	2.43	0.51
60:AX:130:TYR:HB3	60:AX:135:ILE:HD11	1.92	0.51
80:DC:82:SER:OG	80:DC:83:ASP:N	2.43	0.51
4:BE:98:ASN:ND2	4:BE:116:ASP:OD1	2.40	0.51
4:BE:100:ARG:NH2	4:BE:118:GLU:O	2.44	0.51
34:B5:924:A:H2'	34:B5:925:G:C8	2.45	0.51
34:B5:1524:A:N3	34:B5:1590:G:O2'	2.41	0.51
37:AC:11:LEU:HD22	37:AC:168:ALA:HB1	1.91	0.51
38:A1:1497:C:H2'	38:A1:1498:A:C8	2.46	0.51
38:A1:1899:G:O2'	38:A1:2334:U:O4	2.23	0.51
38:A1:3067:C:H3'	54:AR:62:ARG:HH22	1.75	0.51
39:A3:112:G:H2'	39:A3:113:C:C6	2.46	0.51
61:AY:86:THR:HG22	61:AY:96:PRO:HA	1.93	0.51
76:An:15:ARG:HA	76:An:18:ARG:HG2	1.93	0.51
7:BI:76:THR:HG21	7:BI:104:ILE:HD12	1.92	0.51
32:Bf:118:ARG:HH22	32:Bf:134:ASN:N	2.09	0.51
34:B5:29:U:H2'	34:B5:30:G:H8	1.76	0.51
34:B5:626:U:H2'	34:B5:627:C:H6	1.75	0.51
34:B5:1163:A:N3	34:B5:1613:U:O2'	2.38	0.51
38:A1:19:U:H2'	38:A1:20:A:C8	2.46	0.51
49:AM:48:GLY:HA3	49:AM:53:VAL:HB	1.91	0.51
80:DC:577:SER:OG	80:DC:711:ARG:NH1	2.44	0.51
80:DC:758:GLU:OE2	80:DC:767:THR:OG1	2.26	0.51
3:BC:52:THR:OG1	3:BC:54:GLU:OE1	2.27	0.51
22:BP:34:VAL:HG22	22:BP:42:ARG:HG2	1.92	0.51
27:BU:23:ARG:NH2	27:BU:92:ASP:OD2	2.44	0.51
31:Bg:245:PHE:HE1	31:Bg:252:LEU:HD13	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1696:A:H2'	38:A1:1697:A:C8	2.46	0.51
38:A1:1720:U:O4	54:AR:125:LYS:NZ	2.42	0.51
38:A1:2482:U:H2'	38:A1:2483:G:C8	2.46	0.51
45:AH:100:ASN:HD21	80:DC:168:GLN:HE22	1.58	0.51
82:EC:6883:A:H2'	82:EC:6884:G:H4'	1.93	0.51
18:Be:23:LYS:NZ	34:B5:586:G:OP1	2.32	0.51
34:B5:590:C:H2'	34:B5:591:A:C8	2.45	0.51
34:B5:590:C:H2'	34:B5:591:A:H8	1.76	0.51
37:AC:99:MET:HE3	37:AC:102:PRO:HA	1.93	0.51
38:A1:339:C:OP1	38:A1:1380:G:O2'	2.29	0.51
38:A1:370:U:H4'	38:A1:404:G:H5'	1.93	0.51
38:A1:821:U:H2'	38:A1:822:G:H8	1.76	0.51
1:BA:16:LEU:HD12	1:BA:17:LEU:HD12	1.92	0.51
10:BN:64:ARG:NH1	10:BN:68:GLY:O	2.44	0.51
31:Bg:149:ASP:HB3	31:Bg:175:ASP:HB2	1.93	0.51
31:Bg:156:VAL:HG22	31:Bg:169:ILE:HG12	1.93	0.51
34:B5:580:A:O2'	34:B5:582:U:OP1	2.25	0.51
34:B5:895:G:H2'	34:B5:896:U:C6	2.46	0.51
38:A1:1497:C:O2'	38:A1:1602:A:N3	2.41	0.51
41:AD:215:ASP:OD1	41:AD:215:ASP:N	2.44	0.51
60:AX:67:ILE:HD11	60:AX:85:GLN:HB2	1.93	0.51
1:BA:98:ILE:HG21	1:BA:102:PHE:HD1	1.76	0.50
4:BE:121:TYR:OH	4:BE:235:TYR:O	2.26	0.50
31:Bg:83:ALA:HB2	31:Bg:113:VAL:HB	1.91	0.50
34:B5:315:A:N1	34:B5:349:U:O2'	2.38	0.50
35:AA:183:GLY:HA2	38:A1:896:A:H5''	1.94	0.50
36:AB:93:VAL:HG12	36:AB:155:ALA:H	1.76	0.50
38:A1:251:G:H1'	38:A1:253:A:C8	2.46	0.50
38:A1:2465:G:C6	38:A1:2491:A:N6	2.78	0.50
40:A4:112:U:OP1	74:A1:8:ARG:NH1	2.44	0.50
47:AJ:36:VAL:HG13	47:AJ:37:LEU:HD12	1.92	0.50
57:AU:98:THR:HG22	57:AU:104:ARG:HH11	1.76	0.50
62:AZ:50:PRO:HD3	62:AZ:68:ILE:HG12	1.92	0.50
13:BW:23:ARG:HA	13:BW:65:LEU:HB2	1.93	0.50
14:BX:70:LYS:NZ	34:B5:567:A:OP1	2.28	0.50
28:BZ:43:ASP:OD1	28:BZ:44:GLN:N	2.44	0.50
38:A1:1333:C:OP1	53:AQ:2:GLY:N	2.45	0.50
38:A1:2960:C:H2'	38:A1:2961:G:H8	1.75	0.50
60:AX:63:ILE:HD13	60:AX:102:LEU:HD12	1.92	0.50
66:Ad:9:THR:HG23	66:Ad:76:SER:HB3	1.92	0.50
81:V:14:LYS:NZ	81:V:52:LEU:HD13	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:V:120:TRP:HB3	81:V:157:LYS:HD3	1.93	0.50
19:BD:25:PHE:HE1	19:BD:69:LEU:HD13	1.76	0.50
25:BS:86:LEU:HB2	25:BS:89:GLN:HG2	1.92	0.50
34:B5:773:C:O2'	34:B5:787:G:N2	2.43	0.50
34:B5:1041:G:H2'	34:B5:1042:G:C8	2.45	0.50
34:B5:1374:C:H2'	34:B5:1375:A:C8	2.47	0.50
38:A1:1565:G:N2	38:A1:1575:A:N7	2.59	0.50
38:A1:2573:G:OP2	62:AZ:58:GLY:N	2.40	0.50
38:A1:3308:C:O2'	52:AP:69:ARG:O	2.22	0.50
1:BA:126:PRO:HB2	1:BA:152:PRO:HG2	1.94	0.50
8:BJ:3:ARG:O	34:B5:380:U:O2'	2.26	0.50
9:BL:73:GLY:HA3	9:BL:86:ILE:HD12	1.93	0.50
20:BF:111:VAL:HA	20:BF:114:ILE:HG12	1.93	0.50
34:B5:1357:A:H2'	34:B5:1358:G:H8	1.75	0.50
34:B5:1564:U:H2'	34:B5:1565:C:C6	2.46	0.50
35:AA:101:VAL:HG22	35:AA:165:VAL:HG22	1.93	0.50
38:A1:673:U:H2'	38:A1:674:G:C8	2.47	0.50
38:A1:938:C:OP2	63:Aa:26:ARG:NH1	2.44	0.50
38:A1:1595:U:O2'	38:A1:1606:U:O2	2.28	0.50
38:A1:2129:U:H2'	38:A1:2130:G:C8	2.46	0.50
38:A1:2828:G:O2'	46:AI:4:ARG:NH2	2.38	0.50
38:A1:3252:G:H2'	38:A1:3253:G:C8	2.47	0.50
80:DC:638:PRO:HD3	80:DC:644:ASN:HD22	1.76	0.50
1:BA:74:VAL:HG23	1:BA:118:PRO:HB3	1.92	0.50
7:BI:34:ALA:HB2	7:BI:56:ARG:HD2	1.94	0.50
7:BI:48:THR:OG1	7:BI:52:ASN:O	2.29	0.50
10:BN:104:ARG:NH2	34:B5:950:C:O2'	2.35	0.50
25:BS:137:HIS:O	25:BS:141:THR:OG1	2.29	0.50
34:B5:464:A:H4'	34:B5:527:A:H2	1.77	0.50
34:B5:521:A:H2'	34:B5:522:U:C6	2.46	0.50
38:A1:2930:A:H2'	38:A1:2931:C:C6	2.47	0.50
80:DC:495:VAL:HG12	80:DC:504:LEU:HD13	1.92	0.50
82:EC:6809:G:H2'	82:EC:6810:U:C6	2.47	0.50
13:BW:82:LYS:HG3	13:BW:83:ILE:H	1.76	0.50
34:B5:1217:A:H4'	34:B5:1218:G:OP2	2.11	0.50
36:AB:14:LEU:O	38:A1:3009:G:O2'	2.27	0.50
38:A1:307:A:H2'	38:A1:308:A:C8	2.45	0.50
38:A1:1233:G:H2'	38:A1:1234:G:C8	2.47	0.50
38:A1:1334:U:H5''	43:AF:206:LYS:HB3	1.94	0.50
38:A1:1447:G:N7	52:AP:25:SER:OG	2.45	0.50
63:Aa:19:LYS:HB3	63:Aa:25:HIS:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:DC:699:DDE:HAT3	82:EC:6907:G:H1'	1.92	0.50
15:BY:56:SER:HB3	15:BY:74:LEU:HB3	1.93	0.50
25:BS:36:LYS:HD2	34:B5:1567:U:H4'	1.94	0.50
34:B5:1356:U:H2'	34:B5:1357:A:C8	2.47	0.50
34:B5:1671:A:H3'	34:B5:1672:G:H8	1.77	0.50
38:A1:1194:G:H2'	38:A1:1195:A:C8	2.46	0.50
38:A1:1645:U:H3	38:A1:1810:A:H61	1.59	0.50
38:A1:2697:A:H2'	38:A1:2698:G:C8	2.47	0.50
79:E:40:ASN:OD1	79:E:200:ASN:ND2	2.45	0.50
1:BA:6:THR:O	1:BA:191:ARG:NH2	2.45	0.50
6:BH:159:VAL:HG12	6:BH:163:ASP:HB3	1.93	0.50
22:BP:52:LYS:HG3	22:BP:53:PRO:HD3	1.93	0.50
30:Bd:31:ILE:HG21	30:Bd:36:LEU:HD12	1.93	0.50
34:B5:1146:G:H2'	34:B5:1147:A:C8	2.46	0.50
35:AA:67:TYR:OH	38:A1:2525:G:N7	2.34	0.50
36:AB:124:LYS:NZ	38:A1:3297:U:O4	2.45	0.50
38:A1:1812:G:N7	62:AZ:64:LYS:NZ	2.60	0.50
38:A1:2218:G:H2'	38:A1:2219:A:C8	2.47	0.50
38:A1:2351:U:H2'	38:A1:2352:A:H8	1.77	0.50
38:A1:2444:C:H4'	71:AI:63:ASN:HD21	1.77	0.50
81:V:141:VAL:HG22	81:V:156:VAL:HG11	1.94	0.50
8:BJ:110:GLN:HG3	8:BJ:126:ARG:HB2	1.92	0.50
9:BL:130:PRO:O	34:B5:335:U:O2'	2.29	0.50
14:BX:90:ASP:HA	34:B5:568:G:H4'	1.94	0.50
34:B5:27:U:H2'	34:B5:28:A2M:H8	1.93	0.50
34:B5:126:A:N6	34:B5:291:G:C2	2.79	0.50
38:A1:3174:A:H61	68:Af:54:ARG:HH21	1.60	0.50
39:A3:11:A:N6	41:AD:16:PHE:O	2.41	0.50
47:AJ:83:GLY:HA3	47:AJ:127:PHE:CE2	2.47	0.50
50:AN:46:ASP:OD1	50:AN:47:LYS:N	2.44	0.50
61:AY:17:LYS:O	61:AY:21:THR:OG1	2.21	0.50
80:DC:70:ILE:HG13	80:DC:71:LYS:HG2	1.93	0.50
81:V:51:VAL:HG22	81:V:87:VAL:HG22	1.94	0.50
2:BB:89:ASP:HB3	2:BB:223:PHE:HE1	1.77	0.49
3:BC:203:LYS:NZ	34:B5:16:G:O6	2.44	0.49
22:BP:79:HIS:HA	22:BP:97:TYR:HB2	1.94	0.49
23:BQ:75:VAL:HG12	34:B5:1609:U:H5''	1.93	0.49
34:B5:406:U:H2'	34:B5:407:A:C8	2.46	0.49
35:AA:80:GLU:HG3	78:Ap:66:GLY:HA2	1.93	0.49
38:A1:243:G:H3'	38:A1:244:G:C8	2.47	0.49
38:A1:1279:C:H2'	38:A1:1280:C:H6	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1378:U:H2'	38:A1:1379:G:H8	1.77	0.49
38:A1:2474:G:H1'	38:A1:2476:C:H41	1.76	0.49
38:A1:2927:C:H2'	38:A1:2928:C:C6	2.47	0.49
66:Ad:12:TYR:CD1	66:Ad:75:ILE:HD12	2.47	0.49
68:Af:45:LEU:HD11	68:Af:73:ARG:HA	1.93	0.49
80:DC:380:LEU:HD22	80:DC:400:VAL:HG12	1.93	0.49
1:BA:189:VAL:HG23	12:BV:44:ARG:HH22	1.76	0.49
7:BI:26:LYS:HD2	34:B5:399:A:H2'	1.95	0.49
8:BJ:110:GLN:HB2	8:BJ:144:PRO:HB3	1.94	0.49
19:BD:72:LEU:HD21	21:BK:67:THR:HG22	1.93	0.49
25:BS:132:ARG:HH21	25:BS:136:GLN:CD	2.20	0.49
28:BZ:83:LEU:HD11	28:BZ:88:ILE:HD11	1.94	0.49
38:A1:1392:G:H1'	38:A1:1418:A:H61	1.77	0.49
38:A1:3119:U:H4'	75:Am:104:PRO:HG3	1.93	0.49
64:Ab:35:VAL:HB	64:Ab:40:ARG:HD2	1.94	0.49
80:DC:722:PRO:HD2	80:DC:809:LEU:HD11	1.93	0.49
5:BG:77:LEU:HD12	5:BG:95:LYS:HD2	1.94	0.49
5:BG:188:ARG:NH2	34:B5:284:G:O6	2.36	0.49
25:BS:31:ALA:O	25:BS:34:THR:OG1	2.28	0.49
34:B5:161:U:H2'	34:B5:162:A:C8	2.47	0.49
34:B5:406:U:H2'	34:B5:407:A:H8	1.77	0.49
34:B5:925:G:H2'	34:B5:926:A:C8	2.47	0.49
38:A1:351:A:N6	74:Al:37:TYR:O	2.42	0.49
38:A1:939:U:O2'	38:A1:2402:A:N1	2.42	0.49
38:A1:1203:A:H2'	38:A1:1204:A:C8	2.47	0.49
44:AG:183:LYS:HB2	44:AG:194:THR:HG23	1.93	0.49
1:BA:140:ASN:ND2	3:BC:60:SER:O	2.46	0.49
3:BC:201:ASN:ND2	34:B5:1097:U:O4	2.45	0.49
19:BD:60:GLY:HA2	19:BD:65:ARG:HH21	1.77	0.49
20:BF:143:ARG:HD2	29:Bc:55:VAL:HG11	1.93	0.49
26:BT:77:ASN:HB3	26:BT:95:ASP:HB3	1.95	0.49
27:BU:57:ARG:HA	27:BU:89:ARG:HG3	1.95	0.49
34:B5:1297:G:N2	34:B5:1300:A:OP2	2.33	0.49
37:AC:31:ARG:NH2	37:AC:33:ASP:OD2	2.40	0.49
38:A1:631:U:H2'	38:A1:632:G:C8	2.47	0.49
38:A1:1290:A:H2'	38:A1:1291:A:C8	2.47	0.49
38:A1:1551:C:HO2'	38:A1:2170:U:HO2'	1.58	0.49
38:A1:1840:U:H4'	38:A1:1841:A:H5''	1.94	0.49
38:A1:2424:A:OP1	50:AN:90:ASN:ND2	2.37	0.49
47:AJ:49:LYS:HB3	47:AJ:62:ASN:HA	1.94	0.49
48:AL:180:ARG:HD3	71:Ai:11:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:AQ:125:ASP:OD1	53:AQ:126:GLN:N	2.46	0.49
80:DC:404:THR:OG1	80:DC:406:LYS:NZ	2.45	0.49
82:EC:6759:A:H2'	82:EC:6760:A:C8	2.46	0.49
82:EC:6877:C:O2	82:EC:6878:G:N2	2.45	0.49
3:BC:169:LEU:HD23	3:BC:198:THR:HG22	1.94	0.49
18:Be:18:THR:HG21	34:B5:584:C:H1'	1.95	0.49
26:BT:30:VAL:HG12	26:BT:32:GLY:H	1.78	0.49
26:BT:57:ARG:NE	34:B5:1479:A:OP1	2.46	0.49
34:B5:1695:G:H2'	34:B5:1696:G:C8	2.48	0.49
38:A1:1282:G:O5'	81:V:55:LYS:HE2	2.13	0.49
38:A1:2103:U:H2'	38:A1:2104:A:C8	2.48	0.49
38:A1:2588:U:OP1	44:AG:241:LYS:NZ	2.35	0.49
21:BK:93:GLN:OE1	21:BK:93:GLN:N	2.45	0.49
27:BU:36:ASN:OD1	27:BU:37:VAL:N	2.45	0.49
34:B5:58:U:O2'	34:B5:451:A:N3	2.45	0.49
34:B5:772:G:H21	34:B5:774:A:H1'	1.77	0.49
38:A1:1108:U:H2'	38:A1:1109:U:C6	2.48	0.49
38:A1:2228:A:H2'	38:A1:2229:A:C8	2.48	0.49
38:A1:2767:U:H2'	38:A1:2768:U:C6	2.47	0.49
44:AG:163:VAL:HG12	44:AG:166:LEU:HD12	1.94	0.49
69:Ag:86:LYS:O	69:Ag:90:ILE:HG12	2.13	0.49
81:V:96:ILE:O	81:V:100:ILE:HG12	2.12	0.49
81:V:119:ILE:HG12	81:V:180:PRO:HG2	1.93	0.49
6:BH:64:VAL:HG23	6:BH:67:LEU:HD23	1.95	0.49
25:BS:32:LEU:O	25:BS:35:ILE:HG22	2.12	0.49
31:Bg:66:HIS:ND1	31:Bg:67:ILE:HG22	2.28	0.49
31:Bg:207:ASP:OD1	31:Bg:208:GLY:N	2.46	0.49
34:B5:1474:G:H2'	34:B5:1475:A:H8	1.78	0.49
34:B5:1690:G:H2'	34:B5:1691:A:H8	1.78	0.49
38:A1:1174:G:N2	51:AO:87[A]:MET:SD	2.86	0.49
40:A4:150:G:OP1	60:AX:27:ARG:NH2	2.45	0.49
79:E:110:PHE:N	79:E:133:LYS:HG2	2.28	0.49
80:DC:129:VAL:O	80:DC:158:ASN:N	2.40	0.49
20:BF:72:HIS:NE2	34:B5:1610:G:OP1	2.40	0.49
20:BF:112:ARG:HH11	20:BF:115:LYS:HE2	1.78	0.49
34:B5:607:G:H5'	34:B5:613:G:N2	2.27	0.49
34:B5:883:C:H2'	34:B5:884:A:C8	2.48	0.49
34:B5:923:A:H2'	34:B5:924:A:C8	2.47	0.49
34:B5:1210:C:H2'	34:B5:1211:A:H8	1.76	0.49
38:A1:3358:U:H2'	38:A1:3359:A:H8	1.78	0.49
45:AH:92:TYR:HB2	45:AH:142:ASP:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Ad:84:ASP:N	66:Ad:84:ASP:OD1	2.44	0.49
75:Am:104:PRO:HG2	75:Am:107:ALA:HB2	1.95	0.49
79:E:110:PHE:O	79:E:133:LYS:NZ	2.41	0.49
80:DC:681:MET:HE1	80:DC:717:PHE:CD1	2.48	0.49
82:EC:6801:A:C8	82:EC:6884:G:H1'	2.47	0.49
4:BE:31:PRO:HD2	4:BE:38:LEU:HG	1.95	0.49
7:BI:109:PHE:CE2	7:BI:183:ILE:HD11	2.48	0.49
15:BY:9:THR:HG21	15:BY:48:TYR:HE2	1.78	0.49
20:BF:117:THR:HG21	20:BF:194:LEU:HD23	1.95	0.49
25:BS:143:ARG:NH2	34:B5:1462:G:N7	2.61	0.49
34:B5:71:A:H2'	34:B5:72:A:H4'	1.95	0.49
34:B5:130:C:H1'	34:B5:133:U:H5	1.78	0.49
34:B5:1174:C:O2'	34:B5:1196:A:N6	2.46	0.49
38:A1:209:A:H4'	38:A1:211:A:C8	2.48	0.49
57:AU:98:THR:OG1	57:AU:99:LYS:N	2.46	0.49
65:Ac:45:ALA:HB3	65:Ac:48:THR:HG23	1.94	0.49
37:AC:154:THR:OG1	37:AC:252:GLU:HB3	2.13	0.49
37:AC:283:THR:HG21	37:AC:288:ARG:HH21	1.78	0.49
38:A1:792:G:H2'	38:A1:793:C:C6	2.48	0.49
38:A1:1144:U:OP1	38:A1:1367:G:O2'	2.28	0.49
49:AM:50:LYS:HE2	49:AM:85:TRP:CD1	2.47	0.49
60:AX:60:TYR:OH	70:Ah:26:LYS:NZ	2.39	0.49
6:BH:141:ARG:HB2	6:BH:149:ILE:HB	1.95	0.48
7:BI:32:GLN:NE2	34:B5:1727:G:H21	2.11	0.48
13:BW:55:ASP:OD1	13:BW:56:HIS:N	2.46	0.48
19:BD:90:ARG:HH22	19:BD:94:ARG:HH22	1.61	0.48
31:Bg:106:HIS:HE2	31:Bg:132:LYS:HB2	1.78	0.48
33:BM:43:ARG:N	33:BM:47:GLU:OE2	2.46	0.48
34:B5:209:U:H2'	34:B5:210:A:H8	1.77	0.48
34:B5:1170:G:N2	34:B5:1571:C:O2'	2.43	0.48
38:A1:1612:A:H5''	73:Ak:51:LEU:HD22	1.95	0.48
38:A1:1740:U:H4'	38:A1:1741:A:H5'	1.94	0.48
81:V:12:PHE:HA	81:V:15:LEU:HD12	1.94	0.48
3:BC:78:ASP:OD1	3:BC:79:GLU:N	2.46	0.48
4:BE:173:ILE:HD12	4:BE:227:VAL:HG12	1.96	0.48
9:BL:37:ASN:O	34:B5:247:A:O2'	2.28	0.48
10:BN:87:ASP:N	10:BN:87:ASP:OD1	2.46	0.48
25:BS:45:LEU:HD21	25:BS:81:ILE:HD12	1.94	0.48
26:BT:40:SER:OG	26:BT:43:ASN:OD1	2.19	0.48
31:Bg:256:THR:HG21	31:Bg:261:LYS:HG3	1.95	0.48
34:B5:110:U:OP1	34:B5:753:A:O2'	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1592:A:H2'	34:B5:1593:A:C8	2.48	0.48
35:AA:52:SER:HB3	35:AA:191:LEU:HD12	1.95	0.48
36:AB:94:GLU:OE1	36:AB:156:SER:OG	2.27	0.48
38:A1:1081:U:H4'	38:A1:1082:U:H5'	1.94	0.48
38:A1:1940:G:H21	38:A1:3362:A:H8	1.61	0.48
38:A1:2699:G:H5''	56:AT:16:GLN:NE2	2.29	0.48
69:Ag:3:GLN:HE22	69:Ag:29:ILE:HB	1.78	0.48
79:E:67:ILE:HD13	79:E:144:LEU:HD21	1.95	0.48
9:BL:27:THR:HG23	9:BL:30:ARG:H	1.78	0.48
14:BX:112:LYS:NZ	34:B5:1136:U:O4	2.35	0.48
18:Be:57:ASN:ND2	34:B5:588:U:O2	2.42	0.48
31:Bg:200:ASN:ND2	31:Bg:240:VAL:O	2.45	0.48
31:Bg:209:THR:HG23	31:Bg:210:LEU:HD22	1.96	0.48
34:B5:276:C:O2'	34:B5:278:U:OP2	2.26	0.48
34:B5:1254:U:H3'	34:B5:1255:G:H8	1.77	0.48
34:B5:1776:A:H2'	34:B5:1777:G:C8	2.48	0.48
38:A1:109:A:O2'	38:A1:323:A:N6	2.47	0.48
38:A1:567:G:H2'	38:A1:568:G:C8	2.49	0.48
38:A1:952:A:H4'	38:A1:968:G:N2	2.29	0.48
38:A1:1534:A:H2'	38:A1:1535:A:C8	2.48	0.48
38:A1:2152:A:H2'	38:A1:2153:U:H6	1.78	0.48
38:A1:3271:G:C5	42:AE:108:LYS:HE3	2.48	0.48
80:DC:608:PRO:O	80:DC:615:ARG:NH2	2.46	0.48
9:BL:72:THR:H	9:BL:88:ARG:NH1	2.12	0.48
12:BV:25:LYS:HG2	12:BV:26:ALA:H	1.78	0.48
20:BF:218:GLU:HG3	20:BF:222:LYS:NZ	2.27	0.48
21:BK:48:SER:O	21:BK:51:SER:OG	2.22	0.48
34:B5:333:A:H2'	34:B5:334:G:C8	2.48	0.48
34:B5:891:A:H2'	34:B5:892:A:C8	2.48	0.48
34:B5:1628:U:H2'	34:B5:1629:G:C8	2.48	0.48
38:A1:1232:C:O2'	81:V:36:GLN:OE1	2.24	0.48
38:A1:2203:U:H2'	38:A1:2204:C:C6	2.48	0.48
41:AD:60:ILE:HD11	41:AD:93:THR:HA	1.94	0.48
57:AU:22:PRO:HB2	57:AU:28:PHE:HB2	1.95	0.48
64:Ab:20:GLY:O	64:Ab:22:LYS:HG3	2.14	0.48
79:E:14:LYS:HA	79:E:17:LEU:HG	1.94	0.48
79:E:158:GLN:H	79:E:165:LEU:HD22	1.78	0.48
3:BC:92:ALA:HB1	34:B5:1425:A:H5'	1.94	0.48
15:BY:29:HIS:O	15:BY:29:HIS:ND1	2.47	0.48
15:BY:132:ARG:NH2	34:B5:154:G:OP2	2.46	0.48
23:BQ:77:GLN:O	23:BQ:81:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BR:10:LYS:NZ	34:B5:1316:G:O2'	2.46	0.48
24:BR:21:TYR:HE2	24:BR:73:LEU:HD13	1.76	0.48
25:BS:41:ARG:HG2	25:BS:85:PHE:CZ	2.45	0.48
34:B5:1087:A:H2'	34:B5:1088:A:C8	2.48	0.48
34:B5:1552:U:H2'	34:B5:1553:G:C8	2.49	0.48
38:A1:2106:A:H2'	38:A1:2107:A:C8	2.47	0.48
38:A1:3186:A:N3	45:AH:44:THR:OG1	2.44	0.48
69:Ag:51:LEU:HB3	69:Ag:54:ILE:HD12	1.96	0.48
79:E:110:PHE:H	79:E:133:LYS:HG2	1.77	0.48
80:DC:140:GLU:HG2	80:DC:188:ILE:HD13	1.96	0.48
81:V:123:ALA:HA	81:V:152:ILE:HB	1.95	0.48
2:BB:66:VAL:HB	2:BB:86:LEU:HB2	1.93	0.48
2:BB:152:ARG:HB3	34:B5:1799:U:H3	1.77	0.48
4:BE:94:ALA:HB3	15:BY:17:LEU:HD23	1.94	0.48
10:BN:124:ARG:HG2	10:BN:127:ARG:HH22	1.77	0.48
34:B5:1294:G:O2'	34:B5:1321:A:N1	2.46	0.48
38:A1:1235:U:O4	38:A1:1263:A:N6	2.47	0.48
38:A1:1392:G:H1'	38:A1:1418:A:N6	2.29	0.48
38:A1:1447:G:H3'	52:AP:67:ILE:HD11	1.95	0.48
38:A1:2406:C:H2'	38:A1:2407:C:C6	2.48	0.48
38:A1:2413:A:H2'	38:A1:2414:G:H8	1.77	0.48
38:A1:2723:U:H2'	38:A1:2724:OMU:H6	1.96	0.48
55:AS:24:LEU:HD21	56:AT:141:VAL:HG11	1.96	0.48
80:DC:732:GLU:OE2	80:DC:769:LYS:NZ	2.46	0.48
3:BC:146:THR:HG23	3:BC:148:LEU:H	1.79	0.48
7:BI:39:GLY:HA2	7:BI:61:GLU:HG3	1.95	0.48
9:BL:102:LYS:O	14:BX:13:ARG:NH2	2.46	0.48
22:BP:83:MET:HB2	22:BP:116:LEU:HD23	1.95	0.48
31:Bg:297:ASP:HB2	31:Bg:299:GLN:HE22	1.78	0.48
34:B5:50:C:H2'	34:B5:424:C:H41	1.79	0.48
34:B5:445:A:N1	34:B5:462:G:O2'	2.39	0.48
34:B5:1175:U:H2'	34:B5:1176:G:C8	2.49	0.48
38:A1:874:U:N3	38:A1:2978:U:OP1	2.41	0.48
38:A1:1084:A:H2'	38:A1:1085:A:C8	2.48	0.48
38:A1:1119:C:H2'	38:A1:1120:A:C8	2.48	0.48
38:A1:1622:U:H2'	38:A1:1623:G:H8	1.78	0.48
38:A1:2103:U:H2'	38:A1:2104:A:H8	1.78	0.48
38:A1:3050:U:O2'	59:AW:16:GLY:O	2.25	0.48
50:AN:192:LYS:O	50:AN:196:THR:HG23	2.13	0.48
6:BH:12:ALA:HB3	6:BH:13:PRO:HD3	1.95	0.48
30:Bd:32:ARG:NH1	34:B5:1596:C:O2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:209:U:H2'	34:B5:210:A:C8	2.49	0.48
34:B5:407:A:H2'	34:B5:408:C:H6	1.79	0.48
34:B5:428:A:H2'	34:B5:429:G:O4'	2.14	0.48
34:B5:713:A:H2'	34:B5:714:G:H8	1.79	0.48
38:A1:138:U:H2'	38:A1:139:G:H8	1.79	0.48
38:A1:1694:U:H5	38:A1:1752:A:N1	2.12	0.48
41:AD:129:TYR:OH	41:AD:175:HIS:O	2.29	0.48
49:AM:23:ILE:O	49:AM:30:GLY:N	2.45	0.48
61:AY:116:LYS:HG2	61:AY:126:LEU:HD11	1.96	0.48
77:Ao:24:LYS:HB2	77:Ao:73:GLU:HB3	1.95	0.48
80:DC:378:LEU:HD11	80:DC:380:LEU:HD23	1.96	0.48
4:BE:127:LYS:NZ	4:BE:141:THR:O	2.47	0.48
33:BM:45:LEU:HA	33:BM:48:SER:HB3	1.94	0.48
37:AC:266:THR:HG23	37:AC:267:VAL:HG13	1.94	0.48
38:A1:2357:A:H2'	38:A1:2358:A:H8	1.79	0.48
40:A4:57:C:H4'	40:A4:63:G:N7	2.28	0.48
51:AO:27[A]:LEU:O	51:AO:101[A]:ARG:NH1	2.45	0.48
51:AO:46[A]:GLU:HG2	51:AO:49[A]:ARG:HG3	1.96	0.48
3:BC:127:ALA:HA	3:BC:130:ILE:HD12	1.96	0.48
6:BH:64:VAL:HA	6:BH:67:LEU:HD23	1.96	0.48
14:BX:97:ASP:OD1	14:BX:98:GLU:N	2.46	0.48
15:BY:10:ARG:NH1	34:B5:778:G:H22	2.11	0.48
22:BP:81:ARG:HA	22:BP:116:LEU:HD11	1.95	0.48
28:BZ:75:LEU:HD23	28:BZ:78:ILE:HD11	1.95	0.48
34:B5:329:G:H2'	34:B5:330:G:H8	1.78	0.48
34:B5:947:U:H2'	34:B5:948:G:C8	2.48	0.48
34:B5:1178:G:H5'	34:B5:1190:C:H42	1.79	0.48
38:A1:284:A:OP2	77:Ao:41:ARG:NH1	2.45	0.48
38:A1:835:G:O2'	38:A1:857:G:N2	2.34	0.48
38:A1:1419:A:OP1	40:A4:20:U:O2'	2.27	0.48
38:A1:1747:G:H21	73:Ak:2:ALA:HB3	1.79	0.48
38:A1:1827:C:H2'	38:A1:1828:A:C8	2.49	0.48
45:AH:186:PHE:HD2	45:AH:189:GLU:HG3	1.78	0.48
80:DC:27:HIS:HB3	80:DC:30:HIS:NE2	2.29	0.48
81:V:23:LYS:HE3	81:V:193:ASN:HD21	1.78	0.48
1:BA:76:ILE:HD13	1:BA:98:ILE:HB	1.96	0.47
13:BW:101:TYR:HB3	13:BW:112:ASP:HB2	1.96	0.47
18:Be:43:ARG:HE	18:Be:43:ARG:HB2	1.47	0.47
20:BF:140:THR:HB	20:BF:171:ALA:HB1	1.96	0.47
28:BZ:53:GLU:HG3	82:EC:6865:G:H22	1.80	0.47
28:BZ:76:ALA:O	28:BZ:80:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:250:C:H2'	34:B5:251:A:H8	1.78	0.47
34:B5:1055:U:H3	34:B5:1064:G:H1	1.62	0.47
34:B5:1775:U:OP1	76:An:11:ARG:NH2	2.45	0.47
37:AC:294:GLU:OE2	53:AQ:129:VAL:HG23	2.14	0.47
38:A1:715:A:H8	63:Aa:115:LYS:HD3	1.78	0.47
38:A1:1143:A:H5'	38:A1:1368:U:H1'	1.96	0.47
38:A1:1799:A:H2'	38:A1:1800:A:H8	1.79	0.47
38:A1:2338:C:H3'	38:A1:2339:C:H2'	1.96	0.47
81:V:35:SER:HA	81:V:38:MET:HG2	1.95	0.47
1:BA:123:VAL:HG21	1:BA:133:ILE:HD11	1.96	0.47
14:BX:57:LEU:HD11	14:BX:73:ARG:HG3	1.95	0.47
16:Ba:87:ARG:NE	16:Ba:92:ARG:HA	2.28	0.47
19:BD:174:HIS:CE1	34:B5:1277:G:H21	2.31	0.47
31:Bg:108:SER:HB3	31:Bg:127:ARG:HB2	1.96	0.47
34:B5:193:U:O2'	34:B5:195:G:O4'	2.33	0.47
34:B5:609:U:H4'	34:B5:610:G:H5'	1.95	0.47
38:A1:2373:A:N3	38:A1:2824:G:O2'	2.38	0.47
38:A1:2406:C:H2'	38:A1:2407:C:H6	1.79	0.47
38:A1:3160:U:H5''	38:A1:3396:U:H3'	1.96	0.47
39:A3:4:U:H2'	39:A3:5:G:H8	1.79	0.47
41:AD:6:ASP:N	41:AD:6:ASP:OD1	2.46	0.47
80:DC:223:ARG:HG3	80:DC:241:MET:HE1	1.95	0.47
80:DC:380:LEU:HG	80:DC:469:LEU:HB2	1.97	0.47
82:EC:6828:G:H2'	82:EC:6829:A:C8	2.49	0.47
82:EC:6858:A:H4'	82:EC:6859:U:N3	2.29	0.47
7:BI:41:LYS:N	7:BI:61:GLU:OE2	2.47	0.47
16:Ba:87:ARG:NH2	16:Ba:94:ASN:O	2.47	0.47
31:Bg:51:ASP:OD1	31:Bg:51:ASP:N	2.45	0.47
34:B5:1079:U:H2'	34:B5:1080:U:C6	2.48	0.47
38:A1:1523:U:OP1	38:A1:1607:U:N3	2.46	0.47
38:A1:2160:G:H2'	38:A1:2161:G:C8	2.48	0.47
38:A1:2445:A:N6	38:A1:2503:G:O6	2.48	0.47
41:AD:93:THR:O	41:AD:158:ARG:NH1	2.45	0.47
63:Aa:82:ILE:HD11	63:Aa:102:ILE:HG12	1.97	0.47
80:DC:823:ARG:HD2	80:DC:828:MET:HB2	1.95	0.47
7:BI:27:PHE:HB2	34:B5:333:A:N6	2.30	0.47
8:BJ:6:ARG:NE	34:B5:771:A:O2'	2.47	0.47
34:B5:187:G:N2	34:B5:198:A:H62	2.12	0.47
34:B5:1732:A:H2'	34:B5:1733:C:H6	1.80	0.47
35:AA:82:VAL:HG12	35:AA:86:GLN:HE22	1.78	0.47
35:AA:190:ARG:HG3	35:AA:191:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:AB:250:ALA:HB3	38:A1:2880:U:H1'	1.96	0.47
38:A1:629:U:H2'	38:A1:630:A:C8	2.49	0.47
38:A1:1629:U:O2'	38:A1:1630:U:OP1	2.30	0.47
38:A1:2451:G:O2'	38:A1:2452:G:O4'	2.30	0.47
38:A1:2745:G:N2	38:A1:2748:A:OP2	2.40	0.47
80:DC:20:ARG:N	80:DC:99:LEU:O	2.46	0.47
80:DC:735:CYS:HB2	80:DC:739:ALA:HB3	1.95	0.47
1:BA:144:ILE:HG12	1:BA:158:VAL:HB	1.96	0.47
5:BG:139:ASN:ND2	34:B5:143:G:OP2	2.42	0.47
6:BH:14:THR:HG22	6:BH:15:GLU:H	1.80	0.47
34:B5:651:G:N2	34:B5:652:G:O2'	2.47	0.47
38:A1:3066:U:H2'	38:A1:3067:C:C6	2.50	0.47
65:Ac:22:LYS:HG2	65:Ac:93:LEU:HD12	1.95	0.47
80:DC:237:LYS:HB3	80:DC:241:MET:HE2	1.96	0.47
82:EC:6808:G:H2'	82:EC:6809:G:C8	2.49	0.47
1:BA:48:ILE:HG12	1:BA:149:LEU:HD21	1.96	0.47
2:BB:212:VAL:O	2:BB:213:ARG:HG2	2.14	0.47
7:BI:138:ASN:O	7:BI:141:ARG:NH1	2.48	0.47
8:BJ:130:THR:HA	8:BJ:142:ASN:HB2	1.96	0.47
12:BV:74:GLN:HG3	12:BV:83:TRP:HB3	1.95	0.47
16:Ba:51:ARG:NH2	29:Bc:61:ARG:HA	2.30	0.47
34:B5:1061:A:H5''	34:B5:1062:A:H2	1.80	0.47
37:AC:67:THR:HG21	38:A1:2402:A:H2'	1.96	0.47
38:A1:150:A:OP1	50:AN:56:LYS:NZ	2.46	0.47
38:A1:162:G:H2'	38:A1:163:C:H6	1.79	0.47
38:A1:2611:U:H2'	38:A1:2612:U:C6	2.50	0.47
39:A3:52:G:N2	47:AJ:9:MET:SD	2.86	0.47
45:AH:10:ILE:HD11	45:AH:72:LYS:HA	1.97	0.47
1:BA:74:VAL:HG22	1:BA:96:THR:HG23	1.96	0.47
2:BB:87:ARG:HB2	2:BB:101:HIS:HB2	1.97	0.47
6:BH:111:LYS:HG2	34:B5:811:A:N7	2.29	0.47
8:BJ:132:ARG:HH21	15:BY:65:GLY:HA2	1.80	0.47
11:BO:133:ARG:NH1	34:B5:1786:G:OP2	2.47	0.47
13:BW:78:ARG:HB3	13:BW:124:LYS:HB3	1.96	0.47
13:BW:106:THR:HG23	13:BW:108:ALA:H	1.78	0.47
28:BZ:58:ARG:HH21	82:EC:6863:C:H5''	1.79	0.47
34:B5:625:C:O2'	34:B5:939:A:N3	2.38	0.47
34:B5:816:G:H2'	34:B5:817:A:C8	2.50	0.47
34:B5:1441:C:O2'	34:B5:1447:C:N4	2.39	0.47
34:B5:1642:G:H2'	34:B5:1643:U:H6	1.80	0.47
36:AB:250:ALA:HB1	38:A1:2947:G:N3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:AB:251:CYS:SG	38:A1:2943:G:N2	2.88	0.47
38:A1:177:U:O2	38:A1:241:G:N2	2.46	0.47
38:A1:414:U:H2'	38:A1:415:G:C8	2.49	0.47
38:A1:819:U:H2'	38:A1:820:A:H8	1.78	0.47
38:A1:1621:A:H2'	38:A1:1622:U:C6	2.49	0.47
38:A1:1629:U:H1'	62:AZ:115:LYS:HD2	1.96	0.47
38:A1:2376:G:H2'	38:A1:2377:G:C8	2.50	0.47
38:A1:2584:G:O2'	44:AG:240:ASN:OD1	2.24	0.47
40:A4:95:G:O2'	72:Aj:81:GLY:O	2.30	0.47
43:AF:207:LEU:HB3	43:AF:243:MET:HB3	1.97	0.47
44:AG:161:GLU:OE1	50:AN:26:ARG:NH2	2.33	0.47
52:AP:4:TYR:CZ	52:AP:18:ARG:HG3	2.50	0.47
65:Ac:57:GLU:OE1	65:Ac:69:TYR:OH	2.32	0.47
80:DC:108:HIS:HB3	80:DC:109:VAL:H	1.60	0.47
80:DC:736:PRO:HD2	80:DC:791:GLN:HB3	1.97	0.47
81:V:16:ARG:HG2	81:V:66:PHE:CZ	2.50	0.47
1:BA:198:MET:HE3	1:BA:200:ASP:HB2	1.97	0.47
4:BE:49:ARG:NH2	34:B5:448:C:OP1	2.45	0.47
5:BG:102:VAL:HG13	5:BG:106:LEU:HD12	1.96	0.47
22:BP:25:LEU:HD13	22:BP:28:MET:HE2	1.97	0.47
26:BT:78:LYS:HZ3	34:B5:1524:A:H5'	1.80	0.47
31:Bg:38:ARG:NE	31:Bg:67:ILE:HD12	2.30	0.47
34:B5:388:G:OP1	34:B5:423:G:O2'	2.32	0.47
34:B5:625:C:H2'	34:B5:626:U:C6	2.50	0.47
34:B5:1450:U:H2'	34:B5:1451:C:H6	1.79	0.47
38:A1:1074:U:O2'	64:Ab:42:ASN:ND2	2.47	0.47
38:A1:1659:U:H2'	38:A1:1660:C:C6	2.50	0.47
38:A1:1676:A:OP2	57:AU:72:SER:OG	2.24	0.47
38:A1:2810:C:OP2	38:A1:2955:U:O2'	2.32	0.47
38:A1:3273:A:H2'	38:A1:3274:A:C8	2.50	0.47
55:AS:115:ARG:O	55:AS:117:ARG:NH1	2.48	0.47
8:BJ:151:ASP:O	8:BJ:154:LYS:NZ	2.47	0.47
34:B5:1672:G:H2'	34:B5:1673:G:C8	2.50	0.47
38:A1:129:U:H2'	38:A1:130:A:C8	2.50	0.47
38:A1:412:G:H2'	38:A1:413:U:C6	2.50	0.47
38:A1:1506:A:OP2	52:AP:127:ARG:NH1	2.47	0.47
57:AU:20:SER:OG	57:AU:61:THR:OG1	2.33	0.47
61:AY:52:ARG:HG3	61:AY:72:SER:HA	1.97	0.47
80:DC:468:THR:HG23	80:DC:478:MET:HE1	1.97	0.47
1:BA:30:GLN:HE21	1:BA:33:GLN:HG2	1.80	0.47
1:BA:120:LEU:HD13	1:BA:142:PRO:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:142:GLY:N	3:BC:153:SER:O	2.45	0.47
5:BG:126:ASP:OD1	5:BG:126:ASP:N	2.48	0.47
34:B5:107:C:H2'	34:B5:108:A:H8	1.80	0.47
34:B5:706:A:N6	34:B5:731:C:OP2	2.48	0.47
36:AB:238:LEU:HD12	36:AB:246:LEU:HA	1.97	0.47
37:AC:11:LEU:HD21	37:AC:156:LEU:HB2	1.96	0.47
38:A1:1750:A:OP1	73:AK:44:LYS:NZ	2.27	0.47
38:A1:2880:U:OP1	58:AV:47:ASN:ND2	2.42	0.47
2:BB:153:HIS:HE1	34:B5:1044:U:H5''	1.80	0.46
4:BE:52:LEU:HD13	4:BE:54:TYR:CD2	2.50	0.46
6:BH:129:LEU:HD23	6:BH:130:VAL:HG23	1.97	0.46
26:BT:130:ARG:O	26:BT:134:ARG:HG2	2.15	0.46
31:Bg:266:ASP:OD1	31:Bg:267:PRO:HD3	2.14	0.46
34:B5:1160:A:H2'	34:B5:1161:C:C6	2.50	0.46
34:B5:1732:A:H2'	34:B5:1733:C:C6	2.49	0.46
36:AB:294:GLY:HA2	36:AB:359:ILE:HD12	1.96	0.46
38:A1:428:A:H2'	38:A1:429:U:C6	2.50	0.46
38:A1:1232:C:H5	38:A1:1261:G:H2'	1.80	0.46
38:A1:2232:A:H2'	38:A1:2233:A:C8	2.50	0.46
38:A1:3028:G:H4'	80:DC:28:VAL:HG21	1.96	0.46
43:AF:92:ILE:HD11	43:AF:110:ARG:HA	1.96	0.46
53:AQ:22:ASP:HA	53:AQ:27:LYS:HE2	1.95	0.46
58:AV:112:SER:O	58:AV:132:ASN:ND2	2.48	0.46
73:AK:5:ILE:HG23	73:AK:10:GLN:NE2	2.30	0.46
3:BC:83:ILE:HG21	3:BC:121:VAL:HG23	1.97	0.46
3:BC:228:ASN:ND2	12:BV:1:MET:HG3	2.30	0.46
3:BC:235:LEU:HD23	12:BV:52:THR:HG23	1.98	0.46
9:BL:75:VAL:HG21	9:BL:117:VAL:HG11	1.96	0.46
9:BL:99:ARG:HB2	14:BX:12:ALA:HB2	1.96	0.46
25:BS:70:VAL:O	25:BS:74:GLN:HG2	2.14	0.46
27:BU:30:LYS:HG3	27:BU:33:GLN:HB2	1.97	0.46
31:Bg:38:ARG:HE	31:Bg:67:ILE:HD12	1.80	0.46
34:B5:47:A:N7	34:B5:98:U:O2'	2.48	0.46
34:B5:179:A:H3'	34:B5:180:A:H8	1.79	0.46
34:B5:384:G:H2'	34:B5:385:A:C8	2.51	0.46
34:B5:1591:C:H2'	34:B5:1592:A:C8	2.48	0.46
38:A1:1498:A:H2'	38:A1:1499:C:C6	2.50	0.46
38:A1:3322:A:H2'	38:A1:3323:A:H8	1.79	0.46
51:AO:20[A]:ALA:HB2	51:AO:80[A]:PHE:HE1	1.79	0.46
56:AT:18:ASP:OD1	56:AT:19:PHE:N	2.49	0.46
62:AZ:16:GLY:C	62:AZ:18:TYR:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:V:27:VAL:HB	81:V:189:GLN:HB3	1.97	0.46
3:BC:103:VAL:HG12	3:BC:190:LEU:HD12	1.97	0.46
34:B5:520:A:H2'	34:B5:521:A:C8	2.50	0.46
34:B5:883:C:H2'	34:B5:884:A:H8	1.81	0.46
34:B5:1589:C:H2'	34:B5:1590:G:C8	2.51	0.46
36:AB:2:SER:OG	38:A1:2943:G:OP2	2.28	0.46
38:A1:149:U:P	50:AN:49:ARG:HH12	2.38	0.46
38:A1:874:U:OP2	38:A1:1907:C:O2'	2.24	0.46
38:A1:2542:U:H4'	38:A1:2543:U:H5'	1.96	0.46
38:A1:2683:U:H2'	38:A1:2684:C:C6	2.51	0.46
80:DC:414:GLN:HB2	80:DC:477:ASN:HD21	1.80	0.46
80:DC:663:VAL:HG13	80:DC:709:MET:SD	2.56	0.46
5:BG:4:ASN:HB2	5:BG:110:ALA:HA	1.97	0.46
5:BG:173:PRO:HG3	34:B5:66:U:C5	2.50	0.46
25:BS:132:ARG:NH2	34:B5:1544:U:H5''	2.31	0.46
33:BM:140:PHE:O	33:BM:143:GLN:NE2	2.33	0.46
34:B5:1593:A:H2'	34:B5:1594:G:C8	2.51	0.46
37:AC:4:PRO:HD2	37:AC:22:LEU:HB2	1.96	0.46
38:A1:656:A:H2'	38:A1:657:A:C8	2.50	0.46
38:A1:1597:C:H2'	38:A1:1598:G:C8	2.50	0.46
38:A1:1667:A:H2'	38:A1:1668:G:C8	2.50	0.46
63:Aa:114:GLY:O	63:Aa:137:LYS:NZ	2.49	0.46
82:EC:6813:A:H2'	82:EC:6814:G:C8	2.51	0.46
14:BX:48:HIS:CD2	14:BX:105:ALA:HB2	2.51	0.46
34:B5:851:U:O2'	54:AR:170:ARG:NH1	2.47	0.46
34:B5:953:G:H2'	34:B5:954:G:H8	1.79	0.46
36:AB:28:ARG:H	36:AB:28:ARG:HG2	1.60	0.46
36:AB:92:TYR:HB3	36:AB:99:LEU:HG	1.97	0.46
38:A1:144:A:OP1	44:AG:193:LYS:NZ	2.41	0.46
38:A1:1097:G:N7	56:AT:116:ARG:NH2	2.64	0.46
38:A1:1336:U:H2'	38:A1:1337:A:C8	2.51	0.46
38:A1:2465:G:H21	79:E:33:GLU:HG3	1.80	0.46
38:A1:3023:U:H2'	38:A1:3024:A:H8	1.80	0.46
40:A4:142:C:H2'	40:A4:143:U:C6	2.50	0.46
54:AR:98:ARG:NH1	54:AR:132:PHE:O	2.48	0.46
78:Ap:38:ASP:HA	78:Ap:45:LYS:HA	1.97	0.46
82:EC:6815:U:H3'	82:EC:6816:A:H5''	1.97	0.46
3:BC:54:GLU:HG2	12:BV:11:LEU:O	2.15	0.46
3:BC:59:HIS:HA	12:BV:15:ARG:HH12	1.81	0.46
4:BE:180:LEU:HD12	4:BE:228:ILE:HG13	1.98	0.46
12:BV:27:ASP:OD1	12:BV:27:ASP:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BW:31:SER:H	13:BW:34:ILE:HD12	1.81	0.46
22:BP:57:MET:HB3	22:BP:61:ARG:NH1	2.31	0.46
34:B5:407:A:H2'	34:B5:408:C:C6	2.50	0.46
35:AA:181:LYS:HB2	38:A1:860:G:C5	2.50	0.46
38:A1:1492:G:O2'	74:A1:48:LYS:NZ	2.49	0.46
40:A4:71:A:O2'	61:AY:52:ARG:NH1	2.49	0.46
51:AO:168[A]:TYR:HE2	51:AO:172[A]:ARG:HE	1.63	0.46
81:V:104:ARG:HA	81:V:104:ARG:HD2	1.80	0.46
4:BE:11:ARG:NH1	4:BE:21:ASP:O	2.49	0.46
4:BE:87:MET:HB2	4:BE:100:ARG:HD2	1.97	0.46
6:BH:49:ILE:HD12	6:BH:175:LYS:HG2	1.98	0.46
8:BJ:18:PRO:O	8:BJ:23:ARG:NH2	2.45	0.46
8:BJ:39:LYS:HG3	34:B5:592:A:OP1	2.16	0.46
11:BO:111:ARG:HD2	16:Ba:58:VAL:N	2.31	0.46
19:BD:64:ARG:HE	21:BK:91:TYR:HE2	1.62	0.46
24:BR:92:ASP:N	24:BR:92:ASP:OD1	2.44	0.46
34:B5:780:A:H4'	34:B5:781:U:H5''	1.98	0.46
34:B5:1114:G:O2'	34:B5:1130:G:O6	2.30	0.46
34:B5:1279:C:H2'	34:B5:1280:4AC:H6	1.97	0.46
34:B5:1508:U:H2'	34:B5:1509:C:C6	2.51	0.46
38:A1:596:C:O2'	43:AF:165:ASP:OD1	2.33	0.46
38:A1:1678:G:OP2	57:AU:77:LYS:NZ	2.47	0.46
42:AE:56:LYS:NZ	42:AE:101:PHE:O	2.49	0.46
45:AH:69:ARG:HD2	45:AH:72:LYS:HD3	1.97	0.46
1:BA:84:ARG:HH12	1:BA:205:ARG:HD2	1.80	0.46
24:BR:32:LYS:NZ	34:B5:1387:G:OP1	2.31	0.46
27:BU:61:LYS:HB2	27:BU:86:ILE:HB	1.98	0.46
34:B5:513:U:H2'	34:B5:514:G:C8	2.49	0.46
34:B5:775:G:N2	34:B5:786:C:O2	2.48	0.46
38:A1:993:G:N3	38:A1:2637:A:H2'	2.30	0.46
38:A1:1460:A:H2'	38:A1:1461:A:H8	1.81	0.46
38:A1:1785:U:H2'	38:A1:1786:G:C8	2.51	0.46
38:A1:2428:U:H2'	38:A1:2429:G:C8	2.51	0.46
38:A1:2478:C:OP2	38:A1:2480:A:N6	2.38	0.46
38:A1:3044:G:H2'	38:A1:3045:G:C8	2.51	0.46
44:AG:156:ASP:OD1	44:AG:156:ASP:N	2.49	0.46
45:AH:10:ILE:HB	45:AH:53:ILE:HB	1.98	0.46
52:AP:35:ALA:HB2	52:AP:58:ILE:HG23	1.97	0.46
55:AS:42:TRP:CD1	55:AS:53:LYS:HE2	2.51	0.46
81:V:144:LYS:O	81:V:151:GLU:HB2	2.15	0.46
82:EC:6899:C:H2'	82:EC:6900:A:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:82:ARG:HA	2:BB:105:PHE:HA	1.97	0.46
4:BE:89:VAL:HG21	4:BE:119:ALA:HB1	1.97	0.46
5:BG:194:LYS:NZ	34:B5:126:A:O2'	2.49	0.46
7:BI:172:ARG:NH1	34:B5:330:G:OP2	2.49	0.46
20:BF:29:ILE:HG13	20:BF:30:PRO:HD2	1.98	0.46
34:B5:919:A:H2'	34:B5:920:U:C6	2.51	0.46
36:AB:226:PHE:O	38:A1:1886:A:O2'	2.32	0.46
36:AB:284:ARG:NH1	36:AB:293:ASN:O	2.49	0.46
37:AC:281:ILE:HD13	53:AQ:28:LEU:HD12	1.97	0.46
38:A1:273:A:H2'	38:A1:274:G:H8	1.81	0.46
38:A1:1517:G:OP1	74:AI:22:PRO:HG3	2.16	0.46
38:A1:2768:U:H2'	38:A1:2769:A:C8	2.49	0.46
38:A1:3358:U:H2'	38:A1:3359:A:C8	2.51	0.46
40:A4:69:U:H2'	40:A4:70:G:O4'	2.16	0.46
43:AF:121:LYS:HB2	56:AT:133:ALA:HB3	1.98	0.46
55:AS:27:MET:HE2	55:AS:27:MET:HB3	1.82	0.46
1:BA:38:PHE:HB3	1:BA:47:VAL:HG13	1.98	0.46
2:BB:88:VAL:HG11	2:BB:96:LEU:HG	1.98	0.46
7:BI:98:LYS:NZ	34:B5:329:G:OP1	2.39	0.46
24:BR:110:VAL:HG21	24:BR:117:LEU:HD13	1.98	0.46
25:BS:137:HIS:ND1	34:B5:1175:U:OP2	2.49	0.46
30:Bd:15:GLY:O	30:Bd:18:SER:OG	2.29	0.46
32:Bf:99:LYS:HE3	34:B5:1228:G:H1'	1.98	0.46
36:AB:214:MET:HE2	36:AB:279:ASN:HB3	1.98	0.46
38:A1:873:C:H3'	38:A1:874:U:H4'	1.97	0.46
38:A1:1798:A:H2'	38:A1:1799:A:C8	2.51	0.46
38:A1:2106:A:H2'	38:A1:2107:A:H8	1.81	0.46
38:A1:3034:C:H5	45:AH:121:LYS:HB2	1.81	0.46
38:A1:3233:C:H2'	38:A1:3234:A:C8	2.51	0.46
80:DC:20:ARG:NE	80:DC:342:LEU:O	2.47	0.46
80:DC:696:ASP:OD2	82:EC:6906:G:O2'	2.33	0.46
8:BJ:27:GLU:HG2	8:BJ:42:ILE:HG21	1.98	0.45
9:BL:132:SER:OG	34:B5:326:G:OP2	2.33	0.45
14:BX:26:GLU:HB2	14:BX:29:TYR:HB3	1.97	0.45
19:BD:42:THR:OG1	19:BD:43:PRO:HD2	2.15	0.45
32:Bf:105:TYR:OH	34:B5:1253:U:OP2	2.28	0.45
34:B5:800:U:H2'	34:B5:801:G:C8	2.51	0.45
34:B5:1476:C:H2'	34:B5:1477:G:C8	2.51	0.45
36:AB:123:TYR:CZ	36:AB:124:LYS:HG3	2.51	0.45
37:AC:95:ARG:NH1	38:A1:366:A:OP1	2.29	0.45
38:A1:86:G:O2'	38:A1:98:G:O6	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:875:G:O2'	38:A1:1891:A:OP1	2.31	0.45
38:A1:2223:A:H2'	38:A1:2224:A:C8	2.51	0.45
38:A1:2724:OMU:OP2	38:A1:2726:C:N4	2.48	0.45
38:A1:3205:G:OP2	38:A1:3206:C:N4	2.47	0.45
41:AD:85:ARG:NH2	41:AD:250:ASP:O	2.50	0.45
53:AQ:67:ILE:HG12	53:AQ:81:VAL:HG11	1.97	0.45
80:DC:288:ILE:HG22	80:DC:289:MET:HE2	1.98	0.45
2:BB:86:LEU:HB3	2:BB:98:THR:HG21	1.97	0.45
6:BH:104:ARG:HG3	34:B5:803:A:C4	2.51	0.45
10:BN:55:ARG:NH2	17:Bb:51:GLN:OE1	2.49	0.45
20:BF:121:ILE:HG13	20:BF:129:PRO:HB3	1.98	0.45
22:BP:76:VAL:HB	22:BP:94:VAL:HG12	1.99	0.45
26:BT:45:MET:SD	34:B5:1476:C:O2'	2.67	0.45
33:BM:62:LEU:HD13	33:BM:75:VAL:HG21	1.98	0.45
34:B5:751:G:H2'	34:B5:752:A:C8	2.49	0.45
38:A1:799:G:OP2	63:Aa:32:ARG:NH1	2.38	0.45
38:A1:1460:A:H2'	38:A1:1461:A:C8	2.51	0.45
40:A4:26:U:H2'	40:A4:27:U:C6	2.51	0.45
40:A4:67:U:H2'	40:A4:68:G:H8	1.81	0.45
48:AL:80:VAL:HG13	48:AL:85:LEU:HD12	1.99	0.45
80:DC:745:SER:O	80:DC:749:LYS:NZ	2.46	0.45
5:BG:3:LEU:HD11	5:BG:27:PHE:CE2	2.52	0.45
20:BF:45:LYS:HG3	20:BF:46:TRP:CD2	2.51	0.45
20:BF:185:ARG:NH1	34:B5:1471:A:OP2	2.45	0.45
22:BP:111:MET:HE2	25:BS:119:ILE:HD12	1.99	0.45
26:BT:75:LYS:NZ	34:B5:1497:U:O3'	2.50	0.45
34:B5:885:G:H2'	34:B5:886:U:C6	2.51	0.45
34:B5:1524:A:H2'	34:B5:1525:A:C8	2.51	0.45
38:A1:12:A:H2'	38:A1:13:A:C8	2.52	0.45
38:A1:715:A:C8	63:Aa:115:LYS:HD3	2.51	0.45
38:A1:1635:G:N2	38:A1:1638:A:OP2	2.34	0.45
38:A1:2277:C:OP1	76:An:19:LYS:NZ	2.49	0.45
38:A1:2662:G:H2'	38:A1:2663:G:C8	2.51	0.45
61:AY:118:LEU:HD11	61:AY:122:LYS:HE2	1.97	0.45
80:DC:571:SER:HB3	80:DC:720:ALA:HB2	1.97	0.45
7:BI:35:ASN:O	7:BI:59:ARG:NH1	2.47	0.45
13:BW:27:ILE:HB	13:BW:61:ILE:HB	1.97	0.45
27:BU:69:LYS:HG2	27:BU:80:GLU:OE2	2.17	0.45
31:Bg:281:TYR:HD2	31:Bg:287:PRO:HD3	1.80	0.45
34:B5:490:C:N4	34:B5:492:A:O4'	2.50	0.45
34:B5:877:G:H22	34:B5:951:A:H2	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1164:G:H2'	34:B5:1165:G:C8	2.51	0.45
34:B5:1393:C:H2'	34:B5:1394:G:H8	1.81	0.45
37:AC:23:PRO:HD2	37:AC:26:PHE:CD2	2.51	0.45
38:A1:67:A:O2'	38:A1:315:C:O2	2.34	0.45
38:A1:1211:U:O2'	55:AS:113:ARG:NH1	2.47	0.45
38:A1:1235:U:N3	38:A1:1263:A:N7	2.64	0.45
52:AP:67:ILE:HB	52:AP:80:LYS:HD2	1.99	0.45
69:Ag:54:ILE:HD11	69:Ag:78:GLY:HA2	1.98	0.45
80:DC:203:TYR:O	80:DC:208:THR:OG1	2.30	0.45
80:DC:747:LEU:HA	80:DC:750:LYS:HB2	1.99	0.45
1:BA:138:TYR:OH	34:B5:1296:A:OP1	2.27	0.45
8:BJ:159:ALA:HB3	8:BJ:162:SER:HB3	1.98	0.45
16:Ba:33:ASP:N	16:Ba:33:ASP:OD1	2.48	0.45
34:B5:514:G:H1	34:B5:543:C:H5	1.65	0.45
34:B5:1285:U:H4'	34:B5:1286:U:O5'	2.15	0.45
34:B5:1533:C:N4	34:B5:1534:G:O6	2.50	0.45
34:B5:1579:U:H2'	34:B5:1580:C:C6	2.51	0.45
36:AB:303:LYS:NZ	36:AB:359:ILE:O	2.42	0.45
38:A1:89:A:N7	53:AQ:171:LYS:NZ	2.64	0.45
38:A1:775:A:O2'	38:A1:777:U:OP2	2.33	0.45
38:A1:1378:U:H2'	38:A1:1379:G:C8	2.52	0.45
38:A1:2468:A:O2'	38:A1:2477:G:N2	2.50	0.45
38:A1:2471:U:H3	38:A1:2474:G:H22	1.64	0.45
54:AR:170:ARG:NH2	54:AR:173:ARG:O	2.38	0.45
79:E:16:LEU:HD22	79:E:206:VAL:HG22	1.98	0.45
82:EC:6923:C:H2'	82:EC:6924:G:C8	2.52	0.45
1:BA:30:GLN:NE2	1:BA:33:GLN:HG2	2.32	0.45
1:BA:70:PRO:HB2	1:BA:94:GLY:H	1.81	0.45
4:BE:100:ARG:HH21	4:BE:118:GLU:HG3	1.81	0.45
19:BD:31:GLU:HA	19:BD:107:PHE:HE2	1.80	0.45
29:Bc:42:ARG:HH12	29:Bc:61:ARG:HD2	1.81	0.45
31:Bg:155:ARG:HH11	31:Bg:203:THR:HA	1.82	0.45
34:B5:835:U:H2'	34:B5:836:U:H5	1.82	0.45
34:B5:1450:U:H2'	34:B5:1451:C:C6	2.51	0.45
34:B5:1484:G:N2	34:B5:1606:C:O2	2.49	0.45
34:B5:1527:C:H2'	34:B5:1528:U:H6	1.80	0.45
35:AA:68:LYS:HD3	35:AA:70:ARG:HE	1.81	0.45
38:A1:118:U:O2	38:A1:121:A:H5''	2.17	0.45
38:A1:172:G:N2	38:A1:245:U:O2	2.46	0.45
38:A1:631:U:H2'	38:A1:632:G:H8	1.82	0.45
38:A1:994:G:N2	38:A1:995:U:O4	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2222:A:H2'	38:A1:2223:A:C8	2.52	0.45
38:A1:2696:A:N7	38:A1:2758:A:N6	2.65	0.45
38:A1:3214:U:OP2	49:AM:128:ARG:NH1	2.42	0.45
43:AF:89:ILE:HD11	43:AF:229:PHE:HB3	1.99	0.45
56:AT:8:ARG:O	56:AT:11:THR:OG1	2.29	0.45
80:DC:586:ILE:HG12	80:DC:691:VAL:HG12	1.98	0.45
3:BC:125:ILE:O	3:BC:129:ILE:HD12	2.17	0.45
5:BG:14:LYS:HA	5:BG:14:LYS:HD2	1.78	0.45
18:Be:38:LEU:HG	18:Be:42:ARG:HE	1.81	0.45
31:Bg:205:SER:OG	31:Bg:207:ASP:OD1	2.31	0.45
34:B5:545:A:H4'	34:B5:546:U:H5'	1.99	0.45
34:B5:884:A:H2'	34:B5:885:G:H8	1.82	0.45
34:B5:948:G:H2'	34:B5:949:C:C6	2.52	0.45
34:B5:1511:U:H2'	34:B5:1512:G:C8	2.52	0.45
37:AC:101:ALA:HA	38:A1:800:G:H22	1.81	0.45
38:A1:550:A:H3'	38:A1:551:A:H8	1.80	0.45
38:A1:1019:G:H1	38:A1:1033:U:H5''	1.82	0.45
38:A1:1221:A:C8	81:V:61:ARG:HD3	2.52	0.45
38:A1:1643:A:H2'	38:A1:1644:C:C2	2.52	0.45
38:A1:2534:G:H2'	38:A1:2535:A:C8	2.52	0.45
38:A1:2701:U:OP1	56:AT:23:GLY:N	2.39	0.45
38:A1:2812:C:H2'	38:A1:2813:A:C8	2.52	0.45
38:A1:3015:G:H2'	38:A1:3016:A:H8	1.82	0.45
38:A1:3162:C:H2'	38:A1:3163:A:C8	2.49	0.45
38:A1:3295:A:H2'	38:A1:3296:A:C8	2.51	0.45
45:AH:22:SER:OG	45:AH:23:ARG:N	2.46	0.45
49:AM:49:PRO:HG3	49:AM:78:THR:HG23	1.98	0.45
50:AN:5:LYS:HZ1	71:AI:37:THR:HG22	1.82	0.45
54:AR:105:LEU:HD22	54:AR:135:LYS:HG3	1.98	0.45
79:E:120:VAL:HG11	79:E:135:PRO:HG3	1.98	0.45
80:DC:27:HIS:HB3	80:DC:30:HIS:HE2	1.80	0.45
80:DC:704:GLN:O	80:DC:708:THR:OG1	2.27	0.45
81:V:146:ALA:HB3	81:V:151:GLU:HG3	1.99	0.45
4:BE:145:ARG:NH1	34:B5:123:G:O2'	2.50	0.45
15:BY:104:SER:HB3	15:BY:107:GLN:HG2	1.98	0.45
16:Ba:17:HIS:NE2	34:B5:1789:G:OP1	2.44	0.45
17:Bb:56:CYS:O	17:Bb:60:SER:OG	2.28	0.45
21:BK:16:PHE:HE2	21:BK:82:LEU:HD13	1.82	0.45
21:BK:44:LYS:HA	21:BK:47:GLN:HB3	1.97	0.45
34:B5:5:U:H2'	34:B5:6:G:H8	1.81	0.45
34:B5:63:G:O2'	34:B5:170:U:OP1	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:90:C:O2'	34:B5:451:A:OP1	2.34	0.45
36:AB:97:ARG:NH2	38:A1:3244:A:OP1	2.49	0.45
38:A1:2703:A:OP2	41:AD:23:ARG:NH2	2.46	0.45
38:A1:2875:U:O2'	38:A1:2876:C:O5'	2.25	0.45
46:AI:193:ASP:CG	46:AI:194:GLY:H	2.24	0.45
5:BG:56:ASN:OD1	34:B5:153:G:N2	2.42	0.45
5:BG:57:ASP:HA	5:BG:106:LEU:HA	1.97	0.45
11:BO:112:ILE:HG22	16:Ba:56:ALA:O	2.17	0.45
11:BO:125:SER:HB3	34:B5:926:A:H2	1.80	0.45
14:BX:93:LEU:HD21	18:Be:8:LEU:HD12	1.98	0.45
22:BP:25:LEU:HA	22:BP:28:MET:HE2	1.99	0.45
23:BQ:14:LYS:HD3	34:B5:1584:G:N7	2.31	0.45
25:BS:116:LEU:HA	25:BS:119:ILE:HG22	1.99	0.45
31:Bg:117:LYS:O	31:Bg:118:LYS:HG2	2.16	0.45
34:B5:1202:A:N6	34:B5:1457:C:OP1	2.48	0.45
36:AB:308:MET:SD	38:A1:3329:U:H5''	2.57	0.45
38:A1:532:A:H2'	38:A1:533:A:C8	2.52	0.45
38:A1:1329:U:OP1	68:Af:17:GLN:NE2	2.33	0.45
47:AJ:15:GLU:OE1	47:AJ:132:ASN:ND2	2.50	0.45
52:AP:60:PHE:HB3	52:AP:64:ASN:HB3	1.97	0.45
61:AY:74:TYR:HD2	61:AY:77:LYS:HB2	1.81	0.45
80:DC:511:LEU:HD21	80:DC:518:VAL:HG21	1.99	0.45
5:BG:52:ILE:HG23	5:BG:109:LEU:HD21	1.98	0.45
5:BG:140:ASN:HA	5:BG:143:LYS:HG2	1.99	0.45
7:BI:172:ARG:O	7:BI:176:SER:OG	2.31	0.45
20:BF:99:MET:HB2	20:BF:180:ARG:HH12	1.82	0.45
20:BF:118:LEU:HA	20:BF:121:ILE:HG12	1.99	0.45
31:Bg:76:ASP:OD1	31:Bg:76:ASP:N	2.49	0.45
33:BM:117:GLY:HA3	34:B5:1228:G:H22	1.82	0.45
34:B5:229:U:OP2	34:B5:230:C:N4	2.48	0.45
34:B5:1210:C:H2'	34:B5:1211:A:C8	2.51	0.45
38:A1:178:U:H2'	38:A1:179:C:C6	2.52	0.45
38:A1:269:G:OP2	50:AN:44:ARG:NH2	2.50	0.45
38:A1:501:A:H2'	38:A1:502:U:C6	2.52	0.45
38:A1:1243:G:N2	38:A1:1270:A:HO2'	2.15	0.45
38:A1:2344:U:H2'	38:A1:2345:A:C8	2.52	0.45
38:A1:2667:A:OP1	47:AJ:51:ARG:NH2	2.50	0.45
43:AF:151:ARG:HE	43:AF:244:ASN:HA	1.81	0.45
6:BH:114:ARG:O	6:BH:117:THR:OG1	2.33	0.44
8:BJ:126:ARG:HD3	18:Be:33:ARG:NE	2.27	0.44
11:BO:52:ARG:HE	34:B5:905:A:H5''	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BX:37:ALA:O	14:BX:41:SER:OG	2.31	0.44
30:Bd:34:TYR:OH	34:B5:1487:A:OP1	2.32	0.44
30:Bd:45:GLU:OE1	30:Bd:46:LYS:HE3	2.17	0.44
34:B5:340:U:H2'	34:B5:341:A:H8	1.82	0.44
34:B5:431:C:H2'	34:B5:432:G:C8	2.52	0.44
34:B5:1237:G:H2'	34:B5:1238:A:H8	1.82	0.44
36:AB:328:ILE:HD12	36:AB:336:VAL:HG21	1.98	0.44
38:A1:1522:U:H3'	60:AX:113:LEU:HD22	1.99	0.44
39:A3:4:U:H2'	39:A3:5:G:C8	2.52	0.44
39:A3:74:C:H2'	39:A3:75:G:C8	2.52	0.44
41:AD:34:LYS:HA	56:AT:27:LEU:HD11	1.98	0.44
41:AD:151:GLN:HG2	41:AD:159:VAL:HG11	1.99	0.44
62:AZ:33:SER:OG	62:AZ:35:SER:O	2.27	0.44
65:Ac:42:ILE:HD11	65:Ac:67:VAL:HG22	2.00	0.44
6:BH:110:GLN:HG2	34:B5:811:A:N7	2.32	0.44
8:BJ:153:GLU:N	8:BJ:153:GLU:OE1	2.49	0.44
15:BY:61:ARG:HH21	15:BY:62:THR:HG22	1.82	0.44
15:BY:105:ARG:HB3	34:B5:443:C:OP2	2.17	0.44
16:Ba:38:ARG:NH1	34:B5:1798:U:OP2	2.48	0.44
19:BD:29:LEU:HD21	19:BD:69:LEU:HD11	1.97	0.44
34:B5:1291:G:H22	34:B5:1324:G:N2	2.14	0.44
35:AA:132:ASN:HD22	35:AA:151:PRO:HB3	1.82	0.44
35:AA:241:ARG:NH1	38:A1:2155:G:OP1	2.50	0.44
38:A1:1017:C:H1'	38:A1:1035:G:H22	1.83	0.44
38:A1:2526:C:H2'	38:A1:2527:G:H8	1.83	0.44
38:A1:3251:U:H2'	38:A1:3252:G:C8	2.52	0.44
47:AJ:115:LYS:HG3	47:AJ:116:TYR:H	1.82	0.44
49:AM:17:VAL:HG11	49:AM:74:ARG:HA	1.99	0.44
80:DC:803:THR:OG1	80:DC:804:LEU:N	2.50	0.44
3:BC:81:MET:HG3	3:BC:211:LEU:HD11	1.98	0.44
5:BG:139:ASN:HD22	34:B5:143:G:P	2.39	0.44
7:BI:113:PHE:HE1	7:BI:119:GLN:HG2	1.82	0.44
8:BJ:140:ILE:HG12	15:BY:65:GLY:HA3	2.00	0.44
10:BN:129:TYR:HA	10:BN:132:VAL:HG12	1.99	0.44
11:BO:81:VAL:HG11	11:BO:102:LEU:HD13	2.00	0.44
11:BO:136:ARG:HD3	11:BO:136:ARG:H	1.82	0.44
14:BX:57:LEU:HB3	18:Be:4:VAL:HG22	1.99	0.44
19:BD:132:LYS:HB2	19:BD:189:MET:SD	2.58	0.44
20:BF:190:ILE:HA	20:BF:193:THR:HG22	1.99	0.44
22:BP:126:VAL:HG11	34:B5:1458:G:H21	1.82	0.44
34:B5:1590:G:H2'	34:B5:1591:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:305:U:O2	38:A1:2784:G:N2	2.50	0.44
38:A1:341:G:O2'	40:A4:22:U:O4	2.34	0.44
38:A1:1035:G:H2'	38:A1:1036:A:C8	2.52	0.44
38:A1:1542:G:H2'	38:A1:1543:G:C8	2.52	0.44
51:AO:58[A]:LEU:HD21	51:AO:74[A]:ARG:HH12	1.83	0.44
53:AQ:41:ASP:OD1	53:AQ:41:ASP:N	2.50	0.44
53:AQ:126:GLN:HA	53:AQ:129:VAL:HG12	1.98	0.44
56:AT:51:GLY:HA3	56:AT:92:ARG:HG3	1.99	0.44
70:Ah:102:GLU:OE1	70:Ah:105:ARG:NH2	2.50	0.44
80:DC:17:THR:OG1	80:DC:91:GLN:NE2	2.51	0.44
82:EC:6813:A:H2'	82:EC:6814:G:H8	1.83	0.44
82:EC:6888:A:H2'	82:EC:6889:A:H2'	1.99	0.44
1:BA:84:ARG:NH1	24:BR:84:TYR:OH	2.50	0.44
7:BI:84:HIS:NE2	7:BI:97:THR:OG1	2.33	0.44
15:BY:38:ASP:OD1	15:BY:38:ASP:N	2.46	0.44
19:BD:27:ARG:NH2	34:B5:1436:A:OP2	2.45	0.44
27:BU:87:HIS:ND1	34:B5:1383:G:OP1	2.46	0.44
31:Bg:252:LEU:HB3	31:Bg:263:PHE:HB2	1.98	0.44
34:B5:89:G:N2	34:B5:451:A:O3'	2.50	0.44
38:A1:422:A:C2	38:A1:2363:A:H4'	2.53	0.44
38:A1:584:G:OP1	42:AE:82:ARG:NH2	2.35	0.44
38:A1:821:U:H2'	38:A1:822:G:C8	2.53	0.44
38:A1:1597:C:H5'	38:A1:1696:A:H1'	1.99	0.44
47:AJ:21:ILE:HG22	47:AJ:23:VAL:HG13	2.00	0.44
80:DC:180:ARG:HD2	81:V:137:GLN:HG2	1.99	0.44
4:BE:233:LYS:HE2	4:BE:233:LYS:HB2	1.86	0.44
5:BG:2:LYS:HB2	5:BG:108:VAL:HG23	1.99	0.44
7:BI:39:GLY:O	7:BI:59:ARG:HB3	2.17	0.44
12:BV:64:GLU:OE2	17:Bb:3:LEU:HD13	2.17	0.44
34:B5:52:U:H2'	34:B5:53:G:C8	2.52	0.44
34:B5:361:C:H5''	34:B5:378:A:H5'	2.00	0.44
34:B5:1483:A:H2'	34:B5:1484:G:C8	2.52	0.44
36:AB:58:ARG:HA	36:AB:357:LYS:HG3	1.99	0.44
38:A1:87:U:H2'	38:A1:88:A:C8	2.52	0.44
38:A1:271:C:O2	71:Ai:82:ARG:NH2	2.42	0.44
38:A1:531:G:H2'	38:A1:532:A:C8	2.52	0.44
38:A1:662:U:H2'	38:A1:663:OMC:C6	2.52	0.44
38:A1:1010:G:N2	46:AI:193:ASP:OD1	2.49	0.44
38:A1:1553:U:H4'	38:A1:1554:U:H5'	2.00	0.44
38:A1:1831:U:O2'	40:A4:114:G:OP1	2.24	0.44
38:A1:1909:A:H2'	38:A1:1910:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2115:G:H22	38:A1:2120:A:H1'	1.83	0.44
41:AD:93:THR:HG1	41:AD:158:ARG:NH1	2.16	0.44
44:AG:115:ALA:O	44:AG:120:LYS:N	2.50	0.44
51:AO:25[A]:LYS:HA	51:AO:25[A]:LYS:HD2	1.78	0.44
80:DC:373:ASP:OD1	80:DC:373:ASP:N	2.49	0.44
2:BB:137:ILE:HG21	2:BB:172:LEU:HD22	1.98	0.44
5:BG:135:PRO:HB3	5:BG:140:ASN:HB3	2.00	0.44
15:BY:26:ASP:OD1	15:BY:26:ASP:N	2.49	0.44
25:BS:66:LEU:HA	25:BS:69:ILE:HG12	1.98	0.44
31:Bg:239:GLU:O	31:Bg:257:ALA:N	2.50	0.44
35:AA:127:ALA:HB2	35:AA:134:VAL:HG23	1.99	0.44
38:A1:1404:G:N2	38:A1:1407:A:OP2	2.35	0.44
44:AG:25:PRO:HB2	62:AZ:125:GLY:H	1.82	0.44
47:AJ:36:VAL:HG23	47:AJ:39:GLN:HE21	1.83	0.44
63:Aa:75:LEU:HB2	63:Aa:116:GLY:H	1.83	0.44
14:BX:43:PHE:HZ	14:BX:104:LEU:HB2	1.82	0.44
21:BK:23:ALA:O	21:BK:64:TYR:HB2	2.18	0.44
26:BT:39:THR:OG1	34:B5:1478:G:OP1	2.29	0.44
34:B5:1061:A:H3'	34:B5:1062:A:H5''	2.00	0.44
34:B5:1170:G:H21	34:B5:1571:C:H4'	1.83	0.44
34:B5:1533:C:H4'	34:B5:1539:G:C6	2.53	0.44
34:B5:1773:4AC:H5	76:An:2:ARG:HH12	1.83	0.44
35:AA:133:TYR:HE1	35:AA:135:ILE:HD11	1.83	0.44
37:AC:65:TRP:HB3	37:AC:69:ARG:HD3	2.00	0.44
38:A1:63:A:OP1	50:AN:169:LYS:NZ	2.51	0.44
38:A1:1804:A:H2'	38:A1:1805:C:C6	2.53	0.44
38:A1:2609:A:H2'	38:A1:2610:G:C8	2.52	0.44
38:A1:2697:A:H2'	38:A1:2698:G:H8	1.82	0.44
38:A1:2854:U:OP1	46:AI:61:SER:OG	2.27	0.44
38:A1:2897:A:H5''	75:Am:125:LYS:HD2	1.98	0.44
39:A3:16:U:H2'	39:A3:17:A:C8	2.52	0.44
68:Af:8:TYR:CE2	68:Af:99:ARG:HG2	2.52	0.44
71:Ai:84:LYS:O	71:Ai:88:GLU:HG3	2.18	0.44
75:Am:99:CYS:HB2	75:Am:114:LYS:HE3	1.98	0.44
80:DC:563:TYR:O	80:DC:564:ARG:NH1	2.45	0.44
80:DC:718:LEU:HA	80:DC:722:PRO:HG3	1.99	0.44
80:DC:823:ARG:NH1	80:DC:829:LYS:O	2.51	0.44
82:EC:6886:A:H2'	82:EC:6887:G:C8	2.52	0.44
6:BH:111:LYS:O	34:B5:811:A:N6	2.40	0.44
13:BW:107:SER:HA	34:B5:804:A:C8	2.52	0.44
34:B5:950:C:H2'	34:B5:951:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1511:U:H2'	34:B5:1512:G:H8	1.83	0.44
36:AB:259:HIS:CE1	38:A1:2366:C:H5'	2.53	0.44
38:A1:838:G:O6	78:Ap:4:ARG:NH1	2.45	0.44
38:A1:1516:C:OP1	74:Al:46:ARG:NH2	2.51	0.44
38:A1:1555:U:H5'	38:A1:1556:C:OP2	2.18	0.44
38:A1:3182:G:O3'	51:AO:161[A]:LYS:NZ	2.50	0.44
39:A3:49:G:C4	41:AD:58:LYS:HE2	2.53	0.44
39:A3:71:G:H2'	39:A3:72:A:C8	2.53	0.44
79:E:10:ARG:HA	79:E:13:VAL:HG12	1.99	0.44
80:DC:171:LYS:HG2	80:DC:274:ASN:OD1	2.18	0.44
80:DC:429:LYS:HG3	80:DC:430:ALA:H	1.82	0.44
1:BA:74:VAL:HB	1:BA:121:VAL:HG12	2.00	0.44
17:Bb:11:THR:HG22	17:Bb:13:ALA:H	1.83	0.44
19:BD:162:GLN:NE2	19:BD:166:ASP:OD1	2.48	0.44
23:BQ:129:PHE:O	23:BQ:137:ARG:NH1	2.50	0.44
28:BZ:95:HIS:NE2	34:B5:1529:C:OP1	2.42	0.44
34:B5:103:A:H4'	34:B5:105:A:C8	2.52	0.44
34:B5:329:G:H2'	34:B5:330:G:C8	2.53	0.44
36:AB:48:GLY:HA3	36:AB:81:THR:HG22	1.98	0.44
38:A1:264:G:OP1	71:Ai:34:SER:HB2	2.18	0.44
38:A1:649:A2M:OP2	38:A1:2868:U:O2'	2.33	0.44
38:A1:1615:C:H2'	38:A1:1616:U:C6	2.53	0.44
56:AT:18:ASP:HB3	56:AT:21:LYS:HB2	2.00	0.44
63:Aa:90:TYR:CD1	63:Aa:100:PRO:HG3	2.53	0.44
64:Ab:32:LEU:HB3	64:Ab:40:ARG:HE	1.83	0.44
80:DC:154:VAL:HG22	80:DC:337:MET:HE2	2.00	0.44
80:DC:158:ASN:OD1	80:DC:214:GLY:N	2.50	0.44
14:BX:99:ASN:HD21	80:DC:505:VAL:HG22	1.83	0.43
25:BS:117:LYS:NZ	25:BS:124:GLY:O	2.46	0.43
31:Bg:109:ASP:HB2	31:Bg:127:ARG:HD3	2.00	0.43
31:Bg:125:GLY:HA2	31:Bg:131:ILE:HA	2.00	0.43
34:B5:368:U:O2'	34:B5:603:U:O2'	2.34	0.43
34:B5:851:U:OP2	54:AR:173:ARG:NH2	2.51	0.43
34:B5:1474:G:H2'	34:B5:1475:A:C8	2.52	0.43
38:A1:268:A:N1	38:A1:295:A:H5'	2.33	0.43
38:A1:1616:U:H2'	38:A1:1617:G:C8	2.53	0.43
38:A1:2427:U:H2'	38:A1:2428:U:C6	2.53	0.43
38:A1:2429:G:H2'	38:A1:2430:A:C8	2.53	0.43
38:A1:2451:G:H2'	38:A1:2452:G:C8	2.53	0.43
43:AF:176:TYR:CZ	43:AF:197:GLN:HG2	2.53	0.43
45:AH:21:LYS:HG3	45:AH:22:SER:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:AY:51:ARG:HG2	61:AY:52:ARG:H	1.83	0.43
78:Ap:33:GLN:HE21	78:Ap:49:ARG:CZ	2.30	0.43
80:DC:71:LYS:HD3	80:DC:71:LYS:HA	1.65	0.43
3:BC:173:PRO:HG2	8:BJ:57:ARG:HD3	2.01	0.43
14:BX:107:PHE:HE1	14:BX:123:LYS:HB3	1.83	0.43
25:BS:112:ASP:OD1	25:BS:115:ARG:NH2	2.51	0.43
38:A1:170:G:C6	38:A1:250:U:H1'	2.53	0.43
38:A1:1184:A:H2'	38:A1:1185:C:C6	2.53	0.43
38:A1:1805:C:H2'	38:A1:1806:A:C8	2.48	0.43
38:A1:2455:U:O4	38:A1:2457:G:N2	2.52	0.43
38:A1:2526:C:H2'	38:A1:2527:G:C8	2.53	0.43
42:AE:82:ARG:HH21	68:Af:104:PRO:HB2	1.83	0.43
42:AE:102:ASN:ND2	42:AE:104:GLU:OE2	2.51	0.43
51:AO:79[A]:ILE:HG21	51:AO:138[A]:LEU:HD11	2.00	0.43
80:DC:472:SER:OG	80:DC:473:GLU:N	2.50	0.43
5:BG:155:ASP:N	5:BG:155:ASP:OD1	2.50	0.43
25:BS:49:LYS:NZ	25:BS:80:LYS:O	2.51	0.43
25:BS:82:PRO:HG2	26:BT:36:ILE:HG12	2.00	0.43
30:Bd:17:GLY:N	34:B5:1205:C:O2	2.38	0.43
32:Bf:97:LYS:HE2	34:B5:1229:G:H3'	2.00	0.43
34:B5:20:G:H5'	34:B5:571:G:C4	2.53	0.43
34:B5:906:A:H2'	34:B5:907:A:C8	2.54	0.43
34:B5:960:U:H2'	34:B5:961:U:C6	2.53	0.43
34:B5:1519:U:H2'	34:B5:1520:U:C5	2.53	0.43
38:A1:616:G:H2'	38:A1:617:G:C8	2.53	0.43
38:A1:1292:C:O2'	38:A1:1293:U:OP1	2.36	0.43
38:A1:1718:G:H2'	38:A1:1719:G:C8	2.53	0.43
38:A1:1829:G:H5''	38:A1:1830:G:H5'	2.01	0.43
40:A4:142:C:H2'	40:A4:143:U:H6	1.83	0.43
47:AJ:125:MET:HE3	47:AJ:127:PHE:CE1	2.54	0.43
50:AN:84:PRO:HA	50:AN:87:GLN:HG3	1.99	0.43
51:AO:96[A]:LYS:O	51:AO:100[A]:GLU:HG3	2.19	0.43
79:E:77:ALA:HB1	79:E:82:VAL:HG23	2.00	0.43
3:BC:139:ILE:HD13	3:BC:191:ALA:HB1	1.99	0.43
5:BG:94:ARG:NH2	34:B5:1673:G:OP1	2.50	0.43
8:BJ:102:GLU:HA	8:BJ:105:LEU:HD12	2.00	0.43
8:BJ:135:ALA:HA	8:BJ:140:ILE:HA	2.00	0.43
10:BN:54:LEU:HB3	10:BN:60:VAL:HB	1.98	0.43
15:BY:86:GLU:OE2	15:BY:90:ARG:NE	2.51	0.43
25:BS:41:ARG:NH1	26:BT:46:PRO:HG3	2.33	0.43
27:BU:57:ARG:HD2	34:B5:1382:A:N3	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:836:U:H2'	34:B5:837:G:H8	1.83	0.43
34:B5:902:G:H1'	34:B5:907:A:N6	2.33	0.43
34:B5:1142:A:H2'	34:B5:1143:A:C8	2.54	0.43
35:AA:14:SER:OG	38:A1:911:C:OP1	2.35	0.43
38:A1:162:G:H2'	38:A1:163:C:C6	2.51	0.43
38:A1:1035:G:H2'	38:A1:1036:A:H8	1.83	0.43
38:A1:1598:G:H2'	38:A1:1599:G:C8	2.53	0.43
38:A1:2882:U:H2'	38:A1:2883:U:C6	2.53	0.43
38:A1:3015:G:H2'	38:A1:3016:A:C8	2.53	0.43
39:A3:94:C:H2'	39:A3:95:A:C8	2.54	0.43
56:AT:99:SER:OG	56:AT:101:CYS:SG	2.71	0.43
80:DC:726:GLU:N	80:DC:802:SER:O	2.44	0.43
2:BB:156:ALA:HB3	2:BB:161:ILE:HD11	2.00	0.43
5:BG:140:ASN:HA	5:BG:143:LYS:HZ2	1.82	0.43
9:BL:49:ILE:HG22	9:BL:50:GLU:HG2	1.99	0.43
10:BN:73:ARG:HD3	34:B5:859:A:C5	2.53	0.43
11:BO:80:HIS:ND1	11:BO:114:ARG:HB2	2.34	0.43
22:BP:18:ARG:HB2	22:BP:36:LEU:HD21	2.00	0.43
22:BP:111:MET:HA	25:BS:119:ILE:HD11	1.99	0.43
25:BS:23:ASP:OD1	25:BS:23:ASP:N	2.50	0.43
25:BS:39:GLY:H	34:B5:1566:U:H5''	1.83	0.43
27:BU:66:SER:HB2	27:BU:81:THR:HG22	2.01	0.43
31:Bg:180:ALA:HB3	31:Bg:190:ALA:HB3	2.01	0.43
33:BM:37:VAL:HG23	33:BM:38:HIS:CD2	2.53	0.43
34:B5:1156:C:H2'	34:B5:1157:A:C8	2.54	0.43
34:B5:1254:U:H3'	34:B5:1255:G:C8	2.52	0.43
34:B5:1628:U:H2'	34:B5:1629:G:H8	1.83	0.43
38:A1:173:G:H5''	38:A1:173:G:C8	2.53	0.43
38:A1:1560:G:O2'	38:A1:1561:G:O4'	2.30	0.43
38:A1:2352:A:H5''	52:AP:83:TRP:O	2.18	0.43
42:AE:84:VAL:O	68:Af:105:SER:OG	2.25	0.43
46:AI:140:THR:HG21	46:AI:148:VAL:HG21	2.00	0.43
49:AM:113:THR:OG1	49:AM:116:GLU:HG3	2.18	0.43
51:AO:42[A]:ASN:ND2	51:AO:136[A]:THR:O	2.49	0.43
71:AI:5:THR:HG23	71:AI:12:ASN:HB2	2.01	0.43
82:EC:6923:C:H2'	82:EC:6924:G:H8	1.83	0.43
1:BA:49:ASN:HD22	1:BA:52:LYS:HE3	1.82	0.43
2:BB:61:LEU:HD22	2:BB:96:LEU:HD11	2.00	0.43
4:BE:59:ARG:HH12	15:BY:87:PRO:HG3	1.84	0.43
5:BG:56:ASN:HB2	5:BG:108:VAL:HG12	2.01	0.43
7:BI:50:GLY:HA2	34:B5:397:A:H4'	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BI:141:ARG:NH1	7:BI:142:LYS:HG3	2.33	0.43
16:Ba:79:ILE:HD11	34:B5:1795:U:H5'	2.01	0.43
20:BF:73:THR:HG22	23:BQ:47:LYS:NZ	2.34	0.43
26:BT:130:ARG:HG2	34:B5:1359:C:H5''	2.01	0.43
31:Bg:170:ILE:HD13	31:Bg:211:ILE:HG12	2.00	0.43
33:BM:137:MET:HA	33:BM:140:PHE:CZ	2.54	0.43
34:B5:545:A:H1'	34:B5:546:U:C6	2.54	0.43
34:B5:1673:G:H22	34:B5:1728:A:H2	1.67	0.43
36:AB:116:ARG:HB3	36:AB:175:LYS:HG3	1.99	0.43
38:A1:185:C:H5''	61:AY:122:LYS:HG2	1.99	0.43
38:A1:643:U:O2'	38:A1:1153:A:N1	2.50	0.43
38:A1:1134:G:O2'	38:A1:2642:A:N3	2.44	0.43
38:A1:1250:G:H2'	38:A1:1251:A:H8	1.84	0.43
38:A1:2203:U:H2'	38:A1:2204:C:H6	1.82	0.43
38:A1:2444:C:H4'	71:AI:63:ASN:ND2	2.33	0.43
38:A1:2454:G:O5'	38:A1:2484:A:N6	2.51	0.43
40:A4:63:G:H22	40:A4:97:A:H2	1.65	0.43
53:AQ:8:LYS:HB3	53:AQ:11:LYS:HE3	2.01	0.43
57:AU:19:VAL:HG12	57:AU:105:LEU:HD13	1.99	0.43
61:AY:51:ARG:CG	61:AY:52:ARG:H	2.32	0.43
2:BB:61:LEU:HD22	2:BB:96:LEU:HD21	2.01	0.43
6:BH:41:LEU:HD22	6:BH:70:PHE:HD1	1.83	0.43
8:BJ:133:HIS:CE1	34:B5:512:A:H4'	2.53	0.43
16:Ba:8:ASN:HB3	34:B5:1791:A:H3'	1.99	0.43
22:BP:57:MET:HB3	22:BP:61:ARG:HH12	1.82	0.43
34:B5:522:U:H2'	34:B5:523:G:O4'	2.18	0.43
34:B5:599:A:H2'	34:B5:600:U:C6	2.53	0.43
34:B5:1231:U:H2'	34:B5:1232:U:C6	2.54	0.43
34:B5:1404:C:H2'	34:B5:1405:G:C8	2.54	0.43
34:B5:1688:U:H3'	34:B5:1689:A:H8	1.84	0.43
34:B5:1767:G:OP1	34:B5:1770:U:H4'	2.19	0.43
37:AC:40:THR:HG23	38:A1:1426:C:H4'	2.01	0.43
38:A1:173:G:H3'	38:A1:174:C:C6	2.52	0.43
38:A1:210:U:C2	38:A1:230:U:H4'	2.53	0.43
38:A1:584:G:H2'	38:A1:585:A:H8	1.83	0.43
38:A1:1120:A:H2'	38:A1:1121:U:C6	2.53	0.43
38:A1:1221:A:P	81:V:61:ARG:HE	2.42	0.43
38:A1:1708:C:H2'	38:A1:1709:C:H6	1.83	0.43
38:A1:1744:G:H2'	38:A1:1745:C:C6	2.53	0.43
38:A1:1807:G:O2'	38:A1:2559:U:O4	2.28	0.43
38:A1:1834:U:OP2	74:AI:10:LYS:NZ	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2961:G:H2'	38:A1:2962:U:C6	2.53	0.43
38:A1:3000:A:H2'	38:A1:3001:C:C6	2.54	0.43
39:A3:17:A:P	47:AJ:150:ASN:HD21	2.42	0.43
45:AH:79:ILE:HA	45:AH:82:VAL:HG12	1.99	0.43
46:AI:192:ASP:OD1	46:AI:193:ASP:N	2.51	0.43
54:AR:105:LEU:HD23	54:AR:138:LEU:HD23	2.00	0.43
54:AR:181:ARG:NH1	54:AR:182:ASP:OD2	2.52	0.43
55:AS:12:ARG:HB2	55:AS:22:PRO:HB2	2.00	0.43
68:Af:19:SER:OG	68:Af:20:LYS:N	2.52	0.43
2:BB:48:VAL:HG12	2:BB:64:ARG:HH21	1.84	0.43
10:BN:25:TRP:HD1	17:Bb:82:LYS:HZ2	1.66	0.43
13:BW:71:LYS:HB3	13:BW:130:TYR:CZ	2.54	0.43
19:BD:220:PRO:O	31:Bg:193:ILE:HG23	2.19	0.43
23:BQ:31:VAL:HG23	23:BQ:67:VAL:HB	2.01	0.43
34:B5:1527:C:H2'	34:B5:1528:U:C6	2.54	0.43
34:B5:1785:U:H2'	34:B5:1786:G:H8	1.83	0.43
36:AB:315:GLY:HA2	38:A1:3379:C:H4'	1.99	0.43
38:A1:729:C:O2'	53:AQ:79:LYS:NZ	2.50	0.43
38:A1:1257:C:H2'	38:A1:1258:U:O4'	2.19	0.43
38:A1:2428:U:H2'	38:A1:2429:G:H8	1.84	0.43
38:A1:2744:U:H2'	38:A1:2745:G:C8	2.53	0.43
43:AF:102:VAL:HG21	43:AF:129:LEU:HD23	2.01	0.43
50:AN:36:ILE:HD11	50:AN:105:ARG:HB3	2.01	0.43
73:Ak:5:ILE:HG22	73:Ak:54:LEU:HD13	2.00	0.43
80:DC:21:ASN:HB3	80:DC:122:THR:HA	2.00	0.43
4:BE:19:LEU:HD13	34:B5:788:A:C6	2.53	0.43
4:BE:36:HIS:NE2	4:BE:88:ASP:OD2	2.51	0.43
5:BG:5:ILE:HD12	5:BG:16:PHE:CD2	2.54	0.43
15:BY:23:PHE:HE1	15:BY:75:VAL:HG12	1.83	0.43
19:BD:25:PHE:HD1	19:BD:29:LEU:HD23	1.84	0.43
23:BQ:28:LEU:HD21	23:BQ:30:LYS:HD3	2.00	0.43
23:BQ:52:LEU:HA	23:BQ:60:PHE:HE2	1.84	0.43
25:BS:132:ARG:NH1	34:B5:1544:U:H5''	2.33	0.43
29:Bc:67:ARG:HA	29:Bc:67:ARG:HD3	1.82	0.43
31:Bg:183:LEU:HG	31:Bg:186:PHE:HE1	1.84	0.43
38:A1:158:G:H2'	38:A1:159:A:H8	1.84	0.43
38:A1:296:A:N3	38:A1:299:G:O2'	2.51	0.43
38:A1:708:G:N2	38:A1:711:A:OP2	2.45	0.43
38:A1:787:G:H2'	38:A1:788:C:C6	2.54	0.43
38:A1:974:G:H5'	53:AQ:16:ARG:HG3	2.01	0.43
38:A1:1307:G:O2'	38:A1:1308:A:N7	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2508:U:H2'	38:A1:2509:U:C6	2.54	0.43
38:A1:3169:U:H2'	38:A1:3170:A:C8	2.54	0.43
79:E:41:TYR:HE2	79:E:159:LEU:HD21	1.84	0.43
82:EC:6801:A:C6	82:EC:6802:A:H1'	2.54	0.43
4:BE:122:LYS:HD2	4:BE:164:LEU:HD12	2.01	0.43
7:BI:138:ASN:OD1	7:BI:139:ALA:N	2.49	0.43
19:BD:141:LYS:HA	19:BD:147:ALA:HA	2.01	0.43
20:BF:193:THR:HA	20:BF:196:GLU:HG2	2.01	0.43
22:BP:119:PHE:HE1	25:BS:121:ALA:HB2	1.84	0.43
24:BR:107:SER:HA	24:BR:110:VAL:HG12	2.01	0.43
25:BS:29:VAL:HG23	25:BS:30:TYR:CD1	2.53	0.43
26:BT:71:VAL:HG13	26:BT:75:LYS:HB2	2.00	0.43
33:BM:59:LEU:O	33:BM:122:VAL:HA	2.18	0.43
34:B5:222:A:H2'	34:B5:223:U:C6	2.54	0.43
38:A1:176:G:H5''	38:A1:176:G:H8	1.83	0.43
38:A1:238:A:O2'	38:A1:239:G:H5'	2.19	0.43
38:A1:748:U:H2'	38:A1:749:C:C6	2.54	0.43
38:A1:791:A:H2'	38:A1:792:G:H8	1.84	0.43
38:A1:1157:G:H2'	38:A1:1158:A:O4'	2.19	0.43
38:A1:1250:G:H2'	38:A1:1251:A:C8	2.54	0.43
38:A1:1524:A:O2'	38:A1:1526:U:OP1	2.36	0.43
38:A1:1629:U:HO2'	38:A1:1630:U:P	2.41	0.43
38:A1:2986:U:H2'	38:A1:2987:A:H8	1.82	0.43
46:AI:66:GLU:OE1	46:AI:69:ARG:NH2	2.52	0.43
50:AN:103:GLU:OE2	50:AN:118:SER:OG	2.29	0.43
53:AQ:44:PHE:HZ	53:AQ:127:LEU:HD21	1.84	0.43
55:AS:91:TYR:O	55:AS:137:ARG:NH2	2.50	0.43
80:DC:150:ARG:HH11	80:DC:196:VAL:HG21	1.84	0.43
80:DC:567:VAL:HG13	80:DC:717:PHE:CE1	2.54	0.43
82:EC:6918:A:H3'	82:EC:6919:G:H8	1.84	0.43
2:BB:152:ARG:HH21	34:B5:1799:U:H2'	1.83	0.42
14:BX:131:SER:HB2	34:B5:30:G:H4'	2.01	0.42
21:BK:44:LYS:NZ	34:B5:1218:G:OP2	2.52	0.42
34:B5:891:A:H2'	34:B5:892:A:H8	1.83	0.42
34:B5:1164:G:H2'	34:B5:1165:G:H8	1.84	0.42
34:B5:1738:U:H2'	34:B5:1739:C:C6	2.54	0.42
38:A1:107:A:O2'	38:A1:324:A:N3	2.44	0.42
38:A1:560:G:OP1	49:AM:83:LYS:NZ	2.34	0.42
38:A1:640:U:H2'	38:A1:641:C:C6	2.53	0.42
38:A1:815:G:OP2	72:Aj:31:LYS:NZ	2.37	0.42
38:A1:951:A:H5''	38:A1:1143:A:N1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1176:C:H2'	38:A1:1177:G:N2	2.34	0.42
38:A1:3324:C:OP1	66:Ad:19:ARG:NH1	2.45	0.42
62:AZ:70:PRO:HG3	62:AZ:115:LYS:HB2	2.00	0.42
1:BA:66:ALA:HB2	12:BV:37:ALA:HB2	2.02	0.42
1:BA:70:PRO:HB3	1:BA:185:ARG:HH22	1.83	0.42
1:BA:75:ALA:HB3	1:BA:86:VAL:HG13	2.00	0.42
2:BB:82:ARG:NH2	2:BB:188:LEU:O	2.49	0.42
6:BH:4:PRO:HA	6:BH:7:LYS:HB2	2.01	0.42
6:BH:56:LYS:HB2	6:BH:88:ARG:HG2	2.01	0.42
13:BW:16:ASN:ND2	34:B5:1037:C:O2	2.53	0.42
14:BX:70:LYS:HG2	14:BX:93:LEU:HD22	2.01	0.42
21:BK:30:ALA:HA	21:BK:38:LYS:HG3	2.01	0.42
25:BS:13:HIS:CG	25:BS:14:ILE:H	2.36	0.42
32:Bf:138:ARG:NH2	34:B5:1235:C:O2	2.50	0.42
33:BM:126:TRP:CD1	33:BM:126:TRP:H	2.36	0.42
34:B5:368:U:HO2'	34:B5:603:U:HO2'	1.67	0.42
34:B5:512:A:H2'	34:B5:513:U:C6	2.54	0.42
34:B5:549:G:H2'	34:B5:550:A:C8	2.53	0.42
34:B5:1133:A:N3	34:B5:1650:U:O2'	2.47	0.42
38:A1:39:A:H5''	63:Aa:35:ALA:HB2	2.01	0.42
38:A1:949:C:O2'	38:A1:971:G:OP1	2.34	0.42
38:A1:1622:U:H2'	38:A1:1623:G:C8	2.54	0.42
38:A1:1718:G:H2'	38:A1:1719:G:H8	1.83	0.42
38:A1:2775:U:H2'	38:A1:2776:C:C6	2.54	0.42
38:A1:3165:A:H2'	38:A1:3166:C:C6	2.54	0.42
42:AE:64:LEU:HD11	42:AE:76:LEU:HD12	2.01	0.42
53:AQ:55:SER:O	53:AQ:59:ARG:HG2	2.19	0.42
58:AV:57:MET:HE3	58:AV:126:TRP:CH2	2.54	0.42
65:Ac:9:SER:HA	65:Ac:12:GLN:HE22	1.85	0.42
79:E:109:ALA:HB1	79:E:133:LYS:HD3	2.00	0.42
80:DC:27:HIS:ND1	80:DC:138:GLN:HB2	2.33	0.42
80:DC:675:PRO:HG3	80:DC:714:TYR:CD1	2.54	0.42
82:EC:6860:A:H61	82:EC:6870:A:H1'	1.84	0.42
3:BC:137:ILE:HG13	3:BC:138:PRO:HD2	2.01	0.42
3:BC:178:ILE:O	3:BC:185:LYS:HD2	2.20	0.42
5:BG:162:VAL:HG21	5:BG:171:LYS:HE2	2.02	0.42
8:BJ:40:LYS:HB2	8:BJ:40:LYS:HE3	1.81	0.42
24:BR:7:LYS:N	34:B5:1316:G:OP1	2.51	0.42
34:B5:16:G:H2'	34:B5:17:C:C6	2.54	0.42
34:B5:29:U:H2'	34:B5:30:G:C8	2.54	0.42
34:B5:199:G:H2'	34:B5:200:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:816:G:H2'	34:B5:817:A:H8	1.83	0.42
34:B5:925:G:H2'	34:B5:926:A:H8	1.83	0.42
34:B5:1164:G:O2'	34:B5:1612:U:O2	2.33	0.42
34:B5:1322:A:H2'	34:B5:1323:C:C6	2.54	0.42
35:AA:220:GLY:O	38:A1:2245:C:O2'	2.36	0.42
38:A1:835:G:HO2'	38:A1:857:G:H22	1.59	0.42
38:A1:1219:C:O2'	38:A1:1286:A:N1	2.43	0.42
38:A1:2351:U:H2'	38:A1:2352:A:C8	2.54	0.42
42:AE:146:ILE:HA	42:AE:149:ILE:HB	2.00	0.42
55:AS:8:GLN:HB3	55:AS:64:ILE:HD11	2.01	0.42
57:AU:79:LEU:HD23	57:AU:79:LEU:HA	1.89	0.42
79:E:89:ASP:N	79:E:89:ASP:OD1	2.51	0.42
80:DC:27:HIS:HB2	80:DC:139:THR:H	1.83	0.42
80:DC:597:VAL:HG21	80:DC:625:TRP:HE1	1.84	0.42
81:V:89:THR:OG1	81:V:90:ASN:N	2.51	0.42
6:BH:64:VAL:HB	6:BH:94:ALA:HB1	2.01	0.42
23:BQ:93:HIS:HD2	23:BQ:97:VAL:HG11	1.83	0.42
28:BZ:83:LEU:HD23	28:BZ:89:ILE:HD13	2.01	0.42
29:Bc:22:ARG:HG2	34:B5:1619:C:C2	2.55	0.42
34:B5:939:A:H2'	34:B5:940:A:C8	2.54	0.42
34:B5:968:U:H2'	34:B5:969:C:O4'	2.19	0.42
34:B5:1461:C:H1'	82:EC:6914:A:N1	2.34	0.42
34:B5:1595:U:H3	34:B5:1600:A:H2	1.66	0.42
34:B5:1690:G:H2'	34:B5:1691:A:C8	2.54	0.42
37:AC:332:LYS:NZ	38:A1:599:C:OP1	2.37	0.42
38:A1:1039:U:H2'	38:A1:1040:A:C8	2.54	0.42
38:A1:1374:G:O6	63:Aa:10:LYS:NZ	2.45	0.42
38:A1:2367:A:H2'	38:A1:2368:A:C8	2.53	0.42
38:A1:2374:C:N4	38:A1:2941:A:O4'	2.52	0.42
39:A3:38:U:N3	39:A3:41:G:OP2	2.42	0.42
41:AD:41:LYS:HB2	56:AT:68:THR:O	2.19	0.42
48:AL:48:PRO:HA	48:AL:137:GLN:HB2	2.01	0.42
58:AV:126:TRP:HB2	58:AV:129:VAL:HB	2.01	0.42
63:Aa:28:HIS:CD2	63:Aa:32:ARG:HG2	2.55	0.42
63:Aa:88:ASP:OD1	63:Aa:88:ASP:N	2.53	0.42
65:Ac:40:LYS:NZ	65:Ac:93:LEU:O	2.37	0.42
15:BY:41:ARG:HE	15:BY:55:VAL:HG13	1.83	0.42
20:BF:123:VAL:O	28:BZ:58:ARG:NH1	2.53	0.42
33:BM:52:LEU:HB3	33:BM:78:LEU:HB3	2.02	0.42
33:BM:114:LYS:NZ	34:B5:1225:U:OP2	2.53	0.42
34:B5:632:U:O2'	34:B5:1103:U:OP1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:778:G:H2'	34:B5:779:U:H2'	2.02	0.42
35:AA:2:GLY:HA2	38:A1:2608:G:OP1	2.20	0.42
35:AA:144:ASN:OD1	35:AA:144:ASN:N	2.52	0.42
36:AB:92:TYR:HB2	36:AB:157:VAL:HB	2.02	0.42
38:A1:671:U:H2'	38:A1:672:A:H8	1.84	0.42
38:A1:3193:C:H2'	38:A1:3194:C:C6	2.54	0.42
38:A1:3337:G:H2'	38:A1:3338:C:C6	2.55	0.42
40:A4:13:A:O2'	52:AP:121:GLN:O	2.33	0.42
3:BC:188:LEU:HD13	3:BC:196:VAL:HG11	2.00	0.42
4:BE:20:LEU:HD21	4:BE:46:VAL:HG13	2.01	0.42
5:BG:143:LYS:HB3	5:BG:143:LYS:HE3	1.85	0.42
10:BN:54:LEU:HD13	10:BN:60:VAL:HG11	2.01	0.42
20:BF:40:ILE:HD11	23:BQ:54:LEU:HB3	2.01	0.42
31:Bg:34:LEU:HB3	31:Bg:73:LEU:HD21	2.02	0.42
31:Bg:262:VAL:HB	31:Bg:271:VAL:HB	2.01	0.42
34:B5:1181:U:O2	34:B5:1458:G:C2	2.72	0.42
34:B5:1449:U:H2'	34:B5:1450:U:H6	1.84	0.42
37:AC:315:LYS:HA	38:A1:505:G:H5''	2.00	0.42
38:A1:412:G:H2'	38:A1:413:U:H6	1.84	0.42
38:A1:1867:A:H2'	38:A1:1868:G:C8	2.55	0.42
38:A1:2419:A:H2'	38:A1:2420:C:C6	2.54	0.42
38:A1:2455:U:N3	38:A1:2483:G:O2'	2.53	0.42
38:A1:2936:A:H2'	38:A1:2937:G:C8	2.55	0.42
53:AQ:71:LEU:HD13	53:AQ:99:THR:HG21	2.02	0.42
79:E:13:VAL:HG11	79:E:180:VAL:HG12	2.01	0.42
79:E:207:LYS:NZ	79:E:208:SER:O	2.41	0.42
80:DC:285:PHE:CD1	80:DC:320:LEU:HD11	2.55	0.42
80:DC:588:LEU:HD12	80:DC:686:VAL:HG13	2.01	0.42
80:DC:774:VAL:HG11	86:DC:903:SO1:H121	2.01	0.42
1:BA:52:LYS:HG2	12:BV:82:VAL:HG22	2.01	0.42
1:BA:57:LEU:HD21	1:BA:176:LEU:HB3	2.00	0.42
4:BE:68:ARG:HG3	4:BE:76:VAL:HG11	2.02	0.42
17:Bb:51:GLN:HB2	34:B5:871:G:O4'	2.19	0.42
22:BP:85:ILE:HA	22:BP:89:MET:SD	2.59	0.42
25:BS:49:LYS:HD3	25:BS:49:LYS:HA	1.83	0.42
32:Bf:90:LYS:HG2	32:Bf:91:ILE:H	1.84	0.42
34:B5:57:G:H2'	34:B5:58:U:C6	2.55	0.42
34:B5:78:A:H2'	34:B5:79:C:C6	2.55	0.42
34:B5:549:G:H2'	34:B5:550:A:H8	1.85	0.42
34:B5:629:U:H2'	34:B5:630:A:H8	1.85	0.42
34:B5:950:C:O2'	34:B5:951:A:OP1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1641:C:H2'	34:B5:1642:G:C8	2.55	0.42
36:AB:188:ILE:HD13	36:AB:188:ILE:HA	1.88	0.42
38:A1:175:C:H2'	38:A1:176:G:C8	2.55	0.42
38:A1:1246:G:H1'	38:A1:1264:G:C8	2.55	0.42
38:A1:1281:G:H3'	38:A1:1282:G:H21	1.84	0.42
38:A1:1619:A:H2'	38:A1:1620:U:O4'	2.19	0.42
38:A1:2261:G:H1'	38:A1:2262:A:H2	1.84	0.42
38:A1:2534:G:H2'	38:A1:2535:A:H8	1.84	0.42
38:A1:2705:A:N6	56:AT:47:SER:O	2.50	0.42
39:A3:23:A:H2'	39:A3:24:A:C8	2.54	0.42
44:AG:214:LEU:O	44:AG:218:ILE:HG12	2.20	0.42
45:AH:103:ILE:HD11	45:AH:134:ILE:HB	2.02	0.42
70:Ah:6:ALA:O	70:Ah:10:ARG:HG2	2.20	0.42
80:DC:760:ARG:HH11	80:DC:763:THR:HG23	1.84	0.42
81:V:93:LEU:HD22	81:V:190:VAL:HG21	2.02	0.42
1:BA:34:GLU:HG3	1:BA:35:PRO:HD3	2.01	0.42
5:BG:78:THR:HA	5:BG:92:ARG:HG2	2.02	0.42
7:BI:12:SER:HG	7:BI:14:THR:HG1	1.67	0.42
7:BI:83:TYR:OH	7:BI:195:ARG:NE	2.52	0.42
19:BD:191:ASP:HB2	19:BD:194:LYS:HG2	2.01	0.42
22:BP:96:ILE:HG21	22:BP:116:LEU:HD13	2.02	0.42
38:A1:20:A:H2'	38:A1:21:G:C8	2.55	0.42
38:A1:2683:U:H2'	38:A1:2684:C:H6	1.84	0.42
38:A1:2696:A:H2'	38:A1:2697:A:C8	2.55	0.42
38:A1:3041:U:H2'	38:A1:3042:U:C6	2.55	0.42
38:A1:3044:G:H2'	38:A1:3045:G:H8	1.85	0.42
38:A1:3110:C:H2'	38:A1:3111:U:C6	2.55	0.42
41:AD:261:THR:O	41:AD:264:GLN:N	2.51	0.42
44:AG:74:THR:HG21	71:Ai:47:ILE:HG23	2.01	0.42
45:AH:9:GLN:HE22	45:AH:52:LEU:HD21	1.84	0.42
46:AI:193:ASP:OD1	46:AI:194:GLY:N	2.50	0.42
68:Af:9:VAL:HG23	68:Af:100:ILE:HB	2.00	0.42
68:Af:31:LYS:NZ	68:Af:78:SER:O	2.52	0.42
80:DC:412:ARG:HH21	80:DC:426:LEU:HD21	1.84	0.42
80:DC:615:ARG:O	80:DC:619:MET:HG3	2.19	0.42
80:DC:632:LYS:HB3	80:DC:648:ASP:OD1	2.20	0.42
81:V:14:LYS:HE2	81:V:18:TYR:CE1	2.54	0.42
82:EC:6793:A:H2'	82:EC:6795:U:H5'	2.01	0.42
82:EC:6881:U:H2'	82:EC:6882:G:H4'	2.01	0.42
7:BI:81:VAL:HG13	7:BI:91:VAL:HG23	2.02	0.42
8:BJ:112:GLN:O	8:BJ:115:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BN:114:ARG:HA	10:BN:114:ARG:HD3	1.95	0.42
15:BY:57:VAL:HB	15:BY:60:PHE:CE2	2.55	0.42
20:BF:116:HIS:O	20:BF:120:ILE:HD12	2.20	0.42
20:BF:149:VAL:HG12	29:Bc:65:ARG:NH1	2.35	0.42
23:BQ:22:VAL:HG22	23:BQ:65:ILE:HD12	2.01	0.42
25:BS:21:ASN:N	25:BS:21:ASN:OD1	2.53	0.42
33:BM:35:ALA:HB1	33:BM:123:VAL:HG13	2.02	0.42
36:AB:299:ASP:OD2	36:AB:301:THR:HG22	2.20	0.42
38:A1:69:C:OP1	50:AN:178:HIS:ND1	2.31	0.42
38:A1:975:C:H2'	38:A1:976:U:C6	2.55	0.42
38:A1:1783:U:H2'	38:A1:1784:G:C8	2.55	0.42
38:A1:2107:A:H2	38:A1:3344:A:H8	1.67	0.42
38:A1:2471:U:O2	38:A1:2475:G:O6	2.37	0.42
38:A1:2585:G:C6	60:AX:24:LEU:HD21	2.55	0.42
51:AO:40[A]:GLU:HG3	51:AO:40[A]:GLU:O	2.20	0.42
55:AS:95:ARG:HB2	55:AS:140:VAL:HG13	2.01	0.42
63:Aa:59:ARG:HE	63:Aa:59:ARG:HB2	1.69	0.42
68:Af:16:TYR:OH	68:Af:89:LEU:O	2.26	0.42
80:DC:565:GLU:HB3	80:DC:717:PHE:HZ	1.85	0.42
82:EC:6849:A:O2'	82:EC:6850:C:O4'	2.37	0.42
5:BG:32:ILE:HD11	5:BG:63:MET:HE3	2.01	0.42
20:BF:219:ARG:HH21	82:EC:6842:U:H5''	1.84	0.42
24:BR:78:ARG:O	24:BR:82:ASP:HB2	2.20	0.42
28:BZ:37:GLN:NE2	28:BZ:38:HIS:HB2	2.35	0.42
31:Bg:217:ASP:OD1	31:Bg:217:ASP:N	2.53	0.42
34:B5:547:U:H1'	34:B5:596:C:H1'	2.02	0.42
34:B5:766:U:H5'	34:B5:767:U:H5''	2.01	0.42
34:B5:973:A:H4'	38:A1:848:A:C8	2.55	0.42
34:B5:1391:A:H2'	34:B5:1392:U:C6	2.55	0.42
37:AC:107:ARG:HA	38:A1:664:U:H5'	2.01	0.42
38:A1:36:C:H4'	38:A1:808:A:C2	2.55	0.42
38:A1:297:G:OP2	38:A1:297:G:N2	2.41	0.42
38:A1:414:U:H2'	38:A1:415:G:H8	1.84	0.42
38:A1:1506:A:H1'	38:A1:1848:G:O6	2.20	0.42
38:A1:2323:G:O2'	38:A1:2325:G:OP2	2.36	0.42
38:A1:2357:A:H2'	38:A1:2358:A:C8	2.55	0.42
38:A1:2471:U:H3	38:A1:2474:G:N2	2.18	0.42
38:A1:2615:G:H2'	38:A1:2616:C:H6	1.85	0.42
49:AM:32:LEU:HD11	49:AM:94:TRP:CD1	2.55	0.42
51:AO:137[A]:THR:H	51:AO:140[A]:LYS:HZ3	1.68	0.42
53:AQ:67:ILE:HG23	53:AQ:81:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:Af:6:ARG:NH1	68:Af:8:TYR:O	2.51	0.42
80:DC:308:LYS:HD2	80:DC:308:LYS:HA	1.84	0.42
80:DC:733:ILE:HB	80:DC:768:VAL:HB	2.02	0.42
82:EC:6835:U:H5''	82:EC:6848:U:C2	2.55	0.42
7:Bl:56:ARG:NH2	34:B5:331:A:H5''	2.36	0.41
20:BF:111:VAL:HG23	23:BQ:43:ILE:HD13	2.02	0.41
20:BF:183:ALA:HB2	20:BF:193:THR:HG21	2.02	0.41
31:Bg:23:LEU:HD11	31:Bg:33:LEU:HD21	2.02	0.41
33:BM:133:LEU:O	33:BM:136:ILE:HG22	2.19	0.41
34:B5:551:G:H2'	34:B5:552:G:H8	1.84	0.41
34:B5:1144:U:H2'	34:B5:1145:U:C6	2.55	0.41
34:B5:1484:G:H2'	34:B5:1485:C:C6	2.55	0.41
38:A1:219:A:O2'	38:A1:220:G:N2	2.44	0.41
38:A1:273:A:H2'	38:A1:274:G:C8	2.55	0.41
38:A1:584:G:H2'	38:A1:585:A:C8	2.54	0.41
38:A1:1234:G:C8	38:A1:1235:U:H2'	2.55	0.41
38:A1:1389:G:H5''	67:Ae:101:SER:HB3	2.01	0.41
46:AI:130:ASP:OD1	46:AI:133:GLN:HB2	2.20	0.41
46:AI:205:SER:OG	46:AI:208:ASN:OD1	2.38	0.41
49:AM:14:LEU:H	49:AM:19:ARG:NH2	2.18	0.41
51:AO:7[A]:VAL:HB	51:AO:33[A]:ILE:HD13	2.01	0.41
57:AU:81:LYS:HE3	57:AU:90:ARG:HH21	1.85	0.41
58:AV:96:GLU:HG3	59:AW:23:ARG:HA	2.02	0.41
77:Ao:28:TYR:HB3	77:Ao:69:VAL:HB	2.01	0.41
77:Ao:32:LYS:HD2	77:Ao:34:SER:N	2.35	0.41
80:DC:87:LYS:HE3	80:DC:87:LYS:HB3	1.87	0.41
81:V:50:VAL:HG12	81:V:88:PHE:HB2	2.01	0.41
1:BA:105:GLY:N	1:BA:135:GLU:OE2	2.46	0.41
1:BA:148:ASP:OD1	1:BA:149:LEU:N	2.43	0.41
17:Bb:11:THR:O	17:Bb:14:SER:OG	2.35	0.41
19:BD:169:ASP:OD1	19:BD:169:ASP:N	2.49	0.41
25:BS:101:LEU:O	25:BS:105:VAL:HG13	2.20	0.41
34:B5:201:G:H2'	34:B5:202:A:H8	1.85	0.41
34:B5:326:G:H2'	34:B5:327:U:C6	2.55	0.41
34:B5:752:A:O2'	34:B5:753:A:OP1	2.37	0.41
34:B5:1117:U:H2'	34:B5:1118:G:C8	2.56	0.41
37:AC:206:LEU:HD23	37:AC:248:VAL:HG22	2.02	0.41
38:A1:371:G:HO2'	38:A1:396:A:H61	1.60	0.41
38:A1:377:A:H1'	38:A1:392:G:N2	2.35	0.41
38:A1:1153:A:O2'	38:A1:1154:A:H5'	2.20	0.41
38:A1:1340:G:H2'	38:A1:1341:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1660:C:H2'	38:A1:1661:G:H8	1.84	0.41
38:A1:1666:G:H2'	38:A1:1667:A:C8	2.55	0.41
38:A1:2966:G:H2'	38:A1:2967:A:C8	2.55	0.41
43:AF:88:ARG:NH1	43:AF:108:LEU:O	2.43	0.41
47:AJ:107:ASP:HA	47:AJ:124:GLY:HA2	2.01	0.41
75:Am:127:LEU:HD23	75:Am:128:LYS:HB3	2.02	0.41
79:E:115:VAL:HG13	79:E:116:LEU:HD12	2.02	0.41
2:BB:130:SER:HB2	2:BB:180:THR:HG22	2.03	0.41
5:BG:3:LEU:HD11	5:BG:27:PHE:HE2	1.84	0.41
5:BG:18:ILE:HD13	5:BG:24:ILE:HD11	2.02	0.41
11:BO:63:ALA:O	11:BO:67:VAL:HG13	2.19	0.41
20:BF:95:ASN:HD22	34:B5:1612:U:P	2.42	0.41
20:BF:127:GLN:HG3	20:BF:128:ASN:H	1.85	0.41
24:BR:57:LEU:HD23	24:BR:57:LEU:HA	1.87	0.41
29:Bc:9:LEU:HD11	29:Bc:53:ILE:HG22	2.01	0.41
34:B5:1267:G:OP1	34:B5:1435:G:N1	2.52	0.41
36:AB:168:LYS:HB3	36:AB:319:ASN:HD21	1.86	0.41
38:A1:87:U:H2'	38:A1:88:A:H8	1.84	0.41
38:A1:1069:C:H2'	38:A1:1070:U:C6	2.55	0.41
38:A1:1412:G:OP1	67:Ae:105:ARG:NH1	2.42	0.41
38:A1:1571:A:H2'	38:A1:1572:U:O4'	2.20	0.41
38:A1:1831:U:H2'	38:A1:1832:C:C6	2.55	0.41
39:A3:95:A:N3	55:AS:119:ARG:HD2	2.35	0.41
45:AH:36:LYS:HE2	45:AH:36:LYS:HB2	1.82	0.41
46:AI:51:HIS:CD2	46:AI:168:SER:HB2	2.55	0.41
47:AJ:52:TYR:HA	47:AJ:61:ARG:HG2	2.01	0.41
51:AO:108[A]:ILE:HD12	51:AO:160[A]:ARG:CZ	2.50	0.41
54:AR:160:GLU:HA	54:AR:163:ARG:HG2	2.02	0.41
54:AR:170:ARG:HE	54:AR:174:ALA:HB2	1.85	0.41
81:V:26:PHE:HB3	81:V:87:VAL:HB	2.02	0.41
2:BB:117:TRP:HB3	2:BB:153:HIS:HA	2.02	0.41
4:BE:160:VAL:HG12	4:BE:172:PHE:HB3	2.02	0.41
6:BH:104:ARG:HG3	34:B5:803:A:C5	2.55	0.41
9:BL:99:ARG:HG2	14:BX:9:LEU:HA	2.02	0.41
18:Be:14:VAL:O	18:Be:18:THR:HG23	2.20	0.41
20:BF:109:LYS:HE2	20:BF:109:LYS:HB2	1.66	0.41
34:B5:340:U:H2'	34:B5:341:A:C8	2.55	0.41
34:B5:460:A:H3'	34:B5:461:G:H8	1.86	0.41
34:B5:480:G:C6	34:B5:508:U:O2	2.73	0.41
34:B5:1524:A:H2	34:B5:1590:G:H1'	1.86	0.41
36:AB:266:ARG:HH22	38:A1:2392:C:H1'	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:AC:93:MET:HB2	38:A1:658:G:N2	2.34	0.41
38:A1:268:A:C4	50:AN:12:ARG:HG2	2.55	0.41
38:A1:270:U:H2'	38:A1:271:C:H6	1.86	0.41
38:A1:945:C:H2'	38:A1:946:U:C6	2.55	0.41
38:A1:1667:A:H2'	38:A1:1668:G:H8	1.85	0.41
38:A1:1738:C:H1'	69:Ag:52:GLN:HE21	1.83	0.41
38:A1:2138:A:C4	72:Aj:3:LYS:HB3	2.56	0.41
38:A1:2413:A:H2'	38:A1:2414:G:C8	2.53	0.41
38:A1:2631:U:H2'	38:A1:2632:G:H8	1.85	0.41
38:A1:2801:A:O2'	38:A1:2802:A:H2'	2.21	0.41
45:AH:22:SER:O	45:AH:23:ARG:HD3	2.20	0.41
69:Ag:79:SER:HB3	69:Ag:80:ARG:HH11	1.85	0.41
73:Ak:28:ASN:HB2	73:Ak:40:GLN:HG2	2.02	0.41
1:BA:52:LYS:HA	12:BV:82:VAL:HG22	2.01	0.41
4:BE:192:ILE:HG13	4:BE:243:GLY:HA3	2.03	0.41
4:BE:252:ARG:NH1	4:BE:253:ASP:OD1	2.53	0.41
10:BN:92:ILE:HG23	10:BN:141:TYR:HE1	1.84	0.41
19:BD:7:LYS:NZ	34:B5:1516:A:OP2	2.38	0.41
21:BK:29:GLN:OE1	21:BK:39:ASN:ND2	2.54	0.41
25:BS:132:ARG:CZ	34:B5:1544:U:H5''	2.50	0.41
34:B5:327:U:H2'	34:B5:328:A:C8	2.56	0.41
34:B5:521:A:H2'	34:B5:522:U:H6	1.85	0.41
34:B5:1467:C:H2'	34:B5:1468:U:C6	2.55	0.41
36:AB:283:TYR:CZ	36:AB:325:LYS:HB2	2.56	0.41
37:AC:119:ARG:NH2	38:A1:696:C:OP2	2.53	0.41
38:A1:805:OMG:H2'	38:A1:936:A:H61	1.84	0.41
38:A1:1230:G:H4'	81:V:33:VAL:O	2.21	0.41
38:A1:1572:U:O2'	38:A1:1573:G:H8	2.03	0.41
38:A1:1620:U:H2'	38:A1:1621:A:C8	2.55	0.41
38:A1:1925:U:O2'	38:A1:1927:G:N7	2.54	0.41
38:A1:2273:G:O2'	38:A1:2311:G:O6	2.34	0.41
38:A1:3294:A:H2'	38:A1:3295:A:O4'	2.20	0.41
58:AV:45:ARG:HD2	58:AV:46:LEU:H	1.85	0.41
77:Ao:8:ARG:O	77:Ao:23:HIS:N	2.53	0.41
80:DC:641:ASN:N	80:DC:641:ASN:OD1	2.53	0.41
2:BB:219:LYS:HD2	2:BB:220:GLN:H	1.86	0.41
23:BQ:52:LEU:HA	23:BQ:60:PHE:CE2	2.56	0.41
25:BS:8:GLN:NE2	28:BZ:44:GLN:OE1	2.54	0.41
31:Bg:151:VAL:HA	31:Bg:173:GLY:HA2	2.02	0.41
34:B5:779:U:O2'	34:B5:780:A:H5'	2.20	0.41
34:B5:855:A:C2	34:B5:857:U:H1'	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:AB:86:VAL:HG22	36:AB:162:VAL:HG12	2.02	0.41
38:A1:860:G:H5'	38:A1:861:C:H5''	2.02	0.41
38:A1:1088:U:C2	38:A1:1089:G:C8	3.08	0.41
38:A1:1128:U:H2'	38:A1:1129:A:O4'	2.20	0.41
38:A1:1222:G:C8	81:V:57:THR:HG21	2.56	0.41
38:A1:1354:G:H1'	42:AE:9:TRP:NE1	2.35	0.41
38:A1:2152:A:H2'	38:A1:2153:U:C6	2.54	0.41
38:A1:2216:G:H22	38:A1:2229:A:H2	1.69	0.41
38:A1:2407:C:H2'	38:A1:2408:U:H6	1.85	0.41
38:A1:2709:C:H2'	38:A1:2710:C:C6	2.56	0.41
38:A1:3006:A:H2'	38:A1:3007:U:O4'	2.21	0.41
38:A1:3089:C:H2'	38:A1:3090:U:O4'	2.20	0.41
79:E:17:LEU:HD22	79:E:176:GLU:HG3	2.02	0.41
80:DC:610:ASP:HB2	80:DC:615:ARG:HE	1.84	0.41
8:BJ:136:VAL:HA	8:BJ:156:ILE:HD13	2.01	0.41
14:BX:46:SER:HB2	34:B5:435:C:C5	2.56	0.41
25:BS:113:LEU:O	25:BS:117:LYS:HG2	2.21	0.41
25:BS:123:ARG:NH2	34:B5:1546:G:OP1	2.52	0.41
31:Bg:152:SER:H	31:Bg:173:GLY:HA2	1.86	0.41
34:B5:1404:C:H2'	34:B5:1405:G:H8	1.85	0.41
34:B5:1624:C:H2'	34:B5:1625:C:C6	2.55	0.41
36:AB:286:GLY:HA3	36:AB:321:PHE:CE1	2.56	0.41
38:A1:239:G:H4'	38:A1:240:U:OP1	2.21	0.41
38:A1:1597:C:H2'	38:A1:1598:G:H8	1.85	0.41
38:A1:2457:G:H21	38:A1:2483:G:H1'	1.85	0.41
38:A1:2834:G:H2'	38:A1:2835:U:H6	1.85	0.41
39:A3:113:C:H2'	39:A3:114:U:O4'	2.21	0.41
1:BA:118:PRO:HG2	1:BA:141:ILE:HD13	2.03	0.41
13:BW:31:SER:HB2	34:B5:636:A:H5''	2.02	0.41
27:BU:64:LYS:O	30:Bd:33:LYS:NZ	2.44	0.41
34:B5:212:U:H2'	34:B5:213:A:H8	1.86	0.41
34:B5:1071:U:H2'	34:B5:1072:C:C6	2.55	0.41
36:AB:128:LYS:HG3	38:A1:3294:A:H5'	2.03	0.41
38:A1:255:A:H2'	38:A1:256:G:C8	2.55	0.41
38:A1:323:A:H2'	38:A1:324:A:C8	2.55	0.41
38:A1:516:A:H2'	38:A1:517:G:C8	2.55	0.41
38:A1:943:U:H3'	63:Aa:13:GLY:HA2	2.02	0.41
38:A1:1217:A:H2'	38:A1:1218:U:C6	2.55	0.41
38:A1:1613:A:OP1	73:Ak:51:LEU:N	2.40	0.41
38:A1:1793:C:OP2	78:Ap:49:ARG:NH2	2.49	0.41
38:A1:2167:A:H2'	38:A1:2168:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2423:U:H2'	38:A1:2424:A:C8	2.55	0.41
38:A1:2520:A:H2'	38:A1:2521:U:C6	2.56	0.41
38:A1:3267:A:H2'	42:AE:69:PHE:CZ	2.56	0.41
43:AF:83:LEU:HD11	43:AF:116:PHE:HB3	2.01	0.41
72:Aj:27:PHE:HA	72:Aj:34:CYS:HA	2.03	0.41
79:E:41:TYR:CE2	79:E:159:LEU:HD21	2.56	0.41
80:DC:602:GLU:CD	80:DC:682:ARG:HH12	2.28	0.41
82:EC:6806:U:H5''	82:EC:6881:U:C4	2.56	0.41
1:BA:73:VAL:HG22	1:BA:120:LEU:HB3	2.02	0.41
2:BB:26:ARG:HA	2:BB:50:LYS:HE2	2.02	0.41
4:BE:3:ARG:HG2	34:B5:399:A:H4'	2.02	0.41
14:BX:54:LEU:HD11	14:BX:75:GLN:HB2	2.03	0.41
20:BF:100:ASN:O	20:BF:102:ARG:N	2.52	0.41
20:BF:135:ASP:HA	20:BF:138:THR:HG22	2.01	0.41
21:BK:12:HIS:HB3	21:BK:80:LEU:HD21	2.03	0.41
25:BS:121:ALA:O	25:BS:124:GLY:N	2.53	0.41
30:Bd:21:CYS:HB3	30:Bd:26:SER:H	1.86	0.41
31:Bg:133:VAL:HB	31:Bg:142:ALA:HB3	2.03	0.41
31:Bg:245:PHE:CE1	31:Bg:252:LEU:HD13	2.54	0.41
33:BM:129:GLU:OE2	33:BM:134:SER:OG	2.39	0.41
34:B5:206:A:H1'	34:B5:262:U:C2	2.56	0.41
34:B5:872:G:H2'	34:B5:873:U:O4'	2.21	0.41
34:B5:887:A:H2'	34:B5:888:U:H6	1.86	0.41
34:B5:1648:A:H2'	34:B5:1649:G:C8	2.55	0.41
38:A1:174:C:H2'	38:A1:175:C:C6	2.56	0.41
38:A1:177:U:O2	38:A1:241:G:C2	2.74	0.41
38:A1:245:U:H2'	38:A1:246:U:C6	2.56	0.41
38:A1:307:A:H2'	38:A1:308:A:H8	1.86	0.41
38:A1:407:A:C2	40:A4:17:A:H1'	2.56	0.41
38:A1:710:A:H2'	38:A1:711:A:C8	2.56	0.41
38:A1:1001:G:N3	38:A1:1041:U:H5'	2.36	0.41
38:A1:1359:C:H2'	38:A1:1360:C:H6	1.86	0.41
38:A1:2407:C:H2'	38:A1:2408:U:C6	2.56	0.41
38:A1:2429:G:H2'	38:A1:2430:A:H8	1.85	0.41
38:A1:3180:A:C4	51:AO:114[A]:LYS:HA	2.56	0.41
38:A1:3234:A:N6	38:A1:3253:G:H1	2.17	0.41
39:A3:90:U:H2'	39:A3:91:G:O4'	2.20	0.41
40:A4:67:U:H5''	72:Aj:85:LYS:O	2.21	0.41
41:AD:108:ARG:NE	41:AD:253:PHE:HB2	2.35	0.41
49:AM:116:GLU:HB3	51:AO:197[A]:LEU:HD22	2.03	0.41
50:AN:23:GLN:NE2	50:AN:24:ARG:HG3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:AS:27:MET:HG3	55:AS:41:TYR:CE1	2.56	0.41
61:AY:74:TYR:CD2	61:AY:77:LYS:HB2	2.56	0.41
80:DC:171:LYS:HA	80:DC:282:PHE:HE2	1.86	0.41
80:DC:363:ASP:OD1	80:DC:364:ALA:N	2.53	0.41
80:DC:578:LYS:HD3	80:DC:585:ARG:NH2	2.36	0.41
81:V:16:ARG:HG2	81:V:66:PHE:HZ	1.86	0.41
82:EC:6876:A:H5''	82:EC:6878:G:H1'	2.03	0.41
2:BB:30:PHE:N	2:BB:46:THR:O	2.54	0.41
9:BL:36:LYS:HG2	9:BL:60:PHE:O	2.21	0.41
19:BD:11:LEU:HD21	27:BU:29:THR:HG23	2.02	0.41
22:BP:31:GLU:O	22:BP:34:VAL:HG12	2.20	0.41
28:BZ:94:LYS:NZ	34:B5:1531:G:OP1	2.47	0.41
32:Bf:118:ARG:NH1	34:B5:1252:C:OP1	2.54	0.41
33:BM:56:GLU:HG3	33:BM:124:LYS:HZ2	1.86	0.41
34:B5:17:C:H2'	34:B5:18:C:C6	2.56	0.41
34:B5:52:U:H2'	34:B5:53:G:H8	1.85	0.41
34:B5:1109:G:H1	34:B5:1136:U:H3	1.69	0.41
34:B5:1350:U:H2'	34:B5:1351:G:C8	2.56	0.41
34:B5:1389:C:N4	34:B5:1391:A:O4'	2.54	0.41
34:B5:1518:C:H2'	34:B5:1519:U:C6	2.56	0.41
34:B5:1645:G:H2'	34:B5:1646:C:H6	1.86	0.41
36:AB:259:HIS:HB3	38:A1:2987:A:O2'	2.21	0.41
38:A1:784:A:OP2	53:AQ:69:ARG:NH1	2.52	0.41
38:A1:959:C:HO2'	38:A1:2410:U:H3	1.64	0.41
38:A1:1069:C:H2'	38:A1:1070:U:H6	1.86	0.41
38:A1:1432:C:O2'	38:A1:1434:G:OP2	2.37	0.41
38:A1:1757:A:H2'	38:A1:1758:G:C8	2.56	0.41
53:AQ:170:ARG:NH1	63:Aa:57:GLY:O	2.54	0.41
68:Af:53:TYR:CZ	68:Af:65:ARG:HB2	2.56	0.41
2:BB:116:LYS:HG3	34:B5:931:C:H5''	2.02	0.40
3:BC:59:HIS:HA	12:BV:15:ARG:NH1	2.35	0.40
4:BE:29:PRO:HG3	34:B5:448:C:OP1	2.22	0.40
19:BD:131:ALA:HA	19:BD:190:ARG:HA	2.02	0.40
31:Bg:54:PHE:CE2	31:Bg:312:VAL:HG11	2.56	0.40
34:B5:849:C:H2'	34:B5:850:A:H8	1.85	0.40
35:AA:3:ARG:HB3	35:AA:207:VAL:O	2.21	0.40
37:AC:321:LYS:HA	37:AC:324:LEU:HB3	2.03	0.40
38:A1:289:A:H2'	38:A1:290:G:H8	1.86	0.40
38:A1:518:G:OP2	38:A1:518:G:N2	2.35	0.40
38:A1:872:U:H2'	38:A1:873:C:C6	2.56	0.40
38:A1:946:U:H2'	38:A1:947:G:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2433:U:H1'	50:AN:125:SER:HB3	2.03	0.40
38:A1:2515:A:N1	38:A1:2594:C:N4	2.63	0.40
38:A1:3094:A:H2'	38:A1:3095:U:C6	2.56	0.40
41:AD:143:LYS:HE2	41:AD:143:LYS:HB3	1.89	0.40
41:AD:179:ARG:HD3	41:AD:179:ARG:HA	1.84	0.40
43:AF:130:ILE:HD12	43:AF:134:VAL:HG11	2.02	0.40
44:AG:251:LYS:HG3	44:AG:252:ASN:OD1	2.21	0.40
48:AL:123:ILE:HD13	48:AL:123:ILE:HA	1.88	0.40
80:DC:459:ILE:O	80:DC:463:LEU:HD23	2.21	0.40
4:BE:126:VAL:HG13	4:BE:139:VAL:HG13	2.03	0.40
6:BH:67:LEU:HD12	6:BH:71:HIS:NE2	2.36	0.40
9:BL:79:LYS:HB3	34:B5:346:G:H5'	2.03	0.40
20:BF:146:THR:OG1	20:BF:157:ARG:HB3	2.21	0.40
20:BF:219:ARG:HA	20:BF:222:LYS:CE	2.48	0.40
25:BS:41:ARG:NH2	26:BT:36:ILE:O	2.47	0.40
31:Bg:155:ARG:NH1	31:Bg:204:ALA:H	2.20	0.40
34:B5:1393:C:H2'	34:B5:1394:G:C8	2.56	0.40
34:B5:1478:G:H2'	34:B5:1479:A:H8	1.86	0.40
34:B5:1639:OMC:H2'	34:B5:1640:C:O4'	2.21	0.40
36:AB:222:LYS:HE2	36:AB:331:ASN:HB3	2.03	0.40
36:AB:232:ARG:HD3	36:AB:233:TRP:NE1	2.37	0.40
38:A1:13:A:H4'	60:AX:39:LYS:HG2	2.03	0.40
38:A1:432:G:OP1	68:Af:65:ARG:NH2	2.51	0.40
38:A1:1253:U:O2'	38:A1:1263:A:H5''	2.21	0.40
38:A1:2674:A:H5''	47:AJ:105:GLY:HA3	2.03	0.40
43:AF:98:LYS:HG2	43:AF:129:LEU:HD21	2.02	0.40
52:AP:3:ARG:O	52:AP:18:ARG:NH2	2.54	0.40
80:DC:558:PRO:HA	80:DC:559:PRO:HD3	1.97	0.40
81:V:12:PHE:O	81:V:16:ARG:HG3	2.22	0.40
9:BL:78:THR:HA	9:BL:84:ILE:HG22	2.03	0.40
9:BL:155:LYS:HD3	10:BN:83:GLU:HA	2.03	0.40
23:BQ:89:LEU:HD21	23:BQ:105:LEU:HD22	2.02	0.40
28:BZ:91:PRO:HB3	28:BZ:101:TYR:CE1	2.57	0.40
31:Bg:23:LEU:HD21	31:Bg:302:PHE:HB3	2.03	0.40
31:Bg:248:ASN:ND2	31:Bg:249:ARG:HH11	2.17	0.40
34:B5:162:A:C2'	34:B5:163:G:H5'	2.50	0.40
34:B5:990:C:H2'	34:B5:991:G:O4'	2.21	0.40
34:B5:1617:U:H2'	34:B5:1618:C:C6	2.57	0.40
34:B5:1669:U:H2'	34:B5:1670:G:O4'	2.21	0.40
34:B5:1753:A:H2'	34:B5:1754:A:C8	2.56	0.40
35:AA:37:ARG:NH2	38:A1:2525:G:OP2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:AA:180:LEU:HD11	78:Ap:26:VAL:HG21	2.04	0.40
38:A1:226:C:H2'	38:A1:227:G:O4'	2.22	0.40
38:A1:571:U:H2'	38:A1:572:A:H8	1.85	0.40
38:A1:1104:G:H2'	38:A1:1105:A:C8	2.57	0.40
38:A1:1341:U:H2'	38:A1:1342:C:C6	2.56	0.40
38:A1:1562:C:H2'	38:A1:1563:C:C6	2.57	0.40
38:A1:2656:A:H4'	77:Ao:98:LYS:HD2	2.02	0.40
38:A1:2999:U:H2'	38:A1:3000:A:C8	2.57	0.40
39:A3:16:U:H2'	39:A3:17:A:H8	1.86	0.40
47:AJ:93:ASP:HB2	47:AJ:172:LEU:HB2	2.03	0.40
52:AP:67:ILE:HD12	52:AP:82:ARG:CZ	2.52	0.40
61:AY:42:GLN:HE21	61:AY:127:GLU:HB2	1.87	0.40
61:AY:103:LYS:HA	61:AY:103:LYS:HD3	1.94	0.40
62:AZ:136:PHE:O	69:Ag:76:TYR:OH	2.38	0.40
71:Ai:74:LYS:HD2	71:Ai:80:PHE:HD1	1.87	0.40
80:DC:215:LEU:HD12	85:DC:901:GDP:H2'	2.03	0.40
80:DC:607:ASN:O	80:DC:615:ARG:NE	2.55	0.40
80:DC:634:TRP:CG	80:DC:660:LYS:HE3	2.56	0.40
81:V:136:PHE:HE1	81:V:172:LEU:HB2	1.86	0.40
82:EC:6822:U:H2'	82:EC:6823:U:H5''	2.03	0.40
1:BA:30:GLN:HE22	1:BA:32:HIS:HB2	1.86	0.40
4:BE:138:TYR:CD2	4:BE:146:THR:HG23	2.56	0.40
6:BH:35:LYS:HD3	6:BH:35:LYS:HA	1.87	0.40
18:Be:30:PRO:HB2	18:Be:34:ALA:HB3	2.03	0.40
19:BD:164:VAL:O	19:BD:168:ILE:HB	2.22	0.40
26:BT:12:GLN:NE2	34:B5:1529:C:O2	2.54	0.40
27:BU:42:VAL:HA	27:BU:52:LYS:HZ2	1.87	0.40
31:Bg:91:LEU:O	31:Bg:100:TYR:N	2.49	0.40
34:B5:14:C:H2'	34:B5:15:U:C6	2.56	0.40
34:B5:1002:G:O6	34:B5:1003:A:N6	2.54	0.40
36:AB:331:ASN:OD1	36:AB:331:ASN:N	2.55	0.40
36:AB:380:MET:HE3	36:AB:380:MET:HB3	1.89	0.40
38:A1:429:U:H2'	38:A1:430:U:H6	1.86	0.40
38:A1:791:A:H2'	38:A1:792:G:C8	2.57	0.40
38:A1:999:G:H2'	38:A1:1000:C:C6	2.56	0.40
38:A1:1433:A:N7	67:Ae:19:ARG:NH2	2.68	0.40
38:A1:1920:U:O2'	38:A1:1932:A:N7	2.52	0.40
38:A1:2828:G:H5'	46:AI:8:CYS:SG	2.61	0.40
41:AD:173:VAL:O	41:AD:175:HIS:ND1	2.54	0.40
63:Aa:105:LEU:HD12	63:Aa:105:LEU:HA	1.95	0.40
63:Aa:117:ARG:HD3	63:Aa:117:ARG:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:Ae:89:THR:HG22	67:Ae:117:ILE:HG12	2.03	0.40
79:E:117:ILE:HG23	79:E:118:LYS:H	1.87	0.40
82:EC:6828:G:H2'	82:EC:6829:A:H8	1.85	0.40
1:BA:88:LYS:HB3	1:BA:202:TYR:CZ	2.56	0.40
2:BB:140:ILE:HB	2:BB:213:ARG:HD3	2.03	0.40
10:BN:61:THR:HB	34:B5:959:U:C6	2.56	0.40
20:BF:104:ASN:HD22	20:BF:104:ASN:HA	1.69	0.40
34:B5:560:U:H2'	34:B5:561:G:H8	1.87	0.40
34:B5:569:C:H2'	34:B5:570:A:O4'	2.22	0.40
34:B5:918:U:H2'	34:B5:919:A:C8	2.57	0.40
36:AB:95:THR:HG22	36:AB:97:ARG:H	1.86	0.40
38:A1:38:U:H4'	63:Aa:32:ARG:HD2	2.03	0.40
38:A1:1257:C:H4'	81:V:46:ARG:HH22	1.87	0.40
38:A1:2986:U:H2'	38:A1:2987:A:C8	2.56	0.40
40:A4:39:G:H1'	40:A4:104:A:N6	2.37	0.40
44:AG:78:PHE:C	44:AG:80:TYR:H	2.29	0.40
44:AG:162:LEU:HD23	50:AN:7:LEU:HD11	2.02	0.40
55:AS:79:VAL:HG11	55:AS:106:LEU:HD21	2.03	0.40
79:E:35:GLN:H	79:E:205:VAL:HB	1.87	0.40
80:DC:464:LEU:O	80:DC:465:LYS:HG2	2.22	0.40
80:DC:740:VAL:HG21	80:DC:766:PHE:HD2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	204/252 (81%)	181 (89%)	23 (11%)	0	100	100
2	BB	212/255 (83%)	188 (89%)	24 (11%)	0	100	100
3	BC	215/254 (85%)	206 (96%)	9 (4%)	0	100	100
4	BE	258/261 (99%)	233 (90%)	25 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	BG	224/236 (95%)	220 (98%)	4 (2%)	0	100	100
6	BH	182/190 (96%)	168 (92%)	14 (8%)	0	100	100
7	BI	184/200 (92%)	164 (89%)	20 (11%)	0	100	100
8	BJ	183/197 (93%)	171 (93%)	12 (7%)	0	100	100
9	BL	153/156 (98%)	142 (93%)	11 (7%)	0	100	100
10	BN	148/151 (98%)	135 (91%)	13 (9%)	0	100	100
11	BO	125/137 (91%)	111 (89%)	14 (11%)	0	100	100
12	BV	85/87 (98%)	74 (87%)	11 (13%)	0	100	100
13	BW	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
14	BX	142/145 (98%)	131 (92%)	11 (8%)	0	100	100
15	BY	132/135 (98%)	123 (93%)	9 (7%)	0	100	100
16	Ba	95/119 (80%)	82 (86%)	13 (14%)	0	100	100
17	Bb	79/82 (96%)	69 (87%)	10 (13%)	0	100	100
18	Be	58/63 (92%)	52 (90%)	6 (10%)	0	100	100
19	BD	221/240 (92%)	211 (96%)	10 (4%)	0	100	100
20	BF	204/225 (91%)	185 (91%)	19 (9%)	0	100	100
21	BK	94/105 (90%)	85 (90%)	9 (10%)	0	100	100
22	BP	122/142 (86%)	113 (93%)	9 (7%)	0	100	100
23	BQ	139/143 (97%)	134 (96%)	5 (4%)	0	100	100
24	BR	117/136 (86%)	108 (92%)	9 (8%)	0	100	100
25	BS	143/146 (98%)	130 (91%)	13 (9%)	0	100	100
26	BT	139/144 (96%)	128 (92%)	11 (8%)	0	100	100
27	BU	105/121 (87%)	98 (93%)	7 (7%)	0	100	100
28	BZ	67/108 (62%)	64 (96%)	3 (4%)	0	100	100
29	Bc	61/67 (91%)	55 (90%)	6 (10%)	0	100	100
30	Bd	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
31	Bg	310/319 (97%)	278 (90%)	32 (10%)	0	100	100
32	Bf	73/152 (48%)	70 (96%)	3 (4%)	0	100	100
33	BM	122/143 (85%)	111 (91%)	11 (9%)	0	100	100
35	AA	245/254 (96%)	232 (95%)	13 (5%)	0	100	100
36	AB	383/387 (99%)	364 (95%)	19 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	AC	359/362 (99%)	340 (95%)	19 (5%)	0	100	100
41	AD	290/297 (98%)	276 (95%)	14 (5%)	0	100	100
42	AE	152/176 (86%)	143 (94%)	9 (6%)	0	100	100
43	AF	220/244 (90%)	210 (96%)	10 (4%)	0	100	100
44	AG	228/256 (89%)	209 (92%)	19 (8%)	0	100	100
45	AH	188/191 (98%)	171 (91%)	17 (9%)	0	100	100
46	AI	201/221 (91%)	191 (95%)	10 (5%)	0	100	100
47	AJ	167/174 (96%)	150 (90%)	17 (10%)	0	100	100
48	AL	191/199 (96%)	178 (93%)	13 (7%)	0	100	100
49	AM	134/138 (97%)	128 (96%)	6 (4%)	0	100	100
50	AN	201/204 (98%)	192 (96%)	9 (4%)	0	100	100
51	AO	195/199 (98%)	193 (99%)	2 (1%)	0	100	100
52	AP	171/184 (93%)	165 (96%)	6 (4%)	0	100	100
53	AQ	183/186 (98%)	178 (97%)	5 (3%)	0	100	100
54	AR	186/189 (98%)	178 (96%)	8 (4%)	0	100	100
55	AS	170/178 (96%)	162 (95%)	8 (5%)	0	100	100
56	AT	157/160 (98%)	148 (94%)	9 (6%)	0	100	100
57	AU	98/121 (81%)	92 (94%)	6 (6%)	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%)	115 (97%)	4 (3%)	0	100	100
61	AY	124/127 (98%)	118 (95%)	6 (5%)	0	100	100
62	AZ	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
63	Aa	146/149 (98%)	131 (90%)	15 (10%)	0	100	100
64	Ab	56/59 (95%)	50 (89%)	6 (11%)	0	100	100
65	Ac	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
66	Ad	107/113 (95%)	103 (96%)	4 (4%)	0	100	100
67	Ae	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
68	Af	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
69	Ag	110/121 (91%)	107 (97%)	3 (3%)	0	100	100
70	Ah	117/120 (98%)	113 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	Ai	97/100 (97%)	90 (93%)	7 (7%)	0	100	100
72	Aj	85/88 (97%)	80 (94%)	5 (6%)	0	100	100
73	Ak	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
74	Al	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
75	Am	50/128 (39%)	49 (98%)	1 (2%)	0	100	100
76	An	23/25 (92%)	23 (100%)	0	0	100	100
77	Ao	103/106 (97%)	89 (86%)	14 (14%)	0	100	100
78	Ap	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
79	E	215/217 (99%)	198 (92%)	17 (8%)	0	100	100
80	DC	819/842 (97%)	768 (94%)	51 (6%)	0	100	100
81	V	187/312 (60%)	176 (94%)	11 (6%)	0	100	100
All	All	12115/13257 (91%)	11334 (94%)	781 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	110/124 (89%)	110 (100%)	0	100	100
25	BS	128/129 (99%)	128 (100%)	0	100	100
26	BT	113/116 (97%)	113 (100%)	0	100	100
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	134/153 (88%)	134 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	AI	176/187 (94%)	176 (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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	Ao	90/91 (99%)	90 (100%)	0	100	100
78	Ap	71/72 (99%)	71 (100%)	0	100	100
79	E	198/198 (100%)	198 (100%)	0	100	100
80	DC	699/714 (98%)	699 (100%)	0	100	100
81	V	160/254 (63%)	160 (100%)	0	100	100
All	All	10346/11154 (93%)	10346 (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 (180) such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	30	GLN
1	BA	33	GLN
1	BA	49	ASN
1	BA	140	ASN
2	BB	194	ASN
2	BB	209	ASN
3	BC	150	GLN
3	BC	152	HIS
3	BC	201	ASN
3	BC	220	ASN
4	BE	17	HIS
4	BE	157	ASN
4	BE	201	HIS
4	BE	216	ASN
5	BG	119	GLN
5	BG	182	GLN
5	BG	201	GLN
6	BH	11	GLN
6	BH	22	GLN
6	BH	74	GLN
6	BH	89	HIS
7	BI	20	GLN
7	BI	32	GLN
7	BI	87	ASN
7	BI	159	GLN
8	BJ	48	GLN
8	BJ	123	HIS
9	BL	98	ASN

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Mol	Chain	Res	Type
10	BN	21	ASN
10	BN	58	HIS
10	BN	78	ASN
10	BN	105	ASN
12	BV	70	ASN
13	BW	64	GLN
13	BW	70	ASN
14	BX	18	HIS
14	BX	22	ASN
14	BX	63	GLN
14	BX	75	GLN
14	BX	89	ASN
14	BX	94	ASN
15	BY	22	GLN
15	BY	34	ASN
15	BY	77	ASN
18	Be	51	ASN
19	BD	159	HIS
19	BD	165	ASN
19	BD	174	HIS
20	BF	37	GLN
20	BF	63	GLN
20	BF	100	ASN
20	BF	103	ASN
20	BF	104	ASN
20	BF	224	ASN
21	BK	9	ASN
21	BK	13	GLN
21	BK	47	GLN
22	BP	103	ASN
23	BQ	77	GLN
23	BQ	93	HIS
24	BR	62	GLN
25	BS	8	GLN
25	BS	12	GLN
25	BS	25	ASN
25	BS	44	ASN
26	BT	64	HIS
26	BT	77	ASN
27	BU	44	ASN
28	BZ	37	GLN
28	BZ	38	HIS

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Mol	Chain	Res	Type
29	Bc	27	GLN
31	Bg	52	GLN
31	Bg	69	GLN
31	Bg	159	ASN
33	BM	38	HIS
35	AA	47	GLN
35	AA	79	ASN
35	AA	86	GLN
35	AA	132	ASN
35	AA	211	HIS
35	AA	215	ASN
36	AB	121	ASN
36	AB	198	HIS
36	AB	212	ASN
36	AB	313	HIS
36	AB	319	ASN
37	AC	5	GLN
37	AC	9	HIS
37	AC	48	GLN
37	AC	229	ASN
37	AC	260	GLN
41	AD	81	HIS
42	AE	172	HIS
43	AF	64	GLN
43	AF	104	GLN
43	AF	166	ASN
43	AF	194	HIS
43	AF	199	ASN
43	AF	200	ASN
44	AG	28	HIS
45	AH	9	GLN
45	AH	37	ASN
45	AH	51	GLN
45	AH	58	HIS
45	AH	100	ASN
45	AH	116	ASN
45	AH	139	ASN
46	AI	59	GLN
47	AJ	39	GLN
47	AJ	62	ASN
47	AJ	90	GLN
47	AJ	101	ASN

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Mol	Chain	Res	Type
47	AJ	109	HIS
48	AL	103	ASN
48	AL	114	GLN
48	AL	120	GLN
48	AL	129	ASN
48	AL	137	GLN
49	AM	119	GLN
50	AN	86	ASN
52	AP	97	ASN
52	AP	133	HIS
53	AQ	45	ASN
53	AQ	126	GLN
54	AR	66	HIS
54	AR	68	GLN
54	AR	166	ASN
55	AS	62	ASN
55	AS	157	GLN
56	AT	5	HIS
56	AT	103	GLN
56	AT	112	ASN
56	AT	134	GLN
57	AU	87	ASN
58	AV	98	ASN
58	AV	132	ASN
60	AX	85	GLN
61	AY	42	GLN
61	AY	81	GLN
61	AY	98	ASN
62	AZ	78	ASN
64	Ab	42	ASN
66	Ad	57	GLN
66	Ad	87	ASN
67	Ae	13	HIS
67	Ae	20	HIS
67	Ae	71	HIS
68	Af	87	ASN
69	Ag	3	GLN
69	Ag	33	GLN
69	Ag	52	GLN
70	Ah	99	GLN
71	Ai	63	ASN
71	Ai	91	ASN

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Mol	Chain	Res	Type
73	Ak	10	GLN
73	Ak	40	GLN
73	Ak	57	ASN
74	Al	19	GLN
74	Al	33	ASN
74	Al	43	ASN
75	Am	120	GLN
77	Ao	59	HIS
77	Ao	105	GLN
78	Ap	25	GLN
78	Ap	33	GLN
79	E	21	ASN
79	E	119	GLN
79	E	197	ASN
79	E	200	ASN
80	DC	108	HIS
80	DC	461	GLN
80	DC	528	HIS
80	DC	603	ASN
80	DC	607	ASN
80	DC	644	ASN
80	DC	649	GLN
80	DC	654	GLN
81	V	103	ASN
81	V	125	ASN
81	V	193	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	B5	1780/1798 (98%)	420 (23%)	15 (0%)
38	A1	3194/3360 (95%)	573 (17%)	17 (0%)
39	A3	120/121 (99%)	11 (9%)	1 (0%)
40	A4	157/158 (99%)	31 (19%)	0
82	EC	196/202 (97%)	116 (59%)	10 (5%)
All	All	5447/5639 (96%)	1151 (21%)	43 (0%)

All (1151) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	B5	2	A

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Mol	Chain	Res	Type
34	B5	4	C
34	B5	17	C
34	B5	26	A
34	B5	34	G
34	B5	42	G
34	B5	43	A
34	B5	45	U
34	B5	46	A
34	B5	47	A
34	B5	57	G
34	B5	60	U
34	B5	63	G
34	B5	67	A
34	B5	68	A
34	B5	72	A
34	B5	73	U
34	B5	74	U
34	B5	75	U
34	B5	77	U
34	B5	81	G
34	B5	97	C
34	B5	101	U
34	B5	104	A
34	B5	114	C
34	B5	115	G
34	B5	127	G
34	B5	129	U
34	B5	130	C
34	B5	131	C
34	B5	132	U
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	145	A
34	B5	158	U
34	B5	162	A
34	B5	163	G
34	B5	166	C

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Mol	Chain	Res	Type
34	B5	176	C
34	B5	178	U
34	B5	179	A
34	B5	181	A
34	B5	188	A
34	B5	190	C
34	B5	191	C
34	B5	192	U
34	B5	193	U
34	B5	194	U
34	B5	195	G
34	B5	196	G
34	B5	198	A
34	B5	200	A
34	B5	204	G
34	B5	217	A
34	B5	218	A
34	B5	224	C
34	B5	225	A
34	B5	226	A
34	B5	227	U
34	B5	228	G
34	B5	229	U
34	B5	230	C
34	B5	233	C
34	B5	234	G
34	B5	240	U
34	B5	241	U
34	B5	246	G
34	B5	250	C
34	B5	260	U
34	B5	261	U
34	B5	262	U
34	B5	265	A
34	B5	276	C
34	B5	278	U
34	B5	280	U
34	B5	287	G
34	B5	299	A
34	B5	305	C
34	B5	314	C
34	B5	316	A

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Mol	Chain	Res	Type
34	B5	319	U
34	B5	320	U
34	B5	321	C
34	B5	322	G
34	B5	333	A
34	B5	337	G
34	B5	338	C
34	B5	346	G
34	B5	352	A
34	B5	353	A
34	B5	359	A
34	B5	360	A
34	B5	361	C
34	B5	390	G
34	B5	396	G
34	B5	400	A
34	B5	401	A
34	B5	402	C
34	B5	419	G
34	B5	423	G
34	B5	424	C
34	B5	425	A
34	B5	426	G
34	B5	427	C
34	B5	434	G
34	B5	439	U
34	B5	444	C
34	B5	452	A
34	B5	459	G
34	B5	460	A
34	B5	470	A
34	B5	473	A
34	B5	475	A
34	B5	477	A
34	B5	480	G
34	B5	484	C
34	B5	485	A
34	B5	486	G
34	B5	489	C
34	B5	490	C
34	B5	491	C
34	B5	492	A

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Mol	Chain	Res	Type
34	B5	494	U
34	B5	495	C
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	503	G
34	B5	506	A
34	B5	507	U
34	B5	514	G
34	B5	515	A
34	B5	519	C
34	B5	538	A
34	B5	539	G
34	B5	540	G
34	B5	541	A2M
34	B5	542	A
34	B5	544	A
34	B5	549	G
34	B5	555	A
34	B5	557	G
34	B5	558	U
34	B5	559	C
34	B5	562	OMG
34	B5	563	U
34	B5	564	G
34	B5	565	C
34	B5	568	G
34	B5	575	C
34	B5	577	G
34	B5	578	OMU
34	B5	579	A
34	B5	580	A
34	B5	582	U
34	B5	594	A
34	B5	595	G
34	B5	610	G
34	B5	611	U
34	B5	619	A2M
34	B5	620	A

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Mol	Chain	Res	Type
34	B5	621	A
34	B5	622	A
34	B5	623	A
34	B5	624	G
34	B5	634	G
34	B5	635	A
34	B5	638	U
34	B5	639	U
34	B5	650	U
34	B5	652	G
34	B5	655	G
34	B5	656	G
34	B5	658	C
34	B5	677	G
34	B5	678	A
34	B5	681	U
34	B5	683	C
34	B5	694	U
34	B5	696	C
34	B5	697	C
34	B5	698	U
34	B5	704	C
34	B5	705	U
34	B5	709	C
34	B5	711	U
34	B5	712	G
34	B5	713	A
34	B5	715	U
34	B5	716	C
34	B5	717	C
34	B5	718	U
34	B5	719	U
34	B5	721	U
34	B5	722	G
34	B5	725	U
34	B5	726	C
34	B5	727	U
34	B5	728	U
34	B5	730	G
34	B5	731	C
34	B5	732	G
34	B5	733	A

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Mol	Chain	Res	Type
34	B5	735	C
34	B5	740	A
34	B5	741	C
34	B5	753	A
34	B5	755	A
34	B5	765	G
34	B5	766	U
34	B5	774	A
34	B5	775	G
34	B5	778	G
34	B5	781	U
34	B5	782	U
34	B5	783	G
34	B5	784	C
34	B5	789	A
34	B5	794	U
34	B5	807	A
34	B5	814	A
34	B5	815	G
34	B5	819	G
34	B5	820	U
34	B5	821	U
34	B5	823	G
34	B5	832	U
34	B5	833	U
34	B5	836	U
34	B5	839	U
34	B5	840	U
34	B5	846	G
34	B5	851	U
34	B5	859	A
34	B5	863	A
34	B5	877	G
34	B5	886	U
34	B5	895	G
34	B5	898	A
34	B5	899	G
34	B5	906	A
34	B5	907	A
34	B5	923	A
34	B5	933	A
34	B5	935	U

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Mol	Chain	Res	Type
34	B5	951	A
34	B5	960	U
34	B5	966	A
34	B5	973	A
34	B5	988	A
34	B5	992	A
34	B5	993	A
34	B5	1004	U
34	B5	1005	A
34	B5	1020	A
34	B5	1021	C
34	B5	1026	A
34	B5	1028	C
34	B5	1032	G
34	B5	1039	A
34	B5	1040	G
34	B5	1052	U
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	1076	A
34	B5	1083	G
34	B5	1092	A
34	B5	1093	A
34	B5	1097	U
34	B5	1098	U
34	B5	1100	G
34	B5	1138	A
34	B5	1150	G
34	B5	1158	C
34	B5	1159	C
34	B5	1166	A
34	B5	1171	A
34	B5	1173	C
34	B5	1183	A
34	B5	1185	U
34	B5	1186	U
34	B5	1194	A
34	B5	1195	C

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Mol	Chain	Res	Type
34	B5	1196	A
34	B5	1199	G
34	B5	1200	G
34	B5	1201	G
34	B5	1212	G
34	B5	1217	A
34	B5	1218	G
34	B5	1226	A
34	B5	1227	A
34	B5	1228	G
34	B5	1229	G
34	B5	1230	A
34	B5	1243	G
34	B5	1244	A
34	B5	1245	G
34	B5	1246	C
34	B5	1251	U
34	B5	1253	U
34	B5	1256	A
34	B5	1257	U
34	B5	1267	G
34	B5	1268	G
34	B5	1269	OMU
34	B5	1286	U
34	B5	1301	U
34	B5	1314	U
34	B5	1315	U
34	B5	1321	A
34	B5	1338	C
34	B5	1340	U
34	B5	1344	A
34	B5	1345	A
34	B5	1346	A
34	B5	1349	G
34	B5	1352	G
34	B5	1353	U
34	B5	1355	C
34	B5	1362	U
34	B5	1363	U
34	B5	1364	G
34	B5	1366	U
34	B5	1367	G

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Mol	Chain	Res	Type
34	B5	1368	G
34	B5	1370	U
34	B5	1371	A
34	B5	1372	U
34	B5	1373	C
34	B5	1378	U
34	B5	1390	U
34	B5	1398	U
34	B5	1399	C
34	B5	1400	A
34	B5	1402	G
34	B5	1413	U
34	B5	1415	U
34	B5	1426	C
34	B5	1427	A
34	B5	1428	OMG
34	B5	1436	A
34	B5	1447	C
34	B5	1459	C
34	B5	1460	A
34	B5	1461	C
34	B5	1469	A
34	B5	1471	A
34	B5	1481	C
34	B5	1486	G
34	B5	1491	U
34	B5	1492	A
34	B5	1493	A
34	B5	1496	U
34	B5	1506	G
34	B5	1515	A
34	B5	1516	A
34	B5	1520	U
34	B5	1521	G
34	B5	1522	U
34	B5	1523	G
34	B5	1524	A
34	B5	1537	C
34	B5	1540	G
34	B5	1542	G
34	B5	1557	U
34	B5	1559	A

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Mol	Chain	Res	Type
34	B5	1565	C
34	B5	1575	G7M
34	B5	1584	G
34	B5	1601	G
34	B5	1607	G
34	B5	1616	G
34	B5	1619	C
34	B5	1634	C
34	B5	1635	A
34	B5	1636	C
34	B5	1646	C
34	B5	1651	A
34	B5	1657	U
34	B5	1658	G
34	B5	1680	G
34	B5	1682	U
34	B5	1683	C
34	B5	1684	U
34	B5	1688	U
34	B5	1693	A
34	B5	1698	G
34	B5	1700	C
34	B5	1701	A
34	B5	1703	C
34	B5	1711	C
34	B5	1715	G
34	B5	1716	C
34	B5	1717	G
34	B5	1760	G
34	B5	1762	A
34	B5	1766	A
34	B5	1767	G
34	B5	1769	U
34	B5	1773	4AC
34	B5	1780	G
34	B5	1782	MA6
34	B5	1792	G
34	B5	1793	G
34	B5	1794	A
34	B5	1796	C
34	B5	1799	U
38	A1	14	U

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Mol	Chain	Res	Type
38	A1	21	G
38	A1	26	A
38	A1	34	A
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	109	A
38	A1	110	G
38	A1	111	C
38	A1	116	A
38	A1	117	U
38	A1	118	U
38	A1	120	G
38	A1	122	A
38	A1	123	A
38	A1	134	U
38	A1	135	C
38	A1	136	G
38	A1	146	U
38	A1	156	G
38	A1	157	A
38	A1	166	C
38	A1	174	C
38	A1	176	G
38	A1	177	U
38	A1	178	U
38	A1	187	A
38	A1	190	U
38	A1	191	U
38	A1	200	C
38	A1	206	G
38	A1	210	U
38	A1	219	A
38	A1	234	G
38	A1	237	G
38	A1	238	A
38	A1	239	G

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Mol	Chain	Res	Type
38	A1	240	U
38	A1	241	G
38	A1	242	C
38	A1	243	G
38	A1	245	U
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	254	A
38	A1	269	G
38	A1	284	A
38	A1	286	U
38	A1	295	A
38	A1	296	A
38	A1	298	U
38	A1	305	U
38	A1	311	C
38	A1	329	U
38	A1	339	C
38	A1	342	A
38	A1	352	A
38	A1	372	A
38	A1	376	G
38	A1	398	A
38	A1	399	A
38	A1	401	U
38	A1	402	A
38	A1	403	C
38	A1	420	G
38	A1	421	G
38	A1	422	A
38	A1	438	A
38	A1	440	A
38	A1	495	G
38	A1	510	G
38	A1	521	A
38	A1	535	G
38	A1	536	U
38	A1	540	U

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Mol	Chain	Res	Type
38	A1	542	G
38	A1	543	C
38	A1	545	U
38	A1	547	G
38	A1	548	G
38	A1	549	U
38	A1	550	A
38	A1	551	A
38	A1	552	G
38	A1	554	A
38	A1	557	A
38	A1	559	A
38	A1	579	G
38	A1	589	A
38	A1	592	A
38	A1	602	A
38	A1	604	G
38	A1	611	A
38	A1	612	U
38	A1	620	U
38	A1	621	A
38	A1	637	C
38	A1	649	A2M
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	719	U
38	A1	725	G
38	A1	736	A
38	A1	758	C
38	A1	765	C
38	A1	766	U
38	A1	767	U
38	A1	776	U
38	A1	777	U
38	A1	781	G
38	A1	785	G
38	A1	786	A
38	A1	799	G

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Mol	Chain	Res	Type
38	A1	806	A
38	A1	813	G
38	A1	817	A2M
38	A1	818	C
38	A1	830	A
38	A1	849	C
38	A1	857	G
38	A1	861	C
38	A1	874	U
38	A1	879	U
38	A1	896	A
38	A1	897	U
38	A1	907	G
38	A1	908	OMG
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	934	G
38	A1	937	G
38	A1	943	U
38	A1	944	C
38	A1	953	G
38	A1	959	C
38	A1	963	G
38	A1	964	G
38	A1	974	G
38	A1	980	A
38	A1	981	U
38	A1	994	G
38	A1	1000	C
38	A1	1002	A
38	A1	1010	G
38	A1	1014	U
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	1023	C
38	A1	1032	C
38	A1	1034	U
38	A1	1035	G
38	A1	1036	A
38	A1	1045	C
38	A1	1047	A
38	A1	1064	A
38	A1	1072	G
38	A1	1082	U
38	A1	1092	C
38	A1	1093	A
38	A1	1094	U
38	A1	1095	U
38	A1	1097	G
38	A1	1098	A
38	A1	1103	A
38	A1	1104	G
38	A1	1117	G
38	A1	1130	A
38	A1	1131	G
38	A1	1144	U
38	A1	1153	A
38	A1	1154	A
38	A1	1159	A
38	A1	1178	G
38	A1	1179	A
38	A1	1180	A
38	A1	1181	U
38	A1	1182	A
38	A1	1192	C
38	A1	1193	A
38	A1	1201	C
38	A1	1206	G
38	A1	1208	U
38	A1	1219	C
38	A1	1223	A
38	A1	1224	C
38	A1	1228	C
38	A1	1231	A
38	A1	1235	U
38	A1	1236	G

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Mol	Chain	Res	Type
38	A1	1239	C
38	A1	1241	U
38	A1	1242	G
38	A1	1243	G
38	A1	1245	A
38	A1	1246	G
38	A1	1249	G
38	A1	1252	A
38	A1	1256	G
38	A1	1262	G
38	A1	1263	A
38	A1	1265	U
38	A1	1279	C
38	A1	1282	G
38	A1	1283	C
38	A1	1286	A
38	A1	1287	A
38	A1	1293	U
38	A1	1307	G
38	A1	1309	U
38	A1	1317	A
38	A1	1331	U
38	A1	1348	U
38	A1	1349	G
38	A1	1350	A
38	A1	1351	U
38	A1	1352	A
38	A1	1353	U
38	A1	1354	G
38	A1	1355	A
38	A1	1356	U
38	A1	1357	G
38	A1	1386	A
38	A1	1393	A
38	A1	1399	A
38	A1	1400	G
38	A1	1419	A
38	A1	1431	G
38	A1	1434	G
38	A1	1437	OMC
38	A1	1446	A
38	A1	1455	U

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Mol	Chain	Res	Type
38	A1	1481	A
38	A1	1496	C
38	A1	1508	C
38	A1	1523	U
38	A1	1526	U
38	A1	1536	G
38	A1	1539	A
38	A1	1555	U
38	A1	1556	C
38	A1	1558	A
38	A1	1562	C
38	A1	1564	U
38	A1	1565	G
38	A1	1567	U
38	A1	1568	U
38	A1	1569	U
38	A1	1572	U
38	A1	1573	G
38	A1	1574	C
38	A1	1575	A
38	A1	1576	G
38	A1	1579	C
38	A1	1581	C
38	A1	1582	C
38	A1	1583	A
38	A1	1589	A
38	A1	1593	A
38	A1	1605	A
38	A1	1629	U
38	A1	1630	U
38	A1	1642	A
38	A1	1643	A
38	A1	1657	C
38	A1	1683	A
38	A1	1687	U
38	A1	1724	U
38	A1	1734	G
38	A1	1741	A
38	A1	1742	U
38	A1	1750	A
38	A1	1751	G
38	A1	1762	C

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Mol	Chain	Res	Type
38	A1	1763	U
38	A1	1764	U
38	A1	1765	U
38	A1	1766	G
38	A1	1775	G
38	A1	1796	G
38	A1	1797	A
38	A1	1813	A
38	A1	1814	A
38	A1	1815	U
38	A1	1817	G
38	A1	1820	U
38	A1	1821	U
38	A1	1840	U
38	A1	1842	A
38	A1	1846	C
38	A1	1849	C
38	A1	1866	C
38	A1	1878	G
38	A1	1880	U
38	A1	1886	A
38	A1	1893	A
38	A1	1906	G
38	A1	1932	A
38	A1	1946	A
38	A1	1948	G
38	A1	1952	G
38	A1	1953	G
38	A1	1954	G
38	A1	1955	U
38	A1	2094	C
38	A1	2110	G
38	A1	2111	G
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
38	A1	2188	A
38	A1	2197	OMC

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Mol	Chain	Res	Type
38	A1	2201	G
38	A1	2207	A
38	A1	2242	A
38	A1	2249	G
38	A1	2256	A2M
38	A1	2257	C
38	A1	2259	A
38	A1	2260	U
38	A1	2269	U
38	A1	2270	A
38	A1	2272	G
38	A1	2273	G
38	A1	2278	5MC
38	A1	2279	A
38	A1	2280	A2M
38	A1	2281	A2M
38	A1	2282	U
38	A1	2284	C
38	A1	2307	G
38	A1	2308	C
38	A1	2310	U
38	A1	2313	A
38	A1	2314	U
38	A1	2315	G
38	A1	2334	U
38	A1	2335	G
38	A1	2336	U
38	A1	2340	U
38	A1	2356	A
38	A1	2366	C
38	A1	2373	A
38	A1	2374	C
38	A1	2375	G
38	A1	2383	C
38	A1	2388	U
38	A1	2391	G
38	A1	2393	G
38	A1	2397	A
38	A1	2402	A
38	A1	2403	G
38	A1	2404	A
38	A1	2411	U

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Mol	Chain	Res	Type
38	A1	2418	G
38	A1	2435	G
38	A1	2442	G
38	A1	2446	U
38	A1	2448	G
38	A1	2450	G
38	A1	2451	G
38	A1	2453	U
38	A1	2454	G
38	A1	2455	U
38	A1	2456	A
38	A1	2458	A
38	A1	2459	A
38	A1	2460	U
38	A1	2461	A
38	A1	2462	A
38	A1	2467	G
38	A1	2468	A
38	A1	2469	G
38	A1	2474	G
38	A1	2479	C
38	A1	2480	A
38	A1	2481	G
38	A1	2485	A
38	A1	2487	U
38	A1	2489	C
38	A1	2490	C
38	A1	2492	C
38	A1	2493	U
38	A1	2495	C
38	A1	2496	C
38	A1	2497	U
38	A1	2498	U
38	A1	2499	U
38	A1	2500	A
38	A1	2502	A
38	A1	2503	G
38	A1	2505	U
38	A1	2506	U
38	A1	2507	C
38	A1	2514	U
38	A1	2515	A

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Mol	Chain	Res	Type
38	A1	2523	A
38	A1	2524	A
38	A1	2530	G
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	2544	U
38	A1	2549	G
38	A1	2552	C
38	A1	2554	A
38	A1	2561	A
38	A1	2569	A
38	A1	2570	U
38	A1	2571	U
38	A1	2573	G
38	A1	2585	G
38	A1	2593	A
38	A1	2606	G
38	A1	2607	G
38	A1	2614	G
38	A1	2635	A
38	A1	2651	G
38	A1	2652	U
38	A1	2656	A
38	A1	2674	A
38	A1	2677	G
38	A1	2678	A
38	A1	2681	U
38	A1	2688	U
38	A1	2689	A
38	A1	2690	G
38	A1	2691	A
38	A1	2704	A
38	A1	2705	A
38	A1	2714	G
38	A1	2719	U
38	A1	2720	G
38	A1	2728	G
38	A1	2729	OMU

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Mol	Chain	Res	Type
38	A1	2737	C
38	A1	2749	G
38	A1	2752	U
38	A1	2753	G
38	A1	2755	C
38	A1	2773	C
38	A1	2777	G
38	A1	2778	G
38	A1	2796	G
38	A1	2799	A
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	2828	G
38	A1	2842	U
38	A1	2845	A
38	A1	2861	U
38	A1	2871	G
38	A1	2872	A
38	A1	2875	U
38	A1	2876	C
38	A1	2887	A
38	A1	2889	C
38	A1	2898	G
38	A1	2923	U
38	A1	2935	U
38	A1	2936	A
38	A1	2942	C
38	A1	2947	G
38	A1	2977	G
38	A1	2983	C
38	A1	2990	G
38	A1	2997	G
38	A1	3011	A
38	A1	3012	A
38	A1	3022	G
38	A1	3032	A
38	A1	3055	U
38	A1	3056	U

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Mol	Chain	Res	Type
38	A1	3059	G
38	A1	3078	U
38	A1	3080	G
38	A1	3086	A
38	A1	3087	A
38	A1	3092	C
38	A1	3101	G
38	A1	3109	G
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	3153	U
38	A1	3154	C
38	A1	3155	U
38	A1	3156	U
38	A1	3157	U
38	A1	3165	A
38	A1	3170	A
38	A1	3172	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	3198	U
38	A1	3207	U
38	A1	3216	G
38	A1	3217	C
38	A1	3218	A
38	A1	3219	G
38	A1	3224	G
38	A1	3234	A
38	A1	3243	A
38	A1	3246	G
38	A1	3259	U
38	A1	3260	G

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Mol	Chain	Res	Type
38	A1	3263	G
38	A1	3270	U
38	A1	3271	G
38	A1	3275	U
38	A1	3276	G
38	A1	3281	U
38	A1	3289	G
38	A1	3294	A
38	A1	3303	G
38	A1	3304	U
38	A1	3313	U
38	A1	3314	A
38	A1	3316	A
38	A1	3319	U
38	A1	3335	A
38	A1	3342	A
38	A1	3345	G
38	A1	3351	U
38	A1	3352	U
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	3389	U
39	A3	7	G
39	A3	22	A
39	A3	53	U
39	A3	54	U
39	A3	55	A
39	A3	65	G
39	A3	74	C
39	A3	76	A
39	A3	102	A
39	A3	112	G
39	A3	121	U
40	A4	23	U
40	A4	25	G
40	A4	34	U
40	A4	35	C
40	A4	38	U

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Mol	Chain	Res	Type
40	A4	50	C
40	A4	51	G
40	A4	52	A
40	A4	53	A
40	A4	59	A
40	A4	62	C
40	A4	63	G
40	A4	76	C
40	A4	81	U
40	A4	83	C
40	A4	84	C
40	A4	85	G
40	A4	86	U
40	A4	87	G
40	A4	88	A
40	A4	90	U
40	A4	95	G
40	A4	97	A
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
82	EC	6762	U
82	EC	6768	U
82	EC	6769	A
82	EC	6770	U
82	EC	6771	U
82	EC	6772	G
82	EC	6773	G
82	EC	6774	U
82	EC	6775	U
82	EC	6776	A
82	EC	6777	C
82	EC	6778	C
82	EC	6779	C
82	EC	6780	A
82	EC	6781	U
82	EC	6782	C

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Mol	Chain	Res	Type
82	EC	6786	A
82	EC	6788	C
82	EC	6789	G
82	EC	6790	A
82	EC	6791	A
82	EC	6792	A
82	EC	6793	A
82	EC	6794	C
82	EC	6800	G
82	EC	6801	A
82	EC	6802	A
82	EC	6803	C
82	EC	6804	A
82	EC	6805	C
82	EC	6811	G
82	EC	6816	A
82	EC	6817	A
82	EC	6818	G
82	EC	6819	G
82	EC	6820	C
82	EC	6821	U
82	EC	6822	U
82	EC	6823	U
82	EC	6824	C
82	EC	6825	A
82	EC	6831	U
82	EC	6832	G
82	EC	6835	U
82	EC	6836	U
82	EC	6837	G
82	EC	6840	A
82	EC	6841	U
82	EC	6842	U
82	EC	6843	U
82	EC	6844	A
82	EC	6845	G
82	EC	6847	G
82	EC	6848	U
82	EC	6849	A
82	EC	6850	C
82	EC	6852	U
82	EC	6856	C

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Mol	Chain	Res	Type
82	EC	6857	C
82	EC	6858	A
82	EC	6859	U
82	EC	6860	A
82	EC	6864	A
82	EC	6866	C
82	EC	6867	C
82	EC	6870	A
82	EC	6871	A
82	EC	6872	A
82	EC	6873	A
82	EC	6874	A
82	EC	6875	C
82	EC	6877	C
82	EC	6880	G
82	EC	6881	U
82	EC	6882	G
82	EC	6883	A
82	EC	6884	G
82	EC	6888	A
82	EC	6889	A
82	EC	6890	A
82	EC	6895	C
82	EC	6896	A
82	EC	6897	G
82	EC	6902	U
82	EC	6903	U
82	EC	6907	G
82	EC	6908	C
82	EC	6909	A
82	EC	6911	A
82	EC	6912	G
82	EC	6913	U
82	EC	6915	G
82	EC	6916	A
82	EC	6918	A
82	EC	6922	G
82	EC	6925	C
82	EC	6928	G
82	EC	6929	C
82	EC	6934	U
82	EC	6935	G

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Mol	Chain	Res	Type
82	EC	6936	G
82	EC	6938	A
82	EC	6939	C
82	EC	6940	U
82	EC	6941	U
82	EC	6942	A
82	EC	6943	A
82	EC	6944	U
82	EC	6945	U
82	EC	6946	A
82	EC	6947	A
82	EC	6948	U
82	EC	6949	G
82	EC	6953	G
82	EC	6955	U
82	EC	6957	A

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	B5	224	C
34	B5	345	U
34	B5	752	A
34	B5	819	G
34	B5	862	A
34	B5	950	C
34	B5	1217	A
34	B5	1285	U
34	B5	1344	A
34	B5	1369	U
34	B5	1427	A
34	B5	1458	G
34	B5	1521	G
34	B5	1600	A
34	B5	1645	G
38	A1	122	A
38	A1	239	G
38	A1	241	G
38	A1	873	C
38	A1	916	G
38	A1	1092	C
38	A1	1218	U

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Mol	Chain	Res	Type
38	A1	1242	G
38	A1	1292	C
38	A1	1354	G
38	A1	1572	U
38	A1	1629	U
38	A1	2241	U
38	A1	2497	U
38	A1	2506	U
38	A1	2875	U
38	A1	3121	U
39	A3	52	G
82	EC	6789	G
82	EC	6817	A
82	EC	6831	U
82	EC	6844	A
82	EC	6851	G
82	EC	6876	A
82	EC	6889	A
82	EC	6939	C
82	EC	6943	A
82	EC	6952	U

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

68 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
38	OMU	A1	2921	38	19,22,23	1.22	3 (15%)	25,31,34	1.81	5 (20%)
34	OMU	B5	578	34	19,22,23	1.21	2 (10%)	25,31,34	1.79	5 (20%)
34	OMG	B5	1428	34,83	23,26,27	1.21	3 (13%)	32,38,41	1.99	6 (18%)
34	A2M	B5	100	34,83	22,25,26	1.49	4 (18%)	30,36,39	2.10	8 (26%)
38	OMG	A1	805	38	23,26,27	1.18	3 (13%)	32,38,41	2.00	6 (18%)
38	5MC	A1	2278	38,83	19,22,23	1.60	3 (15%)	26,32,35	1.19	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	4AC	B5	1280	34	21,24,25	1.04	1 (4%)	28,34,37	1.13	2 (7%)
34	OMG	B5	562	34	23,26,27	1.20	3 (13%)	32,38,41	2.10	7 (21%)
34	OMC	B5	1639	34	19,22,23	0.76	0	25,31,34	0.81	1 (4%)
38	OMG	A1	908	38	23,26,27	1.21	3 (13%)	32,38,41	2.01	6 (18%)
34	A2M	B5	28	34,83	22,25,26	1.50	4 (18%)	30,36,39	2.14	9 (30%)
38	A2M	A1	2280	38	22,25,26	1.47	4 (18%)	30,36,39	2.08	9 (30%)
34	A2M	B5	541	34	22,25,26	1.52	4 (18%)	30,36,39	2.15	6 (20%)
38	OMC	A1	663	38	19,22,23	0.80	0	25,31,34	0.76	0
38	OMU	A1	2417	38	19,22,23	1.22	3 (15%)	25,31,34	1.80	5 (20%)
34	XSX	B5	1191	34	24,28,29	1.01	1 (4%)	30,40,43	3.76	5 (16%)
38	A2M	A1	1133	38	22,25,26	1.49	4 (18%)	30,36,39	2.10	10 (33%)
34	OMG	B5	1572	34	23,26,27	1.18	3 (13%)	32,38,41	2.02	6 (18%)
34	OMG	B5	1271	34	23,26,27	1.19	3 (13%)	32,38,41	1.92	6 (18%)
38	OMC	A1	2337	38	19,22,23	0.79	0	25,31,34	0.89	1 (4%)
38	5MC	A1	2870	38,83	19,22,23	1.52	3 (15%)	26,32,35	1.28	2 (7%)
34	A2M	B5	436	34	22,25,26	1.52	4 (18%)	30,36,39	2.04	7 (23%)
38	OMG	A1	867	38,83	23,26,27	1.16	3 (13%)	32,38,41	1.96	6 (18%)
34	OMC	B5	414	34	19,22,23	0.83	0	25,31,34	0.97	1 (4%)
38	OMC	A1	2959	38	19,22,23	0.81	0	25,31,34	0.86	1 (4%)
38	OMC	A1	2948	38	19,22,23	0.80	0	25,31,34	0.95	1 (4%)
34	MA6	B5	1782	34	23,26,27	1.50	5 (21%)	33,38,41	2.11	10 (30%)
38	OMG	A1	2791	38	23,26,27	1.20	3 (13%)	32,38,41	1.95	6 (18%)
38	A2M	A1	2946	38,83	22,25,26	1.49	5 (22%)	30,36,39	2.15	10 (33%)
34	G7M	B5	1575	34	23,26,27	2.60	7 (30%)	34,39,42	3.04	17 (50%)
38	OMG	A1	2619	38	23,26,27	1.19	3 (13%)	32,38,41	1.97	6 (18%)
34	A2M	B5	420	34	22,25,26	1.53	4 (18%)	30,36,39	2.08	8 (26%)
38	OMC	A1	650	38	19,22,23	0.79	0	25,31,34	0.81	0
34	OMU	B5	1269	34	19,22,23	1.21	2 (10%)	25,31,34	1.82	5 (20%)
34	OMG	B5	1126	34	23,26,27	1.18	3 (13%)	32,38,41	2.03	6 (18%)
38	OMU	A1	2421	38	19,22,23	1.28	3 (15%)	25,31,34	1.79	5 (20%)
38	A2M	A1	2640	38	22,25,26	1.49	4 (18%)	30,36,39	2.03	8 (26%)
34	MA6	B5	1781	34	23,26,27	1.54	4 (17%)	33,38,41	2.14	9 (27%)
38	A2M	A1	807	38	22,25,26	1.53	5 (22%)	30,36,39	2.03	8 (26%)
38	A2M	A1	817	38,83	22,25,26	1.51	5 (22%)	30,36,39	2.05	8 (26%)
38	OMG	A1	1450	38	23,26,27	1.18	3 (13%)	32,38,41	1.97	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	OMG	A1	2815	38	23,26,27	1.19	3 (13%)	32,38,41	1.98	5 (15%)
38	UR3	A1	2634	38	19,22,23	0.97	0	26,32,35	1.73	3 (11%)
34	A2M	B5	619	34,83	22,25,26	1.49	4 (18%)	30,36,39	2.05	9 (30%)
38	A2M	A1	876	38	22,25,26	1.50	4 (18%)	30,36,39	2.06	7 (23%)
34	A2M	B5	974	34	22,25,26	1.49	4 (18%)	30,36,39	2.07	8 (26%)
38	OMU	A1	2347	38	19,22,23	1.31	4 (21%)	25,31,34	1.86	6 (24%)
34	A2M	B5	796	34	22,25,26	1.50	4 (18%)	30,36,39	2.30	9 (30%)
34	OMC	B5	1007	34	19,22,23	0.79	0	25,31,34	0.82	1 (4%)
38	1MA	A1	2142	38,83	21,25,26	1.33	4 (19%)	30,37,40	1.71	4 (13%)
36	HIC	AB	243	36	10,11,12	1.49	1 (10%)	9,14,16	1.27	2 (22%)
38	A2M	A1	2256	38	22,25,26	1.52	4 (18%)	30,36,39	2.26	9 (30%)
38	A2M	A1	2220	38	22,25,26	1.51	5 (22%)	30,36,39	1.97	9 (30%)
34	4AC	B5	1773	34	21,24,25	1.06	1 (4%)	28,34,37	1.46	5 (17%)
38	OMG	A1	2288	38	23,26,27	1.21	3 (13%)	32,38,41	2.01	6 (18%)
38	OMC	A1	2197	38	19,22,23	0.79	0	25,31,34	0.79	0
38	A2M	A1	2281	38	22,25,26	1.42	5 (22%)	30,36,39	2.28	11 (36%)
38	A2M	A1	1449	38,83	22,25,26	1.51	4 (18%)	30,36,39	2.00	7 (23%)
38	OMU	A1	898	38	19,22,23	1.26	3 (15%)	25,31,34	1.79	4 (16%)
38	OMU	A1	2724	38	19,22,23	1.22	3 (15%)	25,31,34	1.81	6 (24%)
38	OMG	A1	2793	38	23,26,27	1.18	3 (13%)	32,38,41	1.96	6 (18%)
38	OMC	A1	1437	38	19,22,23	0.81	0	25,31,34	1.10	2 (8%)
80	DDE	DC	699	80	18,20,21	0.98	1 (5%)	17,28,30	1.01	1 (5%)
38	OMU	A1	2729	38	19,22,23	1.28	4 (21%)	25,31,34	1.80	5 (20%)
38	A2M	A1	649	38	22,25,26	1.49	4 (18%)	30,36,39	2.03	8 (26%)
38	OMU	A1	1888	38	19,22,23	1.27	4 (21%)	25,31,34	1.85	4 (16%)
38	OMG	A1	2922	38	23,26,27	1.18	3 (13%)	32,38,41	1.98	6 (18%)
38	1MA	A1	645	38,83	21,25,26	1.34	4 (19%)	30,37,40	1.69	6 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	OMU	A1	2921	38	-	0/9/27/28	0/2/2/2
34	OMU	B5	578	34	-	4/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	OMG	B5	1428	34,83	-	3/9/27/28	0/3/3/3
34	A2M	B5	100	34,83	-	0/9/27/28	0/3/3/3
38	OMG	A1	805	38	-	0/9/27/28	0/3/3/3
38	5MC	A1	2278	38,83	-	0/7/25/26	0/2/2/2
34	4AC	B5	1280	34	-	4/11/29/30	0/2/2/2
34	OMG	B5	562	34	-	2/9/27/28	0/3/3/3
34	OMC	B5	1639	34	-	1/9/27/28	0/2/2/2
38	OMG	A1	908	38	-	0/9/27/28	0/3/3/3
34	A2M	B5	28	34,83	-	1/9/27/28	0/3/3/3
38	A2M	A1	2280	38	-	2/9/27/28	0/3/3/3
34	A2M	B5	541	34	-	6/9/27/28	0/3/3/3
38	OMC	A1	663	38	-	1/9/27/28	0/2/2/2
38	OMU	A1	2417	38	-	1/9/27/28	0/2/2/2
34	XSX	B5	1191	34	-	5/16/34/35	0/2/2/2
38	A2M	A1	1133	38	-	0/9/27/28	0/3/3/3
34	OMG	B5	1572	34	-	0/9/27/28	0/3/3/3
34	OMG	B5	1271	34	-	1/9/27/28	0/3/3/3
38	OMC	A1	2337	38	-	0/9/27/28	0/2/2/2
38	5MC	A1	2870	38,83	-	4/7/25/26	0/2/2/2
34	A2M	B5	436	34	-	0/9/27/28	0/3/3/3
38	OMG	A1	867	38,83	-	1/9/27/28	0/3/3/3
34	OMC	B5	414	34	-	1/9/27/28	0/2/2/2
38	OMC	A1	2959	38	-	0/9/27/28	0/2/2/2
38	OMC	A1	2948	38	-	1/9/27/28	0/2/2/2
34	MA6	B5	1782	34	-	5/11/29/30	0/3/3/3
38	OMG	A1	2791	38	-	1/9/27/28	0/3/3/3
38	A2M	A1	2946	38,83	-	1/9/27/28	0/3/3/3
34	G7M	B5	1575	34	-	0/7/25/26	0/3/3/3
38	OMG	A1	2619	38	-	1/9/27/28	0/3/3/3
34	A2M	B5	420	34	-	1/9/27/28	0/3/3/3
38	OMC	A1	650	38	-	0/9/27/28	0/2/2/2
34	OMU	B5	1269	34	-	1/9/27/28	0/2/2/2
34	OMG	B5	1126	34	-	0/9/27/28	0/3/3/3
38	OMU	A1	2421	38	-	1/9/27/28	0/2/2/2
38	A2M	A1	2640	38	-	1/9/27/28	0/3/3/3
34	MA6	B5	1781	34	-	1/11/29/30	0/3/3/3
38	A2M	A1	807	38	-	0/9/27/28	0/3/3/3
38	A2M	A1	817	38,83	-	1/9/27/28	0/3/3/3
38	OMG	A1	1450	38	-	1/9/27/28	0/3/3/3
38	OMG	A1	2815	38	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	UR3	A1	2634	38	-	0/7/25/26	0/2/2/2
34	A2M	B5	619	34,83	-	5/9/27/28	0/3/3/3
38	A2M	A1	876	38	-	0/9/27/28	0/3/3/3
34	A2M	B5	974	34	-	1/9/27/28	0/3/3/3
38	OMU	A1	2347	38	-	0/9/27/28	0/2/2/2
34	A2M	B5	796	34	-	1/9/27/28	0/3/3/3
34	OMC	B5	1007	34	-	0/9/27/28	0/2/2/2
38	1MA	A1	2142	38,83	-	0/7/25/26	0/3/3/3
36	HIC	AB	243	36	-	2/5/6/8	0/1/1/1
38	A2M	A1	2256	38	-	2/9/27/28	0/3/3/3
38	A2M	A1	2220	38	-	1/9/27/28	0/3/3/3
34	4AC	B5	1773	34	-	6/11/29/30	0/2/2/2
38	OMG	A1	2288	38	-	0/9/27/28	0/3/3/3
38	OMC	A1	2197	38	-	6/9/27/28	0/2/2/2
38	A2M	A1	2281	38	-	2/9/27/28	0/3/3/3
38	A2M	A1	1449	38,83	-	0/9/27/28	0/3/3/3
38	OMU	A1	898	38	-	0/9/27/28	0/2/2/2
38	OMU	A1	2724	38	-	1/9/27/28	0/2/2/2
38	OMG	A1	2793	38	-	0/9/27/28	0/3/3/3
38	OMC	A1	1437	38	-	3/9/27/28	0/2/2/2
80	DDE	DC	699	80	-	8/20/21/23	0/1/1/1
38	OMU	A1	2729	38	-	3/9/27/28	0/2/2/2
38	A2M	A1	649	38	-	2/9/27/28	0/3/3/3
38	OMU	A1	1888	38	-	0/9/27/28	0/2/2/2
38	OMG	A1	2922	38	-	0/9/27/28	0/3/3/3
38	1MA	A1	645	38,83	-	2/7/25/26	0/3/3/3

All (196) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1575	G7M	C8-N7	7.48	1.45	1.33
38	A1	2278	5MC	C5-C4	5.70	1.48	1.44
34	B5	1575	G7M	C5-N7	-5.24	1.33	1.39
38	A1	2870	5MC	C5-C4	5.13	1.48	1.44
34	B5	1781	MA6	C5-C4	4.92	1.47	1.39
34	B5	541	A2M	C5-C4	4.88	1.47	1.39
34	B5	436	A2M	C5-C4	4.73	1.47	1.39
34	B5	420	A2M	C5-C4	4.72	1.47	1.39
38	A1	2256	A2M	C5-C4	4.72	1.47	1.39
34	B5	1782	MA6	C5-C4	4.67	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	807	A2M	C5-C4	4.64	1.47	1.39
38	A1	2220	A2M	C5-C4	4.63	1.47	1.39
34	B5	974	A2M	C5-C4	4.63	1.47	1.39
34	B5	28	A2M	C5-C4	4.62	1.47	1.39
38	A1	1449	A2M	C5-C4	4.61	1.47	1.39
38	A1	876	A2M	C5-C4	4.61	1.47	1.39
34	B5	796	A2M	C5-C4	4.60	1.47	1.39
34	B5	619	A2M	C5-C4	4.58	1.47	1.39
38	A1	649	A2M	C5-C4	4.58	1.47	1.39
34	B5	100	A2M	C5-C4	4.57	1.47	1.39
38	A1	2640	A2M	C5-C4	4.57	1.47	1.39
38	A1	817	A2M	C5-C4	4.56	1.47	1.39
38	A1	2946	A2M	C5-C4	4.55	1.47	1.39
38	A1	1133	A2M	C5-C4	4.53	1.47	1.39
38	A1	2280	A2M	C5-C4	4.49	1.47	1.39
38	A1	2281	A2M	C5-C4	4.30	1.46	1.39
34	B5	1575	G7M	C2'-C3'	-3.83	1.43	1.53
34	B5	1575	G7M	C8-N9	3.74	1.45	1.35
34	B5	1575	G7M	C5-C4	3.52	1.47	1.38
38	A1	908	OMG	C5-C4	3.16	1.47	1.38
38	A1	2288	OMG	C5-C4	3.15	1.47	1.38
34	B5	562	OMG	C5-C4	3.15	1.47	1.38
34	B5	1271	OMG	C5-C4	3.14	1.47	1.38
34	B5	1428	OMG	C5-C4	3.14	1.47	1.38
34	B5	1572	OMG	C5-C4	3.13	1.47	1.38
38	A1	1450	OMG	C5-C4	3.09	1.47	1.38
34	B5	1781	MA6	C5-C6	3.09	1.49	1.41
38	A1	2791	OMG	C5-C4	3.07	1.47	1.38
38	A1	2619	OMG	C5-C4	3.06	1.47	1.38
38	A1	645	1MA	C6-N6	3.05	1.35	1.28
38	A1	2142	1MA	C5-C4	3.05	1.47	1.38
38	A1	2793	OMG	C5-C4	3.04	1.47	1.38
38	A1	2815	OMG	C5-C4	3.04	1.47	1.38
38	A1	2922	OMG	C5-C4	3.04	1.47	1.38
34	B5	1126	OMG	C5-C4	3.02	1.47	1.38
38	A1	2142	1MA	C6-N6	3.00	1.35	1.28
38	A1	867	OMG	C5-C4	2.97	1.46	1.38
34	B5	1782	MA6	C5-C6	2.97	1.49	1.41
38	A1	805	OMG	C5-C4	2.95	1.46	1.38
36	AB	243	HIC	CD2-CG	2.95	1.41	1.36
38	A1	645	1MA	C5-C4	2.93	1.46	1.38
38	A1	2421	OMU	C4-N3	-2.93	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	2870	5MC	C6-C5	2.90	1.39	1.34
34	B5	1773	4AC	C4-N4	-2.84	1.35	1.39
38	A1	898	OMU	C4-N3	-2.84	1.33	1.38
34	B5	1280	4AC	C4-N4	-2.81	1.35	1.39
38	A1	2729	OMU	C4-N3	-2.80	1.33	1.38
34	B5	420	A2M	C5-C6	2.79	1.48	1.41
38	A1	2347	OMU	C4-N3	-2.79	1.33	1.38
38	A1	2256	A2M	C5-C6	2.76	1.48	1.41
38	A1	2278	5MC	C6-C5	2.75	1.39	1.34
38	A1	2640	A2M	C5-C6	2.74	1.48	1.41
34	B5	796	A2M	C5-C6	2.74	1.48	1.41
38	A1	1888	OMU	C4-N3	-2.74	1.33	1.38
38	A1	2417	OMU	C4-N3	-2.73	1.33	1.38
34	B5	541	A2M	C5-C6	2.72	1.48	1.41
34	B5	28	A2M	C5-C6	2.72	1.48	1.41
38	A1	2921	OMU	C4-N3	-2.70	1.34	1.38
38	A1	817	A2M	C5-C6	2.70	1.48	1.41
38	A1	2815	OMG	C6-N1	-2.68	1.33	1.38
34	B5	619	A2M	C5-C6	2.67	1.48	1.41
38	A1	1449	A2M	C5-N7	-2.65	1.34	1.39
34	B5	436	A2M	C5-C6	2.65	1.48	1.41
38	A1	807	A2M	C5-C6	2.65	1.48	1.41
38	A1	876	A2M	C5-C6	2.65	1.48	1.41
38	A1	2724	OMU	C4-N3	-2.64	1.34	1.38
38	A1	2791	OMG	C6-N1	-2.64	1.33	1.38
38	A1	2280	A2M	C5-C6	2.64	1.48	1.41
34	B5	100	A2M	C5-C6	2.63	1.48	1.41
38	A1	649	A2M	C5-C6	2.63	1.48	1.41
38	A1	2619	OMG	C6-N1	-2.63	1.33	1.38
34	B5	1269	OMU	C4-N3	-2.61	1.34	1.38
34	B5	974	A2M	C5-C6	2.60	1.48	1.41
38	A1	1133	A2M	C5-C6	2.60	1.48	1.41
34	B5	578	OMU	C4-N3	-2.60	1.34	1.38
38	A1	2288	OMG	C6-N1	-2.59	1.34	1.38
34	B5	1428	OMG	C6-N1	-2.57	1.34	1.38
38	A1	2793	OMG	C6-N1	-2.56	1.34	1.38
38	A1	908	OMG	C6-N1	-2.56	1.34	1.38
38	A1	2946	A2M	C5-C6	2.55	1.48	1.41
34	B5	1126	OMG	C6-N1	-2.54	1.34	1.38
34	B5	562	OMG	C6-N1	-2.53	1.34	1.38
38	A1	2922	OMG	C6-N1	-2.52	1.34	1.38
38	A1	1449	A2M	C5-C6	2.52	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	805	OMG	C6-N1	-2.50	1.34	1.38
38	A1	1450	OMG	C6-N1	-2.50	1.34	1.38
38	A1	2220	A2M	C5-C6	2.50	1.47	1.41
38	A1	807	A2M	C5-N7	-2.50	1.34	1.39
80	DC	699	DDE	CD2-CG	2.49	1.41	1.36
38	A1	876	A2M	C5-N7	-2.48	1.34	1.39
34	B5	1271	OMG	C6-N1	-2.48	1.34	1.38
34	B5	1575	G7M	O3'-C3'	-2.48	1.36	1.43
38	A1	2220	A2M	C5-N7	-2.46	1.34	1.39
38	A1	2347	OMU	C2-N1	2.46	1.42	1.38
38	A1	649	A2M	C5-N7	-2.45	1.34	1.39
38	A1	867	OMG	C6-N1	-2.44	1.34	1.38
38	A1	2946	A2M	C5-N7	-2.44	1.34	1.39
34	B5	420	A2M	C8-N7	2.43	1.36	1.31
38	A1	2640	A2M	C5-N7	-2.41	1.34	1.39
34	B5	1572	OMG	C6-N1	-2.41	1.34	1.38
38	A1	2281	A2M	C5-C6	2.40	1.47	1.41
34	B5	541	A2M	C5-N7	-2.40	1.34	1.39
38	A1	2280	A2M	C5-N7	-2.40	1.34	1.39
34	B5	100	A2M	C5-N7	-2.40	1.34	1.39
34	B5	436	A2M	C5-N7	-2.39	1.34	1.39
38	A1	1133	A2M	C5-N7	-2.37	1.34	1.39
34	B5	619	A2M	C8-N7	2.36	1.36	1.31
38	A1	2921	OMU	C2-N3	-2.35	1.33	1.38
38	A1	2421	OMU	C2-N3	-2.35	1.33	1.38
38	A1	2281	A2M	C5-N7	-2.34	1.34	1.39
38	A1	817	A2M	C5-N7	-2.33	1.34	1.39
38	A1	2256	A2M	C5-N7	-2.33	1.34	1.39
34	B5	974	A2M	C5-N7	-2.33	1.34	1.39
38	A1	898	OMU	C2-N3	-2.33	1.33	1.38
38	A1	2729	OMU	C2-N3	-2.31	1.33	1.38
34	B5	28	A2M	C8-N7	2.31	1.36	1.31
34	B5	619	A2M	C5-N7	-2.31	1.34	1.39
38	A1	2278	5MC	C6-N1	-2.30	1.34	1.38
34	B5	796	A2M	C8-N7	2.30	1.36	1.31
38	A1	2417	OMU	C2-N3	-2.30	1.34	1.38
38	A1	2142	1MA	C5-N7	-2.28	1.34	1.39
38	A1	2347	OMU	C2-N3	-2.28	1.34	1.38
34	B5	1781	MA6	C5-N7	-2.28	1.34	1.39
38	A1	1888	OMU	C2-N3	-2.28	1.34	1.38
34	B5	420	A2M	C5-N7	-2.28	1.34	1.39
38	A1	908	OMG	C5-N7	-2.27	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	100	A2M	C8-N7	2.27	1.36	1.31
34	B5	28	A2M	C5-N7	-2.27	1.34	1.39
34	B5	796	A2M	C5-N7	-2.26	1.35	1.39
34	B5	974	A2M	C8-N7	2.26	1.36	1.31
34	B5	562	OMG	C5-N7	-2.26	1.34	1.39
38	A1	898	OMU	C5-C4	-2.26	1.38	1.43
38	A1	2619	OMG	C5-N7	-2.26	1.34	1.39
38	A1	817	A2M	C8-N7	2.25	1.36	1.31
38	A1	2724	OMU	C5-C4	-2.25	1.38	1.43
38	A1	2256	A2M	C8-N7	2.24	1.36	1.31
34	B5	436	A2M	C8-N7	2.24	1.36	1.31
38	A1	2288	OMG	C5-N7	-2.23	1.34	1.39
34	B5	1782	MA6	C8-N7	2.23	1.36	1.31
38	A1	2946	A2M	C8-N7	2.22	1.36	1.31
38	A1	2281	A2M	C8-N7	2.22	1.36	1.31
38	A1	2870	5MC	C6-N1	-2.22	1.34	1.38
34	B5	1269	OMU	C2-N3	-2.21	1.34	1.38
38	A1	2640	A2M	C8-N7	2.21	1.35	1.31
34	B5	1782	MA6	C5-N7	-2.20	1.35	1.39
34	B5	578	OMU	C2-N3	-2.19	1.34	1.38
38	A1	807	A2M	C8-N7	2.19	1.35	1.31
38	A1	2729	OMU	C5-C4	-2.19	1.39	1.43
38	A1	2724	OMU	C2-N3	-2.19	1.34	1.38
38	A1	645	1MA	C2-N3	2.18	1.34	1.30
38	A1	2347	OMU	C5-C4	-2.18	1.39	1.43
34	B5	1428	OMG	C5-N7	-2.18	1.34	1.39
38	A1	2280	A2M	C8-N7	2.18	1.35	1.31
38	A1	645	1MA	C5-N7	-2.17	1.34	1.39
38	A1	1133	A2M	C8-N7	2.17	1.35	1.31
38	A1	2729	OMU	C2-N1	2.17	1.41	1.38
38	A1	2220	A2M	C4-N9	-2.17	1.33	1.37
38	A1	2142	1MA	C2-N3	2.16	1.34	1.30
38	A1	876	A2M	C8-N7	2.15	1.35	1.31
34	B5	541	A2M	C8-N7	2.15	1.35	1.31
38	A1	2791	OMG	C5-N7	-2.15	1.34	1.39
38	A1	649	A2M	C8-N7	2.14	1.35	1.31
38	A1	805	OMG	C5-N7	-2.13	1.34	1.39
38	A1	2220	A2M	C8-N7	2.13	1.35	1.31
38	A1	2417	OMU	C5-C4	-2.13	1.39	1.43
38	A1	1449	A2M	C8-N7	2.13	1.35	1.31
34	B5	1191	XSX	C2-N1	2.13	1.41	1.38
38	A1	2815	OMG	C5-N7	-2.13	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	2922	OMG	C5-N7	-2.12	1.34	1.39
38	A1	1450	OMG	C5-N7	-2.11	1.34	1.39
38	A1	1888	OMU	C5-C4	-2.10	1.39	1.43
34	B5	1271	OMG	C5-N7	-2.08	1.34	1.39
38	A1	1888	OMU	C2-N1	2.07	1.41	1.38
38	A1	2421	OMU	C5-C4	-2.07	1.39	1.43
34	B5	1126	OMG	C5-N7	-2.07	1.34	1.39
38	A1	817	A2M	C4-N9	-2.07	1.33	1.37
34	B5	1575	G7M	C2'-C1'	-2.07	1.47	1.53
38	A1	2921	OMU	C5-C4	-2.07	1.39	1.43
38	A1	2946	A2M	C4-N9	-2.06	1.33	1.37
38	A1	807	A2M	C4-N9	-2.06	1.33	1.37
38	A1	867	OMG	C5-N7	-2.05	1.35	1.39
34	B5	1781	MA6	C8-N7	2.04	1.35	1.31
34	B5	1572	OMG	C5-N7	-2.04	1.35	1.39
38	A1	2793	OMG	C5-N7	-2.03	1.35	1.39
34	B5	1782	MA6	C4-N9	-2.02	1.33	1.37
38	A1	2281	A2M	C4-N9	-2.01	1.33	1.37

All (385) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1191	XSX	C3-C1-N3	19.14	145.62	112.16
34	B5	1575	G7M	CN7-N7-C8	-7.23	113.83	124.79
38	A1	2634	UR3	C4-N3-C2	-6.89	119.03	124.58
34	B5	562	OMG	C5-C4-N3	-6.70	117.72	128.39
34	B5	541	A2M	C5-C4-N3	-6.69	117.51	126.72
38	A1	2288	OMG	C5-C4-N3	-6.43	118.16	128.39
38	A1	908	OMG	C5-C4-N3	-6.37	118.26	128.39
34	B5	1428	OMG	C5-C4-N3	-6.36	118.27	128.39
38	A1	2619	OMG	C5-C4-N3	-6.28	118.40	128.39
34	B5	1572	OMG	C5-C4-N3	-6.26	118.42	128.39
38	A1	2922	OMG	C5-C4-N3	-6.22	118.48	128.39
38	A1	1450	OMG	C5-C4-N3	-6.22	118.49	128.39
38	A1	2791	OMG	C5-C4-N3	-6.22	118.50	128.39
38	A1	2815	OMG	C5-C4-N3	-6.19	118.54	128.39
34	B5	1575	G7M	N9-C8-N7	-6.19	97.45	112.48
34	B5	796	A2M	C5-C4-N3	-6.15	118.25	126.72
38	A1	2256	A2M	C5-C4-N3	-6.11	118.31	126.72
34	B5	1126	OMG	C5-C4-N3	-6.10	118.68	128.39
38	A1	876	A2M	C5-C4-N3	-6.08	118.35	126.72
38	A1	1449	A2M	C5-C4-N3	-6.03	118.41	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	100	A2M	C5-C4-N3	-6.03	118.41	126.72
34	B5	1271	OMG	C5-C4-N3	-6.01	118.82	128.39
38	A1	805	OMG	C5-C4-N3	-6.00	118.84	128.39
38	A1	2793	OMG	C5-C4-N3	-5.95	118.92	128.39
38	A1	867	OMG	C5-C4-N3	-5.95	118.93	128.39
38	A1	2640	A2M	C5-C4-N3	-5.94	118.54	126.72
38	A1	2280	A2M	C5-C4-N3	-5.94	118.54	126.72
34	B5	28	A2M	C5-C4-N3	-5.92	118.56	126.72
34	B5	420	A2M	C5-C4-N3	-5.88	118.62	126.72
38	A1	649	A2M	C5-C4-N3	-5.83	118.69	126.72
34	B5	974	A2M	C5-C4-N3	-5.83	118.69	126.72
34	B5	1575	G7M	C8-N7-C5	5.82	115.06	107.78
38	A1	817	A2M	C5-C4-N3	-5.79	118.74	126.72
38	A1	807	A2M	C5-C4-N3	-5.78	118.76	126.72
34	B5	436	A2M	C5-C4-N3	-5.75	118.80	126.72
34	B5	1781	MA6	C5-C4-N3	-5.73	118.83	126.72
34	B5	619	A2M	C5-C4-N3	-5.71	118.85	126.72
38	A1	2281	A2M	C5-C4-N3	-5.70	118.86	126.72
38	A1	1133	A2M	C5-C4-N3	-5.69	118.89	126.72
34	B5	1575	G7M	C5-C4-N3	-5.57	117.63	128.15
38	A1	2946	A2M	C5-C4-N3	-5.56	119.06	126.72
34	B5	1575	G7M	N9-C4-N3	5.43	136.81	125.95
38	A1	2142	1MA	C5-C4-N3	-5.39	119.33	127.27
34	B5	1575	G7M	C2-N3-C4	5.37	121.55	112.30
34	B5	562	OMG	C2-N3-C4	5.36	121.54	112.30
34	B5	1782	MA6	C5-C4-N3	-5.36	119.34	126.72
38	A1	2220	A2M	C5-C4-N3	-5.34	119.37	126.72
34	B5	541	A2M	N3-C4-N9	5.32	136.22	127.17
38	A1	645	1MA	C5-C4-N3	-5.25	119.55	127.27
34	B5	562	OMG	N9-C4-N3	5.20	136.35	125.95
34	B5	1572	OMG	C2-N3-C4	5.20	121.25	112.30
38	A1	1450	OMG	C2-N3-C4	5.12	121.12	112.30
34	B5	1428	OMG	C2-N3-C4	5.09	121.07	112.30
38	A1	2288	OMG	C2-N3-C4	5.09	121.06	112.30
34	B5	1773	4AC	N4-C4-N3	5.08	122.11	113.87
38	A1	2815	OMG	C2-N3-C4	5.08	121.05	112.30
38	A1	2619	OMG	C2-N3-C4	5.08	121.05	112.30
38	A1	805	OMG	C2-N3-C4	5.07	121.04	112.30
38	A1	867	OMG	C2-N3-C4	5.05	121.00	112.30
38	A1	2922	OMG	C2-N3-C4	5.04	120.97	112.30
34	B5	1126	OMG	C2-N3-C4	5.02	120.95	112.30
38	A1	908	OMG	C2-N3-C4	5.00	120.91	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2793	OMG	C2-N3-C4	4.94	120.81	112.30
38	A1	2791	OMG	C2-N3-C4	4.94	120.80	112.30
34	B5	1271	OMG	C2-N3-C4	4.92	120.77	112.30
38	A1	2288	OMG	N9-C4-N3	4.85	135.65	125.95
38	A1	2921	OMU	C4-N3-C2	-4.85	120.59	126.61
38	A1	2256	A2M	N3-C4-N9	4.83	135.38	127.17
38	A1	1449	A2M	N3-C4-N9	4.82	135.37	127.17
34	B5	578	OMU	C4-N3-C2	-4.81	120.64	126.61
34	B5	1191	XSX	C4-N3-C2	-4.81	119.01	124.66
38	A1	908	OMG	N9-C4-N3	4.81	135.57	125.95
38	A1	2421	OMU	C4-N3-C2	-4.78	120.68	126.61
34	B5	796	A2M	N3-C4-N9	4.77	135.28	127.17
34	B5	1269	OMU	C4-N3-C2	-4.75	120.72	126.61
38	A1	1888	OMU	C4-N3-C2	-4.72	120.75	126.61
34	B5	100	A2M	N3-C4-N9	4.72	135.20	127.17
38	A1	2281	A2M	N3-C4-N9	4.72	135.19	127.17
38	A1	2417	OMU	C4-N3-C2	-4.71	120.77	126.61
38	A1	898	OMU	C4-N3-C2	-4.69	120.79	126.61
38	A1	1450	OMG	N9-C4-N3	4.68	135.32	125.95
38	A1	876	A2M	N3-C4-N9	4.67	135.12	127.17
38	A1	2791	OMG	N9-C4-N3	4.66	135.28	125.95
38	A1	649	A2M	N3-C4-N9	4.65	135.08	127.17
34	B5	28	A2M	N3-C4-N9	4.65	135.08	127.17
34	B5	974	A2M	N3-C4-N9	4.65	135.07	127.17
38	A1	2280	A2M	N3-C4-N9	4.64	135.06	127.17
38	A1	2724	OMU	C4-N3-C2	-4.63	120.87	126.61
38	A1	2619	OMG	N9-C4-N3	4.62	135.19	125.95
38	A1	2142	1MA	C2-N3-C4	4.60	121.56	112.53
38	A1	1133	A2M	N3-C4-N9	4.57	134.94	127.17
34	B5	420	A2M	N3-C4-N9	4.57	134.94	127.17
34	B5	1572	OMG	N9-C4-N3	4.56	135.08	125.95
38	A1	2640	A2M	N3-C4-N9	4.55	134.91	127.17
38	A1	2729	OMU	C4-N3-C2	-4.53	120.99	126.61
38	A1	2922	OMG	N9-C4-N3	4.52	134.98	125.95
34	B5	436	A2M	N3-C4-N9	4.51	134.83	127.17
38	A1	2793	OMG	N9-C4-N3	4.50	134.95	125.95
38	A1	645	1MA	C2-N3-C4	4.49	121.33	112.53
34	B5	1428	OMG	N9-C4-N3	4.48	134.91	125.95
38	A1	807	A2M	N3-C4-N9	4.48	134.78	127.17
38	A1	2421	OMU	N3-C2-N1	4.48	120.72	114.89
38	A1	1888	OMU	N3-C2-N1	4.47	120.71	114.89
38	A1	2815	OMG	N9-C4-N3	4.47	134.89	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1271	OMG	N9-C4-N3	4.47	134.88	125.95
34	B5	1126	OMG	N9-C4-N3	4.44	134.83	125.95
34	B5	1781	MA6	C2-N1-C6	4.43	122.64	111.83
38	A1	817	A2M	N3-C4-N9	4.42	134.69	127.17
38	A1	2347	OMU	C4-N3-C2	-4.42	121.12	126.61
34	B5	796	A2M	C2'-C1'-N9	-4.39	106.53	113.75
38	A1	805	OMG	N9-C4-N3	4.38	134.72	125.95
34	B5	619	A2M	N3-C4-N9	4.35	134.57	127.17
38	A1	2417	OMU	N3-C2-N1	4.34	120.54	114.89
34	B5	1782	MA6	C2-N1-C6	4.31	122.37	111.83
38	A1	2946	A2M	N3-C4-N9	4.30	134.48	127.17
38	A1	2724	OMU	N3-C2-N1	4.30	120.49	114.89
34	B5	1781	MA6	N3-C4-N9	4.30	134.47	127.17
38	A1	867	OMG	N9-C4-N3	4.29	134.53	125.95
38	A1	2921	OMU	N3-C2-N1	4.28	120.47	114.89
38	A1	898	OMU	N3-C2-N1	4.25	120.43	114.89
38	A1	2870	5MC	C5-C6-N1	-4.23	118.71	123.31
38	A1	2729	OMU	N3-C2-N1	4.22	120.39	114.89
38	A1	2220	A2M	N3-C4-N9	4.21	134.32	127.17
34	B5	1781	MA6	C4-C5-N7	-4.20	105.78	110.58
34	B5	578	OMU	N3-C2-N1	4.12	120.26	114.89
34	B5	1269	OMU	N3-C2-N1	4.11	120.24	114.89
34	B5	1782	MA6	C4-C5-N7	-4.10	105.89	110.58
34	B5	1782	MA6	N3-C4-N9	4.04	134.05	127.17
38	A1	2347	OMU	N3-C2-N1	4.04	120.15	114.89
38	A1	2921	OMU	C5-C4-N3	3.99	120.40	114.80
38	A1	2256	A2M	O2'-C2'-C1'	3.97	116.52	108.99
34	B5	541	A2M	C2-N3-C4	3.96	121.50	111.83
34	B5	796	A2M	C2-N3-C4	3.92	121.41	111.83
34	B5	578	OMU	C5-C4-N3	3.91	120.28	114.80
38	A1	898	OMU	C5-C4-N3	3.90	120.27	114.80
34	B5	1269	OMU	C5-C4-N3	3.85	120.19	114.80
38	A1	2417	OMU	C5-C4-N3	3.83	120.17	114.80
34	B5	1280	4AC	N4-C4-N3	3.82	120.07	113.87
38	A1	2256	A2M	C2-N3-C4	3.81	121.14	111.83
38	A1	2347	OMU	C5-C4-N3	3.81	120.14	114.80
34	B5	28	A2M	C2-N3-C4	3.81	121.13	111.83
38	A1	2729	OMU	C5-C4-N3	3.80	120.12	114.80
38	A1	817	A2M	C2-N3-C4	3.76	121.02	111.83
38	A1	649	A2M	C2-N3-C4	3.76	121.02	111.83
34	B5	100	A2M	C2-N3-C4	3.75	120.98	111.83
38	A1	2640	A2M	C2-N3-C4	3.74	120.97	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	1888	OMU	C5-C4-N3	3.74	120.04	114.80
38	A1	2421	OMU	C5-C4-N3	3.74	120.03	114.80
38	A1	2280	A2M	C2-N3-C4	3.73	120.94	111.83
34	B5	420	A2M	C2-N3-C4	3.72	120.92	111.83
34	B5	619	A2M	C4-C5-N7	-3.70	106.35	110.58
38	A1	876	A2M	C2-N3-C4	3.69	120.85	111.83
38	A1	2724	OMU	C5-C4-N3	3.69	119.97	114.80
34	B5	1782	MA6	C2-N3-C4	3.69	120.85	111.83
38	A1	1449	A2M	C2-N3-C4	3.68	120.81	111.83
34	B5	796	A2M	C4-C5-N7	-3.67	106.38	110.58
34	B5	436	A2M	C2-N3-C4	3.67	120.80	111.83
34	B5	974	A2M	C2-N3-C4	3.67	120.79	111.83
38	A1	2281	A2M	C2-N3-C4	3.67	120.78	111.83
34	B5	1575	G7M	C2'-C1'-N9	3.66	123.43	113.25
34	B5	1781	MA6	C2-N3-C4	3.66	120.76	111.83
38	A1	2640	A2M	C4-C5-N7	-3.64	106.42	110.58
38	A1	817	A2M	C4-C5-N7	-3.63	106.43	110.58
38	A1	1133	A2M	C2-N3-C4	3.63	120.69	111.83
38	A1	2946	A2M	C2-N3-C4	3.62	120.68	111.83
34	B5	619	A2M	C2-N3-C4	3.62	120.67	111.83
38	A1	2281	A2M	C2'-C1'-N9	-3.61	107.80	113.75
34	B5	420	A2M	C4-C5-N7	-3.61	106.45	110.58
38	A1	2280	A2M	C4-C5-N7	-3.61	106.46	110.58
38	A1	2142	1MA	N9-C4-N3	3.60	135.09	126.90
38	A1	876	A2M	C4-C5-N7	-3.56	106.51	110.58
34	B5	28	A2M	C4-C5-N7	-3.56	106.51	110.58
38	A1	2220	A2M	N3-C2-N1	-3.56	123.20	128.58
38	A1	2347	OMU	C1'-N1-C2	3.52	123.91	117.59
38	A1	807	A2M	C4-C5-N7	-3.52	106.56	110.58
38	A1	1133	A2M	C4-C5-N7	-3.48	106.60	110.58
38	A1	2220	A2M	C2-N3-C4	3.48	120.34	111.83
34	B5	1782	MA6	N1-C2-N3	-3.47	123.32	128.58
38	A1	807	A2M	C2-N3-C4	3.47	120.31	111.83
38	A1	2281	A2M	O4'-C1'-N9	3.44	114.70	108.09
38	A1	867	OMG	C6-C5-N7	3.44	136.55	130.29
34	B5	100	A2M	C4-C5-N7	-3.44	106.65	110.58
38	A1	2256	A2M	C4-C5-N7	-3.43	106.66	110.58
38	A1	2634	UR3	C5-C4-N3	3.42	119.55	115.04
34	B5	1575	G7M	CN7-N7-C5	3.42	131.06	126.80
34	B5	974	A2M	C4-C5-N7	-3.39	106.70	110.58
38	A1	645	1MA	N9-C4-N3	3.39	134.62	126.90
34	B5	1126	OMG	C6-C5-N7	3.39	136.46	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	805	OMG	C6-C5-N7	3.38	136.44	130.29
38	A1	649	A2M	C4-C5-N7	-3.37	106.73	110.58
34	B5	796	A2M	N3-C2-N1	-3.37	123.49	128.58
38	A1	2946	A2M	C4-C5-N7	-3.36	106.74	110.58
38	A1	649	A2M	N3-C2-N1	-3.36	123.50	128.58
38	A1	817	A2M	N3-C2-N1	-3.35	123.50	128.58
38	A1	2815	OMG	C6-C5-N7	3.34	136.38	130.29
38	A1	2946	A2M	N3-C2-N1	-3.32	123.56	128.58
34	B5	436	A2M	C4-C5-N7	-3.32	106.79	110.58
34	B5	436	A2M	N3-C2-N1	-3.31	123.56	128.58
34	B5	28	A2M	N3-C2-N1	-3.30	123.59	128.58
38	A1	2946	A2M	C2'-C1'-N9	-3.29	108.33	113.75
34	B5	541	A2M	C4-C5-N7	-3.28	106.83	110.58
34	B5	1572	OMG	C6-C5-N7	3.28	136.26	130.29
34	B5	1575	G7M	O3'-C3'-C4'	3.28	120.51	111.08
34	B5	974	A2M	N3-C2-N1	-3.28	123.62	128.58
38	A1	2220	A2M	C4-C5-N7	-3.27	106.84	110.58
34	B5	1781	MA6	N1-C2-N3	-3.26	123.65	128.58
38	A1	2281	A2M	N3-C2-N1	-3.24	123.67	128.58
38	A1	2793	OMG	C6-C5-N7	3.24	136.18	130.29
38	A1	1133	A2M	N3-C2-N1	-3.21	123.72	128.58
34	B5	1575	G7M	O2'-C2'-C3'	3.21	122.11	111.82
34	B5	1271	OMG	C6-C5-N7	3.21	136.13	130.29
38	A1	2256	A2M	N3-C2-N1	-3.20	123.74	128.58
38	A1	2724	OMU	O4-C4-C5	-3.19	119.65	125.16
38	A1	2280	A2M	N3-C2-N1	-3.19	123.75	128.58
38	A1	1449	A2M	C4-C5-N7	-3.18	106.95	110.58
38	A1	2922	OMG	C6-C5-N7	3.16	136.04	130.29
34	B5	420	A2M	N3-C2-N1	-3.16	123.80	128.58
38	A1	2619	OMG	C6-C5-N7	3.16	136.03	130.29
38	A1	2640	A2M	N3-C2-N1	-3.15	123.82	128.58
34	B5	619	A2M	N3-C2-N1	-3.14	123.82	128.58
34	B5	100	A2M	N3-C2-N1	-3.14	123.83	128.58
38	A1	1449	A2M	N3-C2-N1	-3.13	123.84	128.58
34	B5	541	A2M	N3-C2-N1	-3.12	123.86	128.58
38	A1	2281	A2M	C4-C5-N7	-3.10	107.03	110.58
38	A1	2417	OMU	O4-C4-C5	-3.10	119.81	125.16
38	A1	2921	OMU	O4-C4-C5	-3.10	119.82	125.16
38	A1	1450	OMG	C6-C5-N7	3.09	135.91	130.29
34	B5	1428	OMG	C6-C5-N7	3.08	135.90	130.29
38	A1	1437	OMC	O2-C2-N3	-3.04	117.54	122.33
38	A1	2791	OMG	C6-C5-N7	3.04	135.82	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2347	OMU	O4-C4-C5	-3.04	119.92	125.16
38	A1	876	A2M	N3-C2-N1	-3.03	123.99	128.58
34	B5	1269	OMU	O4-C4-C5	-3.03	119.93	125.16
38	A1	2281	A2M	C4-N9-C8	3.03	108.92	105.74
34	B5	1575	G7M	C8-N9-C4	3.03	114.59	107.09
38	A1	898	OMU	O4-C4-C5	-3.02	119.95	125.16
38	A1	2729	OMU	O4-C4-C5	-3.01	119.97	125.16
38	A1	2278	5MC	C5-C6-N1	-2.98	120.07	123.31
38	A1	2946	A2M	O4'-C1'-N9	2.98	113.81	108.09
38	A1	1888	OMU	O4-C4-C5	-2.97	120.05	125.16
34	B5	1782	MA6	C5-N7-C8	2.96	108.11	103.45
34	B5	578	OMU	O4-C4-C5	-2.95	120.07	125.16
80	DC	699	DDE	CAU-CBW-CBI	-2.95	105.45	111.22
38	A1	2288	OMG	C6-C5-N7	2.95	135.65	130.29
34	B5	1781	MA6	C5-N7-C8	2.93	108.06	103.45
38	A1	908	OMG	C6-C5-N7	2.88	135.53	130.29
34	B5	1782	MA6	C4-N9-C8	2.88	108.76	105.74
38	A1	1133	A2M	C4-N9-C8	2.85	108.73	105.74
34	B5	1191	XSX	C5-C4-N3	2.85	119.58	115.64
34	B5	1773	4AC	C5-C4-N4	-2.84	118.15	122.94
38	A1	1133	A2M	C2'-C1'-N9	-2.82	109.11	113.75
38	A1	2278	5MC	C5-C4-N3	-2.81	118.88	121.75
38	A1	2421	OMU	O4-C4-C5	-2.81	120.32	125.16
34	B5	562	OMG	C6-C5-N7	2.79	135.38	130.29
38	A1	2948	OMC	O2-C2-N3	-2.76	117.98	122.33
38	A1	2278	5MC	O2-C2-N3	-2.72	118.04	122.33
38	A1	807	A2M	N3-C2-N1	-2.72	124.46	128.58
34	B5	1126	OMG	C4-C5-N7	-2.69	106.40	110.67
34	B5	414	OMC	O2-C2-N3	-2.66	118.13	122.33
38	A1	867	OMG	C4-C5-N7	-2.66	106.45	110.67
38	A1	2280	A2M	C5-N7-C8	2.65	107.62	103.45
38	A1	2220	A2M	C2-N1-C6	2.65	123.08	118.73
34	B5	619	A2M	C5-N7-C8	2.64	107.61	103.45
34	B5	1572	OMG	C4-C5-N7	-2.64	106.48	110.67
34	B5	28	A2M	C2'-C1'-N9	-2.64	109.42	113.75
34	B5	28	A2M	C4-N9-C8	2.63	108.50	105.74
38	A1	2815	OMG	C4-C5-N7	-2.63	106.50	110.67
34	B5	974	A2M	C4-N9-C8	2.63	108.50	105.74
34	B5	796	A2M	C5-N7-C8	2.62	107.57	103.45
38	A1	2640	A2M	C5-N7-C8	2.62	107.57	103.45
38	A1	2870	5MC	C5-C4-N3	-2.62	119.07	121.75
38	A1	2922	OMG	C4-C5-N7	-2.61	106.54	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	420	A2M	C5-N7-C8	2.60	107.53	103.45
34	B5	420	A2M	C4-N9-C8	2.60	108.47	105.74
38	A1	2256	A2M	O3'-C3'-C2'	-2.59	103.92	111.19
38	A1	2280	A2M	C4-N9-C8	2.59	108.46	105.74
34	B5	28	A2M	C5-N7-C8	2.59	107.52	103.45
38	A1	805	OMG	C4-C5-N7	-2.58	106.58	110.67
34	B5	1428	OMG	C4-C5-N7	-2.58	106.58	110.67
34	B5	619	A2M	C4-N9-C8	2.58	108.44	105.74
38	A1	2619	OMG	C4-C5-N7	-2.58	106.59	110.67
38	A1	1133	A2M	C5-N7-C8	2.56	107.48	103.45
34	B5	1575	G7M	C1'-N9-C4	-2.55	118.94	126.49
36	AB	243	HIC	NE2-CE1-ND1	-2.53	111.69	112.66
38	A1	876	A2M	C5-N7-C8	2.52	107.41	103.45
38	A1	2791	OMG	C4-C5-N7	-2.52	106.68	110.67
34	B5	974	A2M	C2'-C1'-N9	-2.51	109.61	113.75
34	B5	1782	MA6	C6-C5-N7	2.51	137.44	133.43
34	B5	1271	OMG	C4-C5-N7	-2.51	106.69	110.67
38	A1	817	A2M	C4-N9-C8	2.50	108.37	105.74
34	B5	796	A2M	C4-N9-C8	2.50	108.37	105.74
38	A1	2256	A2M	C5-N7-C8	2.50	107.38	103.45
38	A1	817	A2M	C5-N7-C8	2.49	107.36	103.45
38	A1	2417	OMU	O2-C2-N1	-2.49	119.56	122.80
38	A1	649	A2M	C4-N9-C8	2.48	108.34	105.74
34	B5	1575	G7M	C3'-C2'-C1'	2.48	106.16	101.46
34	B5	100	A2M	C5-N7-C8	2.48	107.35	103.45
38	A1	2288	OMG	C4-C5-N7	-2.48	106.74	110.67
34	B5	974	A2M	C5-N7-C8	2.48	107.34	103.45
38	A1	649	A2M	C5-N7-C8	2.47	107.33	103.45
34	B5	100	A2M	C4-N9-C8	2.45	108.31	105.74
38	A1	2793	OMG	C4-C5-N7	-2.45	106.79	110.67
38	A1	1450	OMG	C4-C5-N7	-2.42	106.84	110.67
38	A1	908	OMG	C4-C5-N7	-2.40	106.86	110.67
38	A1	2281	A2M	C5-N7-C8	2.40	107.23	103.45
34	B5	1269	OMU	O2-C2-N1	-2.40	119.67	122.80
38	A1	2946	A2M	C5-N7-C8	2.40	107.22	103.45
38	A1	2946	A2M	C4-N9-C8	2.40	108.26	105.74
38	A1	807	A2M	C5-N7-C8	2.39	107.20	103.45
38	A1	1437	OMC	C1'-N1-C2	2.39	123.71	118.44
38	A1	807	A2M	C4-N9-C8	2.38	108.24	105.74
34	B5	1575	G7M	C6-C5-N7	2.38	135.16	132.17
38	A1	2220	A2M	C4-N9-C8	2.37	108.23	105.74
34	B5	541	A2M	C5-N7-C8	2.36	107.16	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2640	A2M	C4-N9-C8	2.36	108.22	105.74
38	A1	2337	OMC	O2-C2-N3	-2.35	118.63	122.33
34	B5	1782	MA6	N9-C8-N7	-2.34	110.62	113.94
38	A1	645	1MA	C4-C5-N7	-2.32	106.99	110.67
38	A1	2256	A2M	C4-N9-C8	2.32	108.17	105.74
34	B5	1781	MA6	C4-N9-C8	2.31	108.17	105.74
38	A1	1449	A2M	C5-N7-C8	2.31	107.08	103.45
38	A1	817	A2M	C6-C5-N7	2.31	136.54	132.09
34	B5	436	A2M	C5-N7-C8	2.30	107.07	103.45
34	B5	562	OMG	O6-C6-C5	-2.30	120.46	126.53
38	A1	2724	OMU	C1'-N1-C2	2.30	121.72	117.59
34	B5	1575	G7M	C5-C6-N1	2.29	116.58	111.84
34	B5	562	OMG	C4-C5-N7	-2.29	107.04	110.67
34	B5	1773	4AC	C6-C5-C4	2.28	119.75	117.00
34	B5	619	A2M	C6-C5-N7	2.27	136.46	132.09
34	B5	1575	G7M	O6-C6-C5	-2.26	122.96	128.01
38	A1	876	A2M	C4-N9-C8	2.25	108.10	105.74
34	B5	1575	G7M	O2'-C2'-C1'	2.22	117.75	110.10
34	B5	796	A2M	C6-C5-N7	2.20	136.32	132.09
34	B5	436	A2M	C4-N9-C8	2.19	108.04	105.74
38	A1	2288	OMG	O6-C6-C5	-2.19	120.76	126.53
34	B5	1280	4AC	C6-C5-C4	2.18	119.63	117.00
38	A1	1449	A2M	C4-N9-C8	2.18	108.03	105.74
34	B5	1773	4AC	C1'-N1-C2	2.18	123.25	118.44
34	B5	28	A2M	C6-C5-N7	2.18	136.29	132.09
38	A1	2921	OMU	O2-C2-N1	-2.17	119.97	122.80
34	B5	1191	XSX	C1'-N1-C2	2.17	120.59	117.04
38	A1	2281	A2M	N9-C8-N7	-2.17	110.86	113.94
34	B5	578	OMU	O2-C2-N1	-2.15	120.00	122.80
38	A1	908	OMG	O6-C6-C5	-2.15	120.86	126.53
34	B5	1773	4AC	O2-C2-N3	-2.15	118.95	122.33
38	A1	2793	OMG	O6-C6-C5	-2.14	120.87	126.53
38	A1	2220	A2M	C5-N7-C8	2.14	106.81	103.45
38	A1	2421	OMU	O2-C2-N1	-2.14	120.02	122.80
38	A1	807	A2M	O4'-C1'-N9	2.14	112.19	108.09
38	A1	1133	A2M	C6-C5-N7	2.13	136.20	132.09
34	B5	420	A2M	C6-C5-N7	2.13	136.20	132.09
38	A1	645	1MA	C6-C5-N7	2.12	135.91	132.16
38	A1	2280	A2M	C6-C5-N7	2.12	136.17	132.09
38	A1	2640	A2M	C6-C5-N7	2.11	136.16	132.09
38	A1	805	OMG	O6-C6-C5	-2.11	120.97	126.53
34	B5	1781	MA6	C6-C5-N7	2.11	136.80	133.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2946	A2M	C6-C5-N7	2.11	136.15	132.09
38	A1	2729	OMU	C1'-N1-C2	2.10	121.37	117.59
38	A1	2142	1MA	C4-C5-N7	-2.10	107.33	110.67
34	B5	1572	OMG	O6-C6-C5	-2.10	120.99	126.53
38	A1	2959	OMC	O2-C2-N3	-2.09	119.03	122.33
34	B5	1428	OMG	O6-C6-C5	-2.09	121.01	126.53
38	A1	1450	OMG	O6-C6-C5	-2.09	121.03	126.53
38	A1	649	A2M	C6-C5-N7	2.08	136.10	132.09
38	A1	867	OMG	O6-C6-C5	-2.08	121.05	126.53
38	A1	2724	OMU	O2-C2-N1	-2.07	120.10	122.80
34	B5	1126	OMG	O6-C6-C5	-2.07	121.08	126.53
38	A1	2347	OMU	O2-C2-N3	-2.07	117.68	121.49
38	A1	2220	A2M	C6-C5-N7	2.06	136.06	132.09
38	A1	1133	A2M	N9-C8-N7	-2.06	111.02	113.94
34	B5	1639	OMC	O2-C2-N3	-2.06	119.09	122.33
38	A1	2922	OMG	O6-C6-C5	-2.06	121.11	126.53
34	B5	1191	XSX	C6-N1-C2	-2.06	120.12	121.80
38	A1	2619	OMG	O6-C6-C5	-2.05	121.12	126.53
38	A1	645	1MA	N1-C2-N3	-2.05	123.56	126.00
36	AB	243	HIC	CB-CG-CD2	-2.05	125.01	129.96
34	B5	1007	OMC	O2-C2-N3	-2.05	119.10	122.33
34	B5	619	A2M	N9-C8-N7	-2.05	111.03	113.94
38	A1	2791	OMG	O6-C6-C5	-2.04	121.15	126.53
38	A1	2280	A2M	N9-C8-N7	-2.03	111.06	113.94
34	B5	562	OMG	C5-C6-N1	2.02	118.39	113.25
34	B5	1271	OMG	O6-C6-C5	-2.01	121.21	126.53
34	B5	100	A2M	C2'-C1'-N9	-2.01	110.44	113.75
38	A1	2281	A2M	C6-C5-N7	2.01	135.96	132.09
38	A1	2634	UR3	C3U-N3-C2	2.01	120.83	117.33

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	B5	414	OMC	C1'-C2'-O2'-CM2
34	B5	420	A2M	C1'-C2'-O2'-CM'
34	B5	562	OMG	O4'-C4'-C5'-O5'
34	B5	796	A2M	C1'-C2'-O2'-CM'
34	B5	974	A2M	C1'-C2'-O2'-CM'
34	B5	1191	XSX	C3-C1-N3-C2
34	B5	1191	XSX	C3-C1-N3-C4
34	B5	1191	XSX	N3-C1-C3-C7

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Mol	Chain	Res	Type	Atoms
34	B5	1271	OMG	C1'-C2'-O2'-CM2
34	B5	1428	OMG	C1'-C2'-O2'-CM2
34	B5	1782	MA6	O4'-C4'-C5'-O5'
34	B5	1782	MA6	C3'-C4'-C5'-O5'
34	B5	1782	MA6	C5-C6-N6-C9
80	DC	699	DDE	CBI-CBW-NCB-CAB
80	DC	699	DDE	CBI-CBW-NCB-CAC
80	DC	699	DDE	CBI-CBW-NCB-CAA
80	DC	699	DDE	CAU-CBW-NCB-CAB
80	DC	699	DDE	CAU-CBW-NCB-CAC
80	DC	699	DDE	CAU-CBW-NCB-CAA
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
34	B5	1773	4AC	C5-C4-N4-C7
34	B5	1773	4AC	O7-C7-N4-C4
34	B5	1773	4AC	CM7-C7-N4-C4
38	A1	649	A2M	C1'-C2'-O2'-CM'
38	A1	663	OMC	C1'-C2'-O2'-CM2
38	A1	867	OMG	C1'-C2'-O2'-CM2
38	A1	1437	OMC	C1'-C2'-O2'-CM2
38	A1	2197	OMC	C2'-C1'-N1-C2
38	A1	2197	OMC	C2'-C1'-N1-C6
38	A1	2220	A2M	C1'-C2'-O2'-CM'
38	A1	2256	A2M	C1'-C2'-O2'-CM'
38	A1	2417	OMU	C1'-C2'-O2'-CM2
38	A1	2421	OMU	C1'-C2'-O2'-CM2
38	A1	2619	OMG	C1'-C2'-O2'-CM2
38	A1	2724	OMU	C1'-C2'-O2'-CM2
38	A1	2791	OMG	C1'-C2'-O2'-CM2
38	A1	2946	A2M	C1'-C2'-O2'-CM'
38	A1	2948	OMC	C1'-C2'-O2'-CM2
34	B5	562	OMG	C3'-C4'-C5'-O5'
34	B5	1773	4AC	O4'-C4'-C5'-O5'
38	A1	2729	OMU	C3'-C4'-C5'-O5'
34	B5	541	A2M	O4'-C4'-C5'-O5'
38	A1	1437	OMC	O4'-C4'-C5'-O5'
38	A1	2197	OMC	O4'-C4'-C5'-O5'
38	A1	2280	A2M	O4'-C4'-C5'-O5'
38	A1	2280	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
38	A1	2729	OMU	O4'-C4'-C5'-O5'
80	DC	699	DDE	CE1-CAT-CAU-CBW
34	B5	541	A2M	C3'-C4'-C5'-O5'
34	B5	578	OMU	O4'-C4'-C5'-O5'
34	B5	619	A2M	O4'-C4'-C5'-O5'
34	B5	1773	4AC	C3'-C4'-C5'-O5'
38	A1	1437	OMC	C3'-C4'-C5'-O5'
38	A1	2197	OMC	C3'-C4'-C5'-O5'
34	B5	1191	XSX	N4-C7-C9-O10
34	B5	1782	MA6	N1-C6-N6-C9
34	B5	619	A2M	C3'-C4'-C5'-O5'
38	A1	817	A2M	C4'-C5'-O5'-P
34	B5	1781	MA6	C5-C6-N6-C9
38	A1	2256	A2M	C4'-C5'-O5'-P
38	A1	2870	5MC	C2'-C1'-N1-C6
38	A1	2281	A2M	O4'-C4'-C5'-O5'
34	B5	1191	XSX	N4-C7-C9-O11
34	B5	1639	OMC	O4'-C4'-C5'-O5'
34	B5	619	A2M	C2'-C1'-N9-C8
38	A1	2870	5MC	O4'-C1'-N1-C6
34	B5	541	A2M	C4'-C5'-O5'-P
38	A1	2197	OMC	O4'-C1'-N1-C6
38	A1	2281	A2M	C3'-C4'-C5'-O5'
34	B5	1269	OMU	C3'-C2'-O2'-CM2
80	DC	699	DDE	CAT-CAU-CBW-CBI
34	B5	619	A2M	O4'-C1'-N9-C8
38	A1	2870	5MC	O4'-C1'-N1-C2
36	AB	243	HIC	CA-CB-CG-CD2
38	A1	645	1MA	C2'-C1'-N9-C8
34	B5	28	A2M	C1'-C2'-O2'-CM'
38	A1	2640	A2M	C1'-C2'-O2'-CM'
38	A1	645	1MA	C2'-C1'-N9-C4
38	A1	1450	OMG	C4'-C5'-O5'-P
34	B5	1782	MA6	C5-C6-N6-C10
36	AB	243	HIC	CA-CB-CG-ND1
34	B5	541	A2M	O4'-C1'-N9-C8
34	B5	578	OMU	C3'-C4'-C5'-O5'
34	B5	1428	OMG	O4'-C4'-C5'-O5'
34	B5	1428	OMG	C4'-C5'-O5'-P
34	B5	541	A2M	C2'-C1'-N9-C8
34	B5	619	A2M	C2'-C1'-N9-C4
34	B5	578	OMU	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
38	A1	2870	5MC	C2'-C1'-N1-C2
38	A1	649	A2M	C4'-C5'-O5'-P
38	A1	2729	OMU	C4'-C5'-O5'-P
34	B5	578	OMU	O4'-C1'-N1-C6
34	B5	541	A2M	C2'-C1'-N9-C4
38	A1	2197	OMC	O4'-C1'-N1-C2

There are no ring outliers.

15 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	A1	805	OMG	1	0
34	B5	1280	4AC	3	0
34	B5	1639	OMC	1	0
34	B5	28	A2M	1	0
38	A1	663	OMC	1	0
38	A1	1133	A2M	1	0
34	B5	1575	G7M	1	0
38	A1	650	OMC	1	0
34	B5	974	A2M	1	0
38	A1	2220	A2M	2	0
34	B5	1773	4AC	1	0
38	A1	1449	A2M	1	0
38	A1	2724	OMU	2	0
80	DC	699	DDE	2	0
38	A1	649	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 244 ligands modelled in this entry, 242 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	$\# Z > 2$
85	GDP	DC	901	83	29,30,30	1.14	3 (10%)	45,47,47	1.82	7 (15%)
86	SO1	DC	903	-	34,39,39	0.68	1 (2%)	38,64,64	1.11	5 (13%)

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
85	GDP	DC	901	83	-	0/16/32/32	0/3/3/3
86	SO1	DC	903	-	1/1/15/16	7/21/104/104	0/7/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	DC	901	GDP	C5-C4	3.04	1.47	1.38
86	DC	903	SO1	O14-C5	-2.93	1.19	1.30
85	DC	901	GDP	C6-N1	-2.26	1.34	1.38
85	DC	901	GDP	C5-N7	-2.05	1.35	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	DC	901	GDP	C5-C4-N3	-6.22	118.50	128.39
85	DC	901	GDP	C2-N3-C4	5.16	121.19	112.30
85	DC	901	GDP	N9-C4-N3	4.56	135.07	125.95
86	DC	903	SO1	C12-C6-C2	-3.70	99.36	105.09
85	DC	901	GDP	C6-C5-N7	3.24	136.18	130.29
86	DC	903	SO1	C1-C4-C13	-2.88	115.28	118.36
85	DC	901	GDP	C4-C5-N7	-2.61	106.54	110.67
85	DC	901	GDP	O6-C6-C5	-2.39	120.23	126.53
86	DC	903	SO1	C7-C2-C6	2.35	116.55	112.05
85	DC	901	GDP	C3'-C2'-C1'	2.15	105.54	101.46
86	DC	903	SO1	C18-C9-C16	-2.08	100.87	103.72
86	DC	903	SO1	C24-C18-C9	-2.06	101.11	105.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
86	DC	903	SO1	C4

All (7) torsion outliers are listed below:

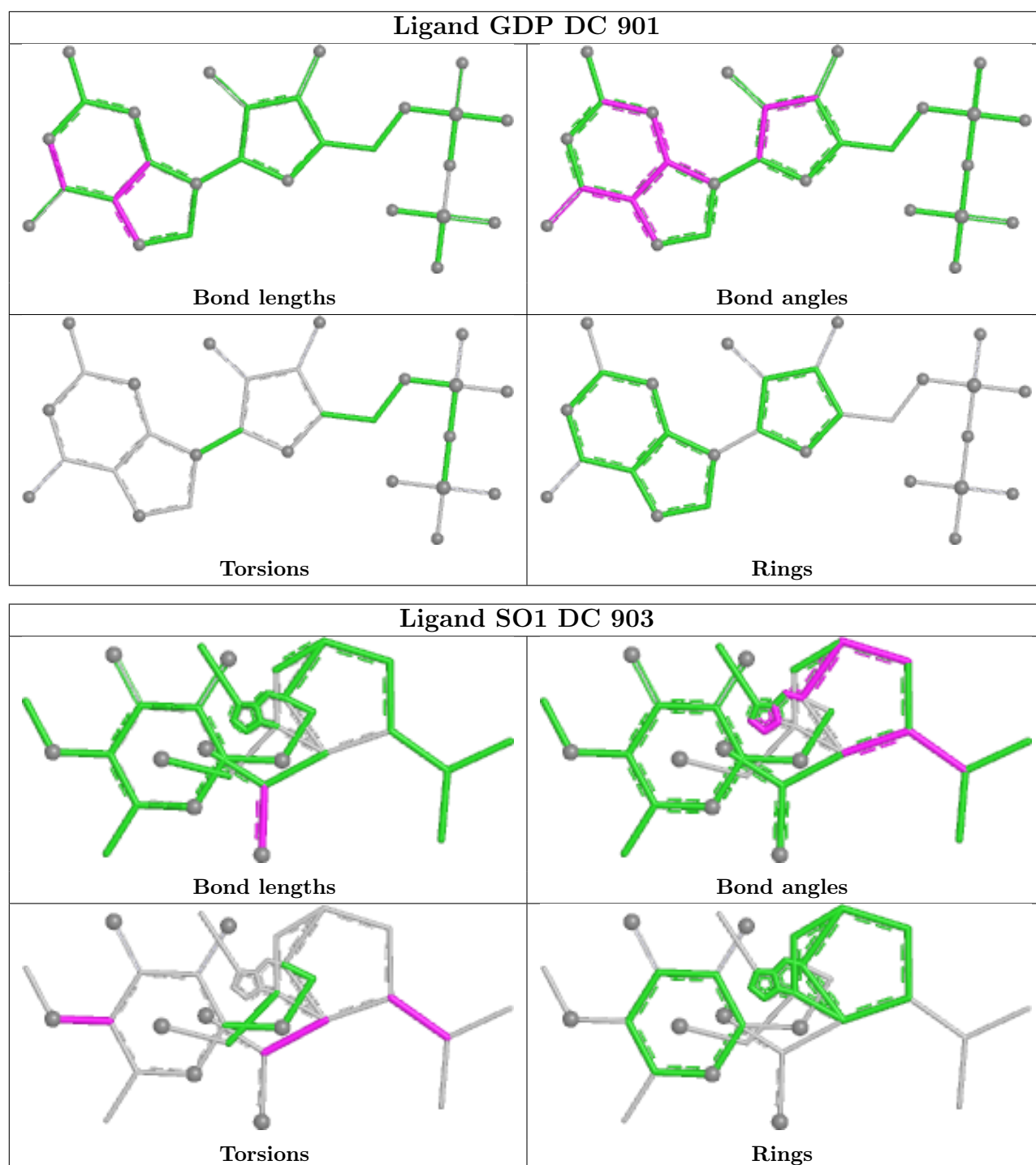
Mol	Chain	Res	Type	Atoms
86	DC	903	SO1	C2-C1-C5-O14
86	DC	903	SO1	C2-C1-C5-O15
86	DC	903	SO1	C21-C13-C4-C12
86	DC	903	SO1	C20-C13-C4-C12
86	DC	903	SO1	C54-C55-O64-C65
86	DC	903	SO1	C21-C13-C4-C1
86	DC	903	SO1	C20-C13-C4-C1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	DC	901	GDP	1	0
86	DC	903	SO1	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.

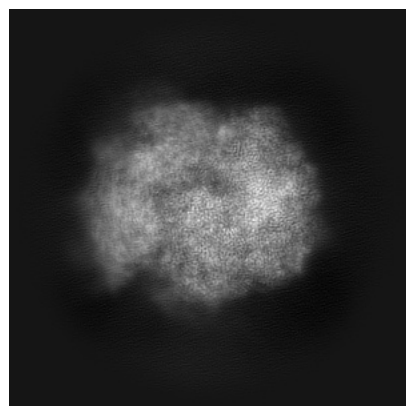
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28633. These allow visual inspection of the internal detail of the map and identification of artifacts.

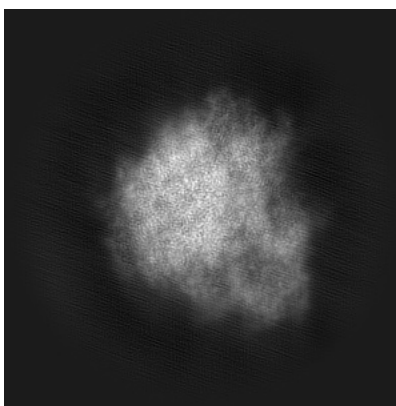
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

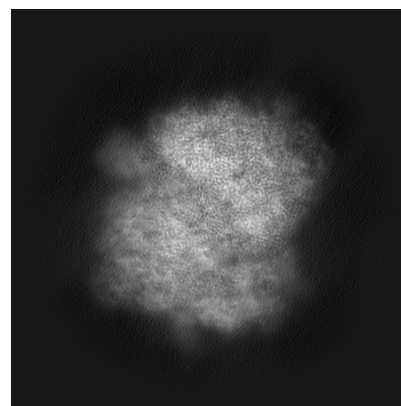
6.1.1 Primary map



X

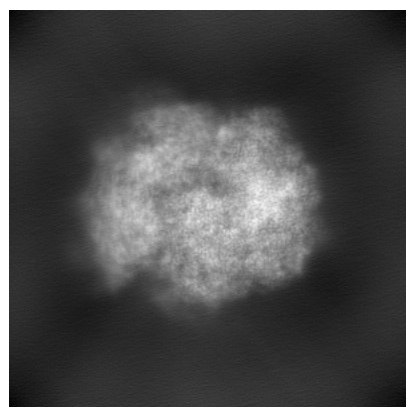


Y

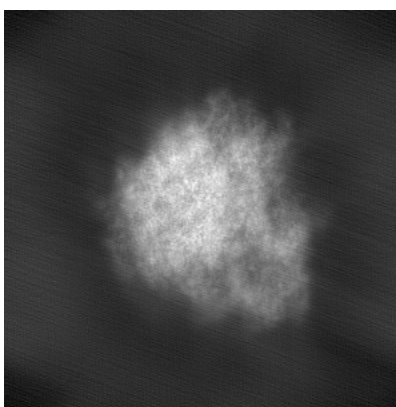


Z

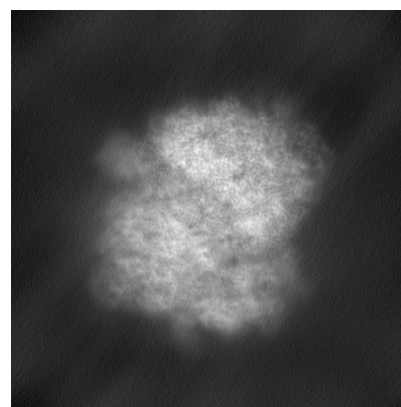
6.1.2 Raw map



X



Y

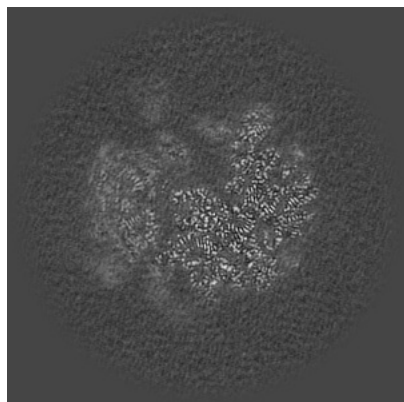


Z

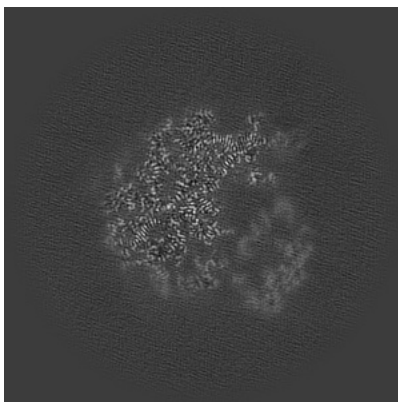
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

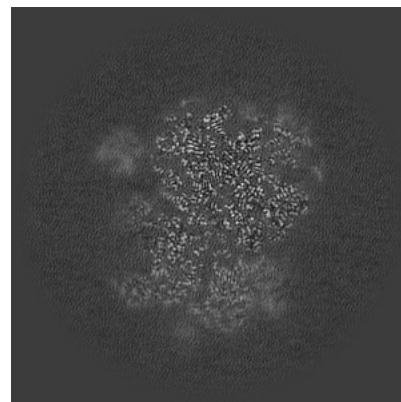
6.2.1 Primary map



X Index: 200

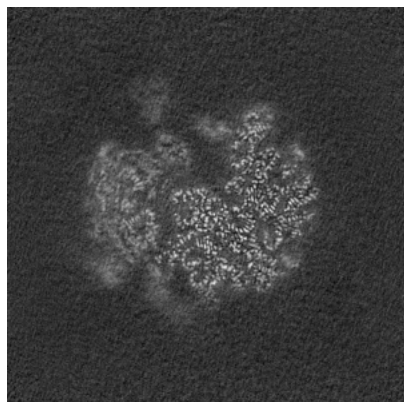


Y Index: 200

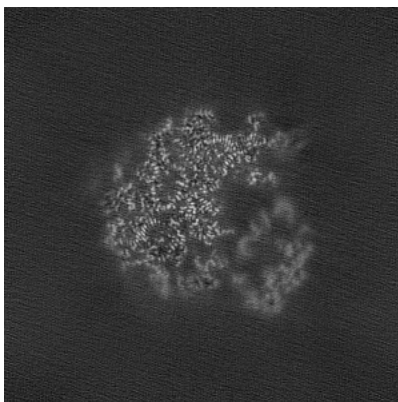


Z Index: 200

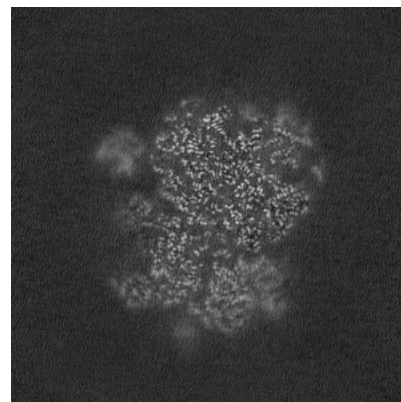
6.2.2 Raw map



X Index: 200



Y Index: 200

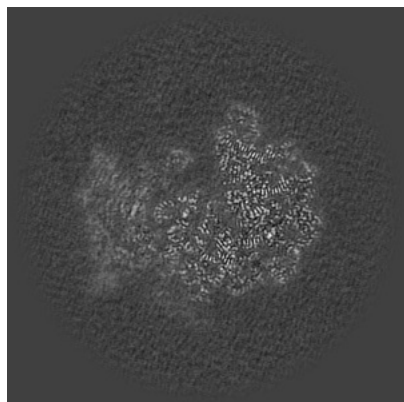


Z Index: 200

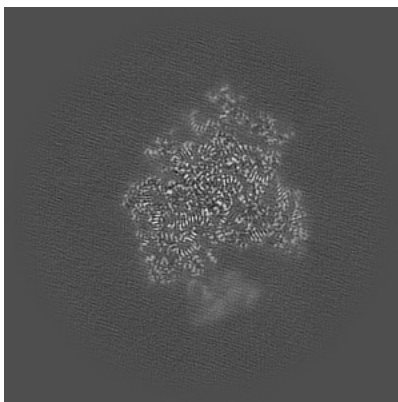
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

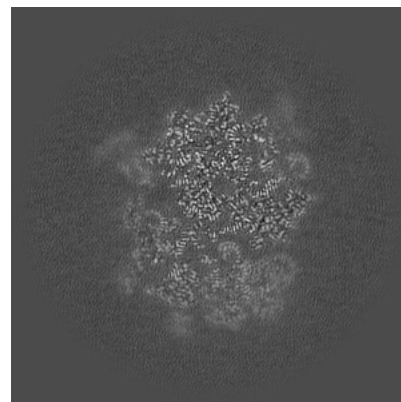
6.3.1 Primary map



X Index: 214

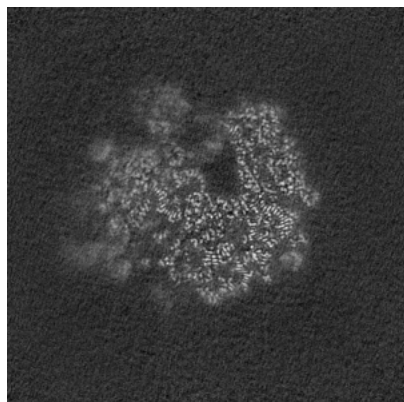


Y Index: 247

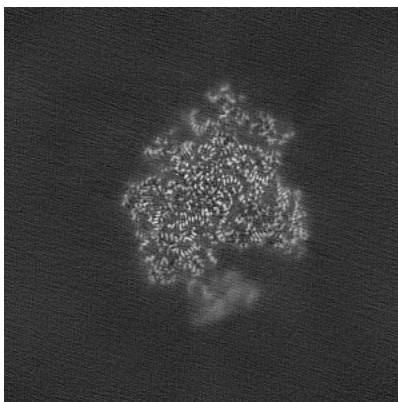


Z Index: 189

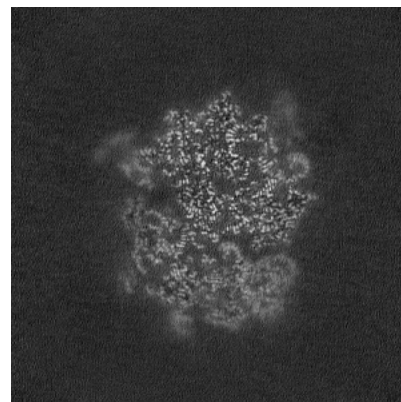
6.3.2 Raw map



X Index: 184



Y Index: 247

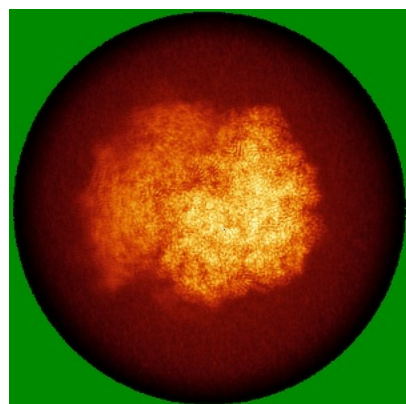


Z Index: 188

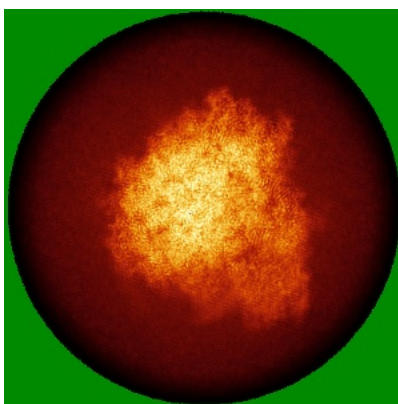
The images above show the largest variance slices of the map in three orthogonal directions.

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

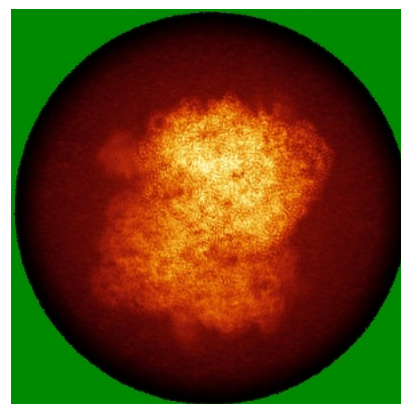
6.4.1 Primary map



X

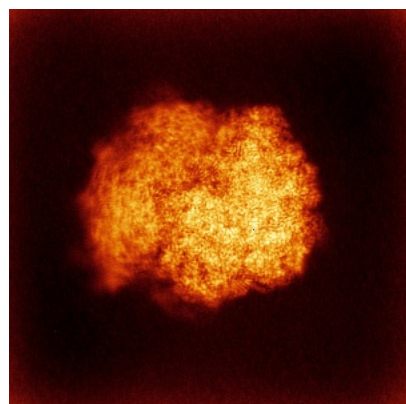


Y

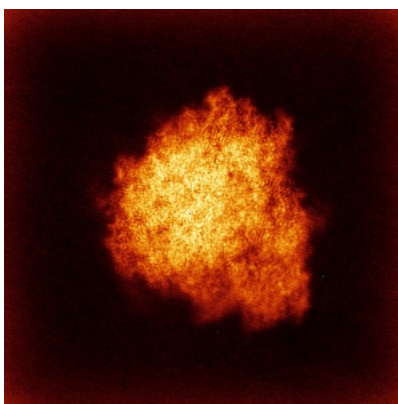


Z

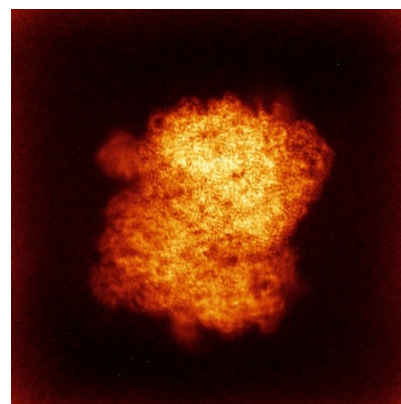
6.4.2 Raw map



X



Y

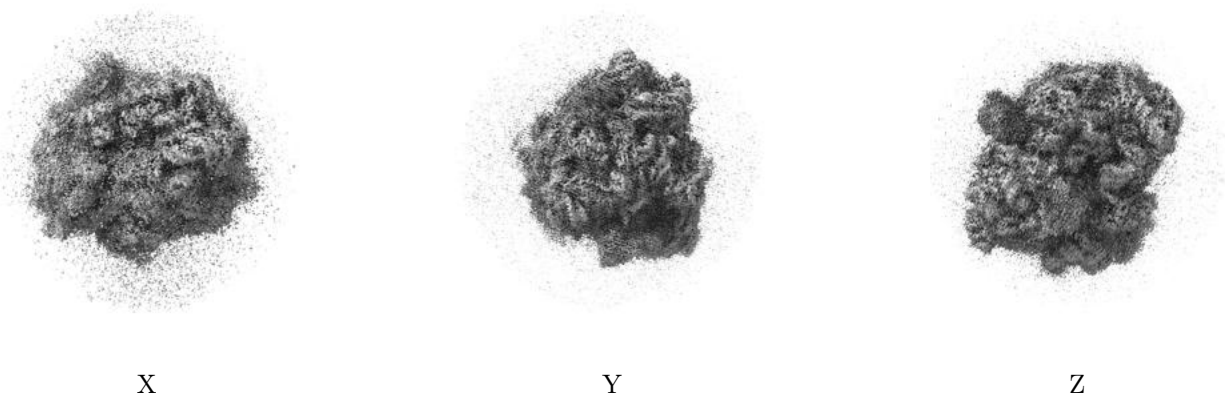


Z

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

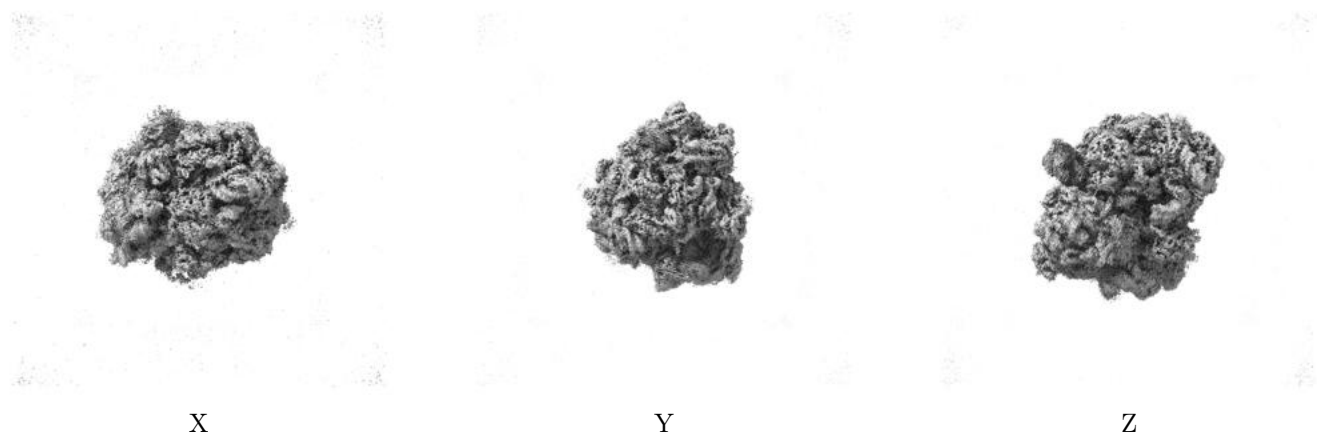
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

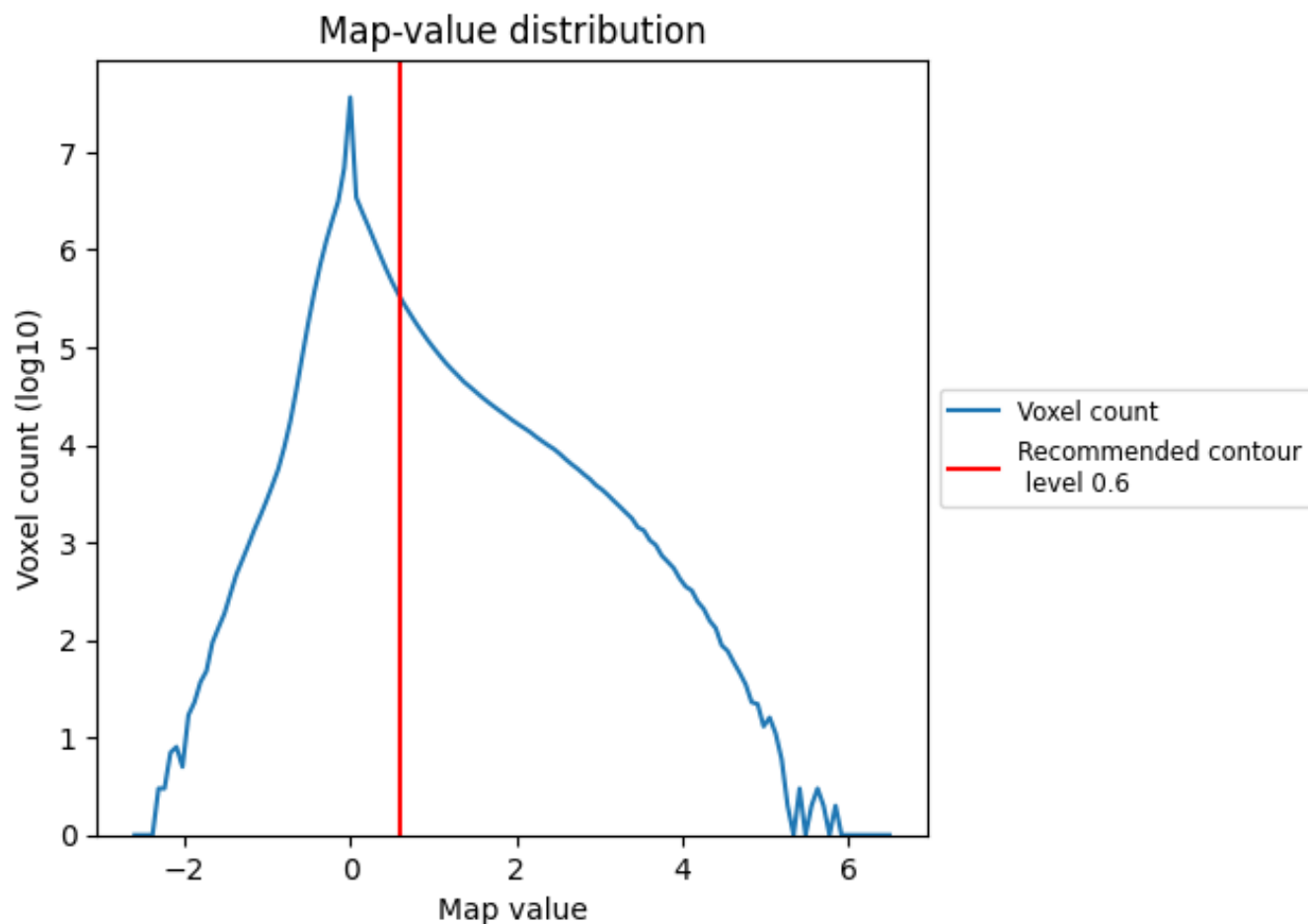
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

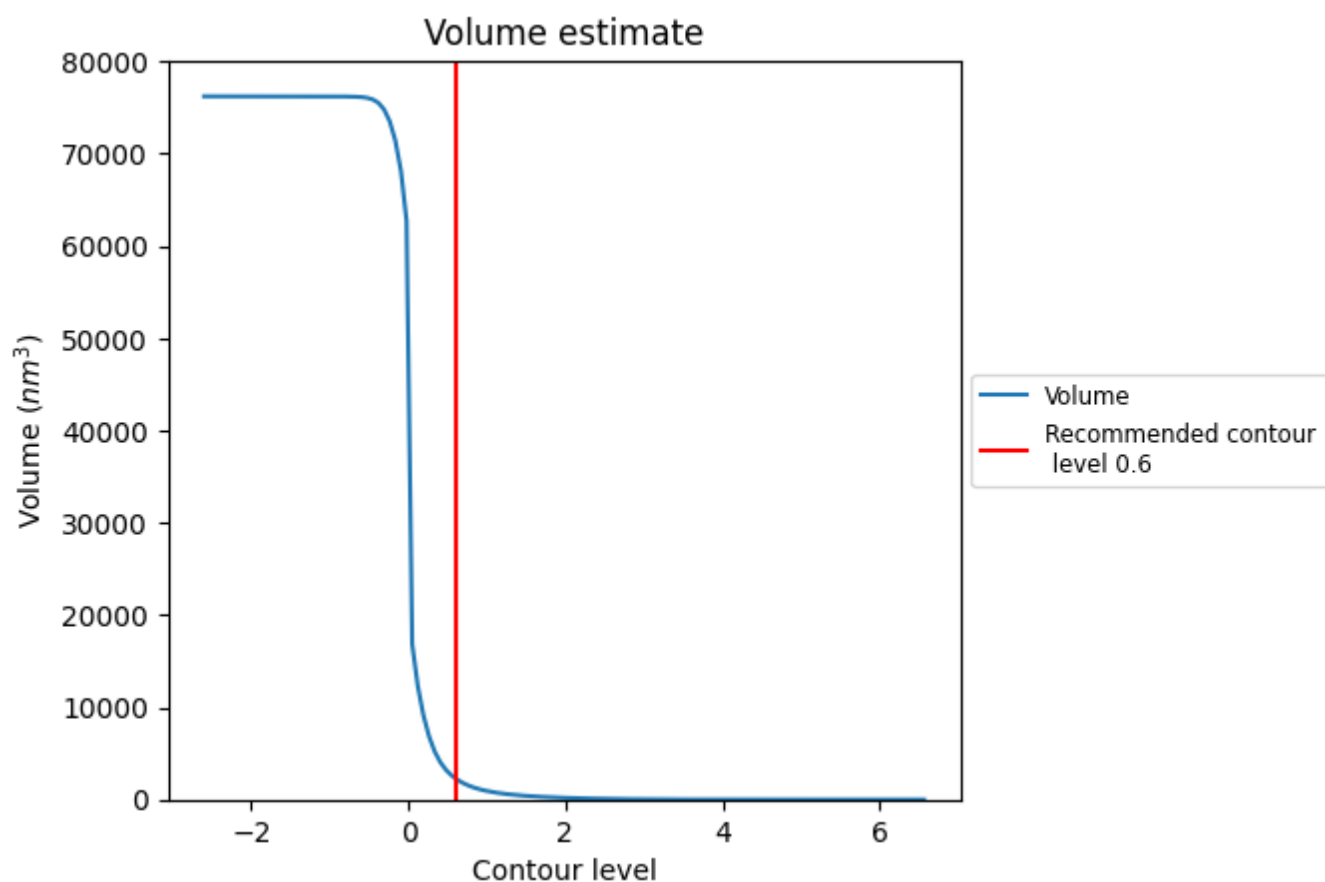
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

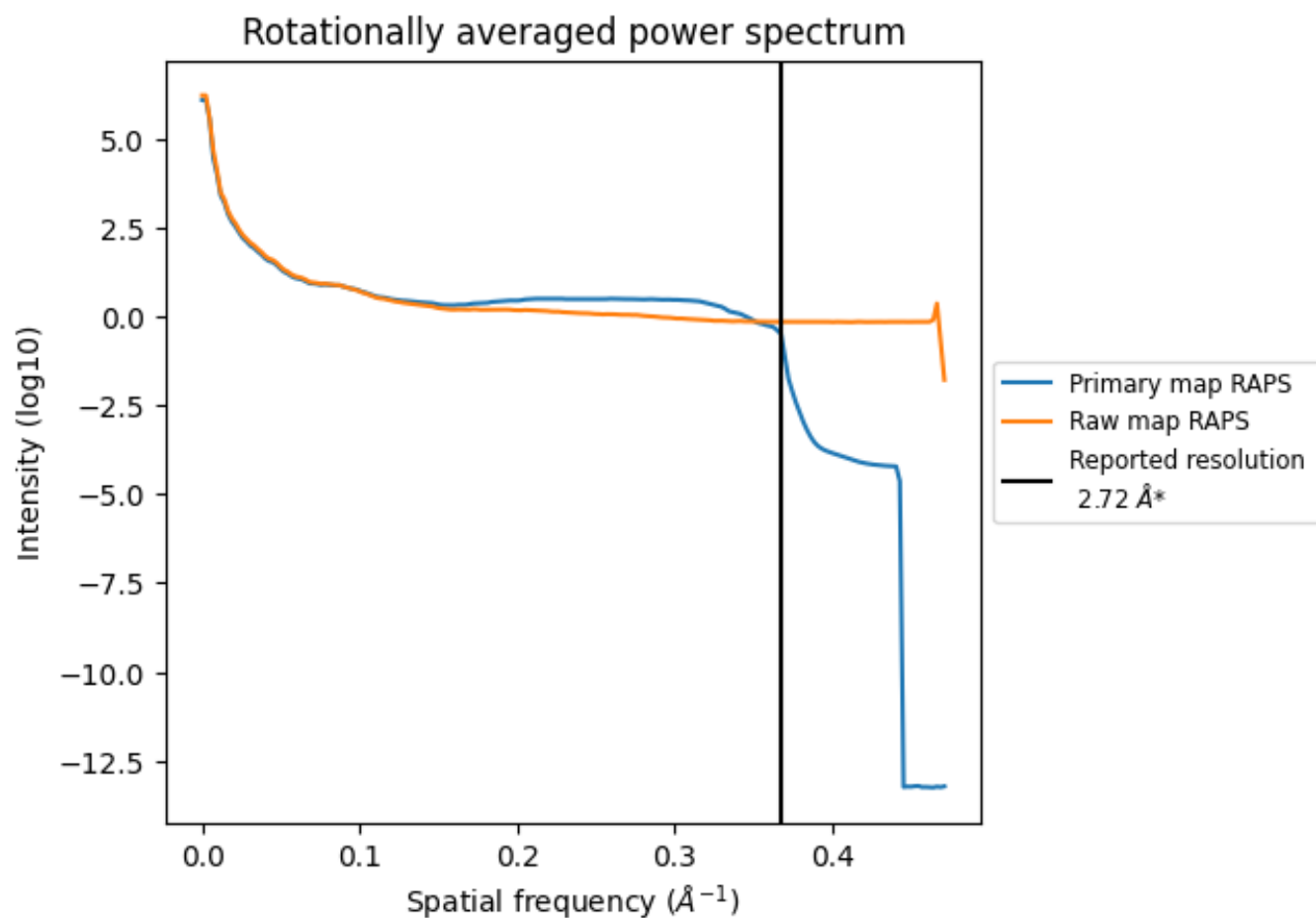
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2308 nm³; this corresponds to an approximate mass of 2085 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 ⓘ

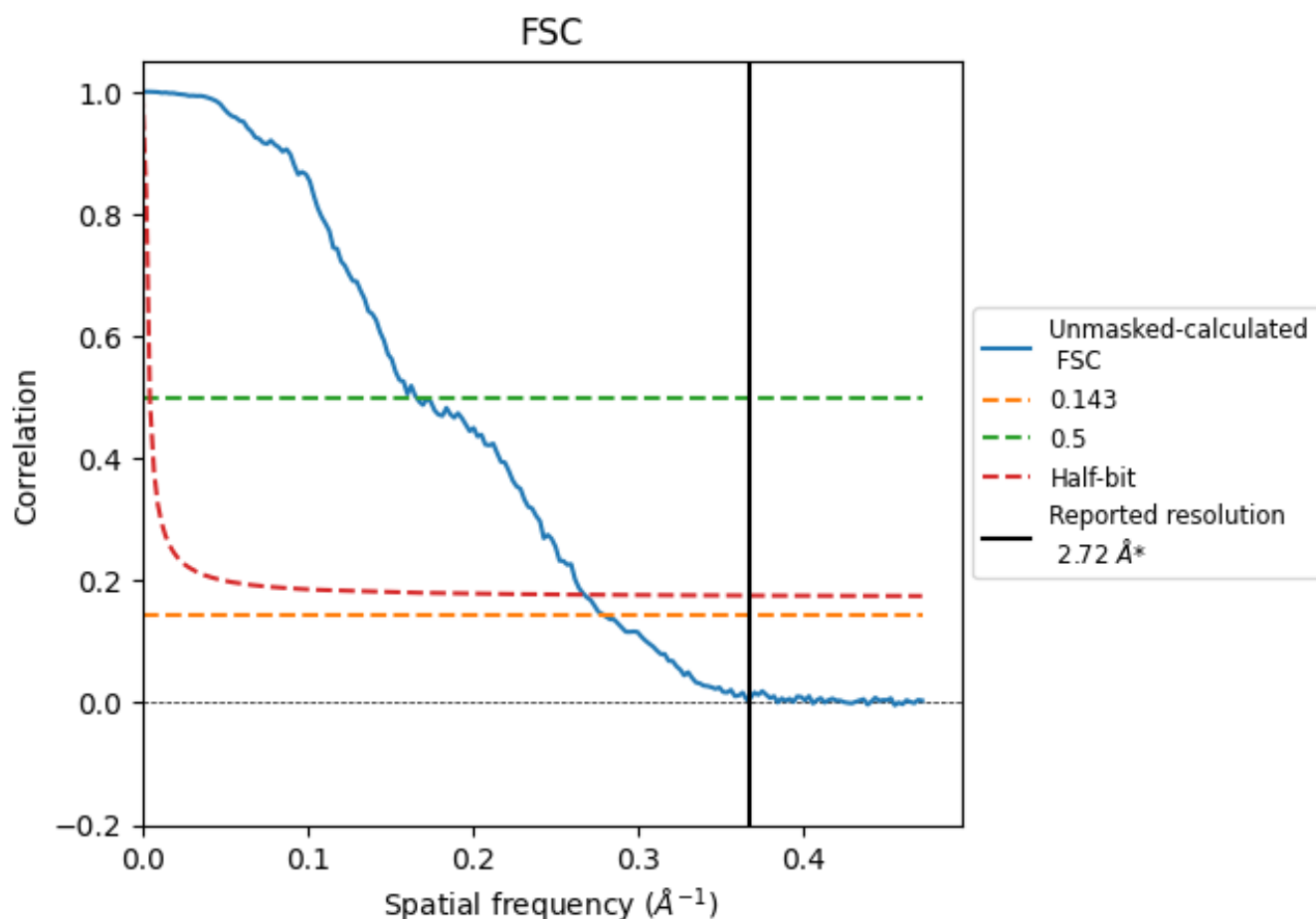


*Reported resolution corresponds to spatial frequency of 0.368 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.368 Å⁻¹

8.2 Resolution estimates [i](#)

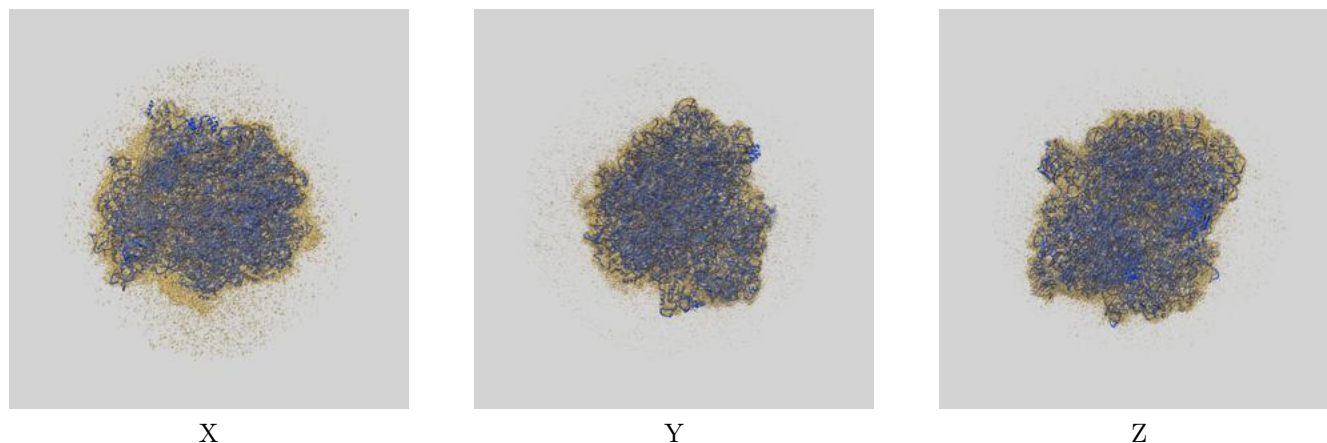
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.58	6.04	3.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.58 differs from the reported value 2.72 by more than 10 %

9 Map-model fit [i](#)

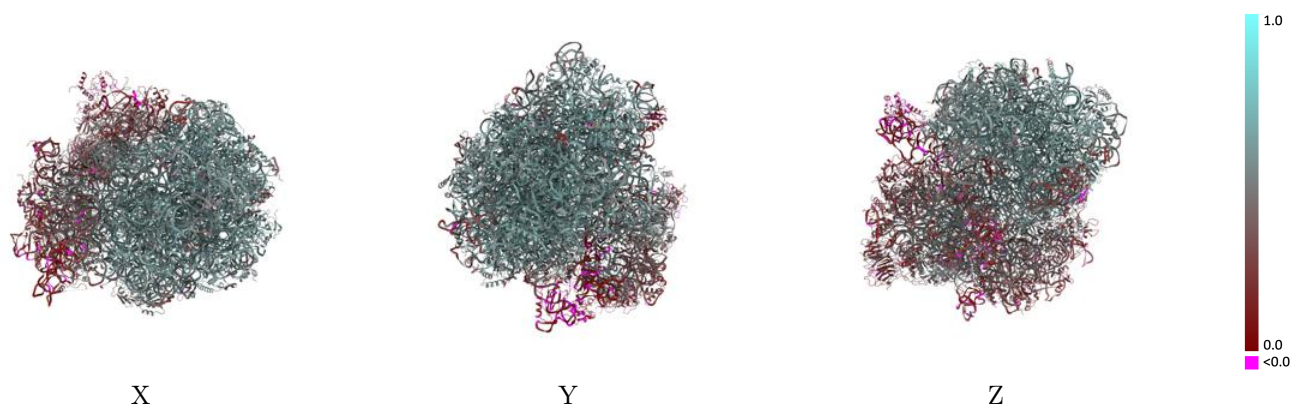
This section contains information regarding the fit between EMDB map EMD-28633 and PDB model 8EVQ. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



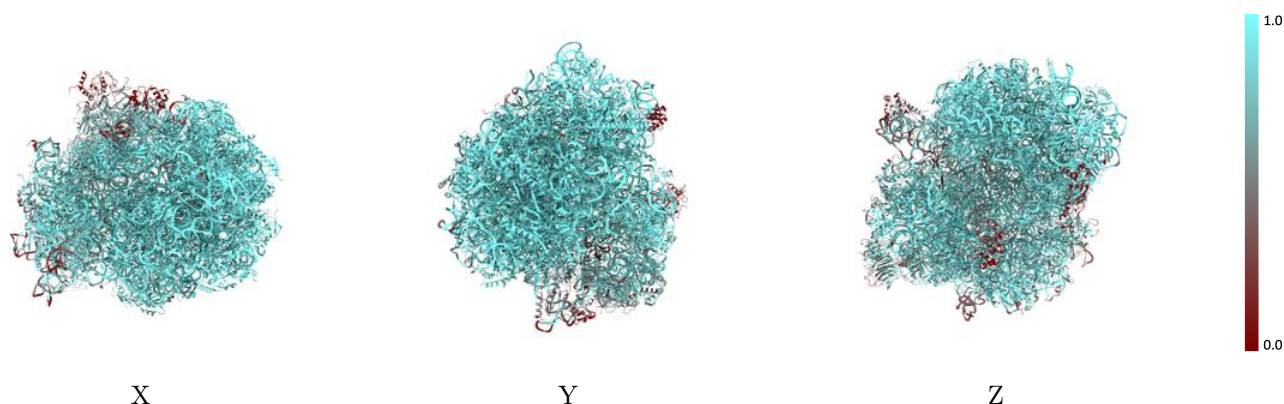
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



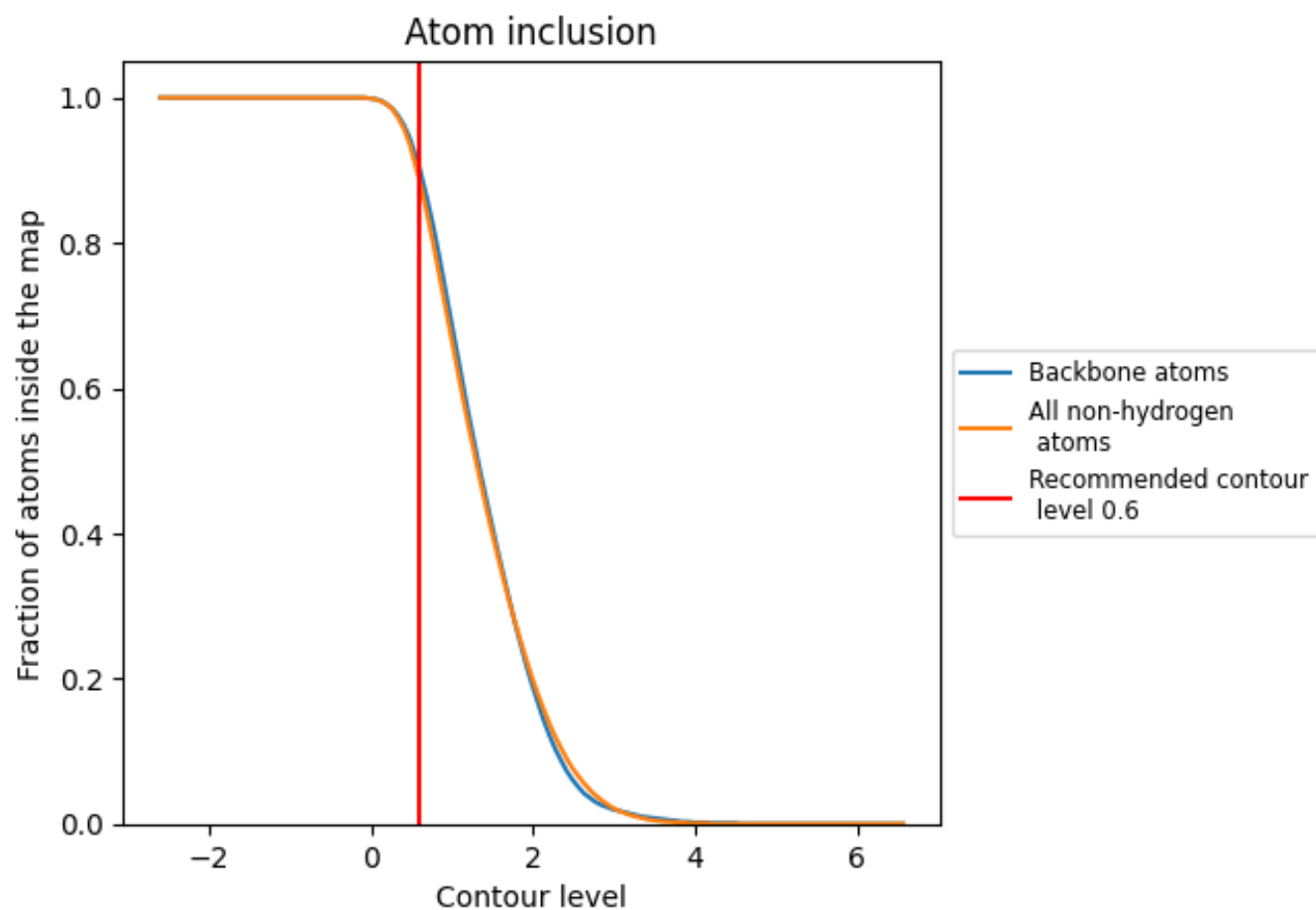
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8860	 0.4870
A1	 0.9680	 0.5710
A3	 0.9920	 0.5790
A4	 0.9820	 0.5940
AA	 0.9740	 0.6210
AB	 0.9630	 0.5830
AC	 0.9640	 0.5870
AD	 0.9080	 0.5130
AE	 0.9380	 0.5380
AF	 0.9710	 0.5980
AG	 0.9170	 0.5510
AH	 0.9420	 0.5730
AI	 0.9640	 0.5820
AJ	 0.8110	 0.4340
AL	 0.9510	 0.5900
AM	 0.9490	 0.5750
AN	 0.9870	 0.6270
AO	 0.9670	 0.5930
AP	 0.9620	 0.5760
AQ	 0.9800	 0.6170
AR	 0.8500	 0.5090
AS	 0.9670	 0.5940
AT	 0.9570	 0.5780
AU	 0.8810	 0.4590
AV	 0.9510	 0.5870
AW	 0.9600	 0.5770
AX	 0.9410	 0.5650
AY	 0.9480	 0.5580
AZ	 0.9220	 0.5440
Aa	 0.9710	 0.6070
Ab	 0.9290	 0.5620
Ac	 0.8880	 0.5490
Ad	 0.9110	 0.5380
Ae	 0.9730	 0.6010
Af	 0.9840	 0.6100



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Chain	Atom inclusion	Q-score
Ag	 0.9250	 0.5740
Ah	 0.9500	 0.5620
Ai	 0.9520	 0.5550
Aj	 0.9860	 0.6150
Ak	 0.7400	 0.4660
Al	 0.9830	 0.5870
Am	 0.9280	 0.5810
An	 0.9530	 0.5560
Ao	 0.9060	 0.5770
Ap	 0.9360	 0.5900
B5	 0.8860	 0.4100
BA	 0.8120	 0.4410
BB	 0.7830	 0.4340
BC	 0.9050	 0.4790
BD	 0.7890	 0.3580
BE	 0.8460	 0.3580
BF	 0.7130	 0.3390
BG	 0.7650	 0.2800
BH	 0.6710	 0.3800
BI	 0.8450	 0.4230
BJ	 0.8310	 0.3500
BK	 0.6600	 0.2670
BL	 0.8150	 0.4430
BM	 0.0840	 0.1490
BN	 0.8610	 0.4860
BO	 0.8430	 0.4800
BP	 0.6570	 0.3210
BQ	 0.8180	 0.3840
BR	 0.5970	 0.2900
BS	 0.7450	 0.3280
BT	 0.7530	 0.3120
BU	 0.6860	 0.3050
BV	 0.8780	 0.4620
BW	 0.9420	 0.5280
BX	 0.8880	 0.4500
BY	 0.7920	 0.3020
BZ	 0.6880	 0.2880
Ba	 0.8740	 0.5090
Bb	 0.7440	 0.4510
Bc	 0.7210	 0.3900
Bd	 0.9170	 0.4040
Be	 0.7360	 0.3000

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Chain	Atom inclusion	Q-score
Bf	 0.1570	 0.1440
Bg	 0.6200	 0.2510
DC	 0.7890	 0.3990
E	 0.3980	 0.1190
EC	 0.5930	 0.1910
V	 0.1270	 0.2200