



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:56 AM UTC

PDB ID : 6S47 / pdb_00006s47
EMDB ID : EMD-10098
Title : Saccharomyces cerevisiae 80S ribosome bound with ABCF protein New1
Authors : Kasari, V.; Pochopien, A.A.; Margus, T.; Murina, V.; Turnbull, K.; Zhou, Y.; Nissan, T.; Graf, M.; Novacek, J.; Atkinson, G.C.; Johansson, M.J.O.; Wilson, D.N.; Hauryliuk, V.
Deposited on : 2019-06-26
Resolution : 3.28 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:

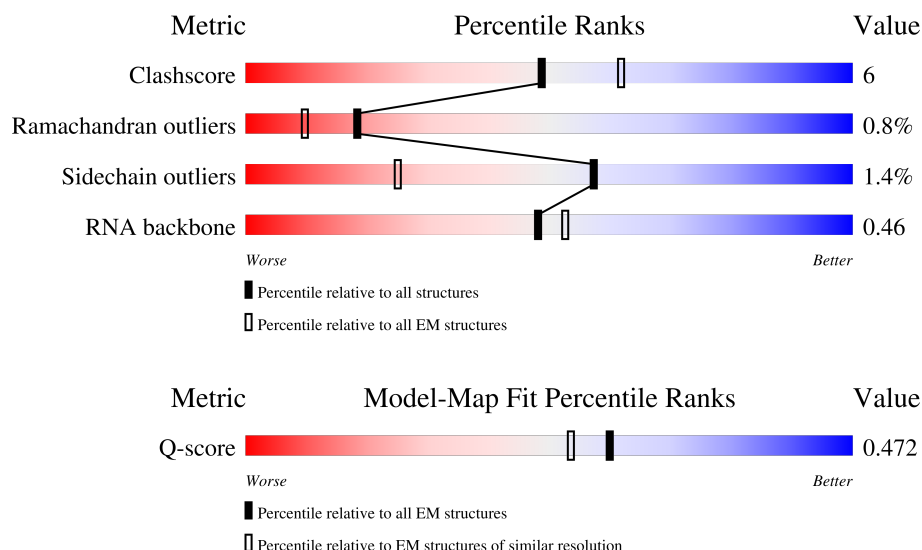
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.28 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.



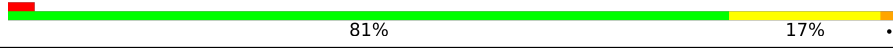
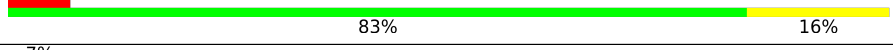
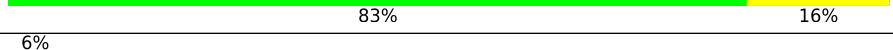
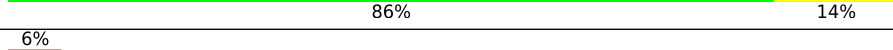
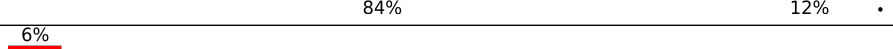
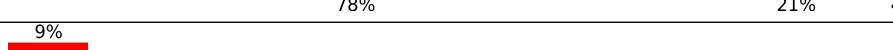
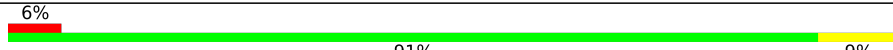
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14492 (2.78 - 3.78)

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	3149	5% 67% 28% .
2	AB	121	77% 21% .
3	AC	158	71% 25% .

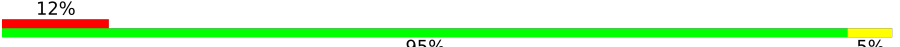
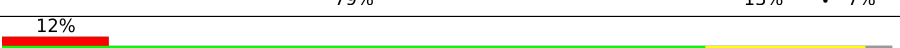
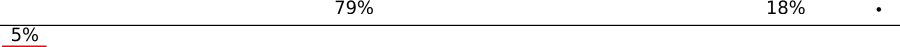
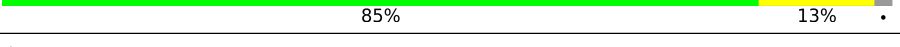
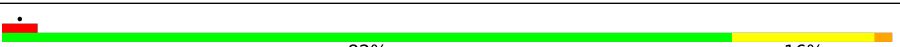
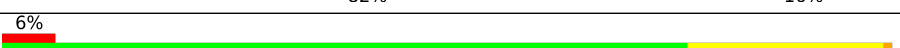
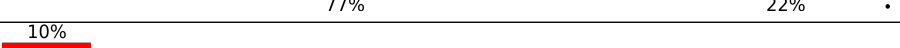
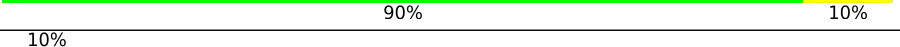
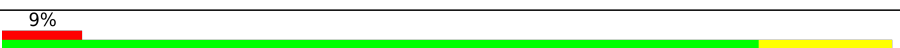
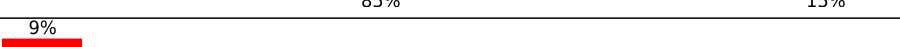
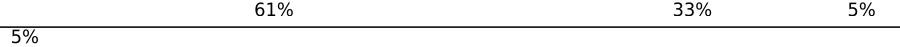
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Mol	Chain	Length	Quality of chain
4	AD	252	
5	AE	386	
6	AF	361	
7	AG	296	
8	AH	175	
9	AI	243	
10	AJ	233	
11	AK	191	
12	AL	220	
13	AM	169	
14	AN	198	
15	AO	137	
16	AP	203	
17	AQ	198	
18	AR	183	
19	AS	185	
20	AT	188	
21	AU	172	
22	AV	159	
23	AW	120	
24	AX	136	
25	AY	155	
26	AZ	141	
27	Aa	126	
28	Ab	135	

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Mol	Chain	Length	Quality of chain
29	Ac	148	
30	Ad	58	
31	Ae	104	
32	Af	112	
33	Ag	129	
34	Ah	106	
35	Ai	121	
36	Aj	119	
37	Ak	99	
38	Al	87	
39	Am	77	
40	An	50	
41	Ao	127	
42	Ap	25	
43	Aq	105	
44	Ar	91	
45	BA	1707	
46	BB	251	
47	BC	254	
48	BD	253	
49	BE	239	
50	BF	260	
51	BG	224	
52	BH	236	
53	BI	189	

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Mol	Chain	Length	Quality of chain
54	BJ	199	
55	BK	196	
56	BL	105	
57	BM	155	
58	BN	142	
59	BO	150	
60	BP	136	
61	BQ	141	
62	BR	142	
63	BS	135	
64	BT	145	
65	BU	143	
66	BV	120	
67	BW	87	
68	BX	129	
69	BY	144	
70	BZ	134	
71	Ba	107	
72	Bb	118	
73	Bc	81	
74	Bd	66	
75	Be	55	
76	Bf	62	
77	Bg	151	
78	Bh	318	

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Mol	Chain	Length	Quality of chain
79	Bi	972	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
80	ATP	Bi	1202	-	-	X	-

2 Entry composition

There are 80 unique types of molecules in this entry. The entry contains 204313 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 RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	3149	Total	C	N	O	P	0	0
			67355	30086	12142	21978	3149		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

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

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	252	Total	C	N	O	S	0	0
			1914	1191	388	334	1		

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

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

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	211	Total	C	N	O	S	0	0
			1705	1083	322	294	6		

- Molecule 13 is a protein called 60S ribosomal protein L11-B.

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

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

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

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	183	Total	C	N	O		
			1420	882	281	257	0	0

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	AT	152	Total	C	N	O		
			1228	763	260	205	0	0

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

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

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

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

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

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

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

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

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AY	61	Total	C	N	O	S	0	0
			509	328	100	80	1		

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AZ	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 27 is a protein called 60S ribosomal protein L26-A.

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

- Molecule 28 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 29 is a protein called 60S ribosomal protein L28.

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

- Molecule 30 is a protein called 60S ribosomal protein L29.

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

- Molecule 31 is a protein called 60S ribosomal protein L30.

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

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Af	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 33 is a protein called 60S ribosomal protein L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 35 is a protein called 60S ribosomal protein L34-A.

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

- Molecule 36 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 37 is a protein called 60S ribosomal protein L36-A.

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

- Molecule 38 is a protein called 60S ribosomal protein L37-A.

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

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 42 is a protein called 60S ribosomal protein L41-B.

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

- Molecule 43 is a protein called 60S ribosomal protein L42-A.

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

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 45 is a RNA chain called 18S rRNA (1707-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BA	1707	Total	C	N	O	P	0	0
			36375	16263	6440	11965	1707		

- Molecule 46 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BB	206	Total	C	N	O	S	0	0
			1577	1014	278	283	2		

- Molecule 47 is a protein called 40S ribosomal protein S1-A.

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

- Molecule 48 is a protein called 40S ribosomal protein S2.

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

- Molecule 49 is a protein called 40S ribosomal protein S3.

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

- Molecule 50 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 51 is a protein called Rps5p.

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

- Molecule 52 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BH	226	Total	C	N	O	S	0	0
			1799	1129	346	321	3		

- Molecule 53 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	BI	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 54 is a protein called 40S ribosomal protein S8-A.

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

- Molecule 55 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 56 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BL	96	Total	C	N	O	S	0	0
			772	499	126	145	2		

- Molecule 57 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BM	155	Total	C	N	O	S	0	0
			1213	774	230	206	3		

- Molecule 58 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BN	124	Total	C	N	O	S	0	0
			890	560	156	172	2		

- Molecule 59 is a protein called 40S ribosomal protein S13.

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

- Molecule 60 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BP	127	Total	C	N	O	S	0	0
			891	545	182	163	1		

- Molecule 61 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BQ	124	Total	C	N	O	S	0	0
			977	622	182	166	7		

- Molecule 62 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	BR	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 63 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BS	120	Total	C	N	O	S	0	0
			926	577	177	170	2		

- Molecule 64 is a protein called 40S ribosomal protein S18-A.

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

- Molecule 65 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	BU	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 66 is a protein called 40S ribosomal protein S20.

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

- Molecule 67 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 68 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 69 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 70 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
70	BZ	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 71 is a protein called 40S ribosomal protein S25-A.

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

- Molecule 72 is a protein called 40S ribosomal protein S26-B.

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

- Molecule 73 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 74 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 75 is a protein called 40S ribosomal protein S29-A.

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

- Molecule 76 is a protein called 40S ribosomal protein S30-A.

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

- Molecule 77 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Bg	57	Total	C	N	O	S	0	0
			444	281	82	77	4		

- Molecule 78 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Bh	318	Total	C	N	O	S	0	0
			2441	1544	419	470	8		

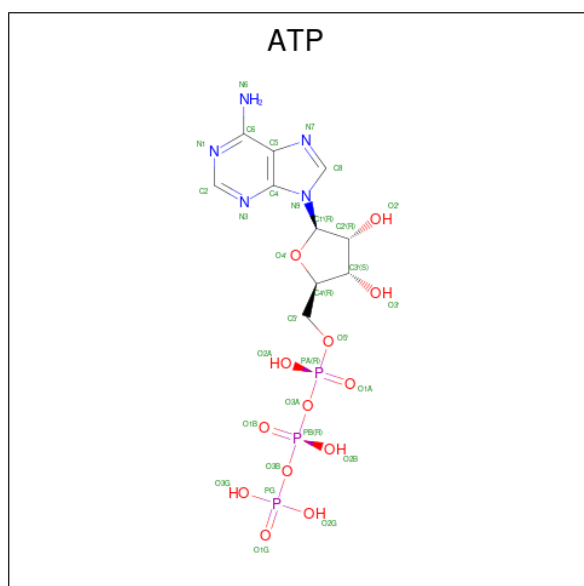
- Molecule 79 is a protein called [NU+] prion formation protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Bi	952	Total	C	N	O	S	0	0
			7512	4763	1271	1450	28		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bi	495	ASP	SER	conflict	UNP Q08972
Bi	713	GLN	GLU	conflict	UNP Q08972
Bi	1058	GLN	GLU	conflict	UNP Q08972

- Molecule 80 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



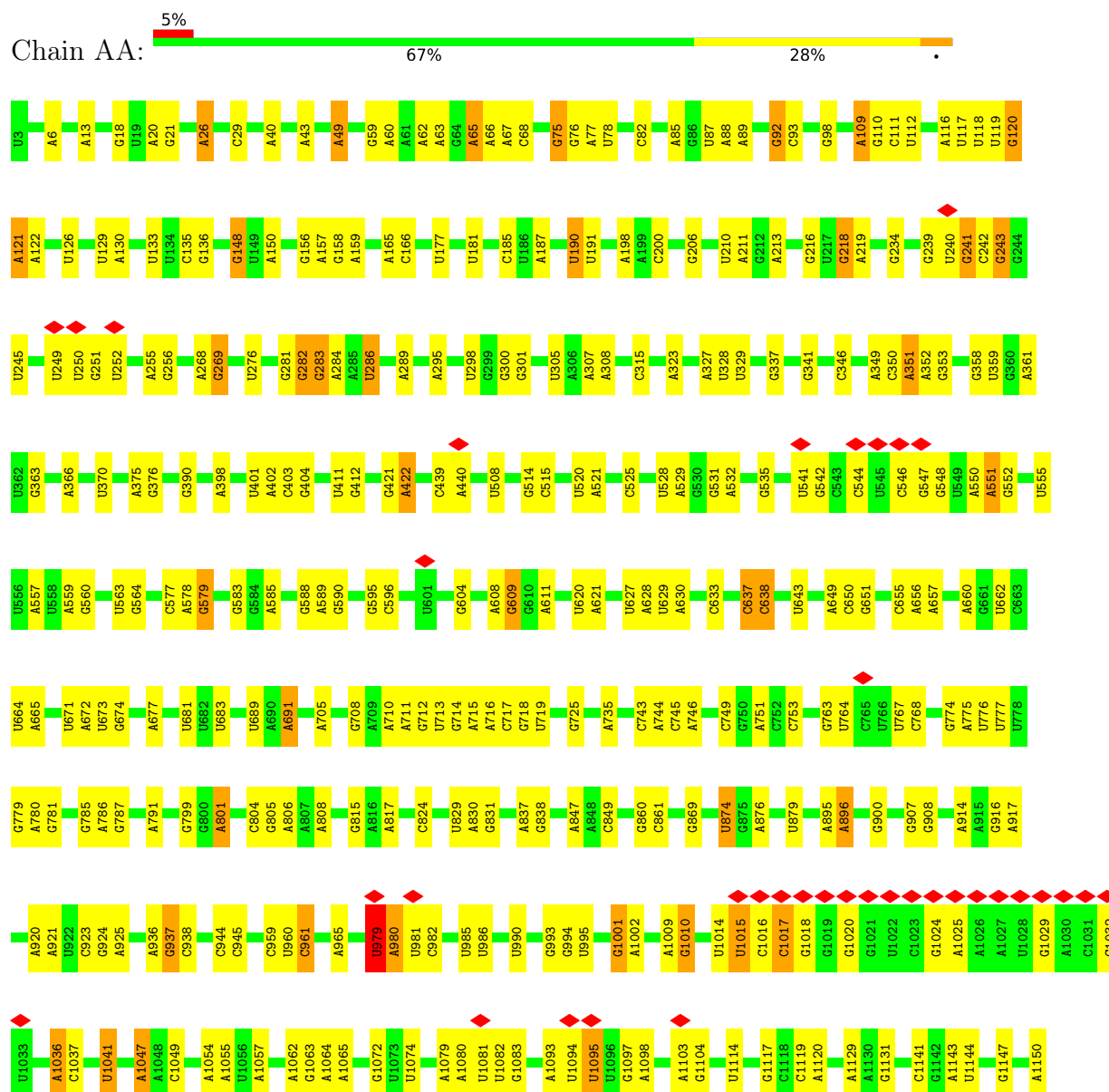
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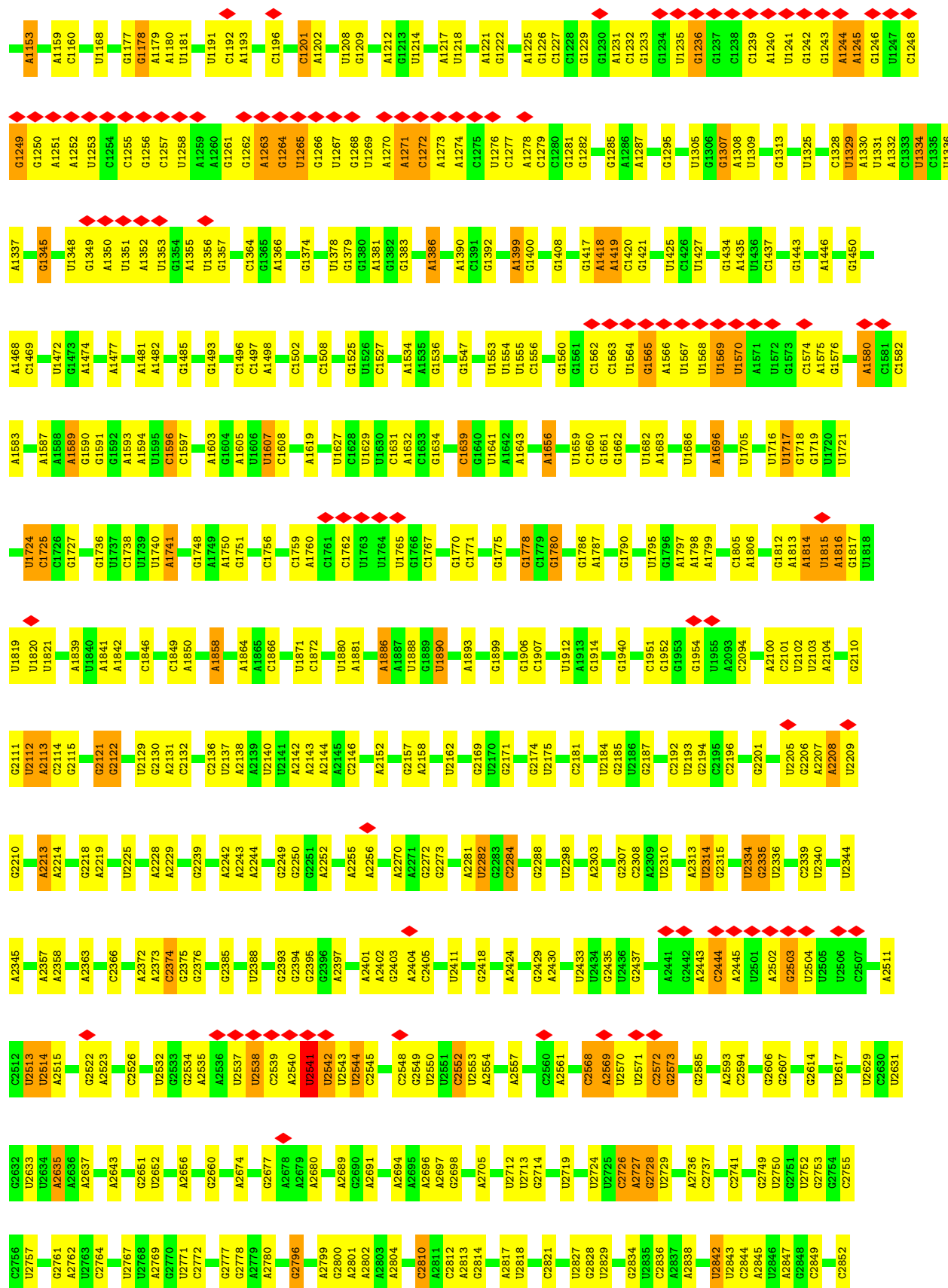
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
80	Bi	1	31	10	5	13	3	0

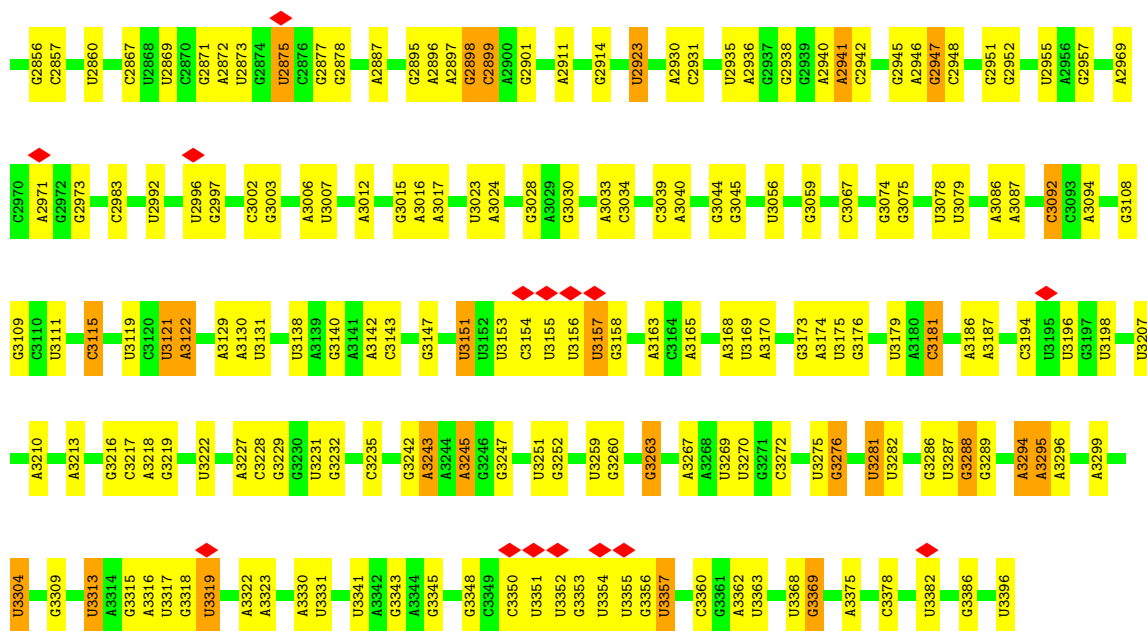
3 Residue-property plots

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: 28S ribosomal RNA







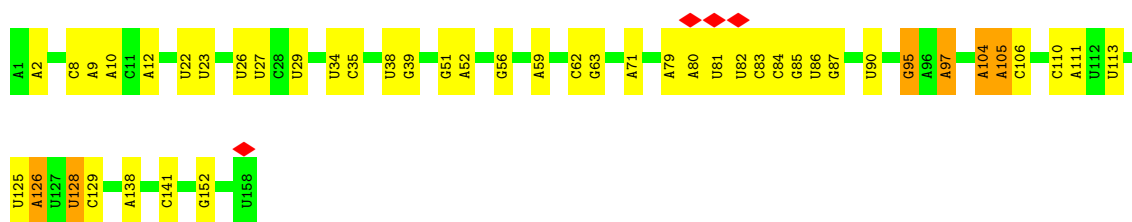
- Molecule 2: 5S ribosomal RNA

Chain AB: 77% 21%



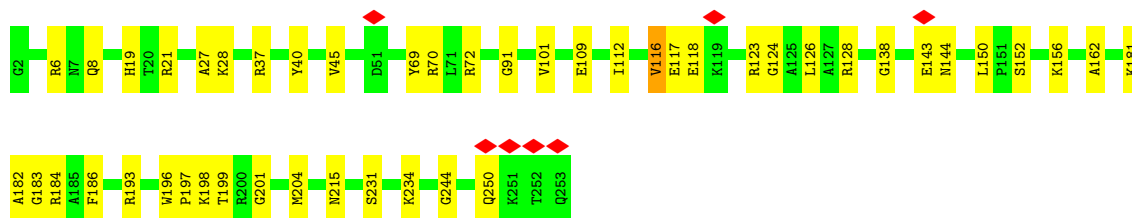
- Molecule 3: 5.8S ribosomal RNA

Chain AC: 71% 25%

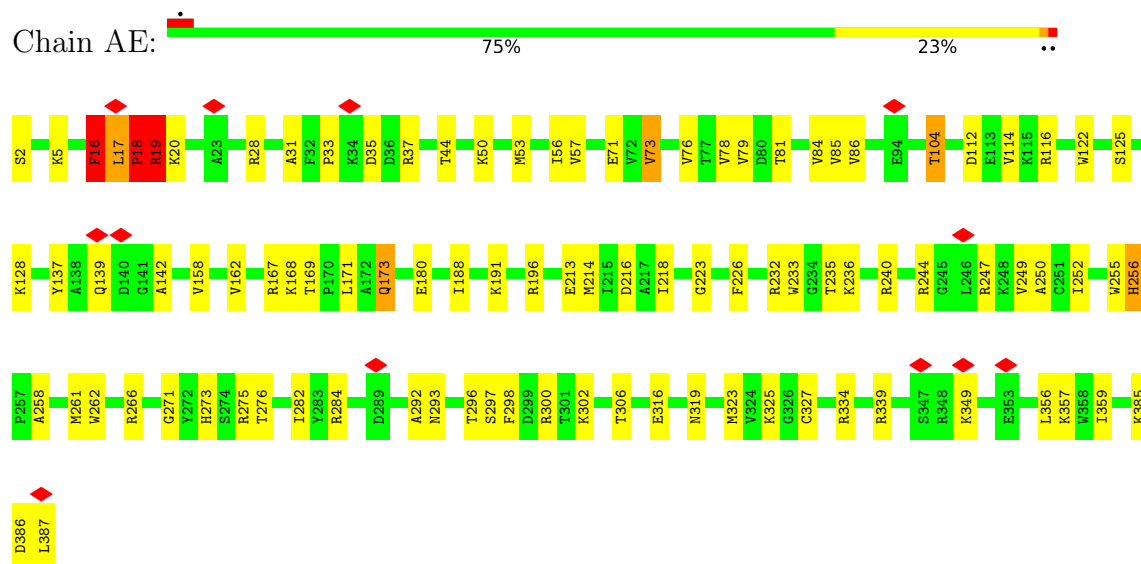


- Molecule 4: 60S ribosomal protein L2-A

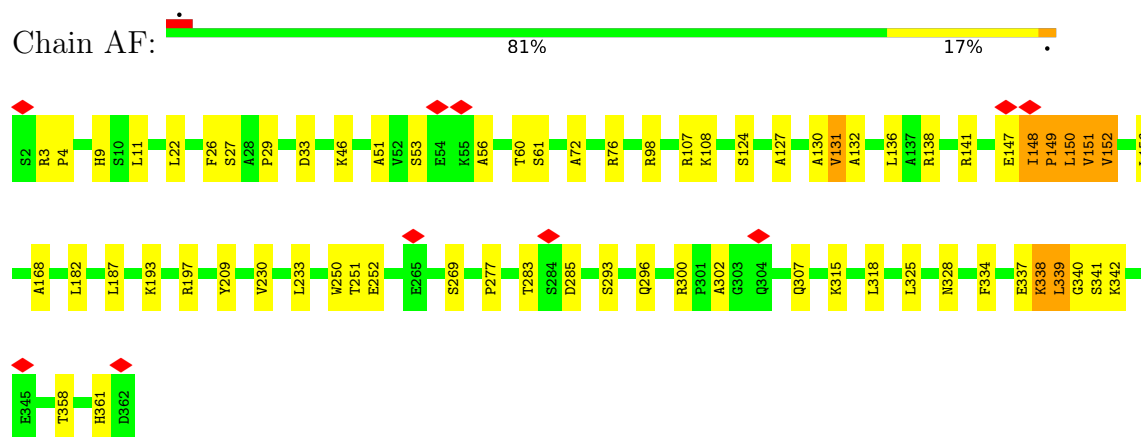
Chain AD: 81% 18%



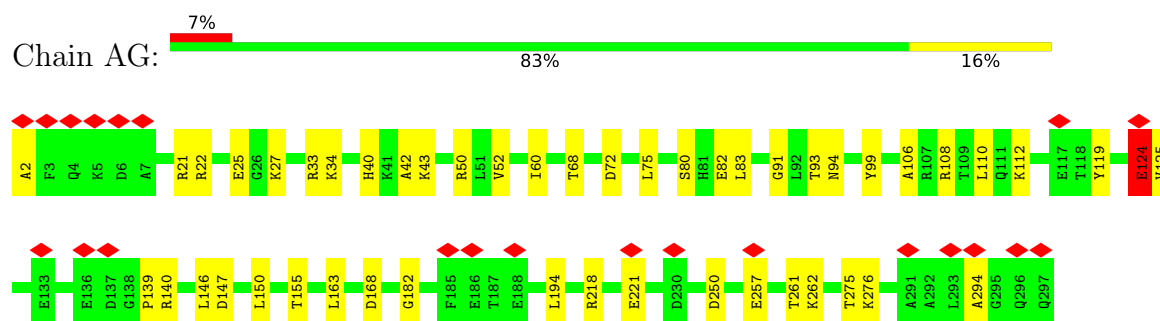
- Molecule 5: 60S ribosomal protein L3



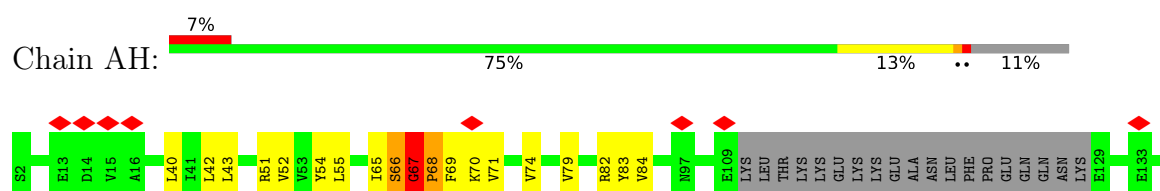
• Molecule 6: 60S ribosomal protein L4-A



• Molecule 7: 60S ribosomal protein L5



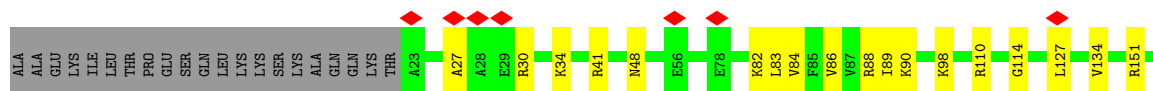
• Molecule 8: 60S ribosomal protein L6-A





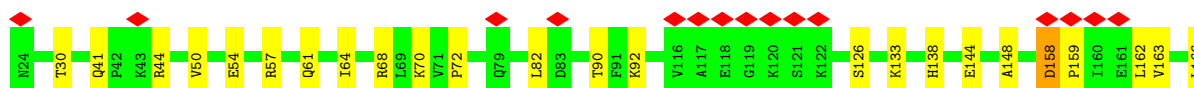
- Molecule 9: 60S ribosomal protein L7-A

Chain AI: 74% 17% 9%



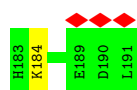
- Molecule 10: 60S ribosomal protein L8-A

Chain AJ: 9% 83% 16%



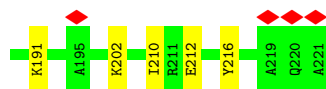
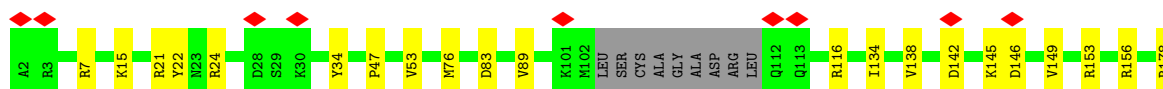
- Molecule 11: 60S ribosomal protein L9-A

Chain AK: 6% 86% 14%

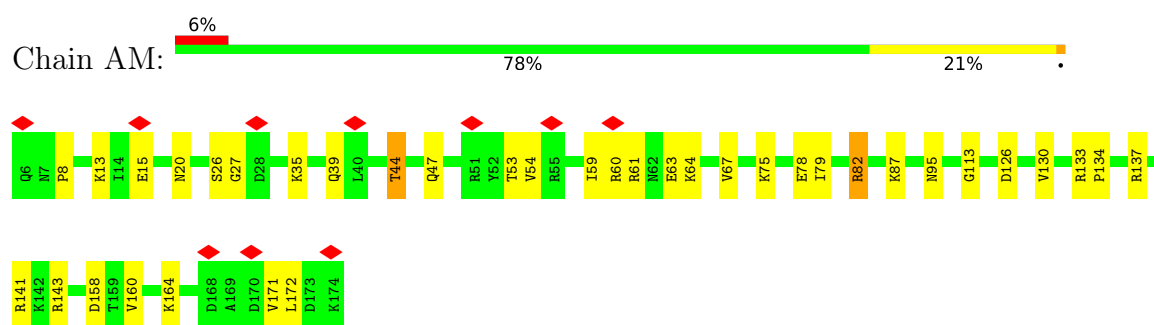


- Molecule 12: 60S ribosomal protein L10

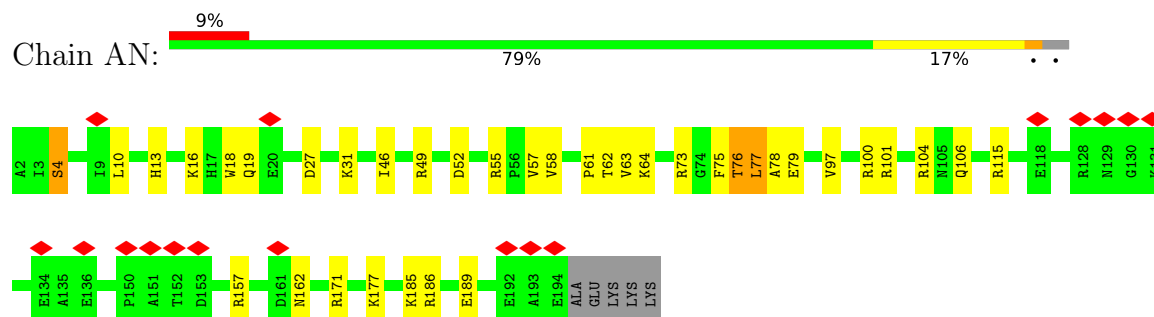
Chain AL: 6% 84% 12%



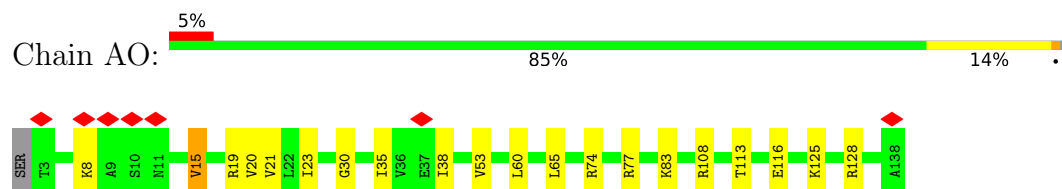
- Molecule 13: 60S ribosomal protein L11-B



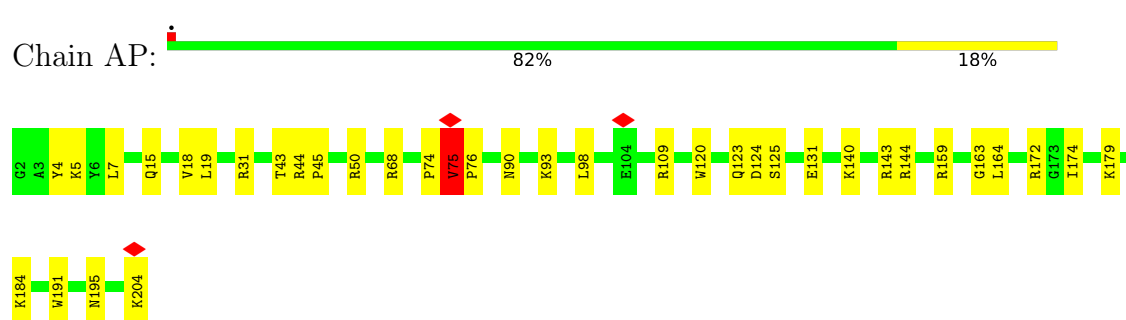
- Molecule 14: 60S ribosomal protein L13-A



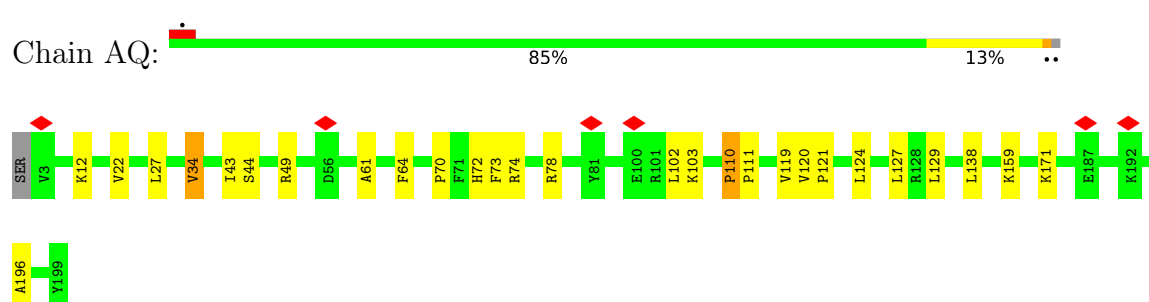
- Molecule 15: 60S ribosomal protein L14-A



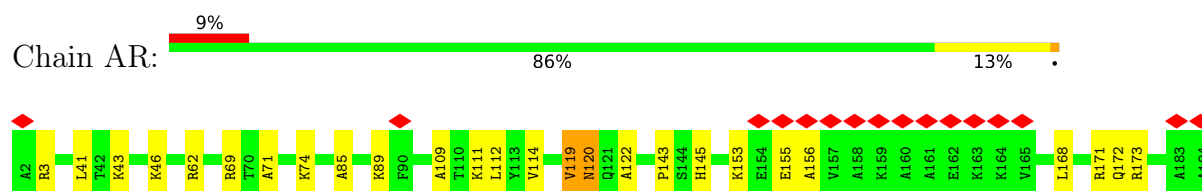
- Molecule 16: 60S ribosomal protein L15-A



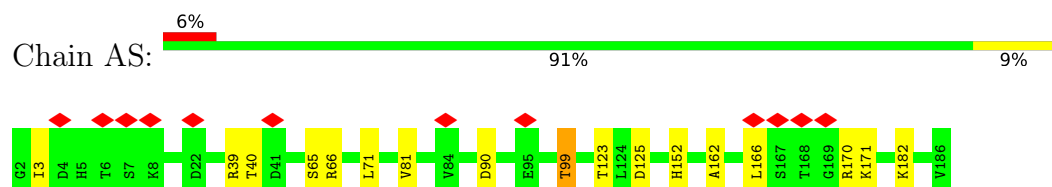
- Molecule 17: 60S ribosomal protein L16-A



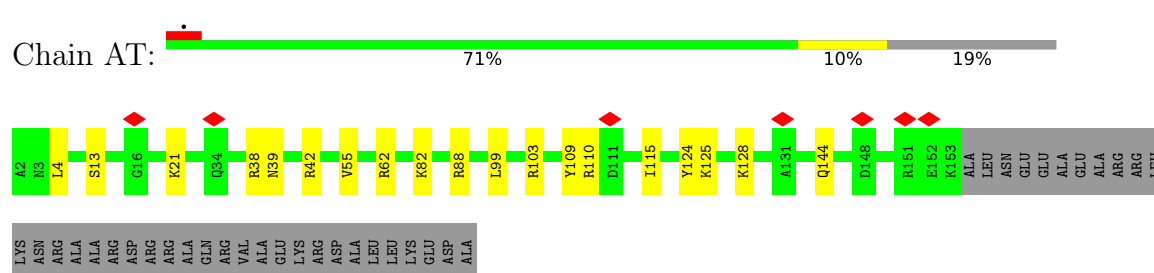
- Molecule 18: 60S ribosomal protein L17-A



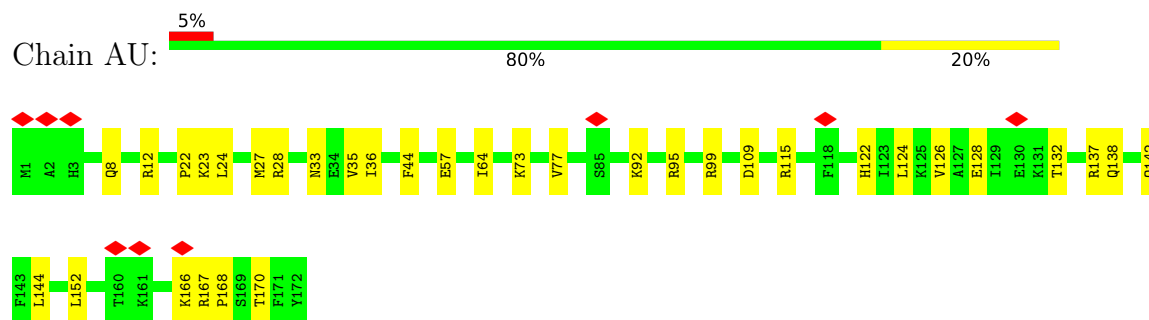
- Molecule 19: 60S ribosomal protein L18-A



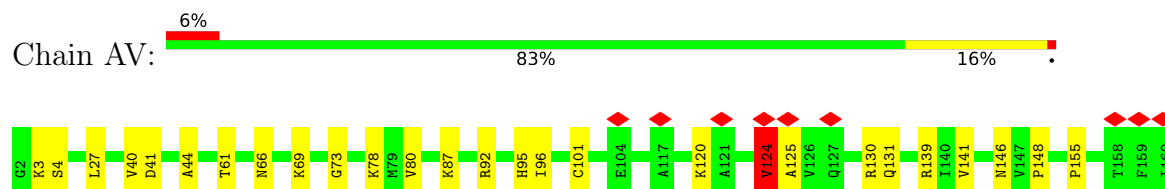
- Molecule 20: 60S ribosomal protein L19-A



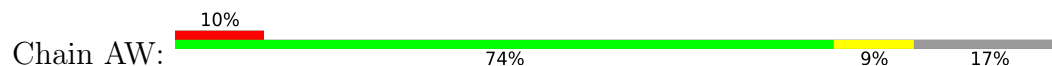
- Molecule 21: 60S ribosomal protein L20-A

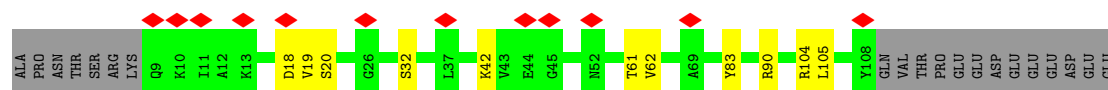


- Molecule 22: 60S ribosomal protein L21-A

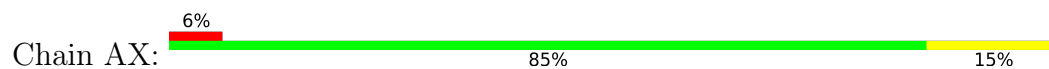


- Molecule 23: 60S ribosomal protein L22-A

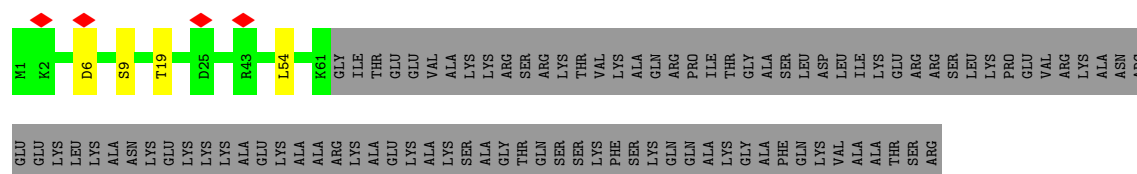




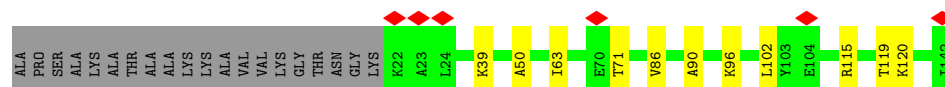
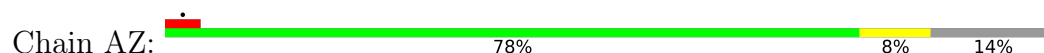
- Molecule 24: 60S ribosomal protein L23-A



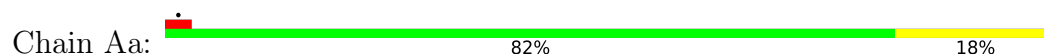
- Molecule 25: 60S ribosomal protein L24-A



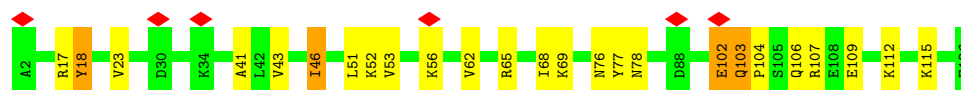
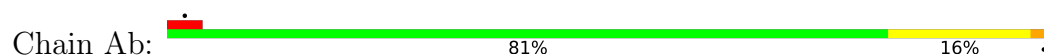
- Molecule 26: 60S ribosomal protein L25



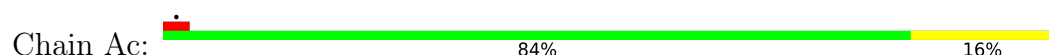
- Molecule 27: 60S ribosomal protein L26-A

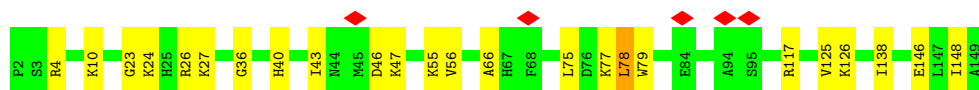


- Molecule 28: 60S ribosomal protein L27-A



- Molecule 29: 60S ribosomal protein L28

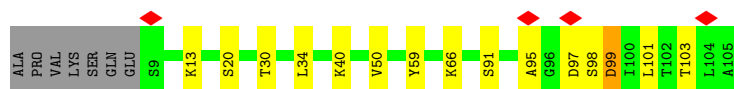
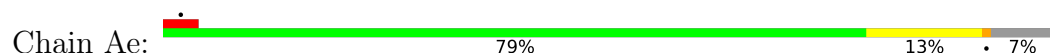




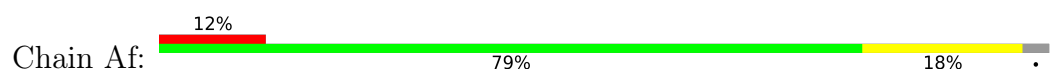
- Molecule 30: 60S ribosomal protein L29



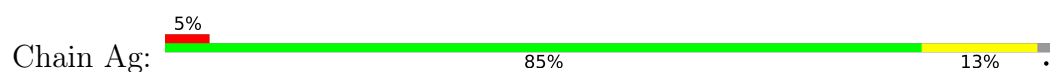
- Molecule 31: 60S ribosomal protein L30



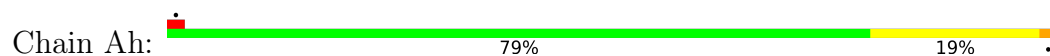
- Molecule 32: 60S ribosomal protein L31-A



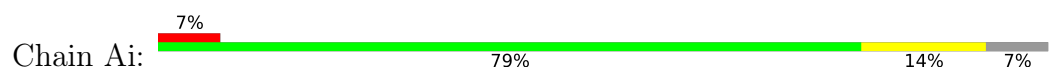
- Molecule 33: 60S ribosomal protein L32



- Molecule 34: 60S ribosomal protein L33-A



- Molecule 35: 60S ribosomal protein L34-A



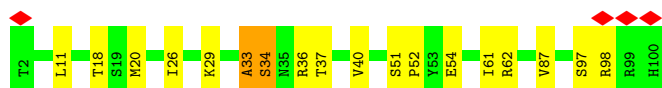
- Molecule 36: 60S ribosomal protein L35-A

Chain Aj:  87% 12%



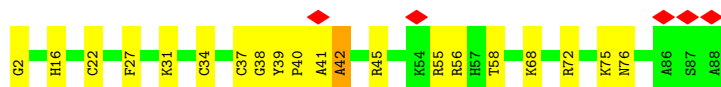
- Molecule 37: 60S ribosomal protein L36-A

Chain Ak:  82% 16%

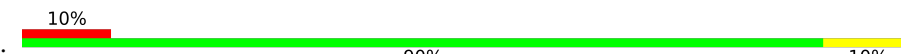


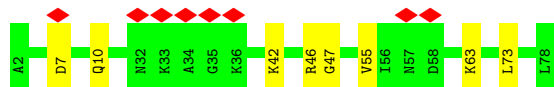
- Molecule 38: 60S ribosomal protein L37-A

Chain Al:  6% 77% 22%



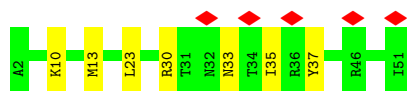
- Molecule 39: 60S ribosomal protein L38

Chain Am:  10% 90% 10%



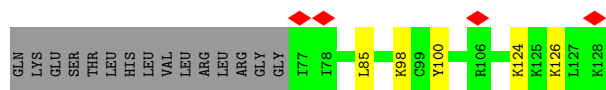
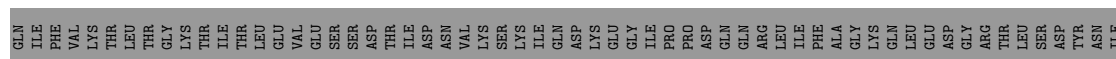
- Molecule 40: 60S ribosomal protein L39

Chain An:  10% 86% 14%



- Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain Ao:  37% 59%

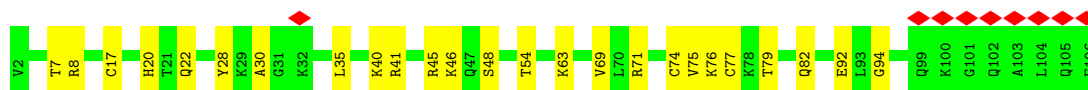
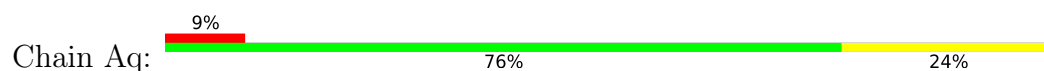


- Molecule 42: 60S ribosomal protein L41-B

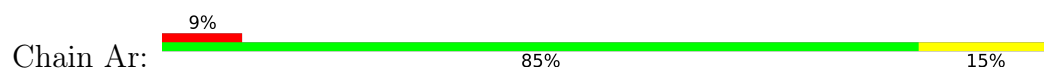
Chain Ap:  40% 80% 20%



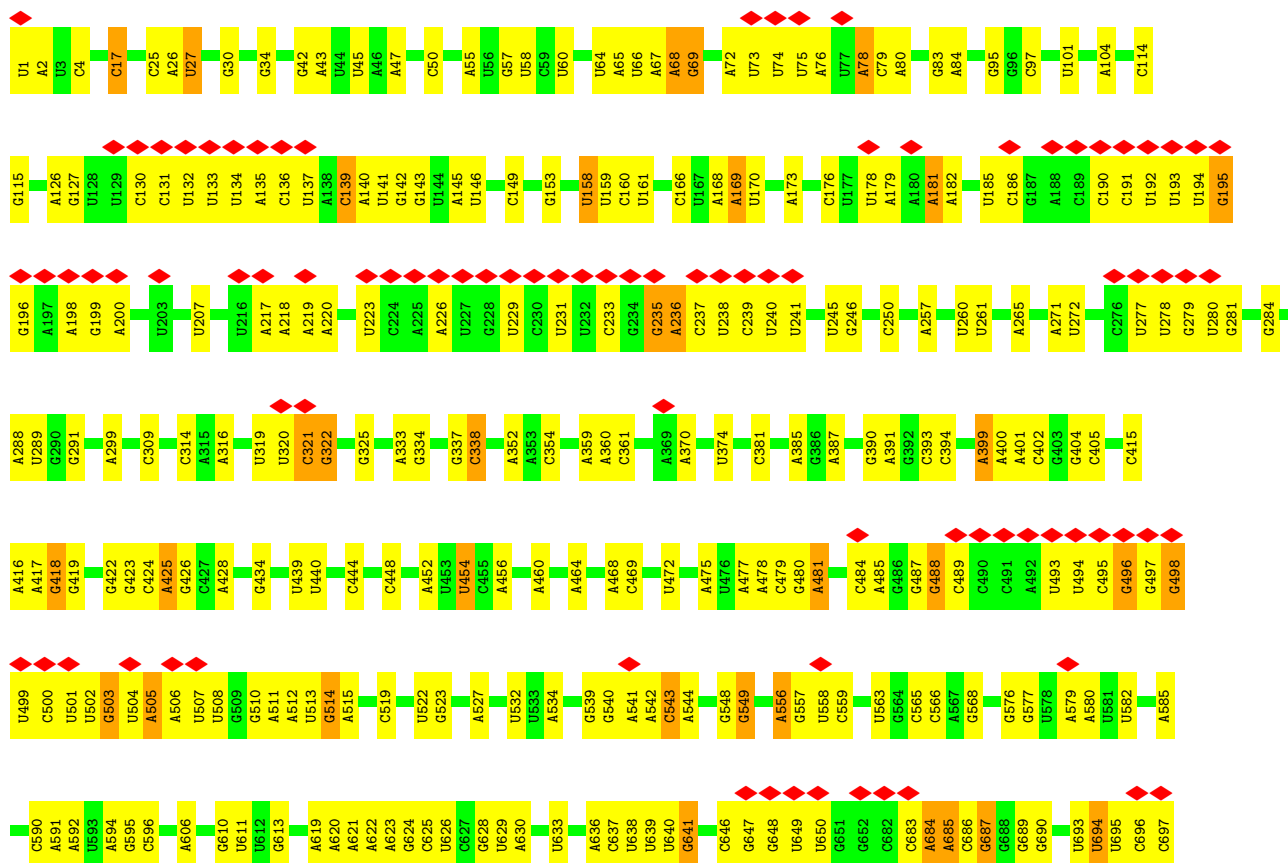
- Molecule 43: 60S ribosomal protein L42-A

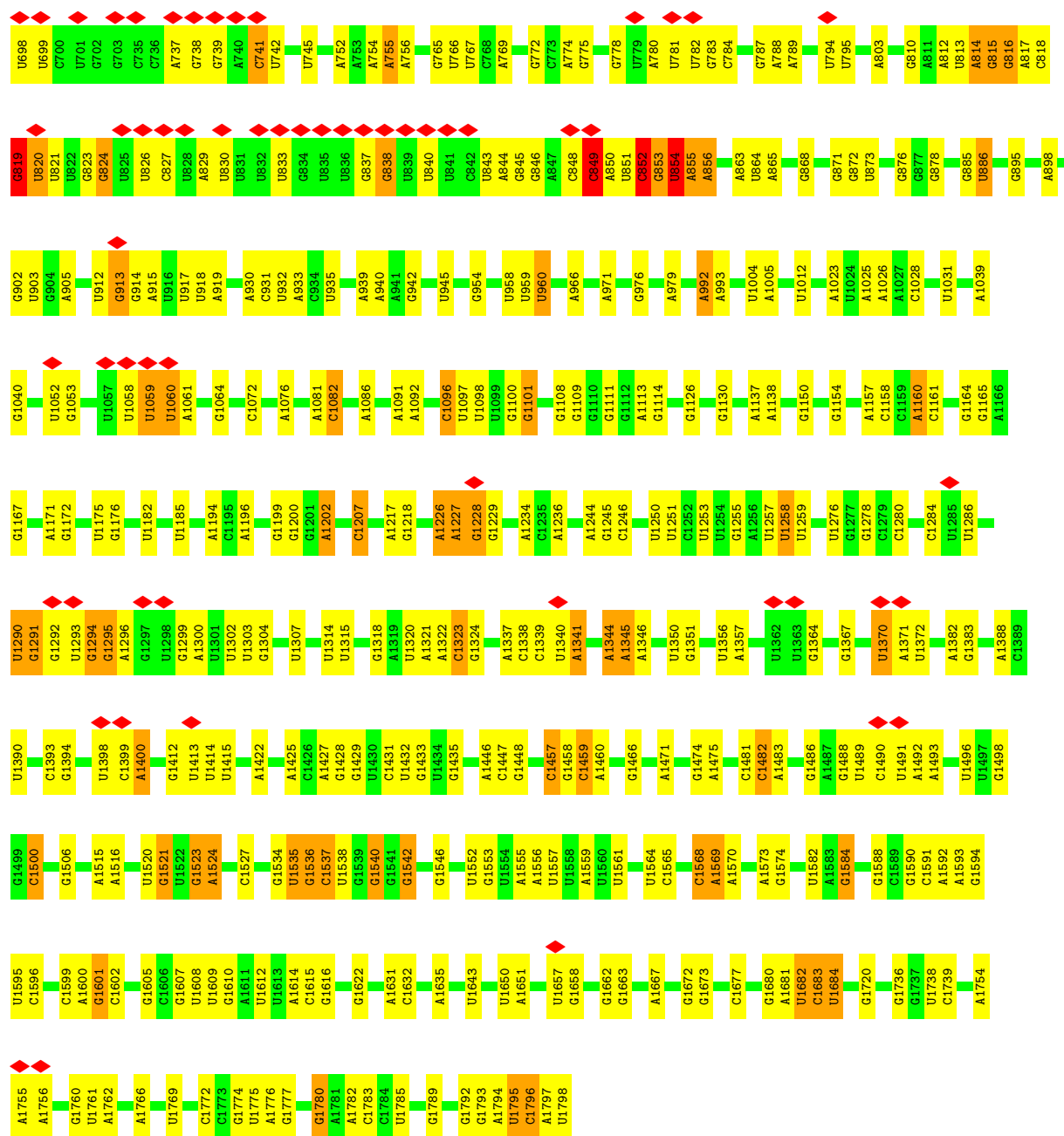


- Molecule 44: 60S ribosomal protein L43-A

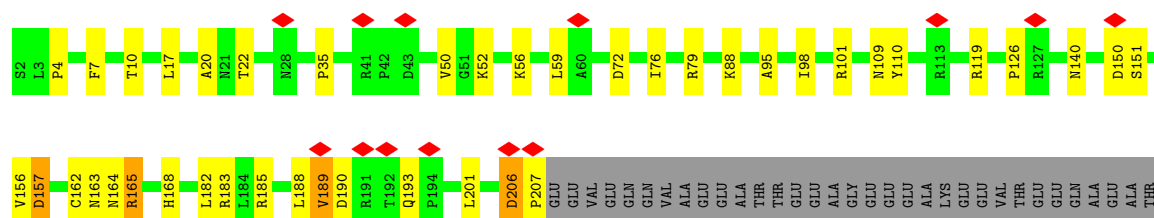


- Molecule 45: 18S rRNA (1707-MER)





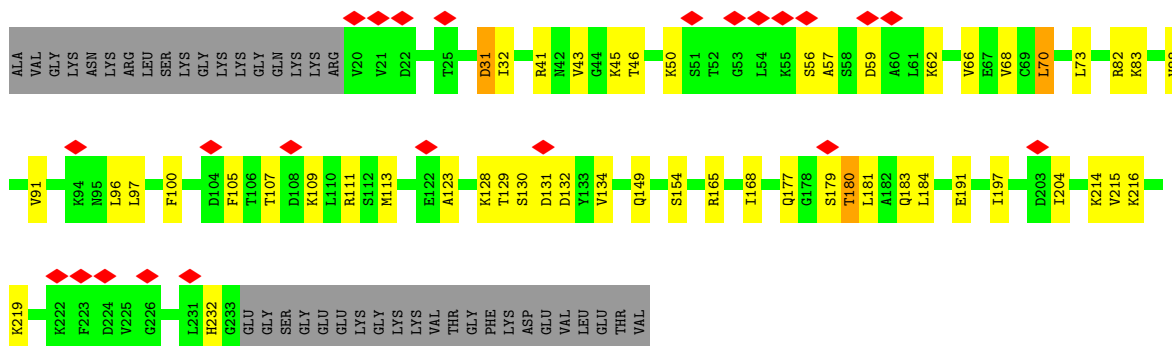
• Molecule 46: 40S ribosomal protein S0-A



GLU
TRP
ALA
GLU
GLU
ASN
ALA
ASP
VAL
GLU
TRP

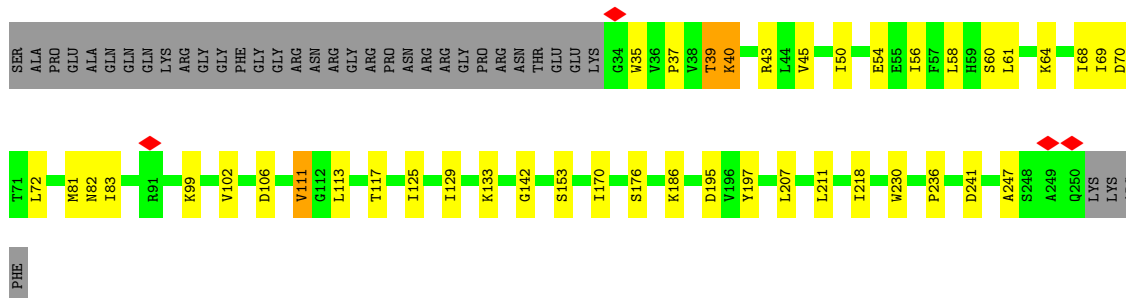
• Molecule 47: 40S ribosomal protein S1-A

Chain BC: 



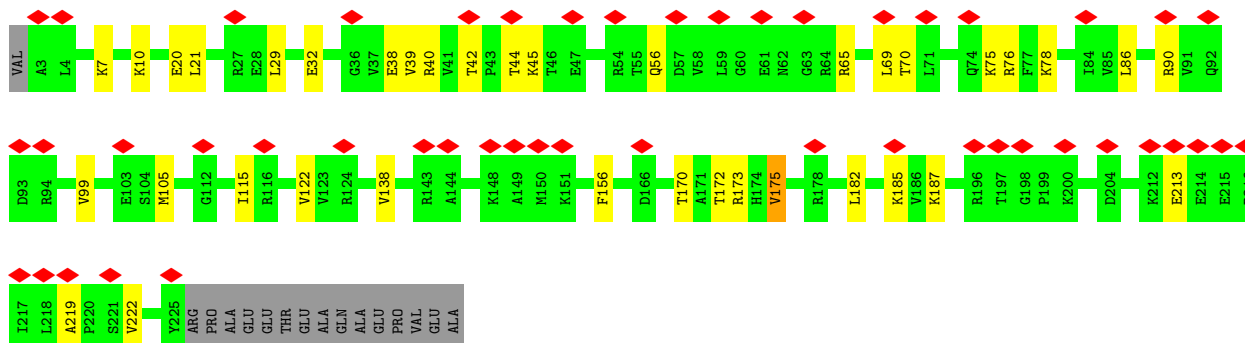
• Molecule 48: 40S ribosomal protein S2

Chain BD: 



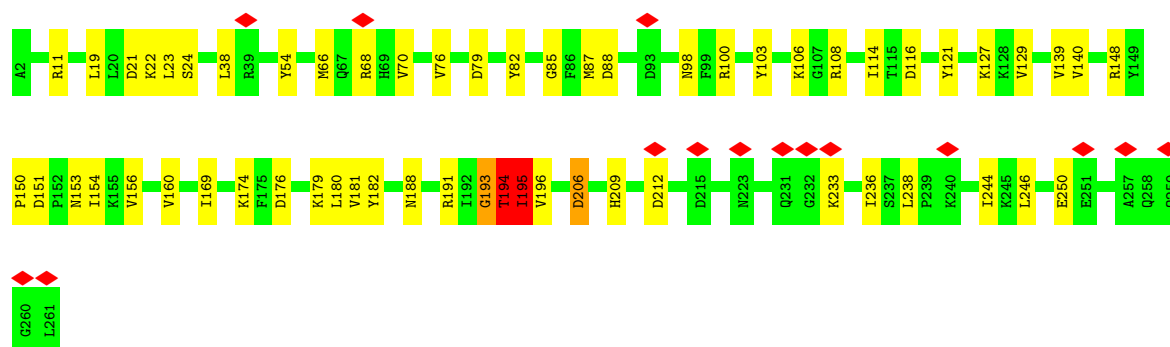
• Molecule 49: 40S ribosomal protein S3

Chain BE: 

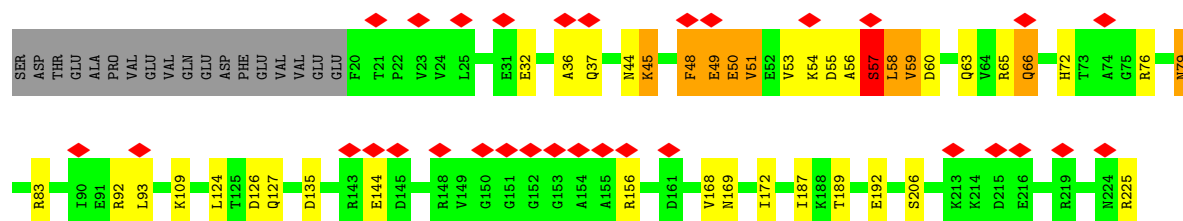
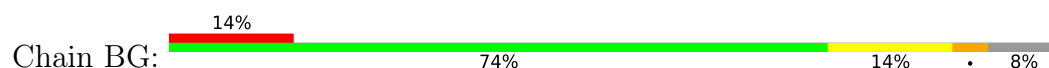


• Molecule 50: 40S ribosomal protein S4-A

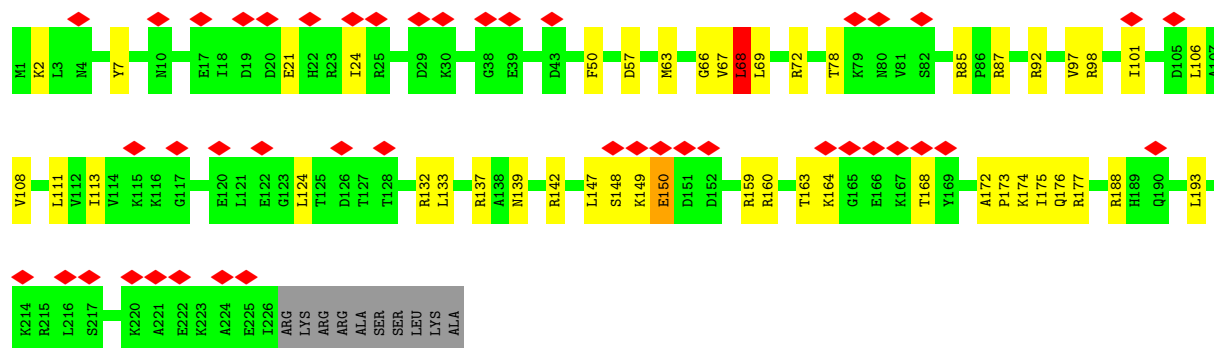
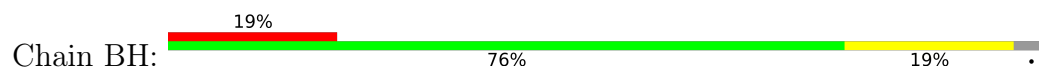
Chain BF: 



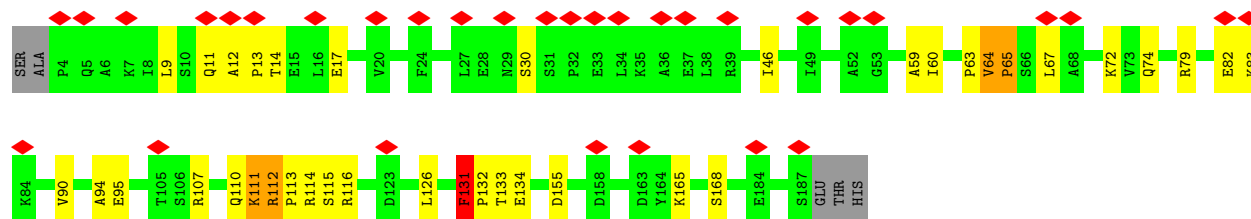
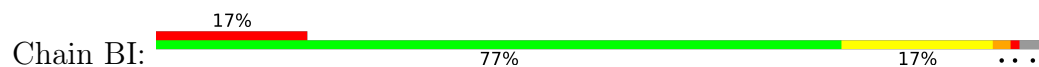
• Molecule 51: Rps5p



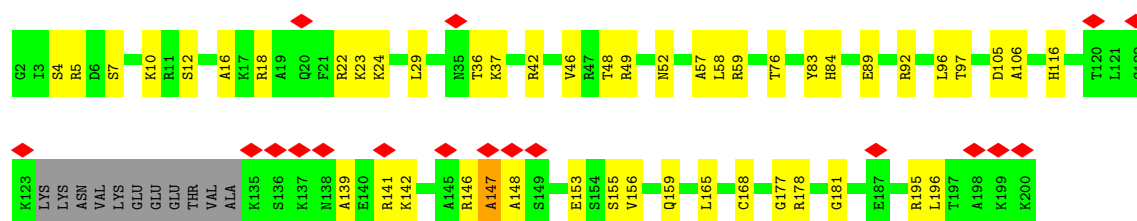
• Molecule 52: 40S ribosomal protein S6-A



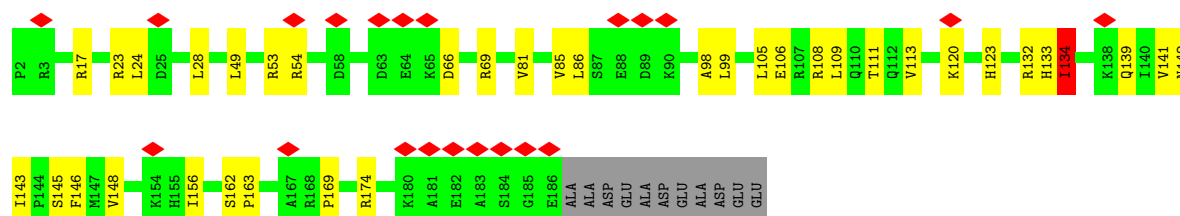
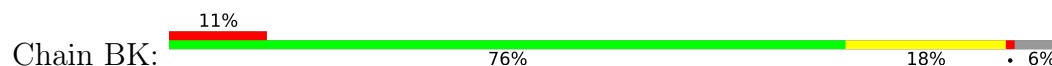
• Molecule 53: 40S ribosomal protein S7-A



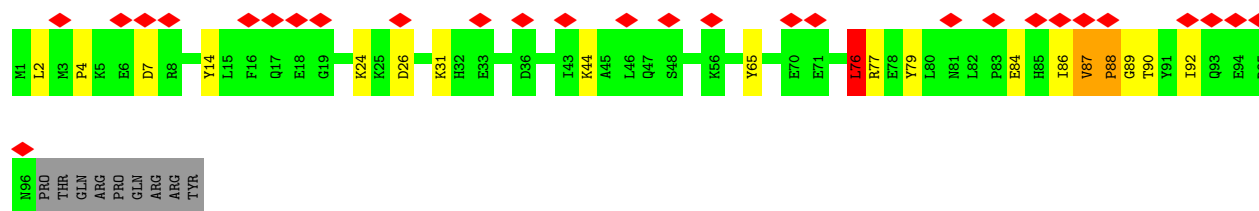
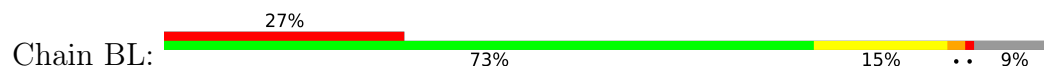
• Molecule 54: 40S ribosomal protein S8-A



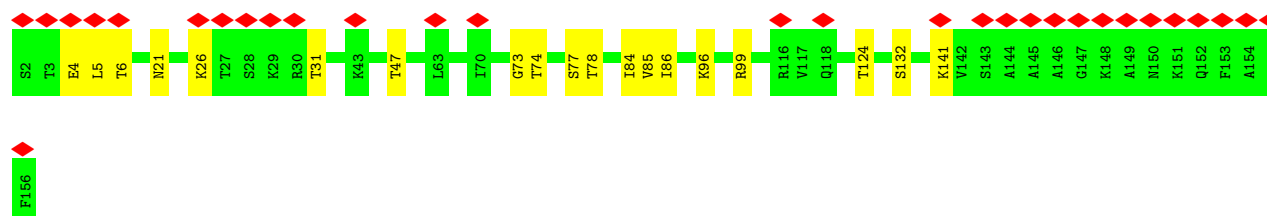
• Molecule 55: 40S ribosomal protein S9-A



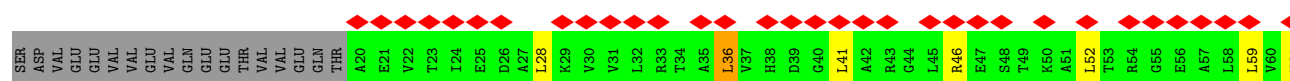
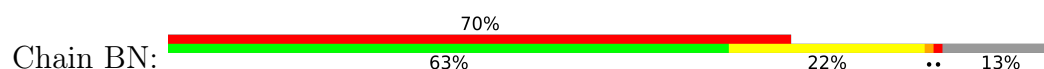
• Molecule 56: 40S ribosomal protein S10-A



• Molecule 57: 40S ribosomal protein S11-A

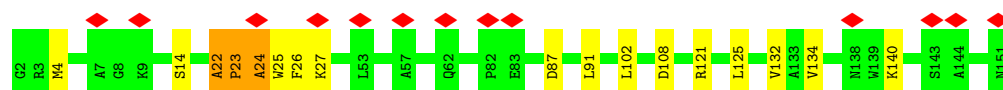
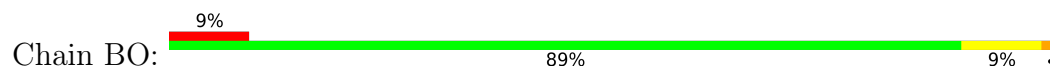


• Molecule 58: 40S ribosomal protein S12

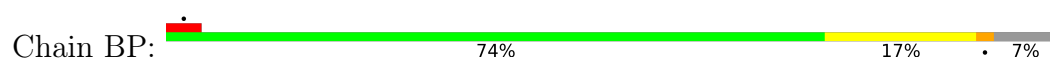




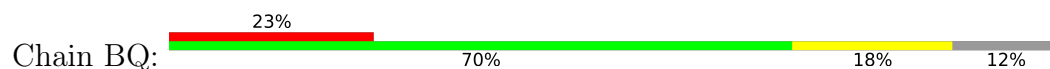
- Molecule 59: 40S ribosomal protein S13



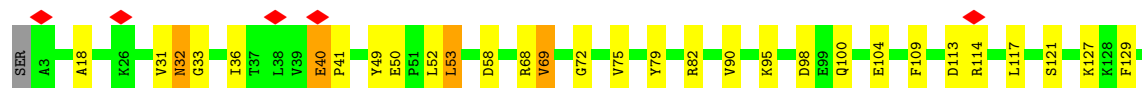
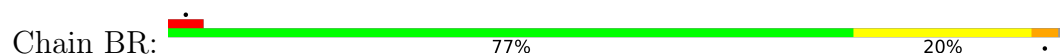
- Molecule 60: 40S ribosomal protein S14-A



- Molecule 61: 40S ribosomal protein S15

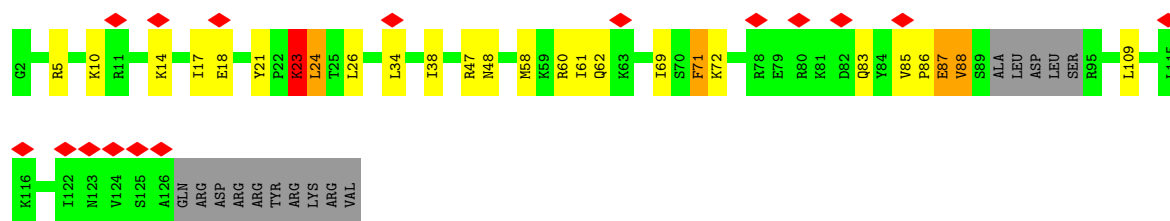


- Molecule 62: 40S ribosomal protein S16-A

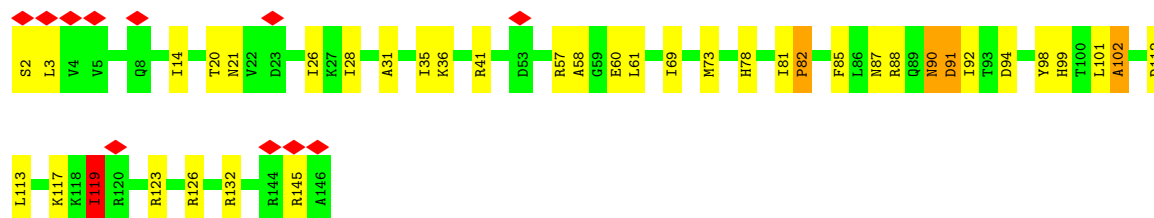
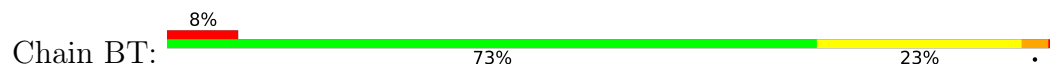


- Molecule 63: 40S ribosomal protein S17-A

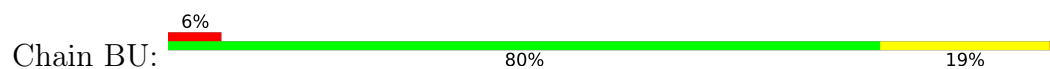




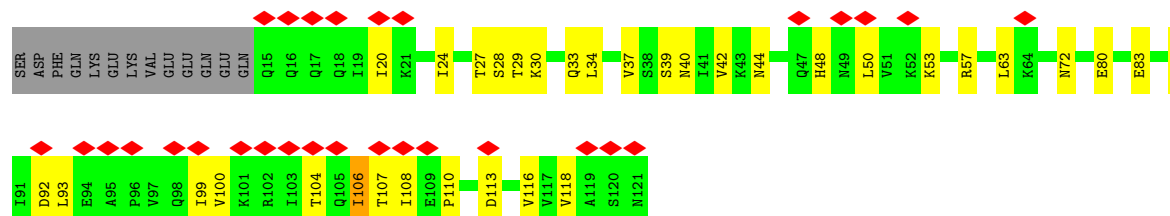
- Molecule 64: 40S ribosomal protein S18-A



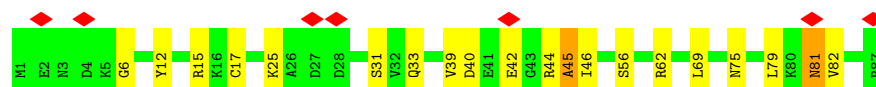
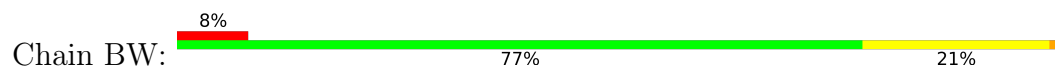
- Molecule 65: 40S ribosomal protein S19-A



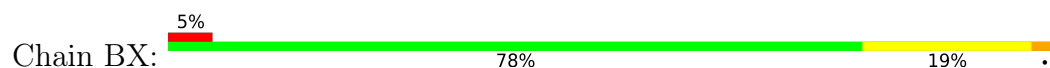
- Molecule 66: 40S ribosomal protein S20



- Molecule 67: 40S ribosomal protein S21-A

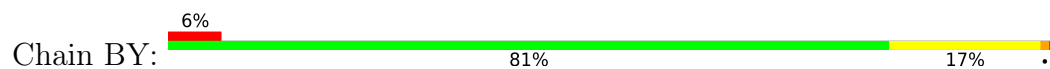


- Molecule 68: 40S ribosomal protein S22-A

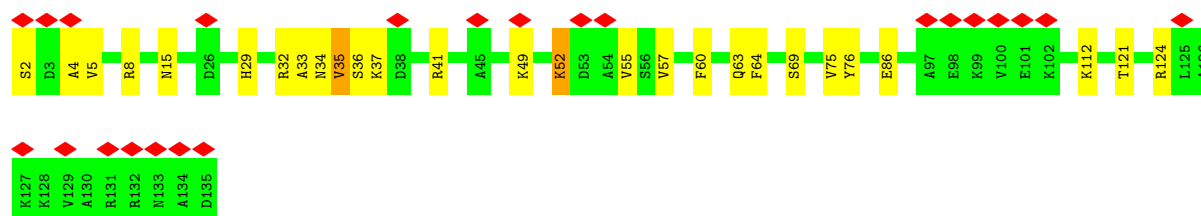
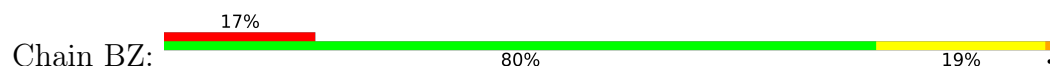




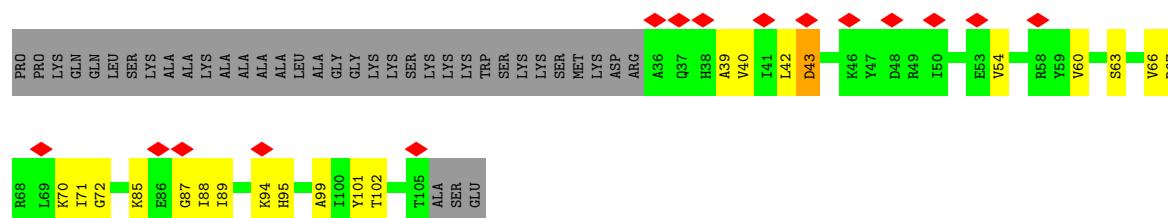
- Molecule 69: 40S ribosomal protein S23-A



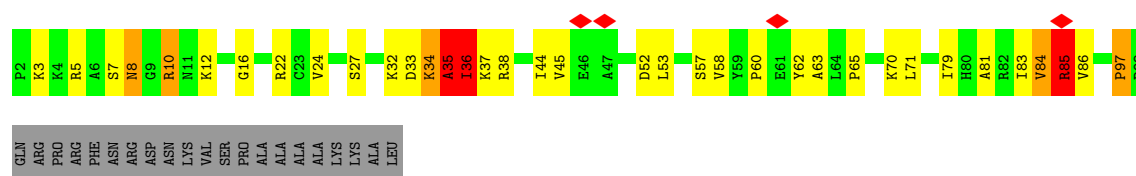
- Molecule 70: 40S ribosomal protein S24-A



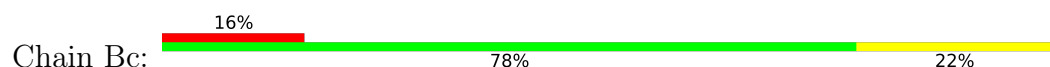
- Molecule 71: 40S ribosomal protein S25-A



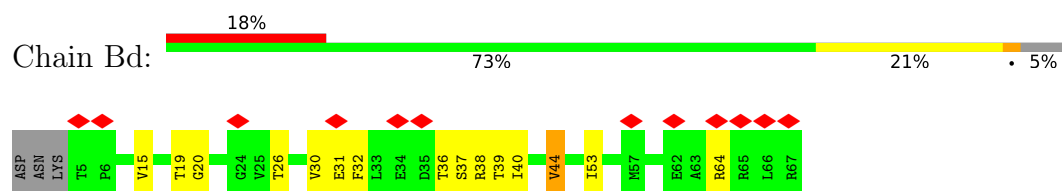
- Molecule 72: 40S ribosomal protein S26-B



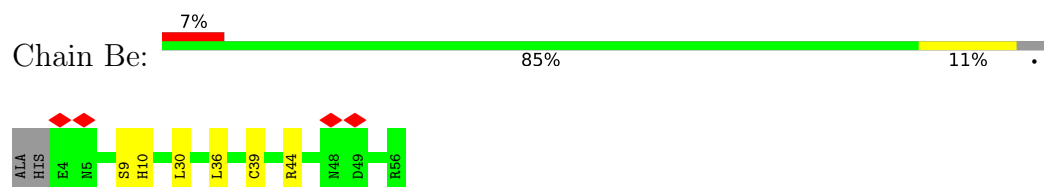
- Molecule 73: 40S ribosomal protein S27-A



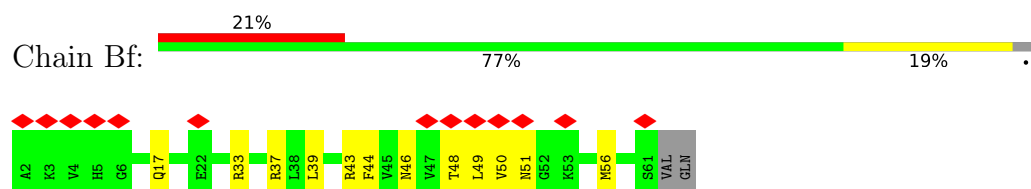
- Molecule 74: 40S ribosomal protein S28-A



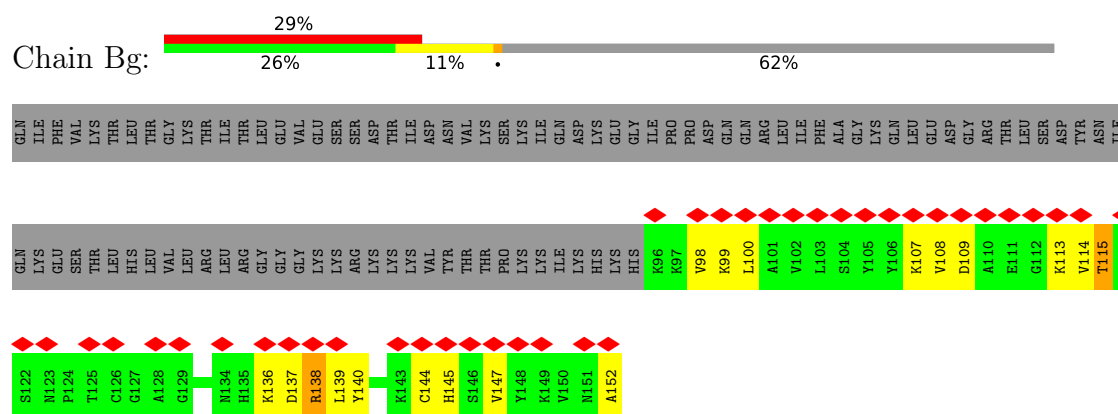
- Molecule 75: 40S ribosomal protein S29-A



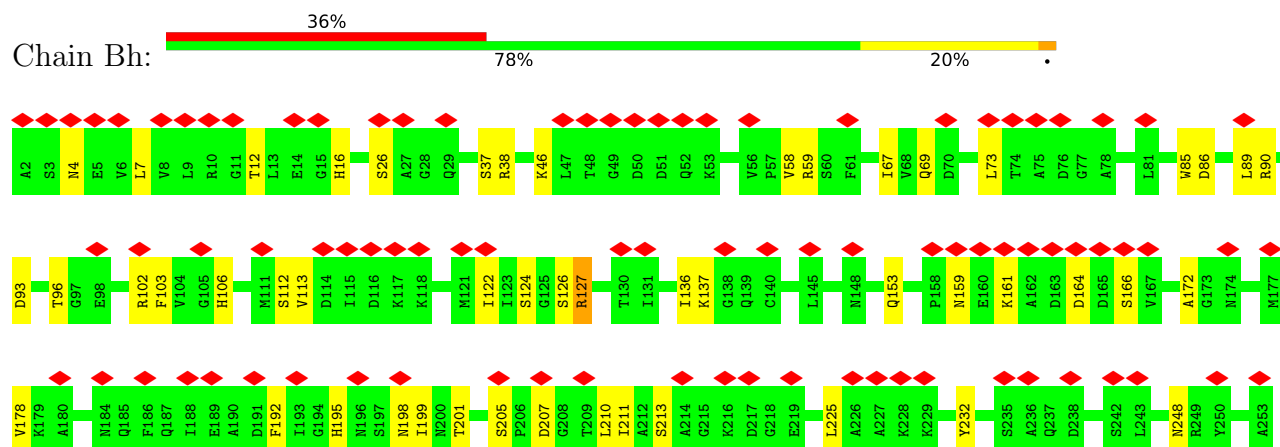
- Molecule 76: 40S ribosomal protein S30-A

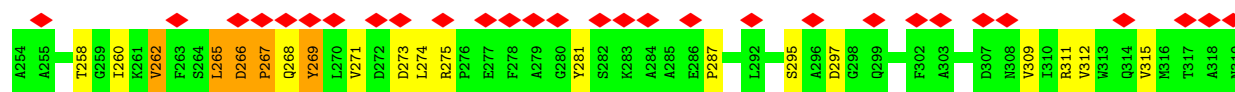


- Molecule 77: Ubiquitin-40S ribosomal protein S31



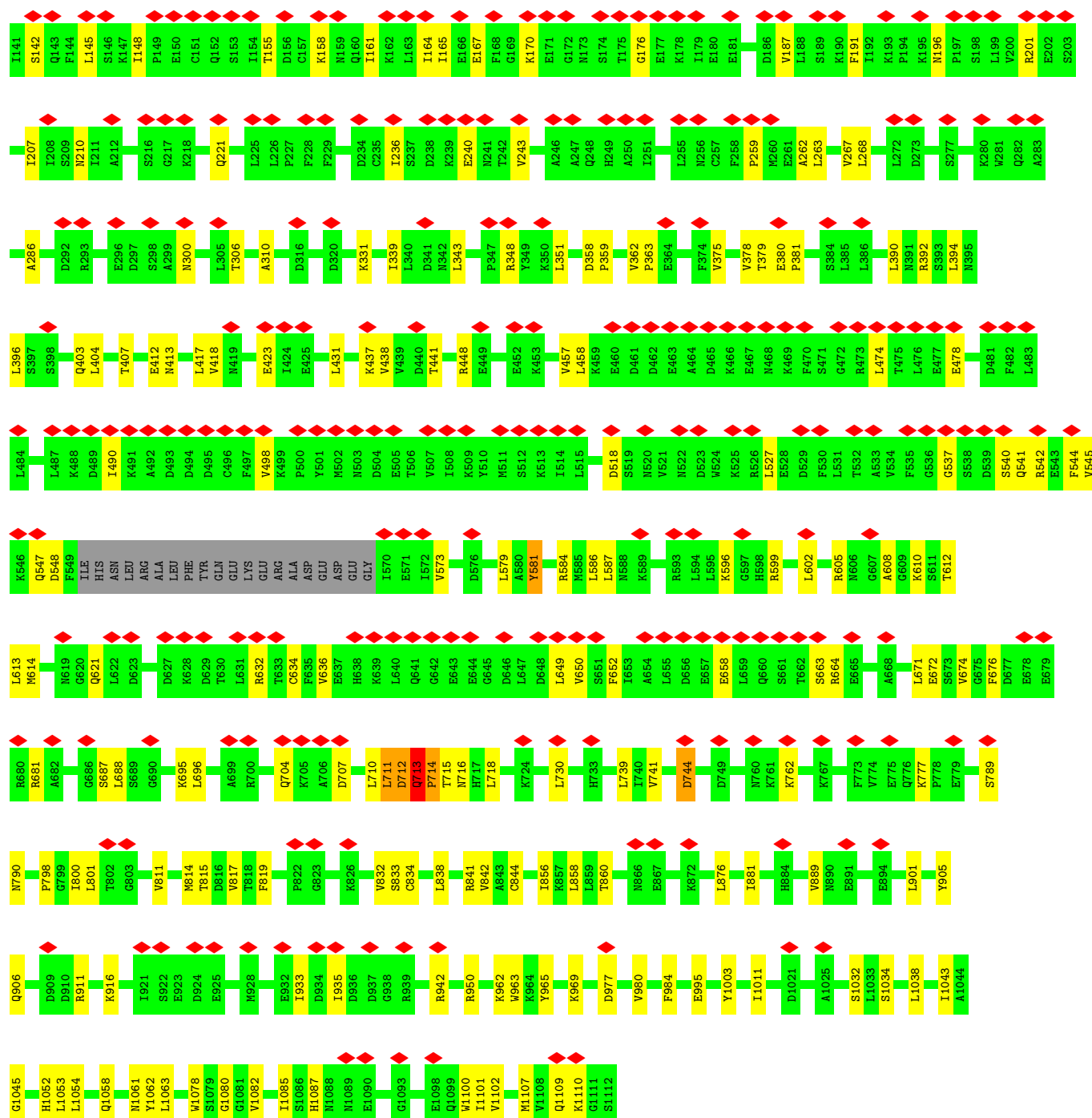
- Molecule 78: Guanine nucleotide-binding protein subunit beta-like protein





• Molecule 79: [NU+] prion formation protein 1

Chain Bi: 27% 78% 19% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48757	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.600	Depositor
Minimum map value	-0.343	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	446.46, 446.46, 446.46	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.063, 1.063, 1.063	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.42	0/75394	0.45	7/117545 (0.0%)
2	AB	0.40	0/2883	0.39	0/4491
3	AC	0.41	0/3746	0.42	0/5832
4	AD	0.45	0/1948	0.68	0/2617
5	AE	0.52	3/3146 (0.1%)	0.89	8/4228 (0.2%)
6	AF	0.42	0/2800	0.74	3/3790 (0.1%)
7	AG	0.39	0/2425	0.77	4/3271 (0.1%)
8	AH	0.36	0/1260	0.71	4/1694 (0.2%)
9	AI	0.41	0/1821	0.70	0/2451
10	AJ	0.36	0/1836	0.67	0/2481
11	AK	0.37	0/1537	0.63	0/2067
12	AL	0.35	0/1741	0.61	0/2335
13	AM	0.47	2/1374 (0.1%)	0.85	1/1842 (0.1%)
14	AN	0.42	0/1568	0.76	0/2106
15	AO	0.36	0/1068	0.66	0/1438
16	AP	0.44	0/1757	0.68	1/2354 (0.0%)
17	AQ	0.37	0/1585	0.60	0/2128
18	AR	0.40	0/1443	0.74	3/1944 (0.2%)
19	AS	0.39	0/1465	0.62	1/1965 (0.1%)
20	AT	0.36	0/1245	0.61	0/1661
21	AU	0.38	0/1481	0.62	0/1990
22	AV	0.40	0/1300	0.67	0/1743
23	AW	0.33	0/812	0.69	0/1099
24	AX	0.38	0/1018	0.59	0/1369
25	AY	0.37	0/521	0.56	0/691
26	AZ	0.37	0/979	0.60	0/1321
27	Aa	0.37	0/1004	0.60	0/1341
28	Ab	0.36	0/1118	0.70	3/1497 (0.2%)
29	Ac	0.46	0/1204	0.83	3/1612 (0.2%)
30	Ad	0.35	0/473	0.65	0/629
31	Ae	0.40	0/751	0.57	0/1008
32	Af	0.38	0/890	0.64	0/1196

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Ag	0.38	0/1041	0.59	0/1394
34	Ah	0.38	0/868	0.54	0/1168
35	Ai	0.41	0/890	0.61	0/1189
36	Aj	0.35	0/978	0.61	0/1301
37	Ak	0.35	0/778	0.71	2/1034 (0.2%)
38	Al	0.42	0/696	0.68	0/923
39	Am	0.33	0/618	0.62	0/826
40	An	0.44	0/443	0.68	0/588
41	Ao	0.36	0/423	0.61	0/562
42	Ap	0.39	0/234	0.67	0/300
43	Aq	0.42	0/860	0.72	0/1136
44	Ar	0.42	0/701	0.66	0/934
45	BA	0.49	0/40685	0.53	14/63392 (0.0%)
46	BB	0.48	0/1617	0.84	2/2215 (0.1%)
47	BC	0.50	0/1735	0.95	0/2335
48	BD	0.54	0/1665	0.73	1/2263 (0.0%)
49	BE	0.58	0/1759	0.80	0/2368
50	BF	0.53	0/2109	0.84	7/2839 (0.2%)
51	BG	0.60	0/1629	0.94	4/2202 (0.2%)
52	BH	0.40	0/1823	0.76	3/2439 (0.1%)
53	BI	0.45	0/1506	0.93	6/2028 (0.3%)
54	BJ	0.52	0/1514	0.82	2/2021 (0.1%)
55	BK	0.48	0/1519	0.78	1/2035 (0.0%)
56	BL	0.62	1/789 (0.1%)	0.90	2/1067 (0.2%)
57	BM	0.50	0/1239	0.74	0/1673
58	BN	0.43	0/898	1.11	5/1220 (0.4%)
59	BO	0.48	0/1215	0.88	5/1638 (0.3%)
60	BP	0.55	0/901	0.97	2/1217 (0.2%)
61	BQ	0.56	0/998	0.87	1/1341 (0.1%)
62	BR	0.63	0/1125	1.23	5/1510 (0.3%)
63	BS	0.49	0/935	0.90	2/1254 (0.2%)
64	BT	0.52	0/1211	0.79	2/1628 (0.1%)
65	BU	0.55	0/1130	0.79	2/1517 (0.1%)
66	BV	0.53	0/865	0.78	2/1169 (0.2%)
67	BW	0.55	0/693	0.85	2/935 (0.2%)
68	BX	0.56	0/1038	0.71	0/1395
69	BY	0.54	0/1139	0.83	0/1518
70	BZ	0.45	0/1087	0.78	0/1449
71	Ba	0.58	0/571	1.12	3/768 (0.4%)
72	Bb	0.54	0/782	0.98	5/1047 (0.5%)
73	Bc	0.51	0/620	0.80	2/838 (0.2%)
74	Bd	0.59	0/499	0.78	0/670
75	Be	0.52	0/452	0.77	0/600

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Bf	0.47	0/483	0.77	0/643
77	Bg	0.40	0/451	1.10	4/603 (0.7%)
78	Bh	0.66	1/2494 (0.0%)	0.81	1/3393 (0.0%)
79	Bi	0.51	10/7649 (0.1%)	0.77	14/10345 (0.1%)
All	All	0.46	17/218948 (0.0%)	0.61	139/320666 (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
4	AD	0	2
5	AE	0	3
6	AF	0	2
7	AG	0	3
8	AH	0	1
9	AI	0	3
11	AK	0	2
14	AN	0	1
15	AO	0	1
17	AQ	0	1
22	AV	0	1
28	Ab	0	1
35	Ai	0	1
36	Aj	0	2
46	BB	0	4
47	BC	0	2
49	BE	0	1
50	BF	0	2
51	BG	0	10
52	BH	0	3
53	BI	0	1
54	BJ	0	1
55	BK	0	2
56	BL	0	4
57	BM	0	1
58	BN	0	5
60	BP	0	2
62	BR	0	2
63	BS	0	3
64	BT	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
67	BW	0	2
69	BY	0	3
70	BZ	0	2
71	Ba	0	4
72	Bb	0	9
77	Bg	0	2
79	Bi	0	1
All	All	0	95

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	Bi	712	ASP	C-O	-17.79	1.04	1.23
79	Bi	712	ASP	CA-C	14.43	1.69	1.53
79	Bi	712	ASP	N-CA	13.20	1.63	1.46
5	AE	18	PRO	CA-C	12.79	1.70	1.52
79	Bi	711	LEU	C-N	10.50	1.47	1.33
79	Bi	713	GLN	C-O	10.46	1.37	1.24
79	Bi	712	ASP	CG-OD1	-9.93	1.06	1.25
79	Bi	712	ASP	CA-CB	8.97	1.64	1.52
79	Bi	713	GLN	CA-C	7.57	1.62	1.52
13	AM	82	ARG	CA-CB	-7.55	1.41	1.53
5	AE	18	PRO	CA-CB	6.89	1.63	1.53
5	AE	18	PRO	C-O	-6.66	1.15	1.24
79	Bi	712	ASP	CB-CG	6.52	1.68	1.52
13	AM	82	ARG	N-CA	-6.27	1.39	1.46
78	Bh	127	ARG	CA-C	-5.69	1.43	1.52
79	Bi	714	PRO	N-CD	-5.61	1.39	1.47
56	BL	65	TYR	CA-CB	-5.47	1.45	1.53

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	BR	40	GLU	CA-C-N	24.14	143.48	119.82
62	BR	40	GLU	C-N-CA	24.14	143.48	119.82
5	AE	18	PRO	CA-C-O	-22.67	79.33	120.60
79	Bi	711	LEU	CA-C-N	15.39	145.93	122.23
79	Bi	711	LEU	C-N-CA	15.39	145.93	122.23
45	BA	855	A	C4'-C3'-O3'	-14.81	87.19	109.40
5	AE	18	PRO	O-C-N	-13.75	104.07	122.64
59	BO	22	ALA	CA-C-N	12.27	135.18	119.84
59	BO	22	ALA	C-N-CA	12.27	135.18	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	Bi	712	ASP	CA-CB-CG	11.62	124.22	112.60
45	BA	854	U	C1'-C2'-O2'	-11.20	95.00	111.80
13	AM	82	ARG	N-CA-CB	-10.69	94.51	110.01
5	AE	17	LEU	N-CA-C	-10.56	99.52	113.25
79	Bi	712	ASP	N-CA-C	10.15	125.54	109.39
5	AE	18	PRO	CA-C-N	10.03	140.70	121.54
5	AE	18	PRO	C-N-CA	10.03	140.70	121.54
79	Bi	714	PRO	N-CD-CG	-9.30	89.25	103.20
45	BA	849	C	C3'-C2'-O2'	8.66	127.59	114.60
51	BG	66	GLN	N-CA-C	8.36	121.79	109.42
79	Bi	713	GLN	CA-C-O	8.22	131.43	120.16
8	AH	70	LYS	CA-C-N	-7.81	115.31	122.97
8	AH	70	LYS	C-N-CA	-7.81	115.31	122.97
50	BF	193	GLY	CA-C-N	7.76	136.35	121.54
50	BF	193	GLY	C-N-CA	7.76	136.35	121.54
29	Ac	47	LYS	CA-C-N	7.70	136.25	121.54
29	Ac	47	LYS	C-N-CA	7.70	136.25	121.54
62	BR	41	PRO	N-CA-C	7.48	123.62	113.98
79	Bi	713	GLN	CB-CA-C	7.45	124.84	110.17
50	BF	194	THR	N-CA-C	7.40	126.56	110.80
51	BG	49	GLU	N-CA-C	-7.33	101.08	110.53
53	BI	131	PHE	N-CA-C	7.19	125.70	109.81
5	AE	19	ARG	N-CA-C	7.15	126.03	110.80
77	Bg	136	LYS	CA-C-N	7.09	135.08	121.54
77	Bg	136	LYS	C-N-CA	7.09	135.08	121.54
56	BL	92	ILE	CA-C-N	6.95	131.67	121.31
56	BL	92	ILE	C-N-CA	6.95	131.67	121.31
79	Bi	713	GLN	CA-C-N	-6.80	111.34	119.84
79	Bi	713	GLN	C-N-CA	-6.80	111.34	119.84
63	BS	23	LYS	CA-C-N	6.68	134.30	121.54
63	BS	23	LYS	C-N-CA	6.68	134.30	121.54
45	BA	849	C	N1-C1'-C2'	-6.67	104.00	114.00
29	Ac	66	ALA	N-CA-C	-6.50	106.30	114.56
51	BG	59	VAL	N-CA-C	-6.45	100.49	109.45
59	BO	27	LYS	CA-C-N	6.37	133.71	121.54
59	BO	27	LYS	C-N-CA	6.37	133.71	121.54
61	BQ	11	VAL	N-CA-C	6.33	112.98	106.21
79	Bi	712	ASP	OD1-CG-OD2	-6.30	107.78	122.90
77	Bg	99	LYS	CA-C-N	6.22	133.42	121.54
77	Bg	99	LYS	C-N-CA	6.22	133.42	121.54
72	Bb	35	ALA	CA-C-N	6.19	133.11	121.97
72	Bb	35	ALA	C-N-CA	6.19	133.11	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AG	124	GLU	CA-C-N	6.14	133.02	121.97
7	AG	124	GLU	C-N-CA	6.14	133.02	121.97
79	Bi	714	PRO	CB-CA-C	6.13	121.68	111.56
45	BA	852	C	C4'-C3'-O3'	-6.09	103.86	113.00
79	Bi	712	ASP	CB-CG-OD2	6.07	132.36	118.40
50	BF	195	ILE	CA-C-N	-6.07	117.03	122.97
50	BF	195	ILE	C-N-CA	-6.07	117.03	122.97
7	AG	43	LYS	CA-C-N	6.00	130.73	121.19
7	AG	43	LYS	C-N-CA	6.00	130.73	121.19
45	BA	853	G	N9-C1'-C2'	5.97	120.95	112.00
71	Ba	43	ASP	N-CA-C	5.92	117.94	110.24
45	BA	819	G	C4'-C3'-O3'	5.92	118.28	109.40
51	BG	51	VAL	N-CA-C	5.82	121.45	109.34
52	BH	67	VAL	CA-C-N	5.82	132.65	121.54
52	BH	67	VAL	C-N-CA	5.82	132.65	121.54
1	AA	282	G	C2'-C3'-O3'	5.80	122.40	113.70
53	BI	30	SER	CA-C-N	5.76	130.67	121.62
53	BI	30	SER	C-N-CA	5.76	130.67	121.62
5	AE	16	PHE	N-CA-C	-5.76	103.84	112.54
59	BO	22	ALA	N-CA-C	5.74	122.50	109.81
66	BV	106	ILE	CA-C-N	5.72	130.97	122.74
66	BV	106	ILE	C-N-CA	5.72	130.97	122.74
16	AP	75	VAL	CA-CB-CG1	5.71	120.10	110.40
67	BW	81	ASN	CA-C-N	5.68	132.20	121.97
67	BW	81	ASN	C-N-CA	5.68	132.20	121.97
58	BN	130	THR	CA-C-N	5.67	132.38	121.54
58	BN	130	THR	C-N-CA	5.67	132.38	121.54
65	BU	88	VAL	CA-C-N	5.66	133.02	121.48
65	BU	88	VAL	C-N-CA	5.66	133.02	121.48
28	Ab	102	GLU	CA-C-N	5.62	135.51	121.80
28	Ab	102	GLU	C-N-CA	5.62	135.51	121.80
1	AA	2541	U	P-O3'-C3'	5.59	128.58	120.20
72	Bb	60	PRO	CA-C-N	5.56	132.16	121.54
72	Bb	60	PRO	C-N-CA	5.56	132.16	121.54
45	BA	1294	G	P-O3'-C3'	5.48	128.41	120.20
48	BD	39	THR	CA-CB-CG2	5.47	119.80	110.50
53	BI	133	THR	CA-C-N	5.47	131.99	121.54
53	BI	133	THR	C-N-CA	5.47	131.99	121.54
52	BH	150	GLU	N-CA-C	-5.45	106.49	114.39
1	AA	1307	G	P-O3'-C3'	5.43	128.35	120.20
18	AR	155	GLU	CA-C-N	5.42	129.38	121.31
18	AR	155	GLU	C-N-CA	5.42	129.38	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BA	498	G	P-O3'-C3'	5.42	128.33	120.20
55	BK	134	ILE	N-CA-C	5.40	120.58	109.34
1	AA	2513	U	P-O3'-C3'	5.40	128.30	120.20
45	BA	1370	U	P-O3'-C3'	5.40	128.30	120.20
58	BN	131	ASP	N-CA-C	5.39	122.27	110.80
50	BF	148	ARG	CA-C-N	5.37	128.63	122.83
50	BF	148	ARG	C-N-CA	5.37	128.63	122.83
73	Bc	2	VAL	CA-C-N	5.36	131.77	121.54
73	Bc	2	VAL	C-N-CA	5.36	131.77	121.54
45	BA	1226	A	C2'-C3'-O3'	5.34	121.72	113.70
58	BN	124	LYS	CA-C-N	5.32	131.71	121.54
58	BN	124	LYS	C-N-CA	5.32	131.71	121.54
6	AF	4	PRO	N-CA-C	5.32	120.84	113.98
6	AF	337	GLU	CA-C-N	5.32	131.69	121.54
6	AF	337	GLU	C-N-CA	5.32	131.69	121.54
1	AA	1815	U	P-O3'-C3'	5.31	128.17	120.20
1	AA	979	U	P-O3'-C3'	5.30	128.15	120.20
62	BR	31	VAL	CA-C-N	5.30	131.66	121.54
62	BR	31	VAL	C-N-CA	5.30	131.66	121.54
1	AA	1607	U	C4'-C3'-O3'	5.29	117.33	109.40
71	Ba	43	ASP	CA-C-N	5.25	127.57	120.38
71	Ba	43	ASP	C-N-CA	5.25	127.57	120.38
79	Bi	714	PRO	CA-C-N	5.20	130.72	122.60
79	Bi	714	PRO	C-N-CA	5.20	130.72	122.60
53	BI	65	PRO	N-CA-C	-5.19	107.40	114.98
5	AE	18	PRO	N-CA-C	5.18	123.15	112.47
60	BP	125	SER	CA-C-N	5.18	129.03	121.31
60	BP	125	SER	C-N-CA	5.18	129.03	121.31
46	BB	95	ALA	CA-C-N	5.15	128.20	120.83
46	BB	95	ALA	C-N-CA	5.15	128.20	120.83
45	BA	139	C	P-O3'-C3'	5.15	127.92	120.20
19	AS	99	THR	N-CA-C	5.13	116.72	110.41
28	Ab	18	TYR	N-CA-C	-5.13	104.80	112.54
37	Ak	33	ALA	CA-C-N	5.11	131.31	121.54
37	Ak	33	ALA	C-N-CA	5.11	131.31	121.54
8	AH	67	GLY	CA-C-N	5.10	126.21	119.84
8	AH	67	GLY	C-N-CA	5.10	126.21	119.84
45	BA	855	A	C5'-C4'-O4'	5.09	116.73	109.10
64	BT	119	ILE	CA-C-N	5.08	129.76	122.40
64	BT	119	ILE	C-N-CA	5.08	129.76	122.40
54	BJ	147	ALA	CA-C-N	5.03	131.15	121.54
54	BJ	147	ALA	C-N-CA	5.03	131.15	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	AR	156	ALA	N-CA-C	5.02	117.38	110.35
72	Bb	36	ILE	N-CA-C	-5.02	98.90	109.34
78	Bh	269	TYR	N-CA-C	5.01	116.69	109.07
45	BA	685	A	C2'-C3'-O3'	5.00	121.20	113.70

There are no chirality outliers.

All (95) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	AD	143	GLU	Peptide
4	AD	250	GLN	Peptide
5	AE	16	PHE	Mainchain
5	AE	18	PRO	Mainchain,Peptide
6	AF	318	LEU	Peptide
6	AF	338	LYS	Peptide
7	AG	124	GLU	Peptide
7	AG	257	GLU	Peptide
7	AG	261	THR	Peptide
8	AH	67	GLY	Mainchain
9	AI	157	ASN	Peptide
9	AI	190	THR	Peptide
9	AI	232	ARG	Peptide
11	AK	20	ILE	Peptide
11	AK	21	LYS	Peptide
14	AN	4	SER	Peptide
15	AO	8	LYS	Peptide
17	AQ	110	PRO	Peptide
22	AV	124	VAL	Peptide
28	Ab	102	GLU	Peptide
35	Ai	80	ARG	Peptide
36	Aj	83	LYS	Peptide
36	Aj	90	ARG	Peptide
46	BB	110	TYR	Peptide
46	BB	156	VAL	Peptide
46	BB	157	ASP	Peptide
46	BB	165	ARG	Peptide
47	BC	177	GLN	Peptide
47	BC	179	SER	Peptide
49	BE	219	ALA	Peptide
50	BF	193	GLY	Peptide
50	BF	194	THR	Peptide
51	BG	126	ASP	Peptide

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Mol	Chain	Res	Type	Group
51	BG	36	ALA	Peptide
51	BG	44	ASN	Peptide
51	BG	48	PHE	Peptide
51	BG	49	GLU	Peptide
51	BG	50	GLU	Peptide
51	BG	56	ALA	Peptide
51	BG	57	SER	Peptide
51	BG	58	LEU	Peptide
51	BG	65	ARG	Peptide
52	BH	148	SER	Peptide
52	BH	150	GLU	Peptide
52	BH	68	LEU	Peptide
53	BI	110	GLN	Peptide
54	BJ	147	ALA	Peptide
55	BK	133	HIS	Peptide
55	BK	163	PRO	Peptide
56	BL	76	LEU	Peptide
56	BL	86	ILE	Peptide
56	BL	87	VAL	Peptide
56	BL	89	GLY	Peptide
57	BM	5	LEU	Peptide
58	BN	110	GLY	Peptide
58	BN	126	TRP	Peptide
58	BN	130	THR	Peptide
58	BN	36	LEU	Peptide
58	BN	83	GLU	Peptide
60	BP	123	SER	Peptide
60	BP	28	VAL	Peptide
62	BR	32	ASN	Peptide
62	BR	40	GLU	Peptide
63	BS	23	LYS	Peptide
63	BS	85	VAL	Peptide
63	BS	86	PRO	Peptide
64	BT	101	LEU	Peptide
64	BT	60	GLU	Peptide
64	BT	81	ILE	Peptide
64	BT	90	ASN	Peptide
64	BT	91	ASP	Peptide
67	BW	45	ALA	Peptide
67	BW	75	ASN	Peptide
69	BY	113	ALA	Peptide
69	BY	130	VAL	Peptide

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Mol	Chain	Res	Type	Group
69	BY	88	PRO	Peptide
70	BZ	33	ALA	Peptide
70	BZ	4	ALA	Peptide
71	Ba	40	VAL	Peptide
71	Ba	42	LEU	Peptide
71	Ba	87	GLY	Peptide
71	Ba	94	LYS	Peptide
72	Bb	10	ARG	Peptide
72	Bb	34	LYS	Peptide
72	Bb	35	ALA	Peptide
72	Bb	63	ALA	Peptide
72	Bb	7	SER	Peptide
72	Bb	81	ALA	Peptide
72	Bb	84	VAL	Peptide
72	Bb	85	ARG	Peptide
72	Bb	97	PRO	Peptide
77	Bg	137	ASP	Peptide
77	Bg	98	VAL	Peptide
79	Bi	1063	LEU	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	67355	0	33848	402	0
2	AB	2579	0	1304	12	0
3	AC	3353	0	1695	21	0
4	AD	1914	0	1981	61	0
5	AE	3075	0	3142	110	0
6	AF	2748	0	2859	87	0
7	AG	2375	0	2325	30	0
8	AH	1239	0	1326	45	0
9	AI	1784	0	1862	25	0
10	AJ	1804	0	1877	28	0
11	AK	1518	0	1585	18	0
12	AL	1705	0	1736	17	0
13	AM	1353	0	1383	29	0
14	AN	1543	0	1608	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	AO	1053	0	1149	12	0
16	AP	1720	0	1779	30	0
17	AQ	1555	0	1659	18	0
18	AR	1420	0	1437	16	0
19	AS	1441	0	1543	12	0
20	AT	1228	0	1314	16	0
21	AU	1445	0	1487	29	0
22	AV	1276	0	1323	19	0
23	AW	796	0	812	7	0
24	AX	1003	0	1048	12	0
25	AY	509	0	537	2	0
26	AZ	964	0	1025	9	0
27	Aa	993	0	1081	15	0
28	Ab	1092	0	1155	16	0
29	Ac	1173	0	1215	17	0
30	Ad	462	0	491	2	0
31	Ae	743	0	797	10	0
32	Af	876	0	912	12	0
33	Ag	1020	0	1090	12	0
34	Ah	850	0	880	47	0
35	Ai	880	0	945	14	0
36	Aj	969	0	1078	12	0
37	Ak	771	0	849	12	0
38	Al	681	0	687	25	0
39	Am	612	0	682	6	0
40	An	436	0	475	4	0
41	Ao	417	0	459	4	0
42	Ap	233	0	284	5	0
43	Aq	847	0	914	19	0
44	Ar	694	0	738	10	0
45	BA	36375	0	18300	262	0
46	BB	1577	0	1567	28	0
47	BC	1709	0	1784	36	0
48	BD	1635	0	1723	27	0
49	BE	1734	0	1817	21	0
50	BF	2068	0	2154	35	0
51	BG	1609	0	1675	24	0
52	BH	1799	0	1879	32	0
53	BI	1481	0	1572	33	0
54	BJ	1489	0	1525	31	0
55	BK	1494	0	1573	21	0
56	BL	772	0	727	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	BM	1213	0	1257	11	0
58	BN	890	0	887	19	0
59	BO	1192	0	1254	27	0
60	BP	891	0	883	20	0
61	BQ	977	0	1002	17	0
62	BR	1105	0	1166	23	0
63	BS	926	0	930	17	0
64	BT	1192	0	1222	24	0
65	BU	1112	0	1124	16	0
66	BV	855	0	917	24	0
67	BW	684	0	672	14	0
68	BX	1021	0	1060	45	0
69	BY	1121	0	1196	45	0
70	BZ	1073	0	1132	19	0
71	Ba	563	0	603	10	0
72	Bb	769	0	818	21	0
73	Bc	610	0	633	9	0
74	Bd	497	0	535	12	0
75	Be	442	0	432	4	0
76	Bf	475	0	525	9	0
77	Bg	444	0	463	11	0
78	Bh	2441	0	2397	43	0
79	Bi	7512	0	7546	141	0
80	Bi	62	0	24	10	0
All	All	204313	0	153350	2019	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 6.

All (2019) 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)
59:BO:23:PRO:HG2	59:BO:26:PHE:CB	1.26	1.65
4:AD:186:PHE:HB2	4:AD:196:TRP:CH2	1.15	1.60
4:AD:186:PHE:CD1	4:AD:196:TRP:HZ3	1.21	1.57
5:AE:16:PHE:CE1	5:AE:275:ARG:NH1	1.83	1.47
4:AD:186:PHE:HB2	4:AD:196:TRP:CZ3	1.50	1.44
34:Ah:103:TYR:CD1	34:Ah:104:PRO:HD3	1.52	1.44
4:AD:186:PHE:CB	4:AD:196:TRP:CZ3	1.99	1.44
4:AD:186:PHE:CB	4:AD:196:TRP:CH2	2.07	1.38
4:AD:186:PHE:CD1	4:AD:196:TRP:CZ3	2.11	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:148:ILE:CG2	6:AF:149:PRO:HD3	1.54	1.37
8:AH:66:SER:O	8:AH:68:PRO:CD	1.72	1.37
59:BO:23:PRO:CG	59:BO:26:PHE:HB2	1.53	1.35
59:BO:23:PRO:O	59:BO:25:TRP:N	1.60	1.34
6:AF:148:ILE:HG23	6:AF:149:PRO:CD	1.58	1.32
8:AH:43:LEU:HD13	34:Ah:102:LEU:O	1.29	1.31
69:BY:63:GLN:CB	69:BY:64:PRO:HD3	1.56	1.31
8:AH:82:ARG:O	34:Ah:104:PRO:HA	1.22	1.29
45:BA:865:A:OP1	68:BX:28:ARG:NH2	1.64	1.27
8:AH:83:TYR:HA	34:Ah:103:TYR:O	1.23	1.26
4:AD:186:PHE:HD1	4:AD:196:TRP:CZ3	1.49	1.22
6:AF:151:VAL:O	6:AF:152:VAL:CG2	1.88	1.22
34:Ah:103:TYR:HD1	34:Ah:104:PRO:CD	1.52	1.20
59:BO:23:PRO:CG	59:BO:26:PHE:CB	2.12	1.20
8:AH:67:GLY:O	8:AH:74:VAL:O	1.60	1.20
8:AH:43:LEU:CD1	34:Ah:102:LEU:O	1.90	1.18
6:AF:151:VAL:O	6:AF:152:VAL:HG23	0.99	1.17
5:AE:16:PHE:CD1	5:AE:275:ARG:NH1	2.13	1.15
4:AD:186:PHE:CG	4:AD:196:TRP:HZ3	1.64	1.15
69:BY:62:LYS:NZ	69:BY:118:PRO:HB3	1.59	1.15
68:BX:6:VAL:HG13	68:BX:29:PRO:HB2	1.18	1.14
5:AE:16:PHE:CE1	5:AE:275:ARG:CZ	2.29	1.14
46:BB:206:ASP:CB	46:BB:207:PRO:CD	2.26	1.13
79:Bi:1034:SER:HB2	80:Bi:1202:ATP:O1B	1.45	1.13
4:AD:186:PHE:CG	4:AD:196:TRP:CZ3	2.34	1.12
59:BO:23:PRO:HG2	59:BO:26:PHE:HB3	1.14	1.12
6:AF:131:VAL:CA	6:AF:148:ILE:HG12	1.79	1.11
59:BO:23:PRO:CB	59:BO:26:PHE:HB2	1.80	1.11
46:BB:206:ASP:CB	46:BB:207:PRO:HD2	1.82	1.09
68:BX:30:SER:OG	68:BX:61:ILE:HG13	1.50	1.09
69:BY:63:GLN:HB3	69:BY:64:PRO:CD	1.80	1.08
5:AE:16:PHE:HE1	5:AE:275:ARG:NH1	1.29	1.08
6:AF:151:VAL:HG12	6:AF:152:VAL:H	1.07	1.08
45:BA:576:G:O6	69:BY:65:ASN:HA	1.52	1.08
69:BY:63:GLN:CB	69:BY:64:PRO:CD	2.30	1.08
5:AE:16:PHE:CD1	5:AE:275:ARG:CZ	2.36	1.07
6:AF:131:VAL:HA	6:AF:148:ILE:HG12	1.17	1.07
13:AM:79:ILE:O	13:AM:82:ARG:HB3	1.52	1.07
69:BY:62:LYS:HZ1	69:BY:118:PRO:HB3	1.04	1.07
6:AF:9:HIS:CD2	6:AF:150:LEU:HD13	1.90	1.07
5:AE:16:PHE:CE1	5:AE:275:ARG:HD3	1.89	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BI:63:PRO:C	53:BI:65:PRO:HD3	1.80	1.06
6:AF:9:HIS:HD2	6:AF:150:LEU:CD1	1.69	1.06
5:AE:17:LEU:HD12	5:AE:262:TRP:HZ3	1.15	1.06
6:AF:132:ALA:HB2	6:AF:148:ILE:HD13	1.29	1.06
4:AD:182:ALA:O	4:AD:196:TRP:CZ2	2.08	1.05
1:AA:3267:A:H2'	8:AH:69:PHE:CZ	1.91	1.04
8:AH:66:SER:C	8:AH:68:PRO:HD3	1.80	1.04
34:Ah:105:SER:OG	34:Ah:107:ILE:HG13	1.57	1.04
45:BA:848:C:H2'	45:BA:849:C:C5'	1.88	1.04
5:AE:17:LEU:HD11	5:AE:262:TRP:CE3	1.92	1.03
5:AE:17:LEU:CD1	5:AE:262:TRP:CZ3	2.41	1.02
45:BA:864:U:H3'	68:BX:28:ARG:HH12	1.23	1.02
8:AH:43:LEU:CD1	34:Ah:103:TYR:HA	1.87	1.02
8:AH:82:ARG:O	34:Ah:104:PRO:CA	2.07	1.01
6:AF:151:VAL:HG12	6:AF:152:VAL:N	1.71	1.01
4:AD:186:PHE:CA	4:AD:196:TRP:CZ3	2.43	1.00
6:AF:132:ALA:CB	6:AF:148:ILE:HD13	1.91	1.00
8:AH:43:LEU:HD13	34:Ah:103:TYR:HA	1.44	0.99
5:AE:17:LEU:HD12	5:AE:262:TRP:CZ3	1.97	0.99
4:AD:196:TRP:HB3	4:AD:197:PRO:HD3	1.42	0.98
5:AE:16:PHE:CZ	5:AE:275:ARG:HD3	1.97	0.98
6:AF:9:HIS:HD2	6:AF:150:LEU:HD13	1.20	0.98
34:Ah:48:ARG:HB2	34:Ah:103:TYR:OH	1.62	0.98
59:BO:23:PRO:HG2	59:BO:26:PHE:HB2	1.01	0.97
1:AA:847:A:OP1	59:BO:140:LYS:HE2	1.65	0.97
8:AH:83:TYR:CA	34:Ah:103:TYR:O	2.13	0.97
45:BA:126:A:H62	45:BA:291:G:H21	0.98	0.97
5:AE:17:LEU:CD1	5:AE:262:TRP:CE3	2.47	0.96
8:AH:67:GLY:HA3	8:AH:74:VAL:HB	1.45	0.96
4:AD:186:PHE:HA	4:AD:196:TRP:CE3	2.01	0.95
13:AM:82:ARG:HG3	79:Bi:1003:TYR:OH	1.65	0.95
45:BA:848:C:H2'	45:BA:849:C:H5''	1.47	0.95
8:AH:66:SER:O	8:AH:68:PRO:HD3	0.76	0.94
3:AC:104:A:H4'	38:Al:42:ALA:HB1	1.50	0.93
45:BA:126:A:H62	45:BA:291:G:N2	1.67	0.93
69:BY:63:GLN:HB3	69:BY:64:PRO:HD3	0.93	0.93
6:AF:151:VAL:C	6:AF:152:VAL:HG23	1.94	0.92
5:AE:16:PHE:CE1	5:AE:275:ARG:CD	2.52	0.91
45:BA:1755:A:C8	69:BY:63:GLN:OE1	2.24	0.91
8:AH:82:ARG:O	34:Ah:103:TYR:O	1.88	0.91
4:AD:196:TRP:HB3	4:AD:197:PRO:CD	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:186:PHE:HA	4:AD:196:TRP:CZ3	2.07	0.89
53:BI:12:ALA:HB3	53:BI:13:PRO:HD3	1.54	0.88
59:BO:23:PRO:HB2	59:BO:26:PHE:HB2	1.52	0.88
4:AD:186:PHE:HB2	4:AD:196:TRP:HH2	1.11	0.88
68:BX:6:VAL:HG13	68:BX:29:PRO:CB	2.02	0.88
78:Bh:266:ASP:CB	78:Bh:267:PRO:HD3	2.04	0.88
6:AF:132:ALA:CA	6:AF:148:ILE:HD13	2.03	0.87
5:AE:16:PHE:CZ	5:AE:275:ARG:CD	2.56	0.87
1:AA:2184:U:C5	4:AD:198:LYS:NZ	2.41	0.87
5:AE:17:LEU:CD1	5:AE:262:TRP:HZ3	1.85	0.85
8:AH:43:LEU:HD13	34:Ah:102:LEU:C	2.01	0.85
5:AE:19:ARG:HA	5:AE:273:HIS:CE1	2.12	0.85
69:BY:62:LYS:CE	69:BY:118:PRO:HB3	2.05	0.85
45:BA:126:A:N6	45:BA:291:G:H21	1.74	0.85
1:AA:2395:G:O4'	5:AE:258:ALA:HB1	1.77	0.84
5:AE:17:LEU:HD11	5:AE:262:TRP:HE3	1.37	0.84
6:AF:151:VAL:CG1	6:AF:152:VAL:H	1.79	0.84
6:AF:9:HIS:CD2	6:AF:150:LEU:CD1	2.55	0.84
1:AA:2184:U:H5	4:AD:198:LYS:NZ	1.74	0.84
68:BX:30:SER:OG	68:BX:61:ILE:CG1	2.26	0.83
4:AD:182:ALA:O	4:AD:196:TRP:CH2	2.31	0.83
4:AD:182:ALA:O	4:AD:196:TRP:HZ2	1.59	0.83
13:AM:113:GLY:H	79:Bi:1003:TYR:HE1	1.25	0.82
5:AE:19:ARG:HD3	5:AE:19:ARG:H	1.45	0.82
53:BI:63:PRO:C	53:BI:65:PRO:CD	2.52	0.82
45:BA:864:U:H3'	68:BX:28:ARG:NH1	1.94	0.81
4:AD:19:HIS:CE1	4:AD:193:ARG:O	2.34	0.81
68:BX:28:ARG:HB3	68:BX:29:PRO:HD3	1.59	0.81
45:BA:848:C:H2'	45:BA:849:C:H5'	1.63	0.81
68:BX:6:VAL:CG1	68:BX:29:PRO:HB2	2.07	0.81
45:BA:848:C:C2'	45:BA:849:C:H5''	2.10	0.81
1:AA:3267:A:OP2	8:AH:69:PHE:HE2	1.65	0.80
13:AM:113:GLY:N	79:Bi:1003:TYR:HE1	1.80	0.79
69:BY:63:GLN:HB2	69:BY:64:PRO:HD3	1.60	0.79
45:BA:848:C:C2'	45:BA:849:C:C5'	2.60	0.79
34:Ah:105:SER:OG	34:Ah:107:ILE:CG1	2.30	0.79
34:Ah:105:SER:C	34:Ah:107:ILE:H	1.90	0.79
69:BY:62:LYS:HZ1	69:BY:118:PRO:CB	1.94	0.78
59:BO:23:PRO:HG2	59:BO:26:PHE:CG	2.16	0.78
38:Al:39:TYR:H	38:Al:40:PRO:HD2	1.49	0.78
4:AD:186:PHE:CA	4:AD:196:TRP:CH2	2.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:Bi:581:TYR:CE2	79:Bi:612:THR:OG1	2.37	0.77
38:Al:22:CYS:HG	38:Al:37:CYS:HG	1.02	0.77
68:BX:27:ILE:HD11	68:BX:61:ILE:HB	1.66	0.77
45:BA:1294:G:H1	45:BA:1303:U:H3	0.79	0.76
45:BA:576:G:O6	69:BY:65:ASN:CA	2.32	0.76
53:BI:63:PRO:HB2	53:BI:65:PRO:HD2	1.68	0.76
79:Bi:581:TYR:HE2	79:Bi:612:THR:OG1	1.66	0.76
47:BC:107:THR:O	47:BC:111:ARG:HB2	1.86	0.75
8:AH:43:LEU:HD11	34:Ah:102:LEU:O	1.86	0.75
53:BI:63:PRO:HB2	53:BI:65:PRO:CD	2.16	0.75
1:AA:3267:A:C8	8:AH:69:PHE:CE2	2.75	0.75
5:AE:16:PHE:CE1	5:AE:275:ARG:NE	2.54	0.75
79:Bi:713:GLN:HB3	79:Bi:716:ASN:ND2	2.01	0.75
80:Bi:1202:ATP:H5'1	80:Bi:1202:ATP:O2B	1.86	0.74
68:BX:28:ARG:HB3	68:BX:29:PRO:CD	2.17	0.74
6:AF:148:ILE:HD12	6:AF:148:ILE:O	1.87	0.74
53:BI:63:PRO:O	53:BI:65:PRO:HD3	1.87	0.73
59:BO:23:PRO:CG	59:BO:26:PHE:CG	2.70	0.73
45:BA:1755:A:H8	69:BY:63:GLN:OE1	1.71	0.73
68:BX:27:ILE:CG1	68:BX:61:ILE:HB	2.18	0.73
78:Bh:266:ASP:HB3	78:Bh:267:PRO:HD3	1.68	0.73
53:BI:64:VAL:N	53:BI:65:PRO:CD	2.50	0.73
34:Ah:48:ARG:CB	34:Ah:103:TYR:OH	2.36	0.73
45:BA:895:G:H1	45:BA:917:U:H3	1.37	0.73
1:AA:1257:C:H42	1:AA:1261:G:N2	1.87	0.73
69:BY:65:ASN:HB2	69:BY:116:ASP:OD2	1.88	0.73
45:BA:647:G:H1	45:BA:687:G:H22	1.36	0.72
65:BU:117:SER:HB3	65:BU:123:ARG:HB2	1.71	0.72
68:BX:30:SER:HG	68:BX:61:ILE:HG13	1.52	0.72
45:BA:848:C:N4	45:BA:849:C:N4	2.37	0.72
69:BY:63:GLN:HB2	69:BY:64:PRO:CD	2.15	0.72
6:AF:131:VAL:HA	6:AF:148:ILE:CG1	2.08	0.72
69:BY:62:LYS:NZ	69:BY:118:PRO:CB	2.49	0.72
7:AG:40:HIS:HD2	7:AG:42:ALA:H	1.38	0.71
72:Bb:12:LYS:HD3	72:Bb:16:GLY:H	1.54	0.71
45:BA:865:A:P	68:BX:28:ARG:HH22	2.09	0.71
1:AA:3267:A:H8	8:AH:69:PHE:CE2	2.07	0.71
45:BA:284:G:N7	52:BH:188:ARG:NH1	2.38	0.71
6:AF:151:VAL:CG1	6:AF:152:VAL:N	2.43	0.71
8:AH:43:LEU:HD13	34:Ah:103:TYR:CA	2.20	0.71
45:BA:868:G:H1	45:BA:960:U:H3	1.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Ah:103:TYR:N	34:Ah:104:PRO:CD	2.53	0.70
45:BA:1294:G:N2	45:BA:1303:U:O2	2.22	0.70
45:BA:1588:G:H1	45:BA:1608:U:H3	1.39	0.70
34:Ah:103:TYR:HD1	34:Ah:104:PRO:HD3	0.63	0.70
79:Bi:379:THR:HG23	79:Bi:381:PRO:HD2	1.73	0.70
1:AA:1603:A:H61	26:AZ:71:THR:HG21	1.55	0.70
1:AA:2138:A:HO2'	38:Al:2:GLY:N	1.88	0.70
6:AF:132:ALA:CA	6:AF:148:ILE:CD1	2.70	0.70
59:BO:23:PRO:C	59:BO:25:TRP:N	2.46	0.69
78:Bh:89:LEU:HB2	78:Bh:103:PHE:HB2	1.73	0.69
5:AE:16:PHE:HE1	5:AE:275:ARG:HH11	0.70	0.69
34:Ah:105:SER:O	34:Ah:107:ILE:N	2.26	0.69
38:Al:39:TYR:N	38:Al:40:PRO:HD2	2.08	0.69
46:BB:206:ASP:CB	46:BB:207:PRO:HD3	2.20	0.68
8:AH:43:LEU:HD12	34:Ah:103:TYR:HA	1.71	0.68
45:BA:864:U:O5'	68:BX:28:ARG:NH1	2.26	0.68
6:AF:131:VAL:C	6:AF:148:ILE:HG12	2.19	0.68
1:AA:2395:G:C4'	5:AE:258:ALA:HB1	2.23	0.68
80:Bi:1202:ATP:H5'1	80:Bi:1202:ATP:PB	2.32	0.68
68:BX:27:ILE:CD1	68:BX:61:ILE:HB	2.24	0.68
79:Bi:1034:SER:HB3	80:Bi:1202:ATP:H3'	1.76	0.68
6:AF:148:ILE:HD12	6:AF:148:ILE:C	2.18	0.68
45:BA:852:C:H6	45:BA:852:C:H5''	1.58	0.68
69:BY:65:ASN:HD22	69:BY:116:ASP:HB3	1.59	0.67
64:BT:78:HIS:O	79:Bi:448:ARG:NH2	2.28	0.67
52:BH:2:LYS:O	52:BH:108:VAL:HA	1.95	0.67
69:BY:63:GLN:NE2	69:BY:63:GLN:HA	2.08	0.67
45:BA:223:U:H3	45:BA:838:G:H1	1.40	0.67
26:AZ:50:ALA:HB1	36:Aj:66:VAL:HG11	1.77	0.66
34:Ah:103:TYR:N	34:Ah:104:PRO:HD2	2.10	0.66
1:AA:1481:A:O2'	1:AA:1858:A:N3	2.28	0.66
66:BV:80:GLU:OE1	75:Be:44:ARG:NH1	2.28	0.66
1:AA:2394:G:N3	5:AE:258:ALA:O	2.28	0.66
65:BU:28:LEU:HD13	65:BU:30:VAL:HG22	1.75	0.66
66:BV:20:ILE:HD11	66:BV:100:VAL:HG21	1.78	0.66
1:AA:2941:A:OP2	5:AE:256:HIS:HB2	1.96	0.66
1:AA:3267:A:H2'	8:AH:69:PHE:CE1	2.30	0.66
5:AE:17:LEU:HB3	5:AE:18:PRO:CD	2.26	0.65
8:AH:67:GLY:CA	8:AH:74:VAL:HB	2.23	0.65
45:BA:1339:C:O2'	45:BA:1341:A:N7	2.28	0.65
1:AA:804:C:OP1	6:AF:98:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:BC:88:VAL:HG11	47:BC:96:LEU:HD12	1.78	0.65
1:AA:2897:A:H2'	1:AA:2899:C:H5''	1.78	0.65
7:AG:50:ARG:NH1	7:AG:147:ASP:OD2	2.29	0.65
12:AL:53:VAL:HG22	12:AL:134:ILE:HG22	1.78	0.65
1:AA:1639:C:OP2	35:Ai:74:ARG:NH2	2.29	0.65
45:BA:522:U:H5''	70:BZ:37:LYS:HG3	1.78	0.65
4:AD:196:TRP:CB	4:AD:197:PRO:HD3	2.23	0.65
17:AQ:73:PHE:HB3	17:AQ:78:ARG:HE	1.61	0.65
68:BX:30:SER:OG	68:BX:61:ILE:CD1	2.45	0.65
45:BA:170:U:H3	45:BA:289:U:HO2'	1.44	0.64
34:Ah:48:ARG:HB2	34:Ah:103:TYR:CZ	2.32	0.64
47:BC:134:VAL:HB	47:BC:219:LYS:HB3	1.78	0.64
4:AD:196:TRP:CB	4:AD:197:PRO:CD	2.73	0.64
1:AA:1257:C:N4	1:AA:1261:G:H22	1.95	0.64
1:AA:2514:U:H5'	10:AJ:68:ARG:HG3	1.80	0.64
6:AF:151:VAL:HG13	6:AF:251:THR:C	2.23	0.64
51:BG:79:ASN:OD1	51:BG:83:ARG:NH1	2.30	0.64
1:AA:2395:G:C1'	5:AE:258:ALA:HB1	2.27	0.64
52:BH:57:ASP:HA	52:BH:106:LEU:HA	1.78	0.64
70:BZ:55:VAL:HG22	70:BZ:75:VAL:HG22	1.79	0.64
45:BA:852:C:H5''	45:BA:852:C:C6	2.33	0.64
47:BC:31:ASP:N	47:BC:31:ASP:OD1	2.31	0.64
1:AA:2875:U:H3	1:AA:2952:G:H1	1.45	0.64
35:Ai:20:ILE:HD12	35:Ai:32:ALA:HB1	1.80	0.64
1:AA:1940:G:H21	1:AA:3362:A:H8	1.44	0.64
74:Bd:36:THR:OG1	74:Bd:37:SER:N	2.31	0.64
45:BA:505:A:N1	45:BA:507:U:N3	2.45	0.63
52:BH:63:MET:SD	52:BH:98:ARG:NH2	2.71	0.63
5:AE:17:LEU:CD1	5:AE:262:TRP:HE3	2.00	0.63
4:AD:112:ILE:HD13	44:Ar:79:VAL:HG22	1.79	0.63
1:AA:2184:U:C6	4:AD:198:LYS:NZ	2.65	0.63
1:AA:2535:A:H61	1:AA:2544:U:H3	1.46	0.63
10:AJ:41:GLN:HE21	10:AJ:44:ARG:HH12	1.44	0.63
17:AQ:22:VAL:HG11	17:AQ:120:VAL:HG11	1.79	0.63
45:BA:1253:U:H3'	58:BN:46:ARG:HH22	1.64	0.63
78:Bh:232:TYR:OH	78:Bh:265:LEU:HD12	1.99	0.63
6:AF:151:VAL:CG1	6:AF:251:THR:C	2.71	0.63
30:Ad:14:ARG:HH22	30:Ad:18:ARG:HH11	1.46	0.63
24:AX:81:GLN:O	24:AX:98:ASN:ND2	2.32	0.63
1:AA:2534:G:H2'	1:AA:2535:A:H8	1.62	0.63
5:AE:16:PHE:HD1	5:AE:275:ARG:NH1	1.90	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:296:THR:HG22	5:AE:298:PHE:H	1.63	0.63
71:Ba:39:ALA:O	71:Ba:72:GLY:N	2.31	0.63
34:Ah:105:SER:C	34:Ah:107:ILE:N	2.57	0.63
45:BA:699:U:H3	45:BA:739:G:H1	1.45	0.63
58:BN:61:VAL:HB	58:BN:121:VAL:HG23	1.79	0.63
47:BC:32:ILE:HD11	47:BC:46:THR:HG23	1.81	0.62
53:BI:131:PHE:HB3	53:BI:132:PRO:HD3	1.79	0.62
1:AA:691:A:OP1	6:AF:46:LYS:NZ	2.31	0.62
55:BK:109:LEU:HB2	55:BK:146:PHE:HB3	1.81	0.62
60:BP:29:HIS:HB2	60:BP:41:ARG:HA	1.81	0.62
1:AA:1888:U:OP1	5:AE:247:ARG:NH1	2.31	0.62
46:BB:162:CYS:SG	46:BB:163:ASN:N	2.71	0.62
5:AE:213:GLU:HB3	5:AE:282:ILE:HD12	1.80	0.62
13:AM:47:GLN:HG2	13:AM:67:VAL:HG12	1.81	0.62
72:Bb:45:VAL:HG11	72:Bb:53:LEU:HD22	1.81	0.62
2:AB:44:C:OP2	13:AM:137:ARG:NH2	2.32	0.62
1:AA:2394:G:N2	5:AE:258:ALA:O	2.32	0.62
4:AD:19:HIS:HE1	4:AD:193:ARG:O	1.83	0.62
5:AE:112:ASP:O	5:AE:116:ARG:HB2	2.00	0.62
8:AH:55:LEU:HD11	8:AH:66:SER:HB3	1.82	0.62
34:Ah:103:TYR:CD1	34:Ah:104:PRO:CD	2.44	0.62
1:AA:2395:G:H4'	5:AE:258:ALA:CB	2.30	0.62
61:BQ:103:ASN:ND2	61:BQ:120:SER:OG	2.33	0.61
69:BY:62:LYS:NZ	69:BY:62:LYS:HB2	2.13	0.61
77:Bg:109:ASP:HB2	77:Bg:113:LYS:HG3	1.82	0.61
18:AR:43:LYS:HA	18:AR:46:LYS:HE2	1.82	0.61
34:Ah:105:SER:OG	34:Ah:107:ILE:CD1	2.47	0.61
47:BC:168:ILE:HG12	47:BC:197:ILE:HD12	1.82	0.61
58:BN:103:LEU:HD11	58:BN:116:VAL:H	1.65	0.61
1:AA:283:G:OP1	43:Aq:45:ARG:NH1	2.31	0.61
1:AA:3267:A:OP2	8:AH:69:PHE:CE2	2.50	0.61
10:AJ:162:LEU:HA	16:AP:7:LEU:HD11	1.81	0.61
45:BA:385:A:H5''	54:BJ:22:ARG:HB3	1.81	0.61
58:BN:36:LEU:HD11	58:BN:102:GLY:HA2	1.82	0.61
1:AA:2895:G:O2'	41:Ao:100:TYR:O	2.18	0.61
1:AA:3138:U:O2'	5:AE:18:PRO:HB2	2.00	0.61
45:BA:1500:C:OP1	65:BU:122:ARG:NH2	2.33	0.61
62:BR:95:LYS:O	78:Bh:59:ARG:NH2	2.33	0.61
79:Bi:610:LYS:HE2	80:Bi:1202:ATP:O2G	2.00	0.61
79:Bi:413:ASN:O	79:Bi:417:LEU:HB2	1.99	0.61
79:Bi:713:GLN:NE2	79:Bi:1061:ASN:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AJ:246:MET:HG3	10:AJ:249:ARG:HH21	1.64	0.61
51:BG:37:GLN:HB3	62:BR:53:LEU:HD13	1.82	0.61
58:BN:73:LYS:NZ	77:Bg:109:ASP:O	2.34	0.61
79:Bi:236:ILE:HG21	79:Bi:286:ALA:HB2	1.83	0.61
6:AF:300:ARG:O	19:AS:39:ARG:NH2	2.34	0.61
6:AF:283:THR:HG22	6:AF:285:ASP:H	1.65	0.61
45:BA:1594:G:OP2	45:BA:1596:C:N4	2.34	0.61
79:Bi:713:GLN:HG3	79:Bi:1062:TYR:HB3	1.83	0.61
1:AA:860:G:OP1	44:Ar:17:ARG:NH1	2.33	0.61
1:AA:1201:C:H42	1:AA:2857:C:H5''	1.65	0.61
73:Bc:36:LYS:HB3	73:Bc:43:ILE:HG22	1.82	0.61
1:AA:965:A:H5''	14:AN:4:SER:HB3	1.82	0.60
5:AE:19:ARG:HD2	5:AE:273:HIS:NE2	2.16	0.60
50:BF:176:ASP:HB2	50:BF:179:LYS:HD2	1.83	0.60
3:AC:104:A:O3'	38:Al:42:ALA:HB2	2.00	0.60
6:AF:132:ALA:HA	6:AF:148:ILE:CD1	2.32	0.60
45:BA:1552:U:OP2	61:BQ:43:ARG:NH2	2.34	0.60
7:AG:294:ALA:HB2	12:AL:210:ILE:HD13	1.82	0.60
52:BH:159:ARG:HG2	52:BH:172:ALA:HB2	1.83	0.60
54:BJ:57:ALA:HB2	54:BJ:177:GLY:HA2	1.83	0.60
1:AA:1390:A:N6	1:AA:1418:A:O2'	2.35	0.60
28:Ab:17:ARG:NH2	28:Ab:18:TYR:OH	2.34	0.60
28:Ab:53:VAL:HG21	28:Ab:62:VAL:HG23	1.83	0.60
47:BC:109:LYS:HE3	47:BC:113:MET:HE2	1.84	0.60
50:BF:87:MET:HE1	50:BF:236:ILE:HD13	1.82	0.60
1:AA:1264:G:N2	1:AA:1265:U:O4	2.35	0.60
1:AA:2821:C:H42	1:AA:2869:U:H3	1.49	0.60
3:AC:104:A:H4'	38:Al:42:ALA:CB	2.30	0.60
4:AD:186:PHE:CD1	4:AD:196:TRP:CE3	2.86	0.60
45:BA:149:C:O2'	52:BH:132:ARG:NH1	2.34	0.60
1:AA:2395:G:H4'	5:AE:258:ALA:HB2	1.83	0.60
50:BF:129:VAL:HG12	50:BF:139:VAL:HG12	1.83	0.60
9:AI:189:ILE:HG23	9:AI:190:THR:HG23	1.83	0.60
51:BG:57:SER:HA	51:BG:59:VAL:H	1.66	0.60
1:AA:937:G:N2	1:AA:961:C:OP1	2.35	0.60
1:AA:1374:G:O6	29:Ac:10:LYS:NZ	2.34	0.60
6:AF:325:LEU:O	9:AI:41:ARG:NH2	2.34	0.60
79:Bi:581:TYR:HE2	79:Bi:612:THR:CB	2.13	0.60
68:BX:27:ILE:HD11	68:BX:61:ILE:CB	2.31	0.60
1:AA:1233:G:H1	1:AA:1255:C:H42	1.50	0.59
1:AA:3275:U:O2'	34:Ah:99:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AQ:72:HIS:O	17:AQ:74:ARG:NH1	2.34	0.59
49:BE:170:THR:HG22	49:BE:187:LYS:HG2	1.84	0.59
6:AF:302:ALA:HA	19:AS:39:ARG:HH12	1.67	0.59
6:AF:361:HIS:O	21:AU:28:ARG:NH2	2.35	0.59
12:AL:21:ARG:O	12:AL:24:ARG:NH1	2.35	0.59
45:BA:1682:U:O4	45:BA:1720:G:N2	2.35	0.59
14:AN:57:VAL:HG23	14:AN:115:ARG:HD2	1.83	0.59
45:BA:207:U:O2	54:BJ:178:ARG:NH1	2.33	0.59
7:AG:75:LEU:O	7:AG:112:LYS:NZ	2.35	0.59
8:AH:68:PRO:HB2	8:AH:71:VAL:HB	1.84	0.59
11:AK:47:LYS:HA	11:AK:53:ILE:HG12	1.84	0.59
66:BV:104:THR:HG22	66:BV:116:VAL:HG21	1.83	0.59
1:AA:1147:G:OP1	33:Ag:47:ARG:NH1	2.36	0.59
1:AA:1682:U:O4	23:AW:90:ARG:NH1	2.35	0.59
46:BB:35:PRO:O	46:BB:52:LYS:NZ	2.34	0.59
61:BQ:98:ASN:ND2	61:BQ:121:ILE:O	2.35	0.59
60:BP:88:GLY:O	60:BP:92:LYS:NZ	2.36	0.59
78:Bh:248:ASN:ND2	78:Bh:297:ASP:O	2.36	0.59
1:AA:1813:A:O2'	1:AA:1816:A:N3	2.36	0.59
3:AC:110:C:C4	38:Al:39:TYR:OH	2.55	0.59
19:AS:170:ARG:NH1	29:Ac:56:VAL:O	2.36	0.59
69:BY:68:ILE:O	69:BY:70:LYS:NZ	2.36	0.59
1:AA:1724:U:O4	20:AT:125:LYS:NZ	2.36	0.59
6:AF:334:PHE:HA	6:AF:339:LEU:HD12	1.84	0.59
17:AQ:61:ALA:HA	17:AQ:70:PRO:HD2	1.83	0.59
54:BJ:12:SER:HB3	54:BJ:18:ARG:HE	1.67	0.59
66:BV:53:LYS:HB3	66:BV:92:ASP:HB2	1.85	0.59
31:Ae:99:ASP:N	31:Ae:99:ASP:OD1	2.33	0.59
54:BJ:7:SER:O	54:BJ:18:ARG:NH1	2.35	0.59
78:Bh:273:ASP:OD2	78:Bh:275:ARG:NH2	2.36	0.59
1:AA:76:G:O2'	14:AN:100:ARG:NH1	2.35	0.58
1:AA:1235:U:H4'	1:AA:1236:G:H5'	1.85	0.58
1:AA:2137:U:OP2	1:AA:2142:A:N6	2.31	0.58
1:AA:801:A:H61	14:AN:19:GLN:HE22	1.51	0.58
6:AF:148:ILE:CB	6:AF:149:PRO:HD3	2.29	0.58
1:AA:831:G:O2'	1:AA:1864:A:N3	2.34	0.58
1:AA:1408:G:OP1	33:Ag:33:ARG:NH2	2.36	0.58
45:BA:772:G:OP1	50:BF:22:LYS:NZ	2.36	0.58
1:AA:2836:C:H5	1:AA:2852:C:H42	1.52	0.58
4:AD:186:PHE:HD1	4:AD:196:TRP:CE3	2.14	0.58
20:AT:21:LYS:HE3	20:AT:55:VAL:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:854:U:OP2	45:BA:854:U:H6	1.87	0.58
1:AA:3092:C:O2'	1:AA:3094:A:OP2	2.20	0.58
68:BX:112:ASP:N	68:BX:112:ASP:OD1	2.31	0.58
1:AA:1245:A:N6	1:AA:1272:C:O2'	2.37	0.58
1:AA:714:G:HO2'	1:AA:753:C:HO2'	1.50	0.58
14:AN:46:ILE:HG22	14:AN:49:ARG:HB2	1.84	0.58
35:AI:87:GLU:OE2	35:AI:91:ARG:NH1	2.36	0.58
45:BA:195:G:O6	54:BJ:141:ARG:NH1	2.36	0.58
45:BA:399:A:OP1	54:BJ:49:ARG:NH2	2.36	0.58
49:BE:42:THR:HG22	66:BV:108:ILE:HG21	1.84	0.58
76:Bf:39:LEU:HD13	76:Bf:43:ARG:HH21	1.69	0.58
1:AA:3242:G:N2	1:AA:3245:A:OP2	2.37	0.58
32:Af:23:VAL:O	32:Af:28:ARG:NH1	2.35	0.58
45:BA:454:U:H5'	50:BF:66:MET:HE3	1.85	0.58
45:BA:639:U:OP1	53:BI:112:ARG:NH2	2.37	0.58
45:BA:1537:C:O2'	45:BA:1540:G:O6	2.20	0.58
63:BS:26:LEU:HD21	63:BS:62:GLN:HG3	1.85	0.58
79:Bi:155:THR:HA	79:Bi:158:LYS:HD2	1.85	0.58
57:BM:73:GLY:HA3	57:BM:86:ILE:HD12	1.86	0.58
58:BN:136:ILE:HA	58:BN:139:HIS:HB3	1.86	0.58
7:AG:218:ARG:NH1	7:AG:221:GLU:OE1	2.37	0.58
13:AM:113:GLY:N	79:Bi:1003:TYR:CE1	2.64	0.58
21:AU:99:ARG:NH1	21:AU:126:VAL:O	2.37	0.58
78:Bh:267:PRO:HG2	78:Bh:269:TYR:HD1	1.68	0.58
1:AA:1257:C:N4	1:AA:1261:G:N2	2.51	0.57
38:Al:34:CYS:HB3	38:Al:38:GLY:CA	2.33	0.57
45:BA:158:U:O2'	45:BA:160:C:OP2	2.21	0.57
21:AU:57:GLU:OE2	22:AV:139:ARG:NH2	2.37	0.57
45:BA:322:G:O2'	54:BJ:10:LYS:NZ	2.37	0.57
45:BA:865:A:OP1	68:BX:28:ARG:CZ	2.46	0.57
45:BA:1535:U:O2'	45:BA:1536:G:N3	2.37	0.57
51:BG:156:ARG:NH1	60:BP:53:ASP:OD1	2.37	0.57
1:AA:3319:U:O4	5:AE:167:ARG:NH1	2.38	0.57
9:AI:88:ARG:HA	9:AI:134:VAL:HG12	1.86	0.57
78:Bh:126:SER:OG	78:Bh:127:ARG:N	2.34	0.57
14:AN:61:PRO:HB2	14:AN:62:THR:HG23	1.86	0.57
20:AT:103:ARG:NH1	20:AT:124:TYR:OH	2.37	0.57
72:Bb:44:ILE:HD11	72:Bb:65:PRO:HG2	1.87	0.57
1:AA:718:G:OP1	29:Ac:117:ARG:NH2	2.37	0.57
50:BF:11:ARG:NH2	50:BF:21:ASP:O	2.38	0.57
74:Bd:64:ARG:NH1	74:Bd:64:ARG:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:Bi:537:GLY:O	79:Bi:542:ARG:NH1	2.37	0.57
79:Bi:672:GLU:HG2	79:Bi:681:ARG:HH12	1.70	0.57
2:AB:17:A:OP1	7:AG:2:ALA:N	2.38	0.57
10:Aj:163:VAL:HA	10:Aj:166:LEU:HD23	1.86	0.57
10:Aj:240:ASN:HA	10:Aj:243:GLN:HB2	1.87	0.57
45:BA:610:G:HO2'	45:BA:613:G:HO2'	1.53	0.57
79:Bi:596:LYS:NZ	79:Bi:707:ASP:OD1	2.37	0.57
1:AA:837:A:OP2	44:Ar:4:ARG:NH1	2.36	0.57
18:AR:111:LYS:HG2	18:AR:153:LYS:HE3	1.87	0.57
49:BE:75:LYS:NZ	56:BL:14:TYR:OH	2.31	0.57
1:AA:370:U:H4'	1:AA:404:G:H5'	1.86	0.57
7:AG:34:LYS:HA	22:AV:27:LEU:HD11	1.87	0.57
11:AK:90:MET:HB2	11:AK:144:ILE:HG22	1.87	0.57
45:BA:741:C:O2	53:BI:107:ARG:NH1	2.36	0.57
72:Bb:52:ASP:OD2	74:Bd:38:ARG:NH1	2.38	0.57
78:Bh:266:ASP:CB	78:Bh:267:PRO:CD	2.81	0.57
5:AE:386:ASP:HB3	5:AE:387:LEU:HD12	1.86	0.57
45:BA:479:C:H4'	55:BK:120:LYS:HE2	1.86	0.57
52:BH:163:THR:HG22	52:BH:168:THR:HG22	1.86	0.57
70:BZ:57:VAL:HB	70:BZ:60:PHE:HE2	1.70	0.57
36:Aj:9:LEU:HB3	36:Aj:17:LEU:HD21	1.87	0.56
38:Al:34:CYS:HB3	38:Al:38:GLY:HA2	1.87	0.56
45:BA:1294:G:O6	45:BA:1303:U:O4	2.23	0.56
79:Bi:145:LEU:HD13	79:Bi:187:VAL:HG11	1.87	0.56
5:AE:31:ALA:O	5:AE:339:ARG:NH1	2.37	0.56
7:AG:146:LEU:HD22	7:AG:163:LEU:HD13	1.86	0.56
19:AS:152:HIS:ND1	19:AS:162:ALA:O	2.38	0.56
79:Bi:390:LEU:HD12	79:Bi:407:THR:HG23	1.87	0.56
1:AA:269:G:OP2	16:AP:44:ARG:NH1	2.37	0.56
1:AA:815:G:OP2	38:Al:31:LYS:NZ	2.33	0.56
1:AA:1481:A:N6	1:AA:1872:C:O2	2.38	0.56
5:AE:292:ALA:HB2	5:AE:302:LYS:HG3	1.87	0.56
59:BO:23:PRO:CG	59:BO:26:PHE:HB3	2.10	0.56
77:Bg:108:VAL:HG12	77:Bg:114:VAL:HG12	1.87	0.56
79:Bi:610:LYS:CE	80:Bi:1202:ATP:O2G	2.54	0.56
1:AA:2181:C:H5''	4:AD:193:ARG:CZ	2.35	0.56
1:AA:2340:U:OP1	5:AE:236:LYS:NZ	2.37	0.56
4:AD:6:ARG:CZ	4:AD:198:LYS:HG3	2.36	0.56
45:BA:1542:G:N2	45:BA:1569:A:OP2	2.38	0.56
65:BU:115:GLU:OE2	65:BU:123:ARG:NH1	2.39	0.56
79:Bi:674:VAL:O	79:Bi:695:LYS:NZ	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:169:A:OP1	52:BH:137:ARG:NH2	2.38	0.56
50:BF:100:ARG:NH2	50:BF:121:TYR:O	2.38	0.56
52:BH:139:ASN:OD1	52:BH:142:ARG:NH1	2.38	0.56
53:BI:63:PRO:O	53:BI:64:VAL:HB	2.05	0.56
54:BJ:116:HIS:O	54:BJ:146:ARG:NH1	2.39	0.56
71:Ba:88:ILE:HG22	71:Ba:89:ILE:HG23	1.87	0.56
79:Bi:348:ARG:HH22	79:Bi:351:LEU:HD13	1.70	0.56
1:AA:799:G:O2'	14:AN:18:TRP:NE1	2.35	0.56
45:BA:1202:A:N6	45:BA:1457:C:OP1	2.33	0.56
46:BB:119:ARG:NH1	48:BD:241:ASP:OD1	2.38	0.56
61:BQ:53:PRO:HB2	61:BQ:57:MET:HG2	1.87	0.56
79:Bi:841:ARG:NH2	79:Bi:1078:TRP:O	2.38	0.56
1:AA:2631:U:OP2	22:AV:4:SER:OG	2.24	0.56
22:AV:120:LYS:HA	22:AV:124:VAL:HG22	1.88	0.56
49:BE:44:THR:OG1	49:BE:45:LYS:NZ	2.39	0.56
55:BK:123:HIS:HD2	76:Bf:33:ARG:HE	1.54	0.56
79:Bi:634:CYS:SG	79:Bi:704:GLN:NE2	2.79	0.56
79:Bi:814:MET:O	79:Bi:833:SER:HA	2.06	0.56
79:Bi:906:GLN:OE1	79:Bi:911:ARG:NH2	2.39	0.56
46:BB:185:ARG:H	67:BW:44:ARG:HA	1.70	0.56
47:BC:123:ALA:HB2	47:BC:165:ARG:HG2	1.87	0.56
80:Bi:1202:ATP:PB	80:Bi:1202:ATP:C5'	2.94	0.56
26:AZ:90:ALA:O	26:AZ:120:LYS:NZ	2.39	0.56
47:BC:131:ASP:HB3	47:BC:180:THR:HG21	1.88	0.56
55:BK:49:LEU:O	55:BK:53:ARG:HB2	2.06	0.56
65:BU:37:VAL:HG11	65:BU:100:ILE:HD11	1.86	0.56
65:BU:118:PRO:HD2	65:BU:123:ARG:HH21	1.71	0.56
1:AA:945:C:OP1	33:Ag:36:LYS:NZ	2.39	0.56
1:AA:2395:G:C4'	5:AE:258:ALA:CB	2.84	0.56
6:AF:132:ALA:N	6:AF:148:ILE:CD1	2.69	0.56
62:BR:50:GLU:OE2	62:BR:82:ARG:NH2	2.39	0.56
74:Bd:26:THR:HB	74:Bd:44:VAL:HG22	1.88	0.56
79:Bi:841:ARG:HH11	79:Bi:1082:VAL:HG22	1.70	0.56
1:AA:938:C:OP2	29:Ac:26:ARG:NH1	2.39	0.55
1:AA:2940:A:O2'	5:AE:256:HIS:O	2.18	0.55
6:AF:151:VAL:HA	6:AF:250:TRP:O	2.05	0.55
32:Af:77:ARG:HD2	32:Af:89:LEU:HD13	1.88	0.55
34:Ah:48:ARG:HB2	34:Ah:103:TYR:CE1	2.41	0.55
44:Ar:46:THR:OG1	44:Ar:57:CYS:SG	2.63	0.55
1:AA:1364:C:H5''	19:AS:3:ILE:HD13	1.87	0.55
1:AA:2878:G:H5''	5:AE:5:LYS:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AH:67:GLY:O	8:AH:74:VAL:C	2.45	0.55
28:Ab:68:ILE:O	28:Ab:115:LYS:NZ	2.34	0.55
32:Af:55:LEU:HB2	32:Af:95:PRO:HD3	1.88	0.55
53:BI:14:THR:HG22	53:BI:17:GLU:OE1	2.06	0.55
1:AA:177:U:O2	1:AA:241:G:O6	2.24	0.55
1:AA:3040:A:H5''	24:AX:12:ARG:HB2	1.86	0.55
2:AB:6:C:O2'	7:AG:50:ARG:NH2	2.39	0.55
2:AB:39:C:H4'	13:AM:44:THR:HG23	1.88	0.55
34:Ah:103:TYR:H	34:Ah:104:PRO:CD	2.19	0.55
68:BX:53:ILE:HD11	73:Bc:25:VAL:HG23	1.88	0.55
4:AD:126:LEU:HD13	4:AD:150:LEU:HD21	1.89	0.55
5:AE:255:TRP:O	5:AE:255:TRP:HD1	1.90	0.55
6:AF:151:VAL:C	6:AF:250:TRP:O	2.49	0.55
45:BA:1096:C:OP2	68:BX:71:LYS:NZ	2.32	0.55
1:AA:353:G:O6	38:Al:55:ARG:NH2	2.40	0.55
78:Bh:258:THR:O	78:Bh:275:ARG:NH1	2.38	0.55
1:AA:1738:C:H1'	35:Ai:52:GLN:HE21	1.71	0.55
79:Bi:671:LEU:HB2	79:Bi:681:ARG:HH11	1.72	0.55
1:AA:68:C:OP2	1:AA:301:G:N2	2.40	0.55
1:AA:120:G:N2	10:AJ:126:SER:O	2.39	0.55
1:AA:2572:C:O2'	1:AA:2573:G:O4'	2.25	0.55
4:AD:116:VAL:HG13	4:AD:126:LEU:HB2	1.89	0.55
16:AP:15:GLN:HB3	37:Ak:52:PRO:HD2	1.87	0.55
47:BC:57:ALA:O	47:BC:62:LYS:NZ	2.40	0.55
69:BY:65:ASN:CB	69:BY:116:ASP:OD2	2.55	0.55
1:AA:1591:G:OP1	35:Ai:16:ARG:NH1	2.40	0.55
1:AA:3267:A:H2'	8:AH:69:PHE:HZ	1.62	0.55
7:AG:106:ALA:O	7:AG:110:LEU:HB2	2.07	0.55
10:AJ:238:LEU:HB2	10:AJ:243:GLN:HE21	1.70	0.55
24:AX:18:PRO:HA	24:AX:51:ALA:HA	1.87	0.55
45:BA:646:C:H2'	45:BA:647:G:C8	2.42	0.55
45:BA:788:A:OP2	50:BF:108:ARG:NH1	2.39	0.55
45:BA:1534:G:OP2	64:BT:57:ARG:NH2	2.39	0.55
63:BS:5:ARG:O	63:BS:10:LYS:NZ	2.38	0.55
78:Bh:122:ILE:HD11	78:Bh:136:ILE:HD12	1.89	0.55
5:AE:284:ARG:NH1	5:AE:293:ASN:O	2.39	0.55
45:BA:848:C:O2'	45:BA:849:C:H5''	2.07	0.55
47:BC:128:LYS:HE3	47:BC:132:ASP:HB3	1.88	0.55
1:AA:3198:U:H1'	11:AK:21:LYS:HB2	1.90	0.54
7:AG:50:ARG:NH2	7:AG:72:ASP:OD2	2.40	0.54
8:AH:55:LEU:HD11	8:AH:66:SER:CB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AW:61:THR:HG23	23:AW:62:VAL:HG23	1.89	0.54
45:BA:646:C:H2'	45:BA:647:G:H8	1.72	0.54
45:BA:1082:C:H1'	67:BW:62:ARG:HH21	1.72	0.54
45:BA:1383:G:H1'	66:BV:57:ARG:HH11	1.73	0.54
57:BM:124:THR:HB	57:BM:141:LYS:HB3	1.88	0.54
63:BS:14:LYS:NZ	63:BS:18:GLU:OE2	2.40	0.54
79:Bi:856:ILE:HG21	79:Bi:1085:ILE:HD11	1.88	0.54
3:AC:29:U:H5''	14:AN:27:ASP:HB3	1.90	0.54
21:AU:8:GLN:HB3	21:AU:64:ILE:HD11	1.88	0.54
35:Ai:29:ILE:HD11	35:Ai:31:ARG:HH21	1.71	0.54
45:BA:959:U:H5''	59:BO:14:SER:HB3	1.88	0.54
49:BE:172:THR:O	49:BE:173:ARG:NH1	2.39	0.54
53:BI:165:LYS:O	53:BI:168:SER:HB2	2.07	0.54
79:Bi:348:ARG:HH12	79:Bi:351:LEU:HD22	1.72	0.54
1:AA:2842:U:OP1	1:AA:2844:C:N4	2.39	0.54
6:AF:132:ALA:N	6:AF:148:ILE:HD13	2.22	0.54
8:AH:82:ARG:O	34:Ah:103:TYR:C	2.51	0.54
68:BX:53:ILE:HG23	68:BX:60:LYS:HB2	1.90	0.54
72:Bb:38:ARG:HH21	72:Bb:83:ILE:HG21	1.72	0.54
1:AA:126:U:OP1	16:AP:144:ARG:NH1	2.40	0.54
1:AA:1778:G:O2'	1:AA:1780:G:OP2	2.26	0.54
3:AC:71:A:O2'	27:Aa:52:ARG:NH2	2.41	0.54
5:AE:168:LYS:O	5:AE:319:ASN:ND2	2.39	0.54
72:Bb:3:LYS:NZ	72:Bb:8:ASN:OD1	2.40	0.54
78:Bh:4:ASN:OD1	78:Bh:4:ASN:N	2.38	0.54
79:Bi:161:ILE:HD12	79:Bi:164:ILE:HB	1.90	0.54
1:AA:791:A:OP1	6:AF:108:LYS:NZ	2.38	0.54
2:AB:53:U:O2'	2:AB:55:A:N7	2.40	0.54
18:AR:172:GLN:NE2	34:Ah:60:ARG:O	2.36	0.54
63:BS:24:LEU:HB3	63:BS:58:MET:HE3	1.90	0.54
13:AM:13:LYS:HD3	13:AM:134:PRO:HD3	1.89	0.54
15:AO:108:ARG:NH2	17:AQ:196:ALA:O	2.41	0.54
20:AT:39:ASN:OD1	20:AT:42:ARG:NH1	2.41	0.54
23:AW:19:VAL:HG12	23:AW:105:LEU:HD22	1.89	0.54
45:BA:161:U:O4	70:BZ:124:ARG:NH2	2.40	0.54
58:BN:74:LEU:HA	77:Bg:108:VAL:HG11	1.90	0.54
79:Bi:540:SER:O	79:Bi:544:PHE:CE2	2.60	0.54
79:Bi:649:LEU:HD21	79:Bi:688:LEU:HD21	1.90	0.54
1:AA:2374:C:N4	1:AA:2941:A:O4'	2.41	0.54
3:AC:126:A:O2'	3:AC:129:C:N4	2.40	0.54
7:AG:80:SER:O	7:AG:83:LEU:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AO:125:LYS:HG2	15:AO:128:ARG:HH21	1.71	0.54
42:Ap:7:LYS:NZ	45:BA:1774:G:OP1	2.31	0.54
52:BH:85:ARG:O	52:BH:87:ARG:NH1	2.41	0.54
61:BQ:15:HIS:HB3	61:BQ:22:LEU:HD12	1.89	0.54
5:AE:57:VAL:HG22	5:AE:73:VAL:HG12	1.89	0.54
17:AQ:27:LEU:HD21	17:AQ:102:LEU:HB2	1.89	0.54
45:BA:992:A:H2	45:BA:1012:U:H3	1.56	0.54
45:BA:1227:A:H4'	45:BA:1228:G:H5''	1.89	0.54
55:BK:139:GLN:HE22	70:BZ:63:GLN:HG3	1.73	0.54
73:Bc:18:LYS:O	73:Bc:29:ARG:NH2	2.41	0.54
79:Bi:744:ASP:OD1	79:Bi:744:ASP:N	2.37	0.54
1:AA:177:U:O2	1:AA:241:G:C6	2.60	0.54
6:AF:293:SER:HA	6:AF:296:GLN:HB2	1.90	0.54
10:AJ:72:PRO:HG3	16:AP:18:VAL:HA	1.88	0.54
45:BA:321:C:N4	45:BA:1667:A:OP1	2.41	0.54
45:BA:1280:C:OP1	75:Be:44:ARG:NH2	2.40	0.54
45:BA:1754:A:OP2	69:BY:62:LYS:HD2	2.07	0.54
50:BF:19:LEU:HD11	50:BF:108:ARG:HD2	1.90	0.54
51:BG:63:GLN:HE22	51:BG:66:GLN:HB2	1.73	0.54
79:Bi:404:LEU:HD23	79:Bi:438:VAL:HG13	1.90	0.54
79:Bi:649:LEU:HG	79:Bi:681:ARG:HA	1.89	0.54
79:Bi:881:ILE:HD13	79:Bi:1043:ILE:HG12	1.89	0.54
1:AA:198:A:N3	1:AA:218:G:O2'	2.39	0.54
1:AA:744:A:OP1	19:AS:66:ARG:NH2	2.40	0.54
1:AA:2284:C:N4	1:AA:2308:C:OP2	2.41	0.54
1:AA:3067:C:H3'	20:AT:62:ARG:HH12	1.73	0.54
51:BG:76:ARG:NH1	62:BR:121:SER:OG	2.41	0.54
55:BK:105:LEU:HD12	55:BK:108:ARG:HD2	1.90	0.54
69:BY:125:VAL:HG12	69:BY:126:LYS:HG3	1.90	0.54
1:AA:284:A:OP2	43:Aq:41:ARG:NH1	2.39	0.53
1:AA:847:A:OP1	59:BO:140:LYS:CE	2.48	0.53
5:AE:17:LEU:N	5:AE:18:PRO:HD2	2.23	0.53
16:AP:163:GLY:O	16:AP:172:ARG:NH1	2.40	0.53
53:BI:113:PRO:HG2	53:BI:116:ARG:HD3	1.88	0.53
66:BV:50:LEU:HD23	66:BV:93:LEU:HB3	1.90	0.53
1:AA:190:U:OP2	27:Aa:40:ARG:NH2	2.40	0.53
5:AE:188:ILE:HD13	5:AE:191:LYS:HD2	1.89	0.53
8:AH:51:ARG:HB3	8:AH:159:LEU:HD23	1.89	0.53
9:AI:156:ILE:HD12	9:AI:161:VAL:HB	1.90	0.53
45:BA:563:U:H4'	76:Bf:17:GLN:HE21	1.73	0.53
68:BX:28:ARG:CB	68:BX:29:PRO:CD	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:BY:65:ASN:HD22	69:BY:116:ASP:CB	2.21	0.53
1:AA:2162:U:OP1	4:AD:234:LYS:NZ	2.41	0.53
1:AA:3151:U:OP1	5:AE:128:LYS:NZ	2.40	0.53
16:AP:140:LYS:NZ	36:Aj:96:GLU:OE2	2.41	0.53
24:AX:14:SER:O	24:AX:81:GLN:NE2	2.38	0.53
24:AX:34:LEU:HD21	24:AX:102:ILE:HG22	1.91	0.53
13:AM:53:THR:HG22	13:AM:61:ARG:H	1.73	0.53
17:AQ:124:LEU:HG	21:AU:168:PRO:HG3	1.91	0.53
45:BA:1483:A:OP2	45:BA:1521:G:N2	2.37	0.53
45:BA:1797:A:OP2	72:Bb:10:ARG:NE	2.39	0.53
49:BE:40:ARG:HG2	66:BV:110:PRO:HB3	1.90	0.53
64:BT:94:ASP:OD2	64:BT:98:TYR:OH	2.27	0.53
1:AA:2395:G:H5''	5:AE:255:TRP:CD1	2.44	0.53
46:BB:59:LEU:HD22	67:BW:79:LEU:HD11	1.90	0.53
53:BI:82:GLU:HG3	53:BI:90:VAL:HG22	1.90	0.53
1:AA:98:G:N7	14:AN:13:HIS:NE2	2.56	0.53
1:AA:363:G:OP2	38:Al:56:ARG:NH2	2.37	0.53
1:AA:643:U:O2'	1:AA:1153:A:N1	2.40	0.53
3:AC:110:C:N4	38:Al:39:TYR:OH	2.42	0.53
8:AH:52:VAL:HG11	8:AH:65:ILE:HD12	1.89	0.53
79:Bi:844:CYS:HB2	79:Bi:1085:ILE:HG13	1.90	0.53
27:Aa:48:LEU:HD13	27:Aa:115:ARG:HH21	1.73	0.53
34:Ah:19:SER:OG	34:Ah:20:LYS:N	2.41	0.53
78:Bh:178:VAL:HB	78:Bh:192:PHE:HB2	1.91	0.53
38:Al:72:ARG:O	38:Al:76:ASN:ND2	2.42	0.53
45:BA:931:C:OP2	72:Bb:70:LYS:NZ	2.39	0.53
45:BA:1236:A:O2'	77:Bg:138:ARG:NH2	2.42	0.53
45:BA:1294:G:N3	45:BA:1322:A:N6	2.56	0.53
49:BE:56:GLN:HB2	49:BE:90:ARG:HH12	1.73	0.53
1:AA:2969:A:N7	4:AD:215:ASN:ND2	2.57	0.53
9:AI:86:VAL:O	9:AI:114:GLY:HA2	2.09	0.53
13:AM:78:GLU:CD	79:Bi:800:ILE:HG21	2.33	0.53
27:Aa:102:SER:OG	27:Aa:103:LYS:NZ	2.42	0.53
45:BA:1595:U:H3	45:BA:1600:A:H2	1.57	0.53
51:BG:58:LEU:HD22	51:BG:168:VAL:HG23	1.90	0.53
54:BJ:76:THR:HB	54:BJ:105:ASP:HB2	1.91	0.53
63:BS:26:LEU:HD23	63:BS:58:MET:HB3	1.90	0.53
66:BV:30:LYS:HD3	66:BV:33:GLN:HE21	1.74	0.53
1:AA:2769:A:OP1	43:Aq:71:ARG:NH2	2.42	0.53
14:AN:157:ARG:NH1	29:Ac:146:GLU:OE2	2.42	0.53
45:BA:864:U:C3'	68:BX:28:ARG:HH12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:1164:G:H2'	45:BA:1165:G:H8	1.74	0.53
51:BG:92:ARG:NH2	51:BG:169:ASN:OD1	2.30	0.53
62:BR:82:ARG:HH22	62:BR:114:ARG:HB2	1.73	0.53
79:Bi:363:PRO:O	79:Bi:403:GLN:NE2	2.41	0.53
1:AA:1244:A:N6	1:AA:1271:A:OP2	2.41	0.52
1:AA:2424:A:OP1	16:AP:90:ASN:ND2	2.39	0.52
6:AF:132:ALA:HA	6:AF:148:ILE:HD11	1.90	0.52
45:BA:903:U:H5''	60:BP:135:ARG:HH21	1.74	0.52
66:BV:37:VAL:HG13	66:BV:107:THR:HB	1.91	0.52
70:BZ:2:SER:HA	70:BZ:32:ARG:HD2	1.91	0.52
79:Bi:358:ASP:N	79:Bi:358:ASP:OD1	2.42	0.52
1:AA:596:C:OP2	9:AI:34:LYS:NZ	2.39	0.52
1:AA:1912:U:N3	1:AA:2122:G:OP2	2.38	0.52
6:AF:3:ARG:NH1	6:AF:27:SER:OG	2.41	0.52
10:AJ:227:ASP:OD1	10:AJ:227:ASP:N	2.42	0.52
45:BA:95:G:HO2'	45:BA:460:A:HO2'	1.58	0.52
45:BA:563:U:O2'	45:BA:566:C:N3	2.43	0.52
45:BA:1278:G:OP1	49:BE:185:LYS:NZ	2.42	0.52
45:BA:1523:G:N7	65:BU:68:ARG:NH1	2.56	0.52
69:BY:141:GLU:OE1	69:BY:144:ARG:NH1	2.40	0.52
43:Aq:17:CYS:SG	43:Aq:77:CYS:N	2.82	0.52
45:BA:1600:A:O2'	45:BA:1602:C:N4	2.42	0.52
49:BE:99:VAL:HG13	49:BE:173:ARG:HH21	1.74	0.52
55:BK:139:GLN:NE2	70:BZ:64:PHE:O	2.42	0.52
5:AE:35:ASP:OD2	5:AE:37:ARG:NH1	2.42	0.52
5:AE:235:THR:HG21	5:AE:249:VAL:HG22	1.91	0.52
54:BJ:37:LYS:H	54:BJ:59:ARG:H	1.56	0.52
69:BY:14:LYS:O	69:BY:18:HIS:HB2	2.09	0.52
72:Bb:24:VAL:HG21	72:Bb:71:LEU:HD12	1.91	0.52
1:AA:1080:A:OP2	7:AG:140:ARG:NH2	2.43	0.52
2:AB:120:C:H41	7:AG:262:LYS:HE3	1.74	0.52
21:AU:12:ARG:HB3	21:AU:24:LEU:HD23	1.91	0.52
39:Am:46:ARG:NH1	39:Am:47:GLY:O	2.42	0.52
62:BR:58:ASP:OD1	62:BR:58:ASP:N	2.40	0.52
66:BV:50:LEU:HD11	66:BV:99:ILE:HG21	1.92	0.52
1:AA:1477:A:OP1	1:AA:3075:G:O2'	2.24	0.52
1:AA:2395:G:H5''	5:AE:255:TRP:NE1	2.25	0.52
45:BA:628:G:H21	45:BA:971:A:H62	1.58	0.52
68:BX:81:VAL:O	68:BX:122:SER:OG	2.27	0.52
79:Bi:161:ILE:HA	79:Bi:164:ILE:HD12	1.90	0.52
1:AA:1381:A:OP1	6:AF:197:ARG:NH1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:82:ARG:NH1	13:AM:113:GLY:HA3	2.25	0.52
17:AQ:12:LYS:O	21:AU:167:ARG:NH2	2.42	0.52
27:Aa:11:ASP:HB3	27:Aa:14:LYS:HB2	1.92	0.52
45:BA:65:A:OP1	52:BH:176:GLN:NE2	2.38	0.52
45:BA:374:U:OP1	57:BM:96:LYS:NZ	2.40	0.52
45:BA:1546:G:OP1	64:BT:123:ARG:NH1	2.42	0.52
45:BA:1561:U:H4'	45:BA:1599:C:H4'	1.91	0.52
71:Ba:63:SER:O	71:Ba:67:ASP:HB2	2.09	0.52
79:Bi:860:THR:OG1	79:Bi:916:LYS:NZ	2.41	0.52
6:AF:338:LYS:O	6:AF:340:GLY:N	2.42	0.52
19:AS:182:LYS:NZ	29:Ac:55:LYS:O	2.43	0.52
45:BA:55:A:OP1	70:BZ:112:LYS:NZ	2.36	0.52
62:BR:18:ALA:HB2	62:BR:69:VAL:HG13	1.92	0.52
62:BR:32:ASN:O	62:BR:68:ARG:NH1	2.42	0.52
1:AA:2617:U:O2'	12:AL:116:ARG:NH2	2.43	0.52
1:AA:2736:A:OP1	22:AV:92:ARG:NH1	2.41	0.52
32:Af:15:ASN:O	32:Af:19:ARG:NH1	2.42	0.52
45:BA:1356:U:H2'	45:BA:1357:A:H8	1.75	0.52
1:AA:3157:U:H4'	1:AA:3158:G:H5'	1.92	0.52
6:AF:151:VAL:CA	6:AF:250:TRP:O	2.58	0.52
20:AT:13:SER:OG	20:AT:38:ARG:NH2	2.42	0.52
48:BD:40:LYS:HB3	48:BD:247:ALA:HB1	1.92	0.52
49:BE:32:GLU:OE2	49:BE:65:ARG:NH2	2.33	0.52
1:AA:63:A:N3	1:AA:78:U:O2'	2.41	0.51
1:AA:1062:A:N3	22:AV:130:ARG:NH2	2.57	0.51
9:AI:234:GLU:O	9:AI:237:ASN:ND2	2.42	0.51
13:AM:15:GLU:HB3	13:AM:130:VAL:HG13	1.91	0.51
25:AY:6:ASP:OD2	25:AY:9:SER:OG	2.27	0.51
65:BU:57:ARG:HG2	65:BU:104:VAL:HG21	1.90	0.51
1:AA:2643:A:OP2	22:AV:3:LYS:NZ	2.43	0.51
1:AA:3108:G:N3	11:AK:163:GLN:NE2	2.53	0.51
10:AJ:171:LYS:NZ	10:AJ:223:ALA:O	2.43	0.51
17:AQ:43:ILE:HD11	17:AQ:138:LEU:HD13	1.91	0.51
27:Aa:55:GLU:HB2	27:Aa:108:LYS:HB3	1.91	0.51
45:BA:1323:C:H3'	45:BA:1324:G:H8	1.75	0.51
61:BQ:18:ARG:NH1	64:BT:90:ASN:O	2.44	0.51
69:BY:62:LYS:CE	69:BY:118:PRO:CB	2.84	0.51
1:AA:2207:A:H4'	45:BA:913:G:C8	2.45	0.51
6:AF:151:VAL:HG11	6:AF:252:GLU:HA	1.92	0.51
15:AO:38:ILE:O	21:AU:95:ARG:NH2	2.41	0.51
33:Ag:86:THR:HG23	33:Ag:115:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:391:A:OP2	54:BJ:23:LYS:NZ	2.39	0.51
47:BC:70:LEU:HA	47:BC:73:LEU:HB3	1.91	0.51
50:BF:98:ASN:ND2	50:BF:116:ASP:OD1	2.41	0.51
79:Bi:392:ARG:HH21	79:Bi:396:LEU:HD11	1.75	0.51
1:AA:268:A:OP1	16:AP:50:ARG:NH1	2.43	0.51
1:AA:801:A:OP1	29:Ac:27:LYS:NZ	2.43	0.51
1:AA:1193:A:OP2	17:AQ:49:ARG:NH1	2.43	0.51
1:AA:3181:C:OP2	17:AQ:171:LYS:NZ	2.37	0.51
5:AE:33:PRO:HD2	5:AE:44:THR:HB	1.93	0.51
24:AX:112:SER:O	24:AX:132:ASN:ND2	2.43	0.51
28:Ab:76:ASN:OD1	28:Ab:78:ASN:ND2	2.44	0.51
45:BA:689:G:H2'	45:BA:690:G:H8	1.75	0.51
45:BA:856:A:N6	53:BI:115:SER:O	2.39	0.51
47:BC:181:LEU:HA	47:BC:184:LEU:HB3	1.92	0.51
54:BJ:4:SER:HB2	54:BJ:24:LYS:HE2	1.92	0.51
1:AA:994:G:N2	1:AA:995:U:O4	2.40	0.51
22:AV:41:ASP:OD1	22:AV:61:THR:OG1	2.27	0.51
45:BA:67:A:N6	45:BA:83:G:O2'	2.43	0.51
45:BA:819:G:H2'	45:BA:819:G:OP2	2.09	0.51
45:BA:930:A:OP1	72:Bb:32:LYS:NZ	2.41	0.51
48:BD:170:ILE:HB	48:BD:197:TYR:HB2	1.91	0.51
73:Bc:67:THR:OG1	73:Bc:70:LYS:O	2.29	0.51
1:AA:1632:A:OP1	28:Ab:69:LYS:NZ	2.43	0.51
6:AF:53:SER:HB3	6:AF:56:ALA:HB2	1.92	0.51
6:AF:72:ALA:O	6:AF:76:ARG:NH1	2.43	0.51
6:AF:328:ASN:OD1	9:AI:48:ASN:ND2	2.40	0.51
37:Ak:51:SER:H	37:Ak:54:GLU:HB2	1.76	0.51
39:Am:7:ASP:HB3	39:Am:10:GLN:HB2	1.93	0.51
45:BA:992:A:O2'	45:BA:1785:U:O2	2.25	0.51
65:BU:105:LEU:HD13	65:BU:122:ARG:HD2	1.93	0.51
74:Bd:32:PHE:HE2	74:Bd:38:ARG:HH21	1.57	0.51
24:AX:104:ASN:OD1	24:AX:108:GLU:N	2.41	0.51
51:BG:57:SER:HB3	74:Bd:53:ILE:HB	1.93	0.51
58:BN:67:THR:HG22	58:BN:68:GLU:HG3	1.92	0.51
58:BN:93:ASP:HB3	58:BN:96:GLN:HB2	1.92	0.51
60:BP:17:ALA:HA	60:BP:30:VAL:HG12	1.93	0.51
79:Bi:581:TYR:N	79:Bi:584:ARG:O	2.41	0.51
1:AA:1427:U:OP2	29:Ac:4:ARG:NH2	2.43	0.51
1:AA:2796:G:N7	43:Aq:63:LYS:NZ	2.55	0.51
3:AC:39:G:O2'	3:AC:105:A:N1	2.42	0.51
8:AH:55:LEU:HD21	8:AH:66:SER:OG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:BL:76:LEU:HA	56:BL:79:TYR:HB3	1.92	0.51
79:Bi:378:VAL:HG23	79:Bi:418:VAL:HG12	1.93	0.51
1:AA:595:G:OP2	9:AI:30:ARG:NH2	2.43	0.51
1:AA:2941:A:P	5:AE:256:HIS:HB2	2.51	0.51
23:AW:18:ASP:HB3	23:AW:104:ARG:HA	1.93	0.51
46:BB:150:ASP:OD2	46:BB:165:ARG:NH2	2.40	0.51
51:BG:53:VAL:HG12	51:BG:55:ASP:H	1.76	0.51
68:BX:30:SER:HG	68:BX:61:ILE:CG1	2.17	0.51
72:Bb:84:VAL:HG13	72:Bb:85:ARG:HD3	1.93	0.51
1:AA:181:U:H4'	38:Al:75:LYS:HD3	1.93	0.51
45:BA:1662:G:H2'	45:BA:1663:G:H8	1.76	0.51
64:BT:2:SER:OG	64:BT:3:LEU:N	2.43	0.51
1:AA:82:C:H4'	16:AP:204:LYS:HE3	1.93	0.50
1:AA:1014:U:H3	1:AA:1036:A:H61	1.57	0.50
6:AF:151:VAL:HG12	6:AF:152:VAL:O	2.12	0.50
9:AI:186:HIS:O	9:AI:190:THR:OG1	2.29	0.50
14:AN:10:LEU:HD23	19:AS:166:LEU:HD11	1.93	0.50
45:BA:1320:U:H3'	46:BB:101:ARG:HH12	1.76	0.50
46:BB:140:ASN:ND2	67:BW:31:SER:O	2.40	0.50
49:BE:10:LYS:NZ	66:BV:113:ASP:OD2	2.42	0.50
50:BF:68:ARG:HD2	50:BF:76:VAL:HG11	1.93	0.50
54:BJ:5:ARG:NH1	54:BJ:29:LEU:O	2.40	0.50
55:BK:108:ARG:HH21	55:BK:145:SER:HB3	1.75	0.50
64:BT:113:LEU:HB3	64:BT:117:LYS:HE3	1.92	0.50
78:Bh:205:SER:HB3	78:Bh:210:LEU:HB2	1.93	0.50
10:AJ:54:GLU:HG2	10:AJ:57:ARG:HH21	1.76	0.50
45:BA:1171:A:H2'	45:BA:1172:G:C8	2.46	0.50
72:Bb:38:ARG:HE	72:Bb:83:ILE:HG13	1.76	0.50
1:AA:148:G:OP2	16:AP:4:TYR:OH	2.22	0.50
1:AA:664:U:H2'	1:AA:665:A:C8	2.47	0.50
1:AA:2534:G:H1	1:AA:2545:C:H42	1.59	0.50
1:AA:3231:U:H2'	1:AA:3232:G:H8	1.75	0.50
11:AK:28:VAL:HG13	11:AK:33:THR:HB	1.92	0.50
26:AZ:63:ILE:HG22	26:AZ:86:VAL:HG12	1.93	0.50
35:Ai:47:CYS:SG	35:Ai:49:SER:OG	2.69	0.50
45:BA:514:G:H1	45:BA:543:C:H5	1.59	0.50
64:BT:35:ILE:HG23	64:BT:102:ALA:HB2	1.93	0.50
79:Bi:614:MET:HE3	79:Bi:710:LEU:HB3	1.93	0.50
1:AA:1231:A:N6	1:AA:1277:C:OP2	2.38	0.50
45:BA:142:G:H22	45:BA:173:A:H2	1.57	0.50
45:BA:354:C:H5''	54:BJ:16:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:BL:24:LYS:HG2	56:BL:26:ASP:HB2	1.93	0.50
60:BP:128:LYS:HZ2	72:Bb:27:SER:HG	1.58	0.50
61:BQ:110:GLU:HB2	64:BT:119:ILE:HD11	1.94	0.50
1:AA:1627:U:H2'	1:AA:1814:A:H62	1.76	0.50
5:AE:297:SER:HA	5:AE:300:ARG:HE	1.75	0.50
38:Al:39:TYR:N	38:Al:40:PRO:CD	2.75	0.50
68:BX:27:ILE:HG13	68:BX:61:ILE:HB	1.93	0.50
1:AA:1249:G:H2'	1:AA:1250:G:H8	1.77	0.50
1:AA:1740:U:H4'	1:AA:1741:A:H5'	1.93	0.50
1:AA:2394:G:C2	5:AE:258:ALA:O	2.65	0.50
1:AA:2660:G:OP1	1:AA:2750:U:O2'	2.29	0.50
1:AA:2931:C:OP1	24:AX:40:LYS:NZ	2.37	0.50
15:AO:23:ILE:O	15:AO:30:GLY:N	2.44	0.50
18:AR:122:ALA:HB3	18:AR:143:PRO:HB2	1.94	0.50
46:BB:76:ILE:HD13	46:BB:98:ILE:HB	1.94	0.50
70:BZ:37:LYS:HD2	70:BZ:57:VAL:HG23	1.92	0.50
1:AA:595:G:H1	1:AA:609:G:H5''	1.75	0.50
1:AA:2940:A:OP2	5:AE:2:SER:N	2.45	0.50
1:AA:3313:U:O5'	5:AE:173:GLN:NE2	2.45	0.50
28:Ab:46:ILE:HD13	28:Ab:68:ILE:HG23	1.92	0.50
45:BA:235:G:H2'	45:BA:236:A:H8	1.77	0.50
47:BC:62:LYS:HE2	47:BC:91:VAL:HG21	1.93	0.50
49:BE:20:GLU:OE2	49:BE:76:ARG:NH2	2.45	0.50
51:BG:54:LYS:NZ	51:BG:135:ASP:OD2	2.44	0.50
59:BO:23:PRO:HG3	59:BO:26:PHE:CG	2.46	0.50
1:AA:1364:C:OP1	9:Al:110:ARG:NH2	2.43	0.50
1:AA:1656:A:OP2	35:Al:37:LYS:NZ	2.45	0.50
1:AA:2780:A:OP1	14:AN:177:LYS:NZ	2.41	0.50
1:AA:3213:A:OP1	15:AO:128:ARG:NH1	2.45	0.50
4:AD:40:TYR:HA	4:AD:91:GLY:HA3	1.93	0.50
45:BA:1474:G:H2'	45:BA:1475:A:H8	1.75	0.50
68:BX:31:SER:OG	68:BX:32:LYS:N	2.45	0.50
72:Bb:10:ARG:HB2	72:Bb:34:LYS:HA	1.93	0.50
79:Bi:343:LEU:HD22	79:Bi:621:GLN:HB3	1.94	0.50
79:Bi:906:GLN:HB2	79:Bi:911:ARG:HH21	1.77	0.50
79:Bi:1054:LEU:HB3	79:Bi:1082:VAL:HG12	1.93	0.50
5:AE:19:ARG:HD3	5:AE:19:ARG:N	2.07	0.50
14:AN:185:LYS:NZ	14:AN:189:GLU:OE2	2.45	0.50
16:AP:5:LYS:HG3	37:Ak:40:VAL:HG11	1.94	0.50
38:Al:34:CYS:HB3	38:Al:38:GLY:H	1.76	0.50
60:BP:125:SER:OG	60:BP:126:THR:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:BV:106:ILE:HG23	66:BV:107:THR:HG23	1.93	0.50
72:Bb:32:LYS:O	72:Bb:37:LYS:NZ	2.35	0.50
1:AA:1719:G:OP1	20:AT:110:ARG:NH2	2.45	0.49
1:AA:1724:U:OP2	20:AT:128:LYS:NZ	2.38	0.49
12:AL:191:LYS:NZ	12:AL:212:GLU:OE1	2.45	0.49
45:BA:878:G:O2'	59:BO:108:ASP:OD1	2.25	0.49
45:BA:979:A:N3	45:BA:1775:U:O2'	2.45	0.49
49:BE:29:LEU:HD21	49:BE:69:LEU:HD11	1.94	0.49
54:BJ:89:GLU:OE2	54:BJ:92:ARG:NH1	2.45	0.49
66:BV:40:ASN:O	66:BV:44:ASN:HB2	2.12	0.49
79:Bi:306:THR:O	79:Bi:310:ALA:HB3	2.12	0.49
1:AA:3169:U:H3	1:AA:3281:U:H3	1.59	0.49
12:AL:21:ARG:NH2	12:AL:22:TYR:OH	2.45	0.49
45:BA:591:A:H5''	55:BK:24:LEU:HD13	1.94	0.49
48:BD:142:GLY:N	48:BD:153:SER:O	2.39	0.49
50:BF:103:TYR:O	50:BF:182:TYR:OH	2.30	0.49
58:BN:97:LEU:O	58:BN:101:ALA:HB2	2.12	0.49
62:BR:36:ILE:HD13	62:BR:52:LEU:HD11	1.93	0.49
68:BX:6:VAL:HG12	68:BX:34:ILE:HD11	1.94	0.49
77:Bg:107:LYS:O	77:Bg:115:THR:OG1	2.30	0.49
1:AA:2724:U:OP1	22:AV:78:LYS:NZ	2.43	0.49
17:AQ:119:VAL:HB	17:AQ:124:LEU:HD21	1.94	0.49
20:AT:99:LEU:HD21	20:AT:103:ARG:HH21	1.76	0.49
45:BA:76:A:N6	45:BA:80:A:O2'	2.44	0.49
45:BA:1291:G:N2	45:BA:1292:G:O6	2.45	0.49
45:BA:1565:C:OP1	64:BT:41:ARG:NH1	2.45	0.49
48:BD:106:ASP:OD1	48:BD:106:ASP:N	2.46	0.49
70:BZ:29:HIS:NE2	70:BZ:69:SER:OG	2.43	0.49
78:Bh:153:GLN:HG3	78:Bh:201:THR:HA	1.93	0.49
79:Bi:819:PHE:HB2	79:Bi:858:LEU:HD11	1.93	0.49
5:AE:19:ARG:C	5:AE:273:HIS:CE1	2.90	0.49
5:AE:169:THR:HG22	5:AE:171:LEU:HG	1.93	0.49
10:AJ:82:LEU:HD13	10:AJ:222:PHE:HE2	1.77	0.49
10:AJ:251:LYS:O	10:AJ:255:SER:OG	2.30	0.49
14:AN:62:THR:O	14:AN:64:LYS:N	2.45	0.49
40:An:10:LYS:HA	40:An:13:MET:HE3	1.93	0.49
45:BA:1294:G:O3'	46:BB:109:ASN:ND2	2.44	0.49
78:Bh:195:HIS:NE2	78:Bh:213:SER:OG	2.39	0.49
79:Bi:636:VAL:HG21	79:Bi:711:LEU:HD23	1.94	0.49
79:Bi:962:LYS:NZ	79:Bi:963:TRP:O	2.40	0.49
1:AA:3348:G:H1	1:AA:3357:U:H3	1.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:70:ARG:HE	4:AD:72:ARG:HD3	1.77	0.49
6:AF:11:LEU:HD21	6:AF:156:LEU:HB2	1.93	0.49
9:AI:27:ALA:HA	9:AI:30:ARG:HB3	1.93	0.49
16:AP:191:TRP:O	16:AP:195:ASN:HB2	2.11	0.49
32:Af:87:ASN:ND2	32:Af:89:LEU:O	2.46	0.49
35:Ai:41:ARG:O	35:Ai:43:LYS:NZ	2.45	0.49
45:BA:1474:G:H2'	45:BA:1475:A:C8	2.47	0.49
45:BA:1677:C:OP1	54:BJ:42:ARG:NH1	2.42	0.49
54:BJ:155:SER:O	54:BJ:159:GLN:NE2	2.45	0.49
57:BM:21:ASN:HD22	57:BM:31:THR:HA	1.76	0.49
63:BS:17:ILE:HG12	63:BS:58:MET:HE2	1.94	0.49
79:Bi:167:GLU:HB2	79:Bi:170:LYS:HE3	1.95	0.49
79:Bi:431:LEU:HD23	79:Bi:458:LEU:HD21	1.93	0.49
1:AA:749:C:H5''	30:Ad:32:LEU:HD12	1.93	0.49
1:AA:1295:G:O2'	21:AU:115:ARG:NH1	2.45	0.49
19:AS:123:THR:OG1	19:AS:125:ASP:OD1	2.29	0.49
52:BH:78:THR:HG23	52:BH:92:ARG:HG2	1.95	0.49
53:BI:13:PRO:HB2	53:BI:14:THR:HB	1.94	0.49
78:Bh:161:LYS:HG2	78:Bh:164:ASP:HB2	1.95	0.49
1:AA:768:C:OP1	14:AN:186:ARG:NH2	2.46	0.49
1:AA:829:U:H3	1:AA:895:A:H62	1.61	0.49
1:AA:1208:U:O2	1:AA:3115:C:N4	2.45	0.49
12:AL:76:MET:HE1	12:AL:138:VAL:HG21	1.95	0.49
13:AM:26:SER:OG	13:AM:27:GLY:N	2.46	0.49
20:AT:109:TYR:HB3	20:AT:115:ILE:HG12	1.94	0.49
31:Ae:13:LYS:HE3	31:Ae:103:THR:HG21	1.94	0.49
45:BA:338:C:H1'	54:BJ:5:ARG:HB2	1.93	0.49
68:BX:15:ASN:ND2	68:BX:72:CYS:O	2.39	0.49
69:BY:65:ASN:ND2	69:BY:116:ASP:HB3	2.24	0.49
1:AA:289:A:O2'	16:AP:93:LYS:O	2.26	0.49
1:AA:1015:U:O2'	1:AA:1017:C:OP2	2.26	0.49
9:AI:88:ARG:NH1	9:AI:90:LYS:O	2.45	0.49
45:BA:65:A:H2	45:BA:84:A:H62	1.58	0.49
45:BA:1064:G:O2'	47:BC:204:ILE:O	2.31	0.49
45:BA:1610:G:OP1	51:BG:72:HIS:NE2	2.40	0.49
47:BC:41:ARG:HH21	47:BC:232:HIS:CD2	2.30	0.49
53:BI:67:LEU:HD21	53:BI:94:ALA:HB2	1.94	0.49
1:AA:1047:A:N3	1:AA:2633:U:O2'	2.46	0.49
1:AA:2185:G:O2'	1:AA:2314:U:OP2	2.25	0.49
8:AH:40:LEU:HD11	8:AH:54:TYR:HB2	1.94	0.49
45:BA:1755:A:H8	69:BY:63:GLN:CD	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:BD:82:ASN:HB2	48:BD:207:LEU:HD23	1.94	0.49
5:AE:17:LEU:HD11	5:AE:262:TRP:CZ3	2.25	0.49
45:BA:1323:C:H3'	45:BA:1324:G:C8	2.47	0.49
69:BY:62:LYS:HB2	69:BY:62:LYS:HZ2	1.78	0.49
1:AA:824:C:O2'	1:AA:1534:A:N3	2.45	0.48
28:Ab:17:ARG:H	35:Ai:74:ARG:HG3	1.76	0.48
36:Aj:85:THR:HG22	36:Aj:88:LEU:H	1.77	0.48
45:BA:1258:U:H4'	56:BL:2:LEU:HB2	1.93	0.48
45:BA:1429:G:N3	66:BV:72:ASN:ND2	2.60	0.48
45:BA:1488:G:H3'	45:BA:1515:A:H61	1.77	0.48
66:BV:28:SER:HB3	66:BV:34:LEU:HD22	1.94	0.48
1:AA:3186:A:N3	11:AK:44:THR:OG1	2.46	0.48
1:AA:3304:U:O3'	5:AE:334:ARG:NH2	2.46	0.48
9:AI:82:LYS:HE2	9:AI:191:VAL:HG22	1.94	0.48
45:BA:1:U:H3	55:BK:54:ARG:HD3	1.77	0.48
45:BA:415:C:O2'	45:BA:418:G:O6	2.25	0.48
3:AC:56:G:OP1	38:Al:68:LYS:NZ	2.36	0.48
5:AE:56:ILE:HG21	5:AE:356:LEU:HD22	1.94	0.48
11:AK:1:MET:HE1	21:AU:138:GLN:HB3	1.95	0.48
14:AN:55:ARG:NH1	14:AN:73:ARG:O	2.43	0.48
16:AP:43:THR:OG1	16:AP:131:GLU:OE1	2.29	0.48
17:AQ:44:SER:HB3	17:AQ:129:LEU:HD11	1.95	0.48
28:Ab:52:LYS:O	28:Ab:65:ARG:NH1	2.47	0.48
48:BD:113:LEU:HD11	48:BD:211:LEU:HB3	1.96	0.48
49:BE:105:MET:HB2	49:BE:122:VAL:HG21	1.95	0.48
49:BE:115:ILE:HD11	49:BE:138:VAL:HG21	1.94	0.48
78:Bh:16:HIS:CE1	78:Bh:37:SER:HB3	2.48	0.48
1:AA:838:G:O6	44:Ar:4:ARG:NH2	2.46	0.48
1:AA:1565:G:N2	1:AA:1574:C:O2	2.39	0.48
1:AA:2282:U:OP1	1:AA:2973:G:O2'	2.30	0.48
1:AA:3147:G:HO2'	5:AE:104:THR:HG1	1.50	0.48
10:AJ:148:ALA:HA	10:AJ:201:THR:HG22	1.94	0.48
14:AN:75:PHE:H	14:AN:97:VAL:HA	1.78	0.48
19:AS:71:LEU:HD22	19:AS:99:THR:HG21	1.95	0.48
34:Ah:105:SER:HG	34:Ah:107:ILE:HG13	1.73	0.48
45:BA:223:U:O2	45:BA:838:G:N2	2.35	0.48
45:BA:789:A:HO2'	50:BF:106:LYS:HZ2	1.59	0.48
50:BF:153:ASN:O	50:BF:174:LYS:NZ	2.45	0.48
50:BF:246:LEU:HB3	50:BF:250:GLU:HB2	1.95	0.48
51:BG:93:LEU:HD12	51:BG:172:ILE:HG23	1.95	0.48
53:BI:12:ALA:N	53:BI:13:PRO:CD	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BI:63:PRO:O	53:BI:64:VAL:CB	2.61	0.48
73:Bc:56:CYS:SG	73:Bc:57:GLU:N	2.86	0.48
1:AA:990:U:H1'	22:AV:101:CYS:HB3	1.96	0.48
1:AA:1639:C:H5'	35:Ai:52:GLN:HG3	1.96	0.48
43:Aq:92:GLU:HG2	43:Aq:94:GLY:H	1.79	0.48
45:BA:885:G:N2	60:BP:123:SER:O	2.45	0.48
48:BD:102:VAL:HG11	48:BD:129:ILE:HG13	1.94	0.48
56:BL:88:PRO:O	56:BL:90:THR:N	2.42	0.48
79:Bi:977:ASP:OD1	79:Bi:977:ASP:N	2.45	0.48
1:AA:655:C:H2'	1:AA:656:A:C8	2.48	0.48
1:AA:2901:G:O2'	1:AA:3024:A:N1	2.45	0.48
3:AC:12:A:H5''	18:AR:3:ARG:HB3	1.96	0.48
12:AL:83:ASP:OD1	12:AL:83:ASP:N	2.47	0.48
45:BA:629:U:H2'	45:BA:630:A:C8	2.49	0.48
45:BA:1290:U:H2'	45:BA:1291:G:H8	1.78	0.48
50:BF:100:ARG:HB2	50:BF:114:ILE:HD13	1.96	0.48
57:BM:99:ARG:NH1	69:BY:7:ARG:O	2.46	0.48
59:BO:132:VAL:HG13	59:BO:134:VAL:HG13	1.95	0.48
79:Bi:437:LYS:O	79:Bi:441:THR:CB	2.62	0.48
1:AA:627:U:H4'	1:AA:1399:A:H1'	1.94	0.48
1:AA:1055:A:N3	2:AB:81:U:O2'	2.43	0.48
9:AI:208:SER:OG	9:AI:209:ASN:N	2.47	0.48
61:BQ:86:VAL:HG22	61:BQ:89:MET:HE3	1.96	0.48
62:BR:49:TYR:HB3	62:BR:53:LEU:HD21	1.95	0.48
69:BY:70:LYS:HB3	69:BY:93:LEU:HD22	1.95	0.48
79:Bi:437:LYS:O	79:Bi:441:THR:HB	2.13	0.48
79:Bi:605:ARG:O	79:Bi:610:LYS:NZ	2.42	0.48
1:AA:508:U:H3	1:AA:583:G:H1	1.61	0.48
21:AU:12:ARG:HD2	21:AU:22:PRO:HD2	1.95	0.48
26:AZ:50:ALA:HB2	36:Aj:77:PRO:HG2	1.95	0.48
31:Ae:98:SER:OG	31:Ae:99:ASP:N	2.46	0.48
45:BA:1591:C:H2'	45:BA:1592:A:H8	1.79	0.48
1:AA:242:C:HO2'	1:AA:243:G:H8	1.62	0.48
1:AA:515:C:O2'	6:AF:342:LYS:O	2.31	0.48
15:AO:21:VAL:HG12	15:AO:65:LEU:HA	1.96	0.48
45:BA:591:A:H2'	45:BA:592:A:C8	2.49	0.48
66:BV:24:ILE:HG12	66:BV:116:VAL:HG22	1.95	0.48
1:AA:286:U:O2'	16:AP:179:LYS:O	2.32	0.48
1:AA:1114:U:OP1	29:Ac:23:GLY:N	2.46	0.48
7:AG:21:ARG:NH1	7:AG:25:GLU:OE1	2.44	0.48
7:AG:119:TYR:OH	7:AG:139:PRO:O	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:133:ARG:NH2	13:AM:158:ASP:OD2	2.38	0.48
45:BA:976:G:N1	45:BA:1023:A:O2'	2.37	0.48
48:BD:45:VAL:HG21	48:BD:68:ILE:HG23	1.95	0.48
53:BI:12:ALA:HB3	53:BI:13:PRO:CD	2.37	0.48
74:Bd:30:VAL:HG23	74:Bd:40:ILE:HG13	1.94	0.48
75:Be:9:SER:OG	75:Be:10:HIS:N	2.46	0.48
79:Bi:608:ALA:HB3	79:Bi:610:LYS:HZ3	1.79	0.48
79:Bi:663:SER:OG	79:Bi:664:ARG:N	2.46	0.48
79:Bi:789:SER:OG	79:Bi:790:ASN:OD1	2.32	0.48
1:AA:585:A:H5''	34:Ah:70:LYS:HE2	1.96	0.47
1:AA:1634:G:N7	28:Ab:17:ARG:NH1	2.62	0.47
1:AA:2157:G:N7	4:AD:152:SER:OG	2.45	0.47
1:AA:2557:A:OP1	4:AD:69:TYR:OH	2.29	0.47
3:AC:8:C:H2'	3:AC:9:A:C8	2.49	0.47
33:Ag:82:LEU:HD11	33:Ag:112:ALA:HB2	1.96	0.47
43:Aq:45:ARG:O	43:Aq:48:SER:OG	2.32	0.47
53:BI:79:ARG:O	53:BI:83:LYS:HB2	2.13	0.47
66:BV:63:LEU:O	66:BV:83:GLU:HA	2.14	0.47
76:Bf:49:LEU:HD12	76:Bf:51:ASN:HD21	1.78	0.47
6:AF:29:PRO:HD2	6:AF:277:PRO:HB2	1.96	0.47
6:AF:151:VAL:HG13	6:AF:250:TRP:O	2.14	0.47
31:Ae:30:THR:HG23	31:Ae:91:SER:HB2	1.96	0.47
50:BF:54:TYR:O	70:BZ:15:ASN:ND2	2.47	0.47
63:BS:61:ILE:HD11	63:BS:69:ILE:HD12	1.97	0.47
78:Bh:7:LEU:HG	78:Bh:315:VAL:HG22	1.96	0.47
78:Bh:266:ASP:HB2	78:Bh:267:PRO:HD3	1.90	0.47
79:Bi:412:GLU:HG2	79:Bi:457:VAL:HG21	1.96	0.47
1:AA:2568:C:O2'	1:AA:2569:A:O4'	2.31	0.47
5:AE:261:MET:HG2	17:AQ:64:PHE:HA	1.96	0.47
6:AF:358:THR:HG21	22:AV:148:PRO:HD2	1.96	0.47
21:AU:77:VAL:HG13	21:AU:126:VAL:HG22	1.96	0.47
26:AZ:115:ARG:HD3	26:AZ:119:THR:HG23	1.95	0.47
45:BA:381:C:O2'	45:BA:755:A:N1	2.43	0.47
45:BA:815:G:H4'	45:BA:815:G:OP2	2.14	0.47
45:BA:1234:A:O2'	77:Bg:145:HIS:O	2.29	0.47
46:BB:88:LYS:NZ	63:BS:83:GLN:OE1	2.47	0.47
51:BG:72:HIS:ND1	62:BR:79:TYR:OH	2.45	0.47
55:BK:28:LEU:HB3	76:Bf:44:PHE:HE2	1.80	0.47
66:BV:48:HIS:O	66:BV:48:HIS:ND1	2.47	0.47
79:Bi:817:VAL:HG22	79:Bi:832:VAL:HG22	1.95	0.47
79:Bi:876:LEU:HD11	79:Bi:1053:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:577:C:O2'	1:AA:579:G:OP1	2.33	0.47
1:AA:979:U:H1'	1:AA:980:A:C8	2.49	0.47
1:AA:1914:G:O2'	20:AT:82:LYS:O	2.29	0.47
11:AK:41:ILE:HD11	11:AK:67:ALA:HB1	1.96	0.47
14:AN:76:THR:HG22	14:AN:101:ARG:HB3	1.95	0.47
18:AR:41:LEU:HD13	18:AR:112:LEU:HD23	1.96	0.47
45:BA:235:G:H2'	45:BA:236:A:C8	2.50	0.47
45:BA:1601:G:OP1	65:BU:86:ARG:NH2	2.46	0.47
47:BC:83:LYS:HB2	47:BC:83:LYS:HE3	1.76	0.47
79:Bi:201:ARG:NH2	79:Bi:240:GLU:OE2	2.47	0.47
1:AA:985:U:H2'	1:AA:986:U:H6	1.79	0.47
10:AJ:158:ASP:OD1	10:AJ:158:ASP:N	2.38	0.47
16:AP:143:ARG:NH2	36:Aj:90:ARG:O	2.46	0.47
24:AX:6:ALA:HB1	24:AX:125:LEU:HG	1.96	0.47
39:Am:42:LYS:HG2	39:Am:55:VAL:HG12	1.96	0.47
56:BL:77:ARG:HD3	56:BL:84:GLU:HA	1.95	0.47
58:BN:81:ASP:OD1	58:BN:81:ASP:N	2.48	0.47
59:BO:91:LEU:HD12	59:BO:125:LEU:HD12	1.95	0.47
1:AA:1256:G:O6	1:AA:1261:G:N2	2.48	0.47
1:AA:1334:U:H5''	9:AI:206:LYS:HB3	1.97	0.47
1:AA:3039:C:OP1	24:AX:88:ARG:NH2	2.47	0.47
1:AA:3243:A:OP1	17:AQ:159:LYS:NZ	2.47	0.47
3:AC:95:G:OP1	38:Al:76:ASN:ND2	2.48	0.47
22:AV:44:ALA:HA	22:AV:95:HIS:HB3	1.97	0.47
45:BA:58:U:OP1	45:BA:456:A:O2'	2.33	0.47
54:BJ:139:ALA:HA	54:BJ:142:LYS:HB2	1.96	0.47
57:BM:21:ASN:OD1	57:BM:21:ASN:N	2.48	0.47
60:BP:131:GLY:O	72:Bb:22:ARG:NH2	2.48	0.47
71:Ba:99:ALA:HB1	71:Ba:101:TYR:HE1	1.78	0.47
79:Bi:375:VAL:HG12	79:Bi:579:LEU:HD13	1.96	0.47
1:AA:185:C:H5''	27:Aa:122:LYS:HG2	1.97	0.47
1:AA:713:U:OP1	14:AN:171:ARG:NH2	2.47	0.47
1:AA:786:A:H4'	1:AA:787:G:H5'	1.97	0.47
1:AA:2437:G:OP1	10:AJ:70:LYS:NZ	2.48	0.47
4:AD:109:GLU:HG2	4:AD:138:GLY:HA2	1.97	0.47
6:AF:132:ALA:N	6:AF:148:ILE:HG12	2.29	0.47
14:AN:52:ASP:N	14:AN:52:ASP:OD1	2.45	0.47
34:Ah:103:TYR:H	34:Ah:104:PRO:HD2	1.77	0.47
38:Al:34:CYS:HB3	38:Al:38:GLY:N	2.30	0.47
40:An:23:LEU:HD11	40:An:35:ILE:HG22	1.97	0.47
45:BA:149:C:OP1	70:BZ:121:THR:OG1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:489:C:N4	45:BA:496:G:O6	2.46	0.47
45:BA:637:C:O2	53:BI:114:ARG:NH2	2.36	0.47
45:BA:772:G:H5'	50:BF:23:LEU:HD23	1.97	0.47
45:BA:1564:U:OP1	65:BU:38:LYS:NZ	2.41	0.47
54:BJ:36:THR:HA	54:BJ:58:LEU:HA	1.96	0.47
54:BJ:37:LYS:HB2	54:BJ:59:ARG:HG2	1.96	0.47
55:BK:85:VAL:HG12	55:BK:99:LEU:HD11	1.97	0.47
64:BT:28:ILE:HD12	64:BT:61:LEU:HD21	1.95	0.47
65:BU:29:GLU:HG3	65:BU:110:LYS:HE3	1.96	0.47
68:BX:38:LEU:HD22	68:BX:47:ILE:HD13	1.97	0.47
78:Bh:267:PRO:HG2	78:Bh:269:TYR:CD1	2.48	0.47
79:Bi:889:VAL:HG21	79:Bi:1038:LEU:HD11	1.95	0.47
1:AA:351:A:N6	40:An:37:TYR:O	2.39	0.47
1:AA:1178:G:N3	1:AA:1328:C:O2'	2.46	0.47
1:AA:2138:A:O2'	38:Al:2:GLY:N	2.46	0.47
1:AA:2810:C:OP2	1:AA:2955:U:O2'	2.29	0.47
6:AF:148:ILE:HG23	6:AF:149:PRO:HD3	0.64	0.47
17:AQ:121:PRO:HA	17:AQ:124:LEU:HD23	1.97	0.47
45:BA:576:G:O6	69:BY:65:ASN:C	2.58	0.47
45:BA:1482:C:O2'	62:BR:72:GLY:O	2.33	0.47
45:BA:1643:U:O2	45:BA:1780:G:N2	2.47	0.47
78:Bh:69:GLN:OE1	78:Bh:85:TRP:NE1	2.47	0.47
1:AA:1795:U:N3	44:Ar:50:GLY:O	2.48	0.47
1:AA:3343:G:H21	1:AA:3362:A:H2	1.63	0.47
7:AG:182:GLY:HA2	7:AG:194:LEU:HD23	1.97	0.47
16:AP:159:ARG:HB3	16:AP:164:LEU:HB2	1.96	0.47
27:Aa:73:VAL:HG13	27:Aa:80:VAL:HG12	1.97	0.47
45:BA:166:C:O2'	52:BH:133:LEU:O	2.31	0.47
45:BA:848:C:N4	45:BA:849:C:H41	2.13	0.47
53:BI:64:VAL:O	53:BI:64:VAL:HG12	2.14	0.47
71:Ba:43:ASP:N	71:Ba:43:ASP:OD1	2.48	0.47
79:Bi:581:TYR:CE2	79:Bi:612:THR:CB	2.98	0.47
79:Bi:834:CYS:HB3	79:Bi:1107:MET:HE1	1.96	0.47
1:AA:2631:U:OP1	1:AA:2757:U:O2'	2.29	0.47
1:AA:2877:G:HO2'	1:AA:2923:U:HO2'	1.59	0.47
46:BB:79:ARG:NH2	46:BB:164:ASN:O	2.48	0.47
61:BQ:15:HIS:CE1	61:BQ:110:GLU:HG2	2.50	0.47
78:Bh:211:ILE:HD11	78:Bh:225:LEU:HD22	1.97	0.47
1:AA:560:G:OP1	15:AO:83:LYS:NZ	2.39	0.46
1:AA:1168:U:O4	1:AA:1329:U:O2'	2.29	0.46
19:AS:65:SER:OG	19:AS:90:ASP:OD2	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Ab:103:GLN:NE2	28:Ab:106:GLN:OE1	2.48	0.46
47:BC:43:VAL:HG13	47:BC:68:VAL:HG11	1.97	0.46
48:BD:40:LYS:HG2	48:BD:43:ARG:HH12	1.80	0.46
50:BF:233:LYS:HE3	50:BF:233:LYS:HB3	1.71	0.46
59:BO:4:MET:HE2	59:BO:121:ARG:HG3	1.97	0.46
64:BT:26:ILE:HG13	64:BT:31:ALA:HB2	1.98	0.46
1:AA:627:U:H2'	1:AA:628:A:C8	2.51	0.46
5:AE:232:ARG:NH1	5:AE:266:ARG:O	2.48	0.46
11:AK:16:VAL:HA	11:AK:28:VAL:O	2.15	0.46
17:AQ:34:VAL:HA	17:AQ:103:LYS:O	2.16	0.46
48:BD:83:ILE:HD11	48:BD:125:ILE:HD11	1.96	0.46
59:BO:23:PRO:O	59:BO:25:TRP:CA	2.54	0.46
64:BT:88:ARG:NH2	64:BT:112:ASP:OD2	2.42	0.46
79:Bi:161:ILE:HG12	79:Bi:207:ILE:HG22	1.97	0.46
79:Bi:714:PRO:HD3	79:Bi:741:VAL:O	2.15	0.46
1:AA:514:G:N3	6:AF:341:SER:OG	2.46	0.46
5:AE:56:ILE:HD12	5:AE:359:ILE:HG12	1.98	0.46
8:AH:43:LEU:CB	34:Ah:103:TYR:HA	2.45	0.46
13:AM:160:VAL:HG13	13:AM:171:VAL:HG21	1.98	0.46
44:Ar:30:GLU:HA	44:Ar:33:GLN:HG2	1.97	0.46
45:BA:1182:U:H4'	61:BQ:124:THR:HB	1.98	0.46
47:BC:32:ILE:HD13	47:BC:66:VAL:HG21	1.97	0.46
63:BS:47:ARG:NH1	63:BS:48:ASN:OD1	2.47	0.46
79:Bi:1100:TRP:CD1	79:Bi:1110:LYS:HG2	2.51	0.46
37:Ak:62:ARG:HH22	37:Ak:98:ARG:HG2	1.80	0.46
45:BA:17:C:O2'	45:BA:1137:A:N1	2.45	0.46
45:BA:143:G:O6	52:BH:177:ARG:NH2	2.48	0.46
45:BA:405:C:O2'	52:BH:92:ARG:O	2.27	0.46
45:BA:592:A:O2'	45:BA:596:C:OP1	2.32	0.46
45:BA:886:U:OP2	47:BC:216:LYS:NZ	2.40	0.46
64:BT:28:ILE:HA	64:BT:58:ALA:HB2	1.97	0.46
79:Bi:544:PHE:HA	79:Bi:547:GLN:HB2	1.96	0.46
1:AA:1214:U:OP2	21:AU:137:ARG:NH2	2.49	0.46
1:AA:1420:C:OP2	6:AF:193:LYS:NZ	2.49	0.46
1:AA:2767:U:O2'	43:Aq:30:ALA:O	2.25	0.46
7:AG:150:LEU:HD12	13:AM:143:ARG:HG3	1.98	0.46
31:Ae:34:LEU:HG	31:Ae:59:TYR:HB3	1.98	0.46
45:BA:1795:U:H5'	72:Bb:79:ILE:HD11	1.97	0.46
51:BG:76:ARG:HH11	62:BR:121:SER:H	1.64	0.46
52:BH:68:LEU:HD23	52:BH:68:LEU:HA	1.75	0.46
63:BS:34:LEU:O	63:BS:38:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:Bi:518:ASP:HB2	79:Bi:527:LEU:HD22	1.97	0.46
1:AA:689:U:O4	6:AF:209:TYR:OH	2.31	0.46
10:AJ:159:PRO:HB2	10:AJ:162:LEU:HD23	1.98	0.46
45:BA:481:A:H61	45:BA:505:A:H62	1.64	0.46
45:BA:1164:G:O2'	45:BA:1612:U:O2	2.31	0.46
45:BA:1683:C:O2'	45:BA:1684:U:O5'	2.32	0.46
61:BQ:75:PRO:HA	61:BQ:93:VAL:O	2.16	0.46
61:BQ:90:ILE:HD11	61:BQ:112:LEU:HD21	1.98	0.46
64:BT:69:ILE:O	64:BT:73:MET:HB2	2.15	0.46
68:BX:111:MET:HE3	68:BX:116:ALA:HA	1.97	0.46
79:Bi:343:LEU:HD13	79:Bi:621:GLN:HA	1.97	0.46
79:Bi:541:GLN:HA	79:Bi:544:PHE:HD2	1.80	0.46
1:AA:49:A:OP1	14:AN:16:LYS:NZ	2.40	0.46
1:AA:2193:U:H5''	1:AA:2194:G:H5'	1.98	0.46
1:AA:3309:G:H1'	18:AR:69:ARG:HD2	1.97	0.46
5:AE:232:ARG:HH11	5:AE:233:TRP:HE1	1.63	0.46
18:AR:109:ALA:HA	18:AR:112:LEU:HD13	1.98	0.46
31:Ae:40:LYS:O	31:Ae:66:LYS:NZ	2.49	0.46
41:Ao:124:LYS:O	41:Ao:126:LYS:NZ	2.48	0.46
57:BM:77:SER:HB3	57:BM:85:VAL:HB	1.97	0.46
76:Bf:43:ARG:NH1	76:Bf:56:MET:SD	2.89	0.46
79:Bi:798:PRO:HB3	79:Bi:1052:HIS:HA	1.98	0.46
79:Bi:1101:ILE:HB	79:Bi:1109:GLN:HB3	1.98	0.46
1:AA:2724:U:OP2	1:AA:2726:C:N4	2.49	0.46
45:BA:30:G:OP1	69:BY:126:LYS:NZ	2.46	0.46
45:BA:503:G:O2'	76:Bf:46:ASN:ND2	2.48	0.46
79:Bi:474:LEU:HD12	79:Bi:478:GLU:HG3	1.98	0.46
1:AA:1907:C:O2	5:AE:240:ARG:NH2	2.44	0.46
32:Af:31:ARG:O	32:Af:35:GLU:N	2.47	0.46
45:BA:1059:U:O2'	45:BA:1060:U:O2	2.34	0.46
48:BD:37:PRO:HG2	48:BD:43:ARG:HG2	1.97	0.46
49:BE:7:LYS:HD2	66:BV:27:THR:HG21	1.98	0.46
58:BN:97:LEU:O	58:BN:101:ALA:CB	2.64	0.46
67:BW:42:GLU:O	67:BW:44:ARG:NH1	2.49	0.46
1:AA:637:C:H2'	1:AA:638:C:C6	2.51	0.46
1:AA:1386:A:H5''	6:AF:141:ARG:HH21	1.81	0.46
1:AA:2635:A:OP2	12:AL:15:LYS:NZ	2.35	0.46
4:AD:186:PHE:N	4:AD:196:TRP:CZ2	2.84	0.46
41:Ao:98:LYS:HB3	41:Ao:98:LYS:HE2	1.75	0.46
43:Aq:74:CYS:HB3	43:Aq:77:CYS:HB2	1.56	0.46
45:BA:68:A:N6	52:BH:132:ARG:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:325:G:OP1	57:BM:132:SER:OG	2.33	0.46
46:BB:188:LEU:HD23	46:BB:188:LEU:HA	1.77	0.46
60:BP:107:ARG:HH22	74:Bd:38:ARG:HH12	1.64	0.46
78:Bh:266:ASP:HB3	78:Bh:267:PRO:CD	2.40	0.46
79:Bi:191:PHE:O	79:Bi:196:ASN:ND2	2.48	0.46
79:Bi:599:ARG:NH1	79:Bi:730:LEU:O	2.49	0.46
1:AA:276:U:O2	16:AP:93:LYS:NZ	2.42	0.45
1:AA:651:G:O2'	1:AA:1435:A:OP1	2.32	0.45
1:AA:673:U:H2'	1:AA:674:G:C8	2.51	0.45
6:AF:148:ILE:CG2	6:AF:149:PRO:CD	2.45	0.45
11:AK:16:VAL:HG12	11:AK:29:GLY:HA3	1.98	0.45
27:Aa:84:LYS:HE3	27:Aa:84:LYS:HB2	1.79	0.45
45:BA:1672:G:H2'	45:BA:1673:G:C8	2.50	0.45
51:BG:76:ARG:NH1	62:BR:121:SER:H	2.14	0.45
72:Bb:33:ASP:OD1	72:Bb:33:ASP:N	2.49	0.45
1:AA:629:U:H2'	1:AA:630:A:C8	2.51	0.45
9:AI:84:VAL:HG21	9:AI:127:LEU:HD21	1.97	0.45
50:BF:139:VAL:HG13	50:BF:150:PRO:HG3	1.98	0.45
66:BV:39:SER:HA	66:BV:42:VAL:HG12	1.97	0.45
78:Bh:90:ARG:HE	78:Bh:102:ARG:HH21	1.63	0.45
1:AA:1474:A:O2'	32:Af:57:GLN:NE2	2.49	0.45
4:AD:118:GLU:OE2	4:AD:156:LYS:NZ	2.50	0.45
8:AH:42:LEU:HD22	8:AH:79:VAL:HG11	1.98	0.45
12:AL:202:LYS:NZ	12:AL:216:TYR:OH	2.44	0.45
13:AM:75:LYS:HA	13:AM:78:GLU:HG2	1.97	0.45
15:AO:15:VAL:HG23	15:AO:35:ILE:HD13	1.99	0.45
26:AZ:63:ILE:HD11	26:AZ:102:LEU:HD12	1.97	0.45
77:Bg:139:LEU:HD13	77:Bg:152:ALA:HB3	1.98	0.45
1:AA:1493:G:OP2	1:AA:1493:G:N2	2.46	0.45
1:AA:3343:G:O2'	1:AA:3362:A:N6	2.49	0.45
4:AD:28:LYS:HD3	4:AD:123:ARG:HE	1.81	0.45
5:AE:218:ILE:HG13	5:AE:276:THR:HG23	1.98	0.45
18:AR:111:LYS:HB3	18:AR:153:LYS:HG3	1.97	0.45
33:Ag:78:ASN:N	33:Ag:78:ASN:OD1	2.46	0.45
47:BC:130:SER:OG	47:BC:131:ASP:N	2.50	0.45
67:BW:42:GLU:HB2	67:BW:44:ARG:HH22	1.80	0.45
1:AA:563:U:H2'	1:AA:564:G:H8	1.81	0.45
5:AE:122:TRP:O	5:AE:125:SER:OG	2.34	0.45
12:AL:47:PRO:HB2	12:AL:178:ARG:HH21	1.81	0.45
14:AN:4:SER:O	14:AN:4:SER:OG	2.30	0.45
45:BA:237:C:H5''	45:BA:238:U:H5'	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:636:A:H5''	68:BX:31:SER:HB2	1.99	0.45
50:BF:24:SER:O	50:BF:24:SER:OG	2.32	0.45
55:BK:66:ASP:HB3	55:BK:69:ARG:HB3	1.99	0.45
59:BO:22:ALA:HA	59:BO:23:PRO:HD3	1.47	0.45
62:BR:90:VAL:HG21	62:BR:117:LEU:HD11	1.98	0.45
68:BX:55:ASP:OD1	68:BX:55:ASP:N	2.43	0.45
1:AA:2213:A:H2'	1:AA:2214:A:C8	2.52	0.45
10:AJ:144:GLU:HA	10:AJ:173:MET:HE3	1.97	0.45
18:AR:119:VAL:HA	18:AR:145:HIS:O	2.16	0.45
45:BA:886:U:OP1	47:BC:214:LYS:NZ	2.48	0.45
58:BN:41:LEU:HD11	58:BN:121:VAL:HB	1.98	0.45
66:BV:24:ILE:O	66:BV:90:TYR:HA	2.17	0.45
71:Ba:70:LYS:HD3	71:Ba:70:LYS:HA	1.82	0.45
72:Bb:57:SER:OG	72:Bb:58:VAL:O	2.27	0.45
72:Bb:79:ILE:HA	72:Bb:84:VAL:HB	1.98	0.45
78:Bh:262:VAL:HG13	78:Bh:271:VAL:HB	1.98	0.45
79:Bi:545:VAL:O	79:Bi:548:ASP:HB2	2.16	0.45
1:AA:3322:A:H2'	1:AA:3323:A:C8	2.51	0.45
5:AE:17:LEU:N	5:AE:18:PRO:CD	2.78	0.45
16:AP:68:ARG:HA	16:AP:98:LEU:HD21	1.98	0.45
49:BE:70:THR:HA	49:BE:86:LEU:HD13	1.98	0.45
53:BI:64:VAL:HG21	53:BI:95:GLU:O	2.16	0.45
65:BU:70:GLN:HE22	65:BU:119:LYS:HE2	1.81	0.45
78:Bh:26:SER:HB2	78:Bh:73:LEU:HD13	1.99	0.45
1:AA:75:G:OP2	14:AN:104:ARG:NH2	2.48	0.45
1:AA:2152:A:HO2'	1:AA:2243:A:HO2'	1.64	0.45
4:AD:6:ARG:NH2	4:AD:198:LYS:HG3	2.31	0.45
6:AF:11:LEU:HD22	6:AF:168:ALA:HB1	1.98	0.45
10:AJ:144:GLU:OE2	37:Ak:36:ARG:NH2	2.50	0.45
29:Ac:36:GLY:HA3	29:Ac:40:HIS:CE1	2.52	0.45
29:Ac:75:LEU:HD23	29:Ac:78:LEU:HD13	1.98	0.45
43:Aq:77:CYS:HB3	43:Aq:79:THR:HG23	1.99	0.45
48:BD:81:MET:HE1	48:BD:186:LYS:HB3	1.97	0.45
51:BG:79:ASN:OD1	51:BG:79:ASN:N	2.40	0.45
62:BR:109:PHE:O	62:BR:113:ASP:N	2.49	0.45
1:AA:117:U:O2'	1:AA:119:U:OP2	2.28	0.45
1:AA:2713:U:O2'	43:Aq:8:ARG:NH1	2.49	0.45
32:Af:41:LYS:NZ	32:Af:47:ASP:OD1	2.41	0.45
34:Ah:14:LEU:HD11	34:Ah:31:LYS:HB2	1.98	0.45
48:BD:39:THR:HG21	48:BD:64:LYS:HB2	1.99	0.45
50:BF:151:ASP:HB3	50:BF:154:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:BV:27:THR:HG23	66:BV:113:ASP:HB3	1.99	0.45
1:AA:528:U:H3	1:AA:564:G:H1	1.65	0.45
1:AA:608:A:OP1	6:AF:315:LYS:NZ	2.48	0.45
1:AA:1257:C:N3	1:AA:1261:G:N1	2.63	0.45
1:AA:2357:A:H2'	1:AA:2358:A:H8	1.81	0.45
5:AE:306:THR:HG21	5:AE:316:GLU:HG3	1.99	0.45
10:AJ:90:THR:HG23	10:AJ:214:LEU:HD21	1.98	0.45
27:Aa:3:LYS:NZ	27:Aa:5:SER:O	2.49	0.45
37:Ak:26:ILE:HD12	37:Ak:29:LYS:HE3	1.99	0.45
45:BA:142:G:H5''	52:BH:139:ASN:HD21	1.82	0.45
45:BA:820:U:O2	45:BA:820:U:O2'	2.31	0.45
47:BC:154:SER:O	47:BC:154:SER:OG	2.32	0.45
67:BW:39:VAL:HG22	67:BW:45:ALA:HB2	1.97	0.45
79:Bi:777:LYS:HB2	79:Bi:777:LYS:HE3	1.79	0.45
1:AA:1886:A:O2'	5:AE:226:PHE:O	2.29	0.44
61:BQ:80:MET:HE2	61:BQ:80:MET:HB3	1.79	0.44
63:BS:21:TYR:HD1	63:BS:58:MET:HE1	1.82	0.44
66:BV:28:SER:OG	66:BV:29:THR:N	2.48	0.44
68:BX:30:SER:HA	68:BX:34:ILE:HD12	1.99	0.44
79:Bi:306:THR:O	79:Bi:310:ALA:CB	2.65	0.44
79:Bi:715:THR:HA	79:Bi:718:LEU:HD12	1.99	0.44
1:AA:1336:U:H2'	1:AA:1337:A:C8	2.52	0.44
1:AA:1717:U:H2'	1:AA:1718:G:C8	2.51	0.44
3:AC:97:A:O2'	36:Aj:59:ASN:ND2	2.48	0.44
7:AG:99:TYR:OH	7:AG:168:ASP:OD2	2.35	0.44
8:AH:40:LEU:HB3	8:AH:84:VAL:HG13	1.99	0.44
11:AK:182:SER:HA	41:Ao:85:LEU:HD11	1.99	0.44
45:BA:66:U:O2	52:BH:160:ARG:NE	2.40	0.44
45:BA:1553:G:N1	45:BA:1556:A:OP2	2.49	0.44
49:BE:175:VAL:HG13	49:BE:182:LEU:HB2	1.99	0.44
50:BF:79:ASP:HB3	50:BF:82:TYR:HB2	1.99	0.44
51:BG:189:THR:OG1	51:BG:192:GLU:OE1	2.32	0.44
51:BG:206:SER:O	51:BG:206:SER:OG	2.32	0.44
55:BK:113:VAL:HG21	55:BK:134:ILE:HD13	1.99	0.44
1:AA:1095:U:O4	22:AV:131:GLN:NE2	2.44	0.44
1:AA:1472:U:H5'	20:AT:4:LEU:HB2	1.98	0.44
4:AD:144:ASN:N	4:AD:144:ASN:OD1	2.50	0.44
23:AW:18:ASP:OD1	23:AW:20:SER:OG	2.27	0.44
45:BA:1400:A:O3'	63:BS:60:ARG:NH1	2.51	0.44
48:BD:230:TRP:CD2	68:BX:68:ARG:HD3	2.52	0.44
51:BG:45:LYS:HA	51:BG:45:LYS:HD3	1.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:BK:106:GLU:O	55:BK:111:THR:OG1	2.35	0.44
79:Bi:632:ARG:NH1	79:Bi:658:GLU:OE2	2.43	0.44
1:AA:550:A:N1	1:AA:551:A:N6	2.66	0.44
2:AB:7:G:OP1	7:AG:33:ARG:NH1	2.49	0.44
5:AE:71:GLU:OE1	5:AE:357:LYS:NZ	2.50	0.44
6:AF:9:HIS:CD2	6:AF:150:LEU:HD12	2.49	0.44
6:AF:151:VAL:HG13	6:AF:250:TRP:C	2.42	0.44
18:AR:71:ALA:O	18:AR:74:LYS:HB2	2.17	0.44
21:AU:124:LEU:HD13	22:AV:155:PRO:HG3	2.00	0.44
45:BA:1344:A:H2'	45:BA:1345:A:C8	2.52	0.44
45:BA:1681:A:C8	52:BH:66:GLY:HA3	2.52	0.44
46:BB:72:ASP:OD1	46:BB:72:ASP:N	2.48	0.44
79:Bi:176:GLY:H	79:Bi:221:GLN:HE22	1.64	0.44
1:AA:358:G:N2	1:AA:361:A:OP2	2.43	0.44
1:AA:2727:A:OP2	1:AA:2728:G:N2	2.46	0.44
45:BA:522:U:H1'	70:BZ:34:ASN:HD21	1.81	0.44
45:BA:694:U:H3'	45:BA:695:U:H6	1.81	0.44
45:BA:1738:U:H2'	45:BA:1739:C:C6	2.52	0.44
47:BC:56:SER:OG	47:BC:59:ASP:OD2	2.32	0.44
50:BF:21:ASP:N	50:BF:21:ASP:OD1	2.50	0.44
50:BF:191:ARG:NH2	50:BF:212:ASP:OD2	2.45	0.44
53:BI:72:LYS:HE2	53:BI:72:LYS:HB3	1.74	0.44
78:Bh:112:SER:OG	78:Bh:113:VAL:N	2.48	0.44
79:Bi:240:GLU:HB2	79:Bi:243:VAL:HG12	1.99	0.44
1:AA:1141:C:O2'	1:AA:1153:A:N3	2.48	0.44
3:AC:27:U:H4'	6:AF:51:ALA:HB3	1.99	0.44
7:AG:22:ARG:HA	7:AG:22:ARG:HD3	1.82	0.44
9:AI:224:ILE:HA	21:AU:36:ILE:HG12	2.00	0.44
10:AJ:246:MET:HE2	10:AJ:246:MET:HB3	1.91	0.44
13:AM:54:VAL:HG12	13:AM:59:ILE:HG12	2.00	0.44
14:AN:106:GLN:HB3	37:Ak:18:THR:HG23	2.00	0.44
15:AO:60:LEU:HD13	21:AU:152:LEU:HD11	1.99	0.44
20:AT:144:GLN:NE2	57:BM:4:GLU:OE1	2.50	0.44
28:Ab:41:ALA:HB2	28:Ab:77:TYR:HE1	1.83	0.44
36:Aj:14:LYS:HD3	36:Aj:14:LYS:HA	1.73	0.44
47:BC:31:ASP:HA	47:BC:45:LYS:HA	1.99	0.44
74:Bd:31:GLU:HB2	74:Bd:39:THR:HG22	1.98	0.44
75:Be:30:LEU:HA	75:Be:39:CYS:HA	2.00	0.44
79:Bi:1058:GLN:NE2	79:Bi:1087:HIS:CE1	2.85	0.44
1:AA:1009:A:H2'	1:AA:1010:G:C8	2.52	0.44
1:AA:1661:G:H2'	1:AA:1662:G:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:2697:A:H2'	1:AA:2698:G:C8	2.53	0.44
1:AA:3313:U:H4'	5:AE:173:GLN:HG2	2.00	0.44
2:AB:4:U:H2'	2:AB:5:G:H8	1.83	0.44
8:AH:43:LEU:CD1	34:Ah:103:TYR:CA	2.76	0.44
9:AI:160:ARG:HG3	9:AI:203:TRP:CD2	2.53	0.44
27:Aa:85:VAL:HG11	27:Aa:99:LEU:HD11	1.98	0.44
28:Ab:51:LEU:HB2	28:Ab:65:ARG:HD2	2.00	0.44
45:BA:689:G:H2'	45:BA:690:G:C8	2.53	0.44
47:BC:149:GLN:HE22	47:BC:154:SER:HB3	1.82	0.44
51:BG:63:GLN:NE2	51:BG:66:GLN:OE1	2.51	0.44
54:BJ:36:THR:OG1	54:BJ:96:LEU:O	2.34	0.44
62:BR:98:ASP:OD1	62:BR:98:ASP:N	2.48	0.44
63:BS:87:GLU:HG2	63:BS:88:VAL:H	1.83	0.44
74:Bd:19:THR:OG1	74:Bd:20:GLY:N	2.51	0.44
79:Bi:586:LEU:HD13	79:Bi:612:THR:HG21	1.99	0.44
1:AA:541:U:H2'	1:AA:542:G:C8	2.52	0.44
3:AC:9:A:H2'	3:AC:10:A:C8	2.53	0.44
5:AE:214:MET:HE3	5:AE:214:MET:HB3	1.80	0.44
6:AF:148:ILE:CD1	6:AF:148:ILE:C	2.86	0.44
6:AF:151:VAL:HG13	6:AF:251:THR:O	2.18	0.44
38:Al:27:PHE:HA	38:Al:34:CYS:HA	1.99	0.44
42:Ap:2:ARG:NH1	45:BA:1772:C:OP2	2.50	0.44
45:BA:939:A:H2'	45:BA:940:A:C8	2.52	0.44
53:BI:13:PRO:HA	53:BI:14:THR:HA	1.70	0.44
54:BJ:84:HIS:NE2	54:BJ:97:THR:OG1	2.33	0.44
55:BK:17:ARG:O	55:BK:23:ARG:NH2	2.50	0.44
78:Bh:137:LYS:HA	78:Bh:137:LYS:HD2	1.65	0.44
1:AA:656:A:H2'	1:AA:657:A:C8	2.53	0.44
1:AA:1378:U:H2'	1:AA:1379:G:H8	1.83	0.44
1:AA:1419:A:H5''	6:AF:193:LYS:NZ	2.33	0.44
1:AA:1497:C:H2'	1:AA:1498:A:H8	1.83	0.44
1:AA:1569:U:H5'	1:AA:1570:U:H5''	2.00	0.44
1:AA:2395:G:C5'	5:AE:255:TRP:CD1	3.01	0.44
1:AA:2948:C:OP1	5:AE:244:ARG:NH1	2.44	0.44
21:AU:33:ASN:OD1	21:AU:33:ASN:N	2.51	0.44
33:Ag:97:ALA:O	33:Ag:105:ARG:NH2	2.51	0.44
36:Aj:73:LYS:HE2	36:Aj:73:LYS:HB3	1.77	0.44
44:Ar:9:GLY:HA3	44:Ar:27:LYS:HE3	2.00	0.44
51:BG:187:ILE:HG12	71:Ba:66:VAL:HG11	1.98	0.44
52:BH:164:LYS:HE3	52:BH:164:LYS:HB3	1.81	0.44
53:BI:46:ILE:HA	53:BI:59:ALA:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:BP:136:ARG:H	60:BP:136:ARG:HD3	1.83	0.44
73:Bc:48:SER:OG	73:Bc:49:HIS:ND1	2.50	0.44
79:Bi:380:GLU:HG2	79:Bi:423:GLU:HG3	2.00	0.44
79:Bi:579:LEU:H	79:Bi:587:LEU:HB2	1.82	0.44
79:Bi:710:LEU:HD23	79:Bi:739:LEU:HD21	2.00	0.44
79:Bi:856:ILE:HD13	79:Bi:1085:ILE:HD13	2.00	0.44
1:AA:327:A:OP2	14:AN:31:LYS:NZ	2.44	0.43
1:AA:3016:A:H2'	1:AA:3017:A:C8	2.53	0.43
4:AD:181:LYS:HB2	4:AD:184:ARG:HG3	2.00	0.43
5:AE:137:TYR:HE2	5:AE:196:ARG:HH12	1.66	0.43
18:AR:120:ASN:OD1	18:AR:120:ASN:N	2.48	0.43
43:Aq:35:LEU:HA	43:Aq:40:LYS:HG2	2.00	0.43
43:Aq:75:VAL:HG23	43:Aq:76:LYS:HD3	2.00	0.43
46:BB:189:VAL:HG12	46:BB:190:ASP:H	1.83	0.43
47:BC:105:PHE:HE2	47:BC:113:MET:HE1	1.83	0.43
54:BJ:48:THR:OG1	54:BJ:52:ASN:O	2.31	0.43
54:BJ:195:ARG:HD3	54:BJ:195:ARG:HA	1.85	0.43
62:BR:82:ARG:HH12	62:BR:114:ARG:HB2	1.83	0.43
67:BW:15:ARG:NH1	67:BW:33:GLN:OE1	2.50	0.43
78:Bh:37:SER:OG	78:Bh:38:ARG:N	2.42	0.43
79:Bi:969:LYS:HB3	79:Bi:969:LYS:HE2	1.75	0.43
1:AA:2553:U:C4	35:Ai:95:ILE:HG12	2.52	0.43
3:AC:26:U:O2'	6:AF:51:ALA:O	2.35	0.43
6:AF:131:VAL:N	6:AF:148:ILE:HG12	2.31	0.43
22:AV:78:LYS:HD3	22:AV:87:LYS:HE3	2.00	0.43
28:Ab:23:VAL:HB	28:Ab:43:VAL:HB	2.00	0.43
34:Ah:49:ILE:HG12	34:Ah:100:ILE:HG13	2.01	0.43
45:BA:1459:C:OP1	64:BT:126:ARG:NH2	2.52	0.43
50:BF:180:LEU:HA	50:BF:194:THR:HA	1.99	0.43
79:Bi:145:LEU:HA	79:Bi:148:ILE:HG12	2.00	0.43
79:Bi:650:VAL:HG23	79:Bi:664:ARG:HH21	1.83	0.43
1:AA:655:C:H2'	1:AA:656:A:H8	1.83	0.43
1:AA:1497:C:H2'	1:AA:1498:A:C8	2.52	0.43
1:AA:3140:G:N7	5:AE:28:ARG:NH2	2.50	0.43
7:AG:52:VAL:HA	7:AG:147:ASP:HB3	2.00	0.43
37:Ak:34:SER:HG	37:Ak:37:THR:H	1.64	0.43
45:BA:27:U:OP1	45:BA:43:A:N6	2.51	0.43
45:BA:428:A:N3	45:BA:440:U:O2'	2.44	0.43
45:BA:810:G:C2	53:BI:111:LYS:HG3	2.53	0.43
45:BA:1498:G:H5''	65:BU:72:GLY:HA3	1.99	0.43
53:BI:46:ILE:HG12	53:BI:60:ILE:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:BX:69:LEU:HD11	68:BX:72:CYS:HB3	2.01	0.43
1:AA:67:A:O2'	1:AA:315:C:O2	2.33	0.43
1:AA:92:G:O5'	43:Aq:46:LYS:NZ	2.52	0.43
1:AA:824:C:H5''	4:AD:21:ARG:HD3	2.00	0.43
1:AA:1864:A:H5'	20:AT:88:ARG:HG2	2.00	0.43
1:AA:2303:A:OP1	42:Ap:23:ARG:NH2	2.52	0.43
1:AA:2429:G:H2'	1:AA:2430:A:C8	2.54	0.43
5:AE:50:LYS:HA	5:AE:79:VAL:HG12	2.01	0.43
11:AK:8:GLN:HB3	11:AK:72:LYS:HD2	2.00	0.43
15:AO:113:THR:HG23	15:AO:116:GLU:H	1.82	0.43
45:BA:633:U:HO2'	68:BX:4:SER:HG	1.66	0.43
45:BA:814:A:O2'	45:BA:816:G:OP1	2.24	0.43
45:BA:1584:G:O2'	45:BA:1610:G:O6	2.32	0.43
45:BA:1754:A:P	69:BY:62:LYS:HD3	2.58	0.43
68:BX:75:ILE:HD13	68:BX:75:ILE:HA	1.75	0.43
78:Bh:38:ARG:HG2	78:Bh:67:ILE:HG23	2.00	0.43
79:Bi:762:LYS:HD3	79:Bi:762:LYS:HA	1.76	0.43
79:Bi:811:VAL:HB	79:Bi:876:LEU:HD22	2.00	0.43
1:AA:243:G:OP1	36:Aj:115:LYS:NZ	2.50	0.43
1:AA:710:A:H2'	1:AA:711:A:C8	2.53	0.43
1:AA:2184:U:H5	4:AD:198:LYS:HZ3	1.61	0.43
5:AE:19:ARG:O	5:AE:273:HIS:HE1	2.02	0.43
7:AG:82:GLU:OE1	7:AG:108:ARG:NH2	2.44	0.43
11:AK:4:ILE:HG12	21:AU:142:GLN:HB3	2.01	0.43
12:AL:142:ASP:OD1	12:AL:142:ASP:N	2.44	0.43
32:Af:61:LYS:HB2	32:Af:61:LYS:HE2	1.84	0.43
42:Ap:15:ARG:NH2	45:BA:1126:G:OP1	2.51	0.43
45:BA:1350:U:H2'	45:BA:1351:G:C8	2.53	0.43
45:BA:1466:G:O2'	45:BA:1602:C:OP1	2.34	0.43
48:BD:60:SER:OG	67:BW:25:LYS:O	2.35	0.43
58:BN:96:GLN:HA	58:BN:99:GLU:HG2	2.00	0.43
64:BT:119:ILE:HD13	64:BT:119:ILE:HA	1.73	0.43
78:Bh:86:ASP:OD1	78:Bh:86:ASP:N	2.44	0.43
79:Bi:942:ARG:HE	79:Bi:965:TYR:HB2	1.83	0.43
1:AA:112:U:OP1	36:Aj:107:LYS:NZ	2.47	0.43
1:AA:650:C:H2'	1:AA:651:G:C8	2.53	0.43
1:AA:805:G:H2'	1:AA:936:A:H61	1.83	0.43
5:AE:252:ILE:HD13	5:AE:252:ILE:HA	1.90	0.43
5:AE:255:TRP:O	5:AE:255:TRP:CD1	2.70	0.43
21:AU:44:PHE:HE1	21:AU:122:HIS:HD2	1.67	0.43
29:Ac:126:LYS:HB3	29:Ac:148:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:568:G:N7	69:BY:69:ARG:NH1	2.52	0.43
47:BC:111:ARG:HD3	47:BC:111:ARG:HA	1.79	0.43
48:BD:236:PRO:O	67:BW:33:GLN:NE2	2.51	0.43
50:BF:206:ASP:N	50:BF:206:ASP:OD1	2.50	0.43
79:Bi:300:ASN:HD22	79:Bi:339:ILE:HB	1.82	0.43
79:Bi:671:LEU:HB3	79:Bi:676:PHE:HB2	2.00	0.43
1:AA:93:C:OP2	1:AA:2764:C:O2'	2.25	0.43
1:AA:307:A:H2'	1:AA:308:A:C8	2.54	0.43
1:AA:2727:A:C2	29:Ac:43:ILE:HG23	2.54	0.43
1:AA:2827:U:O2'	1:AA:2829:U:O4	2.30	0.43
3:AC:38:U:C4	36:Aj:89:ARG:HD3	2.53	0.43
7:AG:91:GLY:O	7:AG:94:ASN:ND2	2.51	0.43
7:AG:250:ASP:N	7:AG:250:ASP:OD1	2.50	0.43
31:Ae:97:ASP:OD1	31:Ae:97:ASP:N	2.44	0.43
37:Ak:61:ILE:HD11	37:Ak:87:VAL:HG13	2.00	0.43
45:BA:181:A:H2'	45:BA:182:A:C8	2.54	0.43
45:BA:1754:A:P	69:BY:62:LYS:CD	3.07	0.43
48:BD:70:ASP:OD1	48:BD:133:LYS:NZ	2.36	0.43
78:Bh:159:ASN:ND2	78:Bh:166:SER:O	2.43	0.43
1:AA:3222:U:H3	1:AA:3263:G:H1	1.66	0.43
3:AC:126:A:O2'	3:AC:128:U:OP1	2.37	0.43
13:AM:35:LYS:HD2	13:AM:39:GLN:HE21	1.84	0.43
13:AM:64:LYS:HE3	13:AM:64:LYS:HB2	1.87	0.43
21:AU:132:THR:HG23	21:AU:144:LEU:HD13	2.00	0.43
32:Af:24:SER:HB3	32:Af:27:LYS:HD2	2.01	0.43
45:BA:472:U:O2'	45:BA:769:A:N3	2.42	0.43
46:BB:7:PHE:HE2	67:BW:39:VAL:HG11	1.83	0.43
47:BC:129:THR:OG1	47:BC:131:ASP:O	2.25	0.43
50:BF:85:GLY:N	50:BF:88:ASP:OD2	2.38	0.43
65:BU:7:ARG:HG2	65:BU:67:MET:HE2	2.00	0.43
79:Bi:664:ARG:HD3	79:Bi:664:ARG:HA	1.84	0.43
79:Bi:687:SER:HB3	80:Bi:1201:ATP:C6	2.53	0.43
8:AH:82:ARG:C	34:Ah:103:TYR:O	2.58	0.43
10:AJ:133:LYS:HD2	10:AJ:138:HIS:HE1	1.83	0.43
15:AO:19:ARG:HG2	15:AO:65:LEU:HD22	2.00	0.43
45:BA:79:C:H1'	52:BH:174:LYS:HD2	2.00	0.43
45:BA:694:U:H5''	45:BA:695:U:H5	1.84	0.43
45:BA:1796:C:OP2	72:Bb:5:ARG:NH2	2.51	0.43
71:Ba:71:ILE:H	71:Ba:71:ILE:HG13	1.52	0.43
73:Bc:51:GLN:HA	73:Bc:66:PRO:HB3	2.01	0.43
79:Bi:602:LEU:HB3	79:Bi:741:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:158:G:H2'	1:AA:159:A:H8	1.84	0.43
1:AA:1119:C:H2'	1:AA:1120:A:H8	1.84	0.43
1:AA:1575:A:N6	1:AA:1576:G:O6	2.52	0.43
1:AA:2196:C:O2'	1:AA:2270:A:N3	2.42	0.43
27:Aa:80:VAL:HG13	27:Aa:101:PRO:HG3	2.00	0.43
45:BA:905:A:H5''	60:BP:52:ARG:HD3	2.01	0.43
45:BA:1171:A:O2'	45:BA:1570:A:N3	2.47	0.43
45:BA:1555:A:O2'	61:BQ:82:ASN:ND2	2.46	0.43
47:BC:62:LYS:HD2	47:BC:96:LEU:HD13	2.01	0.43
52:BH:193:LEU:HD23	52:BH:193:LEU:HA	1.83	0.43
79:Bi:901:LEU:HD23	79:Bi:1011:ILE:HD12	1.99	0.43
1:AA:1057:A:OP1	9:AI:98:LYS:NZ	2.44	0.42
1:AA:1805:C:H2'	1:AA:1806:A:H8	1.84	0.42
1:AA:2228:A:H2'	1:AA:2229:A:C8	2.54	0.42
1:AA:3276:G:O6	18:AR:171:ARG:NH1	2.51	0.42
13:AM:60:ARG:N	13:AM:63:GLU:OE1	2.42	0.42
14:AN:177:LYS:HG3	37:Ak:11:LEU:HD13	1.99	0.42
29:Ac:125:VAL:HG21	29:Ac:138:ILE:HD13	2.01	0.42
45:BA:824:G:C2	45:BA:849:C:C2	3.07	0.42
59:BO:102:LEU:HD23	59:BO:102:LEU:HA	1.87	0.42
70:BZ:76:TYR:OH	70:BZ:86:GLU:OE2	2.33	0.42
1:AA:63:A:H5''	16:AP:174:ILE:HG21	2.00	0.42
1:AA:129:U:H2'	1:AA:130:A:C8	2.54	0.42
1:AA:717:C:OP1	1:AA:751:A:O2'	2.37	0.42
1:AA:1659:U:H3	1:AA:1790:G:H1	1.67	0.42
1:AA:1786:G:H2'	1:AA:1787:A:C8	2.54	0.42
1:AA:2207:A:H2'	1:AA:2208:A:H8	1.84	0.42
1:AA:2444:C:N4	1:AA:2503:G:H21	2.18	0.42
3:AC:141:C:OP1	16:AP:109:ARG:NH2	2.49	0.42
5:AE:17:LEU:CB	5:AE:18:PRO:CD	2.92	0.42
8:AH:66:SER:C	8:AH:68:PRO:CD	2.63	0.42
48:BD:176:SER:N	48:BD:195:ASP:OD1	2.52	0.42
50:BF:188:ASN:HB3	50:BF:191:ARG:HG3	2.00	0.42
50:BF:238:LEU:HD23	50:BF:238:LEU:HA	1.87	0.42
53:BI:12:ALA:CB	53:BI:13:PRO:HD3	2.35	0.42
1:AA:65:A:N1	1:AA:109:A:O2'	2.52	0.42
1:AA:1054:A:H5''	1:AA:2637:A:H61	1.83	0.42
1:AA:1686:U:OP1	23:AW:42:LYS:NZ	2.36	0.42
1:AA:1899:G:O2'	1:AA:2334:U:O4	2.26	0.42
2:AB:4:U:H2'	2:AB:5:G:C8	2.54	0.42
9:AI:178:ILE:HG23	9:AI:183:ASP:HB3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AN:77:LEU:H	14:AN:77:LEU:HG	1.52	0.42
24:AX:79:VAL:HB	24:AX:118:VAL:HG13	2.01	0.42
29:Ac:24:LYS:O	29:Ac:26:ARG:HG2	2.19	0.42
45:BA:625:C:H2'	45:BA:626:U:C6	2.54	0.42
45:BA:902:G:OP1	60:BP:90:ARG:NH1	2.49	0.42
47:BC:41:ARG:HH21	47:BC:232:HIS:HD2	1.68	0.42
48:BD:111:VAL:HG21	48:BD:218:ILE:HD12	2.00	0.42
50:BF:127:LYS:N	50:BF:140:VAL:O	2.49	0.42
62:BR:127:LYS:HA	62:BR:134:ALA:HA	2.02	0.42
62:BR:129:PHE:O	62:BR:137:ARG:NH1	2.52	0.42
79:Bi:331:LYS:HE2	79:Bi:331:LYS:HB2	1.85	0.42
79:Bi:541:GLN:HA	79:Bi:544:PHE:CD2	2.54	0.42
79:Bi:579:LEU:HD22	79:Bi:613:LEU:HD13	2.01	0.42
1:AA:411:U:H2'	1:AA:412:G:C8	2.55	0.42
1:AA:412:G:OP1	18:AR:62:ARG:NH1	2.53	0.42
1:AA:1596:C:H2'	1:AA:1597:C:C6	2.55	0.42
1:AA:2433:U:H1'	16:AP:125:SER:HB3	2.00	0.42
6:AF:187:LEU:HD23	6:AF:187:LEU:HA	1.91	0.42
9:AI:180:SER:OG	9:AI:183:ASP:OD2	2.28	0.42
13:AM:75:LYS:HE2	13:AM:75:LYS:HB3	1.77	0.42
16:AP:19:LEU:HD23	16:AP:19:LEU:HA	1.79	0.42
16:AP:31:ARG:NH1	16:AP:124:ASP:OD2	2.45	0.42
45:BA:549:G:O2'	45:BA:556:A:N1	2.47	0.42
45:BA:844:A:H2'	45:BA:845:G:H8	1.84	0.42
45:BA:1175:U:H2'	45:BA:1176:G:H8	1.84	0.42
45:BA:1295:G:P	46:BB:109:ASN:HD22	2.42	0.42
45:BA:1591:C:H2'	45:BA:1592:A:C8	2.54	0.42
59:BO:23:PRO:CD	59:BO:24:ALA:N	2.81	0.42
79:Bi:142:SER:HB2	79:Bi:145:LEU:HD12	2.01	0.42
79:Bi:950:ARG:HH21	79:Bi:995:GLU:HG2	1.84	0.42
1:AA:1080:A:H5'	7:AG:139:PRO:HB3	2.01	0.42
1:AA:2526:C:OP1	4:AD:37:ARG:NH1	2.45	0.42
1:AA:2828:G:OP2	12:AL:7:ARG:NH2	2.48	0.42
5:AE:20:LYS:HB2	5:AE:20:LYS:HE3	1.86	0.42
6:AF:233:LEU:HD23	6:AF:233:LEU:HA	1.85	0.42
9:AI:151:ARG:NH1	9:AI:206:LYS:O	2.52	0.42
10:AJ:162:LEU:HD21	16:AP:45:PRO:HG2	2.01	0.42
45:BA:523:G:OP2	70:BZ:37:LYS:NZ	2.37	0.42
68:BX:27:ILE:HD11	68:BX:61:ILE:CG2	2.49	0.42
1:AA:874:U:OP2	1:AA:1907:C:O2'	2.32	0.42
1:AA:1336:U:H2'	1:AA:1337:A:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:139:GLN:HE22	5:AE:142:ALA:HB3	1.84	0.42
5:AE:349:LYS:HB3	5:AE:349:LYS:HE2	1.83	0.42
18:AR:85:ALA:O	18:AR:89:LYS:HG3	2.20	0.42
21:AU:166:LYS:H	21:AU:166:LYS:HG2	1.70	0.42
21:AU:167:ARG:HG3	21:AU:168:PRO:HD2	2.00	0.42
42:Ap:16:LYS:HB2	42:Ap:16:LYS:HE3	1.83	0.42
45:BA:918:U:H4'	60:BP:18:ARG:HD3	2.02	0.42
49:BE:78:LYS:HA	49:BE:78:LYS:HD2	1.71	0.42
62:BR:100:GLN:O	62:BR:104:GLU:HG2	2.18	0.42
65:BU:108:LEU:HD23	65:BU:111:ILE:HD11	2.02	0.42
69:BY:41:SER:O	69:BY:43:PHE:N	2.52	0.42
70:BZ:35:VAL:HG23	70:BZ:36:SER:H	1.85	0.42
76:Bf:51:ASN:OD1	76:Bf:51:ASN:N	2.51	0.42
79:Bi:713:GLN:CG	79:Bi:1062:TYR:HB3	2.49	0.42
79:Bi:933:ILE:HD12	79:Bi:984:PHE:HE2	1.85	0.42
1:AA:29:C:H4'	1:AA:62:A:H4'	2.02	0.42
1:AA:89:A:N7	19:AS:171:LYS:NZ	2.57	0.42
1:AA:1235:U:H3	1:AA:1263:A:H62	1.68	0.42
5:AE:78:VAL:HG22	5:AE:323:MET:HG3	2.01	0.42
5:AE:158:VAL:HB	5:AE:191:LYS:HD3	2.02	0.42
6:AF:150:LEU:O	6:AF:250:TRP:HD1	2.02	0.42
16:AP:75:VAL:HA	16:AP:76:PRO:HD3	1.83	0.42
20:AT:99:LEU:HG	20:AT:103:ARG:HE	1.84	0.42
21:AU:73:LYS:HB3	21:AU:128:GLU:HG3	2.01	0.42
31:Ae:20:SER:O	31:Ae:20:SER:OG	2.33	0.42
45:BA:64:U:O2'	45:BA:168:A:N3	2.49	0.42
45:BA:393:C:H2'	45:BA:394:C:C6	2.55	0.42
45:BA:843:U:H2'	45:BA:844:A:C8	2.54	0.42
55:BK:81:VAL:HG23	55:BK:86:LEU:HD23	2.01	0.42
55:BK:169:PRO:HG2	55:BK:174:ARG:HH21	1.84	0.42
56:BL:31:LYS:HD3	56:BL:31:LYS:HA	1.74	0.42
69:BY:41:SER:O	69:BY:41:SER:OG	2.29	0.42
69:BY:142:LYS:O	69:BY:144:ARG:NH1	2.52	0.42
74:Bd:64:ARG:HA	74:Bd:64:ARG:HD2	1.83	0.42
77:Bg:144:CYS:HB3	77:Bg:147:VAL:HG23	2.00	0.42
79:Bi:259:PRO:HD2	79:Bi:262:ALA:HB3	2.01	0.42
1:AA:255:A:H2'	1:AA:256:G:C8	2.55	0.42
1:AA:655:C:H5''	33:Ag:26:HIS:HB2	2.02	0.42
1:AA:1798:A:H2'	1:AA:1799:A:C8	2.55	0.42
1:AA:2174:G:P	4:AD:193:ARG:HH11	2.43	0.42
1:AA:3151:U:H4'	1:AA:3294:A:H1'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AP:120:TRP:HZ2	16:AP:123:GLN:HG2	1.85	0.42
34:Ah:103:TYR:CE1	34:Ah:104:PRO:HD3	2.36	0.42
35:Ai:41:ARG:HE	35:Ai:41:ARG:HB3	1.72	0.42
45:BA:871:G:H2'	45:BA:872:G:C8	2.55	0.42
45:BA:1160:A:H2'	45:BA:1161:C:C6	2.55	0.42
48:BD:50:ILE:HG22	48:BD:72:LEU:HD21	2.01	0.42
50:BF:196:VAL:N	50:BF:209:HIS:O	2.31	0.42
57:BM:26:LYS:HA	57:BM:26:LYS:HD3	1.76	0.42
71:Ba:54:VAL:HG13	71:Ba:60:VAL:HG21	2.02	0.42
79:Bi:1058:GLN:HE21	79:Bi:1087:HIS:CE1	2.37	0.42
1:AA:1631:C:H5''	1:AA:1632:A:H5''	2.00	0.42
1:AA:2103:U:H2'	1:AA:2104:A:C8	2.55	0.42
1:AA:2812:C:H2'	1:AA:2813:A:C8	2.55	0.42
1:AA:3299:A:H61	1:AA:3315:G:H1	1.68	0.42
4:AD:186:PHE:N	4:AD:196:TRP:CH2	2.88	0.42
11:AK:41:ILE:HG23	11:AK:43:VAL:HG13	2.02	0.42
21:AU:22:PRO:O	22:AV:146:ASN:ND2	2.37	0.42
23:AW:32:SER:OG	23:AW:83:TYR:OH	2.36	0.42
49:BE:213:GLU:OE2	63:BS:72:LYS:NZ	2.53	0.42
52:BH:98:ARG:NH1	52:BH:101:ILE:O	2.40	0.42
54:BJ:106:ALA:HB2	54:BJ:165:LEU:HG	2.01	0.42
58:BN:59:LEU:HA	58:BN:87:PRO:HG2	2.02	0.42
64:BT:87:ASN:OD1	64:BT:99:HIS:ND1	2.52	0.42
70:BZ:49:LYS:HE2	70:BZ:49:LYS:HB2	1.83	0.42
71:Ba:85:LYS:HE3	71:Ba:85:LYS:HB2	1.92	0.42
78:Bh:172:ALA:HB1	78:Bh:199:ILE:HB	2.02	0.42
78:Bh:295:SER:OG	78:Bh:297:ASP:OD1	2.31	0.42
79:Bi:1032:SER:HB2	80:Bi:1202:ATP:HN61	1.85	0.42
1:AA:900:G:H1'	1:AA:1589:A:N6	2.35	0.42
1:AA:1251:A:C6	1:AA:1252:A:H1'	2.55	0.42
1:AA:2357:A:H2'	1:AA:2358:A:C8	2.54	0.42
5:AE:81:THR:O	5:AE:81:THR:OG1	2.36	0.42
5:AE:266:ARG:HD3	5:AE:266:ARG:HA	1.88	0.42
8:AH:169:ASP:HB3	8:AH:174:LEU:HD11	2.02	0.42
10:AJ:92:LYS:HE3	10:AJ:92:LYS:HB3	1.84	0.42
32:Af:102:LYS:HB3	32:Af:102:LYS:HE3	1.95	0.42
37:Ak:20:MET:HE2	37:Ak:20:MET:HB3	1.82	0.42
45:BA:97:C:O2	45:BA:425:A:O2'	2.35	0.42
54:BJ:153:GLU:HG2	54:BJ:156:VAL:HG23	2.01	0.42
58:BN:133:LEU:O	58:BN:137:MET:HB2	2.20	0.42
60:BP:30:VAL:H	60:BP:30:VAL:HG22	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:BP:107:ARG:HH22	74:Bd:38:ARG:NH1	2.17	0.42
64:BT:82:PRO:HD2	64:BT:85:PHE:HB2	2.00	0.42
67:BW:17:CYS:HB2	67:BW:56:SER:HB3	2.02	0.42
78:Bh:309:VAL:O	78:Bh:311:ARG:NH1	2.53	0.42
79:Bi:490:ILE:HD12	79:Bi:490:ILE:HA	1.94	0.42
79:Bi:801:LEU:HD13	79:Bi:838:LEU:HD11	2.01	0.42
79:Bi:1034:SER:HB3	80:Bi:1202:ATP:H5'2	2.02	0.42
1:AA:87:U:H2'	1:AA:88:A:C8	2.55	0.41
1:AA:633:C:O2'	34:Ah:21:ARG:O	2.36	0.41
1:AA:2146:C:O3'	4:AD:199:THR:HG23	2.19	0.41
1:AA:2947:G:N3	5:AE:250:ALA:HB1	2.34	0.41
1:AA:3015:G:H2'	1:AA:3016:A:C8	2.55	0.41
6:AF:136:LEU:HD23	6:AF:136:LEU:HA	1.93	0.41
13:AM:20:ASN:HB3	13:AM:126:ASP:HB2	2.01	0.41
16:AP:184:LYS:HB2	16:AP:184:LYS:HE3	1.81	0.41
17:AQ:127:LEU:HD21	21:AU:168:PRO:HB2	2.02	0.41
43:Aq:46:LYS:HE2	43:Aq:54:THR:HB	2.02	0.41
44:Ar:84:ARG:O	44:Ar:88:GLU:HG2	2.20	0.41
47:BC:82:ARG:NH1	47:BC:191:GLU:OE1	2.46	0.41
60:BP:17:ALA:HB3	60:BP:81:VAL:HA	2.02	0.41
64:BT:20:THR:OG1	64:BT:21:ASN:N	2.53	0.41
79:Bi:541:GLN:O	79:Bi:544:PHE:HB2	2.20	0.41
1:AA:359:U:O2'	38:Al:16:HIS:ND1	2.41	0.41
1:AA:411:U:H2'	1:AA:412:G:H8	1.85	0.41
1:AA:671:U:H2'	1:AA:672:A:C8	2.54	0.41
5:AE:284:ARG:HB3	5:AE:323:MET:HB3	2.01	0.41
5:AE:385:LYS:HE3	5:AE:385:LYS:HB2	1.82	0.41
11:AK:152:GLU:O	11:AK:156:GLN:HB2	2.21	0.41
13:AM:160:VAL:HG12	13:AM:164:LYS:HD3	2.02	0.41
18:AR:168:LEU:O	18:AR:173:ARG:NH2	2.53	0.41
22:AV:40:VAL:HG21	22:AV:96:ILE:HD11	2.02	0.41
22:AV:66:ASN:O	22:AV:73:GLY:N	2.42	0.41
34:Ah:68:TRP:CZ3	34:Ah:103:TYR:OH	2.71	0.41
45:BA:419:G:O5'	52:BH:72:ARG:NH2	2.53	0.41
45:BA:487:G:H3'	45:BA:488:G:H5''	2.02	0.41
45:BA:1605:G:OP2	62:BR:127:LYS:NZ	2.53	0.41
48:BD:54:GLU:O	48:BD:58:LEU:HB2	2.20	0.41
51:BG:109:LYS:HZ3	51:BG:109:LYS:HG3	1.62	0.41
54:BJ:168:CYS:O	54:BJ:181:GLY:HA3	2.20	0.41
55:BK:132:ARG:HD2	55:BK:142:ASN:HD22	1.85	0.41
59:BO:87:ASP:OD1	59:BO:87:ASP:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:BT:36:LYS:HB2	64:BT:102:ALA:HA	2.01	0.41
73:Bc:61:THR:HG23	73:Bc:62:ILE:H	1.84	0.41
79:Bi:158:LYS:HA	79:Bi:161:ILE:HG22	2.01	0.41
1:AA:216:G:OP1	27:Aa:16:ARG:NH1	2.54	0.41
6:AF:29:PRO:O	6:AF:124:SER:OG	2.28	0.41
13:AM:82:ARG:NH1	13:AM:113:GLY:CA	2.83	0.41
33:Ag:79:VAL:HG23	33:Ag:111:ARG:HG2	2.02	0.41
35:Ai:58:ARG:HD2	35:Ai:58:ARG:HA	1.87	0.41
40:An:30:ARG:HH21	40:An:33:ASN:HD22	1.68	0.41
45:BA:683:C:H2'	45:BA:684:A:C8	2.55	0.41
45:BA:780:A:C8	70:BZ:8:ARG:HD2	2.56	0.41
45:BA:1556:A:OP1	61:BQ:115:TYR:OH	2.29	0.41
45:BA:1776:A:H2'	45:BA:1777:G:C8	2.55	0.41
45:BA:1785:U:OP1	60:BP:136:ARG:NH2	2.43	0.41
46:BB:20:ALA:HB1	46:BB:168:HIS:HB3	2.02	0.41
60:BP:31:THR:HG22	60:BP:38:THR:HB	2.02	0.41
63:BS:71:PHE:HD1	63:BS:72:LYS:H	1.68	0.41
79:Bi:394:LEU:HD22	79:Bi:438:VAL:HG21	2.02	0.41
79:Bi:610:LYS:HE2	79:Bi:610:LYS:HB2	1.84	0.41
79:Bi:815:THR:O	79:Bi:833:SER:OG	2.28	0.41
1:AA:1366:A:O2'	33:Ag:45:ARG:NH2	2.53	0.41
1:AA:2112:U:H4'	1:AA:2113:A:H5'	2.03	0.41
8:AH:170:LYS:HB3	8:AH:172:HIS:CE1	2.55	0.41
10:AJ:61:GLN:HA	10:AJ:64:ILE:HB	2.03	0.41
21:AU:23:LYS:HD3	21:AU:23:LYS:HA	1.85	0.41
32:Af:47:ASP:OD2	32:Af:86:LYS:NZ	2.54	0.41
34:Ah:20:LYS:HB2	34:Ah:20:LYS:HE2	1.82	0.41
45:BA:1650:U:H2'	45:BA:1651:A:C8	2.55	0.41
48:BD:35:TRP:CE2	48:BD:37:PRO:HB3	2.56	0.41
51:BG:144:GLU:OE1	51:BG:225:ARG:NH2	2.49	0.41
68:BX:22:LYS:HD3	73:Bc:3:LEU:HA	2.01	0.41
69:BY:62:LYS:HE3	69:BY:118:PRO:HG3	2.03	0.41
79:Bi:713:GLN:HA	79:Bi:714:PRO:HD3	1.67	0.41
1:AA:13:A:H4'	26:AZ:39:LYS:HD2	2.02	0.41
1:AA:745:C:H2'	1:AA:746:A:H8	1.84	0.41
1:AA:1001:G:H1'	1:AA:1041:U:H5'	2.03	0.41
1:AA:1249:G:H2'	1:AA:1250:G:C8	2.55	0.41
1:AA:1383:G:O3'	6:AF:138:ARG:NH2	2.53	0.41
1:AA:2129:U:H2'	1:AA:2130:G:C8	2.55	0.41
1:AA:3281:U:H2'	1:AA:3282:U:C6	2.56	0.41
1:AA:3295:A:H2'	1:AA:3296:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:117:GLU:HG2	4:AD:124:GLY:H	1.85	0.41
7:AG:60:ILE:HD11	7:AG:93:THR:HA	2.03	0.41
12:AL:34:TYR:HD2	12:AL:89:VAL:HB	1.85	0.41
21:AU:27:MET:HE2	21:AU:27:MET:HB3	1.85	0.41
45:BA:67:A:O2'	45:BA:69:G:OP1	2.36	0.41
45:BA:1101:G:H5''	68:BX:76:SER:HB3	2.03	0.41
45:BA:1482:C:N4	45:BA:1524:A:OP2	2.40	0.41
45:BA:1789:G:OP2	60:BP:132:ARG:NH2	2.54	0.41
58:BN:90:LYS:HE2	58:BN:90:LYS:HB2	1.85	0.41
63:BS:23:LYS:HG2	78:Bh:198:ASN:HD21	1.85	0.41
64:BT:87:ASN:OD1	64:BT:87:ASN:N	2.48	0.41
77:Bg:113:LYS:H	77:Bg:113:LYS:HG2	1.33	0.41
78:Bh:106:HIS:NE2	78:Bh:124:SER:OG	2.36	0.41
78:Bh:281:TYR:HD2	78:Bh:287:PRO:HD3	1.85	0.41
79:Bi:977:ASP:HA	79:Bi:980:VAL:HG22	2.03	0.41
1:AA:361:A:O3'	38:Al:45:ARG:NH2	2.53	0.41
6:AF:26:PHE:HA	6:AF:127:ALA:HA	2.01	0.41
11:AK:106:LYS:HE3	11:AK:106:LYS:HB3	1.94	0.41
12:AL:146:ASP:O	12:AL:149:VAL:HB	2.20	0.41
14:AN:76:THR:O	14:AN:79:GLU:N	2.44	0.41
26:AZ:96:LYS:HB3	26:AZ:96:LYS:HE3	1.85	0.41
33:Ag:99:ASN:OD1	33:Ag:99:ASN:N	2.45	0.41
34:Ah:17:GLN:O	34:Ah:24:ASN:N	2.52	0.41
46:BB:182:LEU:HA	46:BB:182:LEU:HD23	1.82	0.41
48:BD:99:LYS:HB2	48:BD:117:THR:HG22	2.02	0.41
49:BE:21:LEU:HD23	49:BE:21:LEU:HA	1.87	0.41
55:BK:148:VAL:HG11	55:BK:156:ILE:HD11	2.01	0.41
67:BW:69:LEU:HD23	67:BW:69:LEU:HA	1.82	0.41
69:BY:65:ASN:HD22	69:BY:116:ASP:CG	2.27	0.41
1:AA:20:A:H2'	1:AA:21:G:C8	2.55	0.41
1:AA:118:U:O2	1:AA:121:A:H5'	2.21	0.41
1:AA:2242:A:H5''	4:AD:244:GLY:HA3	2.03	0.41
1:AA:3002:C:O2'	5:AE:180:GLU:OE2	2.32	0.41
1:AA:3033:A:H2'	1:AA:3034:C:H6	1.85	0.41
1:AA:3045:G:H5''	5:AE:19:ARG:NH1	2.35	0.41
2:AB:27:A:O3'	13:AM:141:ARG:NH1	2.53	0.41
4:AD:8:GLN:NE2	4:AD:231:SER:OG	2.53	0.41
4:AD:27:ALA:O	4:AD:128:ARG:NH2	2.36	0.41
5:AE:76:VAL:HG12	5:AE:325:LYS:HA	2.02	0.41
5:AE:168:LYS:HB3	5:AE:319:ASN:HD21	1.86	0.41
6:AF:33:ASP:N	6:AF:33:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AU:92:LYS:NZ	21:AU:109:ASP:OD2	2.41	0.41
27:Aa:31:LEU:HB3	27:Aa:101:PRO:HG2	2.02	0.41
27:Aa:87:LYS:HD2	27:Aa:87:LYS:HA	1.84	0.41
45:BA:478:A:OP1	76:Bf:37:ARG:NH1	2.53	0.41
45:BA:1164:G:H2'	45:BA:1165:G:C8	2.56	0.41
45:BA:1393:C:H2'	45:BA:1394:G:H8	1.86	0.41
56:BL:44:LYS:HA	56:BL:44:LYS:HD3	1.86	0.41
67:BW:40:ASP:HB3	67:BW:46:ILE:HD11	2.03	0.41
78:Bh:46:LYS:HB3	78:Bh:46:LYS:HE3	1.89	0.41
79:Bi:540:SER:O	79:Bi:544:PHE:CD2	2.74	0.41
79:Bi:905:TYR:OH	79:Bi:1045:GLY:O	2.35	0.41
1:AA:1721:U:OP2	20:AT:124:TYR:OH	2.31	0.41
1:AA:2103:U:H2'	1:AA:2104:A:H8	1.85	0.41
1:AA:2552:C:H2'	31:Ae:50:VAL:HG11	2.03	0.41
1:AA:2741:C:O2'	43:Aq:20:HIS:ND1	2.40	0.41
1:AA:3121:U:H1'	1:AA:3122:A:H5''	2.01	0.41
2:AB:84:A:H2'	2:AB:85:G:C8	2.55	0.41
6:AF:151:VAL:CG1	6:AF:250:TRP:O	2.69	0.41
9:AI:223:PHE:HD2	21:AU:35:VAL:HG11	1.86	0.41
13:AM:87:LYS:HD3	13:AM:87:LYS:HA	1.90	0.41
16:AP:50:ARG:HE	16:AP:50:ARG:HB3	1.68	0.41
45:BA:1234:A:N3	77:Bg:140:TYR:OH	2.42	0.41
45:BA:1542:G:H22	45:BA:1568:C:H1'	1.86	0.41
45:BA:1755:A:H8	69:BY:63:GLN:NE2	2.19	0.41
48:BD:56:ILE:HG23	48:BD:61:LEU:HB2	2.03	0.41
53:BI:63:PRO:C	53:BI:64:VAL:HG23	2.45	0.41
78:Bh:93:ASP:HB3	78:Bh:96:THR:HG22	2.03	0.41
1:AA:528:U:H2'	1:AA:529:A:C8	2.55	0.41
1:AA:531:G:H2'	1:AA:532:A:C8	2.56	0.41
1:AA:876:A:H5''	1:AA:1890:U:H5''	2.03	0.41
1:AA:896:A:H5'	4:AD:183:GLY:HA2	2.02	0.41
1:AA:1748:G:OP2	39:Am:42:LYS:NZ	2.52	0.41
1:AA:3251:U:H2'	1:AA:3252:G:C8	2.56	0.41
4:AD:117:GLU:HB2	4:AD:162:ALA:HB1	2.02	0.41
5:AE:16:PHE:CZ	5:AE:275:ARG:HD2	2.48	0.41
5:AE:223:GLY:HA2	5:AE:271:GLY:HA3	2.02	0.41
7:AG:25:GLU:HB2	7:AG:27:LYS:HG3	2.03	0.41
7:AG:275:THR:OG1	7:AG:276:LYS:N	2.54	0.41
8:AH:52:VAL:HG11	8:AH:65:ILE:CD1	2.50	0.41
11:AK:41:ILE:HD12	11:AK:41:ILE:HA	1.94	0.41
12:AL:153:ARG:O	12:AL:156:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:78:GLU:O	13:AM:82:ARG:HB2	2.21	0.41
14:AN:76:THR:O	14:AN:78:ALA:N	2.53	0.41
29:Ac:77:LYS:C	29:Ac:79:TRP:H	2.29	0.41
45:BA:848:C:C4	45:BA:849:C:C5	3.08	0.41
45:BA:1592:A:H2'	45:BA:1593:A:C8	2.55	0.41
45:BA:1609:U:H5''	62:BR:75:VAL:HB	2.02	0.41
46:BB:50:VAL:HG23	63:BS:109:LEU:HD21	2.03	0.41
47:BC:100:PHE:HD2	47:BC:181:LEU:HD12	1.85	0.41
50:BF:181:VAL:HG12	50:BF:194:THR:H	1.86	0.41
52:BH:7:TYR:HD1	52:BH:113:ILE:HB	1.86	0.41
52:BH:50:PHE:HB3	52:BH:111:LEU:HB3	2.03	0.41
57:BM:78:THR:HA	57:BM:84:ILE:HG22	2.03	0.41
58:BN:130:THR:OG1	58:BN:131:ASP:N	2.53	0.41
69:BY:52:ILE:HG12	69:BY:101:GLU:HG2	2.02	0.41
79:Bi:167:GLU:HA	79:Bi:170:LYS:HG3	2.02	0.41
1:AA:26:A:N3	1:AA:328:U:O2'	2.46	0.41
1:AA:1912:U:O2'	1:AA:2121:G:N7	2.52	0.41
1:AA:2344:U:H2'	1:AA:2345:A:C8	2.55	0.41
4:AD:198:LYS:O	4:AD:198:LYS:HG2	2.21	0.41
5:AE:86:VAL:HG22	5:AE:162:VAL:HG12	2.02	0.41
8:AH:55:LEU:HD21	8:AH:145:LEU:HD11	2.03	0.41
12:AL:142:ASP:O	12:AL:145:LYS:HB2	2.20	0.41
24:AX:23:MET:HE1	24:AX:78:VAL:HG22	2.01	0.41
28:Ab:104:PRO:HA	28:Ab:107:ARG:HG3	2.03	0.41
39:Am:63:LYS:HB3	39:Am:63:LYS:HE3	1.86	0.41
45:BA:78:A:H2'	45:BA:79:C:H6	1.85	0.41
45:BA:1171:A:H2'	45:BA:1172:G:H8	1.84	0.41
46:BB:201:LEU:HD12	46:BB:201:LEU:HA	1.92	0.41
50:BF:244:ILE:HD13	50:BF:244:ILE:HA	1.91	0.41
52:BH:21:GLU:HA	52:BH:24:ILE:HD12	2.02	0.41
52:BH:124:LEU:HD13	52:BH:124:LEU:HA	1.94	0.41
55:BK:141:VAL:HG12	55:BK:143:ILE:H	1.86	0.41
64:BT:132:ARG:HD3	64:BT:132:ARG:HA	1.73	0.41
68:BX:27:ILE:H	68:BX:27:ILE:HG12	1.63	0.41
78:Bh:260:ILE:HB	78:Bh:274:LEU:HB2	2.02	0.41
1:AA:255:A:H2'	1:AA:256:G:H8	1.87	0.40
1:AA:664:U:H5'	6:AF:107:ARG:HA	2.02	0.40
1:AA:1119:C:H2'	1:AA:1120:A:C8	2.57	0.40
1:AA:1276:U:H2'	1:AA:1277:C:C6	2.56	0.40
1:AA:3006:A:H2'	1:AA:3007:U:O4'	2.21	0.40
1:AA:3111:U:OP1	11:AK:184:LYS:NZ	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:196:TRP:C	4:AD:196:TRP:CD1	2.99	0.40
4:AD:201:GLY:HA2	4:AD:204:MET:HG3	2.03	0.40
6:AF:22:LEU:HD23	6:AF:22:LEU:HA	1.91	0.40
33:Ag:6:HIS:ND1	33:Ag:7:PRO:O	2.54	0.40
37:Ak:97:SER:OG	37:Ak:98:ARG:N	2.52	0.40
45:BA:641:G:O6	45:BA:693:U:O2	2.39	0.40
45:BA:826:U:H2'	45:BA:827:C:H6	1.86	0.40
47:BC:180:THR:O	47:BC:183:GLN:N	2.54	0.40
59:BO:91:LEU:HD23	59:BO:91:LEU:HA	1.88	0.40
68:BX:30:SER:HG	68:BX:61:ILE:CD1	2.34	0.40
69:BY:3:LYS:HD2	69:BY:3:LYS:HA	1.83	0.40
79:Bi:165:ILE:HD11	79:Bi:210:ASN:HB3	2.03	0.40
1:AA:1660:C:H2'	1:AA:1661:G:C8	2.55	0.40
1:AA:2218:G:H2'	1:AA:2219:A:C8	2.57	0.40
1:AA:2335:G:N2	1:AA:2339:C:O2'	2.54	0.40
1:AA:3368:U:H4'	1:AA:3369:G:H5'	2.03	0.40
5:AE:53:MET:HE1	5:AE:327:CYS:HA	2.03	0.40
9:AI:178:ILE:HD11	9:AI:187:GLU:HG2	2.03	0.40
28:Ab:109:GLU:OE2	28:Ab:112:LYS:NZ	2.55	0.40
39:Am:73:LEU:HD12	39:Am:73:LEU:HA	1.93	0.40
45:BA:334:G:N7	54:BJ:5:ARG:NH2	2.68	0.40
46:BB:56:LYS:HB3	46:BB:56:LYS:HE3	1.91	0.40
46:BB:126:PRO:HG2	46:BB:151:SER:HB2	2.02	0.40
47:BC:50:LYS:HD3	47:BC:50:LYS:HA	1.89	0.40
47:BC:97:LEU:HD12	47:BC:232:HIS:CD2	2.56	0.40
48:BD:211:LEU:HA	48:BD:211:LEU:HD23	1.86	0.40
53:BI:9:LEU:HG	53:BI:11:GLN:O	2.20	0.40
54:BJ:83:TYR:HB2	54:BJ:196:LEU:HD11	2.03	0.40
59:BO:23:PRO:HD2	59:BO:24:ALA:N	2.37	0.40
61:BQ:41:VAL:HG22	61:BQ:84:ILE:HD13	2.03	0.40
79:Bi:359:PRO:HA	79:Bi:362:VAL:HG23	2.03	0.40
1:AA:300:G:H2'	1:AA:301:G:H8	1.86	0.40
1:AA:341:G:O2'	3:AC:22:U:O4	2.29	0.40
1:AA:422:A:C2	1:AA:2363:A:H4'	2.55	0.40
1:AA:1717:U:H3	1:AA:1727:G:H1	1.68	0.40
1:AA:1724:U:H1'	1:AA:1725:C:C6	2.57	0.40
7:AG:40:HIS:CD2	22:AV:69:LYS:HA	2.56	0.40
10:AJ:30:THR:O	10:AJ:30:THR:OG1	2.32	0.40
14:AN:162:ASN:OD1	14:AN:162:ASN:N	2.54	0.40
31:Ae:95:ALA:HB2	31:Ae:101:LEU:HD23	2.03	0.40
43:Aq:7:THR:HB	43:Aq:22:GLN:HE21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:590:C:H2'	45:BA:591:A:C8	2.56	0.40
45:BA:918:U:H2'	45:BA:919:A:C8	2.56	0.40
52:BH:85:ARG:HB3	52:BH:87:ARG:HH12	1.87	0.40
52:BH:147:LEU:HD23	52:BH:147:LEU:HA	1.89	0.40
64:BT:132:ARG:HH21	64:BT:145:ARG:HE	1.69	0.40
70:BZ:41:ARG:HB3	70:BZ:52:LYS:HG3	2.04	0.40
79:Bi:263:LEU:HD12	79:Bi:267:VAL:HG21	2.04	0.40
1:AA:525:C:OP2	15:AO:77:ARG:NH2	2.48	0.40
1:AA:1345:G:H21	6:AF:307:GLN:HE22	1.70	0.40
1:AA:1560:G:N1	1:AA:1580:A:N1	2.70	0.40
1:AA:1569:U:H5''	1:AA:1570:U:C6	2.56	0.40
1:AA:2136:C:O2	1:AA:2143:A:N6	2.55	0.40
1:AA:2538:U:H3	1:AA:2542:U:H3	1.69	0.40
1:AA:2898:G:H5''	1:AA:2899:C:H5'	2.02	0.40
1:AA:3015:G:H2'	1:AA:3016:A:H8	1.86	0.40
1:AA:3044:G:H2'	1:AA:3045:G:C8	2.57	0.40
5:AE:19:ARG:HD2	5:AE:273:HIS:CD2	2.56	0.40
6:AF:60:THR:OG1	6:AF:61:SER:N	2.55	0.40
6:AF:269:SER:O	6:AF:269:SER:OG	2.36	0.40
25:AY:54:LEU:HD12	25:AY:54:LEU:HA	1.86	0.40
29:Ac:117:ARG:HA	29:Ac:117:ARG:HD3	1.93	0.40
43:Aq:28:TYR:HB3	43:Aq:69:VAL:HB	2.03	0.40
43:Aq:82:GLN:HE21	43:Aq:82:GLN:HB2	1.68	0.40
45:BA:78:A:H1'	52:BH:175:ILE:HG12	2.04	0.40
45:BA:1114:G:O2'	45:BA:1130:G:O6	2.27	0.40
45:BA:1202:A:H1'	45:BA:1207:C:H42	1.86	0.40
45:BA:1300:A:H5''	48:BD:117:THR:HG23	2.04	0.40
46:BB:17:LEU:HD22	46:BB:22:THR:HG21	2.04	0.40
56:BL:4:PRO:HG2	56:BL:7:ASP:HB2	2.03	0.40
58:BN:52:LEU:HB3	58:BN:78:LEU:HG	2.04	0.40
79:Bi:164:ILE:HA	79:Bi:167:GLU:HG3	2.04	0.40
79:Bi:652:PHE:HE2	79:Bi:696:LEU:HD21	1.86	0.40
1:AA:1597:C:H5'	1:AA:1696:A:H1'	2.03	0.40
1:AA:2538:U:HO2'	1:AA:2541:U:H3	1.68	0.40
1:AA:3163:A:N6	1:AA:3288:G:O6	2.54	0.40
10:AJ:240:ASN:OD1	10:AJ:240:ASN:N	2.44	0.40
28:Ab:56:LYS:HD2	28:Ab:56:LYS:HA	1.80	0.40
44:Ar:13:LYS:HE3	44:Ar:14:TYR:CZ	2.57	0.40
45:BA:1553:G:O6	61:BQ:40:ARG:NH2	2.54	0.40
46:BB:183:ARG:NH2	46:BB:193:GLN:O	2.54	0.40
50:BF:160:VAL:HG13	50:BF:169:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:Bi:841:ARG:NH1	79:Bi:1080:GLY:O	2.44	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	
4	AD	250/252 (99%)	233 (93%)	17 (7%)	0	100	100
5	AE	384/386 (100%)	359 (94%)	23 (6%)	2 (0%)	24	55
6	AF	359/361 (99%)	320 (89%)	33 (9%)	6 (2%)	7	30
7	AG	294/296 (99%)	266 (90%)	26 (9%)	2 (1%)	18	48
8	AH	152/175 (87%)	142 (93%)	9 (6%)	1 (1%)	18	48
9	AI	220/243 (90%)	204 (93%)	13 (6%)	3 (1%)	9	34
10	AJ	231/233 (99%)	214 (93%)	17 (7%)	0	100	100
11	AK	186/191 (97%)	173 (93%)	13 (7%)	0	100	100
12	AL	207/220 (94%)	194 (94%)	13 (6%)	0	100	100
13	AM	167/169 (99%)	144 (86%)	21 (13%)	2 (1%)	10	37
14	AN	191/198 (96%)	169 (88%)	19 (10%)	3 (2%)	7	31
15	AO	134/137 (98%)	123 (92%)	11 (8%)	0	100	100
16	AP	201/203 (99%)	188 (94%)	11 (6%)	2 (1%)	12	40
17	AQ	195/198 (98%)	185 (95%)	8 (4%)	2 (1%)	12	40
18	AR	181/183 (99%)	165 (91%)	16 (9%)	0	100	100
19	AS	183/185 (99%)	177 (97%)	6 (3%)	0	100	100
20	AT	150/188 (80%)	145 (97%)	5 (3%)	0	100	100
21	AU	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
22	AV	157/159 (99%)	146 (93%)	10 (6%)	1 (1%)	21	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	AW	98/120 (82%)	90 (92%)	8 (8%)	0	100	100
24	AX	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
25	AY	59/155 (38%)	59 (100%)	0	0	100	100
26	AZ	119/141 (84%)	114 (96%)	5 (4%)	0	100	100
27	Aa	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
28	Ab	133/135 (98%)	121 (91%)	11 (8%)	1 (1%)	16	44
29	Ac	146/148 (99%)	129 (88%)	16 (11%)	1 (1%)	18	48
30	Ad	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
31	Ae	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
32	Af	107/112 (96%)	100 (94%)	7 (6%)	0	100	100
33	Ag	125/129 (97%)	122 (98%)	3 (2%)	0	100	100
34	Ah	104/106 (98%)	94 (90%)	9 (9%)	1 (1%)	12	40
35	Ai	110/121 (91%)	106 (96%)	4 (4%)	0	100	100
36	Aj	117/119 (98%)	110 (94%)	7 (6%)	0	100	100
37	Ak	97/99 (98%)	88 (91%)	7 (7%)	2 (2%)	5	26
38	Al	85/87 (98%)	74 (87%)	9 (11%)	2 (2%)	4	24
39	Am	75/77 (97%)	70 (93%)	5 (7%)	0	100	100
40	An	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
41	Ao	50/127 (39%)	48 (96%)	2 (4%)	0	100	100
42	Ap	23/25 (92%)	23 (100%)	0	0	100	100
43	Aq	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
44	Ar	89/91 (98%)	84 (94%)	5 (6%)	0	100	100
46	BB	204/251 (81%)	171 (84%)	31 (15%)	2 (1%)	12	40
47	BC	212/254 (84%)	180 (85%)	32 (15%)	0	100	100
48	BD	215/253 (85%)	196 (91%)	18 (8%)	1 (0%)	24	55
49	BE	221/239 (92%)	207 (94%)	14 (6%)	0	100	100
50	BF	258/260 (99%)	229 (89%)	28 (11%)	1 (0%)	30	60
51	BG	204/224 (91%)	178 (87%)	22 (11%)	4 (2%)	6	27
52	BH	224/236 (95%)	207 (92%)	13 (6%)	4 (2%)	6	30
53	BI	182/189 (96%)	157 (86%)	18 (10%)	7 (4%)	2	16
54	BJ	184/199 (92%)	157 (85%)	26 (14%)	1 (0%)	24	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	BK	183/196 (93%)	156 (85%)	24 (13%)	3 (2%)	7	31
56	BL	94/105 (90%)	76 (81%)	16 (17%)	2 (2%)	5	26
57	BM	153/155 (99%)	140 (92%)	12 (8%)	1 (1%)	18	48
58	BN	122/142 (86%)	90 (74%)	29 (24%)	3 (2%)	4	23
59	BO	148/150 (99%)	138 (93%)	8 (5%)	2 (1%)	9	34
60	BP	125/136 (92%)	109 (87%)	16 (13%)	0	100	100
61	BQ	122/141 (86%)	104 (85%)	17 (14%)	1 (1%)	16	44
62	BR	139/142 (98%)	124 (89%)	14 (10%)	1 (1%)	18	48
63	BS	116/135 (86%)	103 (89%)	9 (8%)	4 (3%)	3	18
64	BT	143/145 (99%)	123 (86%)	16 (11%)	4 (3%)	4	21
65	BU	141/143 (99%)	131 (93%)	9 (6%)	1 (1%)	18	48
66	BV	105/120 (88%)	92 (88%)	13 (12%)	0	100	100
67	BW	85/87 (98%)	71 (84%)	11 (13%)	3 (4%)	3	17
68	BX	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
69	BY	142/144 (99%)	120 (84%)	20 (14%)	2 (1%)	9	34
70	BZ	132/134 (98%)	117 (89%)	12 (9%)	3 (2%)	5	25
71	Ba	68/107 (64%)	56 (82%)	12 (18%)	0	100	100
72	Bb	95/118 (80%)	77 (81%)	12 (13%)	6 (6%)	1	7
73	Bc	79/81 (98%)	67 (85%)	12 (15%)	0	100	100
74	Bd	61/66 (92%)	54 (88%)	7 (12%)	0	100	100
75	Be	51/55 (93%)	48 (94%)	3 (6%)	0	100	100
76	Bf	58/62 (94%)	48 (83%)	10 (17%)	0	100	100
77	Bg	55/151 (36%)	38 (69%)	15 (27%)	2 (4%)	2	17
78	Bh	316/318 (99%)	288 (91%)	27 (8%)	1 (0%)	36	66
79	Bi	948/972 (98%)	857 (90%)	90 (10%)	1 (0%)	48	76
All	All	11821/12759 (93%)	10708 (91%)	1022 (9%)	91 (1%)	18	44

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AE	19	ARG
6	AF	152	VAL
6	AF	339	LEU

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Mol	Chain	Res	Type
14	AN	63	VAL
17	AQ	111	PRO
34	Ah	106	ASN
46	BB	206	ASP
50	BF	195	ILE
51	BG	50	GLU
51	BG	51	VAL
53	BI	64	VAL
53	BI	111	LYS
56	BL	87	VAL
56	BL	88	PRO
59	BO	23	PRO
59	BO	24	ALA
63	BS	24	LEU
63	BS	87	GLU
64	BT	91	ASP
67	BW	82	VAL
69	BY	63	GLN
78	Bh	267	PRO
5	AE	18	PRO
6	AF	149	PRO
9	AI	233	GLU
14	AN	77	LEU
29	Ac	78	LEU
51	BG	127	GLN
52	BH	68	LEU
52	BH	149	LYS
52	BH	173	PRO
53	BI	155	ASP
55	BK	134	ILE
58	BN	130	THR
64	BT	92	ILE
67	BW	81	ASN
70	BZ	5	VAL
72	Bb	35	ALA
72	Bb	36	ILE
77	Bg	100	LEU
77	Bg	138	ARG
37	Ak	33	ALA
38	Al	42	ALA
53	BI	74	GLN
53	BI	131	PHE

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Mol	Chain	Res	Type
53	BI	134	GLU
54	BJ	148	ALA
55	BK	98	ALA
61	BQ	30	THR
64	BT	82	PRO
6	AF	151	VAL
7	AG	124	GLU
9	AI	158	LYS
9	AI	159	GLN
14	AN	76	THR
16	AP	74	PRO
37	AK	34	SER
46	BB	4	PRO
57	BM	6	THR
58	BN	127	GLY
58	BN	131	ASP
62	BR	33	GLY
63	BS	23	LYS
64	BT	102	ALA
69	BY	66	SER
8	AH	68	PRO
17	AQ	110	PRO
38	AI	41	ALA
51	BG	57	SER
65	BU	53	TRP
70	BZ	52	LYS
72	Bb	85	ARG
6	AF	130	ALA
13	AM	172	LEU
22	AV	125	ALA
48	BD	40	LYS
72	Bb	8	ASN
16	AP	75	VAL
28	Ab	103	GLN
79	Bi	713	GLN
7	AG	125	VAL
63	BS	88	VAL
67	BW	6	GLY
72	Bb	86	VAL
6	AF	131	VAL
13	AM	8	PRO
55	BK	162	SER

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Mol	Chain	Res	Type
70	BZ	35	VAL
52	BH	69	LEU
53	BI	112	ARG
72	Bb	97	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	
4	AD	193/194 (100%)	190 (98%)	3 (2%)	55	72
5	AE	319/322 (99%)	309 (97%)	10 (3%)	35	61
6	AF	288/288 (100%)	283 (98%)	5 (2%)	53	71
7	AG	244/244 (100%)	242 (99%)	2 (1%)	73	79
8	AH	134/152 (88%)	133 (99%)	1 (1%)	76	80
9	AI	186/204 (91%)	183 (98%)	3 (2%)	55	72
10	AJ	187/191 (98%)	184 (98%)	3 (2%)	55	72
11	AK	171/171 (100%)	168 (98%)	3 (2%)	51	70
12	AL	177/186 (95%)	177 (100%)	0	100	100
13	AM	147/147 (100%)	145 (99%)	2 (1%)	59	74
14	AN	154/158 (98%)	153 (99%)	1 (1%)	78	82
15	AO	107/108 (99%)	103 (96%)	4 (4%)	30	57
16	AP	175/175 (100%)	175 (100%)	0	100	100
17	AQ	160/161 (99%)	159 (99%)	1 (1%)	78	82
18	AR	140/145 (97%)	137 (98%)	3 (2%)	47	67
19	AS	150/150 (100%)	148 (99%)	2 (1%)	61	75
20	AT	126/153 (82%)	126 (100%)	0	100	100
21	AU	156/156 (100%)	155 (99%)	1 (1%)	78	82
22	AV	136/136 (100%)	133 (98%)	3 (2%)	45	66
23	AW	87/106 (82%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	AX	104/104 (100%)	104 (100%)	0	100	100
25	AY	54/129 (42%)	53 (98%)	1 (2%)	50	69
26	AZ	104/117 (89%)	104 (100%)	0	100	100
27	Aa	109/109 (100%)	108 (99%)	1 (1%)	70	78
28	Ab	115/115 (100%)	114 (99%)	1 (1%)	70	78
29	Ac	118/118 (100%)	117 (99%)	1 (1%)	73	79
30	Ad	46/46 (100%)	46 (100%)	0	100	100
31	Ae	81/87 (93%)	80 (99%)	1 (1%)	63	75
32	Af	92/96 (96%)	91 (99%)	1 (1%)	65	76
33	Ag	109/110 (99%)	109 (100%)	0	100	100
34	Ah	90/90 (100%)	86 (96%)	4 (4%)	25	54
35	Ai	95/103 (92%)	95 (100%)	0	100	100
36	Aj	104/104 (100%)	104 (100%)	0	100	100
37	Ak	81/81 (100%)	81 (100%)	0	100	100
38	Al	70/70 (100%)	69 (99%)	1 (1%)	59	74
39	Am	68/68 (100%)	68 (100%)	0	100	100
40	An	45/45 (100%)	45 (100%)	0	100	100
41	Ao	47/115 (41%)	47 (100%)	0	100	100
42	Ap	23/23 (100%)	23 (100%)	0	100	100
43	Aq	90/90 (100%)	90 (100%)	0	100	100
44	Ar	71/71 (100%)	71 (100%)	0	100	100
46	BB	164/209 (78%)	161 (98%)	3 (2%)	51	70
47	BC	191/223 (86%)	187 (98%)	4 (2%)	47	67
48	BD	176/204 (86%)	174 (99%)	2 (1%)	65	76
49	BE	182/194 (94%)	177 (97%)	5 (3%)	39	63
50	BF	221/221 (100%)	216 (98%)	5 (2%)	44	66
51	BG	173/190 (91%)	167 (96%)	6 (4%)	32	58
52	BH	188/201 (94%)	187 (100%)	1 (0%)	81	83
53	BI	165/169 (98%)	164 (99%)	1 (1%)	78	82
54	BJ	150/160 (94%)	149 (99%)	1 (1%)	76	80
55	BK	158/165 (96%)	158 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	BL	77/98 (79%)	76 (99%)	1 (1%)	61	75
57	BM	129/136 (95%)	127 (98%)	2 (2%)	55	72
58	BN	88/118 (75%)	86 (98%)	2 (2%)	44	66
59	BO	127/127 (100%)	127 (100%)	0	100	100
60	BP	81/104 (78%)	77 (95%)	4 (5%)	22	51
61	BQ	101/117 (86%)	101 (100%)	0	100	100
62	BR	117/118 (99%)	115 (98%)	2 (2%)	53	71
63	BS	94/123 (76%)	93 (99%)	1 (1%)	65	76
64	BT	128/128 (100%)	126 (98%)	2 (2%)	55	72
65	BU	115/115 (100%)	112 (97%)	3 (3%)	40	64
66	BV	100/113 (88%)	99 (99%)	1 (1%)	68	77
67	BW	74/74 (100%)	73 (99%)	1 (1%)	59	74
68	BX	110/110 (100%)	105 (96%)	5 (4%)	24	53
69	BY	119/119 (100%)	115 (97%)	4 (3%)	32	59
70	BZ	112/112 (100%)	112 (100%)	0	100	100
71	Ba	61/88 (69%)	59 (97%)	2 (3%)	33	59
72	Bb	83/99 (84%)	81 (98%)	2 (2%)	43	65
73	Bc	70/70 (100%)	69 (99%)	1 (1%)	59	74
74	Bd	56/59 (95%)	54 (96%)	2 (4%)	31	58
75	Be	47/48 (98%)	46 (98%)	1 (2%)	47	67
76	Bf	51/53 (96%)	49 (96%)	2 (4%)	28	56
77	Bg	48/134 (36%)	47 (98%)	1 (2%)	47	67
78	Bh	260/261 (100%)	252 (97%)	8 (3%)	35	61
79	Bi	840/857 (98%)	830 (99%)	10 (1%)	63	75
All	All	10009/10755 (93%)	9866 (99%)	143 (1%)	57	74

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	AD	45	VAL
4	AD	101	VAL
4	AD	116	VAL
5	AE	16	PHE
5	AE	19	ARG

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Mol	Chain	Res	Type
5	AE	73	VAL
5	AE	84	VAL
5	AE	85	VAL
5	AE	104	THR
5	AE	114	VAL
5	AE	173	GLN
5	AE	216	ASP
5	AE	256	HIS
6	AF	147	GLU
6	AF	148	ILE
6	AF	150	LEU
6	AF	182	LEU
6	AF	230	VAL
7	AG	68	THR
7	AG	155	THR
8	AH	66	SER
9	AI	83	LEU
9	AI	89	ILE
9	AI	239	LEU
10	AJ	50	VAL
10	AJ	158	ASP
10	AJ	229	VAL
11	AK	18	VAL
11	AK	151	VAL
11	AK	157	ASN
13	AM	44	THR
13	AM	95	ASN
14	AN	58	VAL
15	AO	15	VAL
15	AO	20	VAL
15	AO	53	VAL
15	AO	74	ARG
17	AQ	34	VAL
18	AR	114	VAL
18	AR	119	VAL
18	AR	120	ASN
19	AS	40	THR
19	AS	81	VAL
21	AU	170	THR
22	AV	80	VAL
22	AV	124	VAL
22	AV	141	VAL

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Mol	Chain	Res	Type
25	AY	19	THR
27	Aa	59	VAL
28	Ab	46	ILE
29	Ac	46	ASP
31	Ae	99	ASP
32	Af	14	ILE
34	Ah	81	VAL
34	Ah	98	VAL
34	Ah	102	LEU
34	Ah	103	TYR
38	Al	58	THR
46	BB	10	THR
46	BB	157	ASP
46	BB	189	VAL
47	BC	31	ASP
47	BC	70	LEU
47	BC	180	THR
47	BC	215	VAL
48	BD	69	ILE
48	BD	111	VAL
49	BE	38	GLU
49	BE	39	VAL
49	BE	156	PHE
49	BE	175	VAL
49	BE	222	VAL
50	BF	38	LEU
50	BF	70	VAL
50	BF	156	VAL
50	BF	195	ILE
50	BF	206	ASP
51	BG	32	GLU
51	BG	45	LYS
51	BG	48	PHE
51	BG	60	ASP
51	BG	79	ASN
51	BG	124	LEU
52	BH	97	VAL
53	BI	126	LEU
54	BJ	46	VAL
56	BL	76	LEU
57	BM	47	THR
57	BM	74	THR

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Mol	Chain	Res	Type
58	BN	28	LEU
58	BN	121	VAL
60	BP	13	VAL
60	BP	16	VAL
60	BP	43	THR
60	BP	81	VAL
62	BR	53	LEU
62	BR	69	VAL
63	BS	71	PHE
64	BT	14	ILE
64	BT	119	ILE
65	BU	6	VAL
65	BU	28	LEU
65	BU	135	ILE
66	BV	118	VAL
67	BW	12	TYR
68	BX	25	VAL
68	BX	27	ILE
68	BX	28	ARG
68	BX	30	SER
68	BX	53	ILE
69	BY	62	LYS
69	BY	63	GLN
69	BY	83	VAL
69	BY	130	VAL
71	Ba	95	HIS
71	Ba	102	THR
72	Bb	36	ILE
72	Bb	62	TYR
73	Bc	33	LEU
74	Bd	15	VAL
74	Bd	44	VAL
75	Be	36	LEU
76	Bf	48	THR
76	Bf	50	VAL
77	Bg	115	THR
78	Bh	12	THR
78	Bh	58	VAL
78	Bh	207	ASP
78	Bh	262	VAL
78	Bh	265	LEU
78	Bh	266	ASP

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Mol	Chain	Res	Type
78	Bh	268	GLN
78	Bh	312	VAL
79	Bi	268	LEU
79	Bi	498	VAL
79	Bi	573	VAL
79	Bi	581	TYR
79	Bi	712	ASP
79	Bi	713	GLN
79	Bi	744	ASP
79	Bi	842	VAL
79	Bi	935	ILE
79	Bi	1102	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (165) such sidechains are listed below:

Mol	Chain	Res	Type
4	AD	8	GLN
4	AD	19	HIS
4	AD	86	GLN
4	AD	132	ASN
4	AD	209	HIS
4	AD	218	HIS
5	AE	139	GLN
5	AE	173	GLN
5	AE	177	HIS
5	AE	198	HIS
5	AE	211	GLN
5	AE	319	ASN
6	AF	9	HIS
6	AF	196	ASN
6	AF	213	ASN
6	AF	260	GLN
6	AF	291	ASN
6	AF	304	GLN
7	AG	32	GLN
7	AG	40	HIS
8	AH	80	ASN
9	AI	80	GLN
9	AI	186	HIS
9	AI	200	ASN
9	AI	225	GLN
10	AJ	41	GLN

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Mol	Chain	Res	Type
10	AJ	77	GLN
10	AJ	191	ASN
10	AJ	243	GLN
11	AK	64	HIS
11	AK	156	GLN
11	AK	183	HIS
12	AL	12	GLN
12	AL	59	GLN
12	AL	123	HIS
12	AL	162	GLN
13	AM	39	GLN
14	AN	19	GLN
14	AN	37	ASN
14	AN	99	HIS
14	AN	149	GLN
16	AP	138	GLN
16	AP	175	ASN
17	AQ	29	ASN
18	AR	54	HIS
18	AR	97	ASN
19	AS	23	ASN
19	AS	58	ASN
19	AS	145	ASN
20	AT	3	ASN
20	AT	7	GLN
20	AT	34	GLN
20	AT	144	GLN
21	AU	62	ASN
21	AU	63	GLN
21	AU	122	HIS
23	AW	25	ASN
23	AW	87	ASN
24	AX	132	ASN
26	AZ	80	ASN
28	Ab	36	HIS
28	Ab	57	HIS
28	Ab	103	GLN
28	Ab	106	GLN
28	Ab	122	HIS
30	Ad	12	GLN
30	Ad	19	ASN
32	Af	43	HIS

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Mol	Chain	Res	Type
32	Af	57	GLN
33	Ag	104	ASN
35	Ai	11	ASN
37	Ak	92	ASN
38	Al	76	ASN
38	Al	79	GLN
39	Am	67	GLN
40	An	32	ASN
40	An	33	ASN
43	Aq	22	GLN
43	Aq	38	GLN
43	Aq	82	GLN
44	Ar	25	GLN
46	BB	30	GLN
46	BB	46	HIS
46	BB	83	GLN
46	BB	109	ASN
46	BB	163	ASN
47	BC	42	ASN
47	BC	149	GLN
47	BC	199	ASN
47	BC	208	GLN
47	BC	232	HIS
48	BD	87	GLN
48	BD	89	GLN
48	BD	189	GLN
50	BF	17	HIS
50	BF	67	GLN
50	BF	69	HIS
50	BF	188	ASN
50	BF	258	GLN
51	BG	63	GLN
51	BG	103	ASN
51	BG	104	ASN
52	BH	189	HIS
53	BI	22	GLN
53	BI	161	GLN
54	BJ	32	GLN
54	BJ	35	ASN
55	BK	123	HIS
55	BK	139	GLN
56	BL	28	ASN

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Mol	Chain	Res	Type
56	BL	62	GLN
57	BM	138	ASN
59	BO	36	GLN
60	BP	29	HIS
61	BQ	15	HIS
61	BQ	103	ASN
62	BR	62	ASN
62	BR	83	GLN
63	BS	56	HIS
63	BS	62	GLN
64	BT	6	GLN
64	BT	21	ASN
64	BT	25	ASN
64	BT	89	GLN
65	BU	70	GLN
66	BV	17	GLN
66	BV	33	GLN
66	BV	40	ASN
67	BW	7	GLN
69	BY	63	GLN
69	BY	65	ASN
69	BY	79	ASN
70	BZ	34	ASN
71	Ba	44	GLN
71	Ba	82	HIS
72	Bb	43	ASN
75	Be	53	ASN
76	Bf	17	GLN
76	Bf	46	ASN
77	Bg	123	ASN
78	Bh	139	GLN
78	Bh	182	ASN
78	Bh	308	ASN
79	Bi	210	ASN
79	Bi	221	GLN
79	Bi	230	ASN
79	Bi	342	ASN
79	Bi	391	ASN
79	Bi	436	GLN
79	Bi	456	ASN
79	Bi	522	ASN
79	Bi	541	GLN

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Mol	Chain	Res	Type
79	Bi	547	GLN
79	Bi	588	ASN
79	Bi	619	ASN
79	Bi	704	GLN
79	Bi	769	ASN
79	Bi	866	ASN
79	Bi	884	HIS
79	Bi	888	HIS
79	Bi	892	HIS
79	Bi	898	ASN
79	Bi	902	GLN
79	Bi	994	HIS
79	Bi	1087	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	3145/3149 (99%)	649 (20%)	42 (1%)
2	AB	120/121 (99%)	16 (13%)	0
3	AC	157/158 (99%)	31 (19%)	1 (0%)
45	BA	1703/1707 (99%)	437 (25%)	37 (2%)
All	All	5125/5135 (99%)	1133 (22%)	80 (1%)

All (1133) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	A
1	AA	18	G
1	AA	26	A
1	AA	40	A
1	AA	43	A
1	AA	49	A
1	AA	59	G
1	AA	60	A
1	AA	65	A
1	AA	66	A
1	AA	75	G
1	AA	77	A
1	AA	85	A
1	AA	92	G
1	AA	109	A

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Mol	Chain	Res	Type
1	AA	110	G
1	AA	111	C
1	AA	116	A
1	AA	120	G
1	AA	121	A
1	AA	122	A
1	AA	133	U
1	AA	135	C
1	AA	136	G
1	AA	148	G
1	AA	150	A
1	AA	156	G
1	AA	157	A
1	AA	165	A
1	AA	166	C
1	AA	187	A
1	AA	190	U
1	AA	191	U
1	AA	200	C
1	AA	206	G
1	AA	210	U
1	AA	211	A
1	AA	213	A
1	AA	218	G
1	AA	219	A
1	AA	234	G
1	AA	240	U
1	AA	241	G
1	AA	243	G
1	AA	245	U
1	AA	249	U
1	AA	250	U
1	AA	251	G
1	AA	252	U
1	AA	269	G
1	AA	281	G
1	AA	283	G
1	AA	286	U
1	AA	295	A
1	AA	298	U
1	AA	305	U
1	AA	323	A

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Mol	Chain	Res	Type
1	AA	329	U
1	AA	337	G
1	AA	346	C
1	AA	349	A
1	AA	350	C
1	AA	351	A
1	AA	352	A
1	AA	366	A
1	AA	375	A
1	AA	376	G
1	AA	390	G
1	AA	398	A
1	AA	401	U
1	AA	402	A
1	AA	403	C
1	AA	421	G
1	AA	422	A
1	AA	439	C
1	AA	440	A
1	AA	520	U
1	AA	521	A
1	AA	535	G
1	AA	544	C
1	AA	546	C
1	AA	547	G
1	AA	548	G
1	AA	551	A
1	AA	552	G
1	AA	555	U
1	AA	557	A
1	AA	559	A
1	AA	578	A
1	AA	579	G
1	AA	589	A
1	AA	590	G
1	AA	604	G
1	AA	609	G
1	AA	611	A
1	AA	620	U
1	AA	621	A
1	AA	637	C
1	AA	638	C

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Mol	Chain	Res	Type
1	AA	649	A
1	AA	660	A
1	AA	662	U
1	AA	677	A
1	AA	681	U
1	AA	683	U
1	AA	691	A
1	AA	705	A
1	AA	708	G
1	AA	712	G
1	AA	715	A
1	AA	716	A
1	AA	719	U
1	AA	725	G
1	AA	735	A
1	AA	743	C
1	AA	764	U
1	AA	767	U
1	AA	774	G
1	AA	775	A
1	AA	776	U
1	AA	777	U
1	AA	779	G
1	AA	780	A
1	AA	781	G
1	AA	785	G
1	AA	801	A
1	AA	806	A
1	AA	808	A
1	AA	817	A
1	AA	830	A
1	AA	849	C
1	AA	861	C
1	AA	869	G
1	AA	874	U
1	AA	879	U
1	AA	896	A
1	AA	907	G
1	AA	908	G
1	AA	914	A
1	AA	916	G
1	AA	917	A

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Mol	Chain	Res	Type
1	AA	920	A
1	AA	921	A
1	AA	923	C
1	AA	924	G
1	AA	925	A
1	AA	937	G
1	AA	944	C
1	AA	959	C
1	AA	960	U
1	AA	961	C
1	AA	979	U
1	AA	980	A
1	AA	981	U
1	AA	982	C
1	AA	1001	G
1	AA	1002	A
1	AA	1010	G
1	AA	1015	U
1	AA	1016	C
1	AA	1017	C
1	AA	1018	G
1	AA	1020	G
1	AA	1024	G
1	AA	1025	A
1	AA	1029	G
1	AA	1032	C
1	AA	1036	A
1	AA	1037	C
1	AA	1041	U
1	AA	1047	A
1	AA	1049	C
1	AA	1063	G
1	AA	1064	A
1	AA	1065	A
1	AA	1072	G
1	AA	1074	U
1	AA	1079	A
1	AA	1081	U
1	AA	1082	U
1	AA	1083	G
1	AA	1093	A
1	AA	1094	U

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Mol	Chain	Res	Type
1	AA	1095	U
1	AA	1097	G
1	AA	1098	A
1	AA	1103	A
1	AA	1104	G
1	AA	1117	G
1	AA	1129	A
1	AA	1131	G
1	AA	1143	A
1	AA	1144	U
1	AA	1150	A
1	AA	1153	A
1	AA	1159	A
1	AA	1160	C
1	AA	1177	G
1	AA	1178	G
1	AA	1179	A
1	AA	1180	A
1	AA	1181	U
1	AA	1191	U
1	AA	1192	C
1	AA	1196	C
1	AA	1201	C
1	AA	1202	A
1	AA	1209	G
1	AA	1212	A
1	AA	1217	A
1	AA	1218	U
1	AA	1221	A
1	AA	1222	G
1	AA	1225	A
1	AA	1226	G
1	AA	1227	C
1	AA	1229	G
1	AA	1232	C
1	AA	1236	G
1	AA	1239	C
1	AA	1240	A
1	AA	1241	U
1	AA	1242	G
1	AA	1243	G
1	AA	1244	A

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Mol	Chain	Res	Type
1	AA	1245	A
1	AA	1246	G
1	AA	1248	C
1	AA	1249	G
1	AA	1253	U
1	AA	1258	U
1	AA	1262	G
1	AA	1263	A
1	AA	1264	G
1	AA	1265	U
1	AA	1266	G
1	AA	1267	U
1	AA	1268	G
1	AA	1269	U
1	AA	1270	A
1	AA	1271	A
1	AA	1272	C
1	AA	1273	A
1	AA	1274	A
1	AA	1278	A
1	AA	1279	C
1	AA	1281	G
1	AA	1282	G
1	AA	1285	G
1	AA	1287	A
1	AA	1305	U
1	AA	1307	G
1	AA	1308	A
1	AA	1309	U
1	AA	1313	G
1	AA	1325	U
1	AA	1330	A
1	AA	1331	U
1	AA	1332	A
1	AA	1334	U
1	AA	1345	G
1	AA	1348	U
1	AA	1349	G
1	AA	1350	A
1	AA	1351	U
1	AA	1352	A
1	AA	1353	U

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Mol	Chain	Res	Type
1	AA	1355	A
1	AA	1356	U
1	AA	1357	G
1	AA	1386	A
1	AA	1392	G
1	AA	1399	A
1	AA	1400	G
1	AA	1417	G
1	AA	1418	A
1	AA	1419	A
1	AA	1421	G
1	AA	1425	U
1	AA	1434	G
1	AA	1437	C
1	AA	1443	G
1	AA	1446	A
1	AA	1450	G
1	AA	1468	A
1	AA	1469	C
1	AA	1482	A
1	AA	1485	G
1	AA	1496	C
1	AA	1502	C
1	AA	1508	C
1	AA	1525	G
1	AA	1527	C
1	AA	1536	G
1	AA	1547	G
1	AA	1553	U
1	AA	1555	U
1	AA	1556	C
1	AA	1562	C
1	AA	1563	C
1	AA	1564	U
1	AA	1565	G
1	AA	1566	A
1	AA	1567	U
1	AA	1568	U
1	AA	1569	U
1	AA	1570	U
1	AA	1580	A
1	AA	1582	C

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Mol	Chain	Res	Type
1	AA	1583	A
1	AA	1587	A
1	AA	1589	A
1	AA	1590	G
1	AA	1593	A
1	AA	1594	A
1	AA	1596	C
1	AA	1605	A
1	AA	1607	U
1	AA	1608	C
1	AA	1619	A
1	AA	1629	U
1	AA	1639	C
1	AA	1641	U
1	AA	1643	A
1	AA	1656	A
1	AA	1683	A
1	AA	1696	A
1	AA	1705	U
1	AA	1716	U
1	AA	1717	U
1	AA	1724	U
1	AA	1725	C
1	AA	1736	G
1	AA	1741	A
1	AA	1750	A
1	AA	1751	G
1	AA	1756	C
1	AA	1759	C
1	AA	1760	A
1	AA	1762	C
1	AA	1765	U
1	AA	1767	C
1	AA	1770	G
1	AA	1771	C
1	AA	1775	G
1	AA	1778	G
1	AA	1780	G
1	AA	1797	A
1	AA	1812	G
1	AA	1814	A
1	AA	1815	U

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Mol	Chain	Res	Type
1	AA	1816	A
1	AA	1817	G
1	AA	1819	U
1	AA	1820	U
1	AA	1821	U
1	AA	1839	A
1	AA	1841	A
1	AA	1842	A
1	AA	1846	C
1	AA	1849	C
1	AA	1850	A
1	AA	1858	A
1	AA	1866	C
1	AA	1871	U
1	AA	1880	U
1	AA	1881	A
1	AA	1886	A
1	AA	1890	U
1	AA	1893	A
1	AA	1906	G
1	AA	1951	C
1	AA	1952	G
1	AA	1954	G
1	AA	2094	C
1	AA	2100	A
1	AA	2101	C
1	AA	2102	U
1	AA	2110	G
1	AA	2111	G
1	AA	2112	U
1	AA	2113	A
1	AA	2114	C
1	AA	2115	G
1	AA	2121	G
1	AA	2122	G
1	AA	2131	A
1	AA	2132	C
1	AA	2140	U
1	AA	2144	A
1	AA	2158	A
1	AA	2169	G
1	AA	2171	G

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Mol	Chain	Res	Type
1	AA	2175	U
1	AA	2187	G
1	AA	2192	C
1	AA	2201	G
1	AA	2205	U
1	AA	2206	G
1	AA	2208	A
1	AA	2210	G
1	AA	2213	A
1	AA	2225	U
1	AA	2239	G
1	AA	2244	A
1	AA	2249	G
1	AA	2250	G
1	AA	2252	A
1	AA	2255	A
1	AA	2256	A
1	AA	2272	G
1	AA	2273	G
1	AA	2281	A
1	AA	2282	U
1	AA	2284	C
1	AA	2288	G
1	AA	2298	U
1	AA	2307	G
1	AA	2310	U
1	AA	2313	A
1	AA	2314	U
1	AA	2315	G
1	AA	2334	U
1	AA	2335	G
1	AA	2336	U
1	AA	2366	C
1	AA	2373	A
1	AA	2374	C
1	AA	2375	G
1	AA	2376	G
1	AA	2385	G
1	AA	2388	U
1	AA	2393	G
1	AA	2397	A
1	AA	2401	A

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Mol	Chain	Res	Type
1	AA	2402	A
1	AA	2403	G
1	AA	2404	A
1	AA	2405	C
1	AA	2411	U
1	AA	2418	G
1	AA	2435	G
1	AA	2443	A
1	AA	2444	C
1	AA	2445	A
1	AA	2502	A
1	AA	2503	G
1	AA	2504	U
1	AA	2511	A
1	AA	2513	U
1	AA	2514	U
1	AA	2515	A
1	AA	2522	G
1	AA	2523	A
1	AA	2532	U
1	AA	2537	U
1	AA	2538	U
1	AA	2539	C
1	AA	2540	A
1	AA	2541	U
1	AA	2542	U
1	AA	2543	U
1	AA	2544	U
1	AA	2548	C
1	AA	2549	G
1	AA	2550	U
1	AA	2552	C
1	AA	2554	A
1	AA	2561	A
1	AA	2568	C
1	AA	2569	A
1	AA	2570	U
1	AA	2571	U
1	AA	2572	C
1	AA	2573	G
1	AA	2585	G
1	AA	2593	A

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Mol	Chain	Res	Type
1	AA	2594	C
1	AA	2606	G
1	AA	2607	G
1	AA	2614	G
1	AA	2629	U
1	AA	2635	A
1	AA	2651	G
1	AA	2652	U
1	AA	2656	A
1	AA	2674	A
1	AA	2677	G
1	AA	2680	A
1	AA	2689	A
1	AA	2691	A
1	AA	2694	A
1	AA	2696	A
1	AA	2705	A
1	AA	2712	U
1	AA	2714	G
1	AA	2719	U
1	AA	2726	C
1	AA	2727	A
1	AA	2728	G
1	AA	2729	U
1	AA	2737	C
1	AA	2749	G
1	AA	2752	U
1	AA	2753	G
1	AA	2755	C
1	AA	2761	G
1	AA	2762	A
1	AA	2771	U
1	AA	2772	C
1	AA	2777	G
1	AA	2778	G
1	AA	2796	G
1	AA	2799	A
1	AA	2800	G
1	AA	2801	A
1	AA	2802	A
1	AA	2804	A
1	AA	2810	C

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Mol	Chain	Res	Type
1	AA	2814	G
1	AA	2817	A
1	AA	2818	U
1	AA	2834	G
1	AA	2838	A
1	AA	2842	U
1	AA	2843	U
1	AA	2845	A
1	AA	2847	A
1	AA	2849	C
1	AA	2856	G
1	AA	2860	U
1	AA	2867	C
1	AA	2871	G
1	AA	2872	A
1	AA	2873	U
1	AA	2875	U
1	AA	2887	A
1	AA	2896	A
1	AA	2898	G
1	AA	2899	C
1	AA	2911	A
1	AA	2914	G
1	AA	2923	U
1	AA	2930	A
1	AA	2935	U
1	AA	2936	A
1	AA	2938	G
1	AA	2941	A
1	AA	2942	C
1	AA	2945	G
1	AA	2946	A
1	AA	2947	G
1	AA	2951	G
1	AA	2957	G
1	AA	2971	A
1	AA	2983	C
1	AA	2992	U
1	AA	2996	U
1	AA	2997	G
1	AA	3003	G
1	AA	3012	A

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Mol	Chain	Res	Type
1	AA	3023	U
1	AA	3028	G
1	AA	3030	G
1	AA	3056	U
1	AA	3059	G
1	AA	3074	G
1	AA	3078	U
1	AA	3079	U
1	AA	3086	A
1	AA	3087	A
1	AA	3092	C
1	AA	3109	G
1	AA	3115	C
1	AA	3119	U
1	AA	3122	A
1	AA	3129	A
1	AA	3130	A
1	AA	3131	U
1	AA	3142	A
1	AA	3143	C
1	AA	3151	U
1	AA	3153	U
1	AA	3154	C
1	AA	3155	U
1	AA	3156	U
1	AA	3157	U
1	AA	3165	A
1	AA	3168	A
1	AA	3170	A
1	AA	3173	G
1	AA	3174	A
1	AA	3175	U
1	AA	3176	G
1	AA	3179	U
1	AA	3181	C
1	AA	3187	A
1	AA	3194	C
1	AA	3196	U
1	AA	3207	U
1	AA	3210	A
1	AA	3216	G
1	AA	3217	C

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Mol	Chain	Res	Type
1	AA	3218	A
1	AA	3219	G
1	AA	3227	A
1	AA	3229	G
1	AA	3235	C
1	AA	3243	A
1	AA	3245	A
1	AA	3247	G
1	AA	3259	U
1	AA	3260	G
1	AA	3263	G
1	AA	3270	U
1	AA	3272	C
1	AA	3276	G
1	AA	3281	U
1	AA	3286	G
1	AA	3287	U
1	AA	3288	G
1	AA	3289	G
1	AA	3294	A
1	AA	3295	A
1	AA	3304	U
1	AA	3313	U
1	AA	3316	A
1	AA	3317	U
1	AA	3318	G
1	AA	3319	U
1	AA	3330	A
1	AA	3331	U
1	AA	3341	U
1	AA	3345	G
1	AA	3351	U
1	AA	3352	U
1	AA	3353	G
1	AA	3354	U
1	AA	3355	U
1	AA	3356	G
1	AA	3357	U
1	AA	3360	C
1	AA	3363	U
1	AA	3369	G
1	AA	3375	A

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Mol	Chain	Res	Type
1	AA	3378	C
1	AA	3382	U
1	AA	3386	G
1	AA	3396	U
2	AB	7	G
2	AB	10	C
2	AB	13	A
2	AB	22	A
2	AB	29	C
2	AB	41	G
2	AB	54	U
2	AB	55	A
2	AB	65	G
2	AB	74	C
2	AB	76	A
2	AB	91	G
2	AB	99	G
2	AB	102	A
2	AB	112	G
2	AB	121	U
3	AC	2	A
3	AC	23	U
3	AC	34	U
3	AC	35	C
3	AC	51	G
3	AC	52	A
3	AC	59	A
3	AC	62	C
3	AC	63	G
3	AC	79	A
3	AC	80	A
3	AC	81	U
3	AC	82	U
3	AC	83	C
3	AC	84	C
3	AC	85	G
3	AC	86	U
3	AC	87	G
3	AC	90	U
3	AC	95	G
3	AC	97	A
3	AC	104	A

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Mol	Chain	Res	Type
3	AC	105	A
3	AC	106	C
3	AC	111	A
3	AC	113	U
3	AC	125	U
3	AC	126	A
3	AC	128	U
3	AC	138	A
3	AC	152	G
45	BA	2	A
45	BA	4	C
45	BA	17	C
45	BA	25	C
45	BA	26	A
45	BA	27	U
45	BA	34	G
45	BA	42	G
45	BA	45	U
45	BA	47	A
45	BA	50	C
45	BA	57	G
45	BA	60	U
45	BA	68	A
45	BA	69	G
45	BA	72	A
45	BA	73	U
45	BA	74	U
45	BA	75	U
45	BA	78	A
45	BA	101	U
45	BA	104	A
45	BA	114	C
45	BA	115	G
45	BA	127	G
45	BA	130	C
45	BA	131	C
45	BA	132	U
45	BA	133	U
45	BA	134	U
45	BA	135	A
45	BA	136	C
45	BA	137	U

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Mol	Chain	Res	Type
45	BA	140	A
45	BA	141	U
45	BA	145	A
45	BA	146	U
45	BA	153	G
45	BA	158	U
45	BA	159	U
45	BA	169	A
45	BA	176	C
45	BA	178	U
45	BA	179	A
45	BA	181	A
45	BA	185	U
45	BA	186	C
45	BA	190	C
45	BA	191	C
45	BA	192	U
45	BA	193	U
45	BA	194	U
45	BA	195	G
45	BA	196	G
45	BA	198	A
45	BA	199	G
45	BA	200	A
45	BA	217	A
45	BA	218	A
45	BA	219	A
45	BA	220	A
45	BA	226	A
45	BA	229	U
45	BA	231	U
45	BA	233	C
45	BA	235	G
45	BA	236	A
45	BA	239	C
45	BA	240	U
45	BA	241	U
45	BA	245	U
45	BA	246	G
45	BA	250	C
45	BA	257	A
45	BA	260	U

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Mol	Chain	Res	Type
45	BA	261	U
45	BA	265	A
45	BA	271	A
45	BA	272	U
45	BA	277	U
45	BA	278	U
45	BA	279	G
45	BA	280	U
45	BA	281	G
45	BA	288	A
45	BA	299	A
45	BA	309	C
45	BA	314	C
45	BA	316	A
45	BA	319	U
45	BA	320	U
45	BA	321	C
45	BA	322	G
45	BA	333	A
45	BA	337	G
45	BA	338	C
45	BA	352	A
45	BA	359	A
45	BA	360	A
45	BA	361	C
45	BA	370	A
45	BA	387	A
45	BA	390	G
45	BA	399	A
45	BA	400	A
45	BA	401	A
45	BA	402	C
45	BA	404	G
45	BA	416	A
45	BA	417	A
45	BA	418	G
45	BA	422	G
45	BA	423	G
45	BA	424	C
45	BA	425	A
45	BA	426	G
45	BA	434	G

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Mol	Chain	Res	Type
45	BA	439	U
45	BA	444	C
45	BA	448	C
45	BA	452	A
45	BA	454	U
45	BA	464	A
45	BA	468	A
45	BA	469	C
45	BA	475	A
45	BA	477	A
45	BA	480	G
45	BA	481	A
45	BA	484	C
45	BA	485	A
45	BA	488	G
45	BA	493	U
45	BA	494	U
45	BA	495	C
45	BA	496	G
45	BA	497	G
45	BA	498	G
45	BA	499	U
45	BA	500	C
45	BA	501	U
45	BA	502	U
45	BA	504	U
45	BA	505	A
45	BA	506	A
45	BA	508	U
45	BA	510	G
45	BA	511	A
45	BA	513	U
45	BA	514	G
45	BA	515	A
45	BA	519	C
45	BA	527	A
45	BA	532	U
45	BA	534	A
45	BA	539	G
45	BA	540	G
45	BA	541	A
45	BA	542	A

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Mol	Chain	Res	Type
45	BA	543	C
45	BA	544	A
45	BA	548	G
45	BA	549	G
45	BA	556	A
45	BA	557	G
45	BA	558	U
45	BA	559	C
45	BA	565	C
45	BA	577	G
45	BA	579	A
45	BA	580	A
45	BA	582	U
45	BA	585	A
45	BA	594	A
45	BA	595	G
45	BA	606	A
45	BA	611	U
45	BA	619	A
45	BA	620	A
45	BA	621	A
45	BA	622	A
45	BA	623	A
45	BA	624	G
45	BA	638	U
45	BA	640	U
45	BA	641	G
45	BA	648	G
45	BA	649	U
45	BA	650	U
45	BA	684	A
45	BA	686	C
45	BA	687	G
45	BA	694	U
45	BA	696	C
45	BA	697	C
45	BA	698	U
45	BA	737	A
45	BA	738	G
45	BA	741	C
45	BA	742	U
45	BA	745	U

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Mol	Chain	Res	Type
45	BA	752	A
45	BA	754	A
45	BA	755	A
45	BA	756	A
45	BA	765	G
45	BA	766	U
45	BA	767	U
45	BA	774	A
45	BA	775	G
45	BA	778	G
45	BA	781	U
45	BA	782	U
45	BA	783	G
45	BA	784	C
45	BA	787	G
45	BA	794	U
45	BA	795	U
45	BA	803	A
45	BA	812	A
45	BA	813	U
45	BA	814	A
45	BA	815	G
45	BA	816	G
45	BA	817	A
45	BA	818	C
45	BA	819	G
45	BA	820	U
45	BA	821	U
45	BA	823	G
45	BA	824	G
45	BA	829	A
45	BA	830	U
45	BA	833	U
45	BA	837	G
45	BA	838	G
45	BA	840	U
45	BA	846	G
45	BA	849	C
45	BA	850	A
45	BA	851	U
45	BA	852	C
45	BA	853	G

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Mol	Chain	Res	Type
45	BA	854	U
45	BA	855	A
45	BA	856	A
45	BA	863	A
45	BA	873	U
45	BA	876	G
45	BA	886	U
45	BA	898	A
45	BA	912	U
45	BA	913	G
45	BA	914	G
45	BA	915	A
45	BA	932	U
45	BA	933	A
45	BA	935	U
45	BA	942	G
45	BA	945	U
45	BA	954	G
45	BA	958	U
45	BA	960	U
45	BA	966	A
45	BA	992	A
45	BA	993	A
45	BA	1004	U
45	BA	1005	A
45	BA	1025	A
45	BA	1026	A
45	BA	1028	C
45	BA	1031	U
45	BA	1039	A
45	BA	1040	G
45	BA	1052	U
45	BA	1053	G
45	BA	1058	U
45	BA	1059	U
45	BA	1060	U
45	BA	1061	A
45	BA	1072	C
45	BA	1076	A
45	BA	1082	C
45	BA	1086	A
45	BA	1091	A

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Mol	Chain	Res	Type
45	BA	1092	A
45	BA	1096	C
45	BA	1097	U
45	BA	1098	U
45	BA	1100	G
45	BA	1101	G
45	BA	1108	G
45	BA	1109	G
45	BA	1111	G
45	BA	1113	A
45	BA	1138	A
45	BA	1150	G
45	BA	1154	G
45	BA	1158	C
45	BA	1160	A
45	BA	1167	G
45	BA	1185	U
45	BA	1194	A
45	BA	1196	A
45	BA	1199	G
45	BA	1200	G
45	BA	1202	A
45	BA	1207	C
45	BA	1217	A
45	BA	1218	G
45	BA	1227	A
45	BA	1228	G
45	BA	1229	G
45	BA	1244	A
45	BA	1245	G
45	BA	1246	C
45	BA	1250	U
45	BA	1251	U
45	BA	1255	G
45	BA	1257	U
45	BA	1258	U
45	BA	1259	U
45	BA	1276	U
45	BA	1284	C
45	BA	1286	U
45	BA	1290	U
45	BA	1291	G

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Mol	Chain	Res	Type
45	BA	1293	U
45	BA	1295	G
45	BA	1296	A
45	BA	1299	G
45	BA	1302	U
45	BA	1304	G
45	BA	1307	U
45	BA	1314	U
45	BA	1315	U
45	BA	1318	G
45	BA	1321	A
45	BA	1323	C
45	BA	1337	A
45	BA	1338	C
45	BA	1340	U
45	BA	1341	A
45	BA	1344	A
45	BA	1345	A
45	BA	1346	A
45	BA	1364	G
45	BA	1367	G
45	BA	1370	U
45	BA	1371	A
45	BA	1372	U
45	BA	1382	A
45	BA	1388	A
45	BA	1390	U
45	BA	1398	U
45	BA	1399	C
45	BA	1400	A
45	BA	1412	G
45	BA	1413	U
45	BA	1414	U
45	BA	1415	U
45	BA	1422	A
45	BA	1425	A
45	BA	1427	A
45	BA	1428	G
45	BA	1431	C
45	BA	1432	U
45	BA	1433	G
45	BA	1435	G

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Mol	Chain	Res	Type
45	BA	1446	A
45	BA	1447	C
45	BA	1448	G
45	BA	1457	C
45	BA	1458	G
45	BA	1459	C
45	BA	1460	A
45	BA	1471	A
45	BA	1482	C
45	BA	1486	G
45	BA	1489	U
45	BA	1490	C
45	BA	1491	U
45	BA	1492	A
45	BA	1493	A
45	BA	1496	U
45	BA	1500	C
45	BA	1506	G
45	BA	1516	A
45	BA	1520	U
45	BA	1521	G
45	BA	1523	G
45	BA	1524	A
45	BA	1527	C
45	BA	1535	U
45	BA	1536	G
45	BA	1537	C
45	BA	1538	U
45	BA	1540	G
45	BA	1542	G
45	BA	1557	U
45	BA	1559	A
45	BA	1569	A
45	BA	1573	A
45	BA	1574	G
45	BA	1582	U
45	BA	1584	G
45	BA	1590	G
45	BA	1601	G
45	BA	1607	G
45	BA	1614	A
45	BA	1616	G

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Mol	Chain	Res	Type
45	BA	1622	G
45	BA	1631	A
45	BA	1632	C
45	BA	1635	A
45	BA	1657	U
45	BA	1658	G
45	BA	1680	G
45	BA	1682	U
45	BA	1683	C
45	BA	1684	U
45	BA	1736	G
45	BA	1756	A
45	BA	1760	G
45	BA	1761	U
45	BA	1762	A
45	BA	1766	A
45	BA	1769	U
45	BA	1780	G
45	BA	1782	A
45	BA	1783	C
45	BA	1792	G
45	BA	1793	G
45	BA	1794	A
45	BA	1795	U
45	BA	1796	C
45	BA	1798	U

All (80) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	65	A
1	AA	239	G
1	AA	282	G
1	AA	547	G
1	AA	588	G
1	AA	637	C
1	AA	715	A
1	AA	763	G
1	AA	916	G
1	AA	979	U
1	AA	993	G
1	AA	1064	A

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Mol	Chain	Res	Type
1	AA	1094	U
1	AA	1097	G
1	AA	1103	A
1	AA	1307	G
1	AA	1329	U
1	AA	1352	A
1	AA	1355	A
1	AA	1554	U
1	AA	1562	C
1	AA	1607	U
1	AA	1716	U
1	AA	1815	U
1	AA	1816	A
1	AA	1820	U
1	AA	2101	C
1	AA	2112	U
1	AA	2209	U
1	AA	2372	A
1	AA	2513	U
1	AA	2537	U
1	AA	2541	U
1	AA	2771	U
1	AA	2801	A
1	AA	3121	U
1	AA	3218	A
1	AA	3228	C
1	AA	3269	U
1	AA	3316	A
1	AA	3350	C
1	AA	3351	U
3	AC	85	G
45	BA	25	C
45	BA	130	C
45	BA	131	C
45	BA	132	U
45	BA	139	C
45	BA	158	U
45	BA	218	A
45	BA	240	U
45	BA	280	U
45	BA	417	A
45	BA	497	G

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Mol	Chain	Res	Type
45	BA	498	G
45	BA	501	U
45	BA	503	G
45	BA	512	A
45	BA	542	A
45	BA	558	U
45	BA	685	A
45	BA	819	G
45	BA	829	A
45	BA	849	C
45	BA	854	U
45	BA	855	A
45	BA	1081	A
45	BA	1108	G
45	BA	1157	A
45	BA	1226	A
45	BA	1244	A
45	BA	1250	U
45	BA	1344	A
45	BA	1370	U
45	BA	1481	C
45	BA	1568	C
45	BA	1573	A
45	BA	1615	C
45	BA	1657	U
45	BA	1761	U

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	ATP	Bi	1201	-	32,33,33	1.37	5 (15%)	48,52,52	1.72	9 (18%)
80	ATP	Bi	1202	-	32,33,33	1.44	6 (18%)	48,52,52	1.75	9 (18%)

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
80	ATP	Bi	1201	-	-	2/22/38/38	0/3/3/3
80	ATP	Bi	1202	-	-	3/22/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	Bi	1202	ATP	C5-C4	4.64	1.47	1.39
80	Bi	1201	ATP	C5-C4	4.60	1.47	1.39
80	Bi	1202	ATP	C5-C6	2.71	1.48	1.41
80	Bi	1201	ATP	C5-C6	2.61	1.48	1.41
80	Bi	1202	ATP	PA-O3A	2.38	1.62	1.59
80	Bi	1202	ATP	C8-N7	2.36	1.36	1.31
80	Bi	1201	ATP	C5-N7	-2.33	1.34	1.39
80	Bi	1202	ATP	C5-N7	-2.29	1.34	1.39
80	Bi	1202	ATP	PB-O3A	2.26	1.61	1.59
80	Bi	1201	ATP	C8-N7	2.25	1.36	1.31
80	Bi	1201	ATP	C4-N9	-2.05	1.33	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	Bi	1202	ATP	C5-C4-N3	-5.78	118.76	126.72
80	Bi	1201	ATP	C5-C4-N3	-5.59	119.03	126.72
80	Bi	1202	ATP	N3-C4-N9	4.57	134.94	127.17
80	Bi	1201	ATP	N3-C4-N9	4.51	134.84	127.17
80	Bi	1202	ATP	C2-N3-C4	3.69	120.83	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	Bi	1201	ATP	C2-N3-C4	3.63	120.69	111.83
80	Bi	1202	ATP	C4-C5-N7	-3.41	106.68	110.58
80	Bi	1201	ATP	C4-C5-N7	-3.27	106.84	110.58
80	Bi	1201	ATP	N3-C2-N1	-3.24	123.67	128.58
80	Bi	1202	ATP	N3-C2-N1	-3.23	123.70	128.58
80	Bi	1201	ATP	C4-N9-C8	2.78	108.65	105.74
80	Bi	1202	ATP	C4-N9-C8	2.65	108.52	105.74
80	Bi	1202	ATP	C5-N7-C8	2.51	107.39	103.45
80	Bi	1201	ATP	C5-N7-C8	2.35	107.15	103.45
80	Bi	1202	ATP	C3'-C2'-C1'	2.30	105.82	101.46
80	Bi	1201	ATP	C3'-C2'-C1'	2.08	105.41	101.46
80	Bi	1201	ATP	C6-C5-N7	2.07	136.08	132.09
80	Bi	1202	ATP	C6-C5-N7	2.05	136.04	132.09

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
80	Bi	1201	ATP	C5'-O5'-PA-O3A
80	Bi	1202	ATP	PB-O3A-PA-O5'
80	Bi	1201	ATP	C5'-O5'-PA-O1A
80	Bi	1202	ATP	C3'-C4'-C5'-O5'
80	Bi	1202	ATP	O4'-C4'-C5'-O5'

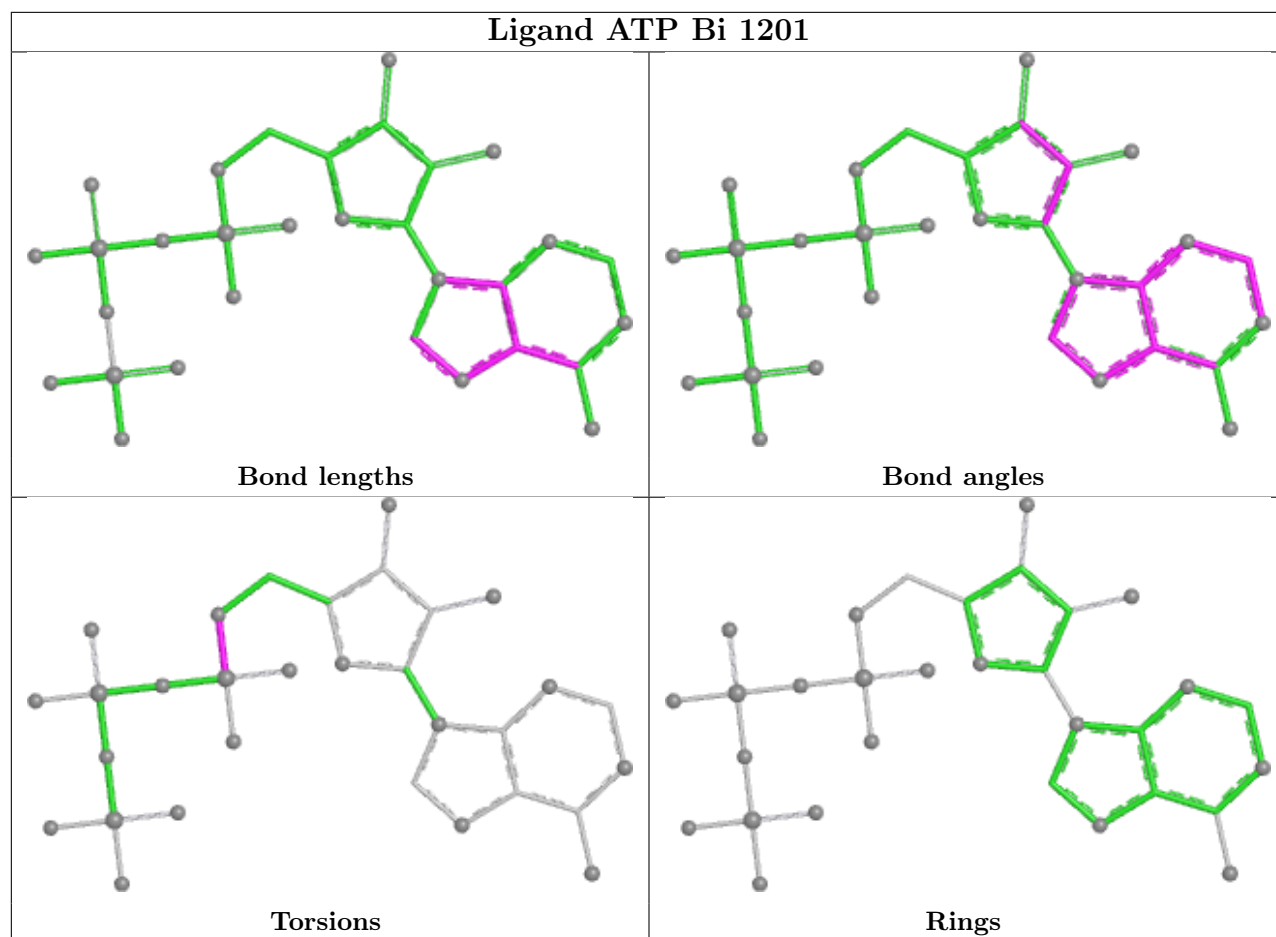
There are no ring outliers.

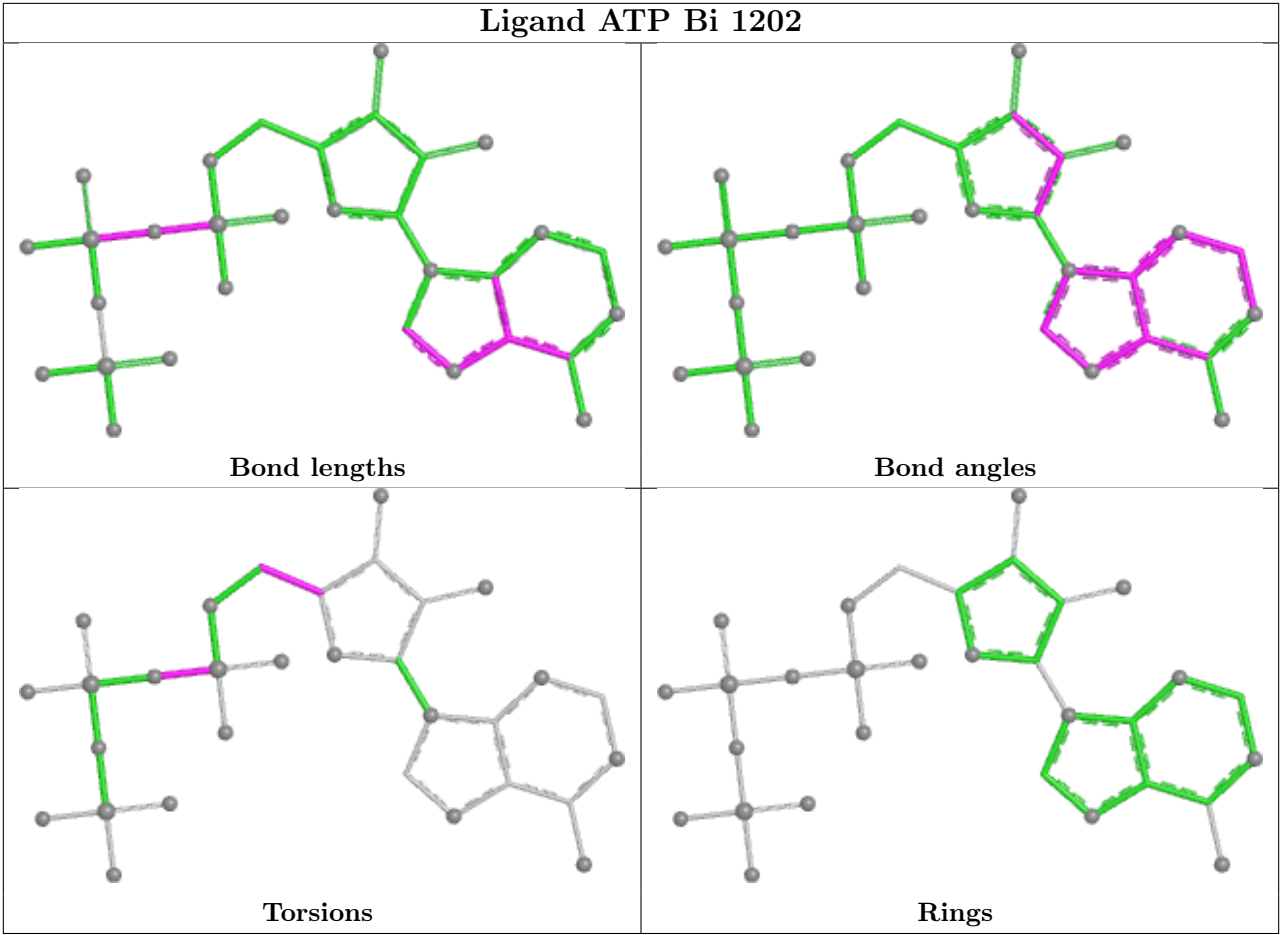
2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	Bi	1201	ATP	1	0
80	Bi	1202	ATP	9	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
1	AA	3
45	BA	3
11	AK	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	1955:U	O3'	2093:A	P	24.80
1	BA	652:G	O3'	682:C	P	17.82
1	BA	703:G	O3'	735:C	P	16.09

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	1685:G	O3'	1717:G	P	15.70
1	AA	2445:A	O3'	2501:U	P	15.05
1	AA	440:A	O3'	494:G	P	13.22
1	AK	167:VAL	C	168:ARG	N	6.38
1	AK	168:ARG	C	169:ASN	N	6.15

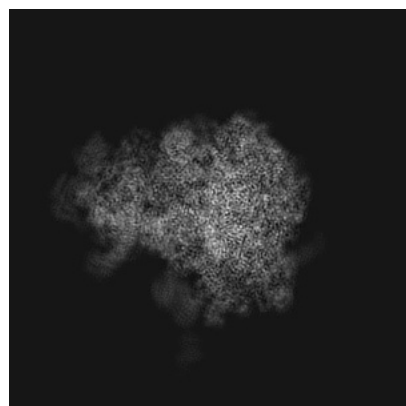
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10098. These allow visual inspection of the internal detail of the map and identification of artifacts.

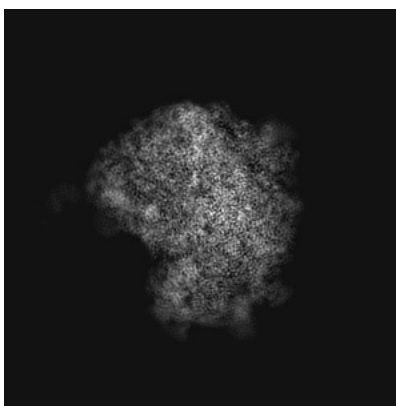
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

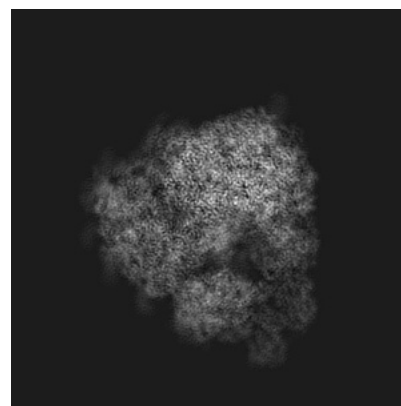
6.1.1 Primary map



X

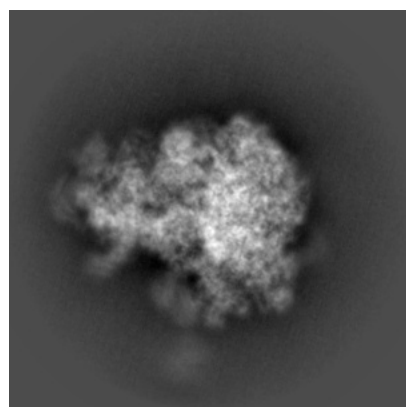


Y

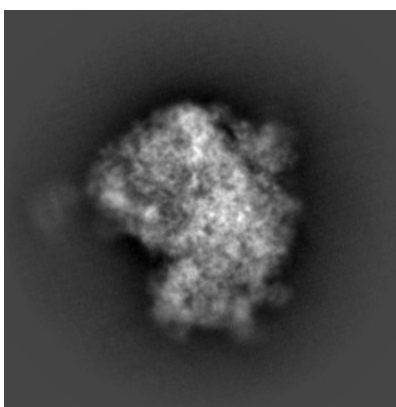


Z

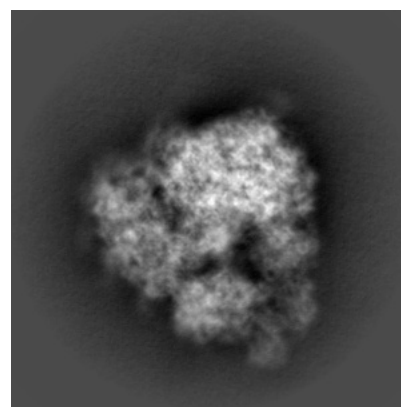
6.1.2 Raw map



X



Y

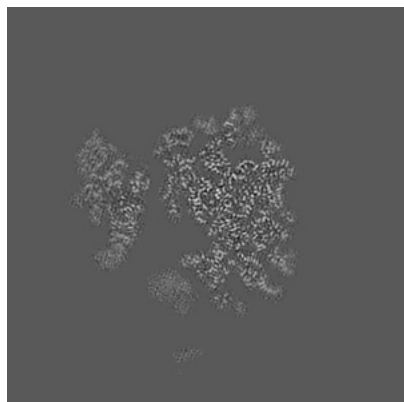


Z

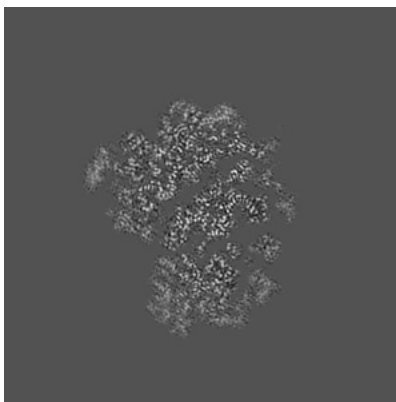
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

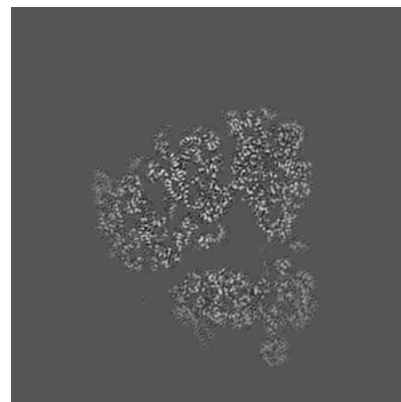
6.2.1 Primary map



X Index: 210

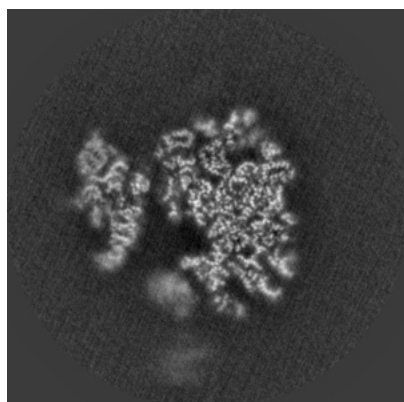


Y Index: 210

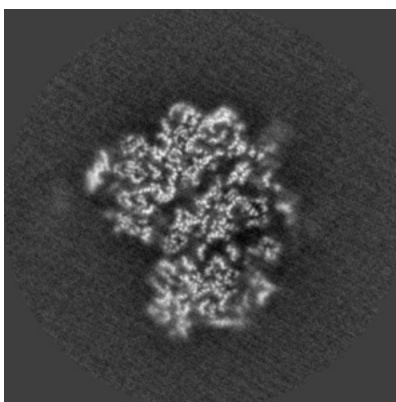


Z Index: 210

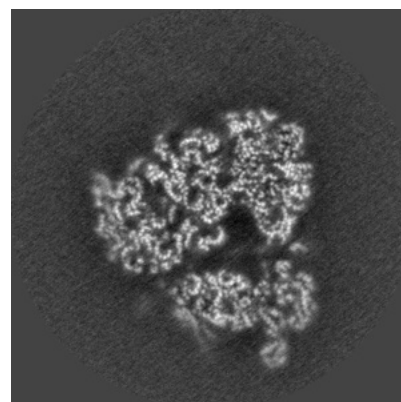
6.2.2 Raw map



X Index: 210



Y Index: 210

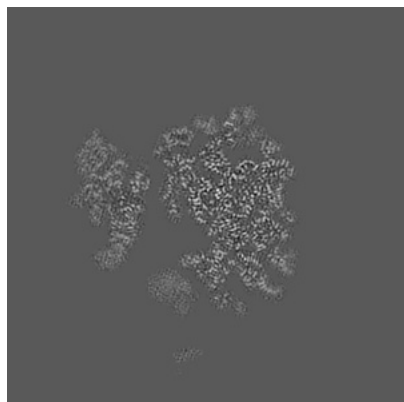


Z Index: 210

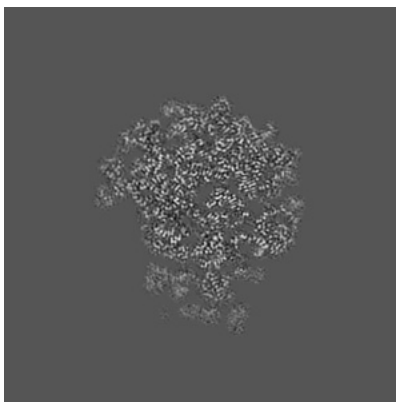
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

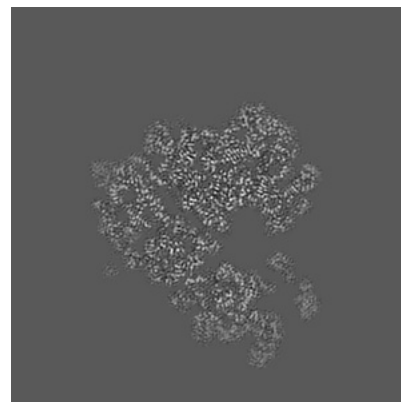
6.3.1 Primary map



X Index: 210

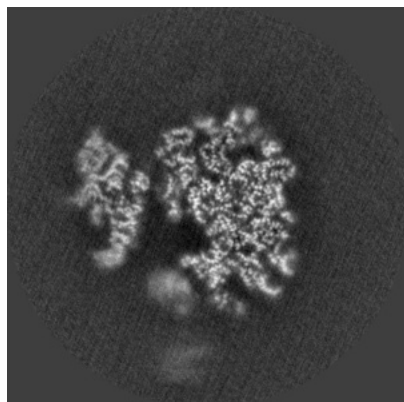


Y Index: 240

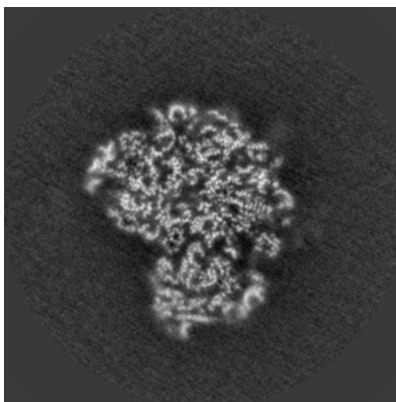


Z Index: 222

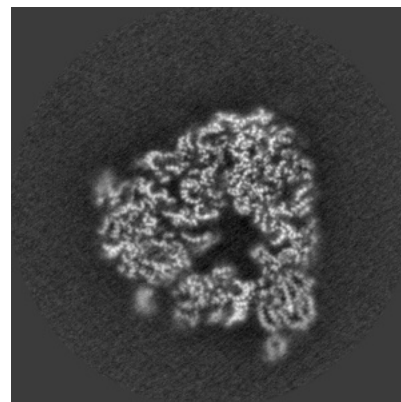
6.3.2 Raw map



X Index: 209



Y Index: 216

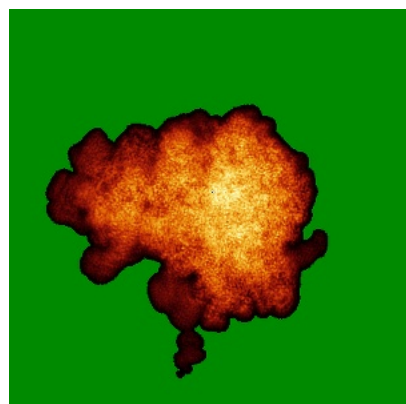


Z Index: 200

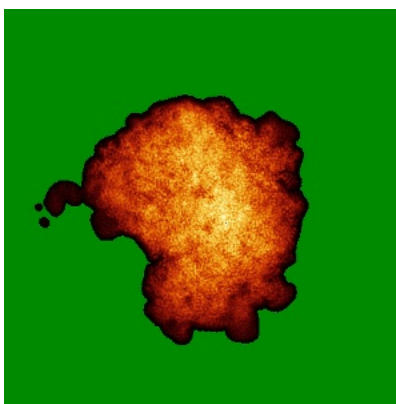
The images above show the largest variance slices of the map in three orthogonal directions.

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

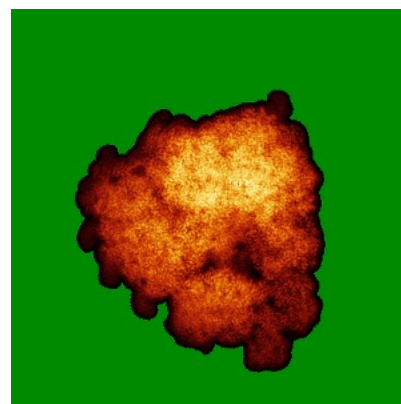
6.4.1 Primary map



X

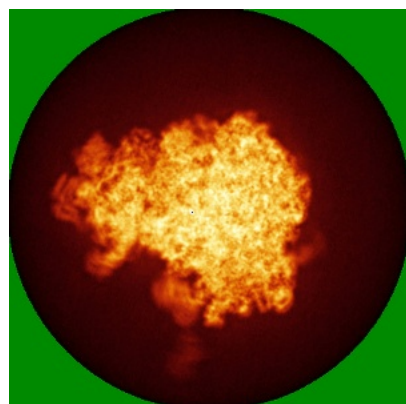


Y

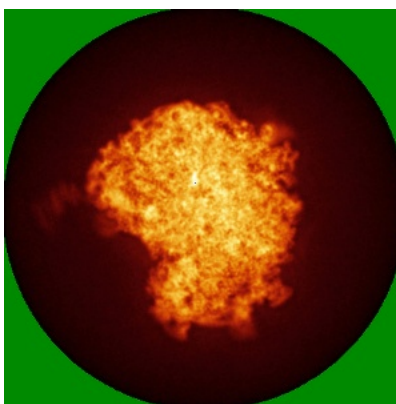


Z

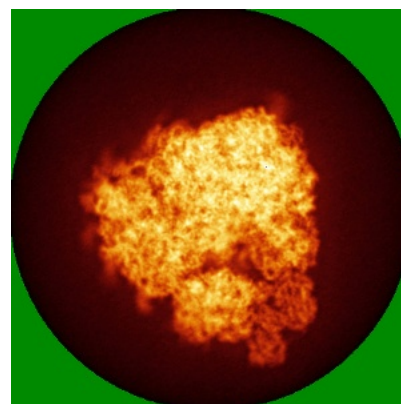
6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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.

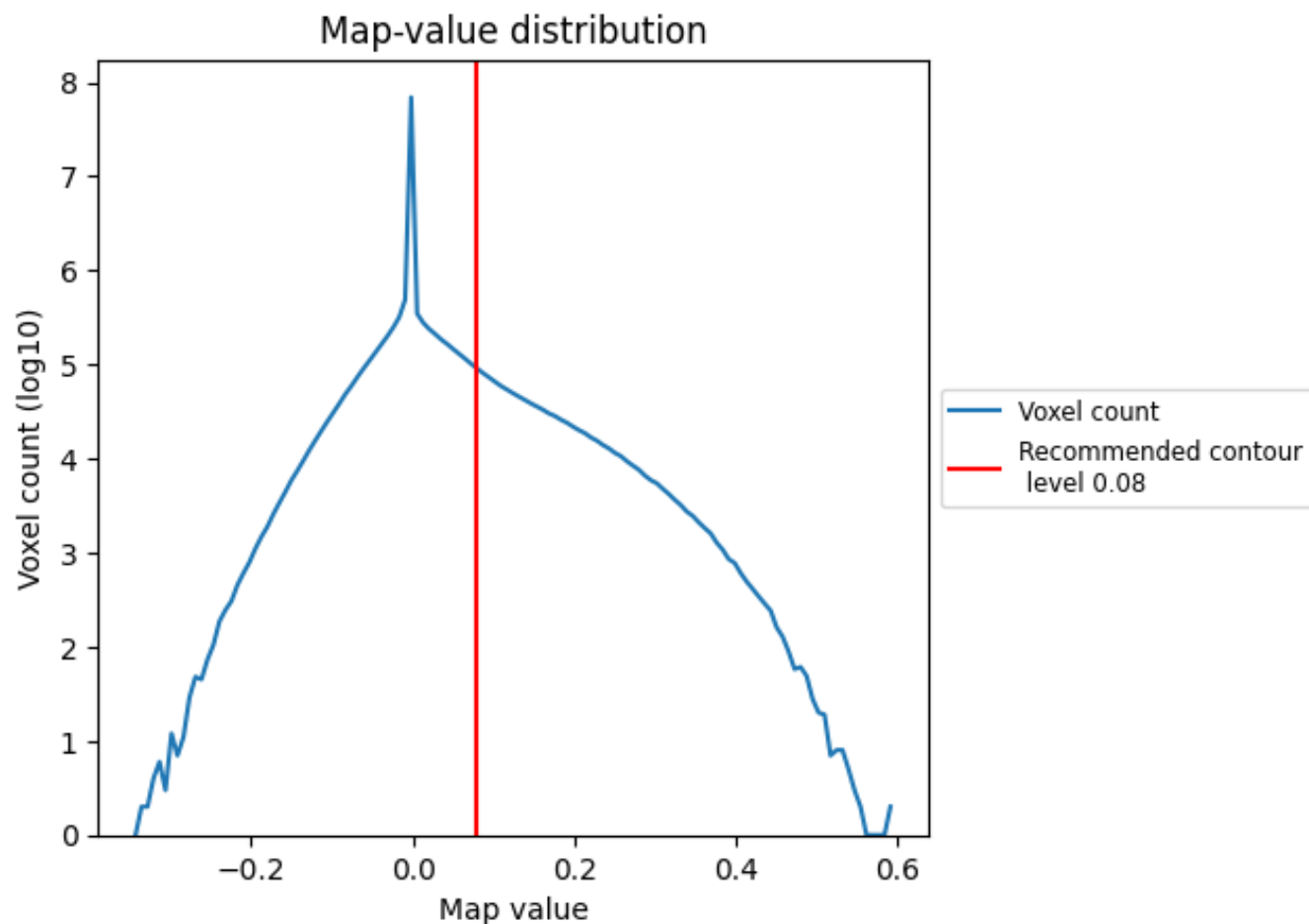
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

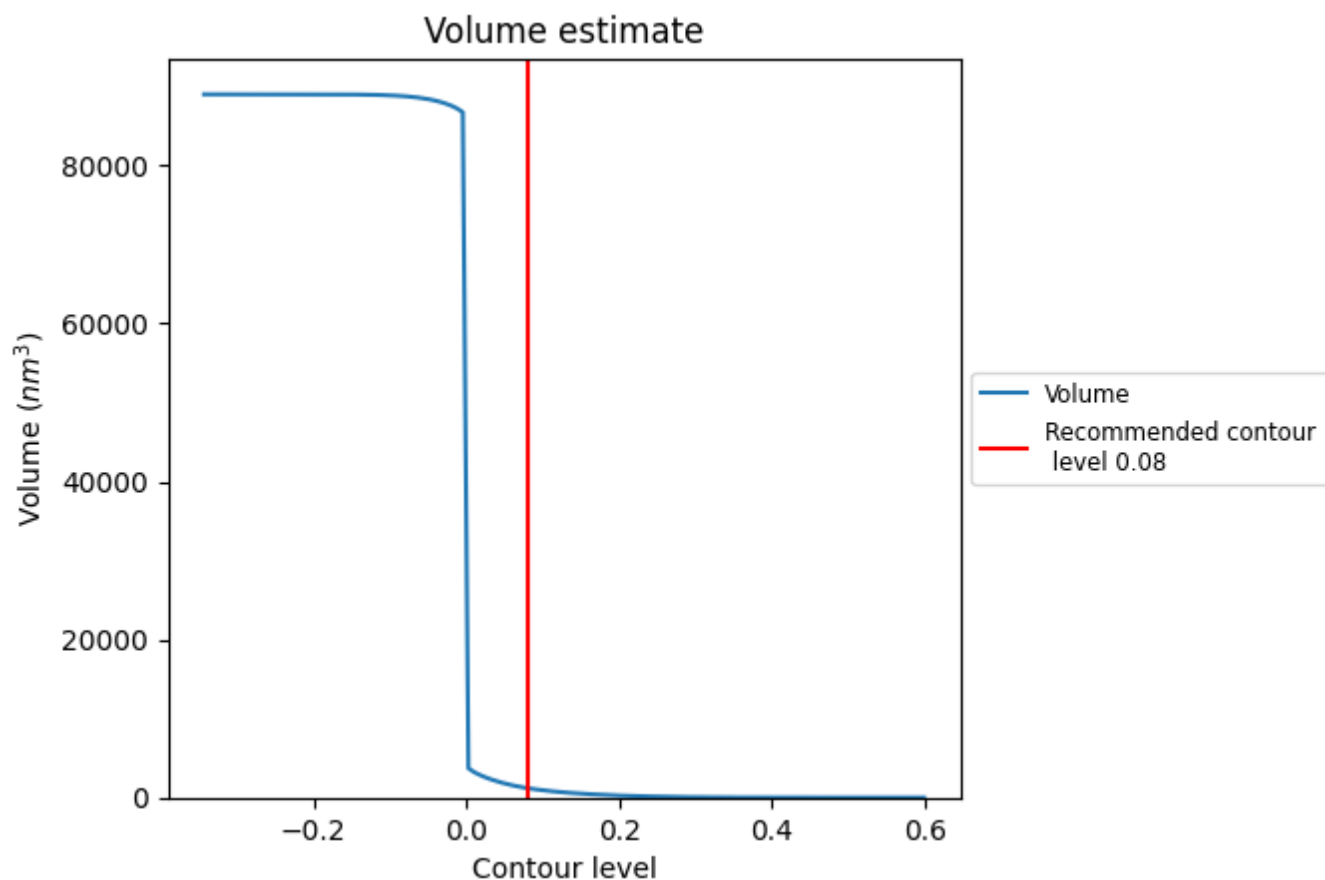
This section contains the results of statistical analysis of the map.

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.

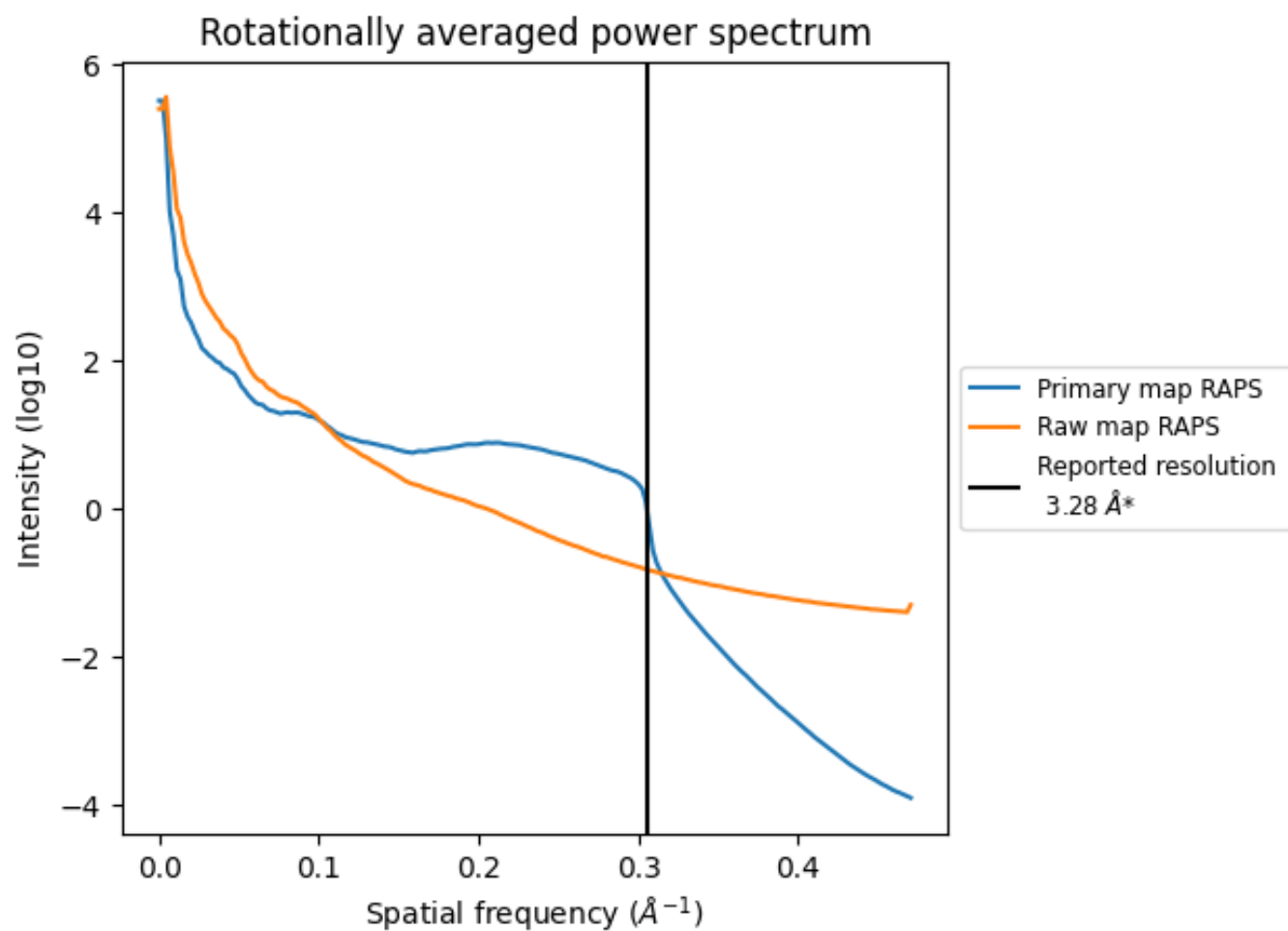
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1193 nm³; this corresponds to an approximate mass of 1078 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 ⓘ

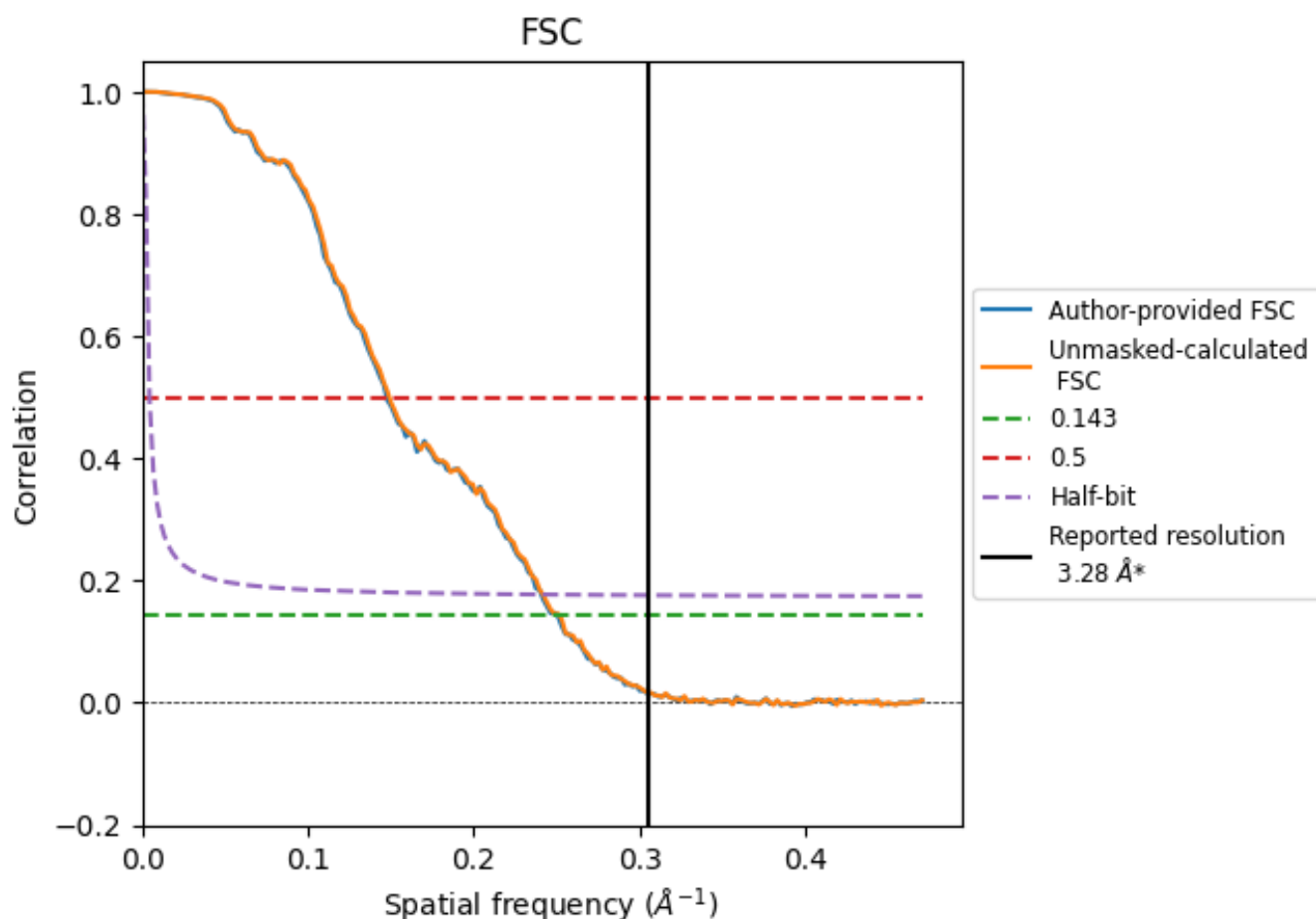


*Reported resolution corresponds to spatial frequency of 0.305 Å⁻¹

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 0.305 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	4.00	6.78	4.15
Unmasked-calculated*	3.98	6.71	4.14

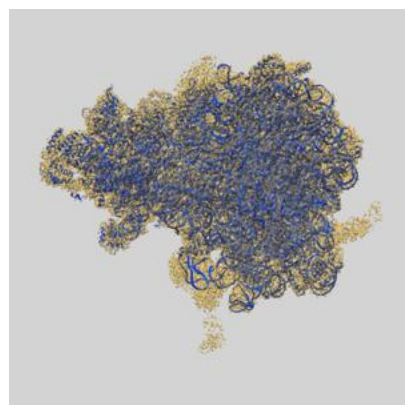
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.00 differs from the reported value 3.28 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 3.28 by more than 10 %

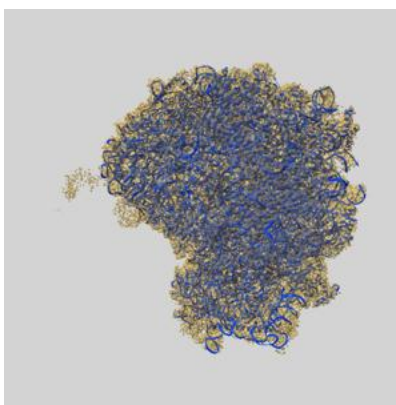
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10098 and PDB model 6S47. Per-residue inclusion information can be found in section 3 on page 20.

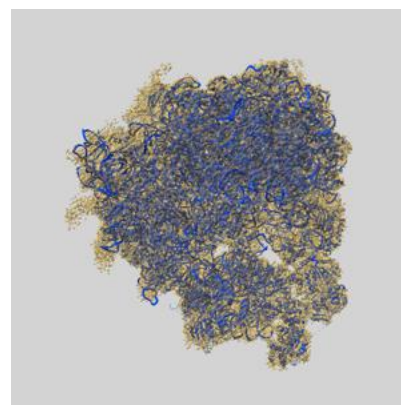
9.1 Map-model overlay [i](#)



X



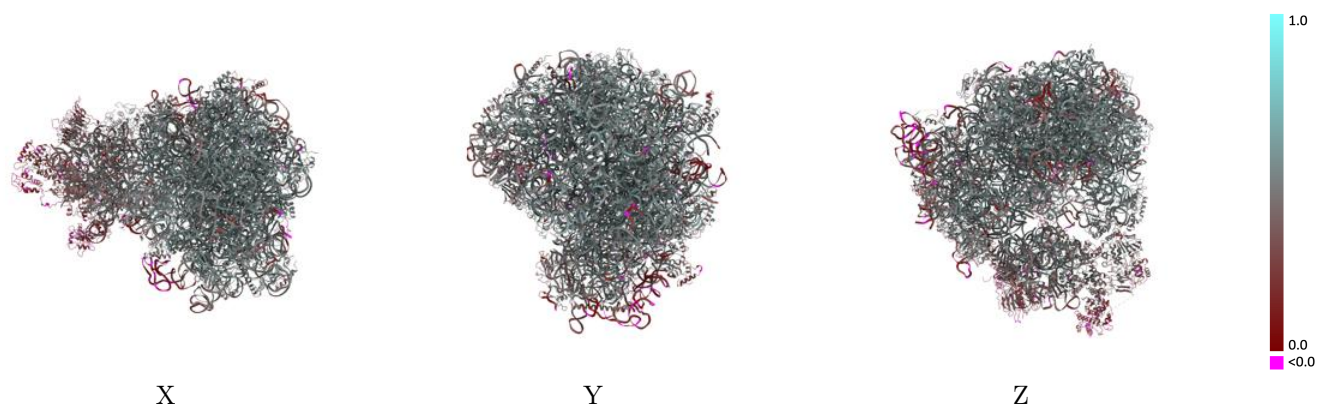
Y



Z

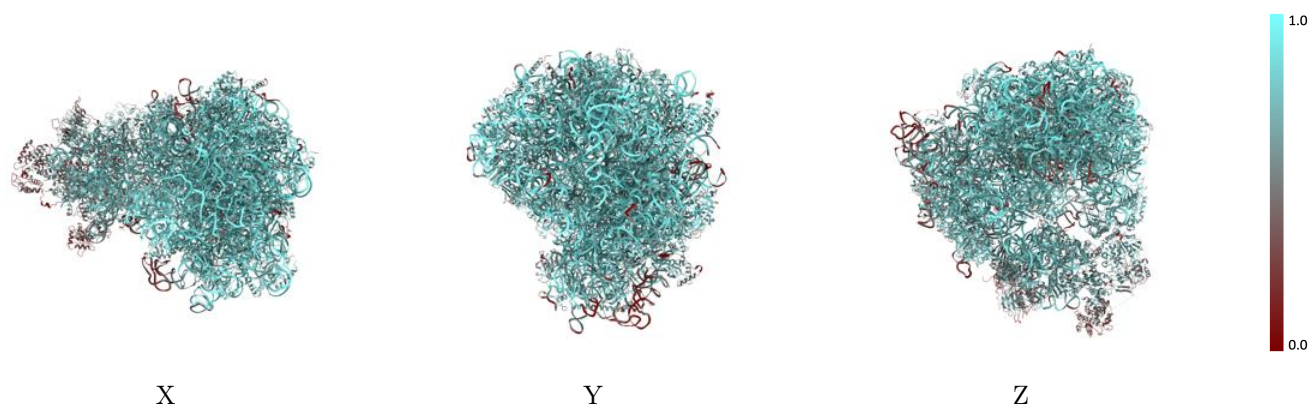
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



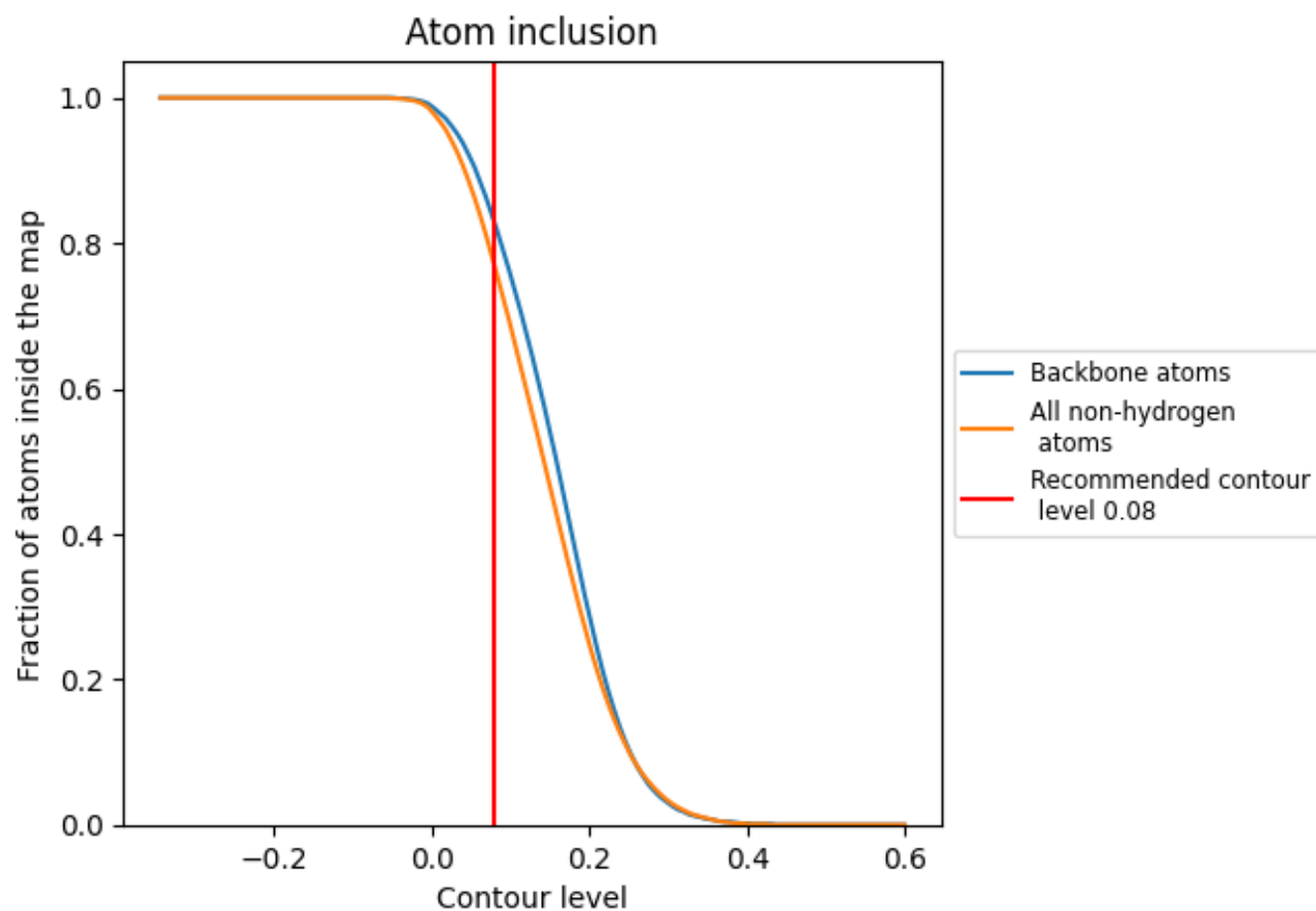
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7690	 0.4720
AA	 0.8610	 0.5000
AB	 0.9050	 0.5110
AC	 0.8880	 0.5190
AD	 0.7740	 0.5370
AE	 0.7640	 0.5160
AF	 0.7650	 0.5130
AG	 0.7260	 0.4730
AH	 0.6940	 0.4770
AI	 0.7420	 0.5110
AJ	 0.6990	 0.4720
AK	 0.6970	 0.4690
AL	 0.7310	 0.5030
AM	 0.6910	 0.4680
AN	 0.7360	 0.5100
AO	 0.7370	 0.4910
AP	 0.7900	 0.5500
AQ	 0.7540	 0.5100
AR	 0.7400	 0.5050
AS	 0.7390	 0.5270
AT	 0.7780	 0.5280
AU	 0.7460	 0.5130
AV	 0.7460	 0.5160
AW	 0.6830	 0.4400
AX	 0.7300	 0.5130
AY	 0.7650	 0.5180
AZ	 0.7470	 0.5130
Aa	 0.7590	 0.5160
Ab	 0.7560	 0.4940
Ac	 0.7810	 0.5340
Ad	 0.6900	 0.4940
Ae	 0.7210	 0.4940
Af	 0.7190	 0.4950
Ag	 0.7150	 0.5300
Ah	 0.7700	 0.5280



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Chain	Atom inclusion	Q-score
Ai	 0.7320	 0.5170
Aj	 0.7550	 0.5150
Ak	 0.7170	 0.4850
Al	 0.7980	 0.5390
Am	 0.6660	 0.4390
An	 0.7450	 0.5330
Ao	 0.7300	 0.4800
Ap	 0.4950	 0.4850
Aq	 0.7070	 0.5040
Ar	 0.7130	 0.5240
BA	 0.8040	 0.4520
BB	 0.7110	 0.4680
BC	 0.6920	 0.4680
BD	 0.7300	 0.4980
BE	 0.5510	 0.3770
BF	 0.7010	 0.4750
BG	 0.6230	 0.4210
BH	 0.5950	 0.3870
BI	 0.5980	 0.3940
BJ	 0.6890	 0.4720
BK	 0.6680	 0.4420
BL	 0.5130	 0.3060
BM	 0.6740	 0.4720
BN	 0.2410	 0.1620
BO	 0.7130	 0.4830
BP	 0.7520	 0.4880
BQ	 0.5670	 0.3520
BR	 0.6890	 0.4470
BS	 0.6320	 0.4070
BT	 0.6780	 0.4290
BU	 0.7090	 0.4500
BV	 0.5390	 0.3590
BW	 0.7110	 0.4770
BX	 0.7510	 0.5260
BY	 0.7150	 0.5010
BZ	 0.6240	 0.4210
Ba	 0.5580	 0.3470
Bb	 0.7500	 0.4760
Bc	 0.6510	 0.4590
Bd	 0.5810	 0.4000
Be	 0.7310	 0.4490
Bf	 0.5770	 0.4060

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Chain	Atom inclusion	Q-score
Bg	 0.2860	 0.1360
Bh	 0.4970	 0.3120
Bi	 0.5360	 0.3310