



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 07:53 PM UTC

PDB ID : 6OLZ / pdb_00006olz
EMDB ID : EMD-0598
Title : Human ribosome nascent chain complex (PCSK9-RNC) stalled by a drug-like molecule with PP tRNA
Authors : Li, W.; Cate, J.H.D.
Deposited on : 2019-04-17
Resolution : 3.90 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:

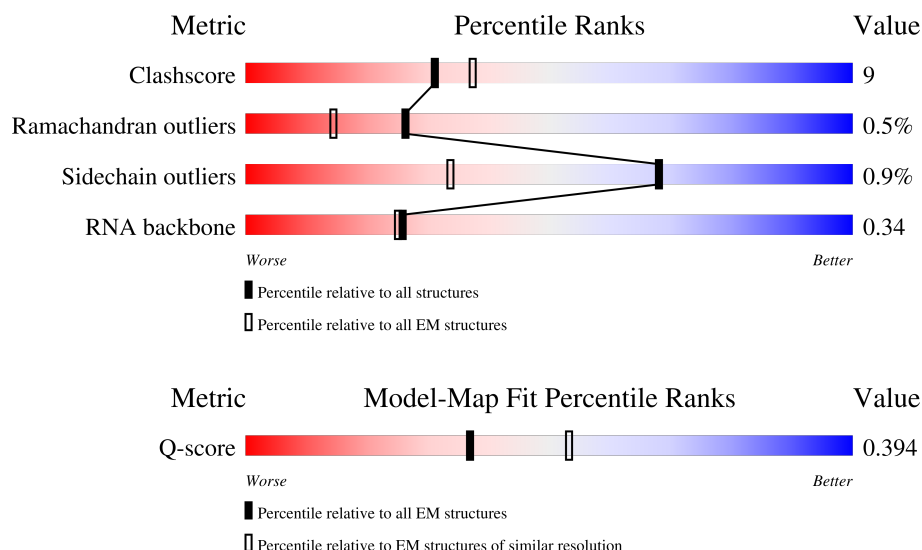
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.90 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	8855 (3.40 - 4.40)

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	AA	248	
2	BA	215	
3	AB	394	

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Mol	Chain	Length	Quality of chain
4	BB	212	
5	AC	363	
6	BC	222	
7	A3	157	
8	A4	119	
9	AD	294	
10	AE	247	
11	AF	234	
12	AG	234	
13	AH	191	
14	AI	211	
15	AJ	169	
16	AL	205	
17	AM	139	
18	AN	203	
19	AO	195	
20	AP	153	
21	AQ	187	
22	AR	181	
23	AS	175	
24	AT	157	
25	AU	99	
26	AV	129	
27	AW	121	
28	AX	117	

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Mol	Chain	Length	Quality of chain
29	AY	127	
30	AZ	134	
31	Aa	147	
32	Ab	118	
33	Ac	103	
34	Ad	106	
35	Ae	129	
36	Af	109	
37	Ag	114	
38	Ah	122	
39	Ai	97	
40	Aj	84	
41	Ak	69	
42	Al	50	
43	Am	50	
44	An	25	
45	Ao	105	
46	Ap	91	
47	At	122	
48	A2	3643	
49	B1	1708	
50	BD	220	
51	BE	257	
52	BF	190	
53	BG	232	

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Mol	Chain	Length	Quality of chain
54	BH	183	
55	BI	207	
56	BJ	179	
57	BK	98	
58	BL	153	
59	BM	120	
60	BN	149	
61	BO	136	
62	BP	120	
63	BQ	139	
64	BR	125	
65	BS	139	
66	BT	143	
67	BU	97	
68	BV	81	
69	BW	129	
70	BX	139	
71	BY	125	
72	BZ	86	
73	Ba	97	
74	Bb	80	
75	Bc	62	
76	Bd	51	
77	Be	55	
78	Bf	73	

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Mol	Chain	Length	Quality of chain
79	Bg	314	 70% 30% 92%
80	Bv	76	 51% 41% 8% 91%
81	Bx	16	 38% 38% 25% 88%
82	A	26	 46% 42% 12% 92%

2 Entry composition

There are 85 unique types of molecules in this entry. The entry contains 214215 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 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BA	215	Total	C	N	O	S	0	0
			1704	1083	298	315	8		

- Molecule 3 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AB	394	Total	C	N	O	S	0	0
			3178	2024	596	544	14		

- Molecule 4 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BB	212	Total	C	N	O	S	0	0
			1722	1093	308	307	14		

- Molecule 5 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AC	363	Total	C	N	O	S	0	0
			2888	1817	577	480	14		

- Molecule 6 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BC	222	Total	C	N	O	S	0	0
			1724	1114	296	304	10		

- Molecule 7 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A3	157	Total	C	N	O	P	0	0
			3337	1489	587	1104	157		

- Molecule 8 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A4	119	Total	C	N	O	P	0	0
			2541	1132	454	836	119		

- Molecule 9 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AD	294	Total	C	N	O	S	0	0
			2392	1510	436	432	14		

- Molecule 10 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AE	226	Total	C	N	O	S	0	0
			1838	1180	350	304	4		

- Molecule 11 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AF	234	Total	C	N	O	S	0	0
			1950	1252	376	313	9		

- Molecule 12 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AG	234	Total	C	N	O	S	0	0
			1880	1197	362	317	4		

- Molecule 13 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AH	191	Total	C	N	O	S	0	0
			1526	960	285	275	6		

- Molecule 14 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AI	208	Total	C	N	O	S	0	0
			1692	1074	327	278	13		

- Molecule 15 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AJ	169	Total	C	N	O	S	0	0
			1353	855	252	240	6		

- Molecule 16 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AL	205	Total	C	N	O	S	0	0
			1657	1036	344	273	4		

- Molecule 17 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 18 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 19 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AO	195	Total	C	N	O	S	0	0
			1606	1034	315	252	5		

- Molecule 20 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 21 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 22 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AR	181	Total	C	N	O	S	0	0
			1517	938	329	241	9		

- Molecule 23 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AS	175	Total	C	N	O	S	0	0
			1449	921	283	234	11		

- Molecule 24 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AT	157	Total	C	N	O	S	0	0
			1284	815	250	214	5		

- Molecule 25 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AU	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

- Molecule 26 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AV	129	Total	C	N	O	S	0	0
			969	613	182	169	5		

- Molecule 27 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AW	121	Total	C	N	O	S	0	0
			989	617	202	167	3		

- Molecule 28 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AX	117	Total	C	N	O	S	0	0
			958	612	180	165	1		

- Molecule 29 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AY	127	Total	C	N	O	S	0	0
			1064	668	216	177	3		

- Molecule 30 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AZ	134	Total	C	N	O	S	0	0
			1103	712	207	181	3		

- Molecule 31 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Aa	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 32 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ab	97	Total	C	N	O	S	0	0
			792	492	175	122	3		

- Molecule 33 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ac	103	Total	C	N	O	S	0	0
			801	508	141	145	7		

- Molecule 34 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ad	106	Total	C	N	O	S	0	0
			879	555	170	152	2		

- Molecule 35 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ae	129	Total	C	N	O	S	0	0
			1064	673	220	166	5		

- Molecule 36 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Af	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 37 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ag	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 38 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ah	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 39 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ai	97	Total	C	N	O	S	0	0
			794	497	168	124	5		

- Molecule 40 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Aj	84	Total	C	N	O	S	0	0
			689	423	152	109	5		

- Molecule 41 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Ak	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 42 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Al	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 43 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Am	50	Total	C	N	O	S	0	0
			411	254	87	64	6		

- Molecule 44 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	An	25	Total	C	N	O	S	0	0
			240	145	64	28	3		

- Molecule 45 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Ao	105	Total	C	N	O	S	0	0
			863	542	175	140	6		

- Molecule 46 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Ap	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 47 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	At	122	Total	C	N	O	S	0	0
			980	607	204	165	4		

- Molecule 48 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	A2	3643	Total	C	N	O	P	0	0
			78102	34781	14290	25388	3643		

- Molecule 49 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B1	1708	Total	C	N	O	P	0	0
			36456	16274	6546	11928	1708		

- Molecule 50 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BD	220	Total	C	N	O	S	0	0
			1709	1090	308	304	7		

- Molecule 51 is a protein called 40S ribosomal protein S4, Y isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BE	257	Total	C	N	O	S	0	0
			2031	1298	381	344	8		

- Molecule 52 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BF	190	Total	C	N	O	S	0	0
			1502	939	285	271	7		

- Molecule 53 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BG	232	Total	C	N	O	S	0	0
			1884	1176	379	322	7		

- Molecule 54 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BH	183	Total	C	N	O	S	0	0
			1479	941	272	265	1		

- Molecule 55 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BI	207	Total	C	N	O	S	0	0
			1696	1064	334	293	5		

- Molecule 56 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BJ	179	Total	C	N	O	S	0	0
			1495	953	299	241	2		

- Molecule 57 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 58 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BL	153	Total	C	N	O	S	0	0
			1258	804	235	213	6		

- Molecule 59 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BM	120	Total	C	N	O	S	0	0
			931	584	164	174	9		

- Molecule 60 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BN	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 61 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BO	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 62 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	BP	120	Total	C	N	O	S	0	0
			999	636	188	168	7		

- Molecule 63 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BQ	139	Total	C	N	O	S	0	0
			1109	704	210	192	3		

- Molecule 64 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	BR	125	Total	C	N	O	S	0	0
			1011	634	187	186	4		

- Molecule 65 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	BS	139	Total	C	N	O	S	0	0
			1154	725	233	195	1		

- Molecule 66 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	BT	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 67 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	BU	97	Total	C	N	O	S	0	0
			769	483	144	138	4		

- Molecule 68 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	BV	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 69 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	BW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 70 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	BX	139	Total	C	N	O	S	0	0
			1080	682	214	181	3		

- Molecule 71 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	BY	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 72 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	BZ	86	Total	C	N	O	S	0	0
			688	442	129	116	1		

- Molecule 73 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Ba	97	Total	C	N	O	S	0	0
			774	481	160	128	5		

- Molecule 74 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bb	80	Total	C	N	O	S	0	0
			625	391	116	111	7		

- Molecule 75 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Bc	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 76 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Bd	51	Total	C	N	O	S	0	0
			427	269	87	66	5		

- Molecule 77 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Be	55	Total	C	N	O	S	0	0
			437	272	96	68	1		

- Molecule 78 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Bf	73	Total	C	N	O	S	0	0
			601	379	115	100	7		

- Molecule 79 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Bg	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 80 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Bv	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

- Molecule 81 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Bx	16	Total	C	N	O	P	0	0
			320	144	32	128	16		

- Molecule 82 is a protein called Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
82	A	26	Total	C	N	O	0	0
			128	76	26	26		

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

Mol	Chain	Residues	Atoms		AltConf
83	AA	1	Total	Mg	0
			1	1	
83	AB	2	Total	Mg	0
			2	2	
83	BC	1	Total	Mg	0
			1	1	

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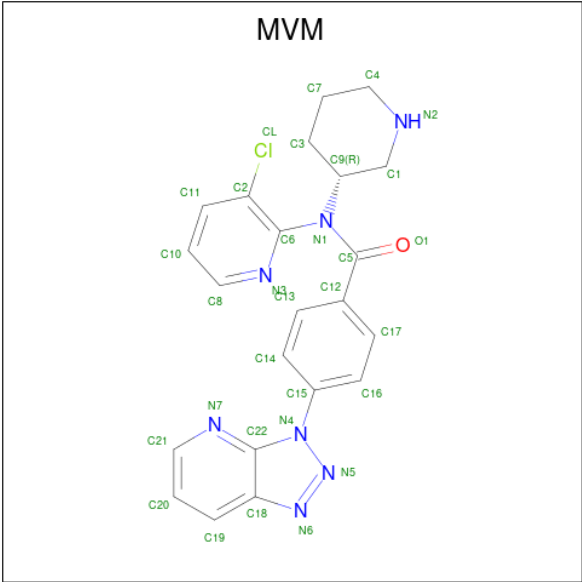
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Mol	Chain	Residues	Atoms		AltConf
83	A3	8	Total 8	Mg 8	0
83	A4	9	Total 9	Mg 9	0
83	AN	1	Total 1	Mg 1	0
83	AP	2	Total 2	Mg 2	0
83	Aa	2	Total 2	Mg 2	0
83	Ae	1	Total 1	Mg 1	0
83	Aj	1	Total 1	Mg 1	0
83	Al	1	Total 1	Mg 1	0
83	An	1	Total 1	Mg 1	0
83	A2	220	Total 220	Mg 220	0
83	B1	73	Total 73	Mg 73	0
83	BI	1	Total 1	Mg 1	0
83	Bv	2	Total 2	Mg 2	0

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

Mol	Chain	Residues	Atoms		AltConf
84	Aj	1	Total 1	Zn 1	0
84	Ao	1	Total 1	Zn 1	0
84	Ap	1	Total 1	Zn 1	0
84	Ba	1	Total 1	Zn 1	0
84	Bd	1	Total 1	Zn 1	0

- Molecule 85 is N-(3-chloropyridin-2-yl)-N-[(3R)-piperidin-3-yl]-4-(3H-[1,2,3]triazolo[4,5-b]pyridin-3-yl)benzamide (CCD ID: MVM) (formula: C₂₂H₂₀ClN₇O).

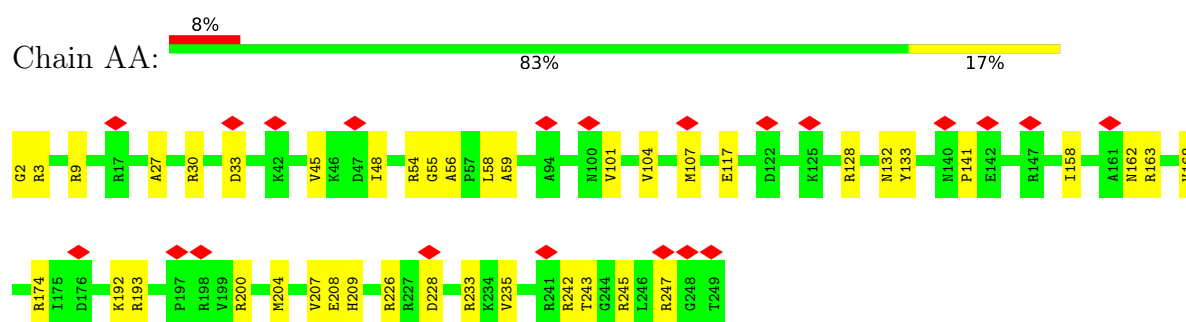


Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
85	A	1	31	22	1	7	1	0

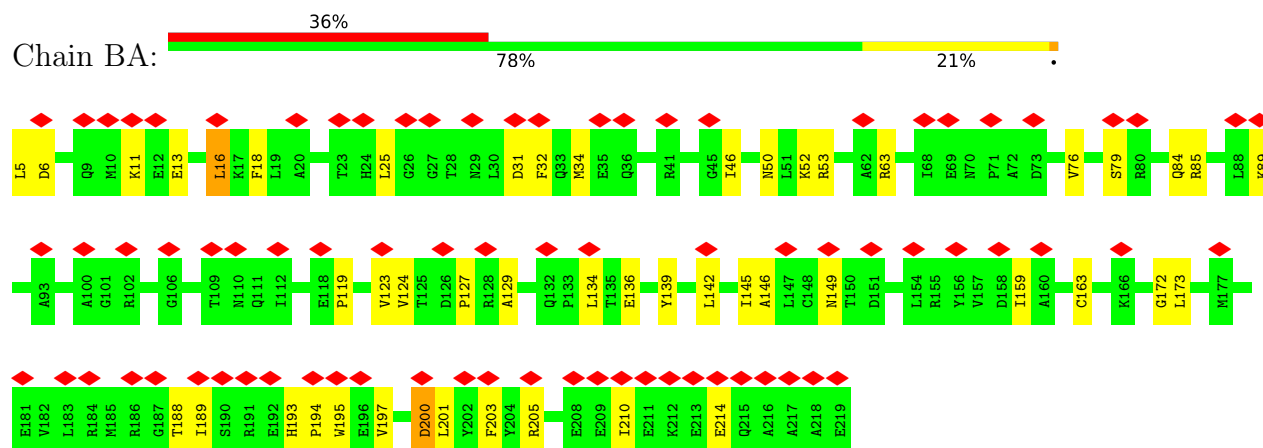
3 Residue-property plots

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

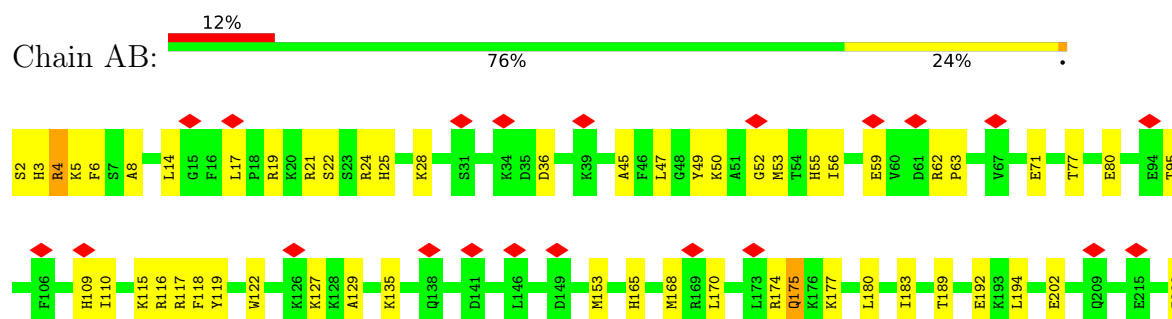
• Molecule 1: 60S ribosomal protein L8

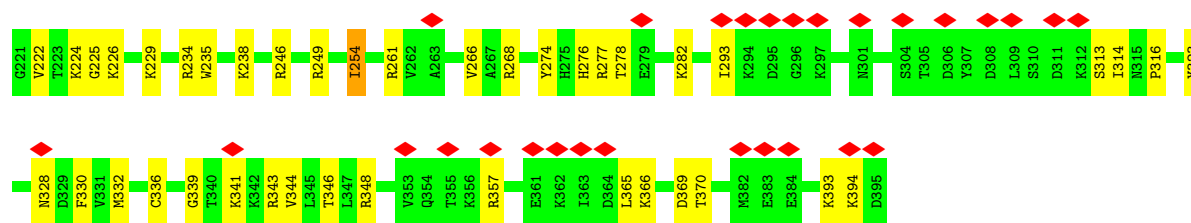


• Molecule 2: 40S ribosomal protein SA

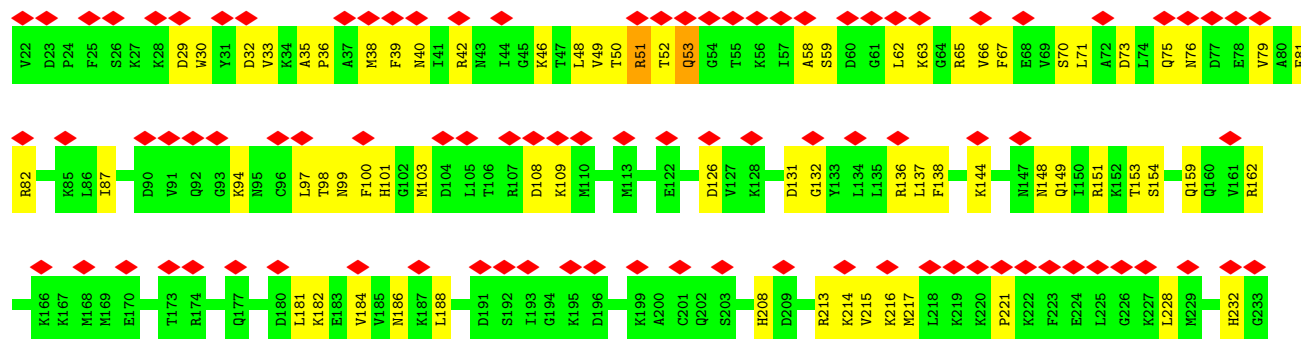
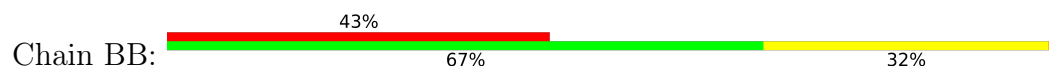


• Molecule 3: 60S ribosomal protein L3

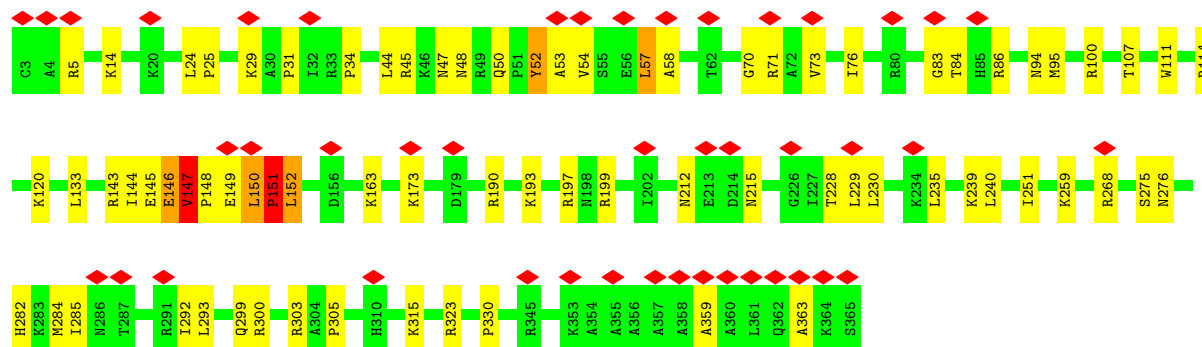
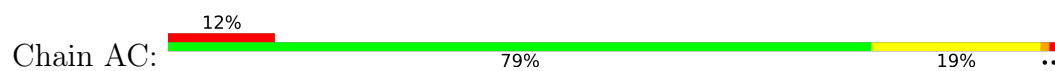




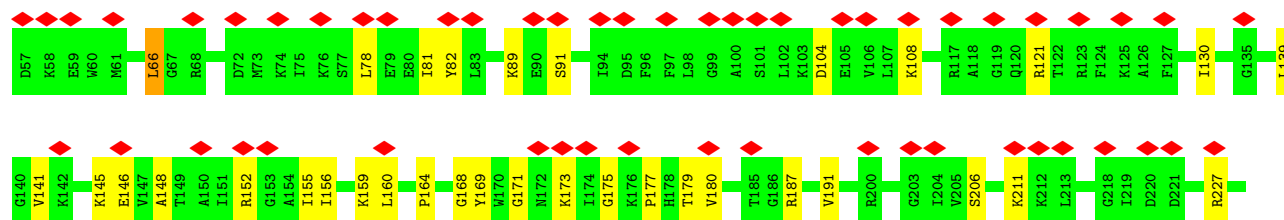
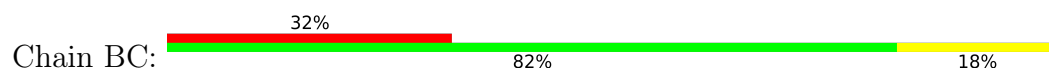
• Molecule 4: 40S ribosomal protein S3a

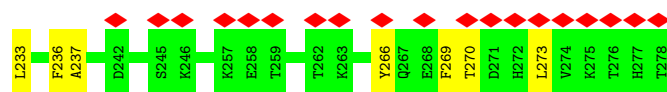


• Molecule 5: 60S ribosomal protein L4

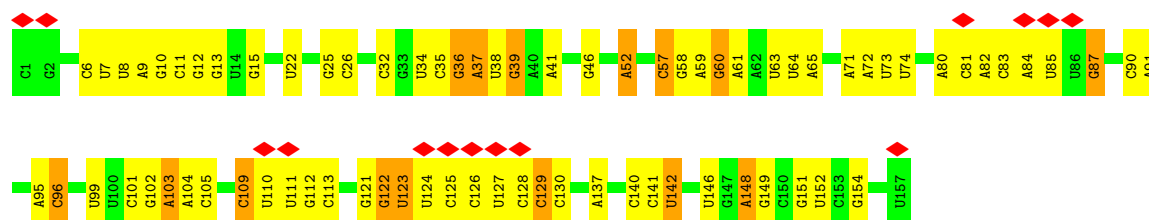


• Molecule 6: 40S ribosomal protein S2

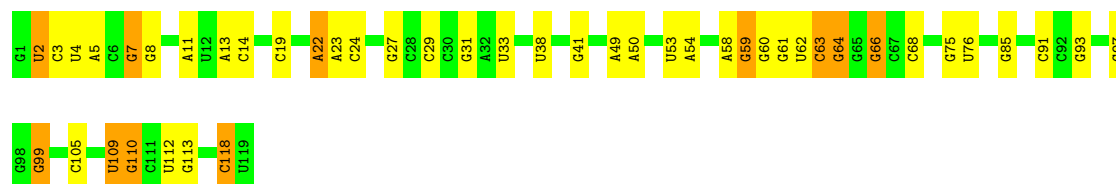




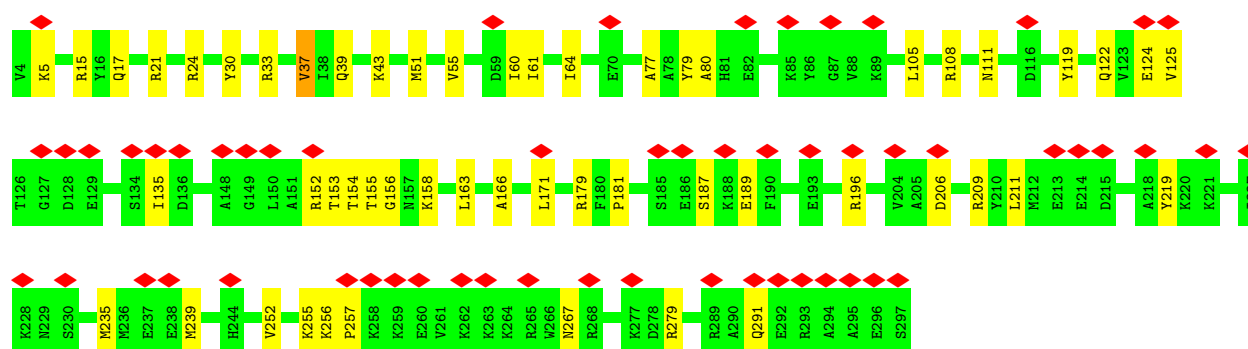
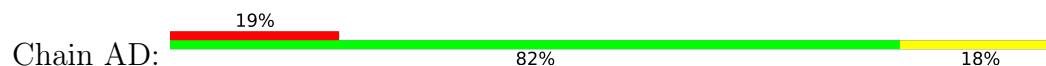
• Molecule 7: 5.8S ribosomal RNA



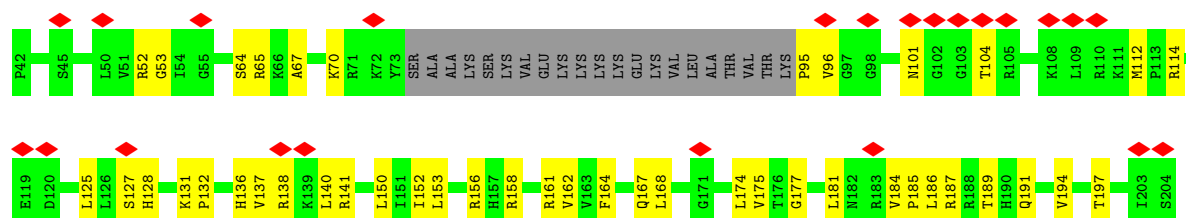
• Molecule 8: 5S ribosomal RNA

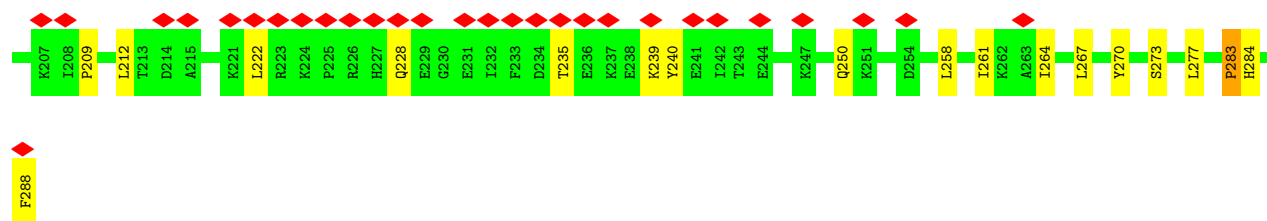


• Molecule 9: 60S ribosomal protein L5

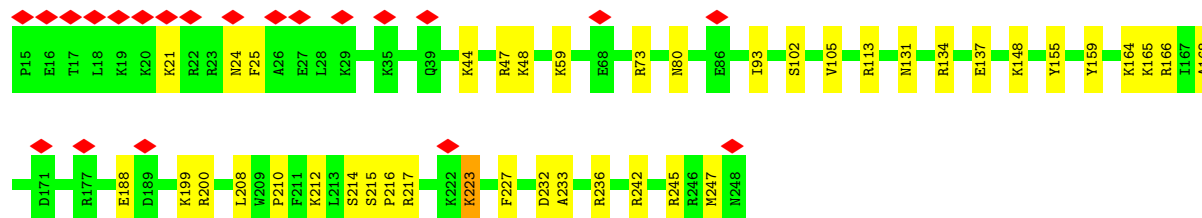
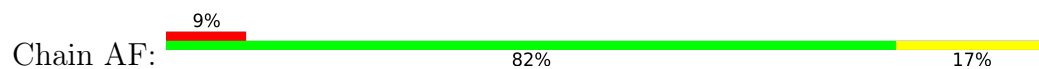


• Molecule 10: 60S ribosomal protein L6

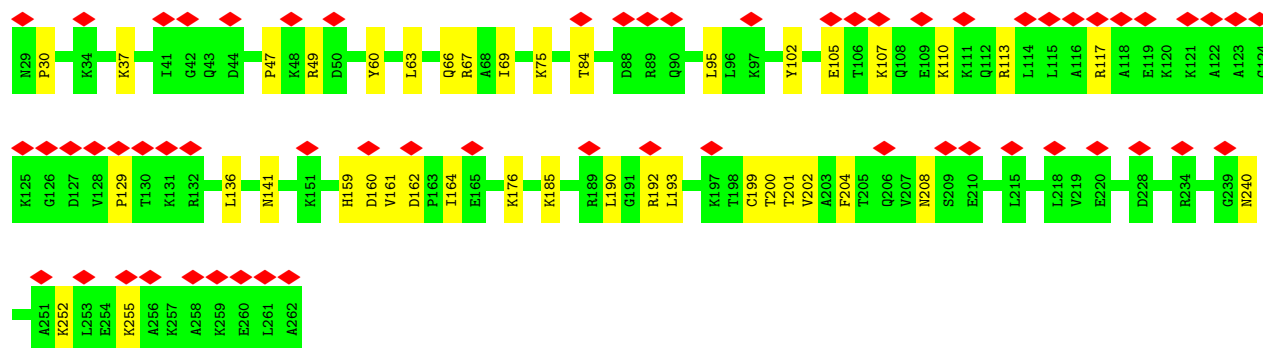
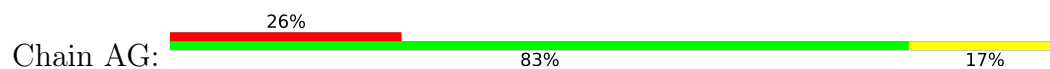




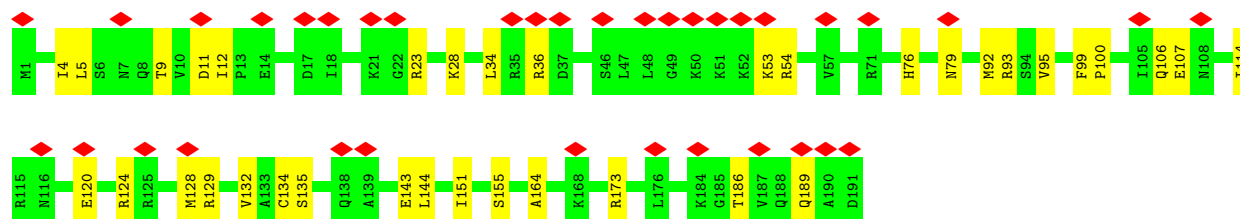
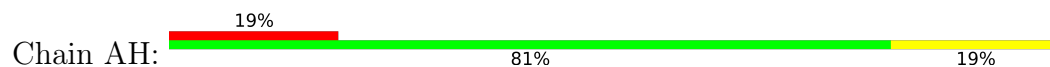
- Molecule 11: 60S ribosomal protein L7



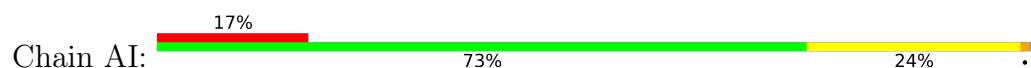
- Molecule 12: 60S ribosomal protein L7a

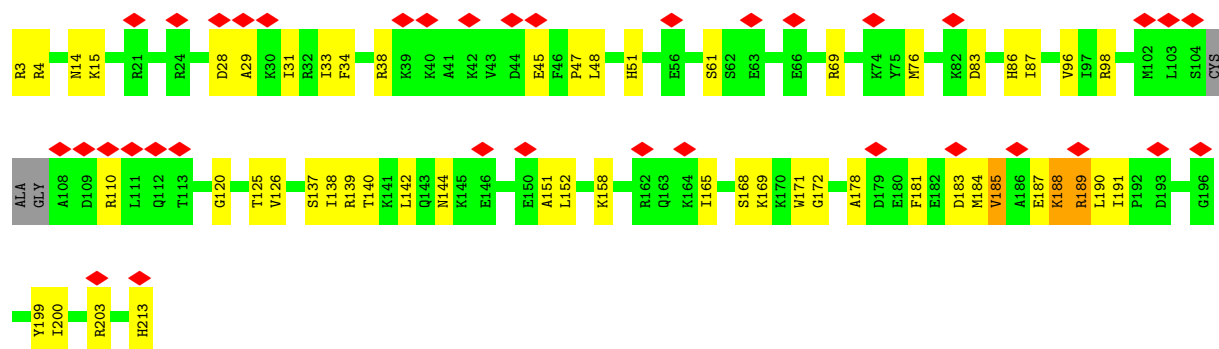


- Molecule 13: 60S ribosomal protein L9



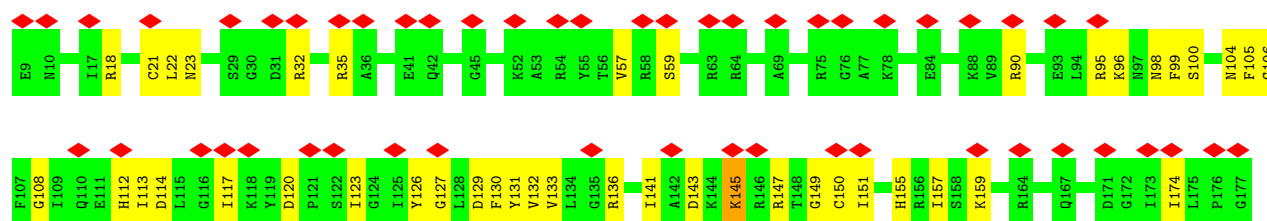
- Molecule 14: 60S ribosomal protein L10





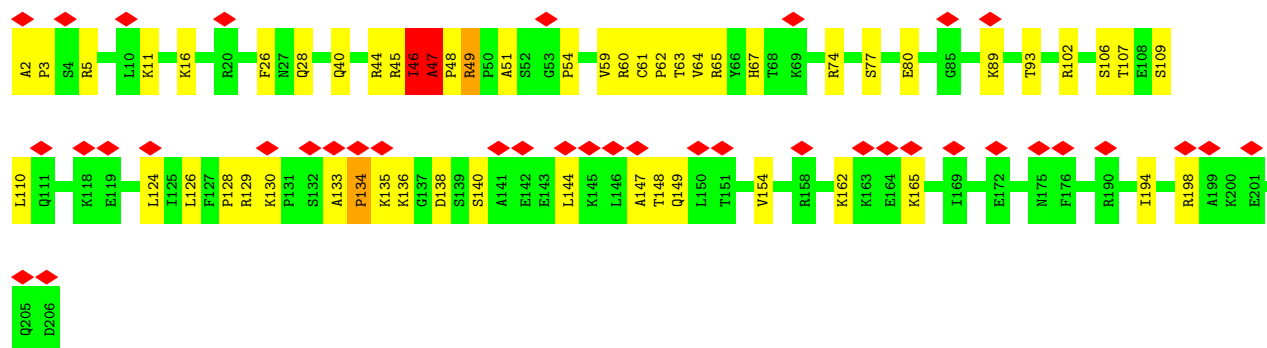
• Molecule 15: 60S ribosomal protein L11

Chain AJ: 30% 75% 25%



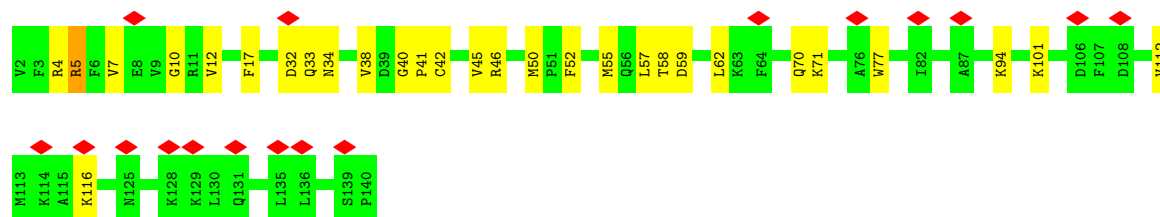
• Molecule 16: 60S ribosomal protein L13

Chain AL: 19% 74% 24%

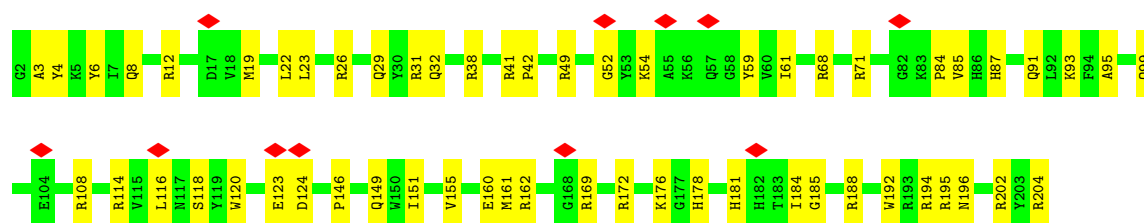
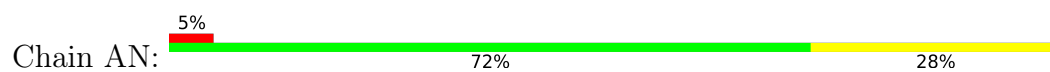


• Molecule 17: 60S ribosomal protein L14

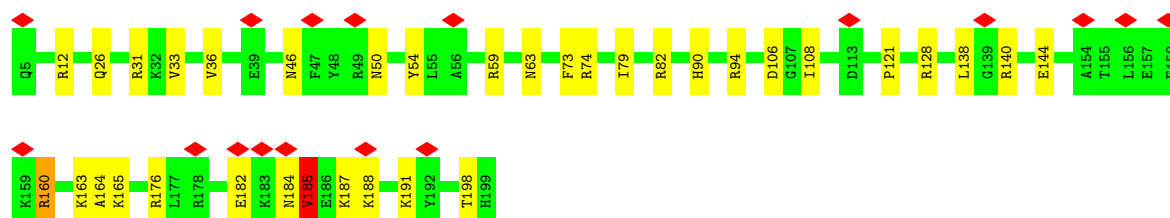
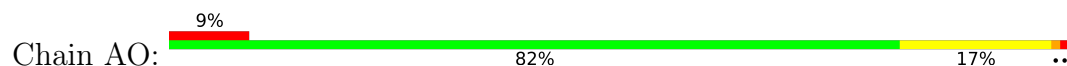
Chain AM: 12% 79% 20%



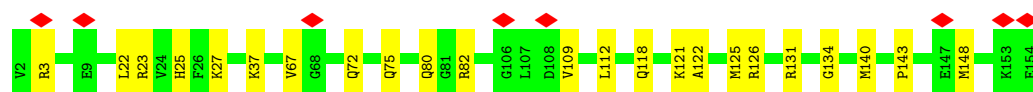
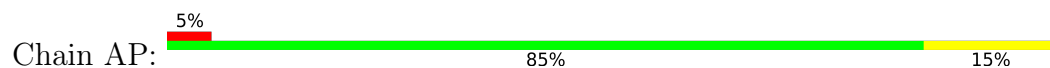
• Molecule 18: 60S ribosomal protein L15



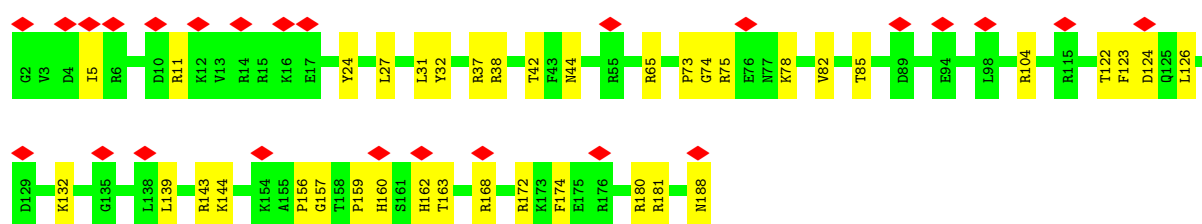
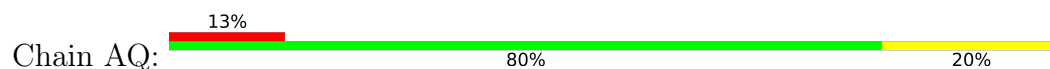
- Molecule 19: 60S ribosomal protein L13a



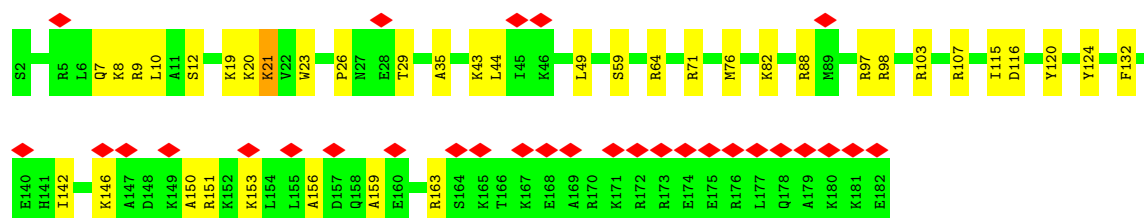
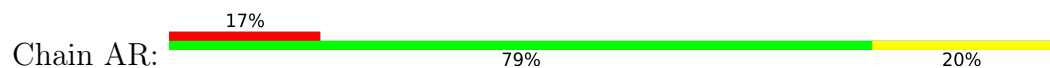
- Molecule 20: 60S ribosomal protein L17



- Molecule 21: 60S ribosomal protein L18

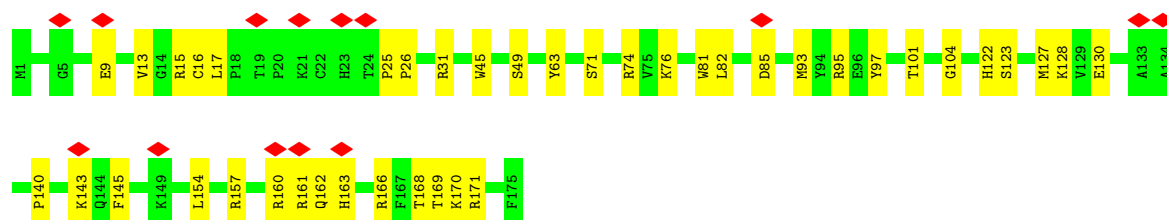


- Molecule 22: 60S ribosomal protein L19



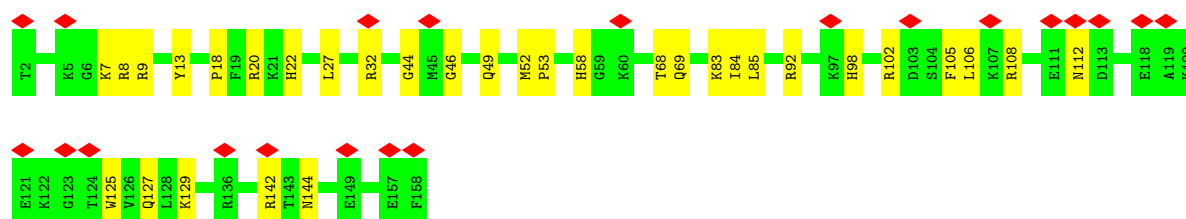
- Molecule 23: 60S ribosomal protein L18a

Chain AS: 



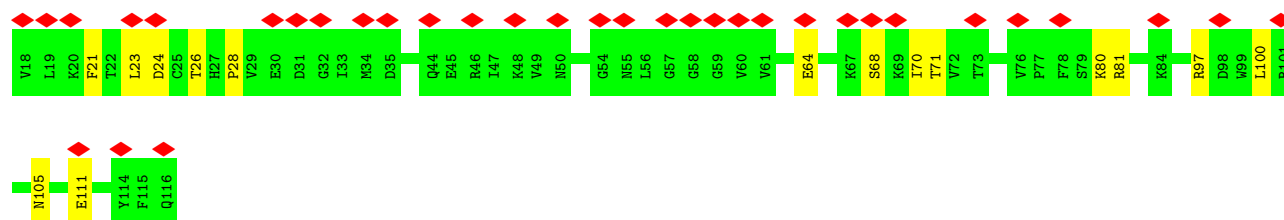
- Molecule 24: 60S ribosomal protein L21

Chain AT: 



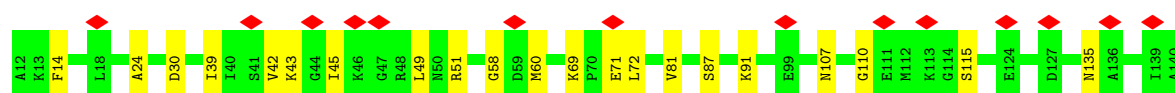
- Molecule 25: 60S ribosomal protein L22

Chain AU: 



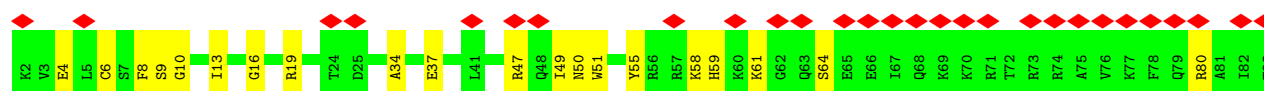
- Molecule 26: 60S ribosomal protein L23

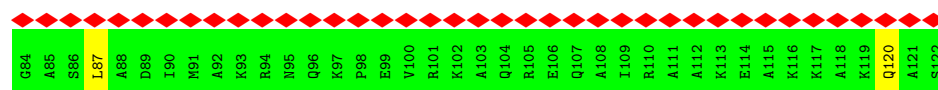
Chain AV: 



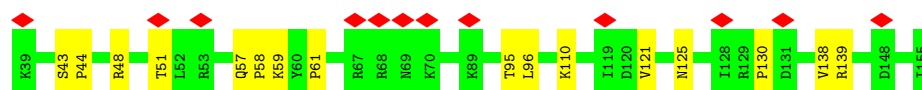
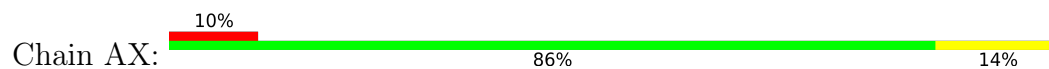
- Molecule 27: 60S ribosomal protein L24

Chain AW: 

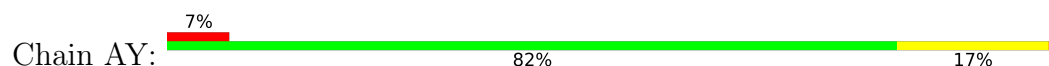




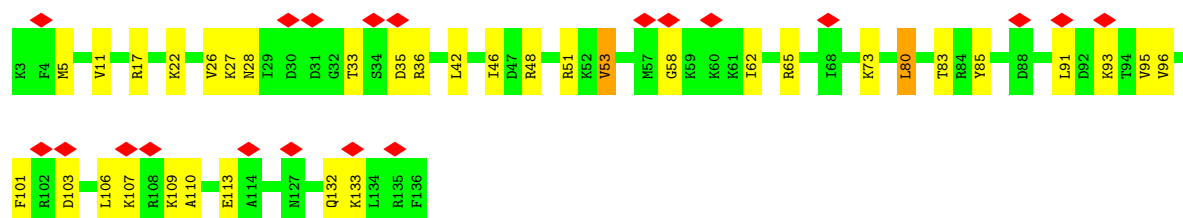
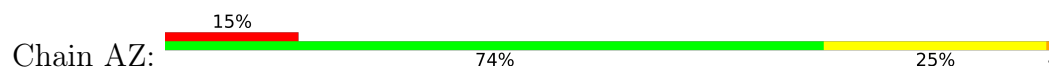
- Molecule 28: 60S ribosomal protein L23a



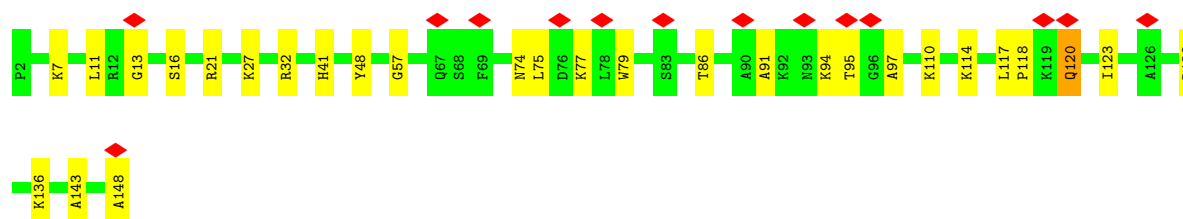
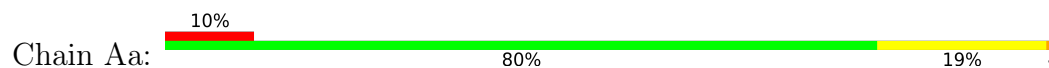
- Molecule 29: 60S ribosomal protein L26



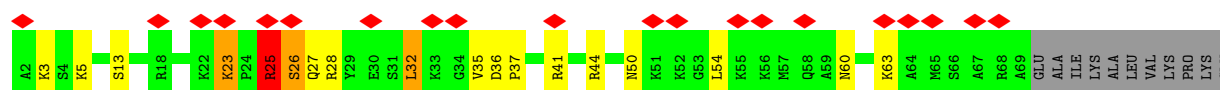
- Molecule 30: 60S ribosomal protein L27

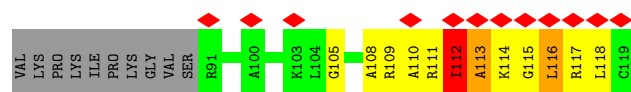


- Molecule 31: 60S ribosomal protein L27a

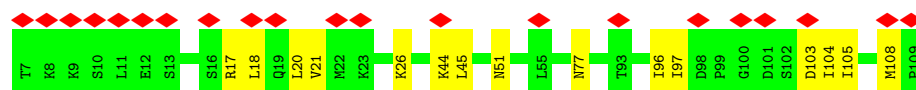
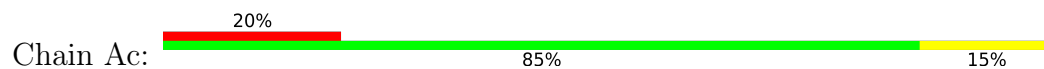


- Molecule 32: 60S ribosomal protein L29

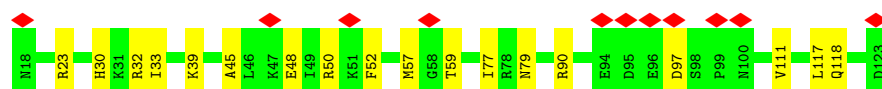
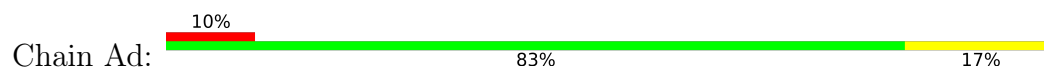




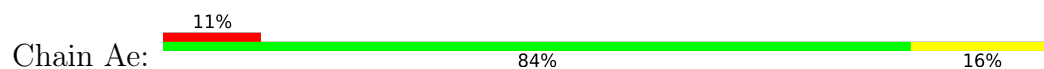
- Molecule 33: 60S ribosomal protein L30



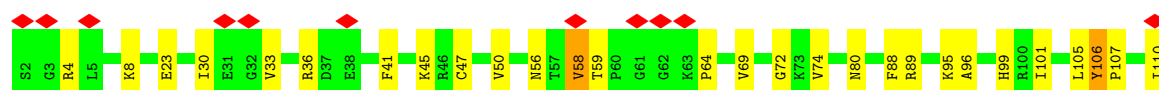
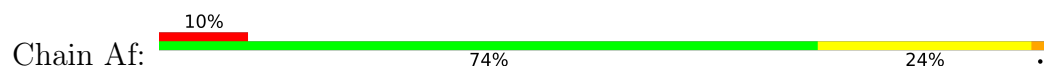
- Molecule 34: 60S ribosomal protein L31



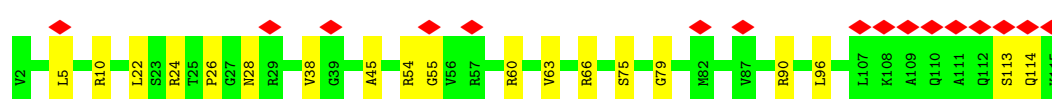
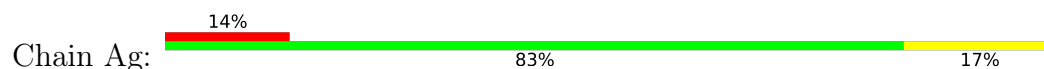
- Molecule 35: 60S ribosomal protein L32



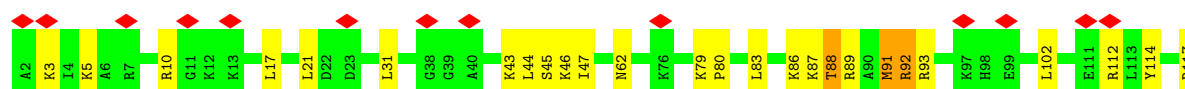
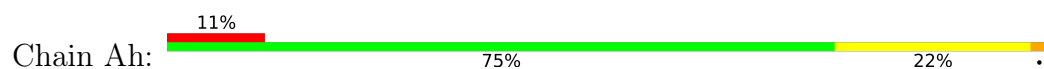
- Molecule 36: 60S ribosomal protein L35a

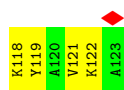


- Molecule 37: 60S ribosomal protein L34

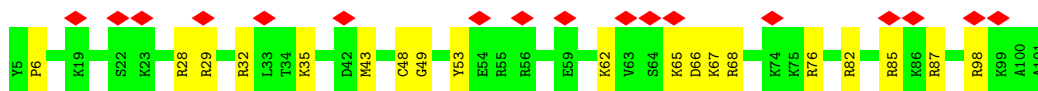
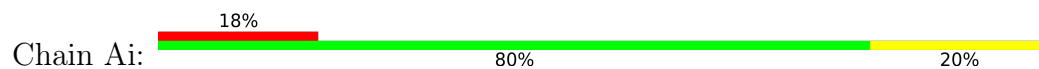


- Molecule 38: 60S ribosomal protein L35

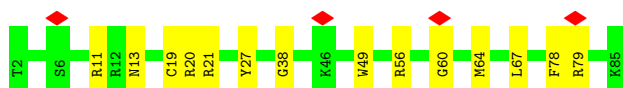
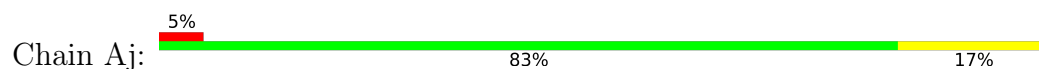




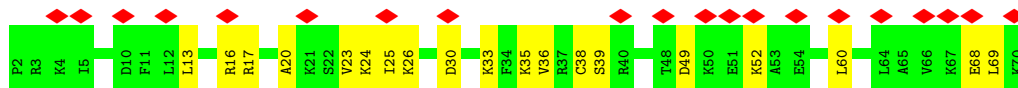
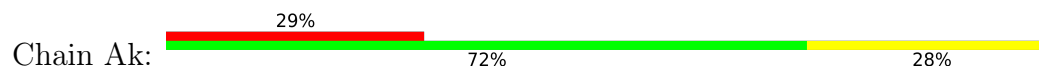
- Molecule 39: 60S ribosomal protein L36



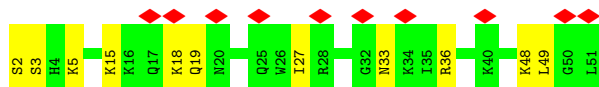
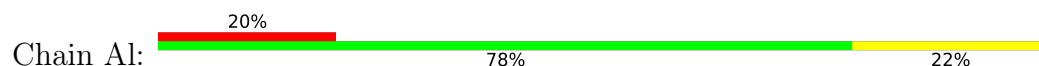
- Molecule 40: 60S ribosomal protein L37



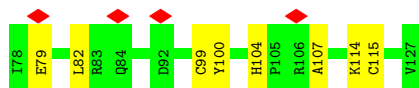
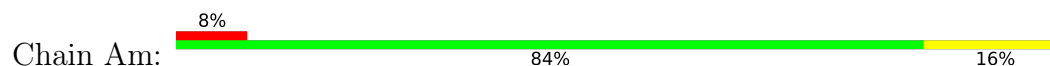
- Molecule 41: 60S ribosomal protein L38



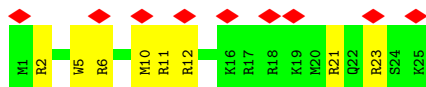
- Molecule 42: 60S ribosomal protein L39



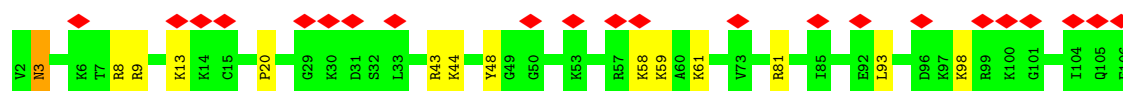
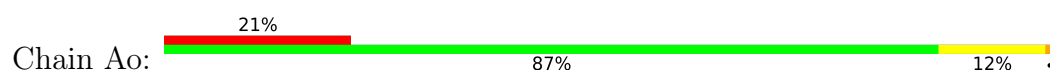
- Molecule 43: 60S ribosomal protein L40



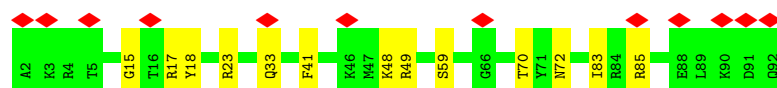
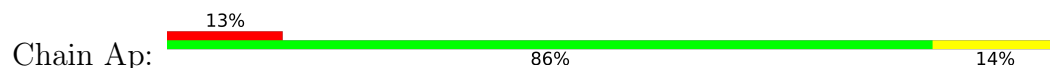
- Molecule 44: 60S ribosomal protein L41



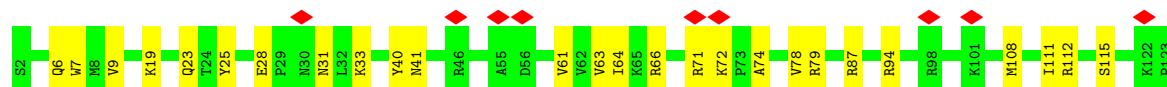
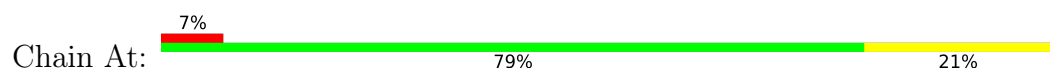
- Molecule 45: 60S ribosomal protein L36a



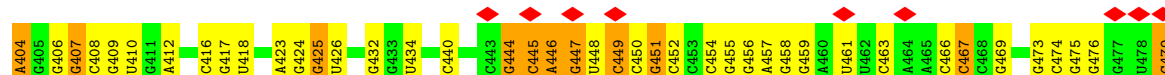
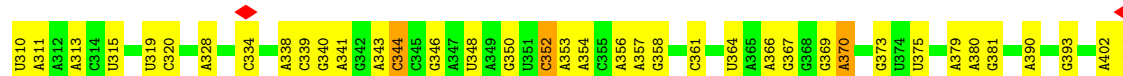
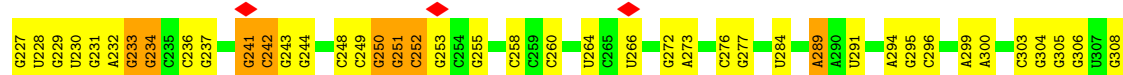
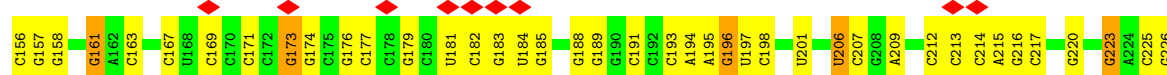
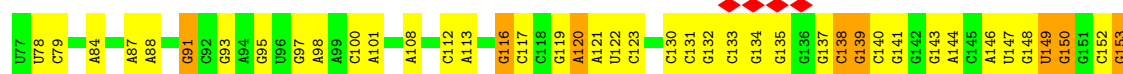
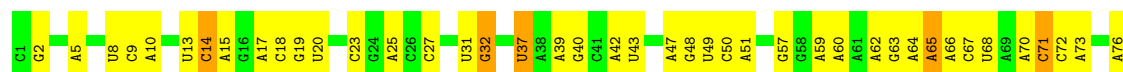
- Molecule 46: 60S ribosomal protein L37a

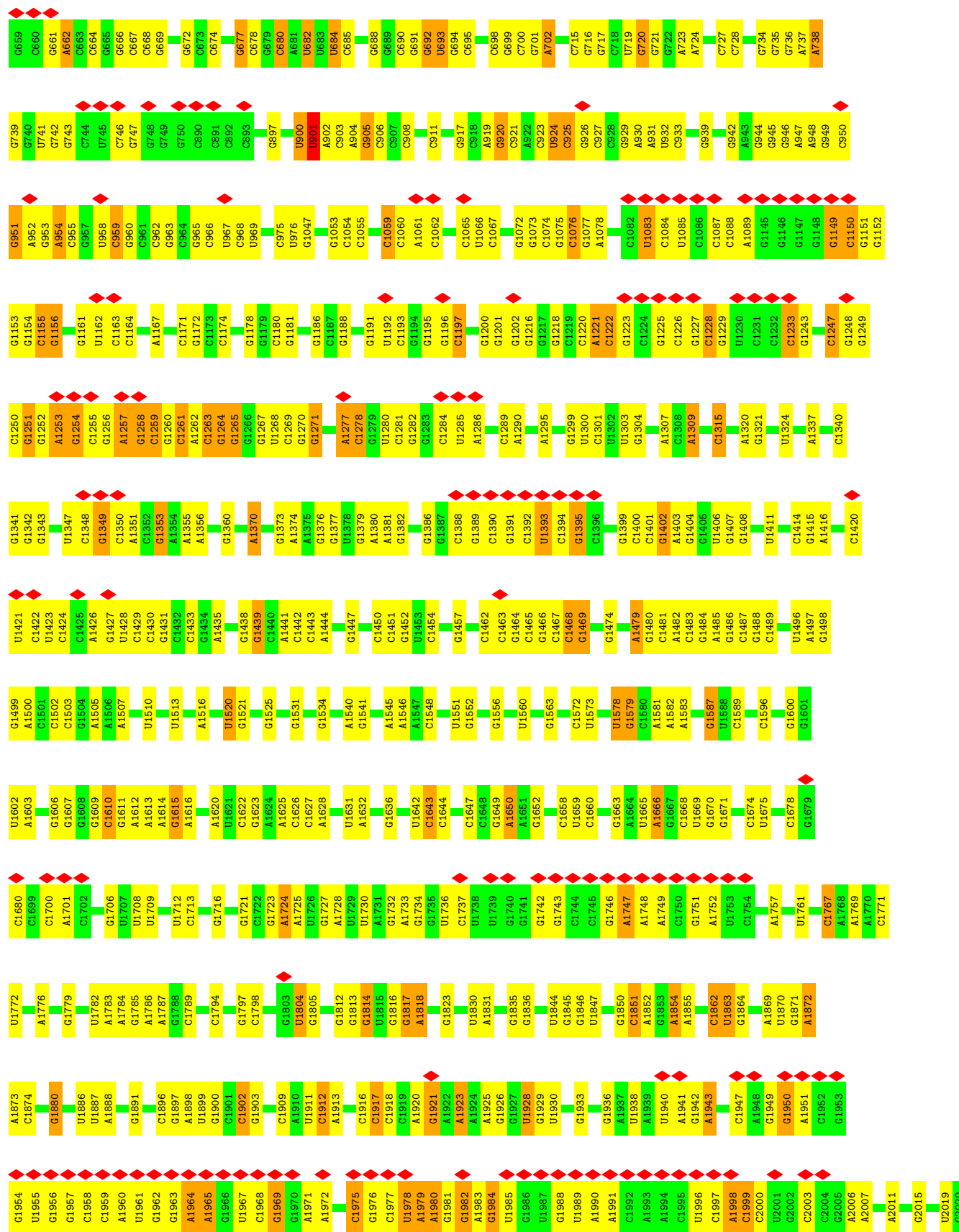


- Molecule 47: 60S ribosomal protein L28

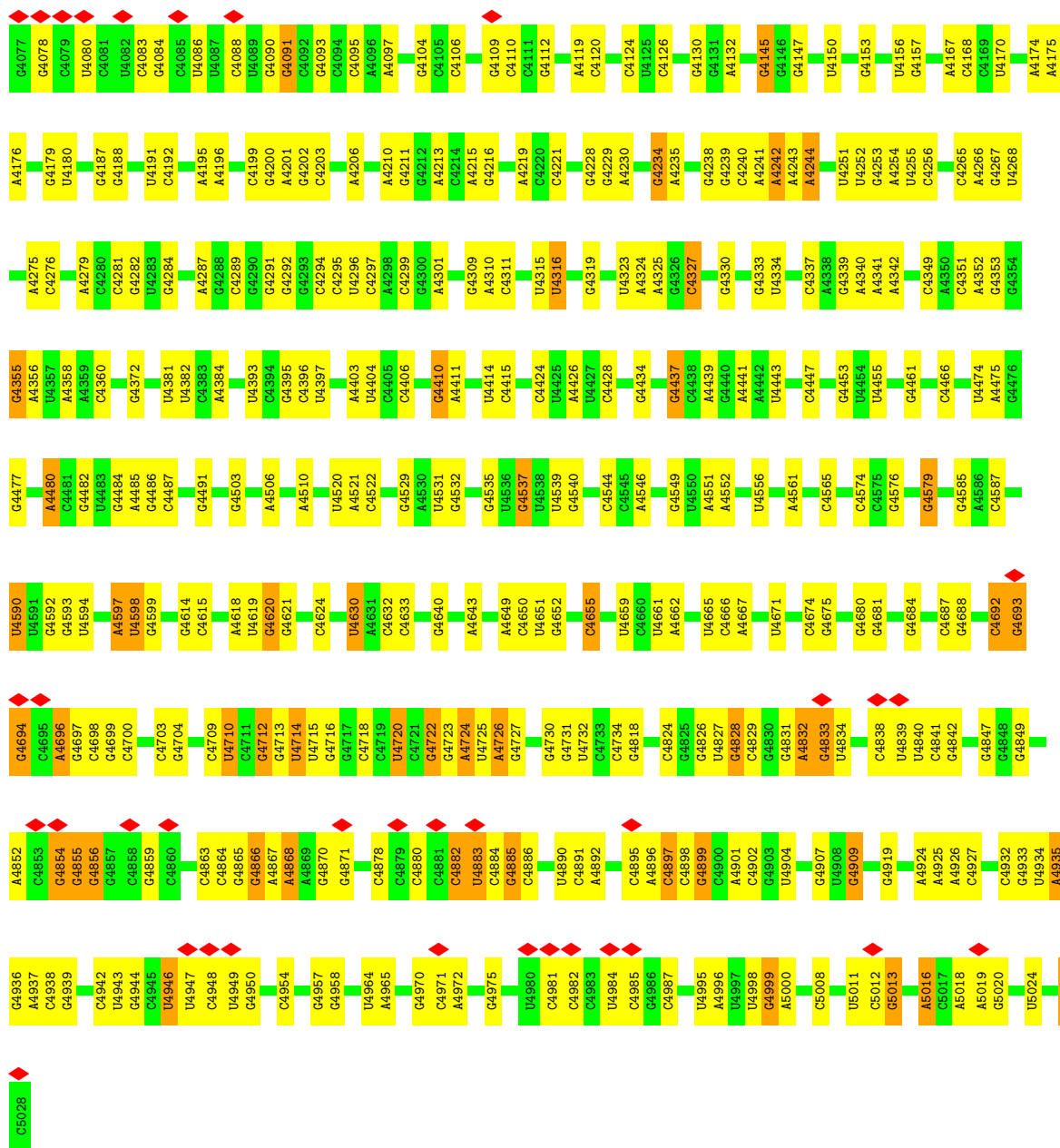


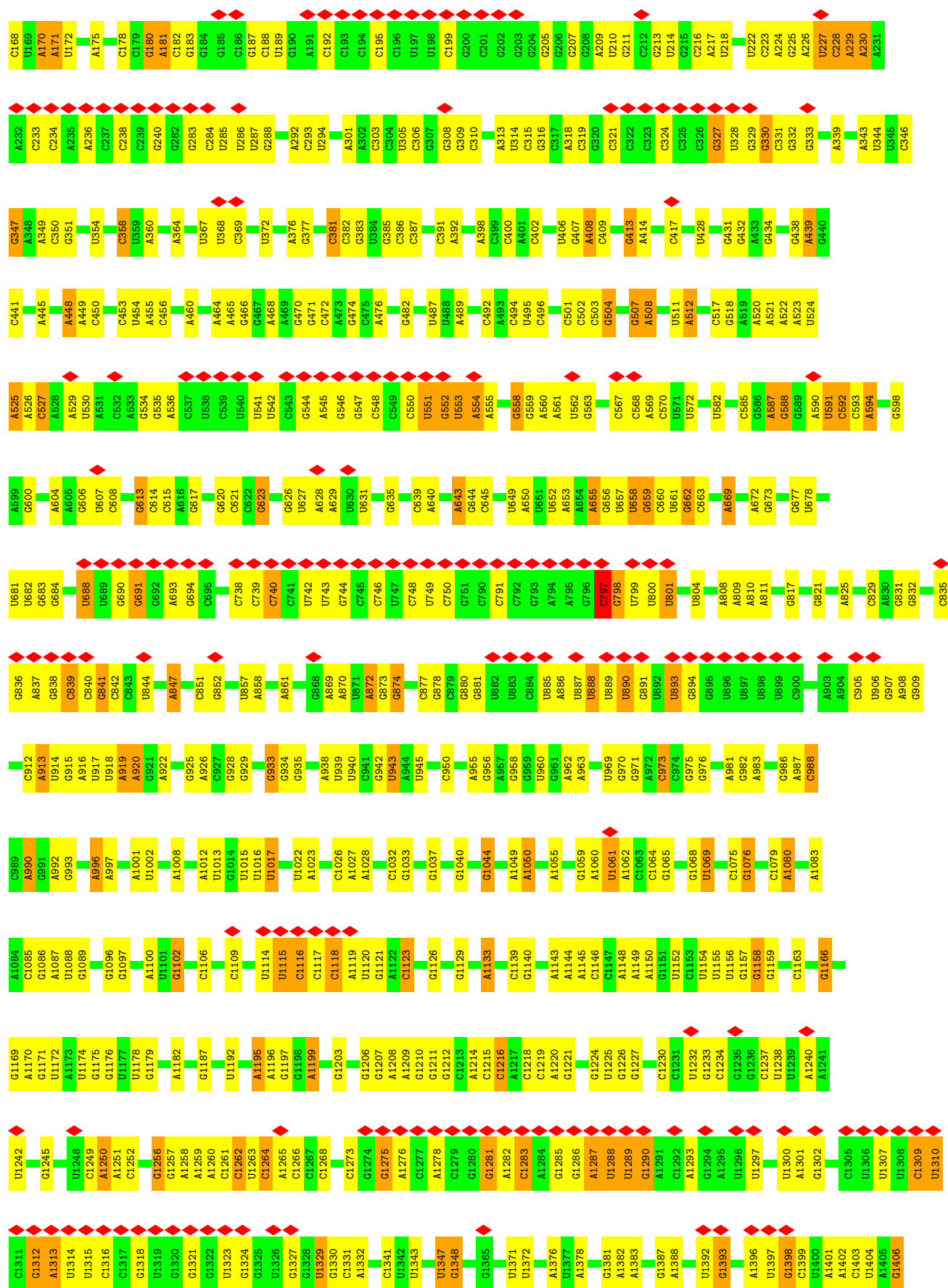
- Molecule 48: 28S ribosomal RNA

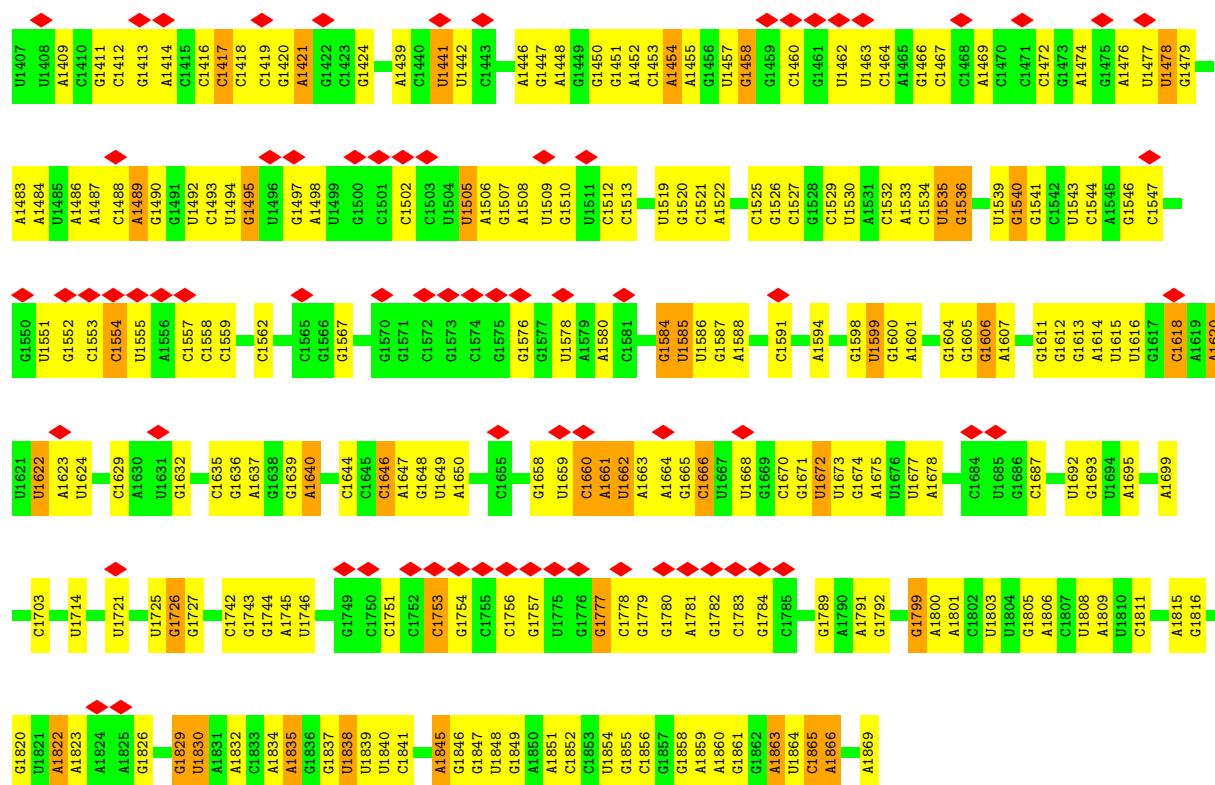




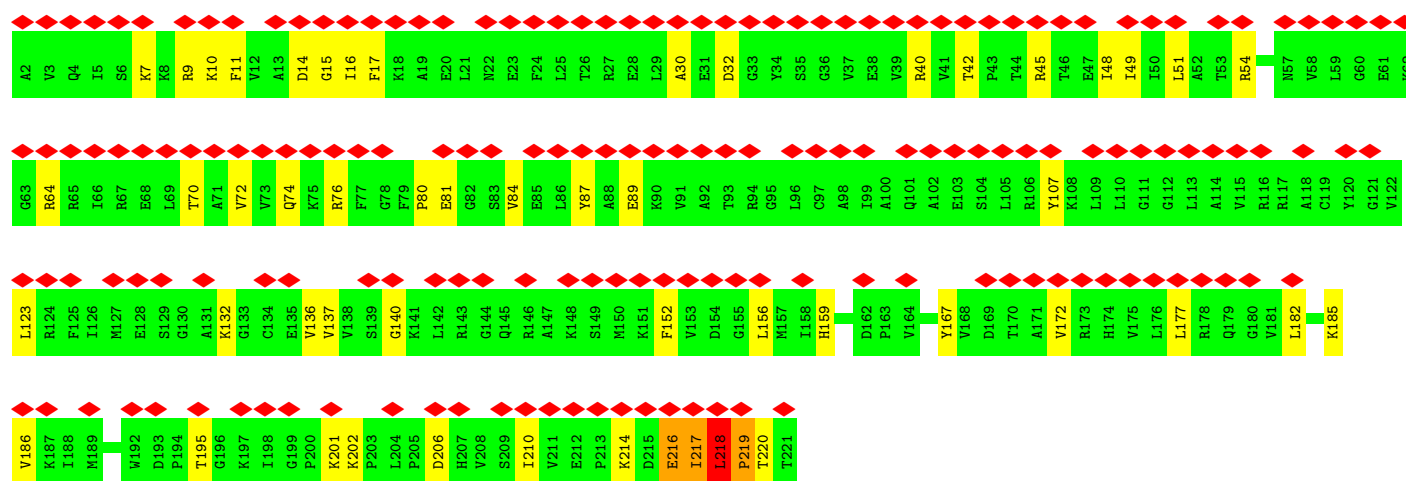
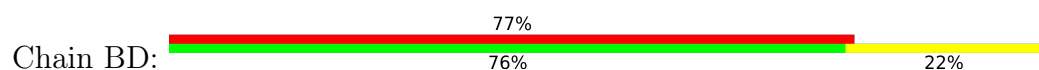




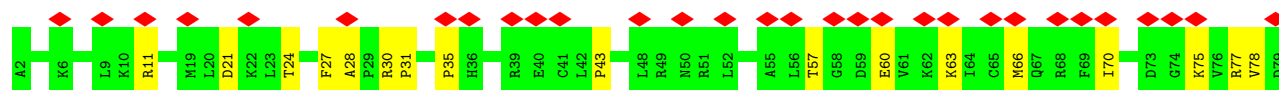
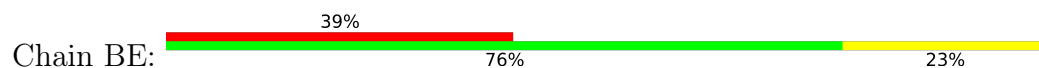




• Molecule 50: 40S ribosomal protein S3

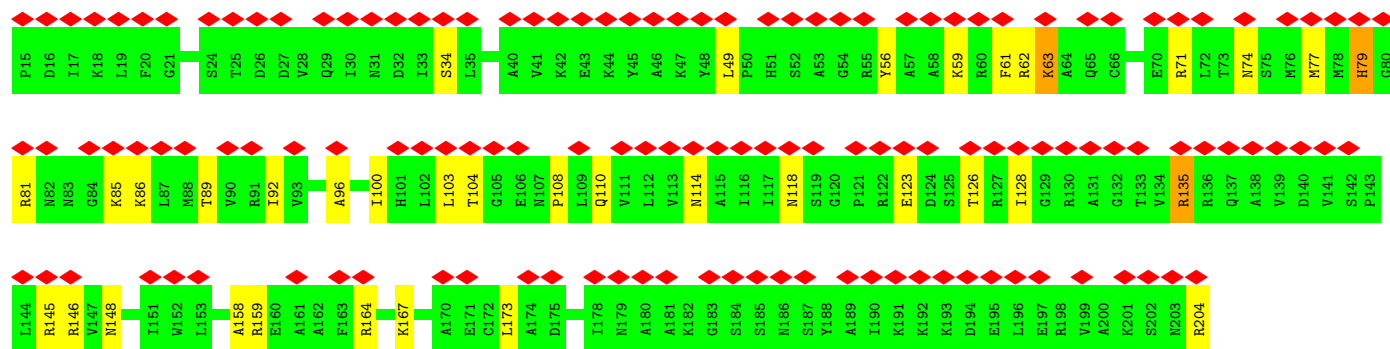
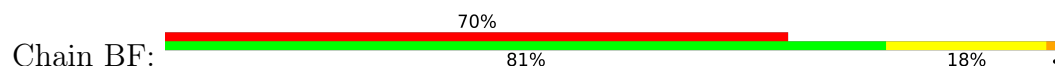


• Molecule 51: 40S ribosomal protein S4, Y isoform 1

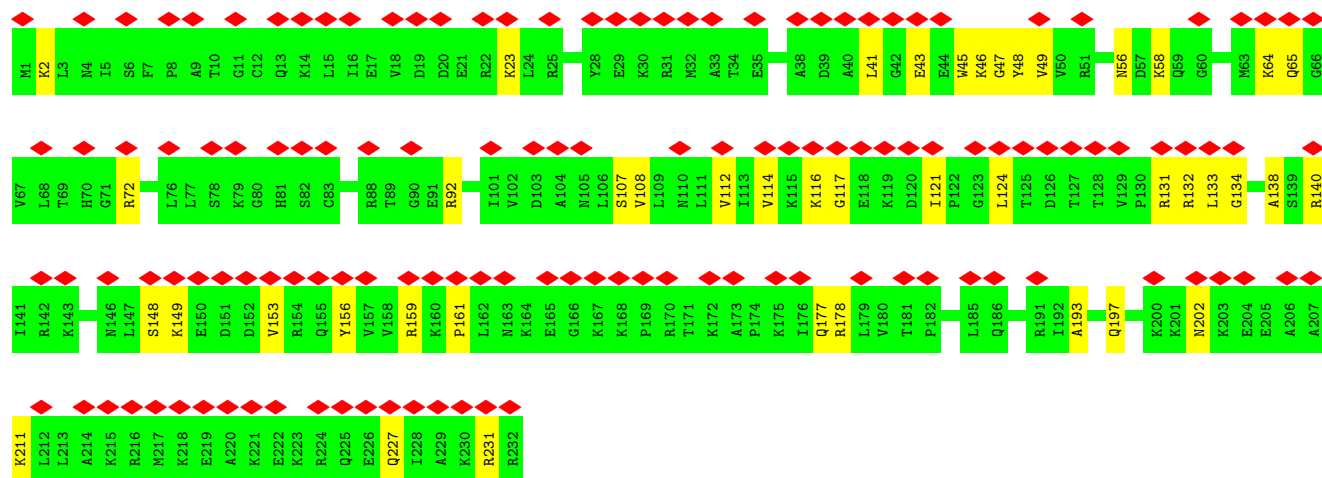
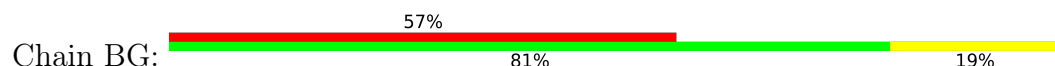




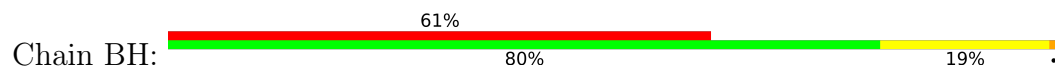
• Molecule 52: 40S ribosomal protein S5

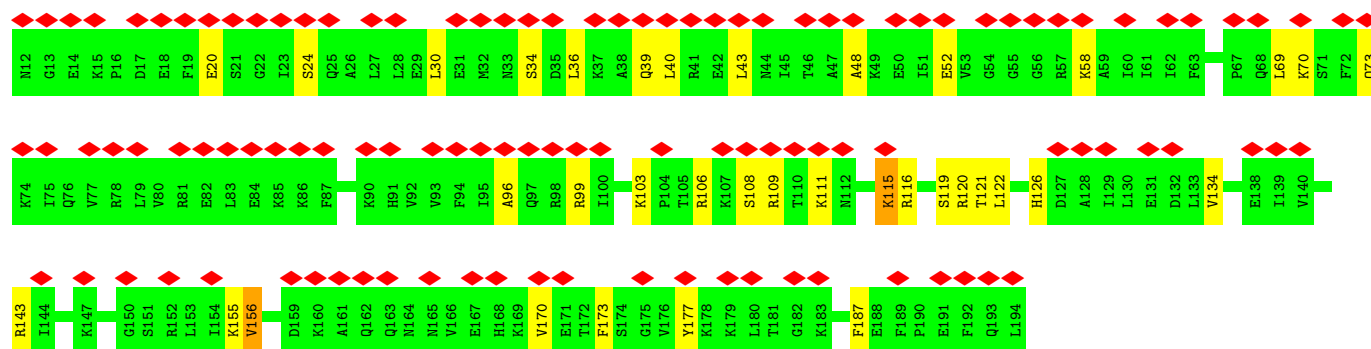


• Molecule 53: 40S ribosomal protein S6

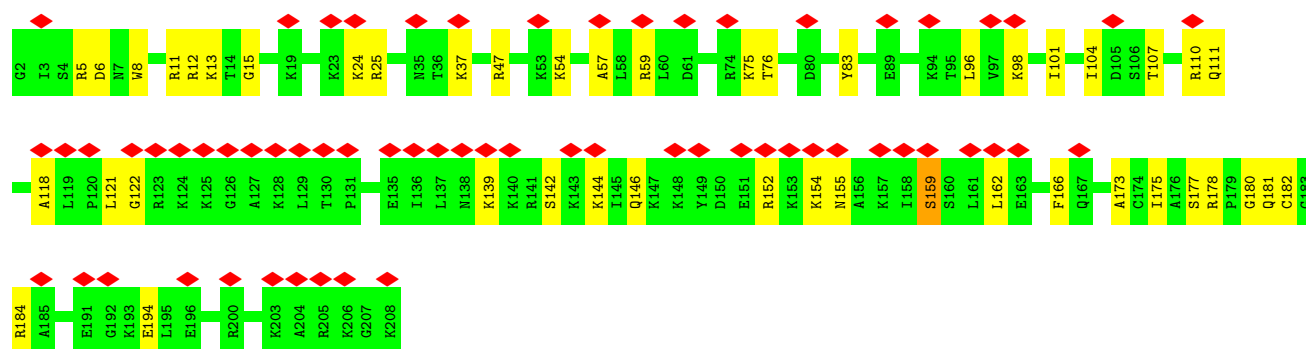
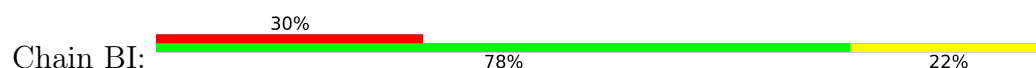


• Molecule 54: 40S ribosomal protein S7

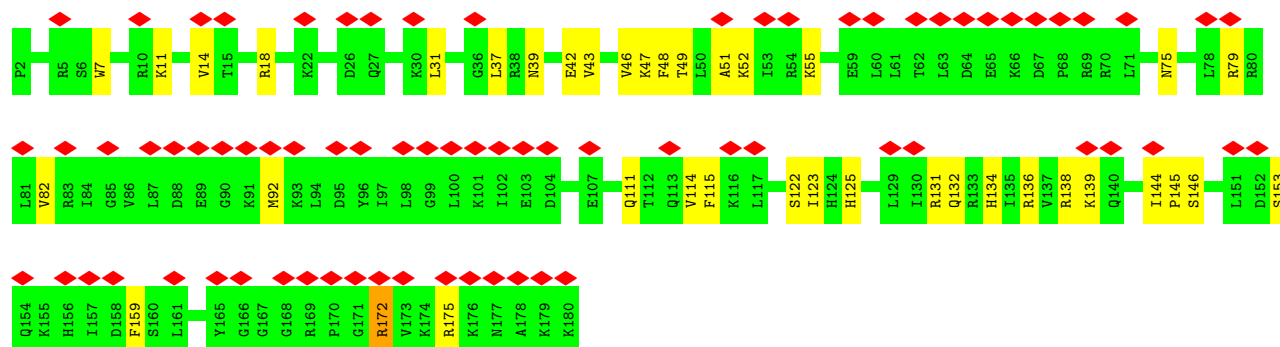
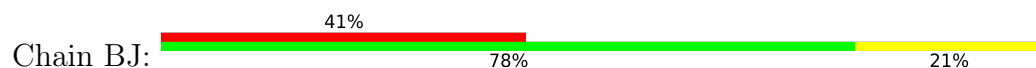




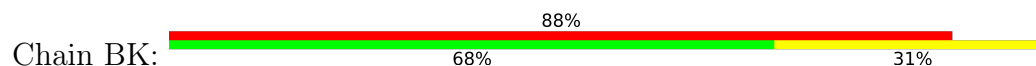
• Molecule 55: 40S ribosomal protein S8



• Molecule 56: 40S ribosomal protein S9

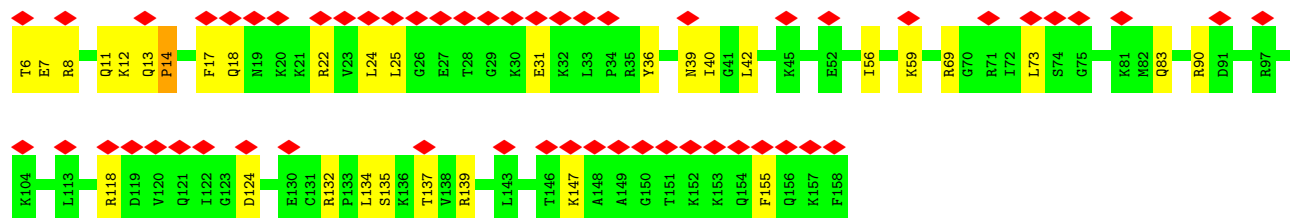
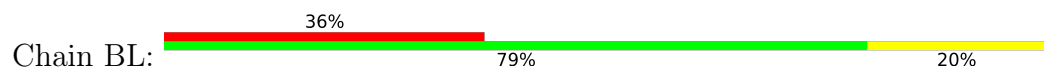


• Molecule 57: 40S ribosomal protein S10

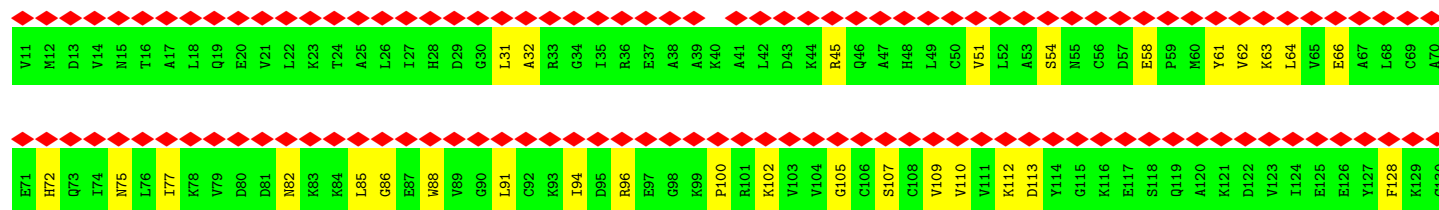




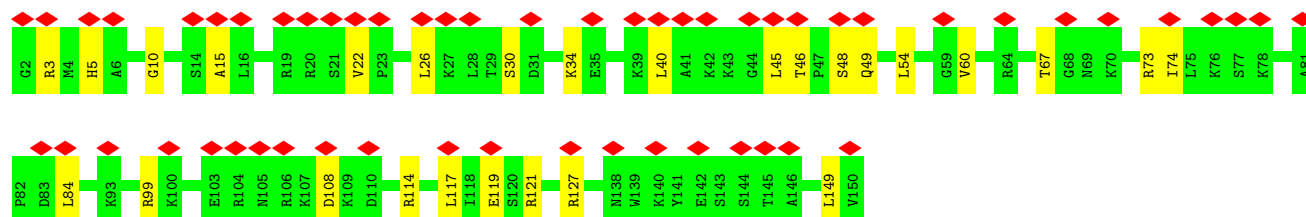
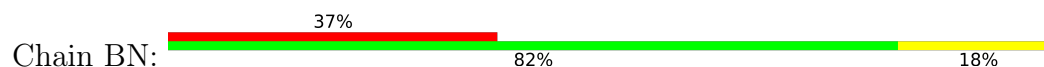
• Molecule 58: 40S ribosomal protein S11



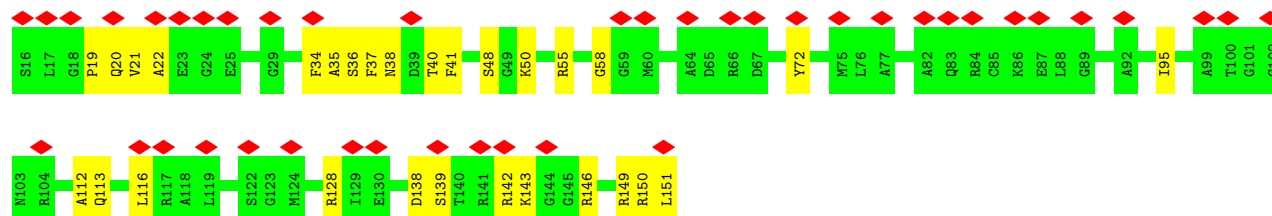
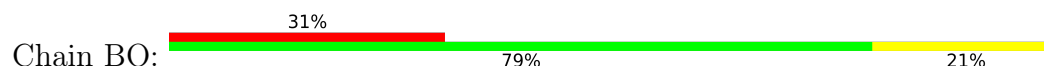
• Molecule 59: 40S ribosomal protein S12



• Molecule 60: 40S ribosomal protein S13



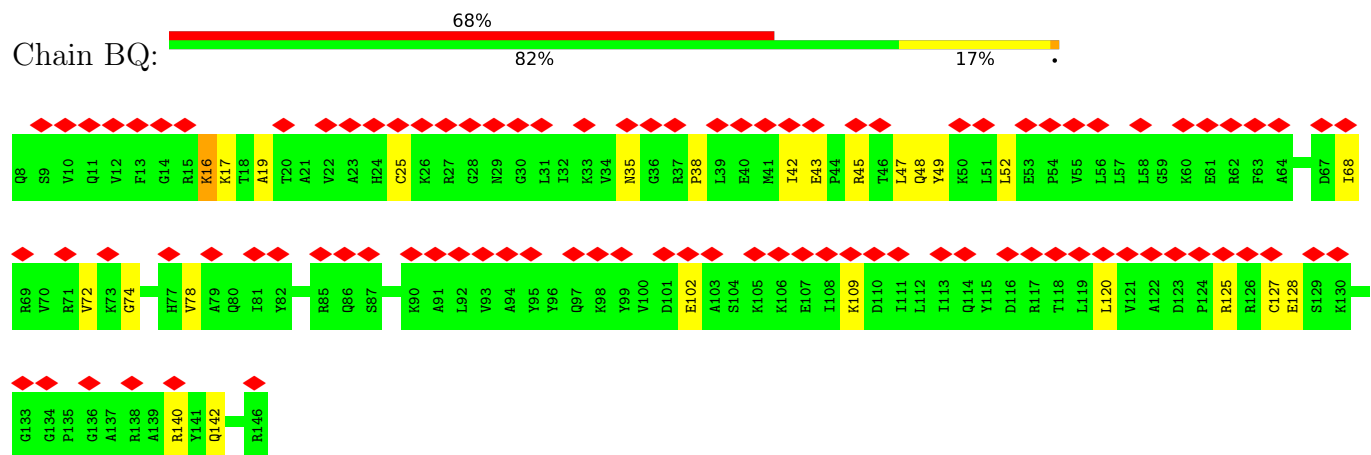
• Molecule 61: 40S ribosomal protein S14



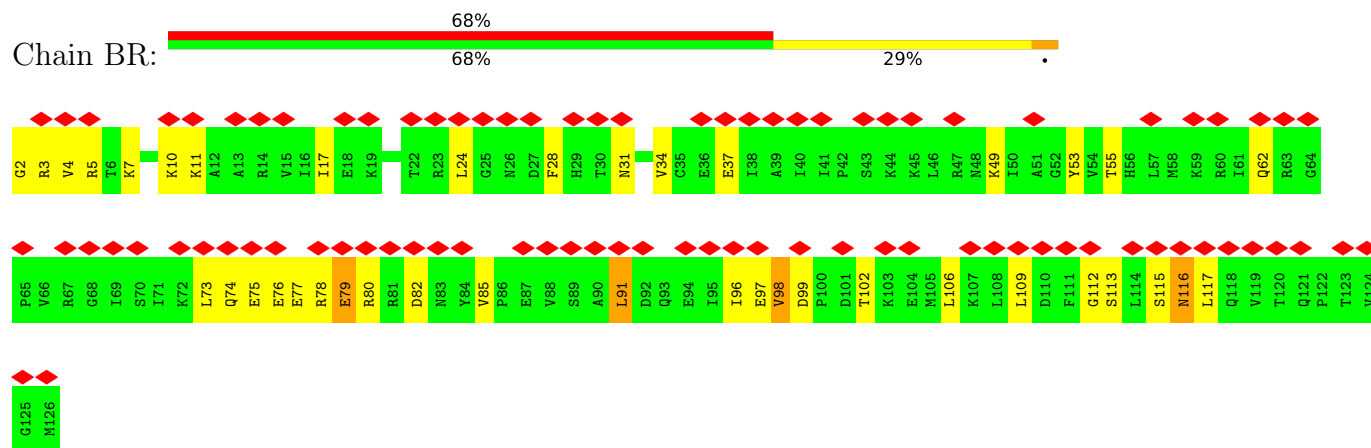
• Molecule 62: 40S ribosomal protein S15



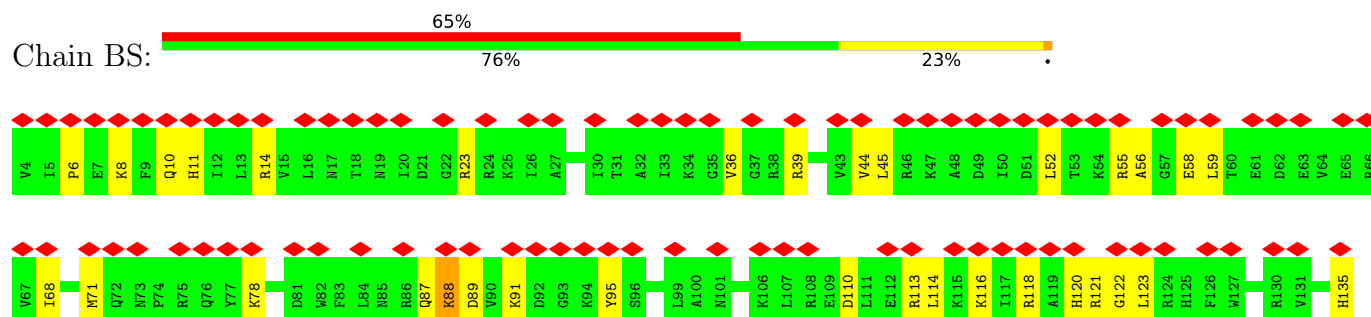
• Molecule 63: 40S ribosomal protein S16



• Molecule 64: 40S ribosomal protein S17

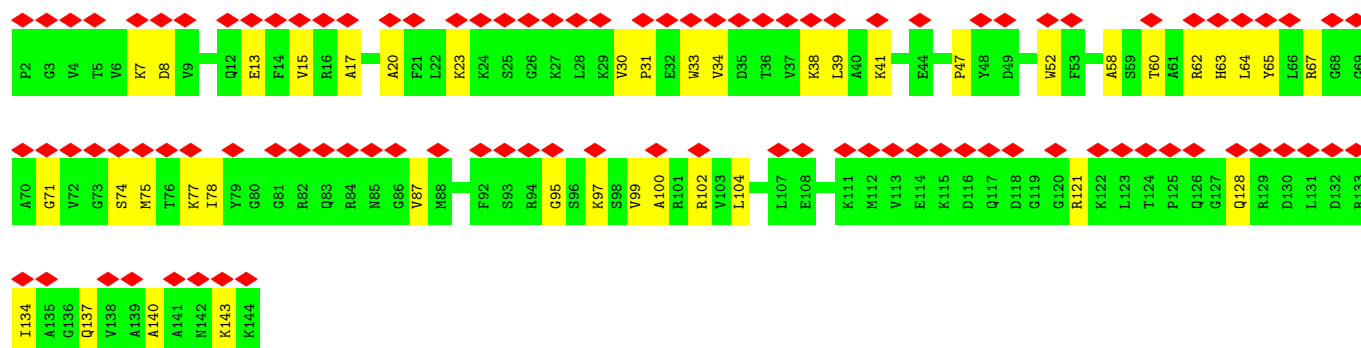
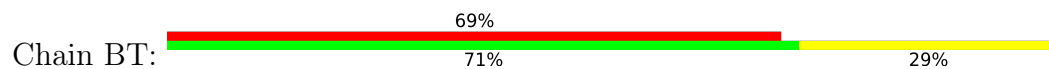


• Molecule 65: 40S ribosomal protein S18

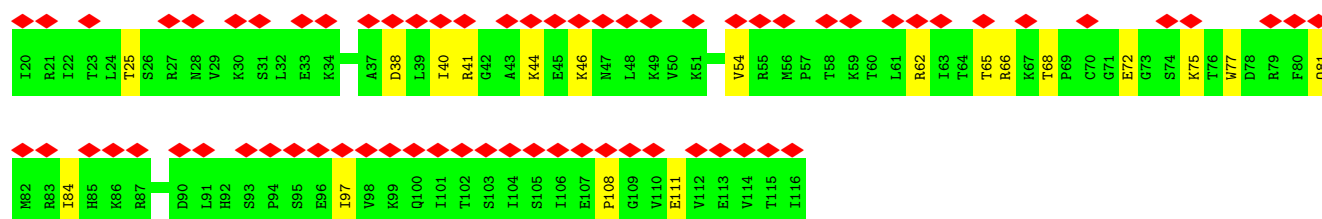
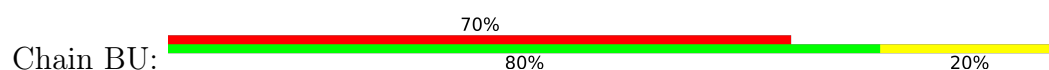




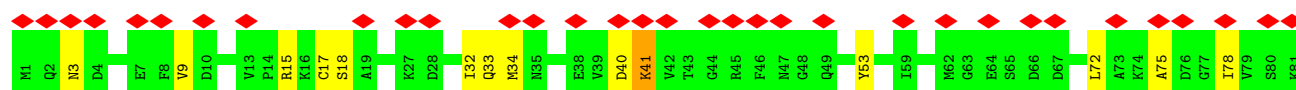
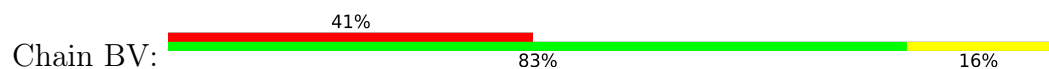
- Molecule 66: 40S ribosomal protein S19



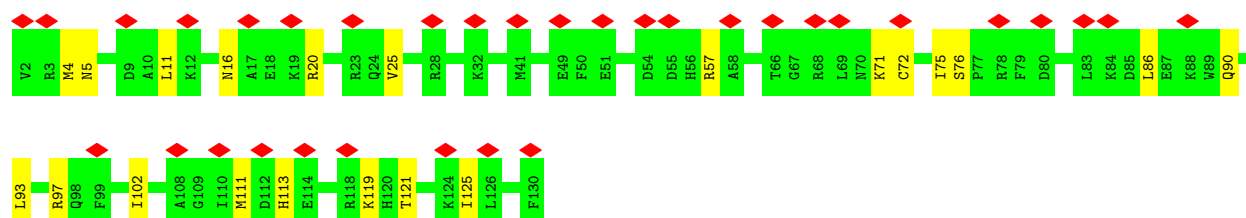
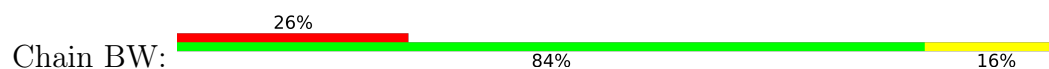
- Molecule 67: 40S ribosomal protein S20



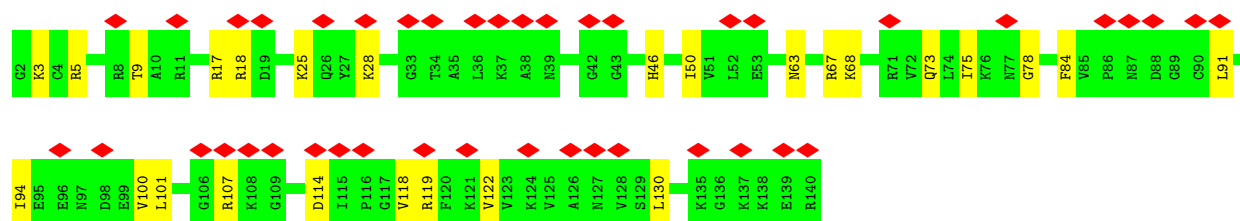
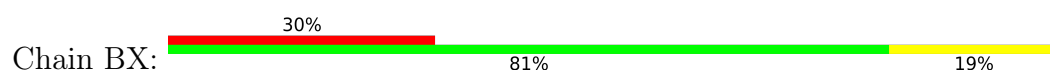
- Molecule 68: 40S ribosomal protein S21



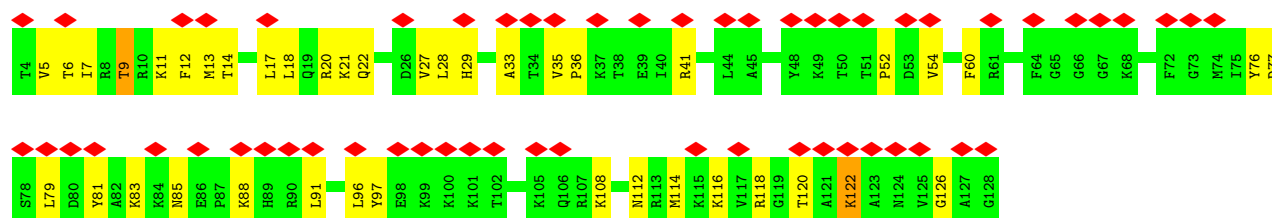
- Molecule 69: 40S ribosomal protein S15a



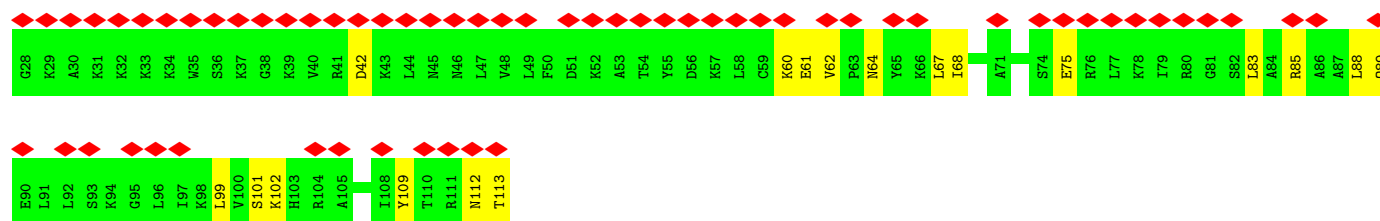
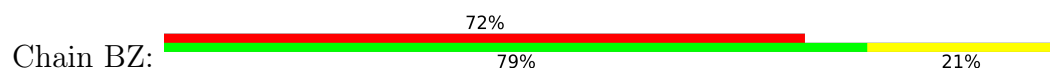
- Molecule 70: 40S ribosomal protein S23



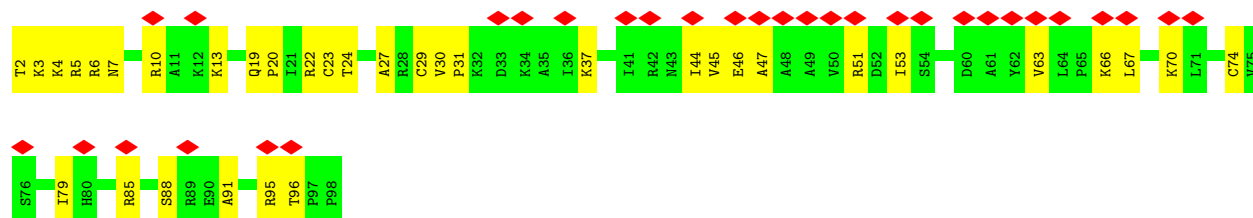
- Molecule 71: 40S ribosomal protein S24



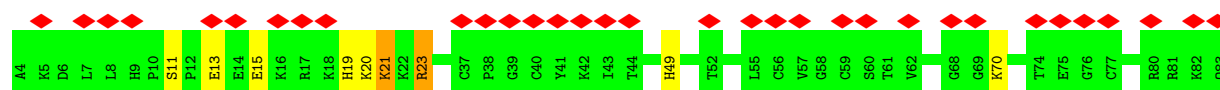
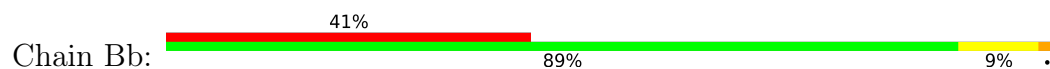
- Molecule 72: 40S ribosomal protein S25



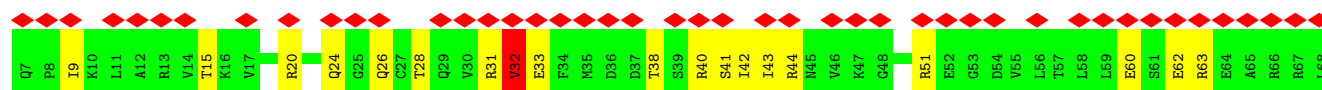
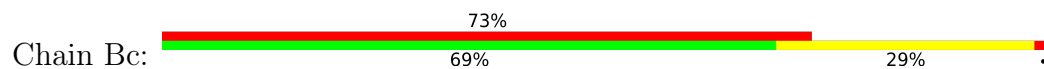
- Molecule 73: 40S ribosomal protein S26



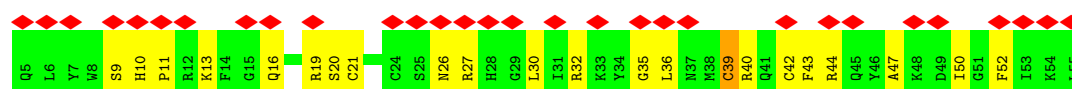
- Molecule 74: 40S ribosomal protein S27



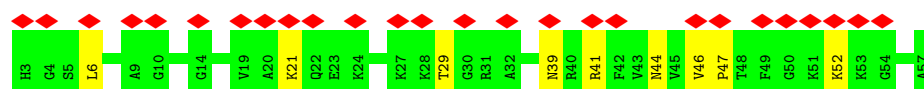
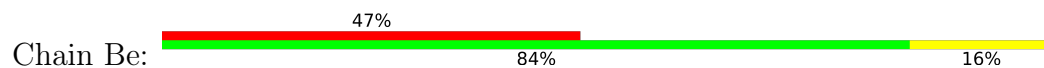
- Molecule 75: 40S ribosomal protein S28



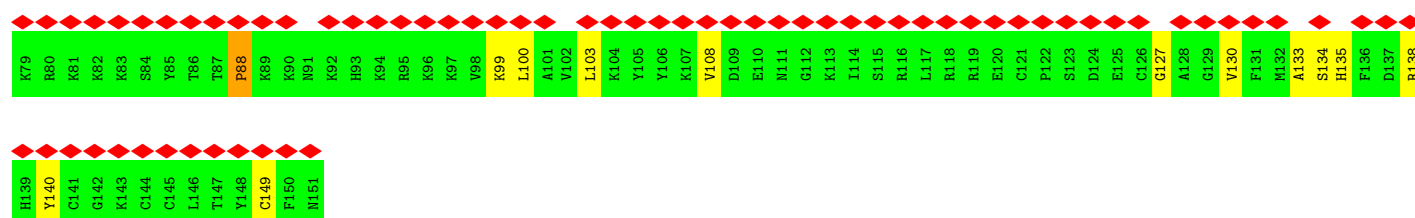
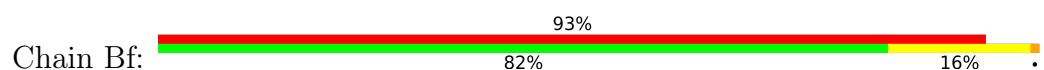
- Molecule 76: 40S ribosomal protein S29



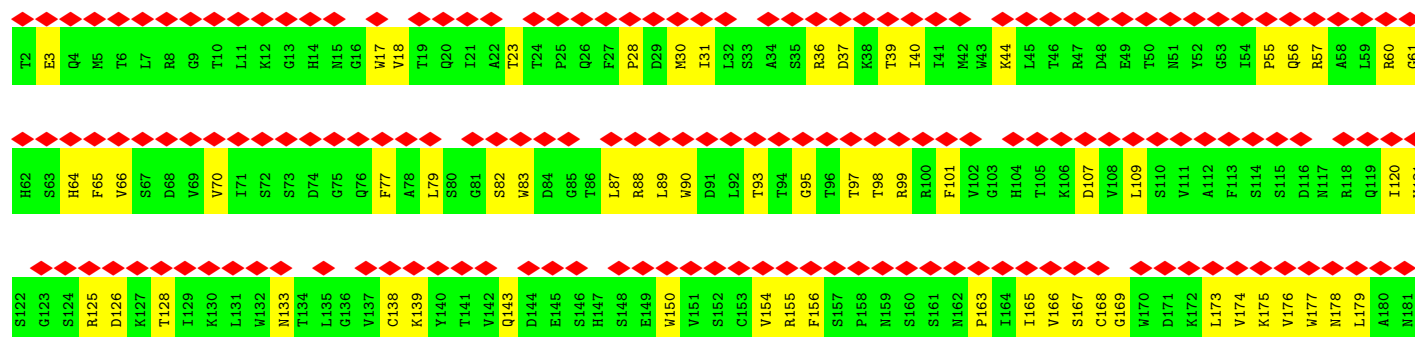
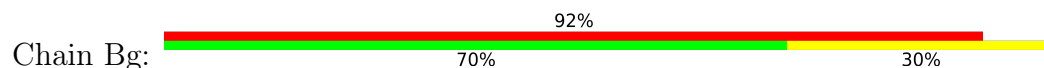
- Molecule 77: 40S ribosomal protein S30

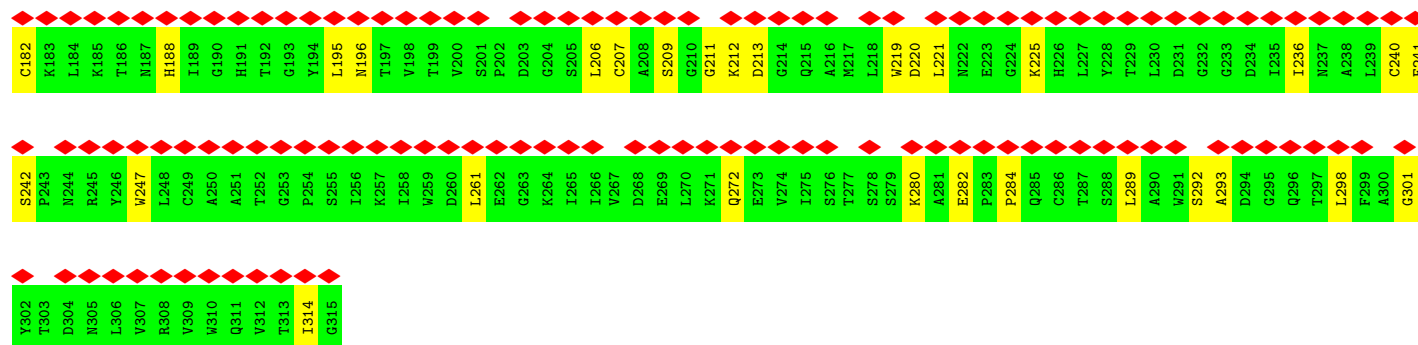


- Molecule 78: Ubiquitin-40S ribosomal protein S27a

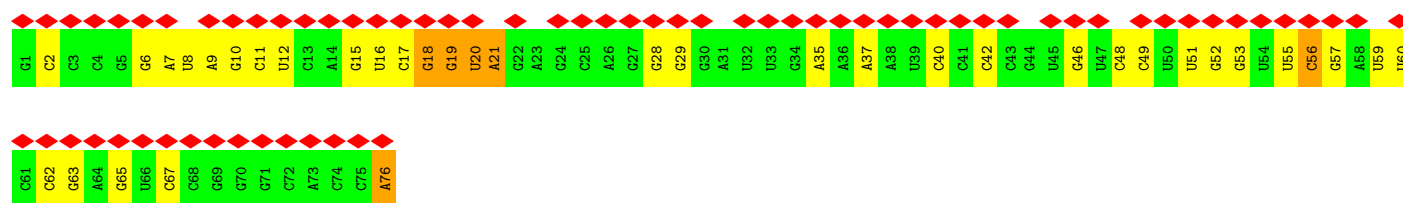
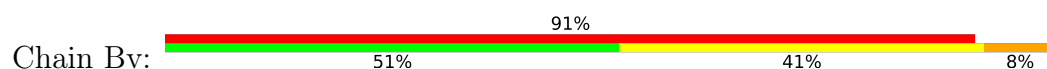


- Molecule 79: Receptor of activated protein C kinase 1

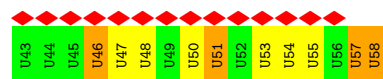
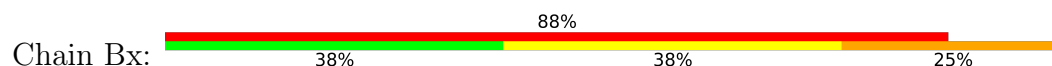




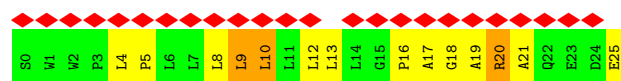
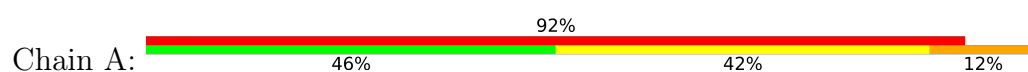
● Molecule 80: tRNA



● Molecule 81: mRNA



● Molecule 82: Proprotein convertase subtilisin/kexin type 9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7214	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.104	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.022	Depositor
Map size ($\text{\AA}$)	488.0, 488.0, 488.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.22, 1.22, 1.22	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.49	0/1936	0.73	0/2596
2	BA	0.39	0/1741	0.73	1/2366 (0.0%)
3	AB	0.48	0/3246	0.76	1/4345 (0.0%)
4	BB	0.38	0/1749	0.78	1/2340 (0.0%)
5	AC	0.52	0/2942	1.06	12/3951 (0.3%)
6	BC	0.40	0/1761	0.70	0/2379
7	A3	0.46	0/3726	0.50	0/5804
8	A4	0.43	0/2839	0.47	0/4425
9	AD	0.41	0/2437	0.74	0/3262
10	AE	0.44	0/1876	0.84	2/2514 (0.1%)
11	AF	0.52	0/1986	0.79	2/2644 (0.1%)
12	AG	0.40	0/1913	0.71	0/2576
13	AH	0.41	0/1545	0.77	0/2077
14	AI	0.45	0/1730	0.73	0/2311
15	AJ	0.38	0/1376	0.74	1/1841 (0.1%)
16	AL	0.53	0/1688	0.92	4/2260 (0.2%)
17	AM	0.44	0/1161	0.71	0/1554
18	AN	0.55	0/1746	0.75	0/2338
19	AO	0.48	0/1638	0.77	3/2191 (0.1%)
20	AP	0.47	0/1268	0.65	0/1701
21	AQ	0.54	0/1537	0.84	1/2052 (0.0%)
22	AR	0.42	0/1533	0.75	0/2025
23	AS	0.44	0/1488	0.72	0/1997
24	AT	0.47	0/1312	0.70	0/1753
25	AU	0.36	0/822	0.70	0/1103
26	AV	0.44	0/983	0.66	0/1319
27	AW	0.40	0/1004	0.79	2/1332 (0.2%)
28	AX	0.42	0/975	0.68	0/1312
29	AY	0.43	0/1081	0.72	0/1439
30	AZ	0.45	0/1126	0.73	0/1502
31	Aa	0.52	0/1191	0.76	2/1591 (0.1%)
32	Ab	4.12	3/804 (0.4%)	1.06	7/1060 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Ac	0.42	0/812	0.65	0/1089
34	Ad	0.48	0/894	0.72	0/1204
35	Ae	0.51	0/1082	0.73	1/1443 (0.1%)
36	Af	0.51	0/895	0.82	0/1198
37	Ag	0.44	0/916	0.82	2/1220 (0.2%)
38	Ah	0.54	0/1023	0.80	1/1351 (0.1%)
39	Ai	0.41	0/805	0.71	0/1065
40	Aj	0.51	0/703	0.83	0/929
41	Ak	0.36	0/575	0.67	0/761
42	Al	0.46	0/454	0.71	0/599
43	Am	0.42	0/417	0.74	0/553
44	An	0.48	0/241	0.88	0/305
45	Ao	0.45	0/877	0.82	3/1156 (0.3%)
46	Ap	0.48	0/718	0.81	2/953 (0.2%)
47	At	0.52	0/995	0.84	0/1334
48	A2	0.55	6/87365 (0.0%)	0.51	8/136272 (0.0%)
49	B1	0.36	0/40767	0.50	2/63536 (0.0%)
50	BD	0.34	0/1736	0.82	4/2338 (0.2%)
51	BE	0.36	0/2072	0.77	5/2793 (0.2%)
52	BF	0.35	0/1524	0.74	0/2048
53	BG	0.34	0/1907	0.73	0/2538
54	BH	0.35	0/1501	0.78	5/2009 (0.2%)
55	BI	0.39	0/1725	0.80	4/2298 (0.2%)
56	BJ	0.39	0/1520	0.76	2/2030 (0.1%)
57	BK	0.35	0/851	0.79	0/1147
58	BL	0.41	0/1281	0.78	0/1710
59	BM	0.33	0/941	0.68	0/1264
60	BN	0.35	0/1226	0.68	0/1649
61	BO	0.40	0/1029	0.72	0/1380
62	BP	0.35	0/1019	0.86	2/1361 (0.1%)
63	BQ	0.36	0/1126	0.78	4/1506 (0.3%)
64	BR	0.33	0/1023	0.83	2/1373 (0.1%)
65	BS	0.34	0/1172	0.77	0/1570
66	BT	0.37	0/1131	0.75	0/1515
67	BU	0.32	0/778	0.72	0/1045
68	BV	0.35	0/623	0.79	1/833 (0.1%)
69	BW	0.42	0/1051	0.75	0/1406
70	BX	0.42	0/1097	0.74	0/1464
71	BY	0.35	0/1032	0.70	0/1371
72	BZ	0.34	0/696	0.77	0/929
73	Ba	0.41	0/786	0.73	0/1053
74	Bb	0.39	0/637	0.74	2/854 (0.2%)
75	Bc	0.31	0/490	0.81	2/656 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Bd	0.37	0/437	0.92	2/580 (0.3%)
77	Be	0.38	0/443	0.75	0/583
78	Bf	0.30	0/613	0.76	0/811
79	Bg	0.31	0/2497	0.70	2/3399 (0.1%)
80	Bv	0.25	0/1813	0.45	0/2823
81	Bx	0.25	0/351	0.50	0/540
82	A	0.28	0/127	1.71	2/175 (1.1%)
All	All	0.53	9/229954 (0.0%)	0.62	97/337979 (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
22	AR	0	1
52	BF	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Ab	112	ILE	N-CA	114.72	2.89	1.46
48	A2	1254	G	N3-C4	46.53	2.28	1.35
48	A2	1254	G	C2-N3	43.80	2.20	1.32
48	A2	1254	G	C5-C6	36.45	2.15	1.42
48	A2	1254	G	N1-C2	35.72	2.09	1.37
48	A2	1254	G	C6-N1	34.69	2.08	1.39
48	A2	1254	G	C5-C4	28.82	1.96	1.38
32	Ab	112	ILE	CA-CB	15.02	1.74	1.54
32	Ab	112	ILE	CA-C	10.04	1.65	1.52

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AC	150	LEU	CA-C-N	27.43	154.13	119.84
5	AC	150	LEU	C-N-CA	27.43	154.13	119.84
50	BD	218	LEU	CA-C-N	12.86	135.91	119.84
50	BD	218	LEU	C-N-CA	12.86	135.91	119.84
82	A	4	LEU	CA-C-N	12.48	135.44	119.84
82	A	4	LEU	C-N-CA	12.48	135.44	119.84
5	AC	150	LEU	C-N-CD	-10.98	79.97	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	Bg	98	THR	N-CA-C	10.60	122.83	111.28
32	Ab	112	ILE	N-CA-C	9.38	128.85	109.34
5	AC	147	VAL	CA-C-N	9.15	129.09	120.03
5	AC	147	VAL	C-N-CA	9.15	129.09	120.03
11	AF	164	LYS	N-CA-C	-8.42	92.87	110.80
50	BD	216	GLU	N-CA-C	8.19	120.21	111.28
38	Ah	45	SER	N-CA-C	-7.44	103.17	111.28
3	AB	175	GLN	N-CA-C	7.36	119.31	111.28
50	BD	217	ILE	N-CA-C	7.36	121.12	108.90
16	AL	47	ALA	CA-C-N	7.18	127.03	119.05
16	AL	47	ALA	C-N-CA	7.18	127.03	119.05
32	Ab	26	SER	N-CA-C	7.16	120.08	108.41
51	BE	213	ALA	CA-C-N	7.05	135.01	121.54
51	BE	213	ALA	C-N-CA	7.05	135.01	121.54
16	AL	49	ARG	CA-C-N	6.83	126.59	119.76
16	AL	49	ARG	C-N-CA	6.83	126.59	119.76
48	A2	1254	G	N3-C4-N9	6.76	146.27	126.00
63	BQ	16	LYS	CA-C-N	6.67	130.07	120.79
63	BQ	16	LYS	C-N-CA	6.67	130.07	120.79
54	BH	115	LYS	CA-C-N	6.58	137.85	121.80
54	BH	115	LYS	C-N-CA	6.58	137.85	121.80
19	AO	94	ARG	N-CA-C	-6.58	105.15	113.43
48	A2	1254	G	C2-N3-C4	6.54	131.53	111.90
21	AQ	5	ILE	N-CA-C	-6.35	105.50	112.80
32	Ab	25	ARG	N-CA-C	6.27	124.16	110.80
63	BQ	48	GLN	CA-C-N	6.25	133.47	121.54
63	BQ	48	GLN	C-N-CA	6.25	133.47	121.54
19	AO	185	VAL	CA-C-N	6.23	133.44	121.54
19	AO	185	VAL	C-N-CA	6.23	133.44	121.54
11	AF	165	LYS	CA-CB-CG	6.21	126.53	114.10
79	Bg	95	GLY	N-CA-C	6.20	120.17	112.73
62	BP	50	ARG	CA-C-N	6.15	133.29	121.54
62	BP	50	ARG	C-N-CA	6.15	133.29	121.54
32	Ab	112	ILE	CB-CA-C	-6.11	101.27	111.29
32	Ab	112	ILE	N-CA-CB	6.10	121.30	111.23
45	Ao	58	LYS	N-CA-C	6.00	118.63	109.62
35	Ae	19	LYS	CA-CB-CG	6.00	126.10	114.10
4	BB	50	THR	N-CA-C	-6.00	100.97	109.96
76	Bd	39	CYS	CA-C-N	5.96	137.00	126.45
76	Bd	39	CYS	C-N-CA	5.96	137.00	126.45
48	A2	1254	G	N1-C2-N3	-5.95	106.04	123.90
37	Ag	45	ALA	CA-C-N	5.83	132.67	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	Ag	45	ALA	C-N-CA	5.83	132.67	121.54
48	A2	1254	G	N3-C4-C5	-5.81	111.16	128.60
55	BI	154	LYS	CA-C-N	5.78	132.58	121.54
55	BI	154	LYS	C-N-CA	5.78	132.58	121.54
51	BE	225	ILE	N-CA-C	5.77	117.47	109.80
5	AC	52	TYR	CA-C-N	5.68	132.40	121.54
5	AC	52	TYR	C-N-CA	5.68	132.40	121.54
46	Ap	59	SER	CA-C-N	5.64	132.32	121.54
46	Ap	59	SER	C-N-CA	5.64	132.32	121.54
75	Bc	32	VAL	CA-C-N	5.63	132.30	121.54
75	Bc	32	VAL	C-N-CA	5.63	132.30	121.54
5	AC	52	TYR	CA-CB-CG	5.61	124.00	113.90
15	AJ	145	LYS	N-CA-C	5.61	117.40	111.28
48	A2	4946	U	P-O3'-C3'	5.57	128.56	120.20
56	BJ	122	SER	CA-C-N	5.57	132.00	121.97
56	BJ	122	SER	C-N-CA	5.57	132.00	121.97
54	BH	108	SER	CA-C-N	5.55	132.13	121.54
54	BH	108	SER	C-N-CA	5.55	132.13	121.54
49	B1	797	C	P-O3'-C3'	5.53	128.49	120.20
68	BV	9	VAL	N-CA-C	-5.52	107.44	112.96
10	AE	283	PRO	CA-C-N	5.50	132.04	121.54
10	AE	283	PRO	C-N-CA	5.50	132.04	121.54
45	Ao	3	ASN	CA-C-N	-5.47	118.57	123.33
45	Ao	3	ASN	C-N-CA	-5.47	118.57	123.33
5	AC	70	GLY	CA-C-N	5.45	131.95	121.54
5	AC	70	GLY	C-N-CA	5.45	131.95	121.54
48	A2	901	U	P-O3'-C3'	5.36	128.24	120.20
31	Aa	120	GLN	CA-C-N	5.34	125.25	119.85
31	Aa	120	GLN	C-N-CA	5.34	125.25	119.85
5	AC	29	LYS	CA-C-N	5.30	129.34	120.86
5	AC	29	LYS	C-N-CA	5.30	129.34	120.86
54	BH	116	ARG	N-CA-C	-5.29	98.12	109.81
48	A2	444	G	O4'-C1'-N9	5.26	116.09	108.20
64	BR	76	GLU	N-CA-C	-5.25	105.64	111.36
49	B1	227	U	P-O3'-C3'	5.25	128.07	120.20
2	BA	200	ASP	N-CA-C	-5.23	106.81	114.39
51	BE	246	LEU	CA-C-N	5.23	133.33	122.41
51	BE	246	LEU	C-N-CA	5.23	133.33	122.41
32	Ab	23	LYS	CA-C-N	5.19	124.81	119.05
32	Ab	23	LYS	C-N-CA	5.19	124.81	119.05
64	BR	79	GLU	N-CA-C	-5.12	105.70	111.28
27	AW	59	HIS	CA-C-N	5.05	131.19	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AW	59	HIS	C-N-CA	5.05	131.19	121.54
55	BI	159	SER	CA-C-N	5.04	128.38	120.82
55	BI	159	SER	C-N-CA	5.04	128.38	120.82
74	Bb	19	HIS	CA-C-N	5.04	131.17	121.54
74	Bb	19	HIS	C-N-CA	5.04	131.17	121.54
48	A2	1254	G	C4-C5-N7	-5.03	95.70	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	AR	21	LYS	Peptide
52	BF	79	HIS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1898	0	1993	30	0
2	BA	1704	0	1704	30	0
3	AB	3178	0	3314	71	0
4	BB	1722	0	1793	87	0
5	AC	2888	0	3064	83	0
6	BC	1724	0	1808	26	0
7	A3	3337	0	1692	50	0
8	A4	2541	0	1284	21	0
9	AD	2392	0	2425	36	0
10	AE	1838	0	1978	59	0
11	AF	1950	0	2093	31	0
12	AG	1880	0	2018	24	0
13	AH	1526	0	1605	24	0
14	AI	1692	0	1744	40	0
15	AJ	1353	0	1386	36	0
16	AL	1657	0	1764	67	0
17	AM	1138	0	1203	52	0
18	AN	1701	0	1749	50	0
19	AO	1606	0	1745	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	AP	1242	0	1269	16	0
21	AQ	1513	0	1628	32	0
22	AR	1517	0	1670	26	0
23	AS	1449	0	1493	48	0
24	AT	1284	0	1352	27	0
25	AU	808	0	831	9	0
26	AV	969	0	1031	13	0
27	AW	989	0	1041	16	0
28	AX	958	0	1029	11	0
29	AY	1064	0	1145	14	0
30	AZ	1103	0	1179	25	0
31	Aa	1162	0	1212	37	0
32	Ab	792	0	853	104	0
33	Ac	801	0	845	9	0
34	Ad	879	0	924	14	0
35	Ae	1064	0	1160	20	0
36	Af	876	0	911	26	0
37	Ag	906	0	1002	15	0
38	Ah	1015	0	1146	62	0
39	Ai	794	0	870	14	0
40	Aj	689	0	717	18	0
41	Ak	569	0	637	13	0
42	Al	444	0	483	10	0
43	Am	411	0	443	8	0
44	An	240	0	289	8	0
45	Ao	863	0	931	10	0
46	Ap	708	0	757	9	0
47	At	980	0	1041	23	0
48	A2	78102	0	39459	824	0
49	B1	36456	0	18411	424	0
50	BD	1709	0	1803	40	0
51	BE	2031	0	2138	43	0
52	BF	1502	0	1557	28	0
53	BG	1884	0	2044	29	0
54	BH	1479	0	1564	24	0
55	BI	1696	0	1784	30	0
56	BJ	1495	0	1613	36	0
57	BK	827	0	854	23	0
58	BL	1258	0	1334	22	0
59	BM	931	0	961	20	0
60	BN	1202	0	1289	21	0
61	BO	1016	0	1039	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	BP	999	0	1046	34	0
63	BQ	1109	0	1174	19	0
64	BR	1011	0	1063	65	0
65	BS	1154	0	1208	63	0
66	BT	1112	0	1146	29	0
67	BU	769	0	837	16	0
68	BV	617	0	622	9	0
69	BW	1034	0	1080	16	0
70	BX	1080	0	1147	21	0
71	BY	1015	0	1086	31	0
72	BZ	688	0	766	11	0
73	Ba	774	0	822	28	0
74	Bb	625	0	646	6	0
75	Bc	488	0	514	13	0
76	Bd	427	0	428	23	0
77	Be	437	0	483	7	0
78	Bf	601	0	623	13	0
79	Bg	2440	0	2396	67	0
80	Bv	1623	0	821	12	0
81	Bx	320	0	161	4	0
82	A	128	0	62	24	0
83	A2	220	0	0	0	0
83	A3	8	0	0	0	0
83	A4	9	0	0	0	0
83	AA	1	0	0	0	0
83	AB	2	0	0	0	0
83	AN	1	0	0	0	0
83	AP	2	0	0	0	0
83	Aa	2	0	0	0	0
83	Ae	1	0	0	0	0
83	Aj	1	0	0	0	0
83	Al	1	0	0	0	0
83	An	1	0	0	0	0
83	B1	73	0	0	0	0
83	BC	1	0	0	0	0
83	BI	1	0	0	0	0
83	Bv	2	0	0	0	0
84	Aj	1	0	0	0	0
84	Ao	1	0	0	0	0
84	Ap	1	0	0	0	0
84	Ba	1	0	0	0	0
84	Bd	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	A	31	0	0	7	0
All	All	214215	0	158232	2784	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 9.

All (2784) 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)
32:Ab:112:ILE:CB	32:Ab:112:ILE:CA	1.74	1.61
31:Aa:79:TRP:HE1	31:Aa:118:PRO:CG	1.15	1.59
62:BP:18:ARG:HH11	65:BS:88:LYS:CD	1.01	1.59
4:BB:138:PHE:CD2	4:BB:213:ARG:NH2	1.69	1.58
82:A:18:GLY:CA	85:A:101:MVM:N6	1.68	1.55
64:BR:102:THR:CG2	64:BR:117:LEU:HD13	1.36	1.52
64:BR:102:THR:HG23	64:BR:117:LEU:CD1	1.36	1.50
49:B1:1611:G:H2'	65:BS:87:GLN:CG	1.43	1.47
31:Aa:79:TRP:NE1	31:Aa:118:PRO:CG	1.71	1.46
82:A:18:GLY:HA2	85:A:101:MVM:N5	1.16	1.46
48:A2:1254:G:C4	48:A2:1254:G:C5	1.96	1.45
17:AM:46:ARG:NH1	48:A2:924:U:H4'	1.12	1.40
32:Ab:110:ALA:O	32:Ab:115:GLY:CA	1.70	1.37
32:Ab:111:ARG:CG	32:Ab:116:LEU:HD11	1.57	1.35
64:BR:74:GLN:O	64:BR:78:ARG:HG3	1.27	1.34
48:A2:1254:G:C5	48:A2:1254:G:C6	2.15	1.34
23:AS:170:LYS:HD2	48:A2:4832:A:P	1.66	1.33
17:AM:46:ARG:HD3	48:A2:924:U:C5'	1.55	1.33
32:Ab:117:ARG:HH21	48:A2:1222:C:C5'	1.39	1.33
17:AM:46:ARG:NH1	48:A2:925:C:O5'	1.62	1.31
49:B1:1611:G:C2'	65:BS:87:GLN:HB2	1.61	1.31
16:AL:47:ALA:HB1	16:AL:48:PRO:CD	1.61	1.31
4:BB:100:PHE:CE2	4:BB:217:MET:CE	2.12	1.30
64:BR:98:VAL:H	64:BR:117:LEU:CD2	1.42	1.30
38:Ah:88:THR:O	38:Ah:92:ARG:CD	1.80	1.30
82:A:18:GLY:CA	85:A:101:MVM:N5	1.90	1.29
32:Ab:116:LEU:HB3	48:A2:1253:A:N3	1.47	1.28
32:Ab:117:ARG:NH2	48:A2:1222:C:P	2.05	1.28
51:BE:184:ILE:HG12	51:BE:224:ASN:O	1.14	1.26
17:AM:46:ARG:NH2	48:A2:925:C:O5'	1.64	1.26
17:AM:46:ARG:NH2	48:A2:925:C:P	2.06	1.26
17:AM:46:ARG:CZ	48:A2:925:C:O5'	1.82	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:BP:18:ARG:NH1	65:BS:88:LYS:HD2	0.91	1.24
82:A:18:GLY:HA2	85:A:101:MVM:N6	0.92	1.23
17:AM:46:ARG:CZ	48:A2:925:C:P	2.26	1.23
17:AM:46:ARG:CZ	48:A2:925:C:OP1	1.88	1.22
31:Aa:79:TRP:CD1	31:Aa:118:PRO:HG2	1.74	1.21
48:A2:1254:G:C6	48:A2:1254:G:N1	2.08	1.21
48:A2:1254:G:C2	48:A2:1254:G:N1	2.09	1.21
32:Ab:110:ALA:C	32:Ab:115:GLY:HA2	1.65	1.21
32:Ab:116:LEU:HB3	48:A2:1253:A:C2	1.75	1.21
32:Ab:111:ARG:C	32:Ab:115:GLY:HA3	1.66	1.20
32:Ab:112:ILE:N	48:A2:1254:G:N3	1.88	1.19
32:Ab:117:ARG:HH22	48:A2:1222:C:P	1.62	1.19
32:Ab:111:ARG:O	48:A2:1254:G:C4	1.96	1.17
17:AM:46:ARG:NH1	48:A2:924:U:C4'	2.08	1.17
23:AS:170:LYS:HD2	48:A2:4832:A:O5'	1.46	1.16
31:Aa:117:LEU:HD12	31:Aa:118:PRO:CD	1.76	1.16
32:Ab:26:SER:HB2	48:A2:1787:A:H61	1.03	1.16
4:BB:51:ARG:O	4:BB:58:ALA:HB2	1.42	1.16
4:BB:100:PHE:CE2	4:BB:217:MET:HE2	1.78	1.16
17:AM:46:ARG:HH11	48:A2:924:U:C4'	1.58	1.15
17:AM:46:ARG:CD	48:A2:924:U:H5'	1.75	1.14
7:A3:36:G:N7	38:Ah:89:ARG:HD3	1.64	1.13
38:Ah:88:THR:O	38:Ah:92:ARG:HD3	0.95	1.13
16:AL:47:ALA:CB	16:AL:48:PRO:CD	2.20	1.12
49:B1:1611:G:C2'	65:BS:87:GLN:CB	2.27	1.12
4:BB:29:ASP:HB2	4:BB:51:ARG:HG3	1.22	1.11
51:BE:185:GLY:O	51:BE:224:ASN:ND2	1.82	1.11
38:Ah:91:MET:HA	38:Ah:91:MET:HE3	1.23	1.11
4:BB:100:PHE:CD2	4:BB:217:MET:CE	2.33	1.11
64:BR:98:VAL:H	64:BR:117:LEU:HD23	1.16	1.11
32:Ab:111:ARG:C	48:A2:1254:G:C4	2.29	1.10
62:BP:18:ARG:HD3	65:BS:88:LYS:HG2	1.13	1.10
32:Ab:26:SER:HB2	48:A2:1787:A:N6	1.65	1.10
56:BJ:136:ARG:NH2	56:BJ:139:LYS:O	1.83	1.10
49:B1:1611:G:H2'	65:BS:87:GLN:HG3	1.15	1.09
15:AJ:145:LYS:CE	48:A2:4203:C:OP2	1.96	1.09
16:AL:47:ALA:HB1	16:AL:48:PRO:HD3	1.10	1.09
64:BR:102:THR:HG22	64:BR:117:LEU:HD13	1.34	1.09
32:Ab:111:ARG:O	32:Ab:115:GLY:CA	1.91	1.09
48:A2:1254:G:C2	48:A2:1254:G:N3	2.20	1.09
5:AC:147:VAL:HG12	5:AC:148:PRO:HD2	1.14	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Ab:117:ARG:NH2	48:A2:1222:C:H5'	1.68	1.08
32:Ab:116:LEU:CB	48:A2:1253:A:N3	2.16	1.08
31:Aa:79:TRP:NE1	31:Aa:118:PRO:HG2	0.75	1.07
32:Ab:111:ARG:HG2	32:Ab:116:LEU:CD1	1.84	1.07
4:BB:138:PHE:HD2	4:BB:213:ARG:NH2	1.17	1.07
31:Aa:79:TRP:CE2	31:Aa:118:PRO:HG2	1.90	1.07
16:AL:77:SER:HB3	16:AL:80:GLU:CG	1.85	1.07
32:Ab:111:ARG:CG	32:Ab:116:LEU:CD1	2.32	1.07
16:AL:77:SER:HB3	16:AL:80:GLU:HG3	1.14	1.06
5:AC:144:ILE:HA	5:AC:147:VAL:CG2	1.85	1.05
32:Ab:117:ARG:HH21	48:A2:1222:C:H5'	1.05	1.05
4:BB:100:PHE:CD2	4:BB:217:MET:HE3	1.90	1.05
49:B1:1611:G:C2'	65:BS:87:GLN:CG	2.34	1.04
4:BB:138:PHE:CE1	4:BB:216:LYS:NZ	2.26	1.04
23:AS:170:LYS:CD	48:A2:4832:A:P	2.45	1.04
49:B1:1611:G:O2'	65:BS:87:GLN:HB2	1.57	1.04
64:BR:73:LEU:O	64:BR:77:GLU:HG2	1.54	1.04
10:AE:140:LEU:HA	10:AE:191:GLN:HE22	1.12	1.04
32:Ab:111:ARG:HG2	32:Ab:116:LEU:HD11	1.09	1.04
64:BR:98:VAL:H	64:BR:117:LEU:HD22	1.21	1.04
49:B1:1612:G:O2'	65:BS:87:GLN:OE1	1.74	1.04
51:BE:184:ILE:CG1	51:BE:224:ASN:O	2.04	1.04
32:Ab:117:ARG:NH2	48:A2:1222:C:C5'	2.16	1.03
14:AI:184:MET:SD	14:AI:189:ARG:HD2	1.98	1.03
31:Aa:91:ALA:HB2	31:Aa:120:GLN:NE2	1.72	1.03
7:A3:36:G:C5	38:Ah:89:ARG:CD	2.36	1.03
49:B1:1611:G:H2'	65:BS:87:GLN:CB	1.87	1.02
62:BP:18:ARG:HD3	65:BS:88:LYS:CG	1.87	1.02
64:BR:74:GLN:HA	64:BR:77:GLU:HB2	1.40	1.02
48:A2:1254:G:C4	48:A2:1254:G:N3	2.28	1.01
51:BE:185:GLY:C	51:BE:224:ASN:ND2	2.17	1.01
16:AL:49:ARG:HH11	38:Ah:118:LYS:HA	1.25	1.00
23:AS:170:LYS:HD2	48:A2:4832:A:OP1	1.58	1.00
64:BR:102:THR:CG2	64:BR:117:LEU:CD1	2.11	1.00
38:Ah:44:LEU:O	38:Ah:47:ILE:HG22	1.61	1.00
49:B1:1611:G:O2'	65:BS:87:GLN:N	1.95	1.00
56:BJ:136:ARG:NH2	56:BJ:139:LYS:C	2.19	1.00
64:BR:96:ILE:O	64:BR:115:SER:OG	1.77	1.00
38:Ah:87:LYS:HD2	40:Aj:78:PHE:CB	1.91	1.00
5:AC:147:VAL:HG12	5:AC:148:PRO:CD	1.90	1.00
62:BP:36:LEU:O	65:BS:88:LYS:HD3	1.62	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:BR:98:VAL:N	64:BR:117:LEU:CD2	2.24	0.99
31:Aa:117:LEU:HD12	31:Aa:118:PRO:HD2	1.40	0.99
4:BB:100:PHE:HE2	4:BB:217:MET:CE	1.63	0.98
32:Ab:112:ILE:N	48:A2:1254:G:C2	2.30	0.98
51:BE:185:GLY:C	51:BE:224:ASN:HD22	1.69	0.98
31:Aa:117:LEU:CD1	31:Aa:118:PRO:HD2	1.92	0.98
48:A2:3875:G:H21	82:A:18:GLY:HA3	1.25	0.98
32:Ab:111:ARG:NH2	48:A2:1248:G:OP2	1.96	0.97
31:Aa:79:TRP:HE1	31:Aa:118:PRO:CD	1.77	0.97
7:A3:36:G:N7	38:Ah:89:ARG:CD	2.27	0.97
64:BR:102:THR:HG23	64:BR:117:LEU:HD11	1.41	0.97
5:AC:144:ILE:HA	5:AC:147:VAL:HG21	1.44	0.97
10:AE:140:LEU:HD11	10:AE:167:GLN:CG	1.95	0.96
32:Ab:117:ARG:HB2	48:A2:1254:G:H1'	1.48	0.96
32:Ab:111:ARG:HG3	32:Ab:116:LEU:HD11	1.44	0.96
5:AC:144:ILE:CG2	5:AC:147:VAL:HG21	1.96	0.95
4:BB:51:ARG:H	4:BB:51:ARG:HD3	1.31	0.95
82:A:19:ALA:O	82:A:21:ALA:N	2.00	0.94
15:AJ:145:LYS:HE3	48:A2:4203:C:OP2	1.29	0.94
16:AL:47:ALA:CB	16:AL:48:PRO:HD2	1.95	0.94
14:AI:189:ARG:HG3	14:AI:190:LEU:H	1.29	0.94
4:BB:29:ASP:CB	4:BB:51:ARG:HG3	1.97	0.94
31:Aa:117:LEU:HD12	31:Aa:118:PRO:HD3	1.45	0.94
82:A:18:GLY:HA3	85:A:101:MVM:N6	1.83	0.94
23:AS:170:LYS:CD	48:A2:4832:A:O5'	2.16	0.94
32:Ab:111:ARG:C	48:A2:1254:G:C6	2.46	0.93
5:AC:144:ILE:C	5:AC:147:VAL:HG23	1.93	0.93
23:AS:170:LYS:CD	48:A2:4832:A:OP1	2.17	0.93
10:AE:140:LEU:HA	10:AE:191:GLN:NE2	1.84	0.93
15:AJ:147:ARG:NH1	15:AJ:147:ARG:HB3	1.84	0.93
4:BB:103:MET:HB3	4:BB:215:VAL:CG1	1.99	0.92
64:BR:98:VAL:N	64:BR:117:LEU:HD23	1.83	0.92
62:BP:18:ARG:HH11	65:BS:88:LYS:HD3	1.35	0.92
4:BB:29:ASP:HB2	4:BB:51:ARG:CG	1.98	0.92
4:BB:51:ARG:O	4:BB:58:ALA:CB	2.17	0.91
5:AC:150:LEU:HB3	5:AC:151:PRO:CD	2.00	0.91
32:Ab:111:ARG:HA	32:Ab:116:LEU:HD13	1.50	0.91
5:AC:71:ARG:NH2	82:A:13:LEU:HA	1.85	0.91
16:AL:47:ALA:CB	16:AL:48:PRO:HD3	1.95	0.91
32:Ab:111:ARG:CA	32:Ab:115:GLY:HA3	1.99	0.91
16:AL:49:ARG:NH1	38:Ah:118:LYS:HA	1.85	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Ab:110:ALA:O	32:Ab:115:GLY:HA2	0.73	0.91
38:Ah:87:LYS:HD2	40:Aj:78:PHE:HB2	1.53	0.91
49:B1:1611:G:C3'	65:BS:87:GLN:HB2	1.99	0.91
4:BB:138:PHE:CZ	4:BB:216:LYS:NZ	2.37	0.91
32:Ab:117:ARG:NH2	48:A2:1222:C:O5'	2.01	0.91
7:A3:36:G:C5	38:Ah:89:ARG:HD3	2.02	0.90
32:Ab:111:ARG:O	32:Ab:115:GLY:HA3	1.11	0.90
17:AM:46:ARG:NH1	48:A2:925:C:P	2.38	0.90
32:Ab:111:ARG:NH1	48:A2:1248:G:OP2	2.05	0.90
38:Ah:91:MET:HA	38:Ah:91:MET:CE	2.02	0.89
17:AM:46:ARG:NH2	48:A2:925:C:OP1	1.97	0.88
49:B1:1611:G:H2'	65:BS:87:GLN:HG2	1.55	0.88
4:BB:100:PHE:CE2	4:BB:217:MET:HE1	2.07	0.88
62:BP:18:ARG:CZ	65:BS:88:LYS:HD2	2.02	0.88
10:AE:131:LYS:O	10:AE:136:HIS:CE1	2.26	0.88
5:AC:144:ILE:O	5:AC:147:VAL:HG23	1.73	0.88
80:Bv:76:A:C3'	82:A:25:GLU:O	2.21	0.88
64:BR:74:GLN:O	64:BR:78:ARG:CG	2.20	0.88
5:AC:145:GLU:C	5:AC:146:GLU:OE1	2.17	0.88
79:Bg:90:TRP:CE3	79:Bg:97:THR:HB	2.09	0.87
10:AE:153:LEU:HD13	36:Af:105:LEU:O	1.74	0.87
48:A2:2617:G:H21	48:A2:2676:A:H62	1.21	0.87
4:BB:103:MET:HB3	4:BB:215:VAL:HG12	1.55	0.87
16:AL:77:SER:CB	16:AL:80:GLU:HG3	2.04	0.87
32:Ab:112:ILE:N	48:A2:1254:G:C4	2.43	0.86
56:BJ:138:ARG:NH2	56:BJ:153:SER:HA	1.90	0.86
5:AC:149:GLU:HB3	47:At:72:LYS:HG3	1.57	0.85
49:B1:1611:G:O2'	65:BS:87:GLN:CB	2.22	0.85
5:AC:147:VAL:CG1	5:AC:148:PRO:HD2	2.05	0.85
64:BR:73:LEU:O	64:BR:77:GLU:CG	2.25	0.85
5:AC:144:ILE:CA	5:AC:147:VAL:CG2	2.55	0.84
16:AL:49:ARG:NH1	38:Ah:117:ARG:O	2.11	0.83
82:A:18:GLY:C	85:A:101:MVM:N5	2.35	0.83
32:Ab:112:ILE:N	48:A2:1254:G:C6	2.46	0.83
16:AL:133:ALA:HA	16:AL:136:LYS:HE3	1.61	0.83
64:BR:98:VAL:HG22	64:BR:117:LEU:HD21	1.61	0.83
79:Bg:88:ARG:HD3	79:Bg:97:THR:HG21	1.60	0.82
4:BB:136:ARG:HD2	4:BB:216:LYS:NZ	1.94	0.82
17:AM:46:ARG:HH12	48:A2:925:C:C5'	1.92	0.82
5:AC:144:ILE:HG23	5:AC:147:VAL:HG21	1.59	0.82
38:Ah:88:THR:HG23	38:Ah:91:MET:HB2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AS:170:LYS:CG	48:A2:4832:A:P	2.68	0.81
16:AL:45:ARG:O	16:AL:46:ILE:O	1.99	0.81
14:AI:189:ARG:HG3	14:AI:190:LEU:N	1.96	0.81
16:AL:133:ALA:CA	16:AL:136:LYS:HE3	2.11	0.81
4:BB:216:LYS:HE3	49:B1:942:G:OP1	1.80	0.80
80:Bv:76:A:H3'	82:A:25:GLU:O	1.80	0.80
23:AS:171:ARG:O	48:A2:4828:G:O6	2.00	0.80
4:BB:136:ARG:HD2	4:BB:216:LYS:HE2	1.65	0.79
62:BP:18:ARG:HH12	65:BS:88:LYS:HD2	1.41	0.79
4:BB:138:PHE:CE2	4:BB:213:ARG:NH2	2.49	0.79
4:BB:103:MET:H	4:BB:215:VAL:HG13	1.48	0.79
10:AE:140:LEU:CA	10:AE:191:GLN:HE22	1.94	0.79
32:Ab:111:ARG:CZ	48:A2:1248:G:OP2	2.30	0.79
5:AC:71:ARG:HH21	82:A:13:LEU:HA	1.47	0.79
7:A3:36:G:C8	38:Ah:89:ARG:HD2	2.18	0.79
49:B1:1611:G:O3'	65:BS:87:GLN:HB2	1.83	0.78
4:BB:136:ARG:HD2	4:BB:216:LYS:CE	2.13	0.78
17:AM:46:ARG:CZ	48:A2:924:U:H4'	2.12	0.78
62:BP:18:ARG:NH1	65:BS:88:LYS:CD	1.83	0.78
5:AC:150:LEU:HB3	5:AC:151:PRO:HD3	1.65	0.78
4:BB:100:PHE:HE2	4:BB:217:MET:HE2	1.23	0.78
45:Ao:59:LYS:NZ	45:Ao:61:LYS:O	2.16	0.78
5:AC:197:ARG:NH2	48:A2:346:G:N7	2.32	0.78
64:BR:97:GLU:HA	64:BR:117:LEU:HD23	1.63	0.78
32:Ab:26:SER:CB	48:A2:1787:A:H61	1.92	0.78
32:Ab:117:ARG:NH2	48:A2:1222:C:OP1	2.16	0.78
49:B1:1611:G:C2'	65:BS:87:GLN:HG3	2.06	0.78
32:Ab:112:ILE:N	48:A2:1254:G:N1	2.32	0.77
5:AC:150:LEU:HB3	5:AC:151:PRO:HD2	1.64	0.77
49:B1:56:G:H1	49:B1:89:C:H41	1.32	0.77
64:BR:98:VAL:CG2	64:BR:117:LEU:CD2	2.62	0.77
64:BR:102:THR:HG23	64:BR:117:LEU:HD13	0.97	0.77
17:AM:40:GLY:H	17:AM:45:VAL:CG1	1.97	0.77
23:AS:85:ASP:H	23:AS:123:SER:HB3	1.49	0.77
16:AL:133:ALA:HA	16:AL:136:LYS:CE	2.15	0.77
17:AM:46:ARG:HD3	48:A2:924:U:H5'	0.80	0.76
16:AL:47:ALA:HB3	16:AL:48:PRO:HD2	1.66	0.76
48:A2:2462:G:H1	48:A2:2474:U:H3	1.33	0.76
4:BB:138:PHE:HD2	4:BB:213:ARG:CZ	1.99	0.76
14:AI:184:MET:HE1	14:AI:190:LEU:HD11	1.66	0.76
38:Ah:87:LYS:CD	40:Aj:78:PHE:CB	2.63	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Ah:89:ARG:NH2	48:A2:20:U:OP2	2.19	0.75
49:B1:1612:G:HO2'	65:BS:87:GLN:CD	1.93	0.75
64:BR:75:GLU:HA	64:BR:78:ARG:HD3	1.69	0.75
56:BJ:136:ARG:NH2	56:BJ:139:LYS:CA	2.50	0.74
16:AL:133:ALA:HA	16:AL:136:LYS:CD	2.17	0.74
21:AQ:156:PRO:HA	21:AQ:163:THR:HG21	1.69	0.74
3:AB:174:ARG:HD2	3:AB:174:ARG:C	2.11	0.74
64:BR:96:ILE:N	64:BR:115:SER:OG	2.20	0.74
56:BJ:136:ARG:NH2	56:BJ:139:LYS:HA	2.03	0.73
17:AM:46:ARG:CD	48:A2:924:U:C5'	2.49	0.73
48:A2:173:G:H22	48:A2:255:G:H1	1.35	0.73
48:A2:451:G:H22	48:A2:691:G:H22	1.36	0.73
32:Ab:112:ILE:HA	48:A2:1254:G:C4	2.23	0.73
17:AM:46:ARG:HH22	48:A2:925:C:P	1.92	0.73
32:Ab:116:LEU:CD1	32:Ab:116:LEU:H	2.02	0.73
55:BI:37:LYS:HB2	55:BI:59:ARG:HG2	1.70	0.73
16:AL:47:ALA:HB1	16:AL:48:PRO:HD2	1.57	0.72
48:A2:3663:A:H62	48:A2:3794:G:H21	1.36	0.72
32:Ab:116:LEU:HD13	32:Ab:116:LEU:H	1.53	0.72
79:Bg:207:CYS:HB3	79:Bg:219:TRP:HB2	1.71	0.72
38:Ah:87:LYS:CD	40:Aj:78:PHE:HB3	2.20	0.72
38:Ah:89:ARG:HA	38:Ah:92:ARG:CZ	2.20	0.72
4:BB:101:HIS:O	4:BB:217:MET:HG2	1.89	0.72
32:Ab:112:ILE:CB	32:Ab:112:ILE:C	2.63	0.72
32:Ab:111:ARG:HG3	32:Ab:116:LEU:CD1	2.07	0.72
32:Ab:116:LEU:O	48:A2:1253:A:O2'	2.05	0.72
64:BR:98:VAL:HG22	64:BR:117:LEU:CD2	2.17	0.72
64:BR:98:VAL:CG2	64:BR:117:LEU:HD21	2.19	0.72
10:AE:141:ARG:H	10:AE:191:GLN:NE2	1.87	0.72
5:AC:149:GLU:HA	47:At:72:LYS:HA	1.72	0.71
32:Ab:116:LEU:HG	48:A2:1252:G:O6	1.89	0.71
38:Ah:91:MET:HE3	38:Ah:91:MET:CA	2.12	0.71
79:Bg:220:ASP:HB3	79:Bg:225:LYS:H	1.52	0.71
49:B1:377:G:H5''	55:BI:98:LYS:HB3	1.72	0.71
82:A:9:LEU:O	82:A:10:LEU:CB	2.38	0.71
4:BB:82:ARG:NH2	4:BB:188:LEU:O	2.24	0.71
5:AC:144:ILE:CA	5:AC:147:VAL:HG21	2.15	0.71
64:BR:98:VAL:N	64:BR:117:LEU:HD22	1.96	0.70
50:BD:218:LEU:HD12	50:BD:219:PRO:HD2	1.73	0.70
4:BB:138:PHE:HE1	4:BB:216:LYS:NZ	1.86	0.70
49:B1:1226:G:H21	49:B1:1640:A:H62	1.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:Bg:77:PHE:HB3	79:Bg:89:LEU:HD11	1.74	0.70
32:Ab:111:ARG:CA	32:Ab:115:GLY:CA	2.69	0.70
3:AB:174:ARG:HD2	3:AB:174:ARG:O	1.90	0.70
14:AI:181:PHE:O	14:AI:185:VAL:HG22	1.92	0.70
31:Aa:79:TRP:CD1	31:Aa:118:PRO:CG	2.48	0.70
80:Bv:51:U:H3	80:Bv:63:G:H1	1.37	0.70
55:BI:110:ARG:HH12	55:BI:122:GLY:HA3	1.56	0.70
64:BR:74:GLN:CA	64:BR:77:GLU:HB2	2.17	0.70
32:Ab:105:GLY:O	32:Ab:108:ALA:HB3	1.92	0.69
49:B1:151:C:N3	49:B1:168:C:N4	2.40	0.69
41:Ak:17:ARG:NH2	41:Ak:38:CYS:SG	2.66	0.69
10:AE:140:LEU:HD11	10:AE:167:GLN:CB	2.22	0.69
4:BB:103:MET:HB3	4:BB:215:VAL:HG11	1.74	0.69
4:BB:151:ARG:NH1	49:B1:1102:G:OP1	2.26	0.69
5:AC:147:VAL:CG1	5:AC:148:PRO:CD	2.65	0.69
5:AC:150:LEU:CB	5:AC:151:PRO:CD	2.64	0.69
79:Bg:89:LEU:O	79:Bg:97:THR:OG1	2.09	0.69
4:BB:100:PHE:HD2	4:BB:217:MET:HE3	1.53	0.69
5:AC:144:ILE:CG2	5:AC:147:VAL:CG2	2.71	0.69
5:AC:152:LEU:HD11	5:AC:251:ILE:HG12	1.72	0.69
24:AT:84:ILE:HD12	32:Ab:23:LYS:HZ3	1.58	0.69
62:BP:18:ARG:HD3	65:BS:88:LYS:CD	2.23	0.69
62:BP:18:ARG:CD	65:BS:88:LYS:CD	2.71	0.69
5:AC:48:ASN:ND2	48:A2:1353:G:OP1	2.18	0.69
73:Ba:88:SER:H	73:Ba:91:ALA:HB3	1.57	0.69
80:Bv:76:A:O3'	82:A:25:GLU:O	2.10	0.69
64:BR:98:VAL:HG23	64:BR:117:LEU:HD22	1.74	0.68
17:AM:40:GLY:H	17:AM:45:VAL:HG13	1.57	0.68
48:A2:2618:U:HO2'	48:A2:2673:G:H1	1.41	0.68
10:AE:140:LEU:HD11	10:AE:167:GLN:HB2	1.75	0.68
24:AT:92:ARG:NH1	48:A2:4275:A:OP1	2.27	0.68
23:AS:170:LYS:HG3	48:A2:4832:A:H5'	1.73	0.68
51:BE:125:LYS:NZ	51:BE:222:LEU:O	2.26	0.68
32:Ab:116:LEU:CA	48:A2:1253:A:N3	2.56	0.68
56:BJ:136:ARG:HH21	56:BJ:139:LYS:C	2.00	0.68
67:BU:46:LYS:HZ2	67:BU:97:ILE:HG23	1.59	0.68
32:Ab:115:GLY:O	48:A2:1254:G:C8	2.46	0.68
4:BB:38:MET:HE1	4:BB:182:LYS:HG2	1.76	0.67
18:AN:108:ARG:HH22	48:A2:2440:G:H5''	1.59	0.67
53:BG:23:LYS:HZ2	53:BG:41:LEU:HG	1.56	0.67
53:BG:159:ARG:HG2	53:BG:161:PRO:HD3	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AE:141:ARG:H	10:AE:191:GLN:HE21	1.39	0.67
4:BB:103:MET:H	4:BB:215:VAL:CG1	2.07	0.67
32:Ab:117:ARG:HD3	48:A2:1254:G:N3	2.10	0.67
16:AL:133:ALA:CB	16:AL:136:LYS:HE3	2.25	0.67
48:A2:4948:C:N3	48:A2:5018:A:N6	2.42	0.67
15:AJ:147:ARG:HB3	15:AJ:147:ARG:HH11	1.58	0.67
49:B1:1598:G:N7	72:BZ:85:ARG:NH2	2.43	0.67
48:A2:2464:U:H3	48:A2:2472:G:H1	1.43	0.66
77:Be:39:ASN:O	77:Be:44:ASN:ND2	2.28	0.66
82:A:19:ALA:O	82:A:20:ARG:C	2.38	0.66
48:A2:177:C:N3	48:A2:252:C:N4	2.39	0.66
7:A3:9:A:H2'	7:A3:10:G:H8	1.61	0.66
48:A2:2673:G:H4'	48:A2:2674:A:H5'	1.76	0.66
70:BX:46:HIS:HB3	70:BX:101:LEU:HD11	1.76	0.66
39:Ai:48:CYS:SG	39:Ai:49:GLY:N	2.68	0.66
34:Ad:50:ARG:NH1	48:A2:2352:C:OP1	2.27	0.66
48:A2:942:G:O2'	48:A2:944:G:N2	2.29	0.66
5:AC:5:ARG:HH21	5:AC:25:PRO:HA	1.59	0.66
32:Ab:111:ARG:CA	32:Ab:116:LEU:HD13	2.24	0.66
65:BS:88:LYS:HB2	65:BS:88:LYS:NZ	2.10	0.66
38:Ah:87:LYS:HD2	40:Aj:78:PHE:HB3	1.77	0.66
17:AM:46:ARG:HH22	48:A2:925:C:C5'	2.09	0.66
32:Ab:112:ILE:CA	32:Ab:112:ILE:CG1	2.73	0.66
46:Ap:33:GLN:HB2	46:Ap:49:ARG:HD3	1.78	0.66
49:B1:913:A:OP2	54:BH:99:ARG:NH1	2.29	0.66
50:BD:218:LEU:HD12	50:BD:219:PRO:CD	2.26	0.66
16:AL:51:ALA:H	16:AL:148:THR:HG23	1.60	0.66
49:B1:1238:U:H4'	62:BP:127:LYS:HB3	1.77	0.66
71:BY:18:LEU:O	71:BY:85:ASN:ND2	2.29	0.66
49:B1:925:G:H1	49:B1:1017:U:H3	1.43	0.65
15:AJ:145:LYS:HE2	48:A2:4203:C:OP2	1.90	0.65
32:Ab:116:LEU:HG	48:A2:1252:G:C6	2.31	0.65
38:Ah:87:LYS:CD	40:Aj:78:PHE:HB2	2.27	0.65
5:AC:145:GLU:O	5:AC:146:GLU:OE1	2.14	0.65
18:AN:195:ARG:HH11	48:A2:98:A:H4'	1.61	0.65
7:A3:36:G:N2	38:Ah:89:ARG:HH22	1.68	0.65
38:Ah:88:THR:C	38:Ah:92:ARG:CD	2.68	0.65
48:A2:410:U:O2'	48:A2:2288:G:N2	2.29	0.65
49:B1:1192:U:OP2	70:BX:119:ARG:NH2	2.29	0.65
53:BG:43:GLU:HG3	53:BG:45:TRP:H	1.60	0.65
64:BR:99:ASP:O	64:BR:117:LEU:HB3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:BF:128:ILE:HB	52:BF:135:ARG:HE	1.62	0.65
61:BO:146:ARG:NH1	73:Ba:29:CYS:SG	2.70	0.65
64:BR:98:VAL:CG2	64:BR:117:LEU:HD22	2.26	0.65
2:BA:188:THR:HG22	2:BA:189:ILE:HG12	1.78	0.65
48:A2:469:G:H22	48:A2:672:G:H22	1.43	0.65
52:BF:71:ARG:NH2	52:BF:148:ASN:OD1	2.30	0.65
10:AE:95:PRO:HA	10:AE:104:THR:HA	1.79	0.65
38:Ah:89:ARG:HA	38:Ah:92:ARG:NE	2.10	0.65
48:A2:1227:G:H4'	48:A2:1251:G:H1'	1.78	0.65
48:A2:1416:A:N6	48:A2:1433:C:O2'	2.30	0.64
64:BR:99:ASP:H	64:BR:117:LEU:HD22	1.62	0.64
3:AB:393:LYS:HD2	48:A2:4998:U:H5'	1.77	0.64
12:AG:159:HIS:HB2	12:AG:185:LYS:HA	1.78	0.64
14:AI:38:ARG:NH2	14:AI:83:ASP:O	2.31	0.64
48:A2:4693:G:H8	48:A2:4694:G:H2'	1.61	0.64
49:B1:885:U:H2'	49:B1:886:A:H8	1.60	0.64
71:BY:13:MET:HB2	71:BY:22:GLN:HB2	1.78	0.64
3:AB:53:MET:HG2	3:AB:77:THR:HG22	1.77	0.64
32:Ab:111:ARG:O	48:A2:1254:G:C6	2.40	0.64
48:A2:4351:C:H2'	48:A2:4352:A:H8	1.62	0.64
49:B1:1230:C:H4'	49:B1:1607:A:H4'	1.79	0.64
17:AM:46:ARG:NE	48:A2:925:C:OP1	2.30	0.64
20:AP:80:GLN:NE2	48:A2:3863:U:O2'	2.31	0.64
10:AE:283:PRO:O	10:AE:284:HIS:ND1	2.30	0.64
17:AM:40:GLY:N	17:AM:45:VAL:CG1	2.59	0.64
35:Ae:36:ARG:NH1	48:A2:1643:C:OP1	2.30	0.64
19:AO:128:ARG:HH22	23:AS:161:ARG:HH11	1.46	0.64
49:B1:1268:C:O2	62:BP:97:TYR:OH	2.16	0.64
3:AB:394:LYS:NZ	48:A2:4958:G:OP1	2.30	0.64
16:AL:60:ARG:NH2	16:AL:67:HIS:O	2.29	0.64
49:B1:1256:G:H3'	76:Bd:30:LEU:HD23	1.80	0.64
10:AE:114:ARG:NH2	48:A2:452:C:OP1	2.31	0.64
17:AM:101:LYS:HD2	19:AO:198:THR:HG21	1.80	0.64
49:B1:1622:U:H5'	65:BS:120:HIS:HE2	1.63	0.64
60:BN:34:LYS:HE3	60:BN:74:ILE:HG23	1.79	0.64
71:BY:20:ARG:HE	71:BY:22:GLN:HE21	1.46	0.64
14:AI:33:ILE:O	14:AI:69:ARG:NH1	2.31	0.64
31:Aa:94:LYS:HG3	31:Aa:95:THR:HG22	1.79	0.64
7:A3:12:G:OP1	20:AP:3:ARG:NH1	2.31	0.64
7:A3:36:G:C5	38:Ah:89:ARG:HD2	2.30	0.63
30:AZ:27:LYS:HB3	30:AZ:42:LEU:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:BR:98:VAL:HG23	64:BR:117:LEU:CD2	2.27	0.63
72:BZ:60:LYS:O	72:BZ:64:ASN:ND2	2.30	0.63
7:A3:15:G:N1	48:A2:412:A:OP2	2.28	0.63
48:A2:4234:G:H22	48:A2:4297:C:H42	1.44	0.63
49:B1:1611:G:HO2'	65:BS:87:GLN:N	1.95	0.63
73:Ba:22:ARG:NH1	73:Ba:27:ALA:O	2.30	0.63
59:BM:86:GLY:HA2	59:BM:91:LEU:HB2	1.81	0.63
79:Bg:3:GLU:HB3	79:Bg:314:ILE:HD13	1.81	0.63
35:Ae:90:MET:HE2	47:At:33:LYS:HE2	1.79	0.63
2:BA:195:TRP:HE1	2:BA:197:VAL:HG12	1.63	0.63
49:B1:507:G:OP1	71:BY:108:LYS:NZ	2.31	0.63
56:BJ:138:ARG:HE	56:BJ:153:SER:HA	1.63	0.63
24:AT:84:ILE:HD12	32:Ab:23:LYS:NZ	2.13	0.63
36:Af:45:LYS:HA	36:Af:107:PRO:CG	2.29	0.63
37:Ag:28:ASN:ND2	48:A2:2616:U:OP1	2.31	0.63
41:Ak:38:CYS:SG	41:Ak:39:SER:N	2.72	0.63
49:B1:1275:G:OP1	49:B1:1506:A:N6	2.32	0.63
2:BA:149:ASN:ND2	2:BA:163:CYS:O	2.31	0.63
10:AE:140:LEU:HD11	10:AE:167:GLN:HG2	1.80	0.63
30:AZ:26:VAL:O	30:AZ:93:LYS:NZ	2.30	0.63
49:B1:1822:A:H3'	49:B1:1823:A:H2'	1.80	0.63
56:BJ:131:ARG:HH21	56:BJ:145:PRO:HG2	1.63	0.63
65:BS:88:LYS:HB2	65:BS:88:LYS:HZ2	1.63	0.63
25:AU:97:ARG:NH1	48:A2:2605:U:O4	2.32	0.63
36:Af:45:LYS:HA	36:Af:107:PRO:HG2	1.78	0.63
23:AS:170:LYS:CD	48:A2:4832:A:C5'	2.76	0.63
49:B1:1307:U:H1'	78:Bf:135:HIS:HD1	1.63	0.63
49:B1:1307:U:O2	78:Bf:135:HIS:ND1	2.32	0.63
1:AA:192:LYS:HB3	1:AA:193:ARG:HE	1.64	0.62
48:A2:2458:G:H2'	48:A2:2459:G:H8	1.63	0.62
49:B1:392:A:O2'	58:BL:83:GLN:NE2	2.31	0.62
49:B1:1152:U:H1'	69:BW:16:ASN:HD21	1.63	0.62
5:AC:144:ILE:HG22	5:AC:147:VAL:CG2	2.29	0.62
21:AQ:11:ARG:NH2	48:A2:1671:G:OP1	2.29	0.62
32:Ab:110:ALA:C	32:Ab:115:GLY:CA	2.48	0.62
49:B1:1281:G:N7	49:B1:1283:C:N4	2.47	0.62
79:Bg:97:THR:HG23	79:Bg:97:THR:O	1.99	0.62
9:AD:155:THR:HG22	9:AD:179:ARG:HD3	1.80	0.62
14:AI:48:LEU:HD23	14:AI:142:LEU:HD12	1.81	0.62
7:A3:39:G:O2'	7:A3:103:A:N6	2.33	0.62
25:AU:64:GLU:HB2	25:AU:71:THR:HB	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A2:416:C:H2'	48:A2:417:G:H8	1.63	0.62
48:A2:1650:A:HO2'	48:A2:1668:C:HO2'	1.46	0.62
49:B1:1065:G:OP1	61:BO:149:ARG:NH2	2.32	0.62
53:BG:138:ALA:HB3	53:BG:178:ARG:HB2	1.80	0.62
5:AC:83:GLY:O	82:A:8:LEU:CB	2.47	0.62
8:A4:59:G:H4'	9:AD:267:ASN:HD21	1.65	0.62
17:AM:71:LYS:NZ	48:A2:727:C:OP2	2.33	0.62
48:A2:904:A:N3	48:A2:905:G:N2	2.46	0.62
49:B1:121:U:OP1	51:BE:77:ARG:NH1	2.33	0.62
58:BL:6:THR:OG1	58:BL:8:ARG:NH1	2.33	0.62
1:AA:54:ARG:NH2	48:A2:3651:U:OP1	2.32	0.62
2:BA:11:LYS:HE3	2:BA:13:GLU:HB3	1.82	0.62
5:AC:144:ILE:CA	5:AC:147:VAL:HG23	2.25	0.62
8:A4:105:C:OP2	14:AI:203:ARG:NH1	2.32	0.62
14:AI:31:ILE:HD12	14:AI:34:PHE:HE1	1.64	0.62
23:AS:95:ARG:NE	23:AS:97:TYR:OH	2.32	0.62
35:Ae:36:ARG:NH2	48:A2:2301:G:OP1	2.32	0.62
38:Ah:112:ARG:NH1	48:A2:171:C:O2	2.32	0.62
49:B1:382:C:H41	55:BI:5:ARG:HH22	1.46	0.62
65:BS:88:LYS:HA	65:BS:95:TYR:HE1	1.64	0.62
50:BD:172:VAL:HG22	50:BD:185:LYS:HG2	1.82	0.62
64:BR:77:GLU:O	64:BR:80:ARG:HB3	2.00	0.62
13:AH:79:ASN:ND2	48:A2:4652:G:OP1	2.33	0.62
16:AL:133:ALA:HB2	16:AL:136:LYS:HE3	1.80	0.62
21:AQ:75:ARG:NH2	48:A2:1439:G:O2'	2.33	0.62
32:Ab:112:ILE:HA	48:A2:1254:G:N3	2.14	0.62
45:Ao:44:LYS:NZ	48:A2:91:G:OP1	2.32	0.62
14:AI:110:ARG:NH1	48:A2:4403:A:OP2	2.33	0.62
17:AM:42:CYS:HB2	17:AM:77:TRP:CZ2	2.31	0.62
49:B1:1324:G:H21	49:B1:1510:G:H5'	1.64	0.62
52:BF:34:SER:HB3	52:BF:146:ARG:HH22	1.65	0.62
62:BP:36:LEU:O	65:BS:88:LYS:CD	2.44	0.61
5:AC:235:LEU:HD22	5:AC:240:LEU:HD11	1.82	0.61
17:AM:41:PRO:HB3	17:AM:70:GLN:HE21	1.65	0.61
22:AR:8:LYS:HD2	22:AR:23:TRP:HE1	1.66	0.61
49:B1:228:C:N4	49:B1:886:A:N3	2.47	0.61
49:B1:650:A:OP2	70:BX:107:ARG:NH1	2.32	0.61
49:B1:1282:A:OP2	59:BM:102:LYS:NZ	2.32	0.61
52:BF:56:TYR:O	52:BF:63:LYS:NZ	2.29	0.61
50:BD:49:ILE:HG12	50:BD:87:TYR:HB2	1.82	0.61
78:Bf:127:GLY:HA2	78:Bf:130:VAL:HB	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AF:155:TYR:OH	11:AF:188:GLU:OE2	2.18	0.61
32:Ab:116:LEU:HD13	32:Ab:116:LEU:N	2.15	0.61
59:BM:32:ALA:HB2	59:BM:112:LYS:HE3	1.81	0.61
5:AC:146:GLU:OE1	5:AC:146:GLU:N	2.33	0.61
17:AM:46:ARG:HH12	48:A2:925:C:H4'	1.65	0.61
49:B1:639:C:OP1	77:Be:41:ARG:NH2	2.33	0.61
49:B1:851:C:H5''	49:B1:852:G:H5'	1.83	0.61
4:BB:100:PHE:CD2	4:BB:217:MET:HE1	2.25	0.61
31:Aa:114:LYS:O	31:Aa:136:LYS:NZ	2.33	0.61
48:A2:117:C:H42	48:A2:152:C:H42	1.47	0.61
75:Bc:44:ARG:NH1	75:Bc:63:ARG:O	2.33	0.61
13:AH:186:THR:O	13:AH:189:GLN:NE2	2.34	0.61
15:AJ:147:ARG:HB3	15:AJ:147:ARG:CZ	2.30	0.61
48:A2:963:G:H1	48:A2:1261:C:H42	1.49	0.61
49:B1:187:G:N7	49:B1:213:G:N2	2.49	0.61
49:B1:1144:A:N3	49:B1:1199:A:O2'	2.33	0.61
63:BQ:42:ILE:HB	63:BQ:45:ARG:HH21	1.64	0.61
69:BW:90:GLN:OE1	69:BW:97:ARG:NH2	2.33	0.61
31:Aa:148:ALA:HB2	39:Ai:6:PRO:HB2	1.82	0.61
34:Ad:57:MET:O	34:Ad:90:ARG:NH1	2.33	0.61
49:B1:1206:G:H1	49:B1:1692:U:H3	1.48	0.61
68:BV:40:ASP:HB3	68:BV:41:LYS:HD3	1.83	0.61
8:A4:2:U:OP1	9:AD:267:ASN:ND2	2.34	0.61
20:AP:27:LYS:NZ	48:A2:2339:A:O2'	2.34	0.61
48:A2:1579:G:N2	85:A:101:MVM:O1	2.32	0.61
60:BN:99:ARG:NH2	60:BN:119:GLU:OE2	2.34	0.61
49:B1:145:G:O6	53:BG:178:ARG:NH2	2.34	0.61
49:B1:990:A:OP2	73:Ba:37:LYS:NZ	2.34	0.61
64:BR:74:GLN:O	64:BR:78:ARG:N	2.34	0.61
3:AB:175:GLN:HE21	3:AB:177:LYS:HB3	1.66	0.60
6:BC:173:LYS:HE3	68:BV:3:ASN:HA	1.81	0.60
23:AS:140:PRO:HA	23:AS:143:LYS:HB3	1.82	0.60
31:Aa:91:ALA:HB2	31:Aa:120:GLN:HE21	1.61	0.60
47:At:87:ARG:NH1	48:A2:682:U:OP1	2.33	0.60
48:A2:4666:C:H2'	48:A2:4667:A:H8	1.64	0.60
49:B1:1225:U:H1'	63:BQ:142:GLN:HE22	1.65	0.60
3:AB:225:GLY:HA3	48:A2:4935:A:H5''	1.83	0.60
17:AM:40:GLY:CA	17:AM:45:VAL:HG12	2.32	0.60
4:BB:101:HIS:O	4:BB:217:MET:CG	2.50	0.60
5:AC:114:ARG:NH2	48:A2:1340:C:O2'	2.33	0.60
30:AZ:33:THR:HB	30:AZ:36:ARG:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:BV:17:CYS:SG	68:BV:18:SER:N	2.75	0.60
1:AA:117:GLU:HB2	1:AA:162:ASN:HB2	1.83	0.60
4:BB:100:PHE:HE2	4:BB:217:MET:HE1	1.50	0.60
5:AC:323:ARG:NH1	48:A2:962:C:O2	2.34	0.60
48:A2:445:C:H2'	48:A2:1277:A:H1'	1.83	0.60
48:A2:1921:G:N2	48:A2:4397:U:OP1	2.34	0.60
49:B1:524:U:H3	49:B1:594:A:H62	1.48	0.60
49:B1:681:U:H4'	70:BX:9:THR:HG22	1.83	0.60
62:BP:18:ARG:CD	65:BS:88:LYS:HD3	2.31	0.60
67:BU:62:ARG:HG2	67:BU:81:GLN:HG2	1.83	0.60
73:Ba:23:CYS:SG	73:Ba:24:THR:N	2.74	0.60
9:AD:111:ASN:HD21	9:AD:252:VAL:HG12	1.67	0.60
15:AJ:113:ILE:HA	15:AJ:117:ILE:HD12	1.82	0.60
16:AL:5:ARG:NH1	48:A2:1666:A:OP2	2.34	0.60
55:BI:11:ARG:NH1	55:BI:15:GLY:O	2.33	0.60
60:BN:15:ALA:HB2	74:Bb:21:LYS:HE3	1.84	0.60
62:BP:18:ARG:HD2	65:BS:88:LYS:HD3	1.83	0.60
7:A3:36:G:C8	38:Ah:89:ARG:CD	2.79	0.60
14:AI:14:ASN:ND2	48:A2:1845:G:OP2	2.33	0.60
39:Ai:29:ARG:HD2	39:Ai:32:ARG:HG3	1.83	0.60
63:BQ:102:GLU:HB2	79:Bg:55:PRO:HB2	1.83	0.60
64:BR:97:GLU:CA	64:BR:117:LEU:HD23	2.31	0.60
10:AE:181:LEU:O	48:A2:4841:C:N4	2.33	0.60
23:AS:170:LYS:HG2	48:A2:4832:A:P	2.40	0.60
29:AY:59:ARG:NH1	48:A2:206:U:OP1	2.35	0.60
49:B1:1584:G:OP1	66:BT:77:LYS:NZ	2.33	0.60
59:BM:82:ASN:ND2	59:BM:107:SER:OG	2.34	0.60
79:Bg:23:THR:HG22	79:Bg:31:ILE:HG23	1.84	0.60
38:Ah:43:LYS:O	38:Ah:46:LYS:HB3	2.01	0.60
48:A2:1382:G:N2	48:A2:1402:G:O2'	2.35	0.60
48:A2:3903:U:H2'	48:A2:3904:G:H8	1.67	0.60
49:B1:525:A:N6	49:B1:587:A:O2'	2.35	0.60
49:B1:878:G:H22	49:B1:908:A:H2	1.49	0.60
57:BK:65:ARG:NH2	76:Bd:20:SER:OG	2.35	0.60
3:AB:336:CYS:HG	48:A2:4587:C:HO2'	1.50	0.60
48:A2:1373:G:N2	48:A2:1376:G:OP2	2.35	0.60
48:A2:2693:G:H2'	48:A2:2694:G:H8	1.66	0.60
48:A2:4355:G:N2	48:A2:4358:A:OP2	2.35	0.60
79:Bg:30:MET:HG3	79:Bg:44:LYS:HG2	1.84	0.60
1:AA:3:ARG:HD2	1:AA:208:GLU:HG2	1.84	0.59
5:AC:100:ARG:NH2	48:A2:1503:C:OP1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AM:46:ARG:HH12	48:A2:925:C:C4'	2.15	0.59
40:Aj:56:ARG:NH2	48:A2:369:G:N7	2.44	0.59
49:B1:810:A:N7	49:B1:851:C:N4	2.50	0.59
49:B1:1406:G:N2	49:B1:1442:U:O4	2.34	0.59
58:BL:13:GLN:HE21	58:BL:18:GLN:HE21	1.48	0.59
64:BR:79:GLU:O	64:BR:82:ASP:N	2.35	0.59
1:AA:226:ARG:HB3	48:A2:3677:C:H5''	1.84	0.59
2:BA:210:ILE:O	2:BA:214:GLU:N	2.33	0.59
22:AR:44:LEU:HD22	22:AR:49:LEU:HD12	1.84	0.59
48:A2:4315:U:H5'	48:A2:4316:U:H5'	1.82	0.59
62:BP:51:ARG:HD2	62:BP:55:SER:HB2	1.82	0.59
79:Bg:195:LEU:HA	79:Bg:211:GLY:HA3	1.84	0.59
10:AE:153:LEU:CD1	36:Af:105:LEU:O	2.49	0.59
48:A2:463:C:N4	48:A2:680:C:O2	2.35	0.59
2:BA:172:GLY:HA3	2:BA:203:PHE:HA	1.84	0.59
4:BB:182:LYS:O	4:BB:186:ASN:ND2	2.35	0.59
10:AE:156:ARG:O	10:AE:158:ARG:NH1	2.34	0.59
48:A2:2618:U:O2'	48:A2:2673:G:N1	2.31	0.59
79:Bg:107:ASP:OD2	79:Bg:125:ARG:NH1	2.34	0.59
5:AC:47:ASN:ND2	48:A2:1356:A:OP1	2.36	0.59
40:Aj:13:ASN:HD21	48:A2:1600:G:H5''	1.67	0.59
49:B1:466:G:O2'	53:BG:72:ARG:NH1	2.34	0.59
35:Ae:14:LYS:NZ	48:A2:2297:G:OP1	2.35	0.59
56:BJ:136:ARG:HH21	56:BJ:139:LYS:CA	2.12	0.59
32:Ab:112:ILE:C	32:Ab:112:ILE:CG2	2.75	0.59
35:Ae:90:MET:HG2	47:At:33:LYS:HG2	1.83	0.59
48:A2:1721:G:N3	48:A2:1724:A:N6	2.51	0.59
64:BR:73:LEU:O	64:BR:77:GLU:CB	2.50	0.59
3:AB:117:ARG:NH1	48:A2:4943:U:OP1	2.35	0.59
10:AE:152:ILE:HD12	10:AE:189:THR:HG21	1.85	0.59
12:AG:66:GLN:HA	12:AG:69:ILE:HD12	1.85	0.59
16:AL:11:LYS:NZ	48:A2:95:G:N7	2.49	0.59
23:AS:81:TRP:HB3	23:AS:127:MET:HE3	1.84	0.59
48:A2:489:C:N3	48:A2:654:G:N2	2.51	0.59
48:A2:4064:G:O2'	48:A2:4066:C:N4	2.36	0.59
49:B1:1618:C:O2'	62:BP:50:ARG:NH2	2.35	0.59
56:BJ:47:LYS:O	56:BJ:51:ALA:N	2.35	0.59
16:AL:129:ARG:HH12	38:Ah:117:ARG:HA	1.67	0.59
32:Ab:116:LEU:HA	48:A2:1253:A:N3	2.17	0.59
42:Al:2:SER:N	48:A2:2386:G:O6	2.36	0.59
43:Am:114:LYS:NZ	48:A2:4447:C:O2'	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:BE:11:ARG:NH1	51:BE:21:ASP:O	2.34	0.59
10:AE:162:VAL:HG12	10:AE:175:VAL:HG12	1.84	0.59
30:AZ:95:VAL:HG11	30:AZ:113:GLU:HG3	1.83	0.59
48:A2:1817:G:OP2	48:A2:1817:G:N2	2.34	0.59
48:A2:2580:A:N6	48:A2:2723:A:OP2	2.36	0.59
49:B1:1611:G:O2'	65:BS:87:GLN:CA	2.51	0.59
52:BF:126:THR:OG1	75:Bc:26:GLN:NE2	2.36	0.59
79:Bg:79:LEU:HD11	79:Bg:120:ILE:HD13	1.85	0.59
5:AC:50:GLN:NE2	48:A2:341:A:O2'	2.36	0.58
39:Ai:66:ASP:OD1	39:Ai:87:ARG:NH1	2.36	0.58
48:A2:2474:U:H2'	48:A2:2475:G:H8	1.68	0.58
49:B1:643:A:OP2	56:BJ:39:ASN:ND2	2.36	0.58
49:B1:832:G:O6	49:B1:842:C:N4	2.36	0.58
7:A3:109:C:H2'	40:Aj:20:ARG:HH22	1.68	0.58
8:A4:62:U:H5'	9:AD:279:ARG:HH12	1.68	0.58
10:AE:177:GLY:HA3	10:AE:184:VAL:HB	1.83	0.58
19:AO:188:LYS:HA	19:AO:191:LYS:HB2	1.85	0.58
44:An:21:ARG:NH1	49:B1:1174:U:OP1	2.36	0.58
49:B1:1387:G:N1	50:BD:206:ASP:OD1	2.36	0.58
49:B1:1591:C:H5''	52:BF:85:LYS:HD3	1.84	0.58
59:BM:63:LYS:HA	59:BM:66:GLU:HG2	1.85	0.58
1:AA:2:GLY:N	48:A2:4147:G:OP1	2.36	0.58
23:AS:170:LYS:CG	48:A2:4832:A:OP2	2.51	0.58
48:A2:1602:U:HO2'	48:A2:2429:G:HO2'	1.49	0.58
48:A2:4016:A:O2'	48:A2:4017:A:N7	2.35	0.58
49:B1:1460:C:H42	49:B1:1466:G:H1	1.50	0.58
49:B1:1540:G:H2'	49:B1:1541:G:H8	1.68	0.58
49:B1:1614:A:OP2	62:BP:42:ARG:NH2	2.36	0.58
54:BH:126:HIS:O	54:BH:177:TYR:OH	2.19	0.58
79:Bg:168:CYS:HA	79:Bg:174:VAL:HA	1.85	0.58
15:AJ:136:ARG:NH1	15:AJ:155:HIS:O	2.36	0.58
17:AM:94:LYS:NZ	48:A2:4829:C:OP2	2.36	0.58
27:AW:6:CYS:SG	27:AW:9:SER:OG	2.59	0.58
32:Ab:41:ARG:NH1	48:A2:1474:G:O2'	2.37	0.58
36:Af:96:ALA:HA	36:Af:99:HIS:HD2	1.67	0.58
45:Ao:3:ASN:ND2	45:Ao:93:LEU:O	2.36	0.58
48:A2:1976:G:O6	48:A2:1981:G:N2	2.37	0.58
57:BK:24:LYS:HE2	57:BK:33:PRO:HB3	1.84	0.58
7:A3:122:G:N2	7:A3:129:C:O2'	2.35	0.58
11:AF:232:ASP:O	11:AF:236:ARG:NH2	2.35	0.58
48:A2:2374:A:O2'	48:A2:2786:A:OP2	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:B1:1622:U:OP1	65:BS:120:HIS:NE2	2.37	0.58
3:AB:116:ARG:O	3:AB:177:LYS:HE3	2.03	0.58
4:BB:214:LYS:NZ	49:B1:943:U:OP1	2.36	0.58
7:A3:46:G:OP1	42:AI:18:LYS:NZ	2.34	0.58
24:AT:84:ILE:CD1	32:Ab:23:LYS:NZ	2.67	0.58
25:AU:81:ARG:NH2	48:A2:2600:A:N7	2.43	0.58
32:Ab:115:GLY:C	48:A2:1254:G:C8	2.82	0.58
48:A2:116:G:H1	48:A2:153:G:H22	1.51	0.58
60:BN:46:THR:HG22	60:BN:48:SER:H	1.68	0.58
3:AB:343:ARG:NH2	48:A2:4935:A:OP1	2.37	0.58
14:AI:98:ARG:HB3	14:AI:120:GLY:HA3	1.86	0.58
29:AY:54:GLU:HB2	29:AY:108:ARG:HB2	1.85	0.58
37:Ag:63:VAL:HG13	37:Ag:66:ARG:HH21	1.69	0.58
48:A2:4284:G:N2	48:A2:4287:A:OP2	2.30	0.58
49:B1:1754:G:H22	49:B1:1777:G:H22	1.52	0.58
67:BU:66:ARG:HH22	67:BU:75:LYS:HG2	1.69	0.58
79:Bg:109:LEU:HG	79:Bg:125:ARG:HH21	1.68	0.58
3:AB:4:ARG:NH1	3:AB:6:PHE:O	2.36	0.58
6:BC:227:ARG:HH12	49:B1:663:C:H4'	1.68	0.58
13:AH:23:ARG:NH1	48:A2:4726:A:OP1	2.36	0.58
33:Ac:51:ASN:ND2	33:Ac:77:ASN:OD1	2.36	0.58
48:A2:2022:A:N7	48:A2:4396:C:O2'	2.36	0.58
3:AB:282:LYS:NZ	3:AB:336:CYS:O	2.36	0.58
14:AI:184:MET:SD	14:AI:189:ARG:CD	2.84	0.58
49:B1:46:A:N7	49:B1:97:U:O2'	2.37	0.58
49:B1:1636:G:O3'	52:BF:164:ARG:NH2	2.37	0.58
3:AB:59:GLU:HB2	3:AB:366:LYS:HE3	1.85	0.58
3:AB:238:LYS:NZ	48:A2:3815:U:OP1	2.32	0.58
22:AR:116:ASP:N	22:AR:116:ASP:OD1	2.35	0.58
23:AS:101:THR:HG23	23:AS:104:GLY:H	1.69	0.58
48:A2:2507:G:H4'	48:A2:2762:A:H4'	1.86	0.58
49:B1:1611:G:OP2	65:BS:121:ARG:NH2	2.37	0.58
55:BI:57:ALA:H	55:BI:180:GLY:HA2	1.68	0.58
58:BL:22:ARG:NH2	58:BL:31:GLU:O	2.37	0.58
58:BL:69:ARG:HH22	58:BL:132:ARG:HA	1.69	0.58
59:BM:51:VAL:HB	59:BM:109:VAL:HB	1.85	0.58
60:BN:3:ARG:NH1	60:BN:10:GLY:O	2.33	0.58
10:AE:156:ARG:NH2	48:A2:4897:C:OP2	2.37	0.57
21:AQ:82:VAL:HG22	21:AQ:139:LEU:HB2	1.84	0.57
22:AR:71:ARG:NH2	48:A2:3576:C:OP1	2.37	0.57
48:A2:3624:A:N6	48:A2:3662:G:O2'	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:B1:1218:C:O2'	75:Bc:24:GLN:NE2	2.36	0.57
5:AC:45:ARG:NH2	48:A2:2274:C:O2'	2.33	0.57
36:Af:36:ARG:HB2	36:Af:80:ASN:HA	1.86	0.57
44:An:10:MET:HE2	49:B1:1172:U:H4'	1.85	0.57
48:A2:2035:U:O2	48:A2:2037:G:N2	2.37	0.57
49:B1:996:A:OP1	60:BN:114:ARG:NH2	2.37	0.57
64:BR:24:LEU:O	79:Bg:212:LYS:NZ	2.37	0.57
9:AD:33:ARG:HE	9:AD:37:VAL:HG21	1.68	0.57
26:AV:69:LYS:HB2	26:AV:72:LEU:HD13	1.85	0.57
30:AZ:26:VAL:HG11	30:AZ:91:LEU:HD23	1.86	0.57
74:Bb:11:SER:OG	74:Bb:13:GLU:OE1	2.21	0.57
4:BB:65:ARG:HD3	61:BO:48:SER:HB2	1.85	0.57
4:BB:98:THR:OG1	4:BB:99:ASN:N	2.38	0.57
16:AL:124:LEU:HA	38:Ah:121:VAL:HG12	1.86	0.57
10:AE:96:VAL:HG13	10:AE:101:ASN:HB3	1.86	0.57
33:Ac:17:ARG:NH1	33:Ac:103:ASP:OD1	2.37	0.57
48:A2:3894:A:OP2	48:A2:4145:G:N2	2.37	0.57
49:B1:880:G:OP2	49:B1:880:G:N2	2.36	0.57
49:B1:1208:A:H2'	49:B1:1209:A:H8	1.69	0.57
19:AO:163:LYS:NZ	48:A2:4867:A:OP1	2.37	0.57
32:Ab:116:LEU:HB3	48:A2:1253:A:H2	1.60	0.57
49:B1:218:U:O2	55:BI:184:ARG:NH2	2.35	0.57
49:B1:1611:G:O3'	65:BS:87:GLN:CB	2.53	0.57
49:B1:1644:C:H4'	63:BQ:140:ARG:HB2	1.86	0.57
49:B1:1860:A:OP2	73:Ba:10:ARG:NH1	2.37	0.57
50:BD:7:LYS:HG3	67:BU:25:THR:HG21	1.87	0.57
38:Ah:80:PRO:HD2	38:Ah:83:LEU:HD12	1.85	0.57
49:B1:1083:A:N7	49:B1:1841:C:O2'	2.36	0.57
54:BH:30:LEU:O	54:BH:34:SER:OG	2.22	0.57
79:Bg:44:LYS:HG3	79:Bg:56:GLN:HG3	1.87	0.57
7:A3:65:A:O2'	38:Ah:10:ARG:NH2	2.38	0.57
9:AD:15:ARG:O	9:AD:17:GLN:NE2	2.38	0.57
15:AJ:18:ARG:NH2	15:AJ:143:ASP:OD2	2.37	0.57
16:AL:28:GLN:OE1	18:AN:202:ARG:NH1	2.37	0.57
49:B1:315:C:OP1	53:BG:177:GLN:NE2	2.37	0.57
50:BD:72:VAL:HG22	57:BK:20:VAL:HG11	1.86	0.57
59:BM:58:GLU:HB2	59:BM:61:TYR:HB2	1.86	0.57
5:AC:268:ARG:NH2	48:A2:487:G:OP1	2.37	0.57
16:AL:49:ARG:HH11	38:Ah:118:LYS:CA	2.08	0.57
19:AO:46:ASN:O	19:AO:50:ASN:ND2	2.37	0.57
48:A2:4938:C:OP2	48:A2:4939:G:N2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:B1:358:C:H5''	70:BX:18:ARG:HD2	1.86	0.57
49:B1:934:G:OP2	49:B1:993:G:N2	2.35	0.57
49:B1:1629:C:OP1	65:BS:39:ARG:NH1	2.36	0.57
9:AD:60:ILE:HG12	9:AD:80:ALA:HB2	1.87	0.57
16:AL:135:LYS:N	16:AL:135:LYS:HD2	2.20	0.57
21:AQ:156:PRO:HG2	31:Aa:48:TYR:HA	1.86	0.57
48:A2:4692:C:H1'	48:A2:4693:G:H2'	1.87	0.57
49:B1:39:A:H5''	56:BJ:7:TRP:HE1	1.70	0.57
22:AR:98:ARG:NH2	22:AR:132:PHE:O	2.38	0.56
49:B1:691:G:N2	49:B1:740:C:O2	2.37	0.56
50:BD:16:ILE:HD11	76:Bd:36:LEU:HD12	1.86	0.56
3:AB:62:ARG:NH2	48:A2:4579:G:OP2	2.25	0.56
4:BB:159:GLN:OE1	4:BB:162:ARG:NH1	2.37	0.56
13:AH:106:GLN:HG2	13:AH:107:GLU:HG2	1.87	0.56
17:AM:5:ARG:NH1	17:AM:59:ASP:OD1	2.37	0.56
25:AU:105:ASN:ND2	25:AU:111:GLU:OE1	2.38	0.56
26:AV:107:ASN:OD1	26:AV:110:GLY:N	2.38	0.56
39:Ai:65:LYS:HG3	39:Ai:67:LYS:H	1.70	0.56
48:A2:3875:G:H21	82:A:18:GLY:CA	2.09	0.56
66:BT:7:LYS:HE3	66:BT:62:ARG:HH21	1.70	0.56
70:BX:67:ARG:NH2	70:BX:114:ASP:OD2	2.33	0.56
17:AM:46:ARG:HH11	48:A2:924:U:H4'	0.74	0.56
18:AN:91:GLN:HB2	45:Ao:48:TYR:HE2	1.70	0.56
22:AR:7:GLN:NE2	22:AR:35:ALA:O	2.37	0.56
48:A2:1451:C:H2'	48:A2:1452:G:H8	1.69	0.56
48:A2:2072:G:O2'	48:A2:2241:G:N2	2.37	0.56
48:A2:4199:C:OP1	48:A2:4289:C:O2'	2.23	0.56
49:B1:801:U:O4	54:BH:106:ARG:NH2	2.38	0.56
49:B1:1209:A:H5'	49:B1:1835:A:H61	1.70	0.56
49:B1:1212:G:H1	49:B1:1687:C:H42	1.52	0.56
49:B1:1495:G:H21	76:Bd:42:CYS:HB3	1.69	0.56
51:BE:197:ASN:ND2	51:BE:198:ARG:O	2.39	0.56
52:BF:110:GLN:HE21	52:BF:114:ASN:HD21	1.53	0.56
53:BG:64:LYS:NZ	53:BG:65:GLN:O	2.35	0.56
64:BR:28:PHE:HA	64:BR:55:THR:HG21	1.86	0.56
2:BA:85:ARG:HH21	2:BA:201:LEU:HA	1.69	0.56
3:AB:170:LEU:O	3:AB:328:ASN:ND2	2.36	0.56
10:AE:141:ARG:N	10:AE:191:GLN:NE2	2.52	0.56
10:AE:222:LEU:O	10:AE:235:THR:OG1	2.22	0.56
49:B1:1286:G:N2	49:B1:1312:G:O6	2.39	0.56
49:B1:1864:U:OP2	73:Ba:4:LYS:NZ	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:BF:100:ILE:HB	52:BF:108:PRO:HB3	1.86	0.56
49:B1:1016:U:OP2	74:Bb:20:LYS:NZ	2.33	0.56
79:Bg:282:GLU:HB3	79:Bg:284:PRO:HD2	1.88	0.56
1:AA:27:ALA:HB3	1:AA:128:ARG:HH21	1.71	0.56
2:BA:79:SER:O	2:BA:84:GLN:NE2	2.38	0.56
4:BB:70:SER:OG	61:BO:128:ARG:NH1	2.38	0.56
10:AE:140:LEU:CD1	10:AE:167:GLN:HB2	2.35	0.56
10:AE:264:ILE:HB	10:AE:267:LEU:HB2	1.88	0.56
49:B1:986:G:OP2	49:B1:988:C:N4	2.38	0.56
49:B1:1283:C:O2'	49:B1:1313:A:N1	2.38	0.56
22:AR:97:ARG:NH2	48:A2:2704:A:OP1	2.38	0.56
30:AZ:36:ARG:NH2	48:A2:2559:U:OP1	2.38	0.56
31:Aa:27:LYS:NZ	48:A2:1500:A:OP1	2.34	0.56
40:Aj:11:ARG:NH1	48:A2:364:U:OP1	2.38	0.56
49:B1:635:G:OP1	77:Be:21:LYS:NZ	2.38	0.56
51:BE:179:ASN:HB2	51:BE:195:ILE:HD12	1.86	0.56
66:BT:65:TYR:HE1	66:BT:128:GLN:HE22	1.53	0.56
74:Bb:15:GLU:O	74:Bb:23:ARG:NH1	2.39	0.56
5:AC:199:ARG:NH2	48:A2:344:C:OP2	2.38	0.56
11:AF:131:ASN:ND2	48:A2:1709:U:OP1	2.38	0.56
21:AQ:65:ARG:NH2	48:A2:1441:A:OP1	2.38	0.56
42:Al:2:SER:N	48:A2:2385:G:N7	2.54	0.56
49:B1:94:G:HO2'	49:B1:508:A:HO2'	1.52	0.56
49:B1:925:G:OP1	60:BN:121:ARG:NH1	2.39	0.56
49:B1:1050:A:H5'	49:B1:1846:G:H21	1.70	0.56
54:BH:52:GLU:HA	54:BH:58:LYS:HA	1.88	0.56
8:A4:63:C:H5'	8:A4:64:G:H5''	1.88	0.56
16:AL:74:ARG:HH12	48:A2:76:A:H8	1.54	0.56
18:AN:12:ARG:NH1	48:A2:273:A:N7	2.54	0.56
32:Ab:27:GLN:NE2	48:A2:1444:A:C1'	2.69	0.56
39:Ai:76:ARG:NH1	48:A2:299:A:OP1	2.37	0.56
48:A2:457:A:H61	48:A2:685:C:H42	1.53	0.56
49:B1:315:C:H2'	49:B1:316:G:H8	1.71	0.56
49:B1:1402:A:N6	49:B1:1441:U:O2'	2.39	0.56
51:BE:127:ARG:HH21	51:BE:142:HIS:HB2	1.71	0.56
66:BT:71:GLY:H	66:BT:74:SER:HB2	1.70	0.56
5:AC:315:LYS:HD2	11:AF:168:ALA:HB1	1.88	0.56
22:AR:64:ARG:NE	48:A2:2595:C:OP1	2.39	0.56
39:Ai:28:ARG:NH2	48:A2:320:C:OP2	2.39	0.56
47:At:33:LYS:NZ	48:A2:2244:G:OP1	2.39	0.56
49:B1:691:G:O6	49:B1:738:C:N4	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:B1:1156:U:OP1	69:BW:71:LYS:NZ	2.35	0.56
49:B1:1392:U:H2'	49:B1:1393:G:H8	1.71	0.56
10:AE:161:ARG:NH1	10:AE:273:SER:OG	2.39	0.55
16:AL:40:GLN:O	16:AL:44:ARG:NE	2.37	0.55
17:AM:7:VAL:HG12	17:AM:57:LEU:HD21	1.88	0.55
24:AT:22:HIS:ND1	48:A2:4240:C:OP2	2.39	0.55
30:AZ:51:ARG:HB2	30:AZ:65:ARG:HD2	1.89	0.55
48:A2:130:C:N4	48:A2:137:G:O6	2.39	0.55
48:A2:3688:A:OP2	48:A2:3706:G:N2	2.39	0.55
49:B1:1233:G:N3	49:B1:1252:C:O2'	2.36	0.55
49:B1:1554:C:H1'	50:BD:76:ARG:HH21	1.71	0.55
50:BD:14:ASP:HA	50:BD:17:PHE:HB3	1.88	0.55
56:BJ:138:ARG:NE	56:BJ:153:SER:HA	2.21	0.55
3:AB:19:ARG:NH2	48:A2:4585:G:OP1	2.38	0.55
15:AJ:150:CYS:SG	15:AJ:151:ILE:N	2.80	0.55
18:AN:31:ARG:NH1	18:AN:124:ASP:OD2	2.39	0.55
49:B1:1219:C:O2'	75:Bc:26:GLN:OE1	2.25	0.55
3:AB:71:GLU:OE2	3:AB:366:LYS:NZ	2.39	0.55
15:AJ:57:VAL:HG12	15:AJ:59:SER:H	1.70	0.55
16:AL:2:ALA:HB1	48:A2:1496:U:H5''	1.88	0.55
18:AN:169:ARG:NH1	48:A2:63:G:OP2	2.37	0.55
21:AQ:32:TYR:HE2	21:AQ:123:PHE:HB3	1.71	0.55
48:A2:1393:U:O2'	48:A2:1797:G:N2	2.39	0.55
48:A2:4883:U:O2'	48:A2:4885:G:N2	2.39	0.55
49:B1:230:A:H5''	49:B1:889:U:H1'	1.88	0.55
49:B1:431:G:H2'	49:B1:432:G:H8	1.71	0.55
3:AB:222:VAL:O	3:AB:343:ARG:NH1	2.39	0.55
4:BB:151:ARG:NH1	4:BB:153:THR:OG1	2.39	0.55
10:AE:65:ARG:NH1	48:A2:1053:G:OP2	2.38	0.55
12:AG:164:ILE:HD12	18:AN:22:LEU:HD11	1.88	0.55
26:AV:51:ARG:NH1	48:A2:3814:C:OP1	2.39	0.55
31:Aa:123:ILE:HG12	31:Aa:143:ALA:HB3	1.88	0.55
48:A2:4592:G:H1	48:A2:4630:U:H3	1.54	0.55
48:A2:4854:G:N2	48:A2:4883:U:O2	2.34	0.55
49:B1:152:U:O2'	53:BG:132:ARG:NH2	2.40	0.55
49:B1:1179:G:N2	49:B1:1182:A:OP2	2.39	0.55
65:BS:120:HIS:HA	65:BS:123:LEU:HB2	1.87	0.55
35:Ae:22:ARG:HD3	35:Ae:31:ILE:HG23	1.88	0.55
42:Al:3:SER:OG	48:A2:2763:C:N4	2.39	0.55
48:A2:3875:G:N2	82:A:18:GLY:HA3	2.08	0.55
49:B1:1208:A:H2'	49:B1:1209:A:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:B1:1490:G:N2	67:BU:72:GLU:OE1	2.39	0.55
59:BM:32:ALA:HB3	59:BM:110:VAL:HB	1.88	0.55
3:AB:316:PRO:HA	3:AB:370:THR:HB	1.89	0.55
14:AI:98:ARG:NH2	48:A2:1846:G:OP2	2.32	0.55
19:AO:54:TYR:OH	19:AO:73:PHE:O	2.25	0.55
24:AT:13:TYR:OH	48:A2:1772:U:OP2	2.24	0.55
32:Ab:112:ILE:CA	48:A2:1254:G:N3	2.69	0.55
38:Ah:112:ARG:NH2	48:A2:258:C:O2'	2.40	0.55
48:A2:2084:G:H2'	48:A2:2085:A:H8	1.71	0.55
48:A2:2541:G:N2	48:A2:2544:A:OP2	2.28	0.55
66:BT:63:HIS:HB3	66:BT:78:ILE:HD13	1.89	0.55
6:BC:145:LYS:HG3	6:BC:146:GLU:HG3	1.89	0.55
48:A2:2567:C:OP1	48:A2:2747:C:O2'	2.24	0.55
49:B1:1658:G:OP2	49:B1:1660:C:N4	2.39	0.55
54:BH:40:LEU:HD23	54:BH:43:LEU:HB3	1.88	0.55
71:BY:79:LEU:HD11	71:BY:96:LEU:HD21	1.89	0.55
72:BZ:88:LEU:HB3	72:BZ:109:TYR:HE2	1.70	0.55
3:AB:118:PHE:O	48:A2:4540:G:O2'	2.25	0.55
23:AS:16:CYS:SG	23:AS:17:LEU:N	2.78	0.55
32:Ab:112:ILE:CA	32:Ab:112:ILE:CG2	2.74	0.55
48:A2:161:G:H1	48:A2:266:U:H3	1.55	0.55
48:A2:1874:C:O2'	48:A2:1917:C:N3	2.39	0.55
49:B1:53:C:OP1	71:BY:112:ASN:ND2	2.37	0.55
59:BM:85:LEU:HA	59:BM:88:TRP:HB2	1.89	0.55
62:BP:53:GLN:HA	62:BP:83:MET:HE1	1.89	0.55
64:BR:62:GLN:HG3	79:Bg:280:LYS:HD3	1.88	0.55
79:Bg:87:LEU:HB2	79:Bg:101:PHE:HB2	1.89	0.55
9:AD:55:VAL:HG13	9:AD:60:ILE:HG22	1.89	0.55
9:AD:125:VAL:HG12	9:AD:196:ARG:HG3	1.89	0.55
45:Ao:43:ARG:NH2	48:A2:284:U:O4	2.40	0.55
47:At:28:GLU:OE1	47:At:41:ASN:ND2	2.40	0.55
49:B1:1416:C:N3	49:B1:1417:C:N4	2.54	0.55
49:B1:1467:C:OP1	64:BR:2:GLY:N	2.39	0.55
52:BF:59:LYS:HB3	52:BF:62:ARG:HB3	1.88	0.55
54:BH:30:LEU:HB3	54:BH:36:LEU:HD12	1.89	0.55
71:BY:5:VAL:HG11	71:BY:35:VAL:HG21	1.89	0.55
9:AD:211:LEU:HB3	9:AD:219:TYR:HB2	1.88	0.55
15:AJ:106:GLY:HA3	15:AJ:131:TYR:HA	1.89	0.55
16:AL:77:SER:HB3	16:AL:80:GLU:CD	2.30	0.55
19:AO:59:ARG:NH2	48:A2:4424:C:OP1	2.40	0.55
48:A2:3932:G:H1	48:A2:3934:A:H3'	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:B1:661:U:OP2	70:BX:3:LYS:NZ	2.40	0.55
65:BS:39:ARG:HH22	66:BT:39:LEU:HB3	1.70	0.55
69:BW:75:ILE:HD12	69:BW:125:ILE:HG21	1.89	0.55
70:BX:100:VAL:HG13	70:BX:122:VAL:HG13	1.88	0.55
79:Bg:128:THR:HG21	79:Bg:143:GLN:HE21	1.70	0.55
9:AD:152:ARG:NH1	9:AD:154:THR:OG1	2.39	0.54
14:AI:184:MET:CE	14:AI:190:LEU:HD11	2.34	0.54
16:AL:80:GLU:OE2	16:AL:102:ARG:NH1	2.34	0.54
16:AL:138:ASP:OD1	16:AL:140:SER:OG	2.25	0.54
24:AT:8:ARG:NH2	48:A2:4295:C:O2	2.40	0.54
48:A2:1869:A:N6	48:A2:3844:G:O2'	2.40	0.54
48:A2:1954:G:N2	48:A2:1975:C:O2	2.40	0.54
48:A2:4484:G:O2'	48:A2:4487:C:OP2	2.24	0.54
49:B1:1854:U:OP1	61:BO:150:ARG:NH1	2.39	0.54
56:BJ:138:ARG:CZ	56:BJ:153:SER:HA	2.37	0.54
70:BX:84:PHE:HB2	70:BX:118:VAL:HG11	1.88	0.54
2:BA:31:ASP:HB3	2:BA:34:MET:HG2	1.88	0.54
48:A2:2827:G:O2'	48:A2:3809:U:O4	2.25	0.54
9:AD:166:ALA:HB1	9:AD:171:LEU:HD12	1.89	0.54
15:AJ:145:LYS:HB3	15:AJ:145:LYS:NZ	2.22	0.54
37:Ag:113:SER:OG	37:Ag:114:GLN:N	2.40	0.54
41:Ak:33:LYS:NZ	48:A2:2672:G:OP2	2.40	0.54
47:At:28:GLU:HG3	47:At:31:ASN:HB2	1.88	0.54
48:A2:2341:U:H2'	48:A2:2342:A:H8	1.72	0.54
49:B1:1060:A:H4'	49:B1:1061:U:H5'	1.90	0.54
49:B1:1714:U:O2	49:B1:1820:G:N2	2.39	0.54
55:BI:142:SER:O	55:BI:146:GLN:N	2.36	0.54
57:BK:50:GLN:HA	57:BK:53:LYS:HE3	1.88	0.54
79:Bg:17:TRP:H	79:Bg:36:ARG:HB2	1.72	0.54
10:AE:187:ARG:NH2	48:A2:4899:G:O3'	2.40	0.54
20:AP:23:ARG:NH2	20:AP:125:MET:SD	2.79	0.54
27:AW:47:ARG:HB3	27:AW:58:LYS:HD2	1.89	0.54
35:Ae:66:THR:HB	35:Ae:69:MET:HG3	1.89	0.54
48:A2:225:C:H42	48:A2:236:C:H42	1.54	0.54
48:A2:451:G:N2	48:A2:691:G:H22	2.05	0.54
48:A2:2834:G:N2	48:A2:2837:A:N1	2.56	0.54
57:BK:81:ASP:OD1	59:BM:96:ARG:NH2	2.40	0.54
3:AB:246:ARG:NH2	48:A2:4520:U:OP2	2.40	0.54
4:BB:100:PHE:HD2	4:BB:217:MET:CE	2.05	0.54
48:A2:2499:C:H5	48:A2:2514:G:H1	1.55	0.54
49:B1:872:A:H2'	49:B1:874:G:H21	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:B1:1536:G:H4'	52:BF:81:ARG:HH21	1.72	0.54
57:BK:7:ASN:HD21	57:BK:40:VAL:HG21	1.71	0.54
9:AD:43:LYS:O	48:A2:1805:G:O2'	2.26	0.54
18:AN:12:ARG:HD2	48:A2:273:A:C5	2.42	0.54
52:BF:114:ASN:O	52:BF:118:ASN:ND2	2.41	0.54
57:BK:23:ALA:HB3	57:BK:67:PHE:HB2	1.89	0.54
59:BM:54:SER:HA	59:BM:62:VAL:HG11	1.88	0.54
9:AD:77:ALA:O	9:AD:108:ARG:NH1	2.38	0.54
9:AD:119:TYR:HE1	9:AD:135:ILE:H	1.54	0.54
47:At:66:ARG:NH1	48:A2:473:G:OP1	2.40	0.54
49:B1:1540:G:H2'	49:B1:1541:G:C8	2.42	0.54
49:B1:1668:U:OP1	67:BU:77:TRP:NE1	2.40	0.54
10:AE:125:LEU:H	48:A2:946:G:H21	1.56	0.54
14:AI:4:ARG:NH1	48:A2:1847:U:OP1	2.37	0.54
16:AL:107:THR:HA	16:AL:110:LEU:HB3	1.89	0.54
18:AN:172:ARG:O	18:AN:188:ARG:NH2	2.41	0.54
30:AZ:73:LYS:NZ	48:A2:2560:A:OP1	2.34	0.54
48:A2:1923:A:OP2	48:A2:2021:A:N6	2.41	0.54
50:BD:167:TYR:OH	50:BD:202:LYS:O	2.22	0.54
5:AC:193:LYS:NZ	48:A2:346:G:OP2	2.41	0.54
15:AJ:114:ASP:OD1	65:BS:14:ARG:NE	2.41	0.54
30:AZ:5:MET:O	30:AZ:28:ASN:ND2	2.41	0.54
31:Aa:117:LEU:CG	31:Aa:118:PRO:HD2	2.37	0.54
39:AI:62:LYS:HD3	39:AI:98:ARG:HH22	1.72	0.54
48:A2:14:C:H2'	48:A2:15:A:H8	1.72	0.54
48:A2:4503:G:N2	48:A2:4506:A:OP2	2.41	0.54
49:B1:91:A:H5'	49:B1:92:A:H5''	1.90	0.54
55:BI:110:ARG:NH2	55:BI:166:PHE:O	2.40	0.54
56:BJ:136:ARG:HG2	56:BJ:159:PHE:HB3	1.88	0.54
76:Bd:11:PRO:HB3	76:Bd:13:LYS:HE2	1.89	0.54
3:AB:189:THR:N	3:AB:192:GLU:OE2	2.39	0.54
12:AG:192:ARG:NH2	48:A2:5:A:O3'	2.38	0.54
30:AZ:96:VAL:HG22	30:AZ:110:ALA:HB1	1.90	0.54
32:Ab:13:SER:OG	48:A2:1706:G:N2	2.41	0.54
51:BE:191:ARG:NH2	51:BE:212:ASP:OD2	2.35	0.54
14:AI:76:MET:HE3	14:AI:151:ALA:HB2	1.89	0.53
27:AW:49:ILE:HD12	48:A2:3586:G:H21	1.73	0.53
27:AW:51:TRP:O	48:A2:4999:G:N2	2.41	0.53
48:A2:920:G:O2'	48:A2:926:G:OP2	2.24	0.53
48:A2:4734:C:N4	48:A2:4818:G:O6	2.40	0.53
52:BF:103:LEU:HD23	52:BF:104:THR:HG23	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:BQ:16:LYS:HB3	63:BQ:19:ALA:HB3	1.89	0.53
17:AM:112:VAL:O	17:AM:116:LYS:N	2.38	0.53
48:A2:959:C:H2'	48:A2:960:G:H8	1.72	0.53
49:B1:838:G:OP1	49:B1:839:C:N4	2.40	0.53
49:B1:1838:U:H5'	61:BO:151:LEU:HD22	1.90	0.53
57:BK:34:GLU:HA	57:BK:41:PRO:HA	1.89	0.53
59:BM:82:ASN:ND2	59:BM:105:GLY:O	2.41	0.53
64:BR:112:GLY:O	64:BR:113:SER:OG	2.24	0.53
24:AT:46:GLY:O	24:AT:49:GLN:NE2	2.41	0.53
50:BD:48:ILE:HD12	50:BD:84:VAL:HG13	1.90	0.53
50:BD:80:PRO:HB2	50:BD:81:GLU:HG2	1.90	0.53
51:BE:176:ASP:O	51:BE:179:ASN:ND2	2.40	0.53
55:BI:194:GLU:OE2	58:BL:11:GLN:NE2	2.41	0.53
62:BP:85:ILE:HD11	62:BP:116:LEU:HG	1.90	0.53
67:BU:68:THR:O	76:Bd:40:ARG:NH1	2.41	0.53
31:Aa:74:ASN:HB3	31:Aa:114:LYS:HG2	1.91	0.53
47:At:7:TRP:NE1	48:A2:2247:A:OP2	2.40	0.53
49:B1:116:U:H3	49:B1:347:G:H1	1.55	0.53
49:B1:1529:C:O2'	66:BT:87:VAL:O	2.25	0.53
49:B1:1659:U:H4'	76:Bd:30:LEU:HB2	1.90	0.53
62:BP:25:LEU:HB3	62:BP:87:PRO:HG2	1.90	0.53
80:Bv:52:G:H2'	80:Bv:53:G:H8	1.74	0.53
2:BA:63:ARG:HH12	68:BV:78:ILE:HG12	1.73	0.53
8:A4:13:A:OP2	8:A4:66:G:N2	2.36	0.53
11:AF:73:ARG:HH22	48:A2:717:G:H5''	1.73	0.53
25:AU:26:THR:HA	25:AU:68:SER:HB2	1.91	0.53
31:Aa:13:GLY:O	35:Ae:39:ARG:NH1	2.42	0.53
48:A2:1320:A:H62	48:A2:2325:C:H5	1.57	0.53
66:BT:30:VAL:HG23	66:BT:34:VAL:HG23	1.90	0.53
32:Ab:44:ARG:NE	48:A2:1447:G:OP1	2.40	0.53
32:Ab:112:ILE:CA	48:A2:1254:G:C4	2.91	0.53
48:A2:1782:U:H2'	48:A2:1783:A:H8	1.74	0.53
51:BE:66:MET:HG2	51:BE:78:VAL:HB	1.89	0.53
58:BL:73:LEU:HD13	58:BL:90:ARG:HH12	1.73	0.53
64:BR:10:LYS:NZ	64:BR:53:TYR:OH	2.36	0.53
66:BT:13:GLU:O	66:BT:17:ALA:N	2.37	0.53
5:AC:133:LEU:HD13	47:At:6:GLN:HE21	1.72	0.53
10:AE:53:GLY:HA3	48:A2:1264:G:H22	1.74	0.53
15:AJ:147:ARG:CZ	15:AJ:147:ARG:CB	2.86	0.53
31:Aa:74:ASN:HD21	48:A2:1370:A:H62	1.56	0.53
49:B1:448:A:H5''	55:BI:25:ARG:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:BM:75:ASN:HB3	59:BM:128:PHE:HE2	1.74	0.53
71:BY:54:VAL:HG22	71:BY:76:TYR:HB2	1.90	0.53
1:AA:242:ARG:NH1	1:AA:243:THR:O	2.42	0.53
10:AE:67:ALA:HB1	10:AE:70:LYS:HE2	1.91	0.53
15:AJ:136:ARG:HG3	15:AJ:157:ILE:HD11	1.90	0.53
17:AM:46:ARG:HH21	48:A2:723:A:H2	1.54	0.53
18:AN:4:TYR:OH	48:A2:149:U:OP2	2.26	0.53
19:AO:140:ARG:NH1	19:AO:144:GLU:OE1	2.42	0.53
48:A2:966:C:O2'	48:A2:969:U:OP2	2.22	0.53
48:A2:1088:C:H2'	48:A2:1089:A:H8	1.73	0.53
49:B1:170:A:OP2	53:BG:140:ARG:NH1	2.42	0.53
49:B1:354:U:OP1	58:BL:90:ARG:NH2	2.42	0.53
49:B1:925:G:N2	49:B1:1017:U:O2	2.38	0.53
49:B1:1649:U:OP1	63:BQ:128:GLU:N	2.39	0.53
50:BD:74:GLN:HG2	50:BD:80:PRO:HA	1.91	0.53
31:Aa:95:THR:HG23	31:Aa:97:ALA:H	1.74	0.53
48:A2:469:G:H1	48:A2:672:G:H1	1.56	0.53
49:B1:377:G:H1	49:B1:387:C:H42	1.56	0.53
50:BD:214:LYS:HG3	50:BD:214:LYS:O	2.09	0.53
3:AB:3:HIS:O	3:AB:5:LYS:N	2.42	0.53
9:AD:5:LYS:NZ	48:A2:4210:A:OP1	2.39	0.53
17:AM:32:ASP:O	17:AM:34:ASN:N	2.42	0.53
28:AX:110:LYS:NZ	28:AX:121:VAL:O	2.41	0.53
38:Ah:17:LEU:O	38:Ah:21:LEU:N	2.41	0.53
48:A2:2372:C:OP2	48:A2:2373:G:N2	2.42	0.53
50:BD:123:LEU:HD11	50:BD:152:PHE:HB3	1.91	0.53
51:BE:80:VAL:HG13	51:BE:81:THR:HG23	1.91	0.53
59:BM:45:ARG:HE	59:BM:72:HIS:HD2	1.55	0.53
4:BB:149:GLN:HE22	4:BB:154:SER:HB3	1.75	0.52
5:AC:54:VAL:O	7:A3:26:C:O2'	2.27	0.52
6:BC:91:SER:HB3	6:BC:156:ILE:HG23	1.89	0.52
7:A3:146:U:O2	28:AX:51:THR:OG1	2.26	0.52
49:B1:104:A:H5'	55:BI:12:ARG:HH12	1.74	0.52
49:B1:1264:C:O2	49:B1:1266:C:N4	2.42	0.52
49:B1:1309:C:H1'	78:Bf:140:TYR:HD2	1.74	0.52
49:B1:1527:C:H5''	63:BQ:142:GLN:HB2	1.89	0.52
49:B1:1616:U:H3	49:B1:1620:A:H62	1.58	0.52
53:BG:49:VAL:O	53:BG:114:VAL:N	2.41	0.52
63:BQ:38:PRO:HG3	66:BT:8:ASP:HA	1.91	0.52
4:BB:73:ASP:N	4:BB:73:ASP:OD1	2.41	0.52
48:A2:1909:C:H42	48:A2:2035:U:H1'	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:B1:406:U:O2'	49:B1:408:A:OP1	2.27	0.52
49:B1:835:C:N4	71:BY:9:THR:O	2.41	0.52
49:B1:1033:G:H1	49:B1:1080:A:HO2'	1.56	0.52
49:B1:1273:C:O2'	49:B1:1275:G:OP1	2.27	0.52
4:BB:131:ASP:OD1	4:BB:131:ASP:N	2.43	0.52
14:AI:140:THR:HB	14:AI:144:ASN:HD22	1.74	0.52
30:AZ:11:VAL:HG11	30:AZ:80:LEU:HD13	1.92	0.52
44:An:12:ARG:NH1	49:B1:1848:U:O4	2.42	0.52
48:A2:4239:G:O2'	48:A2:4244:A:N6	2.42	0.52
49:B1:591:U:OP1	49:B1:593:C:N4	2.42	0.52
49:B1:920:A:O2'	49:B1:922:A:O5'	2.28	0.52
49:B1:1050:A:H62	49:B1:1068:G:H21	1.56	0.52
49:B1:1208:A:O2'	49:B1:1835:A:N1	2.39	0.52
49:B1:1535:U:O4	52:BF:159:ARG:NE	2.38	0.52
49:B1:1539:U:H4'	66:BT:47:PRO:HA	1.91	0.52
71:BY:83:LYS:HG2	71:BY:91:LEU:HD21	1.90	0.52
73:Ba:22:ARG:HD2	73:Ba:27:ALA:HB1	1.92	0.52
79:Bg:163:PRO:HB2	79:Bg:179:LEU:HB2	1.91	0.52
8:A4:59:G:O2'	9:AD:267:ASN:OD1	2.18	0.52
9:AD:51:MET:HE1	9:AD:163:LEU:HA	1.92	0.52
13:AH:95:VAL:HG22	43:Am:82:LEU:HD22	1.91	0.52
14:AI:15:LYS:NZ	48:A2:1844:U:OP1	2.41	0.52
15:AJ:145:LYS:NZ	15:AJ:145:LYS:CB	2.73	0.52
49:B1:524:U:OP1	49:B1:525:A:O2'	2.28	0.52
49:B1:916:A:O2'	60:BN:73:ARG:NH1	2.38	0.52
49:B1:1858:G:OP2	61:BO:146:ARG:NH2	2.36	0.52
50:BD:9:ARG:HH21	76:Bd:35:GLY:HA2	1.75	0.52
61:BO:113:GLN:HE21	73:Ba:46:GLU:HB2	1.74	0.52
73:Ba:44:ILE:HG22	73:Ba:67:LEU:HB2	1.92	0.52
79:Bg:17:TRP:HB2	79:Bg:36:ARG:HD2	1.91	0.52
11:AF:80:ASN:HD21	24:AT:142:ARG:HA	1.74	0.52
13:AH:120:GLU:HG3	48:A2:4574:C:H1'	1.92	0.52
18:AN:68:ARG:NH1	48:A2:296:C:OP1	2.43	0.52
30:AZ:101:PHE:HD1	30:AZ:107:LYS:HE2	1.74	0.52
48:A2:1977:C:H42	48:A2:1981:G:H1	1.56	0.52
48:A2:3724:G:OP2	48:A2:3747:G:O2'	2.28	0.52
49:B1:918:U:O2'	49:B1:919:A:O4'	2.28	0.52
49:B1:1616:U:H5	62:BP:43:ARG:HH12	1.58	0.52
65:BS:88:LYS:NZ	65:BS:88:LYS:CB	2.73	0.52
2:BA:52:LYS:HD2	64:BR:109:LEU:HD11	1.92	0.52
3:AB:109:HIS:N	3:AB:202:GLU:OE2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AR:76:MET:SD	22:AR:88:ARG:NH2	2.82	0.52
23:AS:170:LYS:CE	48:A2:4832:A:OP1	2.57	0.52
53:BG:56:ASN:HB2	53:BG:108:VAL:HB	1.90	0.52
61:BO:35:ALA:HB2	61:BO:112:ALA:HB2	1.92	0.52
79:Bg:272:GLN:HE21	79:Bg:284:PRO:HG3	1.73	0.52
3:AB:55:HIS:ND1	3:AB:369:ASP:OD2	2.40	0.52
4:BB:35:ALA:HB3	4:BB:42:ARG:HA	1.92	0.52
8:A4:60:G:H2'	8:A4:61:G:H8	1.74	0.52
21:AQ:37:ARG:NH1	48:A2:2067:G:OP2	2.42	0.52
48:A2:3668:U:O2	48:A2:3790:G:N2	2.43	0.52
49:B1:1530:U:O2'	49:B1:1606:G:OP1	2.28	0.52
49:B1:1865:C:H1'	73:Ba:7:ASN:HD22	1.74	0.52
53:BG:58:LYS:HA	53:BG:107:SER:HB2	1.91	0.52
79:Bg:166:VAL:HA	79:Bg:176:VAL:HA	1.91	0.52
2:BA:76:VAL:HG22	2:BA:123:VAL:HB	1.92	0.52
12:AG:161:VAL:HG21	12:AG:200:THR:HG23	1.90	0.52
14:AI:168:SER:OG	14:AI:169:LYS:N	2.43	0.52
15:AJ:112:HIS:HD2	15:AJ:126:TYR:H	1.56	0.52
20:AP:122:ALA:HB3	20:AP:143:PRO:HG2	1.91	0.52
31:Aa:21:ARG:NH2	48:A2:1300:U:OP1	2.31	0.52
42:AI:48:LYS:NZ	48:A2:2385:G:O2'	2.40	0.52
48:A2:445:C:H5'	48:A2:446:A:H2	1.75	0.52
49:B1:639:C:H2'	49:B1:640:A:C8	2.45	0.52
49:B1:1245:G:O2'	49:B1:1492:U:OP1	2.26	0.52
49:B1:1288:U:N3	49:B1:1314:U:O4	2.43	0.52
67:BU:38:ASP:OD1	67:BU:41:ARG:NH2	2.42	0.52
73:Ba:2:THR:OG1	73:Ba:3:LYS:N	2.41	0.52
3:AB:153:MET:HB3	3:AB:194:LEU:HD11	1.91	0.52
10:AE:137:VAL:HG22	10:AE:138:ARG:N	2.25	0.52
11:AF:102:SER:HB2	11:AF:105:VAL:HG22	1.92	0.52
13:AH:155:SER:OG	48:A2:4650:C:O2'	2.27	0.52
20:AP:126:ARG:HA	20:AP:140:MET:HG2	1.92	0.52
43:Am:100:TYR:O	48:A2:4434:G:O2'	2.27	0.52
48:A2:1468:C:H2'	48:A2:1469:G:H8	1.74	0.52
6:BC:108:LYS:HD2	6:BC:233:LEU:HD12	1.92	0.52
18:AN:71:ARG:NH1	48:A2:32:G:OP1	2.42	0.52
19:AO:176:ARG:HD3	48:A2:4730:G:H5''	1.92	0.52
31:Aa:117:LEU:CD1	31:Aa:118:PRO:CD	2.56	0.52
39:AI:85:ARG:NH1	48:A2:305:G:OP1	2.43	0.52
49:B1:360:A:H62	49:B1:400:C:H1'	1.74	0.52
49:B1:626:G:N1	81:Bx:51:U:O2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:B1:1636:G:H1'	52:BF:164:ARG:HH12	1.75	0.52
16:AL:126:LEU:HA	38:Ah:119:TYR:HA	1.92	0.51
24:AT:9:ARG:NH2	48:A2:4180:U:OP2	2.43	0.51
35:Ae:30:LYS:HB3	48:A2:1315:C:H5''	1.90	0.51
48:A2:3824:U:O2'	48:A2:4937:A:N3	2.43	0.51
49:B1:181:A:N3	49:B1:182:C:N4	2.58	0.51
49:B1:1451:G:H21	49:B1:1474:A:H61	1.59	0.51
51:BE:35:PRO:HD2	51:BE:83:PRO:HG2	1.91	0.51
61:BO:20:GLN:NE2	61:BO:21:VAL:O	2.41	0.51
6:BC:269:PHE:O	6:BC:273:LEU:N	2.42	0.51
16:AL:16:LYS:NZ	48:A2:97:G:OP1	2.42	0.51
22:AR:103:ARG:NH2	22:AR:124:TYR:OH	2.37	0.51
27:AW:120:GLN:HG3	49:B1:327:G:H5''	1.91	0.51
28:AX:130:PRO:HG3	48:A2:2415:U:C4	2.44	0.51
48:A2:2421:G:H2'	48:A2:2422:G:H8	1.75	0.51
58:BL:24:LEU:HD12	58:BL:25:LEU:HG	1.92	0.51
9:AD:235:MET:O	9:AD:239:MET:N	2.42	0.51
34:Ad:32:ARG:NH1	48:A2:4954:C:OP1	2.43	0.51
44:An:2:ARG:NH2	49:B1:1841:C:OP2	2.42	0.51
45:Ao:81:ARG:NH2	48:A2:4255:U:O2'	2.42	0.51
48:A2:116:G:H22	48:A2:153:G:H22	1.58	0.51
49:B1:453:C:O2'	53:BG:92:ARG:O	2.24	0.51
60:BN:5:HIS:HD2	60:BN:117:LEU:HD22	1.76	0.51
1:AA:54:ARG:HG2	1:AA:56:ALA:H	1.75	0.51
4:BB:138:PHE:HE1	4:BB:216:LYS:HZ1	1.50	0.51
5:AC:293:LEU:O	5:AC:299:GLN:NE2	2.43	0.51
15:AJ:96:LYS:O	15:AJ:159:LYS:NZ	2.36	0.51
48:A2:120:A:N1	48:A2:146:A:O2'	2.42	0.51
49:B1:526:A:H62	49:B1:588:G:H1	1.58	0.51
3:AB:2:SER:O	3:AB:3:HIS:ND1	2.44	0.51
4:BB:103:MET:N	4:BB:215:VAL:CG1	2.73	0.51
10:AE:64:SER:HB3	48:A2:1222:C:H41	1.74	0.51
23:AS:82:LEU:HB2	23:AS:93:MET:HB3	1.92	0.51
26:AV:42:VAL:HG11	26:AV:45:ILE:HD12	1.93	0.51
29:AY:8:THR:O	48:A2:223:G:N2	2.43	0.51
32:Ab:111:ARG:CG	32:Ab:116:LEU:HD13	2.36	0.51
48:A2:51:A:N3	48:A2:1510:U:O2'	2.43	0.51
48:A2:445:C:N4	48:A2:1278:C:O2	2.44	0.51
48:A2:1871:G:H22	48:A2:1920:A:H61	1.59	0.51
49:B1:808:A:OP1	51:BE:188:ASN:ND2	2.44	0.51
49:B1:1079:C:O2'	49:B1:1182:A:N1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:B1:1799:G:OP1	55:BI:24:LYS:NZ	2.43	0.51
53:BG:193:ALA:O	53:BG:197:GLN:N	2.43	0.51
57:BK:3:MET:HB3	57:BK:7:ASN:HB3	1.92	0.51
57:BK:13:GLU:HG3	57:BK:17:LYS:HE3	1.92	0.51
60:BN:54:LEU:HD23	60:BN:60:VAL:HG11	1.93	0.51
78:Bf:133:ALA:HB3	78:Bf:140:TYR:HB3	1.92	0.51
9:AD:187:SER:OG	9:AD:189:GLU:OE1	2.22	0.51
12:AG:107:LYS:HA	12:AG:110:LYS:HB3	1.92	0.51
14:AI:189:ARG:CG	14:AI:190:LEU:H	2.13	0.51
24:AT:125:TRP:NE1	24:AT:127:GLN:OE1	2.43	0.51
27:AW:4:GLU:O	27:AW:13:ILE:N	2.43	0.51
38:Ah:44:LEU:N	38:Ah:44:LEU:HD12	2.25	0.51
43:Am:99:CYS:HB3	43:Am:115:CYS:HB3	1.93	0.51
48:A2:489:C:H2'	48:A2:490:G:H8	1.73	0.51
48:A2:3930:U:H2'	48:A2:3931:A:H8	1.76	0.51
49:B1:1323:U:H3	49:B1:1505:U:H3	1.56	0.51
49:B1:1562:C:OP1	66:BT:74:SER:OG	2.26	0.51
49:B1:1808:U:H2'	49:B1:1809:A:H8	1.76	0.51
64:BR:7:LYS:O	64:BR:11:LYS:N	2.39	0.51
1:AA:55:GLY:HA3	1:AA:174:ARG:HH11	1.75	0.51
14:AI:184:MET:SD	14:AI:190:LEU:CD1	2.99	0.51
18:AN:54:LYS:H	18:AN:59:TYR:HE2	1.58	0.51
48:A2:1784:A:H5''	48:A2:1785:G:H5'	1.93	0.51
49:B1:148:U:O2	49:B1:171:A:N6	2.44	0.51
49:B1:161:U:H5'	71:BY:116:LYS:HD2	1.92	0.51
49:B1:1598:G:N2	49:B1:1599:U:O4	2.35	0.51
54:BH:109:ARG:HH11	54:BH:111:LYS:HA	1.76	0.51
57:BK:22:VAL:HG13	57:BK:35:LEU:HD11	1.92	0.51
81:Bx:57:U:H2'	81:Bx:58:U:H3'	1.93	0.51
1:AA:3:ARG:HH21	48:A2:1615:G:H21	1.59	0.51
3:AB:25:HIS:HA	3:AB:222:VAL:HG21	1.92	0.51
3:AB:56:ILE:HG21	3:AB:365:LEU:HD22	1.92	0.51
3:AB:119:TYR:OH	3:AB:129:ALA:N	2.43	0.51
9:AD:156:GLY:HA2	9:AD:181:PRO:HD3	1.92	0.51
11:AF:214:SER:OG	11:AF:215:SER:N	2.41	0.51
18:AN:114:ARG:NH1	18:AN:151:ILE:O	2.44	0.51
22:AR:120:TYR:O	22:AR:124:TYR:N	2.43	0.51
23:AS:171:ARG:CD	48:A2:4724:A:H61	2.24	0.51
45:Ao:9:ARG:HA	45:Ao:20:PRO:HA	1.93	0.51
48:A2:458:G:H22	48:A2:684:U:H3	1.57	0.51
48:A2:654:G:H2'	48:A2:655:A:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A2:2693:G:H2'	48:A2:2694:G:C8	2.46	0.51
48:A2:3612:U:OP2	48:A2:3617:A:N6	2.43	0.51
49:B1:526:A:N7	49:B1:588:G:N2	2.50	0.51
49:B1:1166:G:N7	70:BX:25:LYS:NZ	2.47	0.51
49:B1:1234:C:H42	49:B1:1525:C:H42	1.58	0.51
13:AH:36:ARG:HH12	13:AH:76:HIS:HD2	1.58	0.51
16:AL:165:LYS:HD2	48:A2:505:C:H5''	1.93	0.51
19:AO:144:GLU:OE2	48:A2:4643:A:O2'	2.28	0.51
32:Ab:109:ARG:HD3	32:Ab:109:ARG:N	2.26	0.51
33:Ac:21:VAL:HG11	33:Ac:96:ILE:HG23	1.93	0.51
40:Aj:49:TRP:O	48:A2:1628:A:O2'	2.29	0.51
48:A2:1060:C:N4	48:A2:1216:G:O6	2.44	0.51
48:A2:1233:C:N4	48:A2:1243:G:O6	2.44	0.51
48:A2:2465:G:H2'	48:A2:2466:G:H8	1.76	0.51
49:B1:460:A:H1'	49:B1:470:G:H22	1.74	0.51
49:B1:1864:U:H5'	73:Ba:79:ILE:HD11	1.92	0.51
51:BE:87:MET:HE2	51:BE:123:LEU:HB2	1.93	0.51
62:BP:60:LEU:HD23	62:BP:76:VAL:HG21	1.93	0.51
3:AB:36:ASP:N	3:AB:36:ASP:OD1	2.41	0.51
3:AB:254:ILE:HG23	3:AB:266:VAL:HG11	1.92	0.51
5:AC:71:ARG:HH22	82:A:13:LEU:CB	2.24	0.51
10:AE:187:ARG:HE	48:A2:4899:G:H4'	1.75	0.51
27:AW:16:GLY:O	48:A2:4590:U:O2'	2.25	0.51
48:A2:123:C:H42	48:A2:144:A:H61	1.57	0.51
48:A2:2090:C:N3	48:A2:2231:G:N1	2.59	0.51
48:A2:4324:A:H2'	48:A2:4325:A:H8	1.76	0.51
49:B1:413:G:H2'	49:B1:414:A:H8	1.75	0.51
53:BG:153:VAL:HG23	53:BG:156:TYR:HB2	1.93	0.51
3:AB:28:LYS:NZ	48:A2:4544:C:OP2	2.35	0.50
4:BB:138:PHE:CG	4:BB:213:ARG:NH2	2.60	0.50
11:AF:199:LYS:HG3	11:AF:200:ARG:HG2	1.93	0.50
15:AJ:145:LYS:HB3	15:AJ:145:LYS:HZ3	1.76	0.50
16:AL:80:GLU:HG2	16:AL:110:LEU:HD12	1.92	0.50
18:AN:8:GLN:HE22	48:A2:272:G:H5''	1.76	0.50
27:AW:34:ALA:HA	27:AW:37:GLU:HB3	1.93	0.50
35:Ae:130:ARG:NH2	48:A2:2284:U:O2	2.44	0.50
37:Ag:10:ARG:NH1	48:A2:2382:A:OP1	2.44	0.50
48:A2:1225:G:OP2	48:A2:1225:G:N2	2.38	0.50
48:A2:3592:A:O2'	48:A2:4620:G:O2'	2.24	0.50
48:A2:4995:U:H2'	48:A2:4996:A:H8	1.76	0.50
49:B1:804:U:O2'	69:BW:121:THR:O	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:B1:1060:A:O2'	49:B1:1062:A:N7	2.41	0.50
49:B1:1232:U:OP2	65:BS:135:HIS:ND1	2.44	0.50
49:B1:1692:U:H2'	49:B1:1693:G:C8	2.46	0.50
50:BD:136:VAL:HG22	50:BD:186:VAL:HG22	1.93	0.50
56:BJ:82:VAL:HG21	56:BJ:92:MET:HE1	1.93	0.50
65:BS:36:VAL:HG11	65:BS:71:MET:HE1	1.93	0.50
79:Bg:28:PRO:HB3	79:Bg:293:ALA:HB2	1.93	0.50
79:Bg:174:VAL:HB	79:Bg:188:HIS:HB2	1.92	0.50
7:A3:83:C:O2	7:A3:87:G:N2	2.44	0.50
18:AN:41:ARG:HD2	48:A2:148:G:C2	2.46	0.50
32:Ab:27:GLN:NE2	48:A2:1444:A:O4'	2.44	0.50
34:Ad:33:ILE:HD11	34:Ad:45:ALA:HB2	1.93	0.50
37:Ag:24:ARG:NH2	48:A2:2592:C:OP1	2.44	0.50
48:A2:1602:U:H2'	48:A2:1603:A:H8	1.76	0.50
48:A2:3588:G:O2'	48:A2:3591:G:N7	2.44	0.50
48:A2:3915:G:N2	48:A2:4039:U:O4	2.32	0.50
49:B1:1778:C:H2'	49:B1:1779:G:C8	2.46	0.50
70:BX:91:LEU:HD21	77:Be:6:LEU:HB3	1.93	0.50
71:BY:114:MET:HE2	71:BY:126:GLY:HA2	1.93	0.50
2:BA:145:ILE:HG12	2:BA:159:ILE:HD12	1.92	0.50
17:AM:45:VAL:HG13	17:AM:45:VAL:O	2.11	0.50
23:AS:170:LYS:CG	48:A2:4832:A:OP1	2.60	0.50
32:Ab:60:ASN:HA	32:Ab:63:LYS:HD2	1.93	0.50
48:A2:217:C:H42	48:A2:232:A:H61	1.59	0.50
48:A2:2739:G:O2'	48:A2:2740:U:O4'	2.29	0.50
49:B1:71:G:OP2	49:B1:72:C:N4	2.44	0.50
49:B1:1559:C:H42	49:B1:1576:G:H1	1.59	0.50
2:BA:89:LYS:HD3	64:BR:82:ASP:HB3	1.93	0.50
3:AB:226:LYS:HB3	3:AB:229:LYS:HD2	1.93	0.50
4:BB:52:THR:O	4:BB:53:GLN:HB2	2.12	0.50
15:AJ:141:ILE:HG22	15:AJ:149:GLY:CA	2.42	0.50
18:AN:84:PRO:HA	18:AN:87:HIS:HD2	1.76	0.50
36:Af:106:TYR:H	36:Af:106:TYR:HD1	1.54	0.50
48:A2:476:G:N2	48:A2:667:C:O2	2.42	0.50
48:A2:4885:G:N2	48:A2:4885:G:OP2	2.44	0.50
49:B1:303:C:H4'	55:BI:75:LYS:HD3	1.93	0.50
49:B1:1268:C:O2'	62:BP:99:GLY:O	2.26	0.50
50:BD:7:LYS:NZ	67:BU:111:GLU:OE1	2.43	0.50
76:Bd:19:ARG:O	76:Bd:27:ARG:NH1	2.44	0.50
79:Bg:89:LEU:HB3	79:Bg:99:ARG:HB3	1.91	0.50
3:AB:249:ARG:NH2	48:A2:3816:A:OP2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AC:275:SER:OG	5:AC:276:ASN:N	2.45	0.50
29:AY:72:GLN:HB2	29:AY:81:TYR:HD2	1.76	0.50
32:Ab:111:ARG:HA	32:Ab:115:GLY:CA	2.41	0.50
46:Ap:33:GLN:OE1	46:Ap:49:ARG:NH1	2.45	0.50
46:Ap:48:LYS:NZ	48:A2:2715:G:OP2	2.35	0.50
48:A2:700:C:H42	48:A2:1270:G:H1	1.58	0.50
48:A2:2381:G:H2'	48:A2:2382:A:H8	1.76	0.50
48:A2:3849:C:N4	48:A2:4480:A:O4'	2.45	0.50
48:A2:3914:A:H2'	48:A2:3915:G:H8	1.77	0.50
49:B1:551:U:N3	49:B1:552:G:O6	2.43	0.50
49:B1:1262:C:H1'	76:Bd:10:HIS:CE1	2.47	0.50
61:BO:95:ILE:HD13	61:BO:116:LEU:HD22	1.93	0.50
19:AO:74:ARG:NH2	48:A2:4674:C:OP1	2.35	0.50
22:AR:151:ARG:HH12	58:BL:118:ARG:HD3	1.77	0.50
24:AT:68:THR:OG1	24:AT:69:GLN:N	2.45	0.50
28:AX:125:ASN:HD22	48:A2:2417:A:H5'	1.76	0.50
48:A2:1725:A:N1	48:A2:1771:C:O2'	2.41	0.50
49:B1:294:U:OP1	58:BL:36:TYR:OH	2.28	0.50
49:B1:1413:G:H2'	49:B1:1414:A:H8	1.77	0.50
56:BJ:37:LEU:HD23	56:BJ:42:GLU:HG3	1.94	0.50
61:BO:142:ARG:HD2	61:BO:143:LYS:H	1.76	0.50
66:BT:104:LEU:HD21	66:BT:121:ARG:HH11	1.77	0.50
4:BB:148:ASN:O	49:B1:1123:C:O2'	2.24	0.50
10:AE:277:LEU:HD11	36:Af:105:LEU:HD11	1.93	0.50
18:AN:172:ARG:HH22	48:A2:62:A:H5'	1.76	0.50
24:AT:83:LYS:HE3	24:AT:85:LEU:HD21	1.93	0.50
28:AX:110:LYS:HG3	28:AX:121:VAL:HB	1.94	0.50
32:Ab:27:GLN:NE2	48:A2:1444:A:H1'	2.27	0.50
36:Af:72:GLY:HA3	36:Af:88:PHE:HA	1.94	0.50
38:Ah:87:LYS:CG	40:Aj:78:PHE:HB3	2.41	0.50
48:A2:3932:G:N1	48:A2:3935:U:OP1	2.42	0.50
49:B1:151:C:OP1	71:BY:120:THR:OG1	2.27	0.50
51:BE:206:ASP:HB2	51:BE:222:LEU:HD12	1.92	0.50
51:BE:212:ASP:OD1	51:BE:216:ASN:N	2.45	0.50
55:BI:177:SER:OG	55:BI:182:CYS:SG	2.70	0.50
16:AL:133:ALA:N	16:AL:134:PRO:HD3	2.27	0.50
35:Ae:37:LYS:HD3	35:Ae:38:PRO:HD2	1.93	0.50
49:B1:104:A:OP1	55:BI:12:ARG:NH1	2.45	0.50
49:B1:1300:U:O2'	62:BP:51:ARG:NH2	2.45	0.50
1:AA:101:VAL:HG22	1:AA:163:ARG:HB3	1.93	0.50
5:AC:190:ARG:NH1	48:A2:2274:C:OP1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A4:68:C:OP1	24:AT:20:ARG:NH2	2.45	0.50
21:AQ:11:ARG:NH1	48:A2:1647:C:O2'	2.45	0.50
22:AR:59:SER:HA	48:A2:2613:C:H5'	1.94	0.50
32:Ab:112:ILE:CA	48:A2:1254:G:C5	2.95	0.50
32:Ab:112:ILE:CA	32:Ab:112:ILE:HB	2.18	0.50
48:A2:216:G:H22	48:A2:233:G:H1	1.59	0.50
48:A2:3754:A:H4'	48:A2:3755:A:H5'	1.93	0.50
49:B1:1508:A:O2'	49:B1:1510:G:N7	2.34	0.50
49:B1:1846:G:H2'	49:B1:1847:G:H8	1.77	0.50
50:BD:64:ARG:HG3	57:BK:94:LEU:HD12	1.93	0.50
73:Ba:45:VAL:HG11	73:Ba:53:ILE:HD12	1.94	0.50
79:Bg:60:ARG:HH11	79:Bg:61:GLY:H	1.59	0.50
4:BB:32:ASP:HB3	4:BB:46:LYS:HG2	1.94	0.49
7:A3:52:A:H62	42:Al:27:ILE:HD13	1.77	0.49
9:AD:21:ARG:HA	9:AD:24:ARG:HH21	1.77	0.49
23:AS:170:LYS:HG2	48:A2:4832:A:OP2	2.13	0.49
48:A2:454:C:H2'	48:A2:455:G:C8	2.47	0.49
48:A2:2634:C:N4	48:A2:2658:G:O6	2.45	0.49
48:A2:4854:G:N7	48:A2:4882:C:N4	2.59	0.49
52:BF:79:HIS:HD2	52:BF:159:ARG:HH11	1.60	0.49
58:BL:135:SER:O	58:BL:139:ARG:NH1	2.45	0.49
63:BQ:47:LEU:HD11	63:BQ:78:VAL:HG22	1.93	0.49
72:BZ:89:GLN:NE2	72:BZ:109:TYR:OH	2.44	0.49
19:AO:106:ASP:N	19:AO:106:ASP:OD1	2.45	0.49
49:B1:502:C:H1'	51:BE:63:LYS:HG2	1.93	0.49
68:BV:72:LEU:HD12	68:BV:75:ALA:HB3	1.94	0.49
12:AG:105:GLU:OE1	12:AG:113:ARG:NH2	2.45	0.49
16:AL:106:SER:O	16:AL:109:SER:OG	2.24	0.49
38:Ah:112:ARG:HG2	48:A2:171:C:H1'	1.95	0.49
48:A2:227:G:N3	48:A2:234:G:N2	2.59	0.49
48:A2:2714:G:H2'	48:A2:2715:G:C8	2.47	0.49
49:B1:15:U:O2'	49:B1:669:A:N6	2.45	0.49
49:B1:229:A:O2'	49:B1:888:U:O2	2.26	0.49
49:B1:1012:A:H5''	60:BN:10:GLY:HA3	1.93	0.49
54:BH:70:LYS:HA	54:BH:73:GLN:HB3	1.95	0.49
57:BK:26:ASP:O	57:BK:42:ASN:ND2	2.38	0.49
57:BK:76:ILE:HD13	57:BK:94:LEU:HD22	1.93	0.49
12:AG:67:ARG:NH2	12:AG:162:ASP:OD1	2.45	0.49
18:AN:184:ILE:HG23	18:AN:194:ARG:HH21	1.78	0.49
23:AS:74:ARG:O	23:AS:76:LYS:NZ	2.44	0.49
48:A2:1951:A:H2	48:A2:1998:A:H62	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A2:3691:G:H1	48:A2:3704:A:H61	1.60	0.49
49:B1:1615:U:OP2	62:BP:43:ARG:NH2	2.45	0.49
49:B1:1664:A:O2'	49:B1:1666:C:N4	2.45	0.49
55:BI:159:SER:HB3	55:BI:162:LEU:HD12	1.93	0.49
56:BJ:111:GLN:O	56:BJ:115:PHE:N	2.44	0.49
62:BP:60:LEU:O	62:BP:64:LYS:N	2.44	0.49
71:BY:77:ASP:HB2	71:BY:81:TYR:HD2	1.78	0.49
75:Bc:38:THR:HG23	75:Bc:40:ARG:HG3	1.94	0.49
9:AD:122:GLN:NE2	9:AD:124:GLU:O	2.37	0.49
9:AD:155:THR:O	9:AD:155:THR:OG1	2.27	0.49
11:AF:223:LYS:HD2	48:A2:1888:A:H4'	1.95	0.49
12:AG:37:LYS:NZ	48:A2:4095:C:OP1	2.44	0.49
13:AH:93:ARG:HD2	43:Am:82:LEU:HD21	1.94	0.49
27:AW:80:ARG:H	53:BG:131:ARG:HH12	1.61	0.49
48:A2:2523:G:OP2	48:A2:2525:G:O2'	2.27	0.49
49:B1:69:C:O2	49:B1:80:G:N2	2.41	0.49
49:B1:926:A:H61	49:B1:1015:U:H3	1.60	0.49
49:B1:1226:G:N1	49:B1:1639:G:OP2	2.35	0.49
64:BR:31:ASN:HA	64:BR:34:VAL:HB	1.95	0.49
4:BB:36:PRO:HG2	4:BB:39:PHE:HE2	1.77	0.49
5:AC:95:MET:SD	5:AC:95:MET:N	2.77	0.49
23:AS:160:ARG:HH21	23:AS:163:HIS:CE1	2.31	0.49
26:AV:24:ALA:HB3	26:AV:39:ILE:HD12	1.95	0.49
29:AY:28:LYS:NZ	48:A2:191:C:OP2	2.35	0.49
31:Aa:7:LYS:HE2	31:Aa:11:LEU:HD11	1.95	0.49
34:Ad:79:ASN:HD22	48:A2:4615:C:H5''	1.77	0.49
48:A2:2091:G:N2	48:A2:2231:G:N3	2.55	0.49
48:A2:2562:C:H2'	48:A2:2563:G:H8	1.77	0.49
48:A2:4251:U:O2'	48:A2:4282:G:O2'	2.30	0.49
48:A2:4537:G:O2'	48:A2:5027:U:OP1	2.25	0.49
48:A2:4696:A:H3'	48:A2:4697:G:H8	1.77	0.49
49:B1:1478:U:H2'	49:B1:1479:G:C8	2.47	0.49
49:B1:1725:U:H2'	49:B1:1726:G:C8	2.48	0.49
49:B1:1743:G:H21	49:B1:1791:A:H62	1.60	0.49
61:BO:36:SER:OG	61:BO:37:PHE:N	2.44	0.49
6:BC:175:GLY:HA2	68:BV:3:ASN:HD22	1.77	0.49
8:A4:23:A:N3	8:A4:118:C:O2'	2.43	0.49
21:AQ:37:ARG:HG3	21:AQ:38:ARG:HG3	1.94	0.49
42:Al:27:ILE:O	42:Al:33:ASN:ND2	2.46	0.49
48:A2:1498:G:H2'	48:A2:1500:A:H62	1.78	0.49
70:BX:68:LYS:HD3	70:BX:91:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A3:142:U:OP1	18:AN:38:ARG:NH2	2.45	0.49
10:AE:70:LYS:NZ	48:A2:1054:C:O2'	2.42	0.49
14:AI:3:ARG:NH1	14:AI:4:ARG:O	2.46	0.49
18:AN:155:VAL:O	18:AN:162:ARG:NH2	2.41	0.49
23:AS:162:GLN:HG2	23:AS:166:ARG:HG2	1.95	0.49
32:Ab:5:LYS:NZ	48:A2:1854:A:OP2	2.33	0.49
48:A2:352:C:H2'	48:A2:353:A:H8	1.78	0.49
48:A2:1406:U:H2'	48:A2:1407:G:H8	1.77	0.49
48:A2:1804:U:H2'	48:A2:1805:G:H8	1.77	0.49
72:BZ:61:GLU:HA	72:BZ:64:ASN:HB2	1.95	0.49
5:AC:152:LEU:HD12	5:AC:152:LEU:O	2.12	0.49
16:AL:133:ALA:CA	16:AL:136:LYS:CE	2.82	0.49
20:AP:109:VAL:HA	20:AP:112:LEU:HD13	1.94	0.49
32:Ab:105:GLY:O	32:Ab:108:ALA:CB	2.61	0.49
48:A2:1964:A:O2'	48:A2:1969:G:O6	2.30	0.49
49:B1:1171:G:O2'	49:B1:1187:G:O6	2.24	0.49
50:BD:177:LEU:HD12	50:BD:182:LEU:HD13	1.95	0.49
51:BE:70:ILE:HD11	71:BY:17:LEU:HD13	1.95	0.49
60:BN:40:LEU:HD12	60:BN:45:LEU:HD12	1.94	0.49
65:BS:10:GLN:NE2	65:BS:56:ALA:O	2.45	0.49
69:BW:75:ILE:HD11	69:BW:93:LEU:HD11	1.95	0.49
12:AG:117:ARG:HD2	12:AG:129:PRO:HG2	1.94	0.49
21:AQ:181:ARG:NH2	48:A2:1374:A:OP1	2.34	0.49
38:Ah:87:LYS:HD2	40:Aj:78:PHE:CG	2.45	0.49
75:Bc:15:THR:N	75:Bc:32:VAL:O	2.43	0.49
79:Bg:30:MET:HE3	79:Bg:44:LYS:HD3	1.95	0.49
13:AH:128:MET:HE2	13:AH:132:VAL:HG13	1.94	0.48
14:AI:96:VAL:HG22	14:AI:125:THR:HG22	1.95	0.48
16:AL:128:PRO:HG3	16:AL:136:LYS:HD2	1.93	0.48
18:AN:176:LYS:NZ	48:A2:65:A:N3	2.60	0.48
24:AT:84:ILE:CD1	32:Ab:23:LYS:HZ3	2.23	0.48
24:AT:108:ARG:O	24:AT:112:ASN:ND2	2.46	0.48
26:AV:14:PHE:HE2	26:AV:91:LYS:HD3	1.78	0.48
29:AY:55:VAL:HG13	29:AY:104:VAL:HG13	1.95	0.48
48:A2:1227:G:H1'	48:A2:1228:C:H5	1.77	0.48
49:B1:1256:G:H1	76:Bd:32:ARG:NH1	2.11	0.48
51:BE:31:PRO:HG3	51:BE:43:PRO:HG3	1.95	0.48
64:BR:37:GLU:HG3	79:Bg:150:TRP:HE1	1.78	0.48
66:BT:33:TRP:CD1	66:BT:34:VAL:HG13	2.47	0.48
66:BT:97:LYS:HA	66:BT:100:ALA:HB3	1.94	0.48
4:BB:97:LEU:HD11	4:BB:232:HIS:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AC:71:ARG:NH2	82:A:13:LEU:CA	2.69	0.48
10:AE:228:GLN:HB2	48:A2:1277:A:H61	1.78	0.48
18:AN:155:VAL:HG12	48:A2:57:G:H4'	1.95	0.48
32:Ab:114:LYS:NZ	32:Ab:114:LYS:HB3	2.28	0.48
34:Ad:30:HIS:NE2	48:A2:4599:G:OP1	2.46	0.48
48:A2:2090:C:N4	48:A2:2091:G:O6	2.46	0.48
50:BD:195:THR:HA	50:BD:201:LYS:HE2	1.94	0.48
76:Bd:40:ARG:HA	76:Bd:43:PHE:HB3	1.95	0.48
79:Bg:57:ARG:NH2	79:Bg:93:THR:O	2.46	0.48
12:AG:190:LEU:HB3	12:AG:199:CYS:HB3	1.95	0.48
22:AR:107:ARG:HH21	48:A2:2644:U:H5'	1.78	0.48
34:Ad:32:ARG:HB3	34:Ad:48:GLU:HG2	1.95	0.48
43:Am:104:HIS:HB3	43:Am:107:ALA:HB2	1.94	0.48
48:A2:67:C:N4	48:A2:319:U:O2'	2.37	0.48
48:A2:2484:C:O3'	48:A2:2485:G:N2	2.46	0.48
48:A2:2623:G:H1	48:A2:2669:C:H42	1.60	0.48
48:A2:4067:G:H2'	48:A2:4068:A:C8	2.48	0.48
49:B1:1454:A:N1	49:B1:1476:A:O2'	2.43	0.48
50:BD:218:LEU:CD1	50:BD:219:PRO:HD2	2.42	0.48
80:Bv:19:G:OP2	80:Bv:57:G:N2	2.36	0.48
3:AB:45:ALA:HB3	3:AB:183:ILE:HG12	1.94	0.48
9:AD:55:VAL:HG11	9:AD:158:LYS:HD2	1.96	0.48
11:AF:48:LYS:NZ	48:A2:1221:A:OP2	2.38	0.48
24:AT:32:ARG:HB3	24:AT:98:HIS:HE1	1.78	0.48
34:Ad:118:GLN:OE1	48:A2:5013:G:N2	2.43	0.48
46:Ap:41:PHE:O	48:A2:2653:A:N6	2.46	0.48
48:A2:1483:C:H4'	48:A2:1484:G:H5'	1.96	0.48
48:A2:2529:G:N2	48:A2:2749:C:N3	2.62	0.48
48:A2:3619:A:H1'	48:A2:3756:A:H61	1.78	0.48
48:A2:3836:A:N6	48:A2:3851:G:O6	2.47	0.48
48:A2:4309:G:H1	48:A2:4327:C:H42	1.62	0.48
49:B1:527:C:O2'	56:BJ:125:HIS:ND1	2.45	0.48
51:BE:104:ASP:N	51:BE:108:ARG:O	2.45	0.48
54:BH:122:LEU:O	54:BH:126:HIS:ND1	2.46	0.48
63:BQ:35:ASN:ND2	63:BQ:72:VAL:O	2.46	0.48
3:AB:168:MET:HG3	3:AB:177:LYS:O	2.13	0.48
7:A3:148:A:H2'	7:A3:149:G:C8	2.49	0.48
14:AI:51:HIS:HB3	14:AI:137:SER:HA	1.95	0.48
36:Af:106:TYR:CD1	36:Af:106:TYR:N	2.73	0.48
48:A2:1812:G:H2'	48:A2:1813:G:C8	2.48	0.48
48:A2:2630:C:O2'	48:A2:2632:C:OP1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:B1:1457:U:H2'	49:B1:1458:G:H8	1.79	0.48
49:B1:1745:A:N6	49:B1:1789:G:O2'	2.46	0.48
79:Bg:121:VAL:HG21	79:Bg:165:ILE:HD13	1.94	0.48
1:AA:133:TYR:HB3	1:AA:168:VAL:HG12	1.96	0.48
2:BA:85:ARG:NE	2:BA:201:LEU:O	2.47	0.48
14:AI:189:ARG:HA	14:AI:200:ILE:HD11	1.94	0.48
16:AL:149:GLN:NE2	38:Ah:121:VAL:O	2.47	0.48
21:AQ:42:THR:HB	48:A2:1411:U:H5''	1.96	0.48
41:Ak:26:LYS:HB2	41:Ak:69:LEU:HD12	1.94	0.48
48:A2:3632:G:H4'	48:A2:3633:A:H5'	1.95	0.48
49:B1:945:U:O2	49:B1:982:G:N2	2.46	0.48
52:BF:167:LYS:NZ	72:BZ:75:GLU:OE1	2.46	0.48
55:BI:178:ARG:HH11	55:BI:181:GLN:HG3	1.79	0.48
76:Bd:47:ALA:HA	76:Bd:50:ILE:HG12	1.96	0.48
79:Bg:138:CYS:SG	79:Bg:139:LYS:N	2.85	0.48
23:AS:170:LYS:CG	48:A2:4832:A:H5'	2.41	0.48
35:Ae:49:PHE:HE1	48:A2:1864:G:H5'	1.78	0.48
44:An:2:ARG:HD2	44:An:5:TRP:CD1	2.49	0.48
48:A2:1669:U:H2'	48:A2:1670:G:H8	1.78	0.48
48:A2:1863:U:OP1	48:A2:2259:G:O2'	2.31	0.48
48:A2:3727:A:H2'	48:A2:3728:G:H8	1.78	0.48
48:A2:4710:U:H3	48:A2:4909:G:H1	1.61	0.48
49:B1:520:A:O2'	49:B1:825:A:N3	2.46	0.48
49:B1:1096:G:OP1	69:BW:20:ARG:NE	2.45	0.48
49:B1:1863:A:OP2	73:Ba:4:LYS:NZ	2.47	0.48
60:BN:54:LEU:HB3	60:BN:60:VAL:HB	1.95	0.48
75:Bc:60:GLU:HG2	75:Bc:62:GLU:H	1.78	0.48
5:AC:163:LYS:NZ	48:A2:220:G:OP1	2.41	0.48
6:BC:206:SER:HB3	6:BC:211:LYS:HB2	1.96	0.48
13:AH:173:ARG:NH2	48:A2:4437:G:OP2	2.47	0.48
23:AS:13:VAL:HG22	23:AS:63:TYR:HB3	1.96	0.48
34:Ad:23:ARG:NH2	48:A2:5016:A:O5'	2.47	0.48
48:A2:179:G:O6	48:A2:251:G:N1	2.47	0.48
48:A2:1430:C:N4	48:A2:1431:G:O6	2.47	0.48
48:A2:4925:A:H2'	48:A2:4926:A:H8	1.79	0.48
49:B1:558:G:H2'	49:B1:559:G:C8	2.49	0.48
49:B1:1013:U:OP1	49:B1:1129:G:O2'	2.28	0.48
49:B1:1289:U:O2'	49:B1:1290:G:O4'	2.32	0.48
49:B1:1546:G:N3	49:B1:1670:C:O2'	2.43	0.48
71:BY:14:THR:HA	71:BY:21:LYS:HG2	1.96	0.48
1:AA:48:ILE:HG22	1:AA:59:ALA:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AC:14:LYS:HA	5:AC:173:LYS:HD3	1.96	0.48
5:AC:76:ILE:HD12	48:A2:2331:U:H5'	1.96	0.48
7:A3:123:U:O2	48:A2:2522:A:O2'	2.30	0.48
10:AE:137:VAL:CG1	48:A2:702:A:H5''	2.43	0.48
10:AE:209:PRO:HB2	10:AE:212:LEU:HD22	1.96	0.48
16:AL:48:PRO:O	16:AL:147:ALA:O	2.32	0.48
23:AS:170:LYS:CD	48:A2:4832:A:H5'	2.43	0.48
33:Ac:108:MET:N	33:Ac:108:MET:SD	2.86	0.48
48:A2:32:G:H1'	48:A2:51:A:H61	1.79	0.48
48:A2:511:C:H2'	48:A2:512:G:H8	1.78	0.48
48:A2:2531:G:H21	48:A2:2745:A:H62	1.62	0.48
48:A2:4722:G:H2'	48:A2:4723:G:H8	1.78	0.48
49:B1:189:U:OP1	55:BI:146:GLN:NE2	2.38	0.48
7:A3:142:U:OP2	18:AN:38:ARG:NH1	2.47	0.48
11:AF:73:ARG:HD3	48:A2:720:G:C6	2.49	0.48
15:AJ:35:ARG:HD3	15:AJ:123:ILE:HA	1.95	0.48
16:AL:45:ARG:O	16:AL:46:ILE:C	2.57	0.48
18:AN:84:PRO:HA	18:AN:87:HIS:CD2	2.48	0.48
30:AZ:33:THR:HB	30:AZ:35:ASP:H	1.79	0.48
38:Ah:44:LEU:N	38:Ah:44:LEU:CD1	2.77	0.48
49:B1:166:A:H5'	53:BG:112:VAL:HG21	1.95	0.48
49:B1:222:U:H5''	58:BL:17:PHE:HB2	1.96	0.48
49:B1:1454:A:H2'	64:BR:3:ARG:HH11	1.79	0.48
62:BP:23:ASP:OD1	62:BP:23:ASP:N	2.38	0.48
64:BR:97:GLU:HA	64:BR:117:LEU:HA	1.95	0.48
4:BB:30:TRP:CE3	61:BO:19:PRO:HB3	2.49	0.47
5:AC:150:LEU:CB	5:AC:151:PRO:HD3	2.37	0.47
6:BC:191:VAL:HG11	6:BC:236:PHE:HD1	1.79	0.47
10:AE:141:ARG:NE	36:Af:110:ILE:OXT	2.47	0.47
11:AF:148:LYS:HB2	48:A2:930:A:H3'	1.95	0.47
32:Ab:112:ILE:CA	48:A2:1254:G:C6	2.97	0.47
35:Ae:49:PHE:CE1	48:A2:1864:G:H5'	2.48	0.47
36:Af:41:PHE:O	36:Af:45:LYS:NZ	2.38	0.47
36:Af:50:VAL:HG22	36:Af:69:VAL:HG22	1.96	0.47
48:A2:289:A:N6	48:A2:4323:U:O2'	2.46	0.47
48:A2:1414:C:H42	48:A2:1435:A:H61	1.62	0.47
48:A2:1581:A:OP1	48:A2:2774:A:N6	2.37	0.47
51:BE:57:THR:HG23	51:BE:60:GLU:H	1.79	0.47
51:BE:179:ASN:OD1	51:BE:230:ASN:ND2	2.47	0.47
53:BG:148:SER:OG	53:BG:149:LYS:N	2.45	0.47
79:Bg:156:PHE:HA	79:Bg:165:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AC:57:LEU:HD22	5:AC:58:ALA:H	1.79	0.47
11:AF:166:ARG:HH22	11:AF:212:LYS:HD3	1.79	0.47
14:AI:171:TRP:HB2	14:AI:178:ALA:HA	1.96	0.47
48:A2:945:G:N2	48:A2:1267:G:OP2	2.47	0.47
48:A2:2714:G:H2'	48:A2:2715:G:H8	1.78	0.47
49:B1:935:G:O2'	60:BN:108:ASP:OD1	2.30	0.47
61:BO:138:ASP:OD1	61:BO:139:SER:N	2.47	0.47
65:BS:39:ARG:NH2	66:BT:39:LEU:HB3	2.29	0.47
67:BU:65:THR:HG23	76:Bd:40:ARG:HB2	1.96	0.47
5:AC:71:ARG:HH22	82:A:13:LEU:HA	1.74	0.47
5:AC:86:ARG:HD2	48:A2:370:A:H4'	1.97	0.47
5:AC:303:ARG:NH2	48:A2:2067:G:OP1	2.46	0.47
19:AO:79:ILE:HG21	19:AO:138:LEU:HD11	1.97	0.47
19:AO:82:ARG:NH1	48:A2:3858:C:OP1	2.48	0.47
48:A2:951:G:N7	48:A2:952:A:N6	2.62	0.47
49:B1:688:U:OP1	54:BH:121:THR:OG1	2.31	0.47
49:B1:1232:U:H3	49:B1:1526:G:H1	1.63	0.47
49:B1:1675:A:O2'	52:BF:74:ASN:O	2.33	0.47
67:BU:65:THR:HG21	76:Bd:44:ARG:HG3	1.96	0.47
4:BB:181:LEU:HA	4:BB:184:VAL:HG22	1.97	0.47
16:AL:63:THR:HB	16:AL:65:ARG:H	1.79	0.47
17:AM:52:PHE:O	23:AS:157:ARG:NH1	2.48	0.47
23:AS:9:GLU:OE2	23:AS:31:ARG:NE	2.45	0.47
23:AS:15:ARG:HB2	23:AS:25:PRO:HB2	1.97	0.47
32:Ab:117:ARG:CD	48:A2:1254:G:N3	2.74	0.47
46:Ap:70:THR:OG1	46:Ap:72:ASN:O	2.30	0.47
48:A2:651:C:N3	48:A2:652:C:N4	2.63	0.47
48:A2:965:G:H1	48:A2:1259:C:H42	1.61	0.47
48:A2:4199:C:H2'	48:A2:4200:G:H8	1.79	0.47
64:BR:98:VAL:HG23	64:BR:102:THR:HG21	1.96	0.47
79:Bg:88:ARG:HG2	79:Bg:97:THR:OG1	2.15	0.47
82:A:19:ALA:C	82:A:21:ALA:N	2.72	0.47
22:AR:26:PRO:O	22:AR:29:THR:OG1	2.31	0.47
34:Ad:111:VAL:HG21	34:Ad:117:LEU:HD11	1.95	0.47
37:Ag:5:LEU:HD11	37:Ag:22:LEU:HD22	1.97	0.47
38:Ah:87:LYS:HG2	40:Aj:78:PHE:HB3	1.97	0.47
48:A2:2398:C:H2'	48:A2:2399:A:H8	1.79	0.47
49:B1:5:U:H2'	49:B1:6:G:H8	1.79	0.47
49:B1:1293:A:O2'	78:Bf:138:ARG:NH2	2.40	0.47
71:BY:91:LEU:HB3	71:BY:96:LEU:HB2	1.96	0.47
80:Bv:20:U:H2'	80:Bv:21:A:H4'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A3:148:A:N3	12:AG:60:TYR:OH	2.39	0.47
8:A4:75:G:O2'	8:A4:99:G:O6	2.24	0.47
17:AM:32:ASP:OD1	17:AM:32:ASP:N	2.44	0.47
26:AV:115:SER:O	26:AV:135:ASN:ND2	2.48	0.47
31:Aa:32:ARG:HD2	48:A2:37:U:H4'	1.96	0.47
36:Af:47:CYS:N	36:Af:72:GLY:O	2.43	0.47
48:A2:198:C:H42	48:A2:209:A:H61	1.61	0.47
48:A2:482:G:H22	48:A2:662:A:H2	1.61	0.47
48:A2:4069:G:H5''	48:A2:4070:C:H5	1.79	0.47
49:B1:559:G:C2	49:B1:561:A:H1'	2.50	0.47
51:BE:125:LYS:H	51:BE:142:HIS:CE1	2.32	0.47
56:BJ:138:ARG:NH2	56:BJ:153:SER:CA	2.67	0.47
3:AB:22:SER:OG	3:AB:24:ARG:O	2.25	0.47
5:AC:114:ARG:HD2	48:A2:1489:C:H5'	1.95	0.47
6:BC:171:GLY:HA3	69:BW:97:ARG:HG2	1.95	0.47
11:AF:47:ARG:HH12	48:A2:962:C:H4'	1.80	0.47
12:AG:102:TYR:OH	12:AG:208:ASN:N	2.45	0.47
15:AJ:141:ILE:HG22	15:AJ:149:GLY:N	2.30	0.47
19:AO:26:GLN:OE1	19:AO:31:ARG:NH1	2.47	0.47
20:AP:134:GLY:O	48:A2:2773:C:N4	2.47	0.47
23:AS:93:MET:HG3	48:A2:1933:G:H4'	1.96	0.47
24:AT:129:LYS:HE3	48:A2:1817:G:H4'	1.97	0.47
47:At:63:VAL:HG22	47:At:79:ARG:HG2	1.96	0.47
48:A2:1303:U:O2'	48:A2:1872:A:N1	2.44	0.47
48:A2:2643:G:H4'	48:A2:2656:G:H4'	1.96	0.47
48:A2:3930:U:H2'	48:A2:3931:A:C8	2.49	0.47
48:A2:4381:U:OP1	48:A2:4437:G:N2	2.46	0.47
48:A2:4722:G:H2'	48:A2:4723:G:C8	2.50	0.47
49:B1:381:C:OP2	55:BI:54:LYS:NZ	2.43	0.47
49:B1:831:G:N7	71:BY:11:LYS:NZ	2.63	0.47
52:BF:158:ALA:HB2	52:BF:173:LEU:HD23	1.96	0.47
55:BI:6:ASP:OD2	55:BI:8:TRP:NE1	2.47	0.47
55:BI:13:LYS:HE3	58:BL:137:THR:HG22	1.96	0.47
59:BM:75:ASN:HB3	59:BM:128:PHE:CE2	2.50	0.47
66:BT:15:VAL:HG22	66:BT:58:ALA:HB1	1.97	0.47
70:BX:94:ILE:HD11	70:BX:130:LEU:HD11	1.96	0.47
73:Ba:95:ARG:HG3	73:Ba:96:THR:H	1.79	0.47
74:Bb:49:HIS:CE1	74:Bb:70:LYS:HB3	2.50	0.47
79:Bg:126:ASP:OD1	79:Bg:128:THR:OG1	2.30	0.47
79:Bg:242:SER:HB3	79:Bg:247:TRP:HB2	1.97	0.47
3:AB:261:ARG:HD2	48:A2:3841:C:H4'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AE:136:HIS:HD2	48:A2:702:A:O4'	1.98	0.47
11:AF:59:LYS:NZ	48:A2:1195:G:OP1	2.38	0.47
14:AI:183:ASP:O	14:AI:187:GLU:OE2	2.33	0.47
17:AM:38:VAL:HG11	17:AM:55:MET:HE1	1.96	0.47
41:Ak:26:LYS:HE3	48:A2:2674:A:H5''	1.97	0.47
48:A2:404:A:O2'	48:A2:408:C:O2'	2.30	0.47
48:A2:511:C:H2'	48:A2:512:G:C8	2.50	0.47
48:A2:1481:C:N4	48:A2:1482:A:N1	2.63	0.47
48:A2:1951:A:H2'	48:A2:1984:G:H22	1.79	0.47
48:A2:2056:G:H2'	48:A2:2057:G:H8	1.79	0.47
48:A2:2390:C:O2'	48:A2:2505:C:O2	2.30	0.47
49:B1:655:A:H4'	49:B1:656:G:H3'	1.97	0.47
54:BH:39:GLN:HE22	54:BH:43:LEU:HD22	1.80	0.47
5:AC:31:PRO:HB3	21:AQ:24:TYR:HE2	1.80	0.47
7:A3:91:A:H5'	29:AY:22:PRO:HB3	1.96	0.47
21:AQ:122:THR:OG1	21:AQ:124:ASP:OD1	2.32	0.47
30:AZ:48:ARG:NH2	48:A2:2554:U:OP1	2.47	0.47
35:Ae:57:ASN:ND2	48:A2:1880:G:O3'	2.48	0.47
41:Ak:20:ALA:HA	41:Ak:38:CYS:HA	1.96	0.47
42:Al:36:ARG:HH22	48:A2:407:G:H5'	1.80	0.47
48:A2:900:U:N3	48:A2:901:U:O4	2.48	0.47
48:A2:1496:U:H2'	48:A2:1497:A:C8	2.50	0.47
48:A2:1943:A:N7	48:A2:2006:A:N6	2.63	0.47
48:A2:2688:C:C4	48:A2:2689:C:H1'	2.50	0.47
49:B1:1332:A:H62	49:B1:1493:C:H42	1.61	0.47
49:B1:1613:G:OP2	62:BP:39:ALA:N	2.46	0.47
6:BC:168:GLY:N	6:BC:179:THR:O	2.39	0.47
12:AG:192:ARG:HD3	12:AG:192:ARG:HA	1.61	0.47
21:AQ:143:ARG:HH12	48:A2:1675:U:H5'	1.80	0.47
36:Af:8:LYS:HD3	48:A2:4714:U:H5'	1.97	0.47
37:Ag:55:GLY:N	48:A2:2662:C:O2'	2.46	0.47
48:A2:108:A:O2'	48:A2:328:A:N6	2.47	0.47
48:A2:116:G:H1	48:A2:153:G:H1	1.63	0.47
48:A2:3931:A:N3	48:A2:4014:U:O2'	2.44	0.47
48:A2:4713:G:N2	48:A2:4907:G:O6	2.39	0.47
49:B1:65:C:N4	53:BG:134:GLY:O	2.37	0.47
49:B1:1116:C:O2'	49:B1:1118:C:N4	2.36	0.47
3:AB:14:LEU:O	48:A2:4549:G:O2'	2.30	0.46
3:AB:254:ILE:HD13	48:A2:3868:G:H4'	1.97	0.46
4:BB:71:LEU:HD22	4:BB:75:GLN:HG2	1.97	0.46
18:AN:195:ARG:NH1	48:A2:98:A:H4'	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AP:131:ARG:HH21	48:A2:1578:U:H2'	1.80	0.46
48:A2:66:A:N6	48:A2:276:C:O2'	2.48	0.46
48:A2:666:G:H2'	48:A2:667:C:H6	1.80	0.46
48:A2:1059:C:H42	48:A2:1218:G:H1	1.63	0.46
49:B1:16:G:H21	49:B1:1195:A:H62	1.62	0.46
49:B1:456:C:O2	49:B1:1800:A:O2'	2.26	0.46
49:B1:1133:A:H4'	73:Ba:13:LYS:HD3	1.97	0.46
59:BM:64:LEU:HD23	78:Bf:108:VAL:HG23	1.97	0.46
61:BO:40:THR:O	61:BO:58:GLY:N	2.47	0.46
7:A3:87:G:OP2	38:Ah:5:LYS:NZ	2.48	0.46
16:AL:129:ARG:HB3	16:AL:130:LYS:HD2	1.96	0.46
18:AN:120:TRP:HZ2	18:AN:123:GLU:HG2	1.80	0.46
19:AO:121:PRO:HD3	23:AS:168:THR:HG22	1.96	0.46
23:AS:170:LYS:HD3	48:A2:4832:A:C5'	2.45	0.46
32:Ab:117:ARG:NH2	48:A2:1222:C:OP2	2.25	0.46
48:A2:1979:A:N3	48:A2:2000:C:O2'	2.42	0.46
48:A2:3798:G:O2'	48:A2:3800:G:OP2	2.29	0.46
48:A2:4170:U:OP1	48:A2:4296:U:O2'	2.33	0.46
48:A2:4970:G:O2'	48:A2:4972:A:OP2	2.33	0.46
49:B1:652:U:H2'	49:B1:653:A:H8	1.80	0.46
49:B1:1507:G:H22	78:Bf:88:PRO:HD2	1.80	0.46
64:BR:96:ILE:C	64:BR:115:SER:OG	2.52	0.46
15:AJ:18:ARG:HB3	15:AJ:133:VAL:HG23	1.97	0.46
15:AJ:21:CYS:SG	48:A2:4221:C:O2'	2.63	0.46
18:AN:146:PRO:HA	18:AN:149:GLN:HG3	1.97	0.46
19:AO:165:LYS:NZ	48:A2:4720:U:O2	2.35	0.46
47:At:111:ILE:O	47:At:115:SER:N	2.38	0.46
48:A2:1520:U:O2'	48:A2:1611:G:OP1	2.28	0.46
48:A2:4439:A:N3	48:A2:4565:C:O2'	2.42	0.46
49:B1:86:C:O2'	49:B1:171:A:N1	2.41	0.46
49:B1:126:G:O2'	49:B1:180:G:N2	2.48	0.46
49:B1:1208:A:OP1	49:B1:1837:G:N2	2.42	0.46
54:BH:69:LEU:HD12	54:BH:96:ALA:HB2	1.97	0.46
56:BJ:111:GLN:HA	56:BJ:114:VAL:HB	1.98	0.46
63:BQ:19:ALA:HA	63:BQ:74:GLY:HA2	1.98	0.46
66:BT:134:ILE:HA	66:BT:137:GLN:HG2	1.97	0.46
79:Bg:196:ASN:ND2	79:Bg:236:ILE:O	2.36	0.46
10:AE:228:GLN:HA	48:A2:447:G:C2	2.51	0.46
16:AL:89:LYS:HD2	38:Ah:114:TYR:HD2	1.81	0.46
16:AL:93:THR:HB	38:Ah:117:ARG:HG2	1.98	0.46
36:Af:56:ASN:HB3	36:Af:64:PRO:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:B1:84:A:H5''	71:BY:122:LYS:HE2	1.97	0.46
49:B1:563:G:H1	49:B1:592:C:H5	1.64	0.46
49:B1:1402:A:H1'	67:BU:54:VAL:HG13	1.97	0.46
52:BF:86:LYS:HA	52:BF:89:THR:HG22	1.98	0.46
80:Bv:52:G:H2'	80:Bv:53:G:C8	2.50	0.46
10:AE:240:TYR:OH	48:A2:4896:A:O3'	2.33	0.46
15:AJ:23:ASN:HB3	15:AJ:129:ASP:HB3	1.97	0.46
18:AN:194:ARG:NH2	48:A2:79:C:OP2	2.48	0.46
32:Ab:111:ARG:HA	32:Ab:116:LEU:N	2.31	0.46
47:At:23:GLN:NE2	47:At:25:TYR:OH	2.46	0.46
48:A2:976:U:O2	48:A2:1047:G:N1	2.41	0.46
48:A2:2626:A:H3'	48:A2:2627:G:H8	1.80	0.46
48:A2:3727:A:H2'	48:A2:3728:G:C8	2.50	0.46
49:B1:1815:A:H3'	49:B1:1816:G:H8	1.80	0.46
57:BK:65:ARG:NH2	76:Bd:21:CYS:O	2.45	0.46
60:BN:5:HIS:HB3	60:BN:117:LEU:HD13	1.98	0.46
64:BR:73:LEU:C	64:BR:77:GLU:HG2	2.35	0.46
69:BW:102:ILE:H	69:BW:113:HIS:HB2	1.80	0.46
2:BA:136:GLU:HA	2:BA:139:TYR:HD2	1.80	0.46
3:AB:268:ARG:NH1	48:A2:3867:C:O2'	2.49	0.46
9:AD:30:TYR:HA	9:AD:33:ARG:HB3	1.96	0.46
15:AJ:90:ARG:NH2	15:AJ:108:GLY:O	2.41	0.46
15:AJ:127:GLY:HA3	48:A2:4213:A:C4	2.51	0.46
18:AN:178:HIS:NE2	48:A2:308:G:OP1	2.48	0.46
30:AZ:11:VAL:HG21	30:AZ:80:LEU:HD22	1.98	0.46
30:AZ:83:THR:HG23	30:AZ:85:TYR:H	1.81	0.46
35:Ae:59:GLY:HA2	48:A2:1880:G:H21	1.80	0.46
48:A2:691:G:H2'	48:A2:692:G:H8	1.81	0.46
48:A2:1784:A:O2'	48:A2:1818:A:OP1	2.34	0.46
48:A2:2599:G:H1	48:A2:2615:U:H3	1.63	0.46
49:B1:431:G:H2'	49:B1:432:G:C8	2.51	0.46
54:BH:20:GLU:HG2	54:BH:48:ALA:HB3	1.96	0.46
4:BB:30:TRP:O	4:BB:94:LYS:NZ	2.47	0.46
6:BC:266:TYR:O	6:BC:270:THR:OG1	2.24	0.46
18:AN:19:MET:HE1	18:AN:23:LEU:HD13	1.98	0.46
28:AX:95:THR:HA	28:AX:139:ARG:HA	1.96	0.46
31:Aa:132:ARG:NH2	48:A2:1450:C:OP1	2.47	0.46
32:Ab:3:LYS:NZ	48:A2:4157:G:O4'	2.39	0.46
48:A2:1748:A:O2'	48:A2:1749:A:O4'	2.32	0.46
49:B1:1726:G:H2'	49:B1:1727:G:H8	1.81	0.46
51:BE:256:LEU:HD21	56:BJ:79:ARG:HH22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:BN:22:VAL:HG21	60:BN:26:LEU:HD23	1.97	0.46
63:BQ:16:LYS:HG3	63:BQ:17:LYS:H	1.80	0.46
63:BQ:109:LYS:HE3	63:BQ:120:LEU:HG	1.98	0.46
70:BX:73:GLN:NE2	70:BX:78:GLY:O	2.49	0.46
5:AC:150:LEU:HD12	5:AC:151:PRO:HD3	1.98	0.46
26:AV:30:ASP:OD1	26:AV:30:ASP:N	2.48	0.46
37:Ag:90:ARG:NH1	48:A2:4091:G:O3'	2.49	0.46
39:Ai:82:ARG:HH12	48:A2:277:G:H1'	1.81	0.46
40:Aj:60:GLY:HA2	40:Aj:64:MET:HE2	1.98	0.46
48:A2:1228:C:H2'	48:A2:1229:G:C8	2.51	0.46
48:A2:1727:G:H2'	48:A2:1728:A:H8	1.81	0.46
48:A2:1727:G:H1	48:A2:1767:C:H42	1.63	0.46
48:A2:4075:G:H5''	48:A2:4076:G:C8	2.51	0.46
48:A2:4698:C:H2'	48:A2:4699:G:C8	2.51	0.46
54:BH:20:GLU:OE2	54:BH:48:ALA:N	2.47	0.46
57:BK:75:GLY:O	57:BK:79:LEU:N	2.48	0.46
69:BW:11:LEU:HD22	69:BW:72:CYS:HB2	1.96	0.46
79:Bg:40:ILE:HD11	79:Bg:66:VAL:HG21	1.98	0.46
1:AA:200:ARG:NE	48:A2:3622:A:OP1	2.46	0.46
4:BB:51:ARG:HD3	4:BB:51:ARG:N	2.14	0.46
5:AC:150:LEU:N	47:At:71:ARG:O	2.41	0.46
10:AE:168:LEU:HD11	10:AE:174:LEU:HD12	1.98	0.46
17:AM:40:GLY:HA3	17:AM:45:VAL:HG12	1.96	0.46
36:Af:4:ARG:HH12	36:Af:8:LYS:HE2	1.80	0.46
48:A2:176:G:O6	48:A2:252:C:N4	2.47	0.46
48:A2:494:G:N2	48:A2:498:G:N3	2.64	0.46
48:A2:1289:C:H2'	48:A2:1290:A:H8	1.80	0.46
48:A2:4410:G:H5''	48:A2:4411:A:H5''	1.96	0.46
49:B1:678:U:OP2	49:B1:1026:C:N4	2.33	0.46
49:B1:1061:U:O2	49:B1:1848:U:O2'	2.34	0.46
49:B1:1075:C:H2'	49:B1:1076:G:C8	2.51	0.46
59:BM:62:VAL:HG23	59:BM:63:LYS:HG3	1.98	0.46
64:BR:102:THR:CG2	64:BR:117:LEU:HD11	2.17	0.46
66:BT:41:LYS:HE3	66:BT:95:GLY:HA2	1.98	0.46
1:AA:247:ARG:HG3	49:B1:1069:U:H4'	1.98	0.46
2:BA:25:LEU:HD13	2:BA:46:ILE:HG21	1.98	0.46
4:BB:97:LEU:HD22	4:BB:98:THR:H	1.81	0.46
8:A4:75:G:N2	8:A4:76:U:O4	2.47	0.46
16:AL:49:ARG:NH1	38:Ah:118:LYS:CA	2.68	0.46
21:AQ:143:ARG:NH1	48:A2:1674:C:O3'	2.49	0.46
48:A2:473:G:H1	48:A2:669:G:H1	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A2:479:C:H4'	48:A2:480:C:H5'	1.98	0.46
48:A2:1855:A:O3'	48:A2:4179:G:N2	2.49	0.46
48:A2:2501:G:H21	48:A2:2690:G:N2	2.14	0.46
49:B1:1383:A:H4'	50:BD:156:LEU:HD11	1.98	0.46
49:B1:1866:A:H1'	73:Ba:95:ARG:HA	1.97	0.46
79:Bg:82:SER:OG	79:Bg:83:TRP:N	2.48	0.46
80:Bv:18:G:H1	80:Bv:55:U:H1'	1.81	0.46
3:AB:21:ARG:HB2	3:AB:274:TYR:HD2	1.81	0.45
4:BB:79:VAL:HG21	4:BB:82:ARG:HD3	1.99	0.45
5:AC:228:THR:HG21	5:AC:239:LYS:HD2	1.98	0.45
8:A4:22:A:N7	8:A4:23:A:N6	2.65	0.45
22:AR:103:ARG:O	22:AR:107:ARG:NH1	2.49	0.45
33:Ac:44:LYS:HB3	33:Ac:105:ILE:HG21	1.98	0.45
48:A2:112:C:H2'	48:A2:113:A:H8	1.81	0.45
48:A2:4539:U:H2'	48:A2:4540:G:H8	1.81	0.45
49:B1:939:U:H2'	49:B1:940:U:H6	1.81	0.45
49:B1:1220:A:N3	49:B1:1677:U:O2'	2.40	0.45
49:B1:1256:G:N2	76:Bd:39:CYS:O	2.48	0.45
49:B1:1447:G:H2'	49:B1:1448:A:H8	1.81	0.45
58:BL:7:GLU:OE1	58:BL:12:LYS:N	2.37	0.45
71:BY:29:HIS:CE1	71:BY:35:VAL:H	2.33	0.45
72:BZ:101:SER:OG	72:BZ:102:LYS:N	2.47	0.45
73:Ba:30:VAL:HG21	73:Ba:74:CYS:HB2	1.98	0.45
6:BC:139:LEU:HD11	6:BC:237:ALA:HB1	1.98	0.45
10:AE:112:MET:HE2	47:At:94:ARG:HH12	1.81	0.45
14:Al:47:PRO:O	14:Al:172:GLY:N	2.49	0.45
16:AL:46:ILE:HB	16:AL:47:ALA:H	1.53	0.45
19:AO:90:HIS:NE2	48:A2:3857:G:OP2	2.48	0.45
27:AW:61:LYS:H	27:AW:64:SER:HB3	1.81	0.45
30:AZ:53:VAL:HG23	30:AZ:62:ILE:HD11	1.99	0.45
48:A2:241:G:H22	48:A2:1349:G:H1	1.63	0.45
49:B1:63:U:O2'	49:B1:170:A:N3	2.45	0.45
49:B1:439:A:HO2'	49:B1:1799:G:HO2'	1.59	0.45
49:B1:1310:U:H5'	78:Bf:130:VAL:HG22	1.99	0.45
49:B1:1648:G:H3'	63:BQ:127:CYS:HA	1.98	0.45
65:BS:68:ILE:HA	65:BS:71:MET:HB2	1.96	0.45
77:Be:52:LYS:H	77:Be:52:LYS:HD2	1.82	0.45
79:Bg:70:VAL:HG13	79:Bg:79:LEU:HB2	1.99	0.45
48:A2:4157:G:O2'	48:A2:4404:U:OP1	2.30	0.45
48:A2:4964:U:H4'	48:A2:4965:A:H5'	1.97	0.45
49:B1:1263:U:H1'	76:Bd:16:GLN:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BD:30:ALA:O	50:BD:107:TYR:OH	2.25	0.45
69:BW:11:LEU:HD23	69:BW:11:LEU:HA	1.82	0.45
72:BZ:99:LEU:HA	72:BZ:109:TYR:HA	1.97	0.45
11:AF:134:ARG:HA	11:AF:137:GLU:HG3	1.98	0.45
15:AJ:99:PHE:HA	15:AJ:105:PHE:HB3	1.99	0.45
15:AJ:100:SER:N	15:AJ:104:ASN:O	2.49	0.45
21:AQ:73:PRO:O	48:A2:1438:G:O2'	2.27	0.45
21:AQ:180:ARG:NH2	48:A2:1479:A:OP1	2.49	0.45
23:AS:71:SER:O	23:AS:76:LYS:NZ	2.49	0.45
35:Ae:26:ASP:OD1	35:Ae:26:ASP:N	2.49	0.45
48:A2:3602:U:O2'	48:A2:3776:U:OP1	2.28	0.45
49:B1:494:C:OP1	51:BE:57:THR:OG1	2.30	0.45
60:BN:84:LEU:HD22	60:BN:149:LEU:HD23	1.99	0.45
3:AB:330:PHE:HE2	3:AB:332:MET:HE3	1.81	0.45
19:AO:182:GLU:HA	19:AO:187:LYS:HZ1	1.81	0.45
31:Aa:110:LYS:NZ	48:A2:1379:G:N7	2.45	0.45
48:A2:466:C:H42	48:A2:677:G:H22	1.65	0.45
48:A2:746:C:H2'	48:A2:747:G:C8	2.51	0.45
48:A2:3672:C:H4'	48:A2:3673:A:H5'	1.99	0.45
49:B1:659:G:O2'	49:B1:662:G:O2'	2.35	0.45
49:B1:1859:A:OP2	73:Ba:10:ARG:NH2	2.50	0.45
64:BR:77:GLU:HA	64:BR:77:GLU:OE1	2.16	0.45
65:BS:110:ASP:OD1	65:BS:113:ARG:NH2	2.48	0.45
75:Bc:41:SER:OG	75:Bc:42:ILE:N	2.49	0.45
14:AI:152:LEU:HB2	14:AI:165:ILE:HD12	1.98	0.45
19:AO:36:VAL:HG12	19:AO:108:ILE:HG12	1.97	0.45
21:AQ:144:LYS:HB3	48:A2:1442:C:H5''	1.99	0.45
47:At:28:GLU:OE2	47:At:31:ASN:ND2	2.50	0.45
48:A2:1572:C:O2	48:A2:1587:G:N2	2.50	0.45
48:A2:2353:A:H2'	48:A2:2354:A:C8	2.51	0.45
48:A2:4058:C:H2'	48:A2:4059:G:C8	2.51	0.45
48:A2:4726:A:H61	48:A2:4826:G:H1	1.62	0.45
49:B1:1249:C:OP2	49:B1:1250:A:O2'	2.34	0.45
49:B1:1451:G:H5'	79:Bg:64:HIS:NE2	2.32	0.45
49:B1:1649:U:H2'	49:B1:1650:A:H8	1.82	0.45
49:B1:1805:G:H2'	49:B1:1806:A:C8	2.51	0.45
54:BH:170:VAL:HG13	54:BH:187:PHE:HB2	1.98	0.45
60:BN:46:THR:HB	60:BN:49:GLN:H	1.82	0.45
62:BP:39:ALA:HA	62:BP:42:ARG:HE	1.82	0.45
76:Bd:16:GLN:O	76:Bd:27:ARG:NH1	2.49	0.45
79:Bg:167:SER:N	79:Bg:175:LYS:O	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:158:ILE:HD12	1:AA:162:ASN:HD21	1.81	0.45
3:AB:276:HIS:O	3:AB:277:ARG:NH1	2.45	0.45
21:AQ:122:THR:O	21:AQ:126:LEU:N	2.48	0.45
23:AS:170:LYS:HG2	48:A2:4832:A:OP1	2.17	0.45
48:A2:734:G:H1	48:A2:908:C:H42	1.63	0.45
48:A2:2713:U:H2'	48:A2:2714:G:C8	2.51	0.45
48:A2:2857:G:H4'	48:A2:3796:A:H5''	1.97	0.45
49:B1:391:C:H2'	49:B1:392:A:H8	1.82	0.45
49:B1:623:G:N7	70:BX:63:ASN:ND2	2.54	0.45
49:B1:1659:U:H1'	76:Bd:30:LEU:HD22	1.97	0.45
49:B1:1743:G:H1'	49:B1:1792:G:N2	2.31	0.45
56:BJ:136:ARG:HH22	56:BJ:139:LYS:C	1.99	0.45
59:BM:77:ILE:HB	59:BM:128:PHE:HE1	1.82	0.45
59:BM:94:ILE:HG22	59:BM:100:PRO:HA	1.99	0.45
80:Bv:55:U:H2'	80:Bv:56:C:H3'	1.98	0.45
4:BB:48:LEU:O	4:BB:49:VAL:CG2	2.64	0.45
4:BB:136:ARG:HD2	4:BB:216:LYS:HZ1	1.78	0.45
5:AC:147:VAL:O	47:At:74:ALA:HB2	2.17	0.45
8:A4:4:U:H2'	8:A4:5:A:H8	1.81	0.45
8:A4:13:A:OP1	8:A4:109:U:O2'	2.33	0.45
8:A4:112:U:H2'	8:A4:113:G:H8	1.82	0.45
10:AE:140:LEU:CA	10:AE:191:GLN:NE2	2.66	0.45
18:AN:93:LYS:O	48:A2:294:A:O2'	2.34	0.45
48:A2:502:G:O2'	48:A2:504:U:OP2	2.32	0.45
48:A2:944:G:O2'	48:A2:2058:C:OP1	2.34	0.45
49:B1:1466:G:N7	64:BR:3:ARG:NH2	2.59	0.45
50:BD:137:VAL:HB	50:BD:185:LYS:HB2	1.99	0.45
65:BS:88:LYS:HA	65:BS:95:TYR:CE1	2.50	0.45
1:AA:9:ARG:NH2	48:A2:1611:G:O6	2.50	0.45
3:AB:278:THR:O	3:AB:278:THR:OG1	2.32	0.45
4:BB:36:PRO:HD3	4:BB:98:THR:HG23	1.98	0.45
5:AC:212:ASN:HD22	5:AC:259:LYS:HD2	1.82	0.45
6:BC:78:LEU:HD12	6:BC:81:ILE:HD12	1.99	0.45
13:AH:11:ASP:OD1	13:AH:11:ASP:N	2.49	0.45
16:AL:46:ILE:H	16:AL:46:ILE:HG12	1.58	0.45
16:AL:47:ALA:HB3	16:AL:48:PRO:CD	2.24	0.45
19:AO:63:ASN:ND2	48:A2:2026:G:OP1	2.43	0.45
30:AZ:103:ASP:OD2	30:AZ:106:LEU:N	2.38	0.45
36:Af:45:LYS:HA	36:Af:107:PRO:HG3	1.99	0.45
48:A2:1076:C:O2	48:A2:1186:G:N2	2.50	0.45
48:A2:3687:C:N3	48:A2:3706:G:O2'	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A2:3939:U:H2'	48:A2:3940:G:H8	1.81	0.45
48:A2:4684:G:OP2	48:A2:4684:G:N2	2.47	0.45
50:BD:40:ARG:HA	67:BU:108:PRO:HB3	1.98	0.45
79:Bg:165:ILE:HG13	79:Bg:177:TRP:HB2	1.99	0.45
79:Bg:213:ASP:OD1	79:Bg:213:ASP:N	2.50	0.45
2:BA:18:PHE:HA	2:BA:173:LEU:HD21	1.98	0.45
3:AB:175:GLN:NE2	3:AB:177:LYS:HB3	2.31	0.45
5:AC:292:ILE:HG21	21:AQ:31:LEU:HD11	1.99	0.45
8:A4:3:C:OP1	8:A4:58:A:O2'	2.27	0.45
8:A4:112:U:H2'	8:A4:113:G:C8	2.52	0.45
10:AE:197:THR:HA	10:AE:288:PHE:HB3	1.98	0.45
15:AJ:174:ILE:HD13	15:AJ:174:ILE:HA	1.82	0.45
20:AP:148:MET:HE2	20:AP:148:MET:HB3	1.79	0.45
21:AQ:172:ARG:HD2	31:Aa:57:GLY:HA3	1.99	0.45
32:Ab:111:ARG:HB3	32:Ab:117:ARG:HG3	1.99	0.45
48:A2:1977:C:N4	48:A2:1978:U:O2	2.49	0.45
48:A2:3741:U:O2'	80:Bv:12:U:O2'	2.26	0.45
48:A2:3933:A:OP1	48:A2:4013:G:N2	2.49	0.45
48:A2:4008:C:O2	48:A2:4020:A:O2'	2.33	0.45
49:B1:981:A:O2'	49:B1:1044:G:OP1	2.26	0.45
49:B1:1753:C:O2	49:B1:1780:G:N2	2.50	0.45
55:BI:83:TYR:HD2	55:BI:101:ILE:HD12	1.81	0.45
71:BY:6:THR:HB	71:BY:28:LEU:HB3	1.99	0.45
2:BA:16:LEU:HD12	64:BR:91:LEU:HD22	1.98	0.44
3:AB:17:LEU:O	3:AB:19:ARG:N	2.50	0.44
11:AF:44:LYS:HZ2	11:AF:44:LYS:HB2	1.82	0.44
15:AJ:32:ARG:O	15:AJ:126:TYR:OH	2.29	0.44
18:AN:85:VAL:HG23	48:A2:43:U:H5''	1.99	0.44
32:Ab:25:ARG:HD2	32:Ab:26:SER:HB3	1.98	0.44
32:Ab:28:ARG:NH1	48:A2:1407:G:O2'	2.50	0.44
48:A2:138:C:H2'	48:A2:139:G:H8	1.82	0.44
48:A2:736:G:O2'	48:A2:738:A:OP2	2.35	0.44
48:A2:4049:C:H2'	48:A2:4050:C:H6	1.81	0.44
49:B1:346:C:O3'	51:BE:30:ARG:NH2	2.50	0.44
49:B1:1513:C:H5''	76:Bd:9:SER:H	1.82	0.44
78:Bf:138:ARG:NH1	78:Bf:149:CYS:SG	2.90	0.44
2:BA:50:ASN:HD21	2:BA:53:ARG:HD2	1.82	0.44
3:AB:117:ARG:HH12	48:A2:4943:U:P	2.39	0.44
5:AC:44:LEU:HD21	5:AC:120:LYS:HE2	1.99	0.44
7:A3:60:G:O6	38:Ah:62:ASN:ND2	2.50	0.44
13:AH:124:ARG:NH1	13:AH:164:ALA:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AL:133:ALA:HA	16:AL:136:LYS:HD3	1.96	0.44
29:AY:79:VAL:HG13	29:AY:98:GLY:HA3	1.99	0.44
48:A2:458:G:N2	48:A2:684:U:H3	2.14	0.44
48:A2:1072:G:H2'	48:A2:1073:G:H8	1.82	0.44
48:A2:2599:G:H2'	48:A2:2600:A:H8	1.81	0.44
48:A2:3703:A:H2'	48:A2:3704:A:C8	2.52	0.44
48:A2:4933:G:O2'	48:A2:4935:A:N6	2.47	0.44
49:B1:156:G:OP1	53:BG:2:LYS:NZ	2.50	0.44
49:B1:195:C:N4	49:B1:205:G:O6	2.50	0.44
49:B1:1495:G:O3'	76:Bd:26:ASN:ND2	2.47	0.44
51:BE:125:LYS:H	51:BE:142:HIS:HE1	1.65	0.44
55:BI:139:LYS:HB3	55:BI:144:LYS:HB2	2.00	0.44
56:BJ:14:VAL:HG23	56:BJ:48:PHE:HB2	2.00	0.44
58:BL:59:LYS:HD3	58:BL:134:LEU:HD23	2.00	0.44
73:Ba:47:ALA:O	73:Ba:51:ARG:NH1	2.50	0.44
79:Bg:17:TRP:N	79:Bg:36:ARG:HB2	2.31	0.44
4:BB:132:GLY:HA3	4:BB:221:PRO:HG3	1.98	0.44
7:A3:57:C:O2	7:A3:61:A:O2'	2.30	0.44
32:Ab:108:ALA:HB3	32:Ab:109:ARG:HE	1.82	0.44
41:Ak:30:ASP:OD1	41:Ak:30:ASP:N	2.49	0.44
45:Ao:8:ARG:NH2	48:A2:4254:A:O2'	2.50	0.44
48:A2:691:G:H2'	48:A2:692:G:C8	2.52	0.44
48:A2:735:G:H2'	48:A2:736:G:C8	2.52	0.44
48:A2:1975:C:H2'	48:A2:1976:G:H8	1.82	0.44
48:A2:2353:A:H2'	48:A2:2354:A:H8	1.82	0.44
49:B1:445:A:H5''	55:BI:47:ARG:HH22	1.82	0.44
49:B1:688:U:H3	54:BH:103:LYS:H	1.65	0.44
66:BT:38:LYS:HD3	66:BT:47:PRO:HG3	1.99	0.44
66:BT:75:MET:HB2	66:BT:121:ARG:HH12	1.82	0.44
80:Bv:28:G:H2'	80:Bv:29:G:H8	1.82	0.44
3:AB:25:HIS:HE1	48:A2:4942:C:H4'	1.81	0.44
3:AB:63:PRO:O	3:AB:357:ARG:NH2	2.50	0.44
3:AB:220:ILE:HD11	3:AB:348:ARG:HE	1.82	0.44
4:BB:48:LEU:C	4:BB:49:VAL:HG23	2.41	0.44
4:BB:108:ASP:OD1	4:BB:109:LYS:N	2.50	0.44
7:A3:6:C:H2'	7:A3:7:U:H6	1.82	0.44
7:A3:80:A:H1'	38:Ah:3:LYS:HD3	2.00	0.44
12:AG:95:LEU:HD11	12:AG:204:PHE:HE2	1.82	0.44
39:Ai:53:TYR:CE1	48:A2:299:A:H5'	2.52	0.44
48:A2:416:C:H2'	48:A2:417:G:C8	2.50	0.44
48:A2:2328:A:H5''	48:A2:2329:U:H5''	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A2:2869:C:H42	48:A2:3582:A:H61	1.64	0.44
48:A2:4480:A:OP1	48:A2:4482:G:O2'	2.27	0.44
49:B1:857:U:H2'	49:B1:858:A:C8	2.53	0.44
49:B1:893:U:H2'	49:B1:894:G:C8	2.52	0.44
49:B1:1648:G:N2	49:B1:1675:A:OP2	2.50	0.44
51:BE:123:LEU:HD22	51:BE:159:THR:HG22	2.00	0.44
55:BI:96:LEU:HD22	55:BI:175:ILE:HD11	2.00	0.44
68:BV:32:ILE:HD12	68:BV:32:ILE:HA	1.74	0.44
4:BB:48:LEU:C	4:BB:49:VAL:CG2	2.91	0.44
9:AD:153:THR:O	9:AD:153:THR:OG1	2.34	0.44
12:AG:47:PRO:HG2	12:AG:49:ARG:HG3	2.00	0.44
35:Ae:57:ASN:N	35:Ae:57:ASN:OD1	2.48	0.44
41:Ak:13:LEU:HD13	41:Ak:16:ARG:HH21	1.83	0.44
48:A2:633:U:H4'	48:A2:634:C:H5'	1.99	0.44
48:A2:4062:G:H3'	48:A2:4063:G:H21	1.81	0.44
49:B1:817:G:H21	49:B1:847:A:H62	1.65	0.44
51:BE:11:ARG:HH12	51:BE:24:THR:HB	1.80	0.44
52:BF:145:ARG:HA	52:BF:148:ASN:HB2	2.00	0.44
53:BG:227:GLN:HB3	53:BG:231:ARG:HH12	1.82	0.44
58:BL:6:THR:HG1	58:BL:8:ARG:NH1	2.14	0.44
61:BO:128:ARG:HA	73:Ba:63:VAL:HG21	1.99	0.44
65:BS:114:LEU:HB3	65:BS:122:GLY:HA3	2.00	0.44
67:BU:40:ILE:HD12	67:BU:44:LYS:HE3	1.98	0.44
72:BZ:68:ILE:HB	72:BZ:109:TYR:HB2	2.00	0.44
2:BA:145:ILE:HG23	2:BA:159:ILE:HB	2.00	0.44
10:AE:161:ARG:HD3	10:AE:270:TYR:CZ	2.53	0.44
22:AR:156:ALA:HB1	58:BL:155:PHE:HE1	1.83	0.44
48:A2:68:U:O2'	48:A2:100:C:O2'	2.23	0.44
48:A2:188:G:H2'	48:A2:189:G:H8	1.81	0.44
48:A2:412:A:O2'	48:A2:2290:C:OP1	2.35	0.44
48:A2:1428:U:H3	48:A2:2079:G:N2	2.15	0.44
48:A2:4007:C:H2'	48:A2:4008:C:C6	2.52	0.44
50:BD:219:PRO:O	50:BD:220:THR:C	2.58	0.44
51:BE:11:ARG:HA	51:BE:28:ALA:HB2	1.98	0.44
2:BA:79:SER:OG	2:BA:129:ALA:O	2.34	0.44
2:BA:201:LEU:HD21	64:BR:85:VAL:HG22	1.99	0.44
5:AC:143:ARG:NH1	48:A2:2279:A:N7	2.65	0.44
11:AF:242:ARG:NH2	48:A2:929:G:OP2	2.50	0.44
13:AH:93:ARG:HA	13:AH:143:GLU:HA	1.98	0.44
13:AH:134:CYS:SG	13:AH:135:SER:N	2.91	0.44
21:AQ:157:GLY:O	21:AQ:188:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AR:82:LYS:O	48:A2:2842:G:O2'	2.34	0.44
24:AT:44:GLY:H	24:AT:58:HIS:CE1	2.35	0.44
24:AT:52:MET:HE2	24:AT:52:MET:HB3	1.80	0.44
28:AX:61:PRO:HD2	38:Ah:80:PRO:HG3	1.99	0.44
44:An:11:ARG:NH2	49:B1:1845:A:OP1	2.36	0.44
49:B1:223:C:H2'	49:B1:224:A:C8	2.53	0.44
49:B1:613:G:N2	49:B1:626:G:OP1	2.50	0.44
49:B1:1781:A:O2'	49:B1:1782:G:O4'	2.29	0.44
52:BF:123:GLU:OE2	52:BF:204:ARG:NH2	2.40	0.44
63:BQ:25:CYS:HA	63:BQ:68:ILE:HG12	1.99	0.44
64:BR:74:GLN:HA	64:BR:77:GLU:CB	2.29	0.44
64:BR:97:GLU:C	64:BR:117:LEU:HD23	2.39	0.44
64:BR:106:LEU:HD23	64:BR:106:LEU:HA	1.85	0.44
66:BT:140:ALA:HA	66:BT:143:LYS:HE3	2.00	0.44
2:BA:127:PRO:HG3	2:BA:146:ALA:HB1	1.99	0.44
7:A3:38:U:N3	38:Ah:86:LYS:HD3	2.33	0.44
9:AD:61:ILE:HG12	9:AD:79:TYR:HD1	1.83	0.44
13:AH:151:ILE:HG23	48:A2:4651:U:H4'	1.99	0.44
22:AR:159:ALA:O	22:AR:163:ARG:N	2.44	0.44
29:AY:15:ARG:NH1	48:A2:226:G:OP1	2.51	0.44
32:Ab:27:GLN:HE22	48:A2:1444:A:C1'	2.31	0.44
45:Ao:13:LYS:HD3	48:A2:4256:C:H4'	2.00	0.44
48:A2:693:U:H2'	48:A2:694:G:H21	1.82	0.44
48:A2:1443:C:H2'	48:A2:1444:A:C8	2.53	0.44
48:A2:1747:A:C5	48:A2:1748:A:H1'	2.53	0.44
49:B1:75:G:O2'	49:B1:77:A:OP1	2.32	0.44
49:B1:1233:G:OP2	65:BS:135:HIS:NE2	2.51	0.44
49:B1:1612:G:C2'	65:BS:87:GLN:OE1	2.25	0.44
49:B1:1830:U:O2'	81:Bx:47:U:OP1	2.36	0.44
52:BF:61:PHE:CG	75:Bc:51:ARG:HD2	2.53	0.44
54:BH:69:LEU:HD23	54:BH:73:GLN:HB2	2.00	0.44
79:Bg:165:ILE:O	79:Bg:177:TRP:N	2.50	0.44
5:AC:150:LEU:CB	5:AC:151:PRO:HD2	2.28	0.44
12:AG:136:LEU:HB2	12:AG:202:VAL:HG13	1.99	0.44
22:AR:9:ARG:O	22:AR:12:SER:OG	2.33	0.44
26:AV:87:SER:HB3	27:AW:19:ARG:HH21	1.82	0.44
29:AY:86:GLN:OE1	29:AY:94:THR:OG1	2.33	0.44
32:Ab:111:ARG:CA	32:Ab:116:LEU:CD1	2.95	0.44
48:A2:1228:C:H42	48:A2:1247:C:N4	2.16	0.44
48:A2:1540:A:H2'	48:A2:1541:G:C8	2.53	0.44
48:A2:2499:C:H2'	48:A2:2500:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:B1:350:C:O2'	49:B1:383:G:N1	2.47	0.44
49:B1:1488:C:H3'	49:B1:1489:A:H4'	2.00	0.44
56:BJ:136:ARG:HG2	56:BJ:159:PHE:HA	1.99	0.44
79:Bg:178:ASN:O	79:Bg:182:CYS:N	2.49	0.44
79:Bg:195:LEU:HD13	79:Bg:209:SER:HB2	2.00	0.44
79:Bg:206:LEU:HD22	79:Bg:261:LEU:HD11	2.00	0.44
1:AA:204:MET:HE2	1:AA:209:HIS:HB2	1.99	0.43
5:AC:24:LEU:HD12	5:AC:25:PRO:HD2	2.00	0.43
11:AF:47:ARG:HA	11:AF:47:ARG:HD3	1.76	0.43
13:AH:99:PHE:HA	13:AH:100:PRO:HD3	1.83	0.43
17:AM:55:MET:HE2	17:AM:55:MET:HB3	1.88	0.43
30:AZ:22:LYS:NZ	30:AZ:132:GLN:O	2.35	0.43
48:A2:1149:G:N3	48:A2:1150:C:O2'	2.51	0.43
48:A2:1155:C:H2'	48:A2:1156:G:H8	1.83	0.43
48:A2:1928:U:O2	48:A2:4655:C:N4	2.51	0.43
49:B1:45:A:H4'	49:B1:46:A:H5'	2.00	0.43
49:B1:520:A:H2'	49:B1:521:A:C8	2.53	0.43
49:B1:1453:C:H2'	49:B1:1454:A:H4'	2.00	0.43
54:BH:156:VAL:HG13	54:BH:187:PHE:HA	2.00	0.43
56:BJ:172:ARG:HB2	56:BJ:175:ARG:HH21	1.82	0.43
66:BT:20:ALA:HA	66:BT:23:LYS:HD3	2.00	0.43
76:Bd:47:ALA:HB1	76:Bd:52:PHE:HB2	2.00	0.43
1:AA:132:ASN:ND2	48:A2:3653:A:H5''	2.33	0.43
5:AC:144:ILE:CB	5:AC:147:VAL:HG21	2.48	0.43
6:BC:66:LEU:HD22	6:BC:66:LEU:HA	1.87	0.43
7:A3:113:C:OP1	48:A2:2757:G:N1	2.47	0.43
11:AF:215:SER:OG	48:A2:1886:U:O2	2.23	0.43
12:AG:252:LYS:HA	12:AG:255:LYS:HE2	1.99	0.43
15:AJ:105:PHE:O	15:AJ:132:VAL:N	2.50	0.43
17:AM:10:GLY:O	17:AM:62:LEU:N	2.42	0.43
17:AM:17:PHE:HB2	48:A2:1902:C:C4	2.53	0.43
29:AY:18:HIS:NE2	48:A2:226:G:O2'	2.50	0.43
34:Ad:97:ASP:N	34:Ad:97:ASP:OD1	2.51	0.43
40:Aj:21:ARG:NH2	40:Aj:38:GLY:O	2.51	0.43
48:A2:339:C:H2'	48:A2:340:G:C8	2.53	0.43
48:A2:1912:C:N4	48:A2:2021:A:O2'	2.43	0.43
48:A2:1949:G:H2'	48:A2:1950:G:C8	2.53	0.43
49:B1:65:C:C4	53:BG:133:LEU:HB3	2.53	0.43
49:B1:976:G:H1'	61:BO:50:LYS:HG2	2.00	0.43
53:BG:48:TYR:HE1	53:BG:117:GLY:HA2	1.83	0.43
72:BZ:112:ASN:HD22	72:BZ:113:THR:H	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Bc:31:ARG:HA	75:Bc:43:ILE:HA	1.99	0.43
3:AB:8:ALA:HB2	26:AV:49:LEU:HD13	2.01	0.43
3:AB:224:LYS:O	3:AB:274:TYR:N	2.44	0.43
6:BC:89:LYS:HD3	6:BC:160:LEU:HD11	1.98	0.43
7:A3:25:G:N3	48:A2:350:G:O2'	2.51	0.43
16:AL:49:ARG:NH1	38:Ah:117:ARG:C	2.75	0.43
17:AM:12:VAL:O	17:AM:58:THR:OG1	2.26	0.43
25:AU:28:PRO:HB3	25:AU:100:LEU:HD21	2.00	0.43
32:Ab:113:ALA:N	48:A2:1254:G:C6	2.86	0.43
36:Af:30:ILE:HG23	36:Af:33:VAL:HB	1.99	0.43
42:Al:5:LYS:O	48:A2:2491:A:N6	2.51	0.43
48:A2:366:A:N1	48:A2:1626:C:O2'	2.42	0.43
48:A2:1149:G:N1	48:A2:1151:G:O2'	2.51	0.43
48:A2:1830:U:O2'	48:A2:1831:A:O4'	2.32	0.43
48:A2:1862:C:H5'	48:A2:2260:U:H1'	1.98	0.43
48:A2:4943:U:H2'	48:A2:4944:G:H8	1.83	0.43
49:B1:652:U:H2'	49:B1:653:A:C8	2.53	0.43
49:B1:1059:G:N2	49:B1:1829:G:O3'	2.51	0.43
49:B1:1532:C:H4'	49:B1:1604:G:H21	1.82	0.43
65:BS:45:LEU:HB3	65:BS:52:LEU:HD11	2.01	0.43
2:BA:124:VAL:HG21	2:BA:134:LEU:HD21	2.01	0.43
6:BC:227:ARG:NH2	49:B1:663:C:O2'	2.40	0.43
10:AE:52:ARG:O	48:A2:1264:G:N1	2.52	0.43
13:AH:12:ILE:HB	13:AH:53:LYS:HB3	2.00	0.43
30:AZ:106:LEU:O	30:AZ:110:ALA:N	2.40	0.43
48:A2:741:U:H2'	48:A2:742:G:H8	1.84	0.43
48:A2:1076:C:H2'	48:A2:1077:G:C8	2.53	0.43
48:A2:2375:A:H5'	48:A2:2785:A:C6	2.53	0.43
48:A2:2822:U:O2'	48:A2:4594:U:OP1	2.30	0.43
48:A2:4192:C:O2'	48:A2:4196:A:N6	2.49	0.43
48:A2:4841:C:H2'	48:A2:4842:G:H8	1.83	0.43
49:B1:1287:A:C6	78:Bf:99:LYS:HB2	2.54	0.43
49:B1:1347:U:H2'	49:B1:1348:G:C8	2.54	0.43
49:B1:1417:C:H42	49:B1:1421:A:H61	1.65	0.43
56:BJ:31:LEU:HD23	56:BJ:43:VAL:HG13	2.00	0.43
56:BJ:46:VAL:O	56:BJ:49:THR:OG1	2.33	0.43
61:BO:34:PHE:HB3	61:BO:41:PHE:HB2	2.00	0.43
66:BT:75:MET:HA	66:BT:78:ILE:HD12	2.00	0.43
67:BU:66:ARG:HH12	67:BU:75:LYS:HB3	1.81	0.43
77:Be:46:VAL:HG23	77:Be:47:PRO:HD3	2.00	0.43
79:Bg:88:ARG:CG	79:Bg:97:THR:OG1	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BA:32:PHE:CG	49:B1:1097:G:H4'	2.54	0.43
4:BB:59:SER:HA	4:BB:62:LEU:HD23	2.01	0.43
5:AC:359:ALA:O	5:AC:363:ALA:N	2.50	0.43
10:AE:150:LEU:HD13	10:AE:194:VAL:HG21	2.01	0.43
11:AF:113:ARG:HB3	11:AF:210:PRO:HG3	2.00	0.43
20:AP:67:VAL:HG22	20:AP:82:ARG:HH21	1.84	0.43
27:AW:8:PHE:HZ	27:AW:49:ILE:HG13	1.82	0.43
39:Ai:76:ARG:HA	39:Ai:76:ARG:HD3	1.86	0.43
40:Aj:79:ARG:HH22	48:A2:248:C:H4'	1.84	0.43
48:A2:189:G:H1	48:A2:244:G:H1	1.66	0.43
48:A2:1171:C:H2'	48:A2:1172:G:H8	1.83	0.43
48:A2:2513:C:H1'	48:A2:2690:G:H1	1.83	0.43
48:A2:2575:G:H2'	48:A2:2576:G:H8	1.82	0.43
48:A2:4485:A:H2'	48:A2:4521:A:H62	1.83	0.43
48:A2:4722:G:N2	48:A2:4727:G:O2'	2.52	0.43
56:BJ:132:GLN:O	56:BJ:134:HIS:N	2.51	0.43
57:BK:29:MET:HG3	57:BK:30:PRO:HD3	1.99	0.43
63:BQ:17:LYS:HE2	63:BQ:17:LYS:HB3	1.80	0.43
1:AA:3:ARG:HD3	48:A2:1610:C:H42	1.83	0.43
4:BB:215:VAL:HG13	4:BB:215:VAL:O	2.16	0.43
5:AC:54:VAL:HG21	5:AC:107:THR:HB	1.99	0.43
12:AG:176:LYS:HD3	39:Ai:43:MET:HG3	2.01	0.43
16:AL:3:PRO:HD2	31:Aa:41:HIS:CE1	2.54	0.43
23:AS:170:LYS:HE3	48:A2:4832:A:OP1	2.19	0.43
36:Af:58:VAL:HB	36:Af:59:THR:H	1.59	0.43
48:A2:242:C:H2'	48:A2:243:G:H8	1.83	0.43
48:A2:474:C:N4	48:A2:475:G:O6	2.51	0.43
48:A2:1083:U:H3	48:A2:1178:G:H1	1.67	0.43
48:A2:1281:C:H2'	48:A2:1282:G:C8	2.53	0.43
48:A2:3702:C:H2'	48:A2:3703:A:C8	2.53	0.43
49:B1:495:U:O2'	51:BE:27:PHE:O	2.32	0.43
49:B1:678:U:OP1	60:BN:127:ARG:NH2	2.51	0.43
49:B1:1144:A:H2'	49:B1:1145:A:C8	2.54	0.43
50:BD:11:PHE:HE2	67:BU:84:ILE:HG23	1.83	0.43
64:BR:99:ASP:N	64:BR:117:LEU:HD22	2.31	0.43
70:BX:25:LYS:HA	70:BX:28:LYS:HE2	1.99	0.43
79:Bg:154:VAL:HG12	79:Bg:167:SER:HA	2.00	0.43
3:AB:95:THR:HG22	48:A2:4868:A:H4'	2.01	0.43
4:BB:81:PHE:CD2	4:BB:82:ARG:HG3	2.54	0.43
6:BC:148:ALA:HB1	6:BC:152:ARG:NH1	2.34	0.43
15:AJ:145:LYS:O	48:A2:4242:A:H2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AN:160:GLU:HG2	18:AN:161:MET:HG3	2.00	0.43
24:AT:105:PHE:HD2	24:AT:106:LEU:HD12	1.83	0.43
32:Ab:112:ILE:CA	48:A2:1254:G:C2	3.01	0.43
48:A2:350:G:N1	48:A2:354:A:OP2	2.48	0.43
48:A2:1153:G:N2	48:A2:1174:C:O2	2.42	0.43
48:A2:1981:G:H5''	48:A2:1982:G:H5'	2.01	0.43
49:B1:658:U:O3'	70:BX:17:ARG:NH2	2.52	0.43
49:B1:831:G:N2	49:B1:844:U:O2	2.52	0.43
49:B1:915:G:OP2	49:B1:915:G:N2	2.41	0.43
51:BE:202:PRO:HB2	58:BL:42:LEU:HD13	2.00	0.43
52:BF:92:ILE:O	52:BF:96:ALA:N	2.49	0.43
6:BC:187:ARG:NH2	49:B1:1143:A:OP2	2.42	0.43
25:AU:23:LEU:HB2	25:AU:70:ILE:HB	2.00	0.43
28:AX:57:GLN:NE2	28:AX:58:PRO:O	2.52	0.43
33:Ac:17:ARG:HB3	33:Ac:104:ILE:HG12	2.01	0.43
36:Af:23:GLU:OE2	48:A2:432:G:N2	2.48	0.43
48:A2:1551:U:H2'	48:A2:1552:G:C8	2.54	0.43
48:A2:1958:C:N4	48:A2:1965:A:OP1	2.51	0.43
48:A2:4597:A:H3'	48:A2:4598:U:H4'	2.00	0.43
49:B1:877:C:H2'	49:B1:878:G:C8	2.53	0.43
49:B1:987:A:H4'	73:Ba:70:LYS:HG3	2.00	0.43
51:BE:104:ASP:HB2	51:BE:110:ALA:HB2	2.01	0.43
56:BJ:136:ARG:CG	56:BJ:159:PHE:HA	2.49	0.43
1:AA:33:ASP:OD1	1:AA:33:ASP:N	2.52	0.43
1:AA:245:ARG:HD2	48:A2:3718:A:N7	2.33	0.43
3:AB:235:TRP:NE1	3:AB:268:ARG:O	2.51	0.43
6:BC:121:ARG:NH2	49:B1:1486:A:O3'	2.52	0.43
13:AH:129:ARG:HD3	13:AH:129:ARG:HA	1.78	0.43
18:AN:42:PRO:HG3	18:AN:61:ILE:HG13	2.01	0.43
23:AS:128:LYS:NZ	23:AS:130:GLU:OE1	2.52	0.43
33:Ac:26:LYS:HG2	33:Ac:97:ILE:HD11	2.00	0.43
43:Am:79:GLU:O	43:Am:82:LEU:N	2.49	0.43
48:A2:194:A:O2'	48:A2:217:C:O2	2.37	0.43
48:A2:1388:C:H42	48:A2:1395:G:H1	1.66	0.43
48:A2:1669:U:H2'	48:A2:1670:G:C8	2.53	0.43
48:A2:4687:C:H2'	48:A2:4688:G:C8	2.54	0.43
49:B1:1158:G:OP1	70:BX:5:ARG:NH1	2.46	0.43
49:B1:1288:U:O4	49:B1:1312:G:O2'	2.34	0.43
49:B1:1830:U:OP2	81:Bx:46:U:O2'	2.30	0.43
51:BE:128:LYS:HA	51:BE:156:VAL:HG13	2.00	0.43
4:BB:126:ASP:OD2	4:BB:136:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BB:136:ARG:CD	4:BB:216:LYS:NZ	2.73	0.43
5:AC:305:PRO:HG3	48:A2:2069:G:C4	2.54	0.43
5:AC:330:PRO:HG2	11:AF:47:ARG:HD2	2.00	0.43
6:BC:148:ALA:HB1	6:BC:152:ARG:HH12	1.83	0.43
18:AN:12:ARG:HA	18:AN:12:ARG:HD3	1.84	0.43
22:AR:43:LYS:NZ	48:A2:2685:G:H22	2.17	0.43
23:AS:168:THR:OG1	23:AS:169:THR:N	2.50	0.43
37:Ag:79:GLY:H	48:A2:2730:G:H4'	1.83	0.43
48:A2:2084:G:H2'	48:A2:2085:A:C8	2.53	0.43
49:B1:582:U:H1'	71:BY:33:ALA:HB2	2.01	0.43
49:B1:1178:U:H2'	49:B1:1179:G:H8	1.84	0.43
49:B1:1692:U:H2'	49:B1:1693:G:H8	1.83	0.43
57:BK:14:LEU:HA	57:BK:17:LYS:HD2	1.99	0.43
63:BQ:49:TYR:HA	63:BQ:52:LEU:HB2	2.00	0.43
3:AB:165:HIS:HB3	3:AB:180:LEU:HD23	2.01	0.42
4:BB:40:ASN:HD22	4:BB:76:ASN:HB2	1.84	0.42
4:BB:48:LEU:O	4:BB:49:VAL:HG22	2.18	0.42
4:BB:103:MET:CB	4:BB:215:VAL:HG12	2.36	0.42
9:AD:64:ILE:HG13	9:AD:105:LEU:HD11	2.01	0.42
13:AH:114:ILE:HB	13:AH:124:ARG:HB3	2.01	0.42
14:AI:86:HIS:HD2	14:AI:139:ARG:HD3	1.85	0.42
14:AI:87:ILE:HB	14:AI:138:ILE:HG12	2.00	0.42
18:AN:23:LEU:HD12	18:AN:23:LEU:HA	1.86	0.42
19:AO:184:ASN:HD22	19:AO:185:VAL:H	1.67	0.42
44:An:6:ARG:NH2	49:B1:1169:G:OP1	2.39	0.42
48:A2:18:C:H2'	48:A2:19:G:C8	2.54	0.42
48:A2:358:G:O2'	48:A2:369:G:O6	2.31	0.42
48:A2:1263:C:O2'	48:A2:1265:G:N7	2.48	0.42
48:A2:2593:C:O2'	48:A2:2787:G:OP1	2.34	0.42
48:A2:4201:A:H2'	48:A2:4202:G:C8	2.54	0.42
49:B1:152:U:H4'	53:BG:132:ARG:HH22	1.84	0.42
49:B1:797:C:H4'	49:B1:798:G:H5'	2.01	0.42
49:B1:1329:U:O4	49:B1:1493:C:O2'	2.30	0.42
49:B1:1543:U:O2'	63:BQ:43:GLU:OE1	2.34	0.42
50:BD:42:THR:HG21	50:BD:45:ARG:HH21	1.84	0.42
64:BR:73:LEU:O	64:BR:77:GLU:HB2	2.18	0.42
66:BT:41:LYS:HE3	66:BT:41:LYS:HB3	1.86	0.42
1:AA:226:ARG:HG3	1:AA:228:ASP:H	1.84	0.42
5:AC:34:PRO:HG3	47:At:9:VAL:HG22	2.00	0.42
7:A3:11:C:H2'	7:A3:12:G:H8	1.83	0.42
7:A3:22:U:O2	48:A2:373:G:N2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A4:7:G:H4'	9:AD:33:ARG:HH22	1.84	0.42
15:AJ:95:ARG:N	15:AJ:98:ASN:OD1	2.52	0.42
31:Aa:75:LEU:HB3	31:Aa:117:LEU:HD13	2.00	0.42
33:Ac:20:LEU:HD23	33:Ac:20:LEU:HA	1.87	0.42
48:A2:1289:C:H2'	48:A2:1290:A:C8	2.54	0.42
48:A2:2638:A:H62	48:A2:2654:G:H21	1.67	0.42
48:A2:3914:A:H2'	48:A2:3915:G:C8	2.53	0.42
49:B1:71:G:H1'	49:B1:79:A:N1	2.33	0.42
49:B1:656:G:H1	49:B1:1156:U:H5	1.67	0.42
49:B1:933:G:N2	73:Ba:19:GLN:HE22	2.17	0.42
49:B1:973:C:O2	61:BO:55:ARG:NH2	2.52	0.42
51:BE:225:ILE:CG2	51:BE:226:PHE:N	2.83	0.42
52:BF:103:LEU:HD12	72:BZ:67:LEU:HD22	2.00	0.42
57:BK:35:LEU:HD23	57:BK:37:ASP:HB2	2.01	0.42
71:BY:18:LEU:HA	71:BY:18:LEU:HD23	1.81	0.42
1:AA:3:ARG:HH11	48:A2:1610:C:H42	1.67	0.42
6:BC:82:TYR:CE1	6:BC:164:PRO:HD3	2.55	0.42
11:AF:227:PHE:N	11:AF:233:ALA:O	2.53	0.42
14:AI:190:LEU:HD21	14:AI:199:TYR:HD1	1.83	0.42
19:AO:12:ARG:NH2	48:A2:4722:G:OP1	2.52	0.42
21:AQ:27:LEU:HA	21:AQ:27:LEU:HD23	1.76	0.42
31:Aa:77:LYS:HE3	48:A2:1484:G:H22	1.84	0.42
32:Ab:32:LEU:HD22	32:Ab:35:VAL:HG21	2.01	0.42
33:Ac:18:LEU:HD23	33:Ac:18:LEU:HA	1.88	0.42
35:Ae:21:ILE:HD11	35:Ae:33:ARG:HB3	2.01	0.42
48:A2:715:C:H2'	48:A2:716:G:C8	2.54	0.42
48:A2:1155:C:H2'	48:A2:1156:G:C8	2.55	0.42
48:A2:1487:C:H2'	48:A2:1488:G:C8	2.54	0.42
49:B1:885:U:H2'	49:B1:886:A:C8	2.47	0.42
49:B1:1483:A:O2'	50:BD:159:HIS:O	2.33	0.42
51:BE:122:LYS:O	51:BE:162:ILE:N	2.47	0.42
65:BS:55:ARG:HB2	65:BS:58:GLU:HG3	2.02	0.42
69:BW:86:LEU:O	69:BW:90:GLN:N	2.49	0.42
79:Bg:207:CYS:HB2	79:Bg:221:LEU:HD22	2.00	0.42
4:BB:33:VAL:HG21	4:BB:67:PHE:CZ	2.54	0.42
4:BB:144:LYS:HG3	4:BB:208:HIS:HD2	1.84	0.42
10:AE:277:LEU:HB3	36:Af:4:ARG:HH21	1.83	0.42
12:AG:63:LEU:HD21	18:AN:32:GLN:HB2	2.01	0.42
13:AH:4:ILE:HG22	13:AH:5:LEU:H	1.83	0.42
16:AL:133:ALA:HA	16:AL:136:LYS:CG	2.48	0.42
17:AM:33:GLN:HB2	23:AS:145:PHE:HZ	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AT:49:GLN:HA	24:AT:52:MET:HE3	2.01	0.42
26:AV:58:GLY:N	26:AV:81:VAL:O	2.44	0.42
32:Ab:118:LEU:HD13	48:A2:1254:G:H4'	2.01	0.42
38:Ah:79:LYS:HE2	38:Ah:79:LYS:HB3	1.88	0.42
48:A2:195:A:H5''	48:A2:233:G:H21	1.84	0.42
48:A2:1347:U:H3	48:A2:1356:A:H61	1.67	0.42
48:A2:2368:A:H2'	48:A2:2369:G:C8	2.55	0.42
48:A2:3932:G:N1	48:A2:3934:A:H3'	2.34	0.42
49:B1:520:A:H2'	49:B1:521:A:H8	1.83	0.42
49:B1:594:A:C8	77:Be:29:THR:HG21	2.53	0.42
49:B1:658:U:H1'	70:BX:17:ARG:HH12	1.85	0.42
49:B1:1148:A:OP1	73:Ba:6:ARG:NH2	2.53	0.42
49:B1:1214:A:O2'	49:B1:1216:C:OP1	2.31	0.42
49:B1:1751:C:N3	49:B1:1782:G:N1	2.66	0.42
58:BL:14:PRO:HG3	58:BL:56:ILE:HG23	2.01	0.42
61:BO:21:VAL:HG12	61:BO:22:ALA:H	1.84	0.42
65:BS:10:GLN:HE22	65:BS:59:LEU:HB3	1.83	0.42
68:BV:15:ARG:NH1	68:BV:33:GLN:HB2	2.34	0.42
71:BY:41:ARG:NH2	71:BY:52:PRO:O	2.52	0.42
79:Bg:240:CYS:SG	79:Bg:241:PHE:N	2.92	0.42
1:AA:233:ARG:O	1:AA:235:VAL:N	2.52	0.42
8:A4:13:A:H1'	8:A4:110:G:C8	2.54	0.42
15:AJ:22:LEU:HD22	15:AJ:130:PHE:CD1	2.54	0.42
22:AR:8:LYS:HE3	22:AR:19:LYS:HG2	2.02	0.42
28:AX:96:LEU:N	28:AX:138:VAL:O	2.52	0.42
48:A2:188:G:H2'	48:A2:189:G:C8	2.54	0.42
48:A2:216:G:N2	48:A2:233:G:H22	2.17	0.42
48:A2:700:C:H2'	48:A2:701:G:H8	1.85	0.42
48:A2:1257:A:H2'	48:A2:1258:G:O4'	2.19	0.42
49:B1:122:G:H2'	49:B1:123:G:C8	2.55	0.42
49:B1:511:U:H2'	49:B1:512:A:C8	2.55	0.42
49:B1:1472:C:N4	49:B1:1476:A:H62	2.17	0.42
50:BD:216:GLU:HG3	50:BD:217:ILE:HG12	2.02	0.42
53:BG:121:ILE:HG21	53:BG:124:LEU:HD23	2.01	0.42
3:AB:47:LEU:HD23	3:AB:346:THR:HG22	2.02	0.42
5:AC:300:ARG:NH2	48:A2:1430:C:OP1	2.52	0.42
9:AD:206:ASP:OD1	9:AD:209:ARG:NH1	2.53	0.42
19:AO:63:ASN:HD21	48:A2:2026:G:P	2.41	0.42
25:AU:24:ASP:HB3	25:AU:111:GLU:HA	2.00	0.42
37:Ag:26:PRO:O	48:A2:2676:A:N6	2.50	0.42
39:Ai:68:ARG:NE	48:A2:3693:G:OP2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:At:64:ILE:HG13	47:At:78:VAL:HG13	2.01	0.42
48:A2:481:G:H2'	48:A2:482:G:C8	2.55	0.42
49:B1:98:C:H42	49:B1:432:G:H1	1.67	0.42
49:B1:1856:C:OP2	61:BO:146:ARG:N	2.52	0.42
49:B1:1865:C:OP2	73:Ba:5:ARG:NH2	2.48	0.42
50:BD:32:ASP:HB3	50:BD:54:ARG:HB2	2.01	0.42
51:BE:185:GLY:CA	51:BE:224:ASN:ND2	2.82	0.42
5:AC:111:TRP:CD1	16:AL:26:PHE:HZ	2.37	0.42
7:A3:13:G:O2'	20:AP:121:LYS:O	2.38	0.42
7:A3:36:G:C4	38:Ah:89:ARG:HD2	2.55	0.42
10:AE:131:LYS:O	10:AE:136:HIS:HE1	1.95	0.42
10:AE:150:LEU:HG	10:AE:164:PHE:HB2	2.02	0.42
11:AF:93:ILE:HG12	11:AF:247:MET:HE1	2.02	0.42
13:AH:92:MET:HB2	13:AH:144:LEU:HB3	2.02	0.42
20:AP:25:HIS:ND1	48:A2:2340:G:O6	2.47	0.42
30:AZ:58:GLY:HA2	30:AZ:62:ILE:HB	2.00	0.42
40:Aj:19:CYS:HB3	40:Aj:27:TYR:HB2	2.02	0.42
46:Ap:18:TYR:HA	48:A2:3606:A:H61	1.85	0.42
47:At:19:LYS:HB2	48:A2:2316:C:H4'	2.02	0.42
48:A2:163:C:H42	48:A2:264:U:H3	1.66	0.42
48:A2:1627:C:H2'	48:A2:1628:A:C8	2.54	0.42
48:A2:2586:C:H2'	48:A2:2587:G:C8	2.55	0.42
49:B1:96:C:H5	49:B1:434:G:H1	1.68	0.42
49:B1:693:A:H2'	49:B1:694:G:C8	2.55	0.42
49:B1:841:G:C8	71:BY:12:PHE:HB3	2.54	0.42
49:B1:890:U:H5'	49:B1:891:G:H5''	2.01	0.42
50:BD:70:THR:HG23	50:BD:84:VAL:HG12	2.01	0.42
54:BH:20:GLU:O	54:BH:24:SER:N	2.41	0.42
55:BI:152:ARG:HA	55:BI:155:ASN:HA	2.01	0.42
66:BT:60:THR:HG22	66:BT:64:LEU:HD23	2.01	0.42
73:Ba:20:PRO:HA	73:Ba:31:PRO:HA	2.02	0.42
79:Bg:289:LEU:HB2	79:Bg:298:LEU:HD11	2.01	0.42
1:AA:174:ARG:NH2	48:A2:3654:C:O2'	2.53	0.42
4:BB:82:ARG:HE	4:BB:103:MET:HE1	1.85	0.42
10:AE:258:LEU:HA	10:AE:261:ILE:HD12	2.02	0.42
11:AF:21:LYS:O	11:AF:25:PHE:N	2.53	0.42
17:AM:50:MET:HE2	17:AM:50:MET:HB3	1.85	0.42
18:AN:26:ARG:HA	18:AN:29:GLN:HB3	2.01	0.42
18:AN:91:GLN:HB2	45:Ao:48:TYR:CE2	2.52	0.42
36:Af:89:ARG:NH2	48:A2:699:G:OP1	2.51	0.42
37:Ag:54:ARG:NH2	48:A2:2632:C:OP1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Ap:83:ILE:HD13	46:Ap:83:ILE:HA	1.88	0.42
48:A2:352:C:H2'	48:A2:353:A:C8	2.54	0.42
48:A2:449:C:H2'	48:A2:450:C:C6	2.54	0.42
48:A2:1307:A:O2'	48:A2:1309:A:OP1	2.34	0.42
48:A2:3581:A:H2'	48:A2:3582:A:H8	1.84	0.42
48:A2:4891:C:H2'	48:A2:4892:A:C8	2.55	0.42
49:B1:1672:U:H2'	49:B1:1673:U:C6	2.54	0.42
50:BD:51:LEU:HG	50:BD:89:GLU:HB2	2.00	0.42
70:BX:17:ARG:HD2	70:BX:17:ARG:HA	1.92	0.42
79:Bg:207:CYS:HB2	79:Bg:221:LEU:HB2	2.00	0.42
1:AA:174:ARG:NH2	48:A2:3654:C:O3'	2.53	0.42
4:BB:137:LEU:HA	4:BB:215:VAL:HA	2.00	0.42
7:A3:37:A:P	38:Ah:92:ARG:HH12	2.42	0.42
13:AH:34:LEU:HD12	13:AH:34:LEU:HA	1.92	0.42
17:AM:46:ARG:HH11	48:A2:924:U:C5'	2.24	0.42
18:AN:49:ARG:NH2	48:A2:150:G:OP2	2.53	0.42
28:AX:48:ARG:NH2	48:A2:2454:G:N7	2.68	0.42
31:Aa:86:THR:HG22	48:A2:504:U:H5'	2.02	0.42
48:A2:423:A:H2'	48:A2:424:G:H8	1.85	0.42
48:A2:1067:C:O2	48:A2:1197:C:N4	2.53	0.42
48:A2:1747:A:H4'	65:BS:118:ARG:HE	1.85	0.42
49:B1:1846:G:H2'	49:B1:1847:G:C8	2.54	0.42
62:BP:124:LYS:HA	62:BP:125:PRO:HD3	1.85	0.42
65:BS:8:LYS:HD2	65:BS:58:GLU:HG2	2.00	0.42
68:BV:34:MET:N	68:BV:53:TYR:O	2.53	0.42
79:Bg:37:ASP:OD1	79:Bg:39:THR:OG1	2.36	0.42
79:Bg:188:HIS:HB3	79:Bg:219:TRP:CD2	2.55	0.42
2:BA:200:ASP:HB3	2:BA:205:ARG:HH22	1.85	0.42
3:AB:80:GLU:OE1	3:AB:323:TYR:OH	2.27	0.42
7:A3:140:C:H2'	7:A3:141:C:C6	2.55	0.42
9:AD:255:LYS:HB3	9:AD:256:LYS:H	1.70	0.42
16:AL:194:ILE:HG22	16:AL:198:ARG:HG3	2.01	0.42
18:AN:23:LEU:HD21	18:AN:120:TRP:HH2	1.85	0.42
22:AR:10:LEU:HD12	22:AR:10:LEU:HA	1.90	0.42
26:AV:71:GLU:HB2	26:AV:72:LEU:HD12	2.02	0.42
36:Af:106:TYR:N	36:Af:107:PRO:CD	2.83	0.42
41:Ak:23:VAL:HG22	41:Ak:36:VAL:HG22	2.00	0.42
41:Ak:25:ILE:HB	41:Ak:68:GLU:HG2	2.02	0.42
49:B1:453:C:H2'	49:B1:454:U:H6	1.84	0.42
49:B1:659:G:O4'	49:B1:662:G:N2	2.52	0.42
79:Bg:169:GLY:N	79:Bg:173:LEU:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AB:174:ARG:C	3:AB:174:ARG:CD	2.85	0.41
7:A3:22:U:OP1	29:AY:11:ARG:NE	2.54	0.41
22:AR:20:LYS:HG3	22:AR:21:LYS:HG3	2.02	0.41
23:AS:160:ARG:NH2	48:A2:4833:G:O6	2.53	0.41
23:AS:170:LYS:HG3	48:A2:4832:A:OP2	2.20	0.41
32:Ab:36:ASP:HA	32:Ab:37:PRO:HD3	1.94	0.41
34:Ad:39:LYS:HD3	34:Ad:77:ILE:HD11	2.02	0.41
38:Ah:31:LEU:HD21	38:Ah:46:LYS:HG3	2.02	0.41
41:Ak:49:ASP:HB3	41:Ak:52:LYS:HB2	2.02	0.41
48:A2:249:C:H2'	48:A2:250:G:C8	2.54	0.41
48:A2:1649:G:N1	48:A2:2260:U:OP2	2.35	0.41
48:A2:3826:C:H2'	48:A2:3827:A:H8	1.85	0.41
48:A2:4855:G:H2'	48:A2:4856:G:H8	1.85	0.41
57:BK:20:VAL:HG13	57:BK:69:TRP:H	1.85	0.41
57:BK:63:ALA:HB3	57:BK:68:TYR:HE2	1.85	0.41
79:Bg:154:VAL:O	79:Bg:155:ARG:NH1	2.48	0.41
3:AB:50:LYS:NZ	3:AB:339:GLY:O	2.39	0.41
3:AB:313:SER:OG	3:AB:314:ILE:N	2.51	0.41
5:AC:285:ILE:N	21:AQ:124:ASP:OD2	2.51	0.41
16:AL:133:ALA:HA	16:AL:136:LYS:HG2	2.01	0.41
24:AT:27:LEU:HD23	24:AT:27:LEU:HA	1.86	0.41
35:Ae:7:LEU:HB3	35:Ae:8:VAL:H	1.69	0.41
48:A2:484:C:H2'	48:A2:485:G:H8	1.84	0.41
49:B1:5:U:H2'	49:B1:6:G:C8	2.53	0.41
49:B1:454:U:H2'	49:B1:455:A:C8	2.56	0.41
49:B1:682:U:O2'	69:BW:4:MET:SD	2.73	0.41
57:BK:3:MET:N	57:BK:3:MET:SD	2.92	0.41
64:BR:97:GLU:HA	64:BR:116:ASN:O	2.19	0.41
65:BS:89:ASP:OD1	65:BS:91:LYS:N	2.48	0.41
66:BT:99:VAL:HA	66:BT:102:ARG:HB3	2.02	0.41
5:AC:284:MET:HE3	21:AQ:124:ASP:HB3	2.02	0.41
6:BC:155:ILE:O	6:BC:159:LYS:HG2	2.20	0.41
7:A3:12:G:H1'	20:AP:118:GLN:HE22	1.85	0.41
7:A3:140:C:H2'	7:A3:141:C:H6	1.84	0.41
7:A3:149:G:N2	48:A2:8:U:O2	2.53	0.41
9:AD:61:ILE:HG12	9:AD:79:TYR:CD1	2.54	0.41
11:AF:217:ARG:NH2	11:AF:245:ARG:O	2.53	0.41
17:AM:4:ARG:HH12	48:A2:4826:G:H1	1.68	0.41
20:AP:37:LYS:NZ	48:A2:418:U:O3'	2.54	0.41
21:AQ:74:GLY:O	21:AQ:78:LYS:NZ	2.53	0.41
24:AT:7:LYS:HB2	24:AT:7:LYS:HE3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Ab:111:ARG:HA	32:Ab:115:GLY:HA3	1.91	0.41
34:Ad:48:GLU:O	34:Ad:52:PHE:N	2.48	0.41
48:A2:1545:A:H2'	48:A2:1546:A:H8	1.84	0.41
48:A2:1980:A:O2'	48:A2:1999:C:O2'	2.28	0.41
49:B1:1106:C:H5''	74:Bb:70:LYS:HE2	2.02	0.41
49:B1:1307:U:O2'	78:Bf:134:SER:O	2.36	0.41
49:B1:1675:A:H1'	52:BF:77:MET:HE3	2.02	0.41
71:BY:35:VAL:HA	71:BY:36:PRO:HD3	1.94	0.41
71:BY:118:ARG:HA	71:BY:122:LYS:HZ2	1.84	0.41
3:AB:52:GLY:HA2	3:AB:341:LYS:HE2	2.02	0.41
5:AC:84:THR:OG1	48:A2:361:C:O2	2.37	0.41
6:BC:104:ASP:HB3	6:BC:130:ILE:HG22	2.02	0.41
7:A3:64:U:H2'	7:A3:65:A:H8	1.86	0.41
9:AD:39:GLN:HE21	9:AD:43:LYS:HB2	1.86	0.41
11:AF:216:PRO:O	48:A2:1886:U:O2'	2.38	0.41
24:AT:8:ARG:NH1	24:AT:52:MET:SD	2.92	0.41
34:Ad:57:MET:HB2	34:Ad:59:THR:HG22	2.02	0.41
36:Af:88:PHE:HZ	36:Af:101:ILE:HD13	1.85	0.41
41:Ak:35:LYS:HE3	48:A2:2675:A:H62	1.86	0.41
46:Ap:85:ARG:NH2	49:B1:938:A:O2'	2.54	0.41
48:A2:1228:C:H42	48:A2:1247:C:H42	1.66	0.41
48:A2:2378:G:O2'	48:A2:2801:G:O2'	2.37	0.41
48:A2:3623:A:H2'	48:A2:3624:A:C5	2.56	0.41
49:B1:907:G:H2'	49:B1:908:A:C8	2.55	0.41
50:BD:76:ARG:HB2	57:BK:22:VAL:HG21	2.01	0.41
64:BR:5:ARG:HG2	64:BR:49:LYS:HD2	2.02	0.41
71:BY:7:ILE:HG12	71:BY:27:VAL:HG22	2.01	0.41
82:A:17:ALA:O	82:A:18:GLY:C	2.64	0.41
16:AL:61:CYS:HA	16:AL:62:PRO:HD3	1.80	0.41
20:AP:72:GLN:O	20:AP:75:GLN:NE2	2.53	0.41
21:AQ:160:HIS:O	21:AQ:162:HIS:N	2.53	0.41
31:Aa:117:LEU:HG	31:Aa:118:PRO:HD2	2.02	0.41
48:A2:4078:G:O2'	48:A2:4080:U:O4	2.34	0.41
49:B1:85:A:OP1	71:BY:122:LYS:NZ	2.51	0.41
49:B1:1115:U:H1'	49:B1:1116:C:C4	2.55	0.41
53:BG:211:LYS:HE3	53:BG:211:LYS:HB2	1.87	0.41
54:BH:143:ARG:N	54:BH:155:LYS:O	2.52	0.41
58:BL:124:ASP:HB2	58:BL:147:LYS:HB3	2.02	0.41
73:Ba:66:LYS:HE2	73:Ba:66:LYS:HB2	1.90	0.41
79:Bg:64:HIS:HD1	79:Bg:65:PHE:H	1.66	0.41
6:BC:179:THR:OG1	6:BC:180:VAL:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A3:36:G:H22	38:Ah:89:ARG:HH22	1.62	0.41
21:AQ:168:ARG:HH11	21:AQ:174:PHE:HE1	1.69	0.41
27:AW:87:LEU:HD23	27:AW:87:LEU:HA	1.92	0.41
29:AY:26:ARG:NE	29:AY:78:TYR:OH	2.53	0.41
38:Ah:91:MET:CE	38:Ah:91:MET:CA	2.85	0.41
48:A2:1665:U:H2'	48:A2:1666:A:C8	2.56	0.41
48:A2:2583:C:H42	48:A2:2714:G:H1	1.67	0.41
48:A2:3864:C:H42	48:A2:4529:G:H1	1.68	0.41
48:A2:4687:C:H2'	48:A2:4688:G:H8	1.86	0.41
49:B1:572:U:H5''	71:BY:60:PHE:H	1.85	0.41
49:B1:1033:G:N1	49:B1:1080:A:O2'	2.52	0.41
49:B1:1286:G:H4'	49:B1:1313:A:H62	1.85	0.41
49:B1:1646:C:H4'	49:B1:1647:A:H5'	2.02	0.41
50:BD:218:LEU:HA	50:BD:219:PRO:HD3	1.33	0.41
62:BP:16:THR:OG1	65:BS:91:LYS:O	2.37	0.41
4:BB:103:MET:CB	4:BB:215:VAL:CG1	2.84	0.41
7:A3:9:A:H2'	7:A3:10:G:C8	2.50	0.41
8:A4:93:G:H21	23:AS:122:HIS:CD2	2.38	0.41
18:AN:185:GLY:HA2	48:A2:78:U:H5''	2.03	0.41
22:AR:115:ILE:HD12	22:AR:142:ILE:HG23	2.03	0.41
48:A2:225:C:H2'	48:A2:226:G:H8	1.86	0.41
48:A2:294:A:H2'	48:A2:295:G:H8	1.85	0.41
48:A2:481:G:H2'	48:A2:482:G:H8	1.86	0.41
48:A2:1747:A:C5	65:BS:116:LYS:HG2	2.55	0.41
48:A2:2556:C:H2'	48:A2:2557:G:H8	1.86	0.41
49:B1:3:C:O2	56:BJ:18:ARG:NH2	2.54	0.41
49:B1:439:A:O2'	49:B1:1799:G:O2'	2.29	0.41
49:B1:1648:G:O4'	63:BQ:125:ARG:NH2	2.54	0.41
50:BD:140:GLY:HA3	50:BD:182:LEU:HG	2.03	0.41
54:BH:119:SER:OG	54:BH:120:ARG:NH1	2.54	0.41
4:BB:66:VAL:HA	4:BB:87:ILE:HA	2.03	0.41
7:A3:152:U:O2'	12:AG:160:ASP:OD2	2.37	0.41
10:AE:186:LEU:HD13	10:AE:250:GLN:HG2	2.03	0.41
12:AG:75:LYS:HG2	12:AG:240:ASN:HB2	2.02	0.41
24:AT:102:ARG:HA	24:AT:105:PHE:HB3	2.02	0.41
36:Af:99:HIS:CE1	48:A2:4712:G:H5''	2.55	0.41
48:A2:242:C:H2'	48:A2:243:G:C8	2.56	0.41
49:B1:24:C:OP1	56:BJ:11:LYS:NZ	2.44	0.41
49:B1:1398:G:H21	79:Bg:61:GLY:HA2	1.86	0.41
55:BI:104:ILE:HD12	55:BI:173:ALA:HB3	2.02	0.41
58:BL:39:ASN:OD1	58:BL:40:ILE:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Bc:26:GLN:H	75:Bc:26:GLN:HG2	1.63	0.41
78:Bf:100:LEU:HD12	78:Bf:103:LEU:HG	2.02	0.41
79:Bg:18:VAL:HB	79:Bg:301:GLY:HA3	2.02	0.41
2:BA:5:LEU:HB3	2:BA:6:ASP:H	1.69	0.41
3:AB:122:TRP:CH2	3:AB:127:LYS:HG3	2.55	0.41
3:AB:293:ILE:H	3:AB:293:ILE:HG13	1.66	0.41
4:BB:36:PRO:HA	4:BB:232:HIS:CD2	2.56	0.41
4:BB:228:LEU:O	4:BB:232:HIS:ND1	2.45	0.41
5:AC:94:ASN:HD21	48:A2:1502:C:H4'	1.86	0.41
9:AD:291:GLN:HE22	14:AI:213:HIS:HB3	1.85	0.41
12:AG:190:LEU:HD13	12:AG:190:LEU:HA	1.82	0.41
14:AI:28:ASP:OD1	14:AI:29:ALA:N	2.54	0.41
14:AI:38:ARG:NH1	14:AI:45:GLU:OE1	2.50	0.41
17:AM:40:GLY:CA	17:AM:45:VAL:CG1	2.99	0.41
17:AM:46:ARG:HD3	48:A2:924:U:C4'	2.36	0.41
18:AN:99:GLN:NE2	18:AN:118:SER:OG	2.48	0.41
18:AN:178:HIS:HA	18:AN:181:HIS:NE2	2.36	0.41
19:AO:160:ARG:O	19:AO:164:ALA:N	2.54	0.41
23:AS:45:TRP:O	23:AS:49:SER:OG	2.29	0.41
37:Ag:66:ARG:HD3	48:A2:2518:C:H5''	2.03	0.41
47:At:108:MET:O	47:At:112:ARG:HG2	2.20	0.41
48:A2:27:C:H4'	48:A2:60:A:C2	2.56	0.41
48:A2:469:G:N2	48:A2:672:G:H22	2.15	0.41
48:A2:1582:A:N6	82:A:12:LEU:CB	2.84	0.41
48:A2:1734:G:N2	48:A2:1761:U:O2	2.54	0.41
48:A2:1789:C:O2	48:A2:1814:G:N2	2.50	0.41
48:A2:2531:G:N2	48:A2:2745:A:H62	2.19	0.41
48:A2:2838:G:N2	48:A2:3808:C:O2	2.35	0.41
48:A2:3667:C:N4	48:A2:3668:U:O4	2.54	0.41
48:A2:3903:U:H2'	48:A2:3904:G:C8	2.50	0.41
48:A2:4015:G:N1	48:A2:4018:A:OP2	2.52	0.41
48:A2:4539:U:H2'	48:A2:4540:G:C8	2.55	0.41
49:B1:919:A:H4'	69:BW:57:ARG:HD3	2.03	0.41
49:B1:1227:G:N2	49:B1:1635:C:O2'	2.54	0.41
49:B1:1324:G:N2	49:B1:1510:G:H5'	2.34	0.41
49:B1:1387:G:H3'	49:B1:1388:A:H8	1.86	0.41
49:B1:1460:C:N4	49:B1:1466:G:H1	2.17	0.41
50:BD:132:LYS:O	50:BD:156:LEU:N	2.54	0.41
51:BE:163:ASP:OD1	51:BE:164:LEU:N	2.54	0.41
51:BE:252:ARG:HH22	56:BJ:75:ASN:ND2	2.19	0.41
52:BF:49:LEU:HD23	52:BF:49:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:BH:52:GLU:HG3	54:BH:58:LYS:HB3	2.03	0.41
55:BI:107:THR:HG23	55:BI:111:GLN:HE22	1.86	0.41
60:BN:84:LEU:HD12	60:BN:84:LEU:HA	1.95	0.41
61:BO:38:ASN:OD1	61:BO:38:ASN:N	2.53	0.41
62:BP:34:MET:HG3	62:BP:45:LEU:HD13	2.03	0.41
75:Bc:20:ARG:NH1	75:Bc:28:THR:OG1	2.54	0.41
6:BC:169:TYR:CZ	6:BC:177:PRO:HG3	2.56	0.41
7:A3:41:A:N6	7:A3:102:G:O2'	2.47	0.41
10:AE:132:PRO:HG3	48:A2:1271:G:C6	2.56	0.41
10:AE:239:LYS:NZ	48:A2:4897:C:O2	2.43	0.41
18:AN:204:ARG:NH1	48:A2:1324:U:O3'	2.54	0.41
21:AQ:44:ASN:HD21	21:AQ:132:LYS:HA	1.86	0.41
23:AS:154:LEU:HD23	23:AS:154:LEU:HA	1.93	0.41
24:AT:144:ASN:OD1	24:AT:144:ASN:N	2.54	0.41
26:AV:43:LYS:HG3	26:AV:60:MET:HE3	2.02	0.41
27:AW:6:CYS:SG	27:AW:10:GLY:N	2.77	0.41
44:An:23:ARG:NH1	48:A2:3778:A:OP1	2.53	0.41
48:A2:1428:U:H3	48:A2:2079:G:H22	1.69	0.41
48:A2:3741:U:H2'	48:A2:3742:C:C6	2.57	0.41
48:A2:4486:G:OP1	48:A2:4521:A:N6	2.53	0.41
48:A2:4932:C:N4	48:A2:4933:G:O6	2.53	0.41
49:B1:677:G:N1	49:B1:1027:A:OP2	2.52	0.41
49:B1:1585:U:H6	66:BT:67:ARG:HH12	1.66	0.41
49:B1:1661:A:O2'	49:B1:1662:U:O4'	2.39	0.41
64:BR:17:ILE:HD12	64:BR:17:ILE:HA	1.88	0.41
71:BY:88:LYS:HD2	71:BY:97:TYR:CZ	2.56	0.41
3:AB:49:TYR:CE1	3:AB:344:VAL:HG22	2.57	0.40
7:A3:60:G:O6	7:A3:96:C:O2'	2.39	0.40
11:AF:247:MET:HE2	11:AF:247:MET:HB3	1.93	0.40
14:AI:61:SER:HA	14:AI:126:VAL:HG12	2.03	0.40
18:AN:192:TRP:NE1	18:AN:196:ASN:HD22	2.20	0.40
21:AQ:85:THR:HG21	21:AQ:104:ARG:HH21	1.86	0.40
31:Aa:16:SER:OG	48:A2:2262:G:OP1	2.39	0.40
43:Am:104:HIS:CE1	48:A2:4659:U:H5'	2.56	0.40
48:A2:473:G:H2'	48:A2:474:C:C6	2.56	0.40
48:A2:1851:C:H2'	48:A2:1852:A:H8	1.87	0.40
48:A2:2556:C:H2'	48:A2:2557:G:C8	2.56	0.40
48:A2:4855:G:H2'	48:A2:4856:G:C8	2.56	0.40
49:B1:321:C:H42	49:B1:330:G:H1	1.68	0.40
49:B1:877:C:H2'	49:B1:878:G:H8	1.86	0.40
56:BJ:31:LEU:HD12	56:BJ:31:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:BJ:144:ILE:HG22	56:BJ:146:SER:H	1.85	0.40
59:BM:113:ASP:OD1	59:BM:113:ASP:N	2.51	0.40
3:AB:234:ARG:HA	3:AB:234:ARG:HD2	1.77	0.40
12:AG:141:ASN:N	48:A2:149:U:O4	2.54	0.40
18:AN:52:GLY:HA3	18:AN:116:LEU:HD21	2.03	0.40
25:AU:21:PHE:CE1	25:AU:80:LYS:HB3	2.56	0.40
27:AW:50:ASN:HA	27:AW:55:TYR:CE2	2.57	0.40
27:AW:120:GLN:HG3	49:B1:327:G:H3'	2.03	0.40
30:AZ:17:ARG:HD3	37:Ag:75:SER:HB3	2.03	0.40
30:AZ:46:ILE:HD12	30:AZ:46:ILE:HA	1.93	0.40
32:Ab:116:LEU:HD22	32:Ab:117:ARG:N	2.37	0.40
35:Ae:37:LYS:N	48:A2:1644:C:OP1	2.47	0.40
38:Ah:89:ARG:O	38:Ah:93:ARG:HD3	2.21	0.40
42:Al:15:LYS:O	42:Al:19:GLN:HG2	2.21	0.40
47:At:31:ASN:ND2	47:At:40:TYR:O	2.53	0.40
48:A2:466:C:H2'	48:A2:467:C:C6	2.56	0.40
48:A2:954:A:H2	48:A2:2073:A:H2	1.70	0.40
48:A2:2499:C:H2'	48:A2:2500:G:H8	1.86	0.40
48:A2:4168:C:O2'	48:A2:4297:C:O2'	2.28	0.40
48:A2:4556:U:O2	48:A2:4579:G:N2	2.54	0.40
49:B1:906:U:H2'	49:B1:907:G:H8	1.86	0.40
53:BG:47:GLY:HA3	53:BG:116:LYS:HD2	2.02	0.40
56:BJ:55:LYS:HD3	56:BJ:55:LYS:HA	1.85	0.40
61:BO:72:TYR:HB2	75:Bc:63:ARG:HH21	1.86	0.40
65:BS:11:HIS:O	65:BS:23:ARG:HB3	2.21	0.40
65:BS:44:VAL:HG11	65:BS:71:MET:HG2	2.03	0.40
66:BT:38:LYS:HD2	66:BT:52:TRP:CD1	2.57	0.40
79:Bg:292:SER:OG	79:Bg:293:ALA:N	2.51	0.40
2:BA:193:HIS:ND1	2:BA:194:PRO:O	2.55	0.40
3:AB:135:LYS:HE3	3:AB:135:LYS:HB2	1.93	0.40
10:AE:53:GLY:HA3	48:A2:1264:G:N2	2.35	0.40
14:AI:61:SER:OG	48:A2:4393:U:OP1	2.24	0.40
16:AL:59:VAL:HG22	16:AL:102:ARG:HH21	1.86	0.40
18:AN:3:ALA:HA	18:AN:6:TYR:HD2	1.86	0.40
19:AO:108:ILE:N	48:A2:4868:A:N1	2.67	0.40
21:AQ:65:ARG:HD3	48:A2:1483:C:H3'	2.03	0.40
22:AR:150:ALA:HA	22:AR:153:LYS:HG2	2.03	0.40
23:AS:25:PRO:HA	23:AS:26:PRO:HD3	1.88	0.40
28:AX:43:SER:HA	28:AX:44:PRO:HD3	1.90	0.40
48:A2:196:G:N2	48:A2:231:G:H1	2.19	0.40
48:A2:425:G:C8	48:A2:3859:G:H2'	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A2:743:G:O6	48:A2:897:G:N1	2.54	0.40
48:A2:2081:C:O2	48:A2:2082:G:N1	2.54	0.40
48:A2:3916:A:N6	48:A2:4037:U:O4	2.54	0.40
49:B1:57:U:H5'	49:B1:504:G:H21	1.86	0.40
49:B1:122:G:H2'	49:B1:123:G:H8	1.86	0.40
49:B1:553:U:H5'	49:B1:554:A:H4'	2.03	0.40
49:B1:1159:G:P	69:BW:76:SER:HB3	2.61	0.40
49:B1:1725:U:H2'	49:B1:1726:G:H8	1.86	0.40
50:BD:11:PHE:O	50:BD:15:GLY:N	2.54	0.40
52:BF:59:LYS:H	52:BF:62:ARG:HD2	1.86	0.40
54:BH:134:VAL:HG22	54:BH:173:PHE:CE2	2.57	0.40
55:BI:178:ARG:HD2	55:BI:181:GLN:HG3	2.02	0.40
60:BN:30:SER:HB2	60:BN:67:THR:HG23	2.03	0.40
69:BW:111:MET:HE1	69:BW:119:LYS:HE3	2.03	0.40
1:AA:104:VAL:HA	1:AA:107:MET:HE3	2.02	0.40
2:BA:119:PRO:HG2	2:BA:142:LEU:HD22	2.04	0.40
3:AB:110:ILE:O	3:AB:115:LYS:NZ	2.54	0.40
11:AF:113:ARG:NH1	11:AF:208:LEU:O	2.55	0.40
16:AL:64:VAL:HG12	48:A2:71:C:H5'	2.03	0.40
16:AL:144:LEU:HD23	38:Ah:122:LYS:H	1.87	0.40
37:Ag:38:VAL:O	37:Ag:60:ARG:NH2	2.54	0.40
41:Ak:24:LYS:HB3	41:Ak:69:LEU:HD11	2.03	0.40
48:A2:1074:C:H2'	48:A2:1075:G:C8	2.57	0.40
49:B1:925:G:H2'	49:B1:926:A:H8	1.85	0.40
49:B1:1265:A:O2'	49:B1:1327:G:OP2	2.24	0.40
49:B1:1743:G:N2	49:B1:1791:A:H62	2.19	0.40
53:BG:43:GLU:O	53:BG:46:LYS:HG3	2.22	0.40
1:AA:30:ARG:O	1:AA:163:ARG:NH2	2.53	0.40
11:AF:159:TYR:HB3	11:AF:166:ARG:HE	1.86	0.40
13:AH:9:THR:HG23	13:AH:54:ARG:HD2	2.03	0.40
14:AI:189:ARG:HB2	14:AI:189:ARG:HH11	1.86	0.40
16:AL:162:LYS:HE3	16:AL:162:LYS:HB2	1.91	0.40
29:AY:58:VAL:HG22	29:AY:59:ARG:HE	1.86	0.40
30:AZ:65:ARG:HA	30:AZ:65:ARG:HD3	1.92	0.40
30:AZ:106:LEU:HA	30:AZ:109:LYS:HB3	2.04	0.40
32:Ab:50:ASN:HA	32:Ab:54:LEU:HD21	2.04	0.40
37:Ag:96:LEU:HD23	37:Ag:96:LEU:HA	1.85	0.40
46:Ap:15:GLY:O	46:Ap:23:ARG:NH1	2.54	0.40
48:A2:1451:C:H2'	48:A2:1452:G:C8	2.54	0.40
48:A2:1545:A:H2'	48:A2:1546:A:C8	2.55	0.40
48:A2:4461:G:C2	48:A2:4491:G:H1'	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A2:4841:C:H2'	48:A2:4842:G:C8	2.57	0.40
48:A2:4866:G:H21	48:A2:4870:G:H2'	1.87	0.40
48:A2:4925:A:H2'	48:A2:4926:A:C8	2.56	0.40
49:B1:1453:C:H5	49:B1:1476:A:H2	1.70	0.40
70:BX:50:ILE:HD12	70:BX:75:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	246/248 (99%)	216 (88%)	29 (12%)	1 (0%)	30	64
2	BA	213/215 (99%)	193 (91%)	20 (9%)	0	100	100
3	AB	392/394 (100%)	352 (90%)	39 (10%)	1 (0%)	36	69
4	BB	210/212 (99%)	175 (83%)	34 (16%)	1 (0%)	24	59
5	AC	361/363 (99%)	323 (90%)	32 (9%)	6 (2%)	7	35
6	BC	220/222 (99%)	196 (89%)	24 (11%)	0	100	100
9	AD	292/294 (99%)	261 (89%)	30 (10%)	1 (0%)	36	69
10	AE	222/247 (90%)	184 (83%)	35 (16%)	3 (1%)	9	38
11	AF	232/234 (99%)	201 (87%)	30 (13%)	1 (0%)	30	64
12	AG	232/234 (99%)	208 (90%)	23 (10%)	1 (0%)	30	64
13	AH	189/191 (99%)	172 (91%)	17 (9%)	0	100	100
14	AI	204/211 (97%)	181 (89%)	21 (10%)	2 (1%)	12	45
15	AJ	167/169 (99%)	146 (87%)	21 (13%)	0	100	100
16	AL	203/205 (99%)	174 (86%)	26 (13%)	3 (2%)	8	37
17	AM	137/139 (99%)	119 (87%)	18 (13%)	0	100	100
18	AN	201/203 (99%)	172 (86%)	28 (14%)	1 (0%)	24	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AO	193/195 (99%)	183 (95%)	10 (5%)	0	100	100
20	AP	151/153 (99%)	142 (94%)	9 (6%)	0	100	100
21	AQ	185/187 (99%)	165 (89%)	19 (10%)	1 (0%)	24	59
22	AR	179/181 (99%)	170 (95%)	9 (5%)	0	100	100
23	AS	173/175 (99%)	153 (88%)	20 (12%)	0	100	100
24	AT	155/157 (99%)	131 (84%)	22 (14%)	2 (1%)	9	40
25	AU	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
26	AV	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
27	AW	119/121 (98%)	103 (87%)	16 (13%)	0	100	100
28	AX	115/117 (98%)	104 (90%)	11 (10%)	0	100	100
29	AY	125/127 (98%)	116 (93%)	9 (7%)	0	100	100
30	AZ	132/134 (98%)	116 (88%)	16 (12%)	0	100	100
31	Aa	145/147 (99%)	124 (86%)	21 (14%)	0	100	100
32	Ab	93/118 (79%)	81 (87%)	9 (10%)	3 (3%)	3	25
33	Ac	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
34	Ad	104/106 (98%)	91 (88%)	13 (12%)	0	100	100
35	Ae	127/129 (98%)	107 (84%)	20 (16%)	0	100	100
36	Af	107/109 (98%)	96 (90%)	11 (10%)	0	100	100
37	Ag	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
38	Ah	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
39	Ai	95/97 (98%)	81 (85%)	13 (14%)	1 (1%)	11	43
40	Aj	82/84 (98%)	75 (92%)	7 (8%)	0	100	100
41	Ak	67/69 (97%)	62 (92%)	5 (8%)	0	100	100
42	Al	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
43	Am	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
44	An	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
45	Ao	103/105 (98%)	92 (89%)	11 (11%)	0	100	100
46	Ap	89/91 (98%)	78 (88%)	11 (12%)	0	100	100
47	At	120/122 (98%)	106 (88%)	14 (12%)	0	100	100
50	BD	218/220 (99%)	193 (88%)	23 (11%)	2 (1%)	14	47
51	BE	255/257 (99%)	231 (91%)	23 (9%)	1 (0%)	30	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	BF	188/190 (99%)	163 (87%)	25 (13%)	0	100	100
53	BG	230/232 (99%)	197 (86%)	33 (14%)	0	100	100
54	BH	181/183 (99%)	158 (87%)	22 (12%)	1 (1%)	21	55
55	BI	205/207 (99%)	170 (83%)	34 (17%)	1 (0%)	24	59
56	BJ	177/179 (99%)	157 (89%)	19 (11%)	1 (1%)	21	55
57	BK	96/98 (98%)	77 (80%)	18 (19%)	1 (1%)	12	45
58	BL	151/153 (99%)	131 (87%)	19 (13%)	1 (1%)	18	53
59	BM	118/120 (98%)	110 (93%)	8 (7%)	0	100	100
60	BN	147/149 (99%)	129 (88%)	18 (12%)	0	100	100
61	BO	134/136 (98%)	116 (87%)	18 (13%)	0	100	100
62	BP	118/120 (98%)	100 (85%)	16 (14%)	2 (2%)	7	35
63	BQ	137/139 (99%)	121 (88%)	16 (12%)	0	100	100
64	BR	123/125 (98%)	107 (87%)	15 (12%)	1 (1%)	16	50
65	BS	137/139 (99%)	117 (85%)	19 (14%)	1 (1%)	18	53
66	BT	141/143 (99%)	126 (89%)	14 (10%)	1 (1%)	18	53
67	BU	95/97 (98%)	87 (92%)	8 (8%)	0	100	100
68	BV	79/81 (98%)	72 (91%)	6 (8%)	1 (1%)	9	40
69	BW	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
70	BX	137/139 (99%)	124 (90%)	13 (10%)	0	100	100
71	BY	123/125 (98%)	113 (92%)	10 (8%)	0	100	100
72	BZ	84/86 (98%)	71 (84%)	12 (14%)	1 (1%)	10	41
73	Ba	95/97 (98%)	84 (88%)	10 (10%)	1 (1%)	11	43
74	Bb	78/80 (98%)	68 (87%)	10 (13%)	0	100	100
75	Bc	60/62 (97%)	52 (87%)	6 (10%)	2 (3%)	3	24
76	Bd	49/51 (96%)	38 (78%)	11 (22%)	0	100	100
77	Be	53/55 (96%)	45 (85%)	8 (15%)	0	100	100
78	Bf	71/73 (97%)	61 (86%)	9 (13%)	1 (1%)	9	38
79	Bg	312/314 (99%)	273 (88%)	39 (12%)	0	100	100
82	A	24/26 (92%)	16 (67%)	3 (12%)	5 (21%)	0	1
All	All	11199/11402 (98%)	9901 (88%)	1246 (11%)	52 (0%)	26	59

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AB	4	ARG
5	AC	53	ALA
5	AC	151	PRO
14	AI	189	ARG
16	AL	46	ILE
16	AL	47	ALA
32	Ab	25	ARG
50	BD	219	PRO
62	BP	51	ARG
82	A	5	PRO
82	A	10	LEU
82	A	20	ARG
5	AC	152	LEU
10	AE	128	HIS
18	AN	95	ALA
32	Ab	112	ILE
39	Ai	35	LYS
57	BK	41	PRO
58	BL	14	PRO
72	BZ	42	ASP
82	A	9	LEU
5	AC	57	LEU
14	AI	188	LYS
24	AT	53	PRO
32	Ab	113	ALA
56	BJ	123	ILE
66	BT	31	PRO
5	AC	52	TYR
5	AC	73	VAL
11	AF	223	LYS
24	AT	18	PRO
51	BE	150	PRO
54	BH	115	LYS
55	BI	118	ALA
68	BV	41	LYS
73	Ba	85	ARG
82	A	16	PRO
4	BB	53	GLN
9	AD	257	PRO
10	AE	127	SER
16	AL	134	PRO
21	AQ	159	PRO
62	BP	125	PRO

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Mol	Chain	Res	Type
75	Bc	33	GLU
10	AE	185	PRO
50	BD	218	LEU
64	BR	4	VAL
75	Bc	32	VAL
1	AA	141	PRO
78	Bf	88	PRO
65	BS	6	PRO
12	AG	30	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	190/190 (100%)	187 (98%)	3 (2%)	55	69
2	BA	180/180 (100%)	179 (99%)	1 (1%)	78	80
3	AB	343/343 (100%)	342 (100%)	1 (0%)	86	85
4	BB	193/193 (100%)	191 (99%)	2 (1%)	68	75
5	AC	302/302 (100%)	295 (98%)	7 (2%)	44	63
6	BC	188/188 (100%)	186 (99%)	2 (1%)	65	74
9	AD	248/248 (100%)	247 (100%)	1 (0%)	84	83
10	AE	202/220 (92%)	202 (100%)	0	100	100
11	AF	203/203 (100%)	202 (100%)	1 (0%)	81	82
12	AG	199/199 (100%)	196 (98%)	3 (2%)	57	70
13	AH	170/170 (100%)	169 (99%)	1 (1%)	78	80
14	AI	178/179 (99%)	174 (98%)	4 (2%)	45	64
15	AJ	142/142 (100%)	141 (99%)	1 (1%)	76	78
16	AL	171/171 (100%)	168 (98%)	3 (2%)	51	67
17	AM	118/118 (100%)	117 (99%)	1 (1%)	73	77
18	AN	171/171 (100%)	171 (100%)	0	100	100
19	AO	168/168 (100%)	165 (98%)	3 (2%)	51	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AP	134/134 (100%)	133 (99%)	1 (1%)	76	78
21	AQ	164/164 (100%)	164 (100%)	0	100	100
22	AR	160/160 (100%)	159 (99%)	1 (1%)	78	80
23	AS	156/156 (100%)	156 (100%)	0	100	100
24	AT	138/138 (100%)	138 (100%)	0	100	100
25	AU	89/89 (100%)	89 (100%)	0	100	100
26	AV	100/100 (100%)	100 (100%)	0	100	100
27	AW	100/100 (100%)	100 (100%)	0	100	100
28	AX	105/105 (100%)	104 (99%)	1 (1%)	68	75
29	AY	119/119 (100%)	115 (97%)	4 (3%)	32	55
30	AZ	117/117 (100%)	114 (97%)	3 (3%)	40	60
31	Aa	120/120 (100%)	120 (100%)	0	100	100
32	Ab	79/98 (81%)	77 (98%)	2 (2%)	42	62
33	Ac	88/88 (100%)	87 (99%)	1 (1%)	65	74
34	Ad	97/97 (100%)	97 (100%)	0	100	100
35	Ae	115/115 (100%)	115 (100%)	0	100	100
36	Af	88/88 (100%)	84 (96%)	4 (4%)	24	49
37	Ag	98/98 (100%)	98 (100%)	0	100	100
38	Ah	109/109 (100%)	105 (96%)	4 (4%)	30	53
39	Ai	83/83 (100%)	83 (100%)	0	100	100
40	Aj	71/71 (100%)	70 (99%)	1 (1%)	59	71
41	Ak	64/64 (100%)	63 (98%)	1 (2%)	55	69
42	Al	47/47 (100%)	46 (98%)	1 (2%)	47	65
43	Am	46/46 (100%)	46 (100%)	0	100	100
44	An	24/24 (100%)	24 (100%)	0	100	100
45	Ao	93/93 (100%)	92 (99%)	1 (1%)	65	74
46	Ap	74/74 (100%)	73 (99%)	1 (1%)	59	71
47	At	106/106 (100%)	105 (99%)	1 (1%)	70	75
50	BD	183/183 (100%)	181 (99%)	2 (1%)	65	74
51	BE	220/220 (100%)	216 (98%)	4 (2%)	51	67
52	BF	160/160 (100%)	158 (99%)	2 (1%)	61	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	BG	202/202 (100%)	201 (100%)	1 (0%)	81	82
54	BH	164/164 (100%)	163 (99%)	1 (1%)	78	80
55	BI	179/179 (100%)	177 (99%)	2 (1%)	65	74
56	BJ	160/160 (100%)	158 (99%)	2 (1%)	61	71
57	BK	89/89 (100%)	89 (100%)	0	100	100
58	BL	138/138 (100%)	138 (100%)	0	100	100
59	BM	102/102 (100%)	101 (99%)	1 (1%)	68	75
60	BN	130/130 (100%)	130 (100%)	0	100	100
61	BO	106/106 (100%)	106 (100%)	0	100	100
62	BP	109/109 (100%)	108 (99%)	1 (1%)	70	75
63	BQ	115/115 (100%)	115 (100%)	0	100	100
64	BR	113/113 (100%)	110 (97%)	3 (3%)	39	60
65	BS	121/121 (100%)	119 (98%)	2 (2%)	53	68
66	BT	113/113 (100%)	113 (100%)	0	100	100
67	BU	90/90 (100%)	90 (100%)	0	100	100
68	BV	65/65 (100%)	65 (100%)	0	100	100
69	BW	112/112 (100%)	110 (98%)	2 (2%)	51	67
70	BX	111/111 (100%)	111 (100%)	0	100	100
71	BY	107/107 (100%)	105 (98%)	2 (2%)	50	66
72	BZ	75/75 (100%)	73 (97%)	2 (3%)	39	60
73	Ba	84/84 (100%)	84 (100%)	0	100	100
74	Bb	72/72 (100%)	70 (97%)	2 (3%)	38	59
75	Bc	55/55 (100%)	54 (98%)	1 (2%)	51	67
76	Bd	45/45 (100%)	45 (100%)	0	100	100
77	Be	44/44 (100%)	44 (100%)	0	100	100
78	Bf	66/66 (100%)	66 (100%)	0	100	100
79	Bg	272/272 (100%)	271 (100%)	1 (0%)	84	83
All	All	9752/9790 (100%)	9660 (99%)	92 (1%)	68	75

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	45	VAL

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Mol	Chain	Res	Type
1	AA	58	LEU
1	AA	207	VAL
2	BA	16	LEU
3	AB	254	ILE
4	BB	51	ARG
4	BB	63	LYS
5	AC	146	GLU
5	AC	147	VAL
5	AC	151	PRO
5	AC	215	ASN
5	AC	229	LEU
5	AC	230	LEU
5	AC	282	HIS
6	BC	66	LEU
6	BC	141	VAL
9	AD	37	VAL
11	AF	24	ASN
12	AG	84	THR
12	AG	193	LEU
12	AG	201	THR
13	AH	28	LYS
14	AI	158	LYS
14	AI	185	VAL
14	AI	188	LYS
14	AI	191	ILE
15	AJ	120	ASP
16	AL	46	ILE
16	AL	54	PRO
16	AL	154	VAL
17	AM	5	ARG
19	AO	33	VAL
19	AO	160	ARG
19	AO	185	VAL
20	AP	22	LEU
22	AR	146	LYS
28	AX	59	LYS
29	AY	2	LYS
29	AY	71	VAL
29	AY	74	TYR
29	AY	79	VAL
30	AZ	53	VAL
30	AZ	80	LEU

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Mol	Chain	Res	Type
30	AZ	133	LYS
32	Ab	32	LEU
32	Ab	116	LEU
33	Ac	45	LEU
36	Af	58	VAL
36	Af	74	VAL
36	Af	95	LYS
36	Af	106	TYR
38	Ah	88	THR
38	Ah	91	MET
38	Ah	92	ARG
38	Ah	102	LEU
40	Aj	67	LEU
41	Ak	60	LEU
42	Al	49	LEU
45	Ao	98	LYS
46	Ap	17	ARG
47	At	61	VAL
50	BD	10	LYS
50	BD	210	ILE
51	BE	75	LYS
51	BE	153	VAL
51	BE	221	ARG
51	BE	238	LEU
52	BF	63	LYS
52	BF	135	ARG
53	BG	202	ASN
54	BH	156	VAL
55	BI	76	THR
55	BI	121	LEU
56	BJ	52	LYS
56	BJ	172	ARG
59	BM	31	LEU
62	BP	126	VAL
64	BR	91	LEU
64	BR	98	VAL
64	BR	116	ASN
65	BS	78	LYS
65	BS	88	LYS
69	BW	5	ASN
69	BW	25	VAL
71	BY	9	THR

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Mol	Chain	Res	Type
71	BY	122	LYS
72	BZ	62	VAL
72	BZ	83	LEU
74	Bb	21	LYS
74	Bb	23	ARG
75	Bc	9	ILE
79	Bg	133	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (181) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	50	HIS
1	AA	132	ASN
1	AA	209	HIS
1	AA	216	HIS
1	AA	218	HIS
2	BA	113	GLN
2	BA	131	HIS
2	BA	149	ASN
3	AB	25	HIS
3	AB	204	GLN
3	AB	376	HIS
4	BB	40	ASN
4	BB	76	ASN
4	BB	149	GLN
4	BB	208	HIS
5	AC	38	ASN
5	AC	50	GLN
5	AC	61	GLN
5	AC	85	HIS
5	AC	94	ASN
5	AC	215	ASN
5	AC	299	GLN
6	BC	134	ASN
6	BC	178	HIS
6	BC	267	GLN
9	AD	39	GLN
9	AD	57	ASN
9	AD	111	ASN
9	AD	191	ASN
9	AD	198	HIS
9	AD	244	HIS

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Mol	Chain	Res	Type
10	AE	136	HIS
10	AE	190	HIS
10	AE	191	GLN
10	AE	211	HIS
10	AE	279	ASN
11	AF	24	ASN
11	AF	146	ASN
12	AG	43	GLN
12	AG	90	GLN
12	AG	149	ASN
13	AH	189	GLN
14	AI	14	ASN
14	AI	86	HIS
14	AI	144	ASN
14	AI	147	HIS
14	AI	166	HIS
15	AJ	104	ASN
16	AL	149	GLN
16	AL	159	ASN
16	AL	175	ASN
17	AM	56	GLN
17	AM	70	GLN
18	AN	8	GLN
18	AN	37	HIS
18	AN	86	HIS
18	AN	87	HIS
18	AN	109	HIS
18	AN	145	ASN
18	AN	158	HIS
18	AN	196	ASN
18	AN	199	GLN
18	AN	201	HIS
19	AO	65	ASN
19	AO	180	GLN
19	AO	184	ASN
20	AP	40	HIS
20	AP	75	GLN
20	AP	80	GLN
20	AP	118	GLN
21	AQ	7	HIS
21	AQ	44	ASN
21	AQ	77	ASN

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Mol	Chain	Res	Type
21	AQ	93	GLN
23	AS	23	HIS
23	AS	66	GLN
23	AS	77	ASN
23	AS	122	HIS
24	AT	3	ASN
24	AT	98	HIS
25	AU	50	ASN
25	AU	105	ASN
26	AV	135	ASN
27	AW	45	ASN
27	AW	63	GLN
28	AX	57	GLN
28	AX	107	HIS
29	AY	4	ASN
29	AY	20	ASN
29	AY	40	GLN
29	AY	96	HIS
31	Aa	67	GLN
31	Aa	74	ASN
31	Aa	89	ASN
31	Aa	120	GLN
32	Ab	58	GLN
33	Ac	15	ASN
34	Ad	79	ASN
36	Af	56	ASN
36	Af	65	ASN
36	Af	99	HIS
37	Ag	73	HIS
40	Aj	13	ASN
42	Al	19	GLN
42	Al	43	HIS
43	Am	109	ASN
43	Am	120	ASN
45	Ao	3	ASN
45	Ao	45	GLN
46	Ap	34	HIS
47	At	4	HIS
47	At	6	GLN
47	At	41	ASN
47	At	83	ASN
50	BD	74	GLN

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Mol	Chain	Res	Type
50	BD	101	GLN
51	BE	36	HIS
51	BE	197	ASN
51	BE	216	ASN
51	BE	230	ASN
52	BF	79	HIS
52	BF	114	ASN
52	BF	203	ASN
53	BG	13	GLN
53	BG	56	ASN
53	BG	163	ASN
53	BG	186	GLN
53	BG	202	ASN
54	BH	39	GLN
54	BH	162	GLN
54	BH	165	ASN
54	BH	193	GLN
55	BI	64	ASN
56	BJ	75	ASN
56	BJ	124	HIS
56	BJ	134	HIS
56	BJ	140	GLN
56	BJ	177	ASN
57	BK	7	ASN
57	BK	44	HIS
57	BK	61	GLN
58	BL	11	GLN
58	BL	18	GLN
58	BL	19	ASN
58	BL	83	GLN
59	BM	72	HIS
59	BM	82	ASN
60	BN	5	HIS
60	BN	105	ASN
60	BN	123	HIS
61	BO	32	HIS
62	BP	54	HIS
62	BP	79	HIS
63	BQ	142	GLN
64	BR	31	ASN
64	BR	56	HIS
65	BS	17	ASN

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Mol	Chain	Res	Type
65	BS	19	ASN
65	BS	76	GLN
66	BT	105	GLN
69	BW	5	ASN
69	BW	16	ASN
70	BX	61	GLN
70	BX	92	ASN
70	BX	127	ASN
71	BY	15	ASN
71	BY	22	GLN
71	BY	29	HIS
72	BZ	89	GLN
72	BZ	112	ASN
73	Ba	7	ASN
74	Bb	9	HIS
75	Bc	24	GLN
76	Bd	41	GLN
76	Bd	45	GLN
79	Bg	20	GLN
79	Bg	133	ASN
79	Bg	143	GLN
79	Bg	187	ASN
79	Bg	272	GLN
79	Bg	305	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
48	A2	3626/3643 (99%)	1021 (28%)	12 (0%)
49	B1	1701/1708 (99%)	533 (31%)	6 (0%)
7	A3	156/157 (99%)	49 (31%)	1 (0%)
8	A4	118/119 (99%)	29 (24%)	0
80	Bv	75/76 (98%)	28 (37%)	0
81	Bx	15/16 (93%)	9 (60%)	0
All	All	5691/5719 (99%)	1669 (29%)	19 (0%)

All (1669) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A3	8	U
7	A3	32	C

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Mol	Chain	Res	Type
7	A3	34	U
7	A3	35	C
7	A3	36	G
7	A3	37	A
7	A3	39	G
7	A3	52	A
7	A3	57	C
7	A3	58	G
7	A3	59	A
7	A3	60	G
7	A3	63	U
7	A3	71	A
7	A3	72	A
7	A3	73	U
7	A3	74	U
7	A3	81	C
7	A3	82	A
7	A3	84	A
7	A3	85	U
7	A3	87	G
7	A3	90	C
7	A3	95	A
7	A3	96	C
7	A3	99	U
7	A3	101	C
7	A3	103	A
7	A3	104	A
7	A3	105	C
7	A3	109	C
7	A3	110	U
7	A3	111	U
7	A3	112	G
7	A3	121	G
7	A3	122	G
7	A3	123	U
7	A3	124	U
7	A3	125	C
7	A3	126	C
7	A3	127	U
7	A3	128	C
7	A3	129	C
7	A3	130	C

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Mol	Chain	Res	Type
7	A3	137	A
7	A3	142	U
7	A3	148	A
7	A3	151	G
7	A3	154	G
8	A4	2	U
8	A4	7	G
8	A4	8	G
8	A4	11	A
8	A4	14	C
8	A4	19	C
8	A4	22	A
8	A4	24	C
8	A4	27	G
8	A4	29	C
8	A4	31	G
8	A4	33	U
8	A4	38	U
8	A4	41	G
8	A4	49	A
8	A4	50	A
8	A4	53	U
8	A4	54	A
8	A4	59	G
8	A4	63	C
8	A4	64	G
8	A4	66	G
8	A4	85	G
8	A4	91	C
8	A4	97	G
8	A4	99	G
8	A4	109	U
8	A4	110	G
8	A4	118	C
48	A2	2	G
48	A2	9	C
48	A2	10	A
48	A2	13	U
48	A2	14	C
48	A2	17	A
48	A2	23	C
48	A2	25	A

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Mol	Chain	Res	Type
48	A2	32	G
48	A2	37	U
48	A2	39	A
48	A2	40	G
48	A2	42	A
48	A2	47	A
48	A2	48	G
48	A2	49	U
48	A2	50	C
48	A2	59	A
48	A2	64	A
48	A2	65	A
48	A2	70	A
48	A2	71	C
48	A2	72	C
48	A2	73	A
48	A2	84	A
48	A2	87	A
48	A2	88	A
48	A2	91	G
48	A2	93	G
48	A2	101	A
48	A2	116	G
48	A2	119	G
48	A2	120	A
48	A2	121	A
48	A2	122	U
48	A2	131	C
48	A2	132	G
48	A2	133	C
48	A2	134	G
48	A2	135	G
48	A2	138	C
48	A2	139	G
48	A2	140	C
48	A2	141	G
48	A2	143	G
48	A2	147	U
48	A2	149	U
48	A2	150	G
48	A2	153	G
48	A2	156	C

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Mol	Chain	Res	Type
48	A2	157	G
48	A2	158	G
48	A2	161	G
48	A2	167	C
48	A2	169	C
48	A2	173	G
48	A2	174	G
48	A2	181	U
48	A2	182	C
48	A2	183	G
48	A2	184	U
48	A2	185	G
48	A2	193	C
48	A2	196	G
48	A2	197	U
48	A2	201	U
48	A2	206	U
48	A2	207	C
48	A2	212	C
48	A2	213	C
48	A2	214	C
48	A2	215	A
48	A2	223	G
48	A2	228	U
48	A2	229	G
48	A2	230	U
48	A2	233	G
48	A2	234	G
48	A2	237	G
48	A2	241	G
48	A2	242	C
48	A2	250	G
48	A2	251	G
48	A2	252	C
48	A2	253	G
48	A2	260	C
48	A2	289	A
48	A2	291	U
48	A2	300	A
48	A2	303	C
48	A2	304	G
48	A2	306	G

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Mol	Chain	Res	Type
48	A2	309	G
48	A2	310	U
48	A2	311	A
48	A2	313	A
48	A2	315	U
48	A2	334	C
48	A2	338	A
48	A2	343	A
48	A2	344	C
48	A2	348	U
48	A2	352	C
48	A2	356	A
48	A2	357	A
48	A2	367	G
48	A2	370	A
48	A2	375	U
48	A2	379	A
48	A2	380	A
48	A2	381	G
48	A2	390	A
48	A2	393	G
48	A2	402	A
48	A2	403	G
48	A2	404	A
48	A2	406	G
48	A2	407	G
48	A2	409	G
48	A2	425	G
48	A2	426	U
48	A2	434	U
48	A2	440	C
48	A2	444	G
48	A2	445	C
48	A2	446	A
48	A2	447	G
48	A2	448	U
48	A2	449	C
48	A2	451	G
48	A2	456	G
48	A2	459	G
48	A2	461	U
48	A2	467	C

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Mol	Chain	Res	Type
48	A2	479	C
48	A2	480	C
48	A2	481	G
48	A2	489	C
48	A2	492	C
48	A2	493	G
48	A2	495	C
48	A2	496	C
48	A2	497	C
48	A2	498	G
48	A2	505	C
48	A2	506	U
48	A2	507	U
48	A2	508	U
48	A2	509	C
48	A2	513	C
48	A2	633	U
48	A2	635	G
48	A2	645	C
48	A2	646	G
48	A2	649	C
48	A2	651	C
48	A2	652	C
48	A2	654	G
48	A2	655	A
48	A2	658	G
48	A2	661	G
48	A2	662	A
48	A2	664	C
48	A2	668	C
48	A2	674	C
48	A2	677	G
48	A2	678	C
48	A2	680	C
48	A2	682	U
48	A2	684	U
48	A2	688	G
48	A2	690	C
48	A2	692	G
48	A2	693	U
48	A2	695	C
48	A2	698	C

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Mol	Chain	Res	Type
48	A2	702	A
48	A2	719	U
48	A2	720	G
48	A2	721	G
48	A2	724	A
48	A2	728	C
48	A2	737	A
48	A2	738	A
48	A2	739	G
48	A2	900	U
48	A2	901	U
48	A2	902	A
48	A2	903	C
48	A2	905	G
48	A2	906	C
48	A2	911	C
48	A2	917	G
48	A2	919	A
48	A2	920	G
48	A2	921	C
48	A2	923	C
48	A2	924	U
48	A2	925	C
48	A2	927	C
48	A2	931	A
48	A2	932	U
48	A2	933	C
48	A2	939	G
48	A2	947	A
48	A2	948	A
48	A2	949	G
48	A2	950	C
48	A2	951	G
48	A2	953	G
48	A2	954	A
48	A2	955	C
48	A2	958	U
48	A2	959	C
48	A2	967	U
48	A2	968	C
48	A2	975	C
48	A2	1055	C

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Mol	Chain	Res	Type
48	A2	1059	C
48	A2	1061	A
48	A2	1062	C
48	A2	1065	C
48	A2	1066	U
48	A2	1076	C
48	A2	1078	A
48	A2	1083	U
48	A2	1084	C
48	A2	1085	U
48	A2	1087	C
48	A2	1149	G
48	A2	1150	C
48	A2	1152	G
48	A2	1154	G
48	A2	1155	C
48	A2	1156	G
48	A2	1161	G
48	A2	1162	U
48	A2	1163	C
48	A2	1164	C
48	A2	1167	A
48	A2	1180	C
48	A2	1181	G
48	A2	1188	G
48	A2	1191	G
48	A2	1192	U
48	A2	1193	C
48	A2	1196	G
48	A2	1197	C
48	A2	1200	G
48	A2	1201	G
48	A2	1202	G
48	A2	1220	C
48	A2	1221	A
48	A2	1222	C
48	A2	1223	G
48	A2	1226	C
48	A2	1228	C
48	A2	1233	C
48	A2	1247	C
48	A2	1249	G

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Mol	Chain	Res	Type
48	A2	1250	C
48	A2	1251	G
48	A2	1253	A
48	A2	1255	C
48	A2	1256	G
48	A2	1257	A
48	A2	1258	G
48	A2	1259	C
48	A2	1260	G
48	A2	1261	C
48	A2	1262	A
48	A2	1263	C
48	A2	1264	G
48	A2	1265	G
48	A2	1268	U
48	A2	1269	C
48	A2	1271	G
48	A2	1277	A
48	A2	1278	C
48	A2	1280	U
48	A2	1284	C
48	A2	1285	U
48	A2	1286	A
48	A2	1295	A
48	A2	1299	G
48	A2	1301	C
48	A2	1304	G
48	A2	1309	A
48	A2	1315	C
48	A2	1321	G
48	A2	1337	A
48	A2	1341	G
48	A2	1342	G
48	A2	1343	G
48	A2	1348	C
48	A2	1349	G
48	A2	1350	C
48	A2	1351	A
48	A2	1353	G
48	A2	1355	A
48	A2	1360	G
48	A2	1370	A

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Mol	Chain	Res	Type
48	A2	1377	G
48	A2	1380	A
48	A2	1381	A
48	A2	1386	G
48	A2	1389	G
48	A2	1390	C
48	A2	1391	G
48	A2	1392	C
48	A2	1393	U
48	A2	1394	C
48	A2	1395	G
48	A2	1399	G
48	A2	1400	C
48	A2	1401	C
48	A2	1402	G
48	A2	1403	A
48	A2	1404	G
48	A2	1408	G
48	A2	1415	G
48	A2	1420	C
48	A2	1421	U
48	A2	1422	C
48	A2	1423	U
48	A2	1424	C
48	A2	1426	A
48	A2	1427	G
48	A2	1429	C
48	A2	1439	G
48	A2	1454	C
48	A2	1457	G
48	A2	1462	C
48	A2	1463	C
48	A2	1464	G
48	A2	1465	C
48	A2	1466	G
48	A2	1467	C
48	A2	1468	C
48	A2	1469	G
48	A2	1479	A
48	A2	1480	G
48	A2	1485	A
48	A2	1486	G

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Mol	Chain	Res	Type
48	A2	1499	G
48	A2	1505	A
48	A2	1507	A
48	A2	1513	U
48	A2	1516	A
48	A2	1520	U
48	A2	1521	G
48	A2	1525	G
48	A2	1531	G
48	A2	1534	G
48	A2	1548	C
48	A2	1556	G
48	A2	1560	U
48	A2	1563	G
48	A2	1573	U
48	A2	1578	U
48	A2	1579	G
48	A2	1583	A
48	A2	1587	G
48	A2	1589	C
48	A2	1596	C
48	A2	1606	G
48	A2	1607	G
48	A2	1609	G
48	A2	1610	C
48	A2	1612	A
48	A2	1613	A
48	A2	1614	A
48	A2	1615	G
48	A2	1616	A
48	A2	1620	A
48	A2	1622	C
48	A2	1623	G
48	A2	1625	A
48	A2	1631	U
48	A2	1632	A
48	A2	1636	G
48	A2	1642	U
48	A2	1643	C
48	A2	1650	A
48	A2	1652	G
48	A2	1658	C

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Mol	Chain	Res	Type
48	A2	1659	U
48	A2	1660	C
48	A2	1663	G
48	A2	1666	A
48	A2	1678	C
48	A2	1680	C
48	A2	1700	C
48	A2	1701	A
48	A2	1708	U
48	A2	1712	U
48	A2	1713	C
48	A2	1716	G
48	A2	1723	G
48	A2	1724	A
48	A2	1730	U
48	A2	1732	G
48	A2	1733	A
48	A2	1736	U
48	A2	1737	C
48	A2	1742	G
48	A2	1743	G
48	A2	1746	G
48	A2	1747	A
48	A2	1751	G
48	A2	1752	A
48	A2	1757	A
48	A2	1767	C
48	A2	1769	A
48	A2	1776	A
48	A2	1779	G
48	A2	1786	A
48	A2	1794	C
48	A2	1798	C
48	A2	1804	U
48	A2	1814	G
48	A2	1816	G
48	A2	1817	G
48	A2	1818	A
48	A2	1823	G
48	A2	1835	G
48	A2	1836	G
48	A2	1850	G

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Mol	Chain	Res	Type
48	A2	1851	C
48	A2	1854	A
48	A2	1862	C
48	A2	1863	U
48	A2	1870	U
48	A2	1872	A
48	A2	1873	A
48	A2	1880	G
48	A2	1887	U
48	A2	1891	G
48	A2	1896	C
48	A2	1897	G
48	A2	1898	A
48	A2	1899	U
48	A2	1900	G
48	A2	1902	C
48	A2	1903	G
48	A2	1911	U
48	A2	1912	C
48	A2	1913	A
48	A2	1916	C
48	A2	1917	C
48	A2	1918	C
48	A2	1921	G
48	A2	1923	A
48	A2	1925	A
48	A2	1926	G
48	A2	1928	U
48	A2	1929	G
48	A2	1930	U
48	A2	1936	G
48	A2	1938	U
48	A2	1940	U
48	A2	1941	A
48	A2	1942	G
48	A2	1943	A
48	A2	1947	C
48	A2	1950	G
48	A2	1955	U
48	A2	1956	G
48	A2	1957	G
48	A2	1959	C

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Mol	Chain	Res	Type
48	A2	1960	A
48	A2	1961	U
48	A2	1962	G
48	A2	1963	G
48	A2	1964	A
48	A2	1965	A
48	A2	1967	U
48	A2	1968	C
48	A2	1969	G
48	A2	1971	A
48	A2	1972	A
48	A2	1975	C
48	A2	1978	U
48	A2	1979	A
48	A2	1980	A
48	A2	1982	G
48	A2	1983	A
48	A2	1984	G
48	A2	1985	U
48	A2	1988	G
48	A2	1989	U
48	A2	1990	A
48	A2	1991	A
48	A2	1996	U
48	A2	1997	C
48	A2	1998	A
48	A2	1999	C
48	A2	2003	C
48	A2	2007	A
48	A2	2011	A
48	A2	2015	G
48	A2	2019	U
48	A2	2023	A
48	A2	2025	U
48	A2	2027	G
48	A2	2029	U
48	A2	2036	G
48	A2	2037	G
48	A2	2043	C
48	A2	2050	A
48	A2	2051	U
48	A2	2065	C

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Mol	Chain	Res	Type
48	A2	2069	G
48	A2	2073	A
48	A2	2074	G
48	A2	2076	G
48	A2	2077	U
48	A2	2078	G
48	A2	2082	G
48	A2	2084	G
48	A2	2087	C
48	A2	2088	G
48	A2	2091	G
48	A2	2092	G
48	A2	2237	C
48	A2	2238	G
48	A2	2239	C
48	A2	2243	C
48	A2	2246	U
48	A2	2247	A
48	A2	2257	G
48	A2	2258	A
48	A2	2268	C
48	A2	2275	G
48	A2	2277	U
48	A2	2279	A
48	A2	2280	G
48	A2	2282	C
48	A2	2288	G
48	A2	2292	A
48	A2	2295	G
48	A2	2298	C
48	A2	2308	U
48	A2	2321	G
48	A2	2325	C
48	A2	2327	G
48	A2	2330	C
48	A2	2339	A
48	A2	2340	G
48	A2	2343	G
48	A2	2348	U
48	A2	2352	C
48	A2	2358	A
48	A2	2363	U

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Mol	Chain	Res	Type
48	A2	2366	G
48	A2	2370	G
48	A2	2375	A
48	A2	2376	G
48	A2	2400	G
48	A2	2401	C
48	A2	2405	U
48	A2	2416	C
48	A2	2417	A
48	A2	2420	C
48	A2	2426	U
48	A2	2429	G
48	A2	2432	A
48	A2	2439	A
48	A2	2442	G
48	A2	2446	U
48	A2	2447	U
48	A2	2449	C
48	A2	2452	A
48	A2	2453	G
48	A2	2454	G
48	A2	2467	C
48	A2	2468	C
48	A2	2469	U
48	A2	2473	U
48	A2	2478	C
48	A2	2480	C
48	A2	2482	G
48	A2	2483	C
48	A2	2484	C
48	A2	2485	G
48	A2	2486	A
48	A2	2490	A
48	A2	2492	A
48	A2	2499	C
48	A2	2509	U
48	A2	2523	G
48	A2	2524	U
48	A2	2525	G
48	A2	2527	C
48	A2	2532	A
48	A2	2533	U

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Mol	Chain	Res	Type
48	A2	2545	G
48	A2	2555	G
48	A2	2560	A
48	A2	2561	A
48	A2	2565	G
48	A2	2566	A
48	A2	2567	C
48	A2	2568	C
48	A2	2569	G
48	A2	2580	A
48	A2	2584	G
48	A2	2585	G
48	A2	2601	G
48	A2	2606	C
48	A2	2617	G
48	A2	2619	G
48	A2	2632	C
48	A2	2640	U
48	A2	2642	G
48	A2	2646	C
48	A2	2648	C
48	A2	2652	G
48	A2	2653	A
48	A2	2665	G
48	A2	2666	U
48	A2	2673	G
48	A2	2674	A
48	A2	2675	A
48	A2	2676	A
48	A2	2682	G
48	A2	2684	G
48	A2	2686	U
48	A2	2687	U
48	A2	2689	C
48	A2	2690	G
48	A2	2691	G
48	A2	2699	C
48	A2	2700	G
48	A2	2704	A
48	A2	2705	G
48	A2	2719	U
48	A2	2720	U

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Mol	Chain	Res	Type
48	A2	2722	A
48	A2	2723	A
48	A2	2734	A
48	A2	2737	G
48	A2	2740	U
48	A2	2741	G
48	A2	2742	U
48	A2	2743	A
48	A2	2745	A
48	A2	2746	U
48	A2	2766	A
48	A2	2767	U
48	A2	2769	U
48	A2	2773	C
48	A2	2776	C
48	A2	2778	G
48	A2	2782	U
48	A2	2785	A
48	A2	2794	A
48	A2	2805	U
48	A2	2806	G
48	A2	2814	A
48	A2	2822	U
48	A2	2824	A
48	A2	2829	A
48	A2	2831	U
48	A2	2832	C
48	A2	2834	G
48	A2	2835	C
48	A2	2837	A
48	A2	2842	G
48	A2	2846	C
48	A2	2854	C
48	A2	2858	A
48	A2	2860	A
48	A2	2863	G
48	A2	2876	G
48	A2	2881	G
48	A2	3570	A
48	A2	3572	C
48	A2	3576	C
48	A2	3579	A

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Mol	Chain	Res	Type
48	A2	3586	G
48	A2	3591	G
48	A2	3596	G
48	A2	3597	G
48	A2	3601	A
48	A2	3602	U
48	A2	3606	A
48	A2	3612	U
48	A2	3613	A
48	A2	3614	A
48	A2	3615	U
48	A2	3619	A
48	A2	3627	A
48	A2	3633	A
48	A2	3643	G
48	A2	3644	C
48	A2	3646	G
48	A2	3649	G
48	A2	3651	U
48	A2	3656	C
48	A2	3659	U
48	A2	3663	A
48	A2	3665	U
48	A2	3683	A
48	A2	3686	U
48	A2	3688	A
48	A2	3700	U
48	A2	3704	A
48	A2	3707	A
48	A2	3721	G
48	A2	3724	G
48	A2	3731	A
48	A2	3732	C
48	A2	3733	U
48	A2	3738	C
48	A2	3741	U
48	A2	3744	U
48	A2	3747	G
48	A2	3748	G
48	A2	3751	G
48	A2	3754	A
48	A2	3755	A

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Mol	Chain	Res	Type
48	A2	3756	A
48	A2	3761	U
48	A2	3774	A
48	A2	3781	C
48	A2	3782	G
48	A2	3783	C
48	A2	3784	A
48	A2	3788	A
48	A2	3789	U
48	A2	3790	G
48	A2	3795	A
48	A2	3800	G
48	A2	3809	U
48	A2	3810	G
48	A2	3811	U
48	A2	3814	C
48	A2	3822	U
48	A2	3829	C
48	A2	3836	A
48	A2	3838	A
48	A2	3840	C
48	A2	3847	A
48	A2	3848	A
48	A2	3849	C
48	A2	3850	G
48	A2	3851	G
48	A2	3853	C
48	A2	3856	G
48	A2	3860	G
48	A2	3861	A
48	A2	3866	G
48	A2	3868	G
48	A2	3872	A
48	A2	3876	A
48	A2	3877	A
48	A2	3878	G
48	A2	3879	A
48	A2	3885	U
48	A2	3886	U
48	A2	3889	G
48	A2	3894	A
48	A2	3909	G

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Mol	Chain	Res	Type
48	A2	3918	A
48	A2	3922	G
48	A2	3935	U
48	A2	3937	A
48	A2	3943	A
48	A2	3944	G
48	A2	4005	G
48	A2	4009	G
48	A2	4011	C
48	A2	4012	G
48	A2	4013	G
48	A2	4014	U
48	A2	4016	A
48	A2	4018	A
48	A2	4019	U
48	A2	4027	C
48	A2	4029	C
48	A2	4033	U
48	A2	4034	C
48	A2	4035	G
48	A2	4037	U
48	A2	4038	U
48	A2	4040	U
48	A2	4041	U
48	A2	4046	G
48	A2	4047	A
48	A2	4058	C
48	A2	4065	G
48	A2	4067	G
48	A2	4068	A
48	A2	4069	G
48	A2	4070	C
48	A2	4071	C
48	A2	4072	C
48	A2	4074	A
48	A2	4076	G
48	A2	4083	C
48	A2	4084	G
48	A2	4086	U
48	A2	4088	C
48	A2	4090	G
48	A2	4091	G

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Mol	Chain	Res	Type
48	A2	4093	G
48	A2	4097	A
48	A2	4104	G
48	A2	4106	C
48	A2	4109	G
48	A2	4110	C
48	A2	4112	G
48	A2	4119	A
48	A2	4120	C
48	A2	4124	C
48	A2	4126	C
48	A2	4130	G
48	A2	4132	A
48	A2	4145	G
48	A2	4150	U
48	A2	4153	G
48	A2	4156	U
48	A2	4167	A
48	A2	4174	A
48	A2	4175	A
48	A2	4176	A
48	A2	4187	G
48	A2	4188	G
48	A2	4191	U
48	A2	4195	A
48	A2	4206	A
48	A2	4211	G
48	A2	4215	A
48	A2	4216	G
48	A2	4219	A
48	A2	4228	G
48	A2	4229	G
48	A2	4230	A
48	A2	4234	G
48	A2	4235	A
48	A2	4238	G
48	A2	4241	A
48	A2	4242	A
48	A2	4243	A
48	A2	4244	A
48	A2	4252	U
48	A2	4253	G

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Mol	Chain	Res	Type
48	A2	4265	C
48	A2	4266	A
48	A2	4267	G
48	A2	4268	U
48	A2	4276	C
48	A2	4279	A
48	A2	4281	C
48	A2	4291	G
48	A2	4292	G
48	A2	4294	C
48	A2	4299	C
48	A2	4301	A
48	A2	4310	A
48	A2	4311	C
48	A2	4316	U
48	A2	4319	G
48	A2	4327	C
48	A2	4330	G
48	A2	4333	G
48	A2	4334	U
48	A2	4337	C
48	A2	4339	G
48	A2	4340	A
48	A2	4341	A
48	A2	4342	A
48	A2	4349	C
48	A2	4353	G
48	A2	4355	G
48	A2	4356	A
48	A2	4360	C
48	A2	4372	G
48	A2	4382	U
48	A2	4384	A
48	A2	4395	G
48	A2	4406	C
48	A2	4410	G
48	A2	4414	U
48	A2	4415	C
48	A2	4426	A
48	A2	4428	C
48	A2	4437	G
48	A2	4441	A

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Mol	Chain	Res	Type
48	A2	4443	U
48	A2	4453	G
48	A2	4455	U
48	A2	4466	C
48	A2	4474	U
48	A2	4475	A
48	A2	4477	G
48	A2	4480	A
48	A2	4510	A
48	A2	4522	C
48	A2	4531	U
48	A2	4532	G
48	A2	4535	G
48	A2	4537	G
48	A2	4546	A
48	A2	4551	A
48	A2	4552	A
48	A2	4561	A
48	A2	4576	G
48	A2	4579	G
48	A2	4590	U
48	A2	4593	G
48	A2	4597	A
48	A2	4598	U
48	A2	4614	G
48	A2	4618	A
48	A2	4619	U
48	A2	4620	G
48	A2	4621	G
48	A2	4624	C
48	A2	4630	U
48	A2	4632	C
48	A2	4633	C
48	A2	4640	G
48	A2	4649	A
48	A2	4655	C
48	A2	4662	A
48	A2	4665	U
48	A2	4671	U
48	A2	4675	G
48	A2	4680	G
48	A2	4681	G

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Mol	Chain	Res	Type
48	A2	4692	C
48	A2	4693	G
48	A2	4694	G
48	A2	4696	A
48	A2	4700	C
48	A2	4703	C
48	A2	4704	G
48	A2	4709	C
48	A2	4710	U
48	A2	4712	G
48	A2	4714	U
48	A2	4715	U
48	A2	4716	G
48	A2	4718	C
48	A2	4720	U
48	A2	4722	G
48	A2	4724	A
48	A2	4725	U
48	A2	4726	A
48	A2	4731	G
48	A2	4732	U
48	A2	4824	C
48	A2	4827	U
48	A2	4828	G
48	A2	4831	G
48	A2	4832	A
48	A2	4833	G
48	A2	4834	U
48	A2	4838	C
48	A2	4839	U
48	A2	4840	U
48	A2	4847	G
48	A2	4849	G
48	A2	4852	A
48	A2	4854	G
48	A2	4855	G
48	A2	4856	G
48	A2	4859	G
48	A2	4863	C
48	A2	4864	C
48	A2	4865	G
48	A2	4866	G

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Mol	Chain	Res	Type
48	A2	4868	A
48	A2	4871	G
48	A2	4878	C
48	A2	4880	C
48	A2	4882	C
48	A2	4883	U
48	A2	4884	C
48	A2	4885	G
48	A2	4886	C
48	A2	4890	U
48	A2	4895	C
48	A2	4897	C
48	A2	4898	C
48	A2	4899	G
48	A2	4901	A
48	A2	4902	C
48	A2	4904	U
48	A2	4909	G
48	A2	4919	G
48	A2	4924	A
48	A2	4927	C
48	A2	4934	U
48	A2	4935	A
48	A2	4936	G
48	A2	4946	U
48	A2	4947	U
48	A2	4949	U
48	A2	4950	G
48	A2	4957	G
48	A2	4971	C
48	A2	4975	G
48	A2	4981	C
48	A2	4982	C
48	A2	4984	U
48	A2	4985	C
48	A2	4987	C
48	A2	4999	G
48	A2	5000	A
48	A2	5008	C
48	A2	5011	U
48	A2	5012	C
48	A2	5013	G

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Mol	Chain	Res	Type
48	A2	5016	A
48	A2	5019	A
48	A2	5020	G
48	A2	5024	U
48	A2	5027	U
49	B1	4	C
49	B1	16	G
49	B1	20	G
49	B1	23	G
49	B1	33	G
49	B1	41	G
49	B1	44	U
49	B1	46	A
49	B1	49	C
49	B1	51	U
49	B1	54	A
49	B1	59	U
49	B1	61	A
49	B1	62	G
49	B1	65	C
49	B1	67	C
49	B1	70	G
49	B1	71	G
49	B1	72	C
49	B1	73	C
49	B1	74	G
49	B1	77	A
49	B1	82	G
49	B1	89	C
49	B1	91	A
49	B1	100	U
49	B1	101	U
49	B1	103	A
49	B1	104	A
49	B1	109	U
49	B1	110	U
49	B1	113	G
49	B1	114	G
49	B1	115	U
49	B1	116	U
49	B1	122	G
49	B1	125	C

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Mol	Chain	Res	Type
49	B1	126	G
49	B1	142	C
49	B1	143	U
49	B1	146	G
49	B1	147	A
49	B1	153	G
49	B1	154	U
49	B1	155	G
49	B1	157	U
49	B1	159	A
49	B1	160	U
49	B1	161	U
49	B1	162	C
49	B1	170	A
49	B1	171	A
49	B1	172	U
49	B1	175	A
49	B1	178	C
49	B1	180	G
49	B1	181	A
49	B1	183	G
49	B1	188	C
49	B1	192	C
49	B1	199	C
49	B1	207	G
49	B1	209	A
49	B1	210	U
49	B1	211	G
49	B1	214	U
49	B1	217	A
49	B1	225	G
49	B1	226	A
49	B1	227	U
49	B1	228	C
49	B1	229	A
49	B1	230	A
49	B1	233	C
49	B1	234	C
49	B1	236	A
49	B1	238	C
49	B1	240	G
49	B1	283	G

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Mol	Chain	Res	Type
49	B1	284	C
49	B1	285	U
49	B1	286	U
49	B1	287	U
49	B1	288	G
49	B1	292	A
49	B1	293	C
49	B1	301	A
49	B1	305	U
49	B1	306	C
49	B1	308	G
49	B1	309	G
49	B1	310	C
49	B1	313	A
49	B1	314	U
49	B1	318	A
49	B1	319	C
49	B1	324	C
49	B1	327	G
49	B1	328	U
49	B1	329	G
49	B1	330	G
49	B1	331	C
49	B1	332	G
49	B1	333	G
49	B1	339	A
49	B1	343	A
49	B1	344	U
49	B1	347	G
49	B1	349	A
49	B1	351	G
49	B1	358	C
49	B1	364	A
49	B1	367	U
49	B1	368	U
49	B1	369	C
49	B1	372	U
49	B1	376	A
49	B1	381	C
49	B1	385	G
49	B1	386	C
49	B1	398	A

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Mol	Chain	Res	Type
49	B1	402	C
49	B1	407	G
49	B1	408	A
49	B1	409	C
49	B1	413	G
49	B1	417	C
49	B1	428	U
49	B1	438	G
49	B1	439	A
49	B1	441	C
49	B1	448	A
49	B1	449	A
49	B1	450	C
49	B1	464	A
49	B1	465	A
49	B1	468	A
49	B1	471	G
49	B1	472	C
49	B1	474	G
49	B1	476	A
49	B1	482	G
49	B1	487	U
49	B1	489	A
49	B1	492	C
49	B1	496	C
49	B1	501	C
49	B1	503	C
49	B1	504	G
49	B1	507	G
49	B1	508	A
49	B1	512	A
49	B1	517	C
49	B1	518	G
49	B1	522	A
49	B1	523	A
49	B1	525	A
49	B1	527	C
49	B1	529	A
49	B1	530	U
49	B1	534	G
49	B1	535	G
49	B1	536	A

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Mol	Chain	Res	Type
49	B1	541	U
49	B1	542	U
49	B1	544	G
49	B1	545	A
49	B1	546	G
49	B1	547	G
49	B1	548	C
49	B1	550	C
49	B1	551	U
49	B1	552	G
49	B1	553	U
49	B1	554	A
49	B1	555	A
49	B1	558	G
49	B1	560	A
49	B1	562	U
49	B1	567	C
49	B1	568	C
49	B1	569	A
49	B1	570	C
49	B1	585	C
49	B1	587	A
49	B1	588	G
49	B1	590	A
49	B1	591	U
49	B1	592	C
49	B1	594	A
49	B1	598	G
49	B1	600	G
49	B1	604	A
49	B1	606	G
49	B1	607	U
49	B1	608	C
49	B1	613	G
49	B1	614	C
49	B1	615	C
49	B1	617	G
49	B1	620	G
49	B1	621	C
49	B1	623	G
49	B1	627	U
49	B1	628	A

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Mol	Chain	Res	Type
49	B1	629	A
49	B1	631	U
49	B1	643	A
49	B1	644	G
49	B1	645	C
49	B1	649	U
49	B1	655	A
49	B1	657	U
49	B1	658	U
49	B1	659	G
49	B1	660	C
49	B1	662	G
49	B1	669	A
49	B1	672	A
49	B1	673	G
49	B1	683	G
49	B1	684	G
49	B1	688	U
49	B1	690	G
49	B1	691	G
49	B1	739	C
49	B1	740	C
49	B1	742	U
49	B1	743	U
49	B1	744	G
49	B1	746	C
49	B1	748	C
49	B1	749	U
49	B1	750	C
49	B1	791	C
49	B1	797	C
49	B1	798	G
49	B1	799	U
49	B1	800	U
49	B1	801	U
49	B1	809	A
49	B1	811	A
49	B1	821	G
49	B1	829	C
49	B1	836	G
49	B1	837	A
49	B1	839	C

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Mol	Chain	Res	Type
49	B1	840	C
49	B1	841	G
49	B1	847	A
49	B1	861	A
49	B1	870	A
49	B1	872	A
49	B1	873	G
49	B1	874	G
49	B1	881	G
49	B1	887	U
49	B1	888	U
49	B1	890	U
49	B1	893	U
49	B1	905	C
49	B1	909	G
49	B1	912	C
49	B1	913	A
49	B1	914	U
49	B1	917	U
49	B1	919	A
49	B1	920	A
49	B1	928	G
49	B1	929	G
49	B1	933	G
49	B1	943	U
49	B1	950	C
49	B1	955	A
49	B1	956	G
49	B1	958	G
49	B1	960	U
49	B1	962	A
49	B1	963	A
49	B1	969	U
49	B1	970	G
49	B1	971	G
49	B1	973	C
49	B1	975	G
49	B1	983	A
49	B1	988	C
49	B1	990	A
49	B1	992	A
49	B1	996	A

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Mol	Chain	Res	Type
49	B1	997	A
49	B1	1001	A
49	B1	1002	U
49	B1	1008	A
49	B1	1017	U
49	B1	1022	U
49	B1	1023	A
49	B1	1028	A
49	B1	1032	C
49	B1	1037	G
49	B1	1040	G
49	B1	1044	G
49	B1	1049	A
49	B1	1050	A
49	B1	1055	A
49	B1	1061	U
49	B1	1064	C
49	B1	1069	U
49	B1	1076	G
49	B1	1080	A
49	B1	1085	C
49	B1	1086	G
49	B1	1087	A
49	B1	1088	U
49	B1	1089	G
49	B1	1100	A
49	B1	1102	G
49	B1	1109	C
49	B1	1114	U
49	B1	1115	U
49	B1	1116	C
49	B1	1117	C
49	B1	1118	C
49	B1	1119	A
49	B1	1120	U
49	B1	1121	G
49	B1	1123	C
49	B1	1126	G
49	B1	1133	A
49	B1	1139	C
49	B1	1140	G
49	B1	1146	C

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Mol	Chain	Res	Type
49	B1	1149	A
49	B1	1150	A
49	B1	1154	U
49	B1	1155	U
49	B1	1157	G
49	B1	1158	G
49	B1	1163	C
49	B1	1166	G
49	B1	1170	A
49	B1	1175	G
49	B1	1176	G
49	B1	1195	A
49	B1	1196	A
49	B1	1197	G
49	B1	1199	A
49	B1	1203	G
49	B1	1207	G
49	B1	1210	G
49	B1	1211	G
49	B1	1215	C
49	B1	1216	C
49	B1	1221	G
49	B1	1224	G
49	B1	1237	C
49	B1	1240	A
49	B1	1242	U
49	B1	1250	A
49	B1	1251	A
49	B1	1256	G
49	B1	1257	G
49	B1	1258	A
49	B1	1259	A
49	B1	1260	A
49	B1	1261	C
49	B1	1262	C
49	B1	1264	C
49	B1	1275	G
49	B1	1276	A
49	B1	1278	A
49	B1	1281	G
49	B1	1283	C
49	B1	1285	G

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Mol	Chain	Res	Type
49	B1	1287	A
49	B1	1288	U
49	B1	1289	U
49	B1	1290	G
49	B1	1297	U
49	B1	1301	A
49	B1	1302	G
49	B1	1309	C
49	B1	1310	U
49	B1	1312	G
49	B1	1313	A
49	B1	1315	U
49	B1	1316	C
49	B1	1318	G
49	B1	1321	G
49	B1	1329	U
49	B1	1330	G
49	B1	1331	C
49	B1	1341	C
49	B1	1343	U
49	B1	1347	U
49	B1	1348	G
49	B1	1371	U
49	B1	1372	U
49	B1	1376	A
49	B1	1378	A
49	B1	1381	G
49	B1	1382	A
49	B1	1393	G
49	B1	1396	A
49	B1	1397	U
49	B1	1398	G
49	B1	1399	C
49	B1	1401	A
49	B1	1403	C
49	B1	1404	U
49	B1	1406	G
49	B1	1409	A
49	B1	1411	G
49	B1	1412	C
49	B1	1417	C
49	B1	1418	C

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Mol	Chain	Res	Type
49	B1	1419	C
49	B1	1420	G
49	B1	1421	A
49	B1	1424	G
49	B1	1439	A
49	B1	1441	U
49	B1	1446	A
49	B1	1450	G
49	B1	1452	A
49	B1	1454	A
49	B1	1455	A
49	B1	1458	G
49	B1	1462	U
49	B1	1463	U
49	B1	1464	C
49	B1	1469	A
49	B1	1477	U
49	B1	1478	U
49	B1	1484	A
49	B1	1487	A
49	B1	1489	A
49	B1	1494	U
49	B1	1495	G
49	B1	1497	G
49	B1	1498	A
49	B1	1502	C
49	B1	1505	U
49	B1	1509	U
49	B1	1512	C
49	B1	1519	U
49	B1	1520	G
49	B1	1521	C
49	B1	1522	A
49	B1	1533	A
49	B1	1534	C
49	B1	1535	U
49	B1	1536	G
49	B1	1540	G
49	B1	1544	C
49	B1	1547	C
49	B1	1551	U
49	B1	1552	G

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Mol	Chain	Res	Type
49	B1	1553	C
49	B1	1554	C
49	B1	1555	U
49	B1	1557	C
49	B1	1558	C
49	B1	1567	G
49	B1	1578	U
49	B1	1580	A
49	B1	1584	G
49	B1	1585	U
49	B1	1586	U
49	B1	1587	G
49	B1	1588	A
49	B1	1594	A
49	B1	1599	U
49	B1	1600	G
49	B1	1601	A
49	B1	1605	G
49	B1	1606	G
49	B1	1618	C
49	B1	1620	A
49	B1	1622	U
49	B1	1623	A
49	B1	1624	U
49	B1	1632	G
49	B1	1637	A
49	B1	1640	A
49	B1	1646	C
49	B1	1660	C
49	B1	1661	A
49	B1	1662	U
49	B1	1663	A
49	B1	1665	G
49	B1	1666	C
49	B1	1671	G
49	B1	1672	U
49	B1	1674	G
49	B1	1678	A
49	B1	1695	A
49	B1	1699	A
49	B1	1703	C
49	B1	1721	U

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Mol	Chain	Res	Type
49	B1	1726	G
49	B1	1742	C
49	B1	1744	G
49	B1	1746	U
49	B1	1753	C
49	B1	1756	C
49	B1	1757	G
49	B1	1777	G
49	B1	1783	C
49	B1	1784	G
49	B1	1799	G
49	B1	1801	A
49	B1	1803	U
49	B1	1811	C
49	B1	1822	A
49	B1	1826	G
49	B1	1829	G
49	B1	1830	U
49	B1	1832	A
49	B1	1834	A
49	B1	1835	A
49	B1	1838	U
49	B1	1839	U
49	B1	1840	U
49	B1	1845	A
49	B1	1849	G
49	B1	1851	A
49	B1	1852	C
49	B1	1855	G
49	B1	1861	G
49	B1	1863	A
49	B1	1865	C
49	B1	1866	A
49	B1	1869	A
80	Bv	2	C
80	Bv	6	G
80	Bv	7	A
80	Bv	8	U
80	Bv	9	A
80	Bv	10	G
80	Bv	11	C
80	Bv	15	G

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Mol	Chain	Res	Type
80	Bv	16	U
80	Bv	17	C
80	Bv	18	G
80	Bv	19	G
80	Bv	20	U
80	Bv	21	A
80	Bv	35	A
80	Bv	37	A
80	Bv	40	C
80	Bv	42	C
80	Bv	46	G
80	Bv	48	C
80	Bv	49	C
80	Bv	56	C
80	Bv	59	U
80	Bv	60	U
80	Bv	62	C
80	Bv	65	G
80	Bv	67	C
80	Bv	76	A
81	Bx	46	U
81	Bx	48	U
81	Bx	50	U
81	Bx	51	U
81	Bx	53	U
81	Bx	54	U
81	Bx	55	U
81	Bx	57	U
81	Bx	58	U

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A3	109	C
48	A2	31	U
48	A2	71	C
48	A2	901	U
48	A2	947	A
48	A2	1161	G
48	A2	1222	C
48	A2	2407	A
48	A2	3755	A

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Mol	Chain	Res	Type
48	A2	4333	G
48	A2	4661	U
48	A2	4865	G
48	A2	4946	U
49	B1	160	U
49	B1	216	C
49	B1	227	U
49	B1	797	C
49	B1	869	A
49	B1	1398	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 332 ligands modelled in this entry, 331 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
85	MVM	A	101	-	35,35,35	1.95	7 (20%)	44,49,49	3.16	19 (43%)

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	MVM	A	101	-	-	6/20/28/28	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	A	101	MVM	N4-N5	-7.32	1.30	1.38
85	A	101	MVM	C5-N1	5.72	1.45	1.37
85	A	101	MVM	C6-N1	2.73	1.45	1.39
85	A	101	MVM	O1-C5	-2.18	1.18	1.22
85	A	101	MVM	C2-CL	2.09	1.78	1.73
85	A	101	MVM	C1-C9	2.07	1.54	1.52
85	A	101	MVM	C7-C3	-2.03	1.48	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	A	101	MVM	C15-N4-C22	-10.67	121.07	130.55
85	A	101	MVM	C15-N4-N5	9.34	127.66	119.25
85	A	101	MVM	N7-C22-N4	6.53	133.22	125.88
85	A	101	MVM	C6-N1-C5	-4.76	117.24	122.94
85	A	101	MVM	N3-C6-N1	4.26	120.91	116.35
85	A	101	MVM	C19-C18-N6	4.06	135.79	130.50
85	A	101	MVM	C7-C3-C9	3.83	118.09	110.81
85	A	101	MVM	C14-C15-N4	-3.78	115.89	119.93
85	A	101	MVM	C18-C22-N7	-3.77	122.00	127.18
85	A	101	MVM	C8-N3-C6	3.16	122.20	115.05
85	A	101	MVM	C21-N7-C22	2.92	121.65	115.05
85	A	101	MVM	C12-C5-N1	2.49	121.66	118.36
85	A	101	MVM	C17-C12-C13	2.37	121.58	118.57
85	A	101	MVM	C6-N1-C9	2.34	121.88	118.40
85	A	101	MVM	C1-C9-N1	-2.34	110.29	116.16
85	A	101	MVM	O1-C5-C12	-2.19	115.94	120.29
85	A	101	MVM	C20-C21-N7	-2.13	120.04	123.42
85	A	101	MVM	C22-N4-N5	2.09	111.26	110.25
85	A	101	MVM	C6-C2-CL	-2.06	119.56	121.50

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	A	101	MVM	C16-C15-N4-C22
85	A	101	MVM	C14-C15-N4-C22

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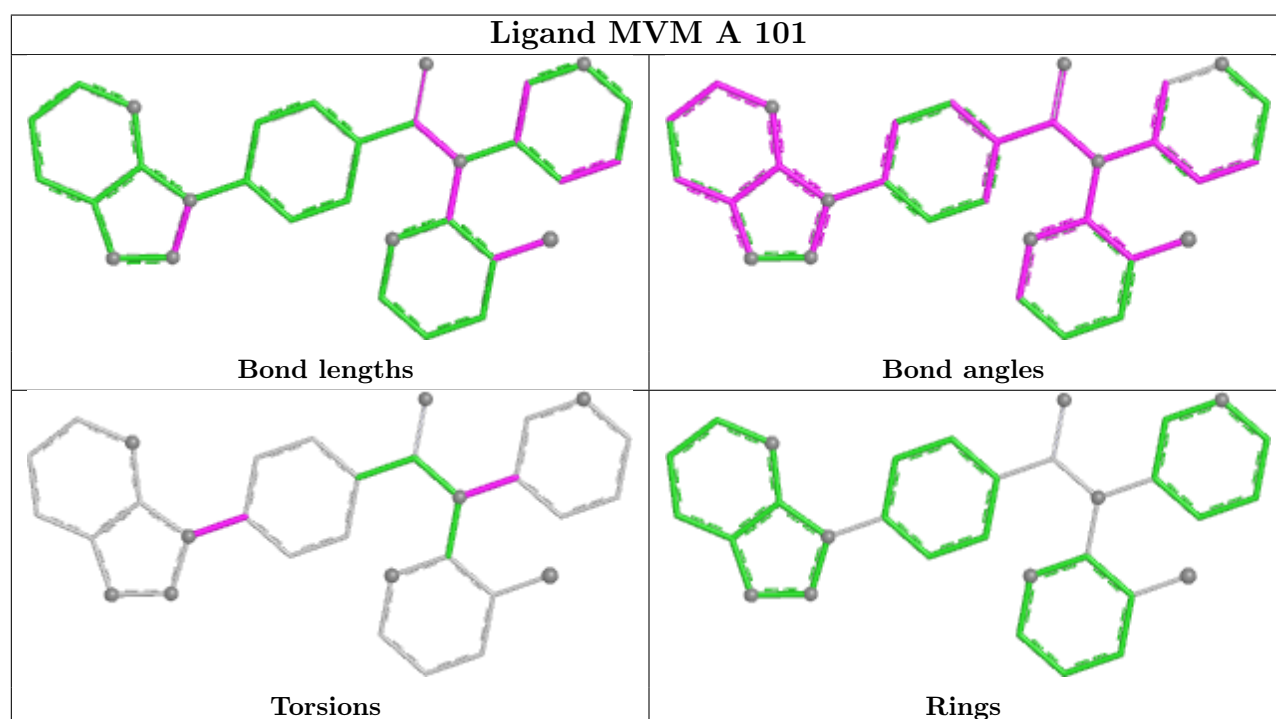
Mol	Chain	Res	Type	Atoms
85	A	101	MVM	C16-C15-N4-N5
85	A	101	MVM	C14-C15-N4-N5
85	A	101	MVM	C3-C9-N1-C5
85	A	101	MVM	C3-C9-N1-C6

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	A	101	MVM	7	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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	A2	16
49	B1	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A2	3923:A	O3'	3930:U	P	31.28
1	B1	126:G	O3'	141:A	P	22.59
1	A2	2231:G	O3'	2235:C	P	21.97
1	A2	3948:C	O3'	4004:G	P	18.85
1	B1	1426:U	O3'	1438:A	P	18.66
1	A2	1680:C	O3'	1699:C	P	18.34
1	A2	517:C	O3'	629:G	P	18.29
1	B1	751:G	O3'	790:C	P	17.33
1	A2	4734:C	O3'	4818:G	P	17.05
1	A2	2881:G	O3'	3569:C	P	16.41
1	A2	750:G	O3'	890:C	P	16.33
1	B1	696:G	O3'	737:G	P	15.56
1	A2	976:U	O3'	1047:G	P	15.44
1	B1	1757:G	O3'	1775:U	P	15.15
1	A2	1233:C	O3'	1243:G	P	14.69
1	A2	2093:C	O3'	2228:C	P	14.13
1	A2	1089:A	O3'	1145:G	P	14.10
1	B1	240:G	O3'	282:G	P	13.82
1	A2	955:C	O3'	957:G	P	8.96
1	A2	2229:C	O3'	2231:G	P	8.58
1	A2	1202:G	O3'	1216:G	P	8.51
1	A2	962:C	O3'	963:G	P	5.47

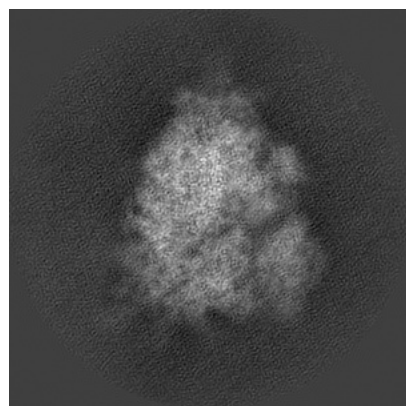
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0598. These allow visual inspection of the internal detail of the map and identification of artifacts.

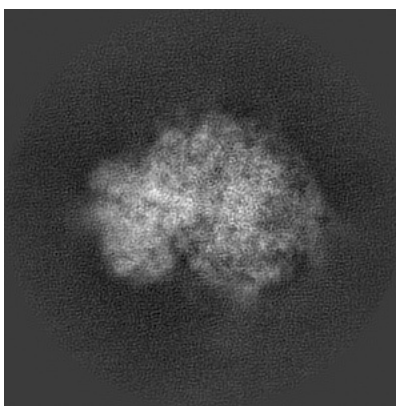
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

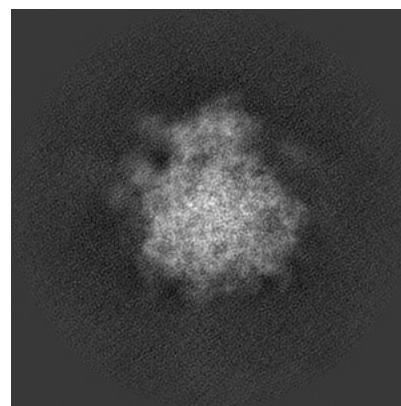
6.1.1 Primary map



X

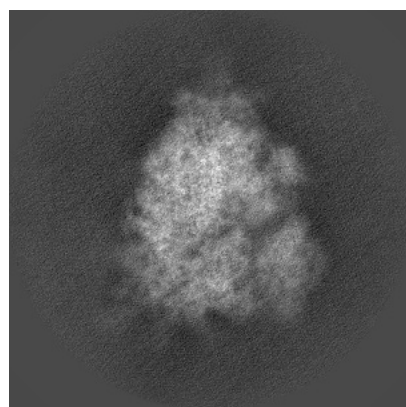


Y

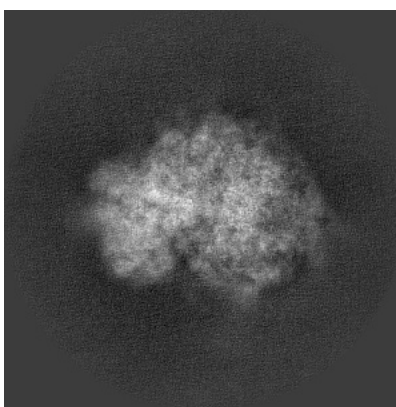


Z

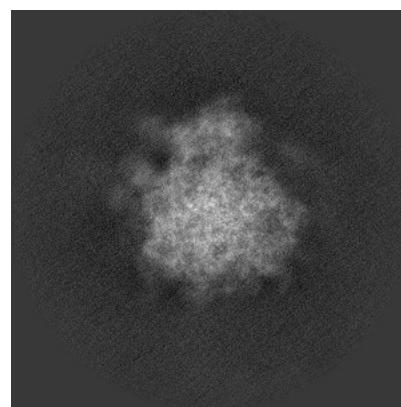
6.1.2 Raw map



X



Y

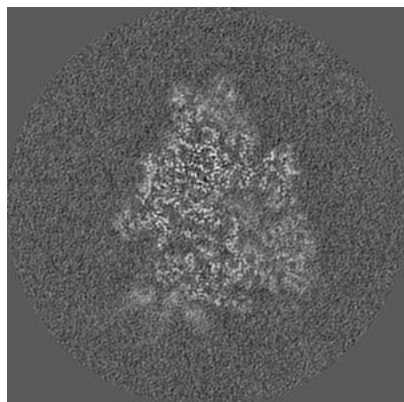


Z

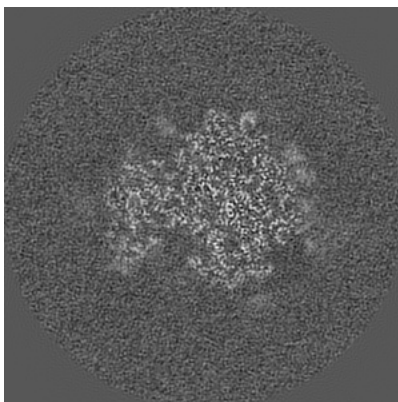
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

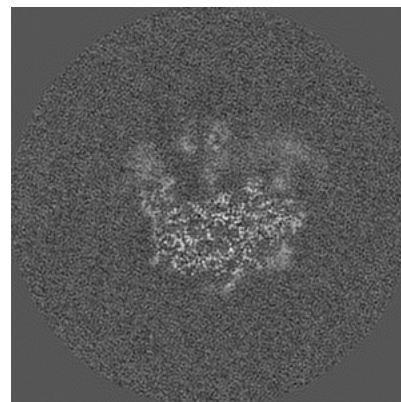
6.2.1 Primary map



X Index: 200

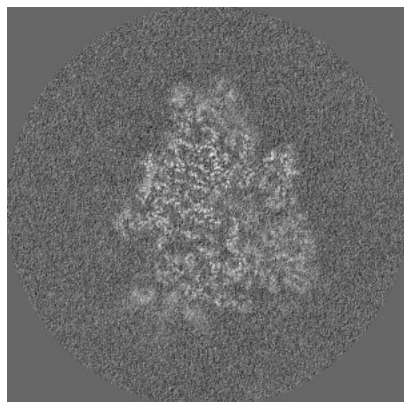


Y Index: 200

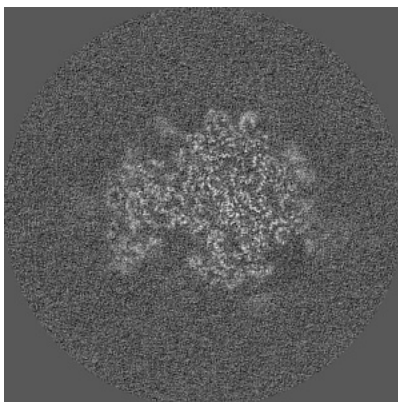


Z Index: 200

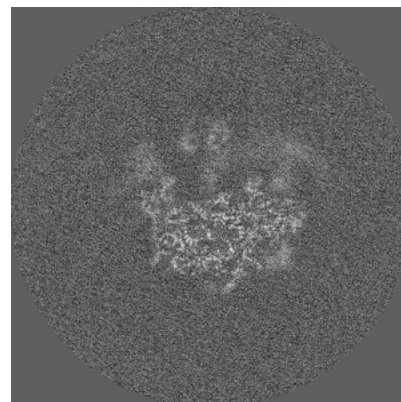
6.2.2 Raw map



X Index: 200



Y Index: 200

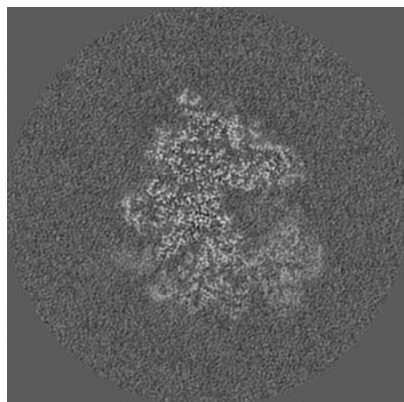


Z Index: 200

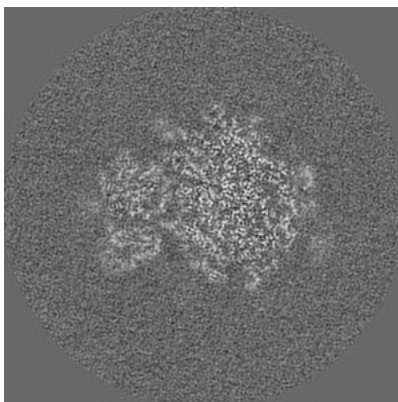
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

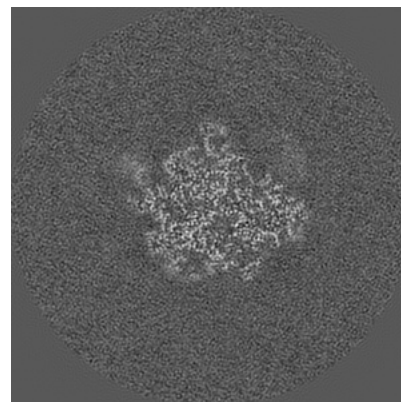
6.3.1 Primary map



X Index: 217

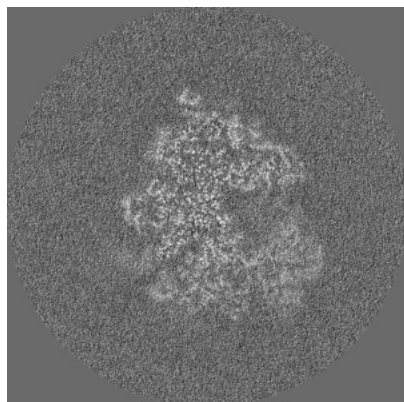


Y Index: 194

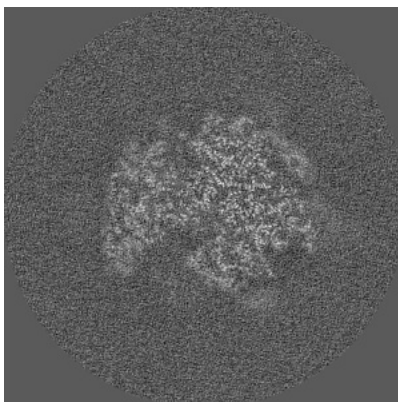


Z Index: 220

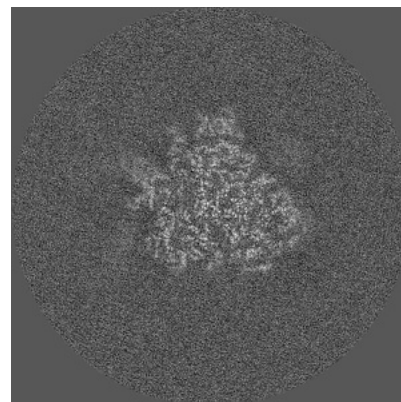
6.3.2 Raw map



X Index: 217



Y Index: 205

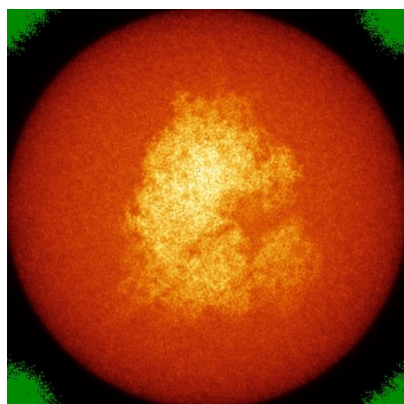


Z Index: 228

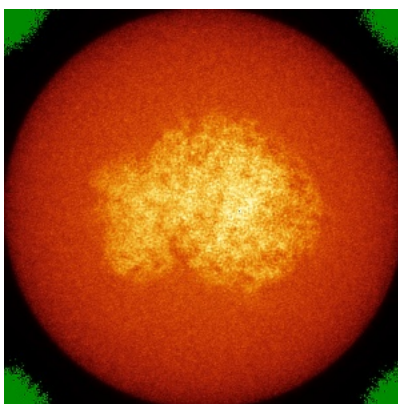
The images above show the largest variance slices of the map in three orthogonal directions.

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

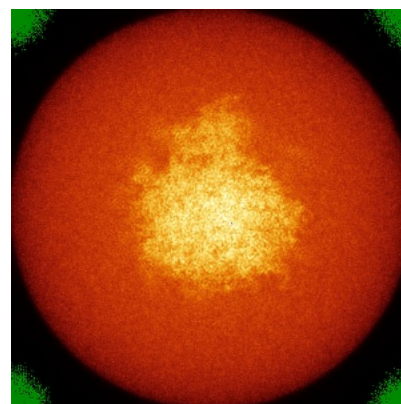
6.4.1 Primary map



X

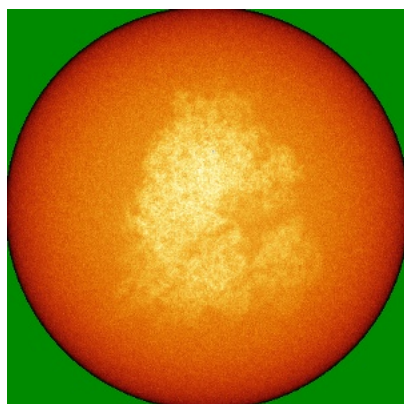


Y

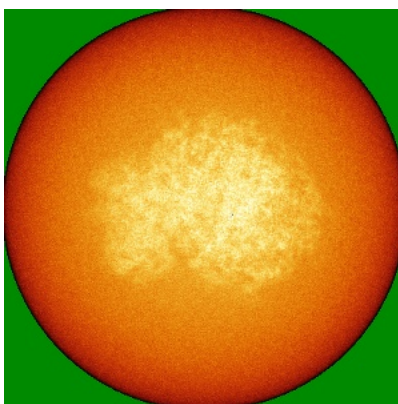


Z

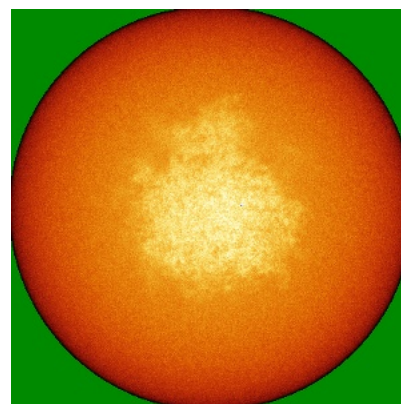
6.4.2 Raw map



X



Y

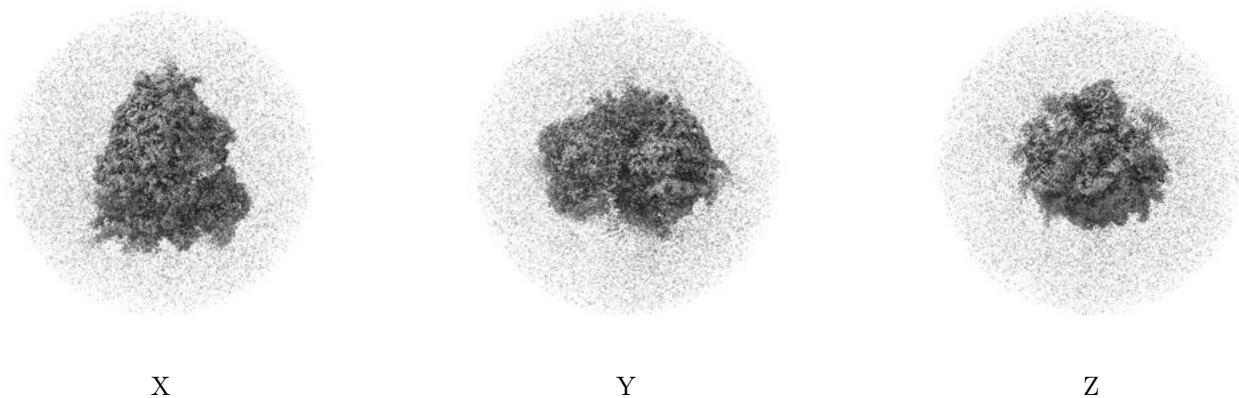


Z

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.

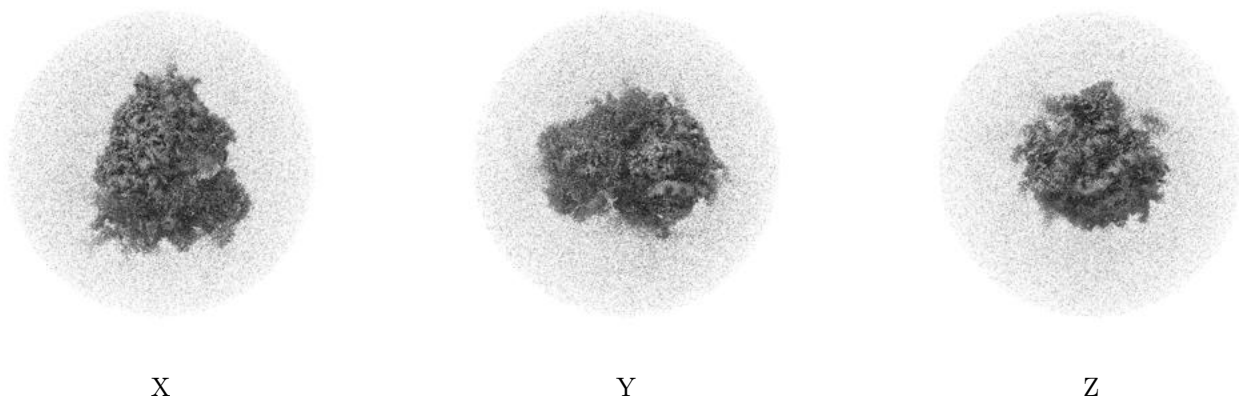
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. 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.

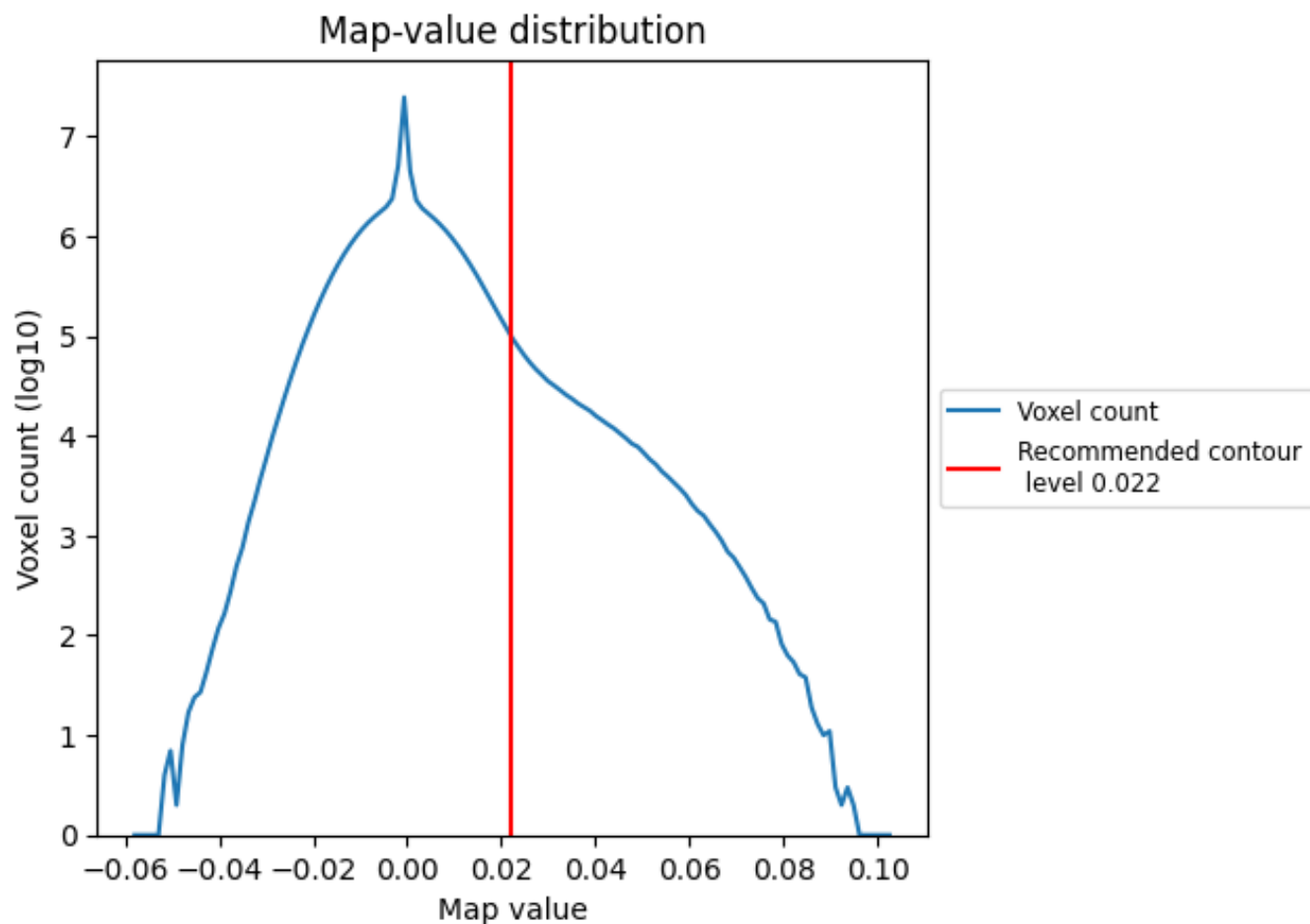
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

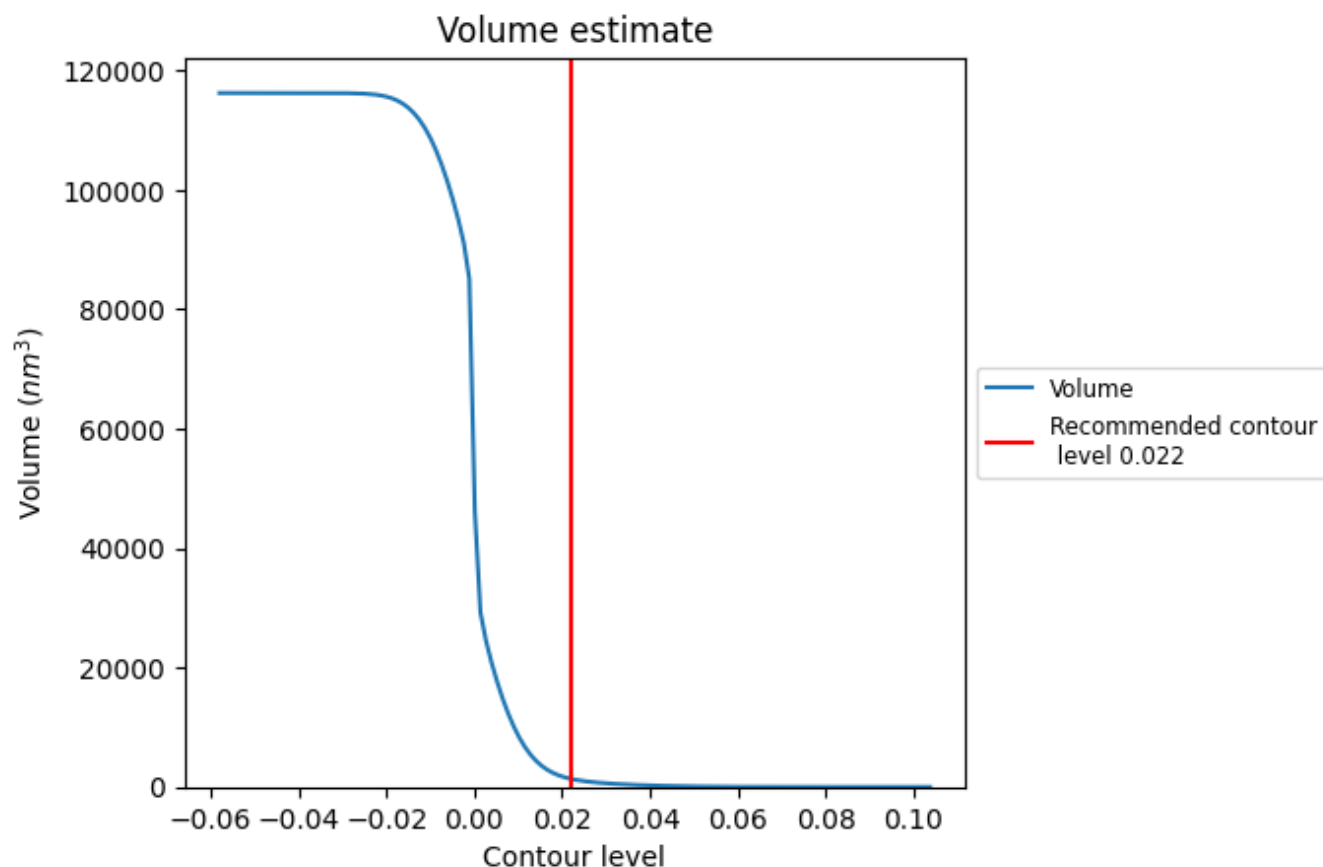
This section contains the results of statistical analysis of the map.

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.

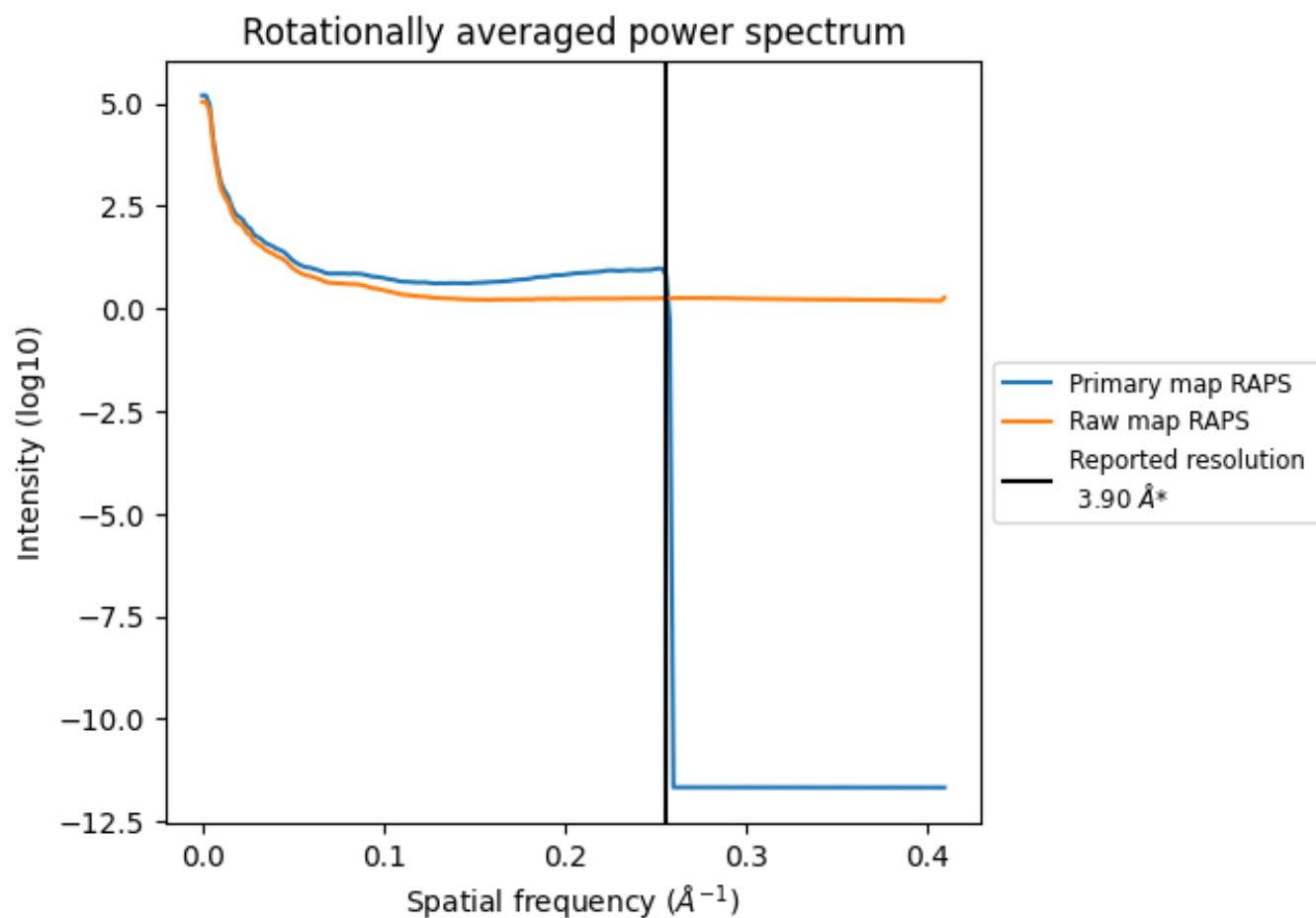
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1361 nm³; this corresponds to an approximate mass of 1230 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 ⓘ

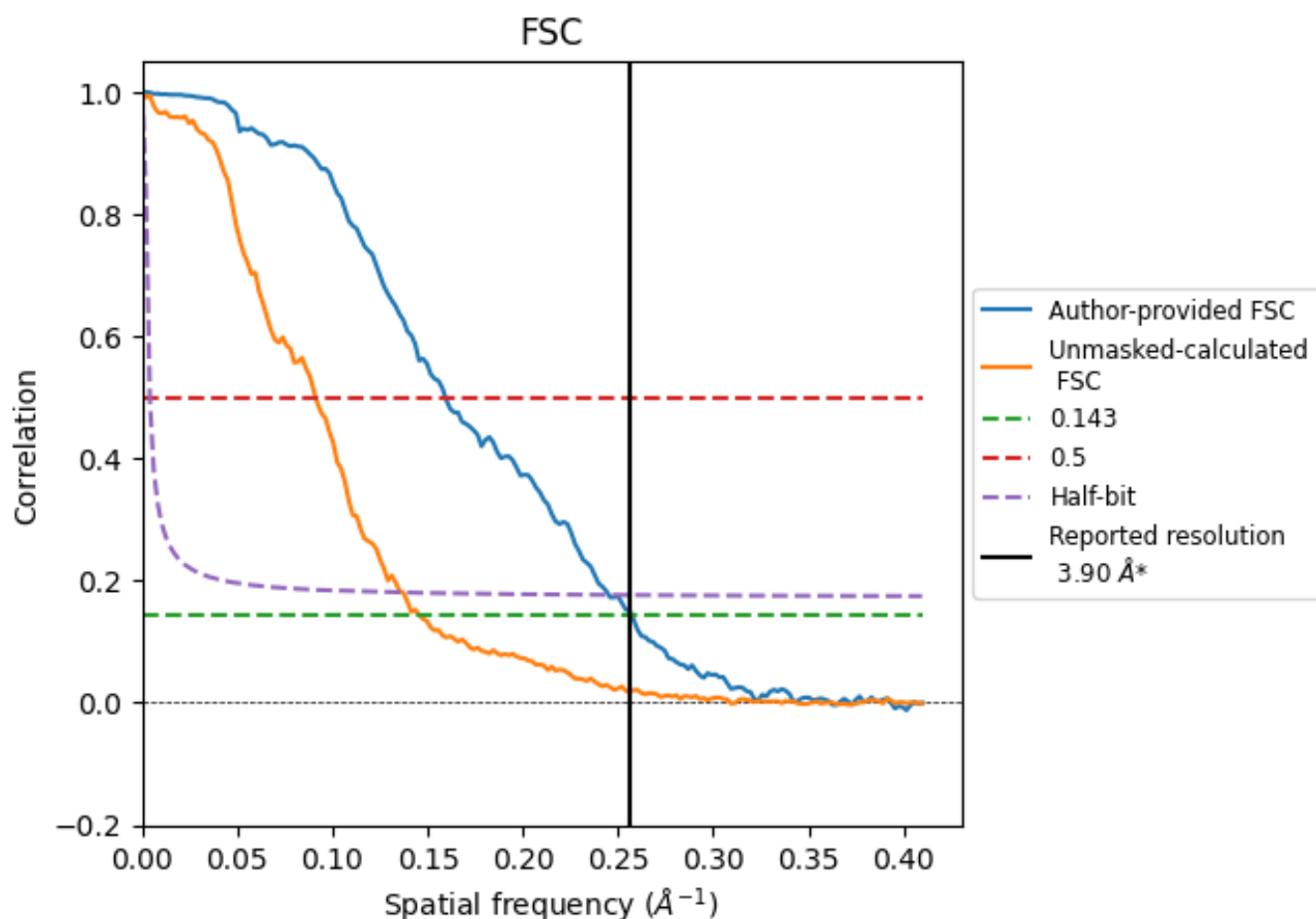


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

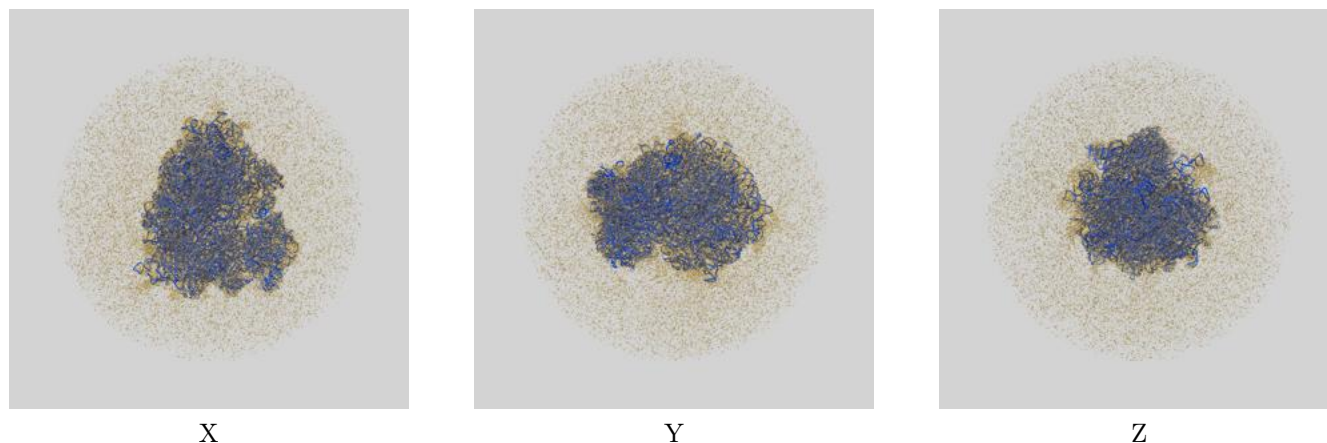
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.89	6.27	4.08
Unmasked-calculated*	6.86	10.96	7.30

*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 6.86 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

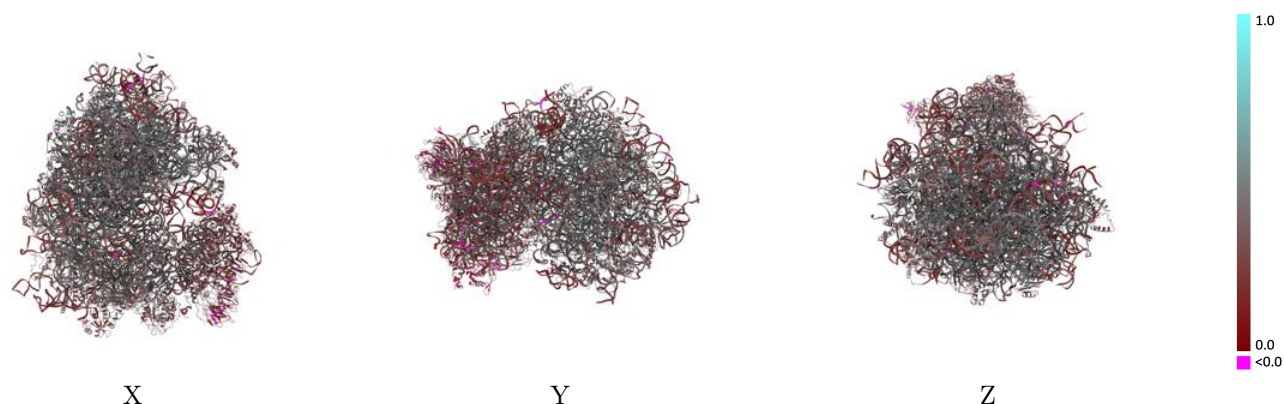
This section contains information regarding the fit between EMDB map EMD-0598 and PDB model 6OLZ. Per-residue inclusion information can be found in [section 3](#) on [page 21](#).

9.1 Map-model overlay [i](#)



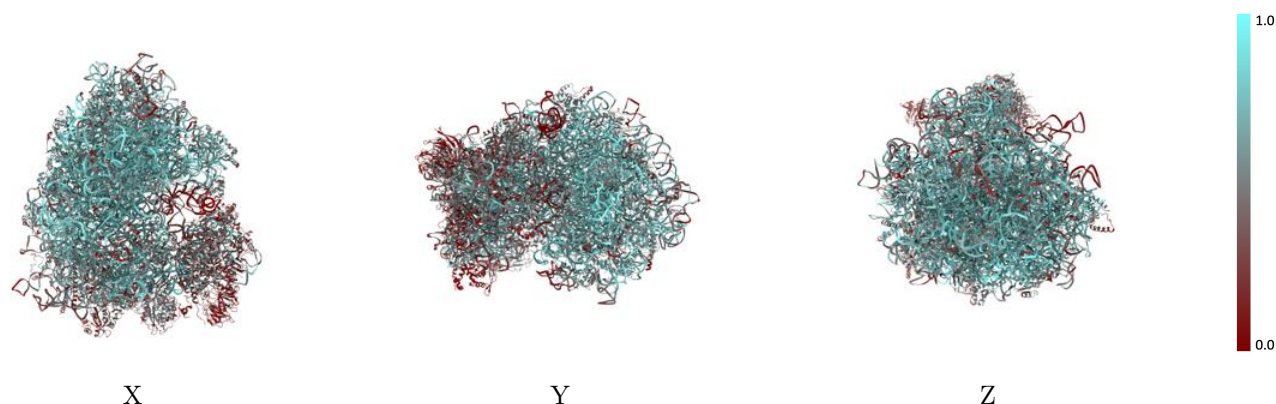
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



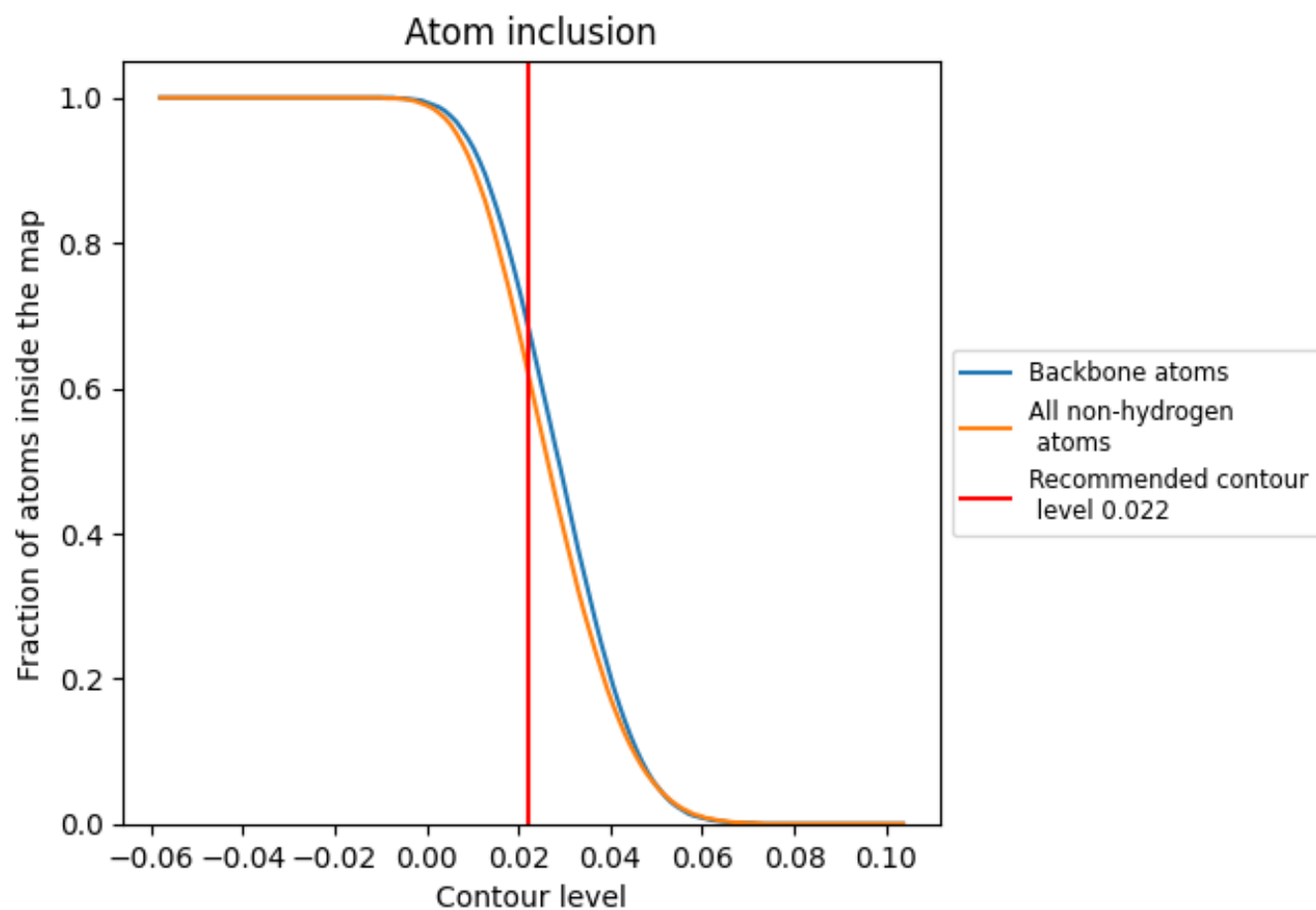
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 62% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6240	 0.3940
A	 0.2520	 0.3190
A2	 0.7480	 0.4090
A3	 0.7580	 0.4190
A4	 0.8400	 0.4390
AA	 0.6540	 0.4800
AB	 0.6310	 0.4530
AC	 0.6540	 0.4610
AD	 0.5620	 0.3920
AE	 0.5300	 0.3990
AF	 0.6220	 0.4410
AG	 0.5420	 0.4000
AH	 0.5620	 0.4300
AI	 0.5920	 0.4410
AJ	 0.5140	 0.3780
AL	 0.5930	 0.4140
AM	 0.6250	 0.4380
AN	 0.6920	 0.4760
AO	 0.6330	 0.4560
AP	 0.6660	 0.4730
AQ	 0.6440	 0.4640
AR	 0.5940	 0.4170
AS	 0.6480	 0.4620
AT	 0.6090	 0.4610
AU	 0.5110	 0.3850
AV	 0.6180	 0.4720
AW	 0.3680	 0.3430
AX	 0.6280	 0.4480
AY	 0.6480	 0.4620
AZ	 0.6010	 0.4220
Aa	 0.6750	 0.4650
Ab	 0.5330	 0.3850
Ac	 0.5540	 0.4100
Ad	 0.6220	 0.4460
Ae	 0.6570	 0.4720



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Chain	Atom inclusion	Q-score
Af	 0.6400	 0.4720
Ag	 0.6110	 0.4530
Ah	 0.6110	 0.4220
Ai	 0.6020	 0.4130
Aj	 0.7160	 0.4890
Ak	 0.5080	 0.3880
Al	 0.5850	 0.4380
Am	 0.6370	 0.4520
An	 0.5270	 0.4190
Ao	 0.6230	 0.4480
Ap	 0.6100	 0.4430
At	 0.6580	 0.4510
B1	 0.6440	 0.3640
BA	 0.4470	 0.3730
BB	 0.4620	 0.3870
BC	 0.4960	 0.3990
BD	 0.2440	 0.2790
BE	 0.4570	 0.3800
BF	 0.3020	 0.3080
BG	 0.3640	 0.3210
BH	 0.3390	 0.3290
BI	 0.5160	 0.4110
BJ	 0.4450	 0.3500
BK	 0.2030	 0.2460
BL	 0.4870	 0.4030
BM	 0.0440	 0.1750
BN	 0.4890	 0.3940
BO	 0.4960	 0.4110
BP	 0.2920	 0.2920
BQ	 0.3180	 0.2950
BR	 0.2880	 0.2990
BS	 0.3140	 0.2870
BT	 0.2930	 0.2630
BU	 0.2850	 0.2960
BV	 0.4330	 0.3670
BW	 0.5260	 0.4170
BX	 0.5180	 0.4040
BY	 0.4190	 0.3250
BZ	 0.2400	 0.2770
Ba	 0.5190	 0.4030
Bb	 0.4800	 0.4030
Bc	 0.2530	 0.3040

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Chain	Atom inclusion	Q-score
Bd	 0.3440	 0.3100
Be	 0.4240	 0.3860
Bf	 0.1100	 0.2150
Bg	 0.1370	 0.2190
Bv	 0.2000	 0.2750
Bx	 0.1250	 0.2270