



Full wwPDB EM Validation Report ⓘ

Aug 3, 2026 – 01:01 pm BST

PDB ID : 9SRB / pdb_00009srb
EMDB ID : EMD-55136
Title : Cryo-EM structure of P. abyssi 70S ribosome in complex with hibernation factor HibA and SBDS
Authors : Madru, C.M.; Bourgeois, G.B.; Mechulam, Y.M.; Schmitt, E.S.
Deposited on : 2025-09-24
Resolution : 2.30 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:

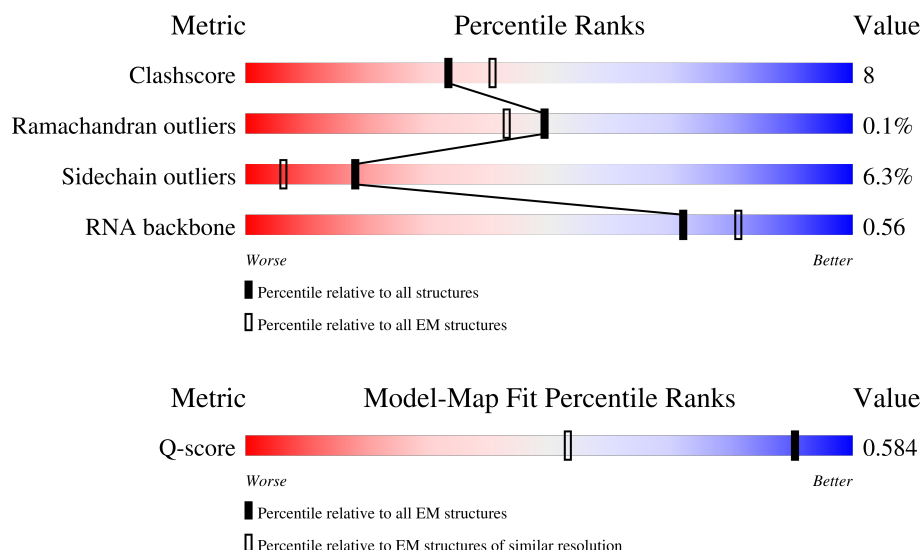
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 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	4254 (1.80 - 2.80)

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	1	3018	
2	2	1512	
3	3	128	

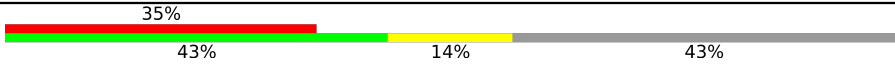
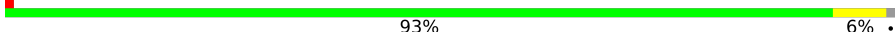
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Mol	Chain	Length	Quality of chain
4	A	236	
5	H	392	
6	AA	199	
7	AB	202	
8	AC	63	
9	AD	180	
10	AE	243	
11	AF	236	
12	AG	125	
13	AH	215	
14	AI	130	
15	AJ	127	
16	AK	135	
17	AL	102	
18	AM	137	
19	AN	147	
20	AP	56	
21	AQ	158	
22	AR	113	
23	AS	67	
24	AU	150	
25	AV	99	
25	B6	99	
26	AW	65	
27	AX	71	

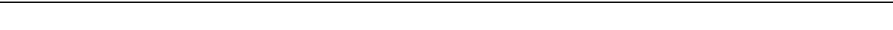
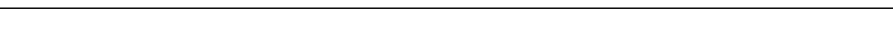
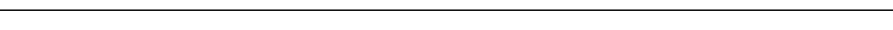
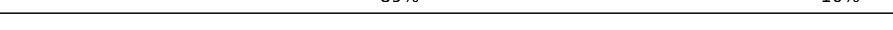
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Mol	Chain	Length	Quality of chain
28	AY	51	
29	AZ	210	
30	A0	37	
31	A3	123	
31	B4	123	
31	BG	123	
32	AT	132	
33	AO	148	
34	BB	239	
35	BY	155	
36	BO	203	
37	BC	361	
38	B5	82	
38	BK	82	
39	BL	147	
40	Bf	51	
41	BU	121	
42	Bb	130	
43	Be	62	
44	BE	188	
45	Ba	94	
46	BT	86	
47	BW	68	
48	Bi	83	
49	BI	142	

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Mol	Chain	Length	Quality of chain
50	BR	97	 86% 12% ..
51	BQ	151	 83% 15% ..
52	BV	67	 85% 9% 6%
53	Bj	94	 94% 6%
54	BD	255	 86% 13% .
55	BF	184	 81% 18% ..
56	BZ	99	 77% 21% ..
57	BP	120	 89% 11%
58	BM	194	 89% 10% .
59	BS	155	 87% 12% .
60	Bd	91	 90% 10%
61	BN	181	 81% 17% .
62	Bg	51	 78% 16% 6%
63	Bc	87	 89% 10% .
64	BJ	141	 86% 13% .
65	Bl	77	 84% 16%
66	Bk	65	 85% 12% .
67	BA	219	 48% 58% 39% ..

2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 173872 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 rRNA 23S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	3018	Total	C	N	O	P	0	0
			65181	29055	12094	21014	3018		

- Molecule 2 is a RNA chain called rRNA 16S.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1496	Total	C	N	O	P	0	0
			32291	14408	5957	10430	1496		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	126	Total	C	N	O	P	0	0
			2703	1203	498	876	126		

- Molecule 4 is a protein called Ribosome maturation protein SDO1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	235	Total	C	N	O	S	0	0
			1900	1216	334	346	4		

- Molecule 5 is a protein called Dehydrogenase.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	386	Total	C	N	O	S	0	0
			3074	1962	535	567	10		

- Molecule 6 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AA	188	Total	C	N	O	S	0	0
			1531	993	268	266	4		

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AB	196	Total	C	N	O	S	0	0
			1571	1017	269	281	4		

- Molecule 8 is a protein called Zn-ribbon RNA-binding protein involved in translation.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AC	57	Total	C	N	O	S	0	0
			449	285	80	76	8		

- Molecule 9 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AD	173	Total	C	N	O	S	0	0
			1452	913	280	255	4		

- Molecule 10 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AE	242	Total	C	N	O	S	0	0
			1983	1281	358	339	5		

- Molecule 11 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AF	229	Total	C	N	O	S	0	0
			1808	1147	334	320	7		

- Molecule 12 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AG	124	Total	C	N	O	S	0	0
			977	621	178	176	2		

- Molecule 13 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AH	214	Total	C	N	O	S	0	0
			1725	1095	323	300	7		

- Molecule 14 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AI	129	Total	C	N	O	S	0	0
			1034	668	184	180	2		

- Molecule 15 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AJ	125	Total	C	N	O	S	0	0
			986	612	205	169			

- Molecule 16 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AK	135	Total	C	N	O	S	0	0
			1073	673	207	189	4		

- Molecule 17 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AL	100	Total	C	N	O	S	0	0
			809	502	157	147	3		

- Molecule 18 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AM	127	Total	C	N	O	S	0	0
			955	591	190	172	2		

- Molecule 19 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AN	146	Total	C	N	O	S	0	0
			1148	727	224	194	3		

- Molecule 20 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AP	55	Total	C	N	O	S	0	0
			455	288	95	67	5		

- Molecule 21 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AQ	157	Total	C	N	O	S	0	0
			1305	833	249	219	4		

- Molecule 22 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AR	108	Total	C	N	O	S	0	0
			893	567	173	150	3		

- Molecule 23 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AS	64	Total	C	N	O	S	0	0
			541	343	104	93	1		

- Molecule 24 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AU	149	Total	C	N	O		0	0
			1223	790	221	212			

- Molecule 25 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AV	96	Total	C	N	O	S	0	0
			808	528	129	148	3		
25	B6	94	Total	C	N	O	S	0	0
			790	516	125	146	3		

- Molecule 26 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AW	61	Total	C	N	O	S	0	0
			470	294	91	80	5		

- Molecule 27 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	AX	65	Total	C	N	O	0	0
			516	316	103	97		

- Molecule 28 is a protein called 30S ribosomal protein S27ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AY	29	Total	C	N	O	S	0	0
			227	141	44	37	5		

- Molecule 29 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AZ	196	Total	C	N	O	S	0	0
			1541	983	284	270	4		

- Molecule 30 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	A0	36	Total	C	N	O	S	0	0
			343	218	84	39	2		

- Molecule 31 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	A3	122	Total	C	N	O	S	0	0
			933	594	156	180	3		
31	BG	122	Total	C	N	O	S	0	0
			932	594	156	179	3		
31	B4	122	Total	C	N	O	S	0	0
			933	594	156	180	3		

- Molecule 32 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AT	130	Total	C	N	O	S	0	0
			1057	675	201	174	7		

- Molecule 33 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AO	138	Total	C	N	O	S	0	0
			1116	700	221	190	5		

- Molecule 34 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BB	238	Total	C	N	O	S	0	0
			1838	1163	354	317	4		

- Molecule 35 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BY	154	Total	C	N	O	S	0	0
			1235	783	234	212	6		

- Molecule 36 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BO	198	Total	C	N	O	S	0	0
			1607	1024	302	279	2		

- Molecule 37 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BC	360	Total	C	N	O	S	0	0
			2870	1843	522	494	11		

- Molecule 38 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	B5	81	Total	C	N	O	S	0	0
			614	388	116	108	2		
38	BK	80	Total	C	N	O	S	0	0
			607	383	115	107	2		

- Molecule 39 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BL	147	Total	C	N	O	S	0	0
			1149	720	224	202	3		

- Molecule 40 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Bf	50	Total	C	N	O	S	0	0
			435	275	99	60	1		

- Molecule 41 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BU	121	Total	C	N	O	S	0	0
			1011	638	198	170	5		

- Molecule 42 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Bb	129	Total	C	N	O	S	0	0
			1095	702	221	171	1		

- Molecule 43 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Be	61	Total	C	N	O	S	0	0
			503	312	112	75	4		

- Molecule 44 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BE	185	Total	C	N	O	S	0	0
			1485	934	277	265	9		

- Molecule 45 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Ba	94	Total	C	N	O	S	0	0
			778	503	147	127	1		

- Molecule 46 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BT	86	Total	C	N	O	S	0	0
			696	451	118	126	1		

- Molecule 47 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BW	68	Total	C	N	O	S	0	0
			565	349	111	99	6		

- Molecule 48 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Bi	82	Total	C	N	O	S	0	0
			620	389	129	97	5		

- Molecule 49 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BI	142	Total	C	N	O	S	0	0
			1148	734	217	194	3		

- Molecule 50 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BR	96	Total	C	N	O	S	0	0
			797	507	164	125	1		

- Molecule 51 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BQ	150	Total	C	N	O	S	0	0
			1265	795	261	203	6		

- Molecule 52 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BV	63	Total	C	N	O	S	0	0
			532	339	103	84	6		

- Molecule 53 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Bj	94	Total	C	N	O	S	0	0
			789	502	163	119	5		

- Molecule 54 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BD	255	Total	C	N	O	S	0	0
			2026	1290	388	343	5		

- Molecule 55 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BF	183	Total	C	N	O	S	0	0
			1456	943	251	261	1		

- Molecule 56 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	BZ	98	Total	C	N	O		
			749	486	122	141	0	0

- Molecule 57 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	BP	120	Total	C	N	O	S	
			971	610	188	170	3	0

- Molecule 58 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	BM	193	Total	C	N	O	S	
			1588	1014	318	251	5	0

- Molecule 59 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	BS	154	Total	C	N	O	S	
			1247	786	246	211	4	0

- Molecule 60 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms				AltConf	Trace
60	Bd	91	Total	C	N	O	S	
			759	477	163	109	10	0

- Molecule 61 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	BN	178	Total	C	N	O	S	
			1452	920	281	246	5	0

- Molecule 62 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	Bg	48	Total	C	N	O	S	
			387	243	80	60	4	0

- Molecule 63 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Bc	87	Total	C	N	O	S	0	0
			684	435	132	115	2		

- Molecule 64 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	BJ	140	Total	C	N	O	S	0	0
			1066	664	214	185	3		

- Molecule 65 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Bl	77	Total	C	N	O	S	0	0
			659	425	120	113	1		

- Molecule 66 is a protein called C2H2-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Bk	63	Total	C	N	O	S	0	0
			528	339	108	78	3		

- Molecule 67 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	BA	215	Total	C	N	O	S	0	0
			1675	1065	301	304	5		

- Molecule 68 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
68	1	164	Total	Mg	0
			164	164	
68	2	65	Total	Mg	0
			65	65	
68	3	1	Total	Mg	0
			1	1	
68	AD	1	Total	Mg	0
			1	1	
68	AK	1	Total	Mg	0
			1	1	
68	AN	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
68	BB	2	Total 2	Mg 2	0
68	Bb	1	Total 1	Mg 1	0
68	BD	1	Total 1	Mg 1	0
68	BM	1	Total 1	Mg 1	0
68	BS	1	Total 1	Mg 1	0
68	Bc	1	Total 1	Mg 1	0

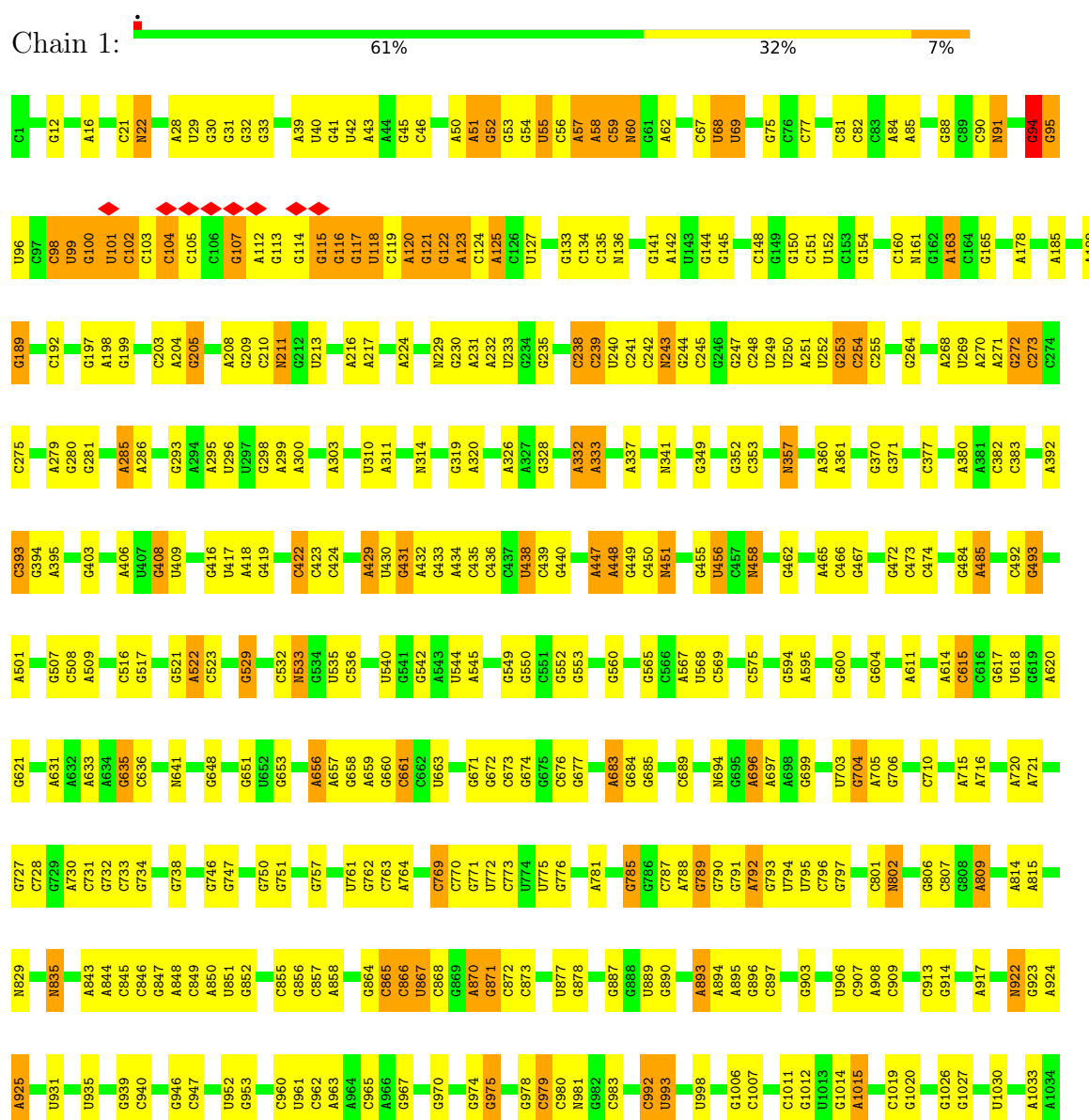
- Molecule 69 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
69	AC	2	Total 2	Zn 2	0
69	AF	1	Total 1	Zn 1	0
69	AP	1	Total 1	Zn 1	0
69	AR	1	Total 1	Zn 1	0
69	AW	1	Total 1	Zn 1	0
69	Be	1	Total 1	Zn 1	0
69	Bi	1	Total 1	Zn 1	0
69	BV	1	Total 1	Zn 1	0
69	Bj	1	Total 1	Zn 1	0
69	Bd	1	Total 1	Zn 1	0
69	Bg	1	Total 1	Zn 1	0
69	Bk	1	Total 1	Zn 1	0

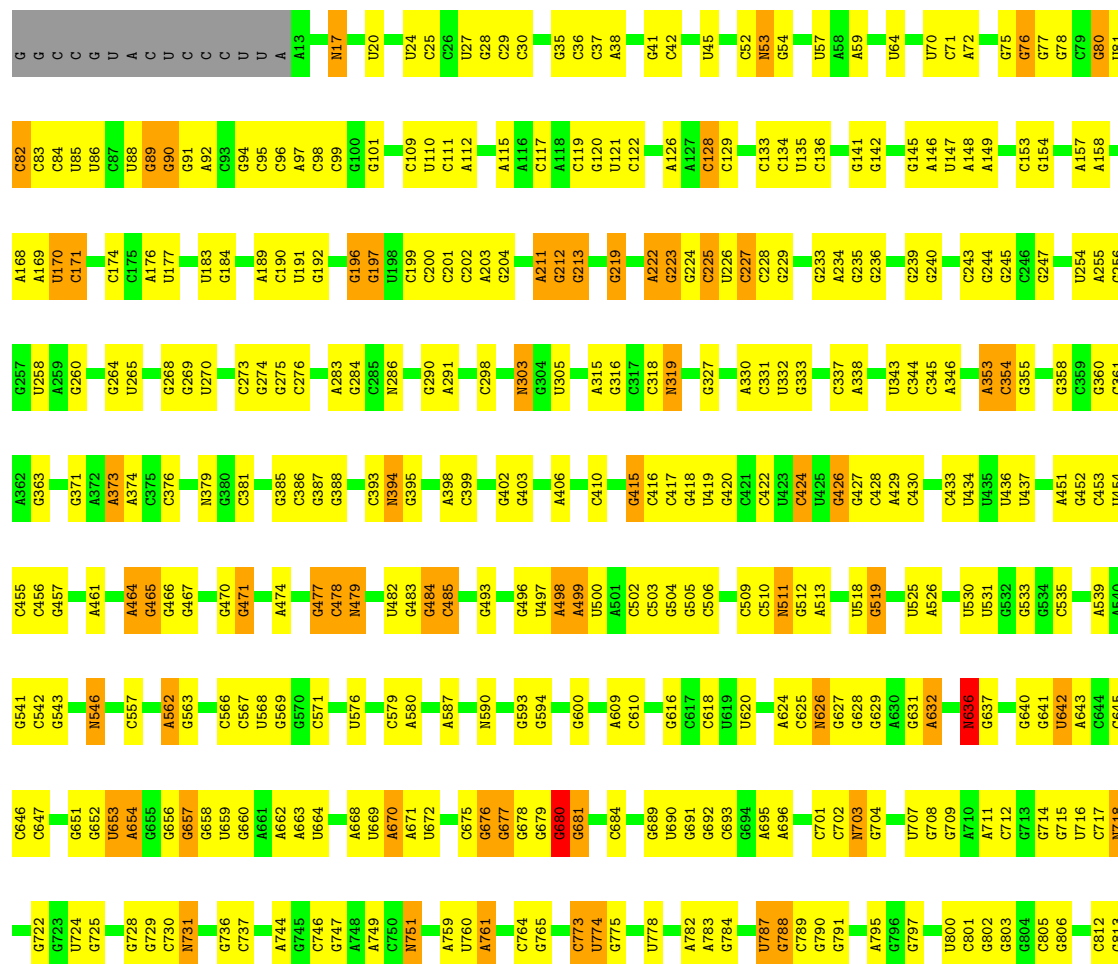
3 Residue-property plots [i](#)

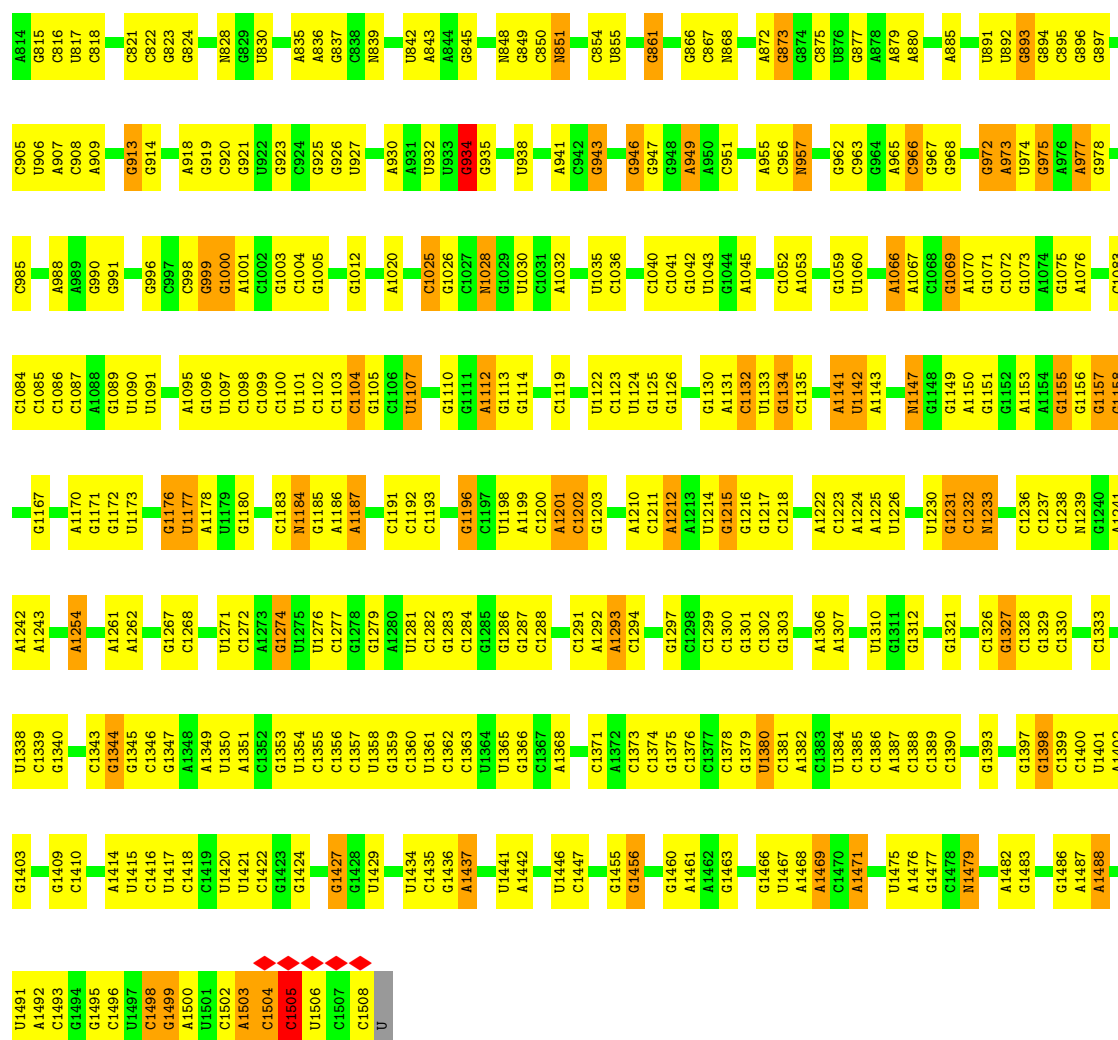
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: rRNA 23S



G2397	A2398	G2399	C2400	C2401	G2402	C2405	A2406	U2407	G2408	G2409	G2410	A2411	G2412	G2416	C2417	G2418	C2419	A2420	G2421	U2422	C2426	G2427	C2428	G2429	G2430	C2431	A2438	A2446	A2447	A2448	A2455	C2456	A2457	G2468	G2469	C2470	A2471	C2472	U2473	U2474	G2477	C2478	A2488	N2495	G2496	G2497	A2498	A2499			
U2208	G2209	A2211	U2212	G2213	U2232	G2233	U2234		C2242		N2249	G2253	G2254	G2255	A2256		U2259	U2265	G2266	G2267	C2268	G2269	G2270	G2271	G2272	G2273	G2276	G2277	G2278	G2281	N2287	G2288	G2291	G2292		A2295	A2300	G2301	A2302	G2303	C2304	C2305	C2306	G2309	G2310	A2311	G2312	G2313	U2314	U2315	
A2109	A2110	U2118	A2119	G2120	A2121	U2128	G2129	A2130	A2131	N2136	G2137	G2138	A2142	A2143	G2144	G2145	G2146	G2147	G2148	A2153	A2154	G2155	U2156	A2157	G2162	G2163	U2166	U2167	A2168	A2169	G2170	G2171	U2172	A2173	A2177	A2178	A2179	U2180	U2181	G2182	C2183	U2184	U2196	G2197	G2198	U2390	G2391	G2392	G2393	U2394	U2395
G2009	C2010	A2011	G2012	G2020		N2027	G2028	A2029		U2035	A2040	A2041	A2042	A2043	C2044	A2045	A2046	A2047	U2050	G2051	C2052	G2055	C2056	U2057	A2058	G2059	N2062	A2065	A2066	G2067	U2077	G2078	G2081	C2082	N2083	G2084	A2085		C2093	C2094	A2095	G2098	C2099		G2102	U2103	A2104	G2108			
A1883	N1884	N1885		C1890	A1891	G1895	C1896	C1897	C1898	G1901	G1905	A1908		A1914	U1920	G1921	U1922	C1923	G1928	A1929	G1932	C1933	N1934	G1938	G1939	G1942	G1943	G1950	C1951	N1962	G1972	A1976	G1987	U1992	G1993	C1994	G1995	U1996	A1997	A1998	C1999	C2000	N2001								
A1768	A1769	C1773	G1774	A1775	G1776	A1777	C1778	N1780	G1781	G1782	G1783	A1787	A1788	G1789	C1790	G1791	U1796		C1799	C1805	G1806	U1807	U1808	A1809	G1810	U1816	A1824	G1830	G1831	A1840	A1841	A1842	A1843	C1847	U1848	U1856	U1857	U1862	N1867	G1873	G1874	N1878	G1879								
G1678		C1681	A1685	A1686	C1687	G1688	C1689	G1692	N1695	G1696	A1697	A1698	G1699	G1700	G1703	A1704	C1705	G1706	C1707	G1710	G1711	G1712	G1713	G1714	U1715	G1729	U1731	G1732	A1733	G1734	G1735	G1739	A1742	A1743	A1748	C1754	N1755	G1756	G1759	A1760	U1762	G1763	C1764	N1765	A1767	U1767					
G1574	A1575	C1576	A1577	G1578	G1579	C1580	A1591	G1592	C1593	N1594	G1598	U1601	G1606	A1612	A1613	C1616	N1617	G1618	A1621	G1625	C1626	G1630	C1631	G1632	C1633	A1639	A1640	A1641	A1645	A1646	A1647	C1648	U1653	A1657	C1660	C1661	N1662	C1666	N1667	G1668	A1676	G1677									
G1411	A1412	C1413	C1414	C1415	C1421	A1422	C1423	G1433	C1443	N1460	G1470	A1471	G1478	C1479	C1480	G1481	A1484	U1487	C1488	G1493	C1498	G1499	C1509	C1514	G1524	U1533	A1545	A1546	U1547	C1548	C1549	N1550	N1554	N1557	A1560	C1561	C1566	A1567	G1568												
G1323	A1324	A1325	C1326	A1327	A1328	G1329	C1330	C1331	U1332	U1333	A1339	A1340	A1343	G1344	U1345	G1346	C1347	A1350	A1351	C1352	A1353	G1354	C1355	U1356	A1357	A1358	C1359	C1360	C1361	G1362	U1363	C1364	G1365	A1366	G1367	G1368	C1371	G1387	A1388	C1389	G1392	G1393	C1394	U1395	C1396	A1397	C1401	G1406			
A1235	G1240	C1241	C1242	N1243	A1250	A1251	G1252	G1253	C1254	A1258	A1259	A1261	U1262	G1263	G1266	G1272	C1278	U1279	C1280	C1281	A1282	A1283	A1284	U1288	G1289	N1293	G1296	C1297	C1298	U1299	U1300	A1301	G1302	A1303	C1304	A1305	G1306	G1307	G1308	G1309	G1310	G1311	A1316	G1317	G1318	C1319	A1322				
G1138	C1139	G1140	A1141	A1142	A1143	G1144	C1145	C1146	C1147	A1148	C1149	C1154	C1155	U1159	C1160	A1161	A1162	A1163	C1164	G1168	C1171	C1172	C1173	A1174	G1177	C1178	C1179	G1180	G1186	G1187	C1093	G1094	G1095	G1096	A1101	G1110	G1111	A1115	G1116	C1117	A1118	G1129	U1130	G1131	C1132	A1133	G1134				





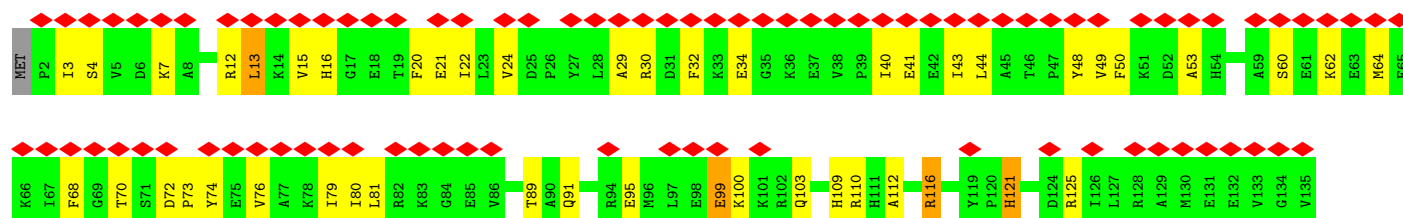
• Molecule 3: rRNA 5S

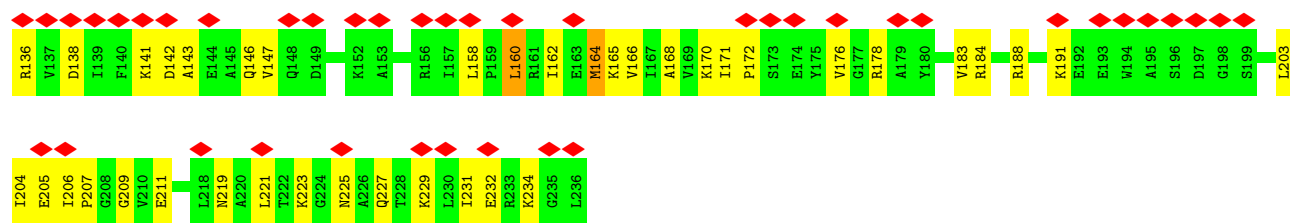
Chain 3: 69% 24% 5% .



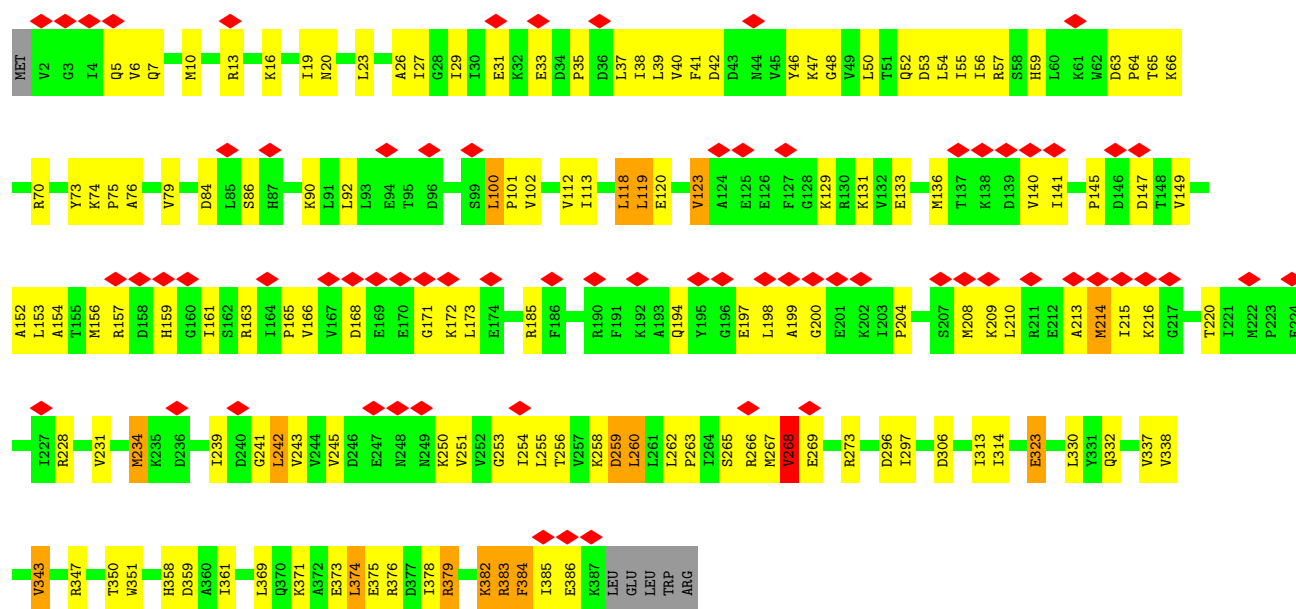
• Molecule 4: Ribosome maturation protein SDO1 homolog

Chain A: 55% 63% 34% .

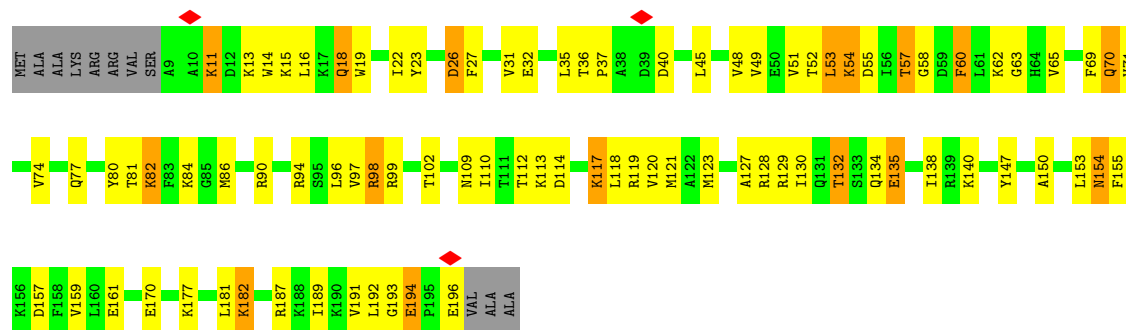




• Molecule 5: Dehydrogenase



• Molecule 6: 30S ribosomal protein S3Ae



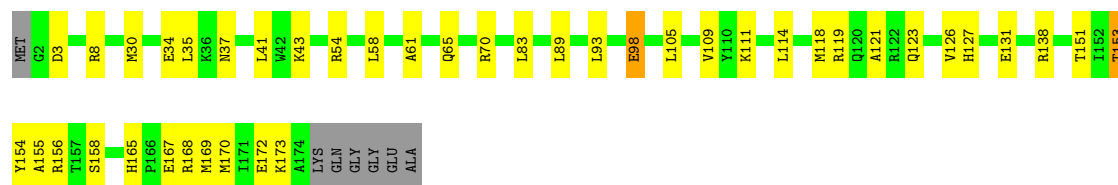
• Molecule 7: 30S ribosomal protein S2



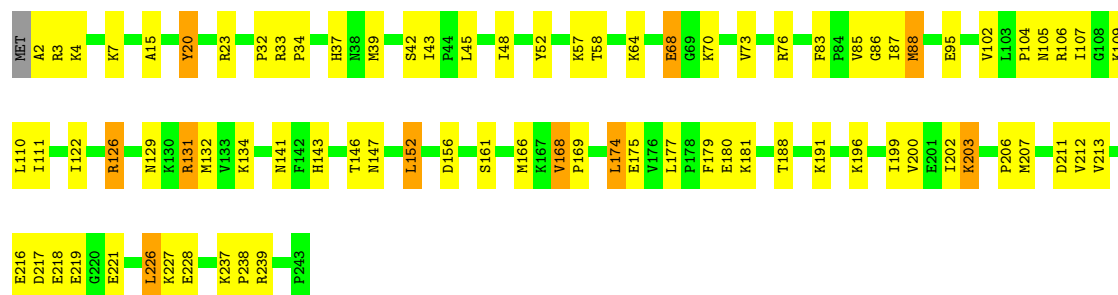
- Molecule 8: Zn-ribbon RNA-binding protein involved in translation



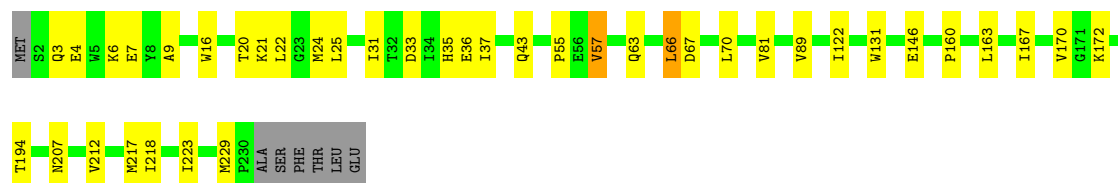
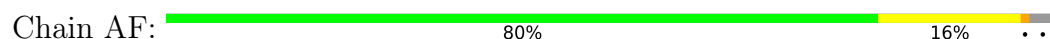
- Molecule 9: 30S ribosomal protein S4



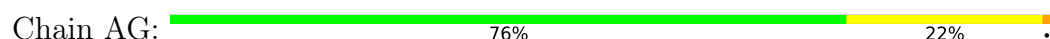
- Molecule 10: 30S ribosomal protein S4e

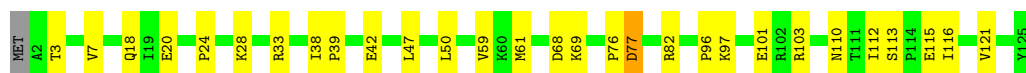


- Molecule 11: 30S ribosomal protein S5



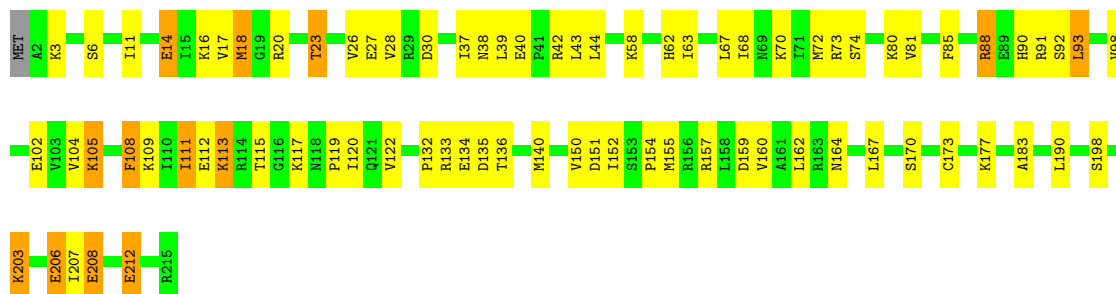
- Molecule 12: 30S ribosomal protein S6e





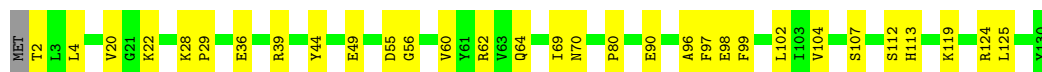
- Molecule 13: 30S ribosomal protein S7

Chain AH: 63% 31% 6%



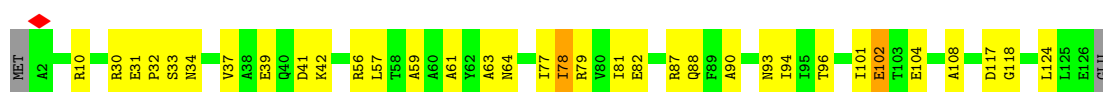
- Molecule 14: 30S ribosomal protein S8

Chain AI: 75% 24%



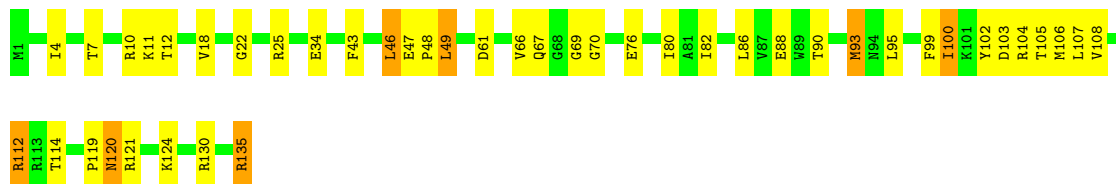
- Molecule 15: 30S ribosomal protein S8e

Chain AJ: 72% 25%



- Molecule 16: 30S ribosomal protein S9

Chain AK: 67% 27% 5%



- Molecule 17: 30S ribosomal protein S10

Chain AL: 59% 32% 7%





- Molecule 18: 30S ribosomal protein S11

Chain AM: 64% 24% 5% 7%



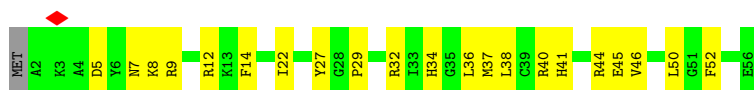
- Molecule 19: 30S ribosomal protein S12

Chain AN: 86% 12% ..



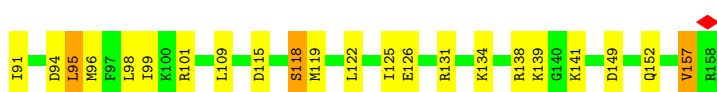
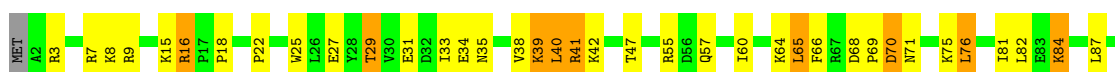
- Molecule 20: 30S ribosomal protein S14 type Z

Chain AP: 61% 38% .



- Molecule 21: 30S ribosomal protein S15

Chain AQ: 62% 30% 8% .



- Molecule 22: Small ribosomal subunit protein uS17

Chain AR: 72% 22% . .



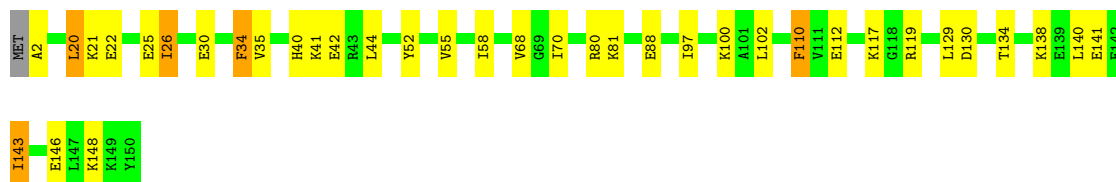
- Molecule 23: 30S ribosomal protein S17e

Chain AS: 57% 34% . .



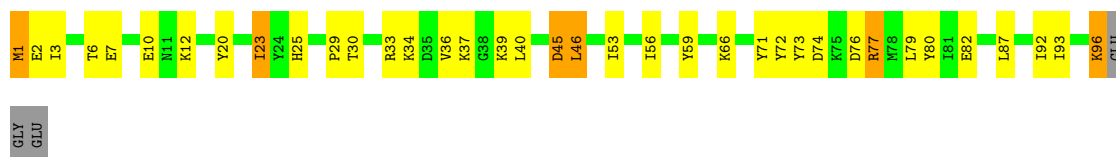
- Molecule 24: 30S ribosomal protein S19e

Chain AU: 75% 21% . .



- Molecule 25: 30S ribosomal protein S24e

Chain AV: 60% 31% 6% .



- Molecule 25: 30S ribosomal protein S24e

Chain B6: 82% 10% 5% .



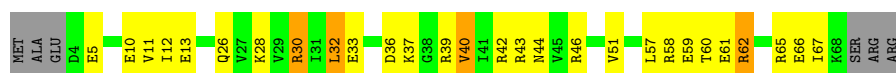
- Molecule 26: 30S ribosomal protein S27e

Chain AW: 51% 38% 5% 6%



- Molecule 27: 30S ribosomal protein S28e

Chain AX: 52% 34% 6% 8%



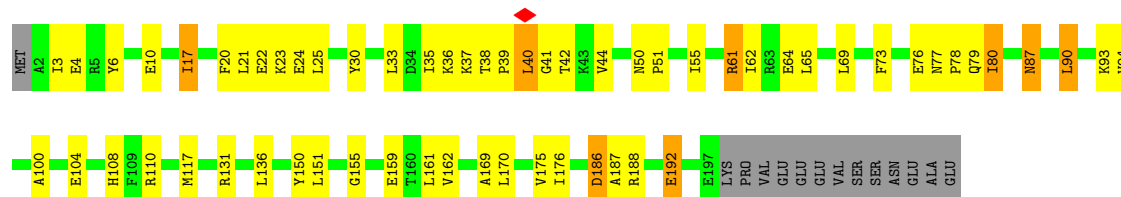
- Molecule 28: 30S ribosomal protein S27ae

Chain AY: 35% 43% 14% 43%



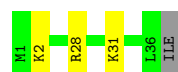
- Molecule 29: 30S ribosomal protein S3

Chain AZ: 64% 25% 7%



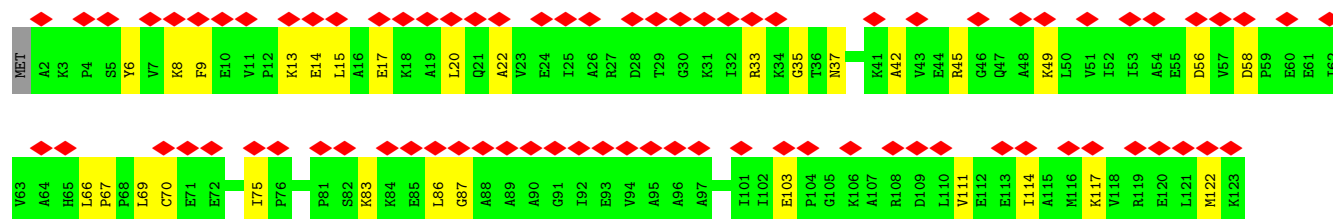
- Molecule 30: Small ribosomal subunit protein eS32

Chain A0: 89% 8%



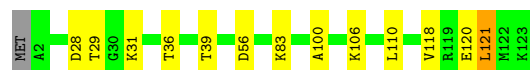
- Molecule 31: 50S ribosomal protein L7Ae

Chain A3: 64% 75% 24%



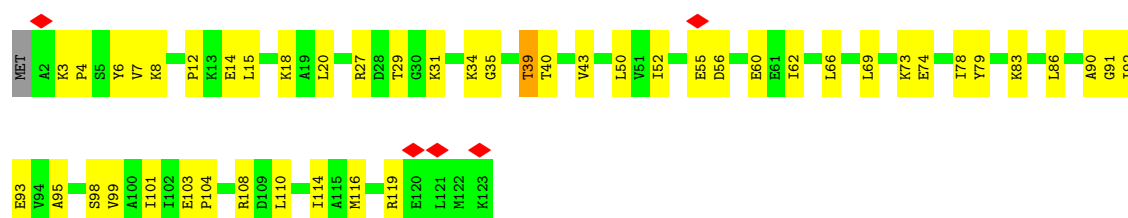
- Molecule 31: 50S ribosomal protein L7Ae

Chain BG: 89% 10%

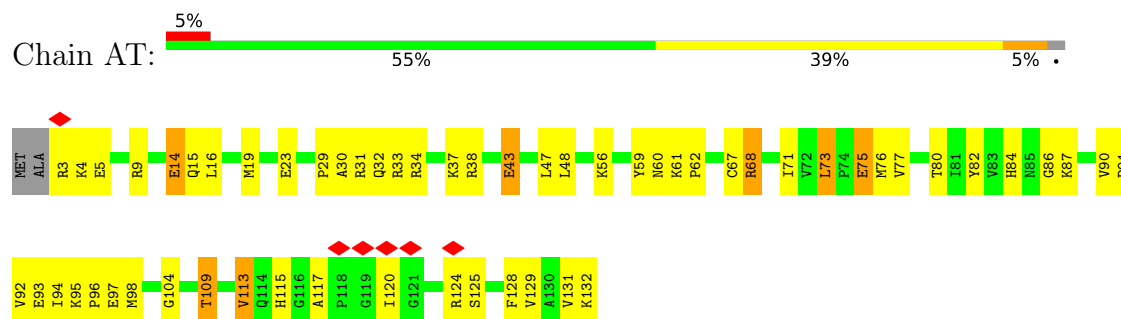


- Molecule 31: 50S ribosomal protein L7Ae

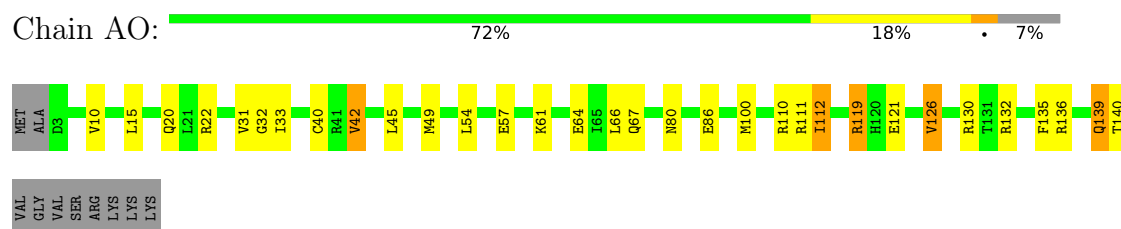
Chain B4: 61% 37%



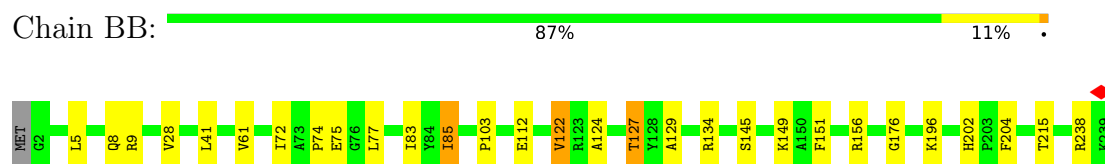
- Molecule 32: 30S ribosomal protein S19



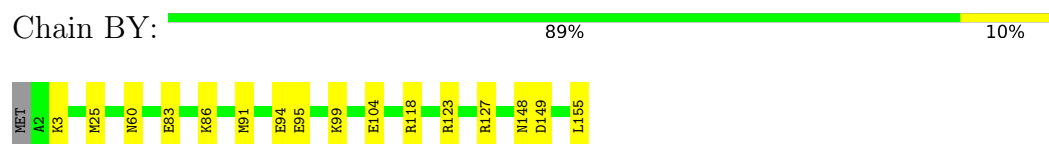
- Molecule 33: 30S ribosomal protein S13



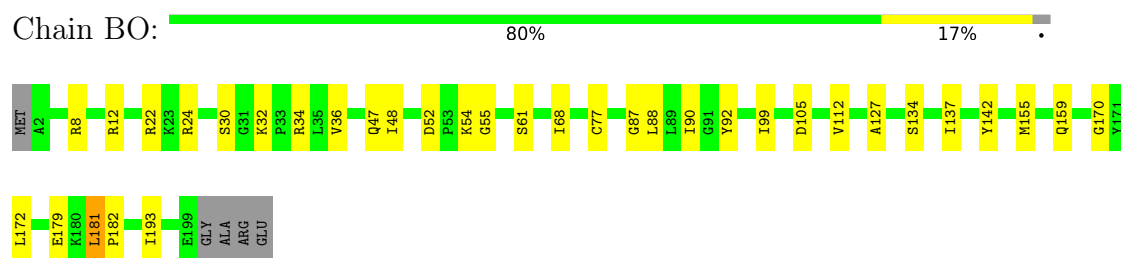
- Molecule 34: Large ribosomal subunit protein uL2



- Molecule 35: Large ribosomal subunit protein uL30

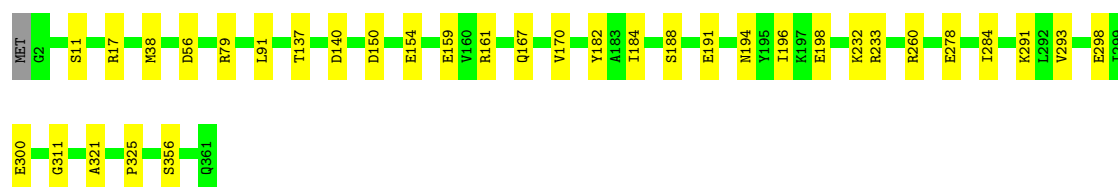


- Molecule 36: Large ribosomal subunit protein uL18

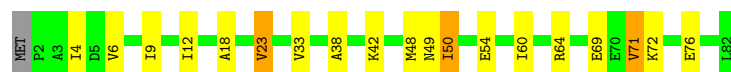
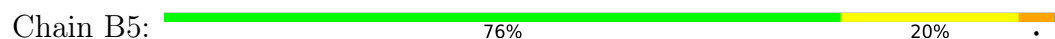


- Molecule 37: Large ribosomal subunit protein uL3

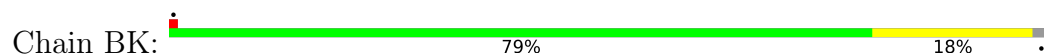




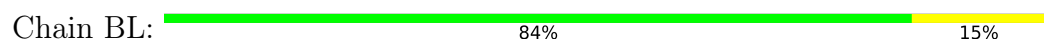
- Molecule 38: Large ribosomal subunit protein eL14



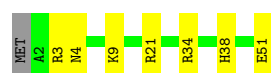
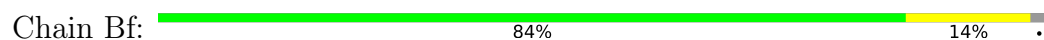
- Molecule 38: Large ribosomal subunit protein eL14



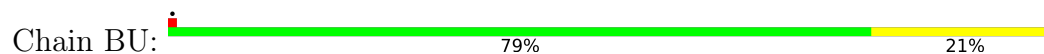
- Molecule 39: Large ribosomal subunit protein uL15



- Molecule 40: Large ribosomal subunit protein eL39



- Molecule 41: Large ribosomal subunit protein uL24



- Molecule 42: Large ribosomal subunit protein eL32



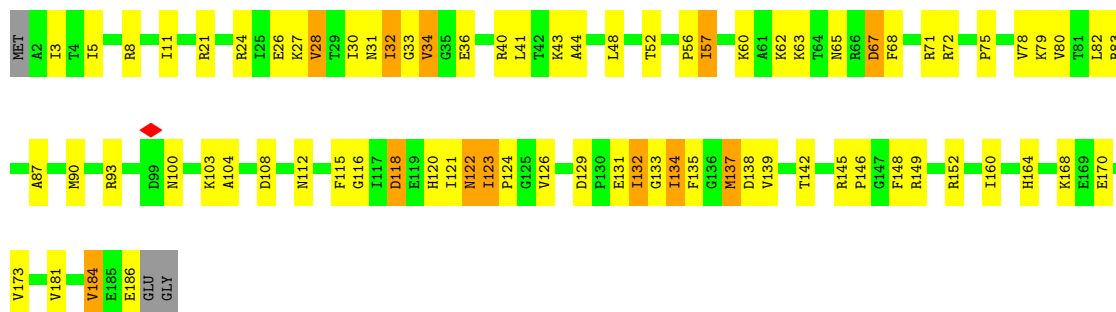
- Molecule 43: Large ribosomal subunit protein eL37

Chain Be:  81% 18%



- Molecule 44: Large ribosomal subunit protein uL5

Chain BE:  57% 35% 6%



- Molecule 45: Large ribosomal subunit protein eL31

Chain Ba:  82% 18%

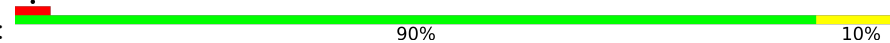


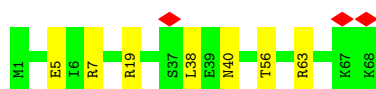
- Molecule 46: Large ribosomal subunit protein uL23

Chain BT:  87% 12%



- Molecule 47: Large ribosomal subunit protein uL29

Chain BW:  90% 10%



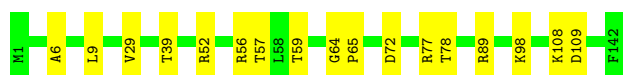
- Molecule 48: Large ribosomal subunit protein eL43

Chain Bi:  93% 6%



- Molecule 49: Large ribosomal subunit protein uL13

Chain BI:  88% 12%



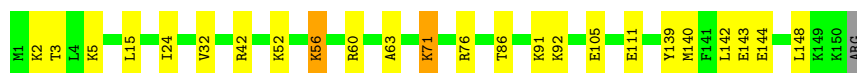
- Molecule 50: Large ribosomal subunit protein eL21

Chain BR:  86% 12% ..



- Molecule 51: Large ribosomal subunit protein eL19

Chain BQ:  83% 15% ..

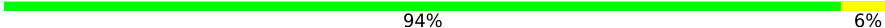


- Molecule 52: Large ribosomal subunit protein eL24

Chain BV:  85% 9% 6%



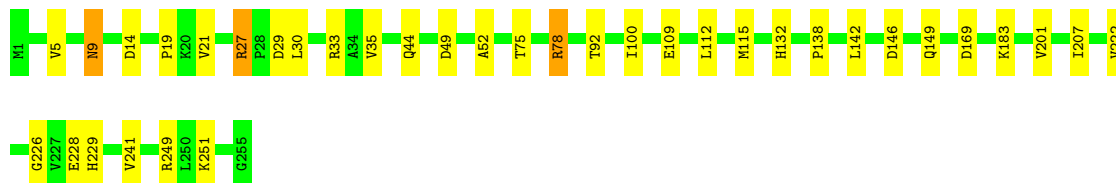
- Molecule 53: Large ribosomal subunit protein eL42

Chain Bj:  94% 6%



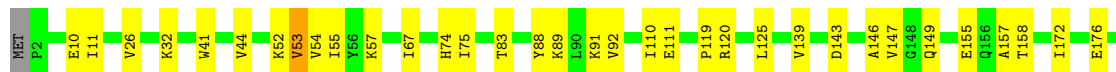
- Molecule 54: Large ribosomal subunit protein uL4

Chain BD:  86% 13% .



- Molecule 55: Large ribosomal subunit protein uL6

Chain BF:  81% 18% ..



F184

- Molecule 56: Large ribosomal subunit protein eL30

Chain BZ:  77% 21% ..



- Molecule 57: Large ribosomal subunit protein eL18

Chain BP:  89% 11%



- Molecule 58: Large ribosomal subunit protein eL15

Chain BM:  89% 10% .



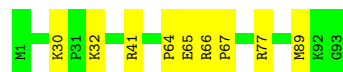
- Molecule 59: Large ribosomal subunit protein uL22

Chain BS:  87% 12% .



- Molecule 60: Large ribosomal subunit protein eL34

Chain Bd:  90% 10%



- Molecule 61: Large ribosomal subunit protein uL16

Chain BN:  81% 17% .



- Molecule 62: Large ribosomal subunit protein eL40

Chain Bg:  78% 16% 6%



- Molecule 63: Large ribosomal subunit protein eL33

Chain Bc:  89% 10% .



- Molecule 64: Large ribosomal subunit protein uL14

Chain BJ:  86% 13% .



- Molecule 65: Large ribosomal subunit protein eL20

Chain Bl:  84% 16%



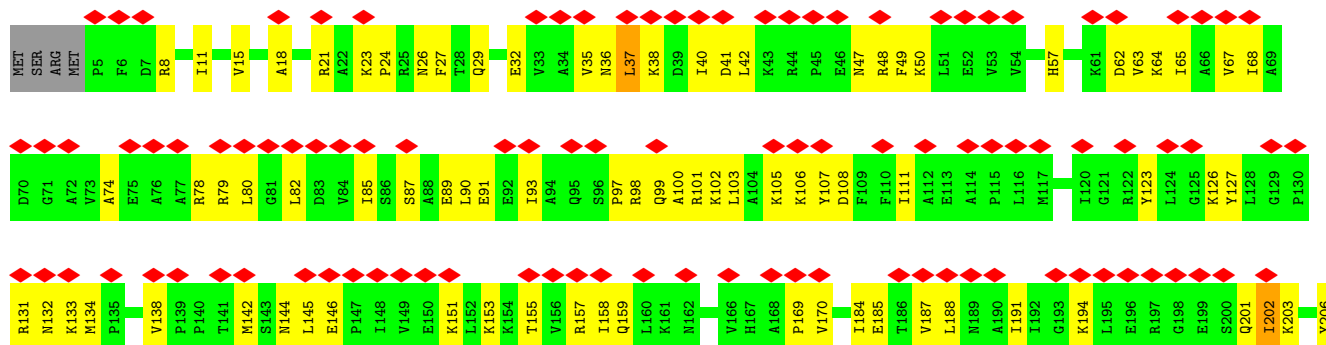
- Molecule 66: C2H2-type domain-containing protein

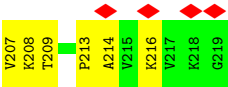
Chain Bk:  85% 12% .



- Molecule 67: Large ribosomal subunit protein uL1

Chain BA:  48% 58% 39% ..





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.014	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0009	Depositor
Map size ($\text{\AA}$)	302.04, 302.04, 302.04	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83900005, 0.83900005, 0.83900005	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4AC, B8H, OMU, 6MZ, OMC, A2M, 5MC, MA6, UR3, MG, ZN, OMG, LHH

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	1	0.17	2/70601 (0.0%)	0.31	2/110066 (0.0%)
2	2	0.19	2/34435 (0.0%)	0.38	0/53681
3	3	0.15	0/2995	0.34	0/4669
4	A	0.13	0/1934	0.35	0/2598
5	H	0.12	0/3120	0.32	0/4209
6	AA	0.24	0/1557	0.43	0/2087
7	AB	0.17	0/1602	0.31	0/2165
8	AC	0.19	0/463	0.35	0/628
9	AD	0.13	0/1476	0.28	0/1980
10	AE	0.18	0/2032	0.36	0/2742
11	AF	0.14	0/1838	0.28	0/2478
12	AG	0.12	0/993	0.28	0/1329
13	AH	0.17	0/1762	0.37	0/2366
14	AI	0.14	0/1055	0.31	0/1415
15	AJ	0.13	0/995	0.28	0/1327
16	AK	0.14	0/1089	0.39	0/1459
17	AL	0.19	0/817	0.35	0/1097
18	AM	0.14	0/973	0.38	0/1311
19	AN	0.12	0/1165	0.27	0/1547
20	AP	0.13	0/465	0.30	0/613
21	AQ	0.15	0/1333	0.35	0/1791
22	AR	0.18	0/916	0.33	0/1237
23	AS	0.12	0/548	0.24	0/725
24	AU	0.19	0/1253	0.33	0/1689
25	AV	0.17	0/826	0.34	0/1108
25	B6	0.10	0/808	0.27	0/1086
26	AW	0.13	0/476	0.31	0/641
27	AX	0.13	0/518	0.33	0/694
28	AY	0.12	0/235	0.36	0/315
29	AZ	0.16	0/1563	0.32	0/2099
30	A0	0.14	0/349	0.28	0/451
31	A3	0.11	0/945	0.34	0/1274

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	B4	0.16	0/945	0.36	0/1274
31	BG	0.11	0/944	0.25	0/1274
32	AT	0.16	0/1077	0.35	0/1439
33	AO	0.17	0/1135	0.35	0/1526
34	BB	0.13	0/1882	0.28	0/2538
35	BY	0.11	0/1254	0.26	0/1677
36	BO	0.12	0/1645	0.27	0/2209
37	BC	0.12	0/2933	0.27	0/3943
38	B5	0.11	0/619	0.29	0/830
38	BK	0.11	0/611	0.28	0/819
39	BL	0.12	0/1167	0.30	0/1552
40	Bf	0.12	0/443	0.25	0/589
41	BU	0.11	0/1027	0.26	0/1368
42	Bb	0.12	0/1120	0.25	0/1494
43	Be	0.13	0/514	0.26	0/676
44	BE	0.17	0/1509	0.37	0/2022
45	Ba	0.12	0/793	0.26	0/1064
46	BT	0.12	0/705	0.24	0/945
47	BW	0.09	0/566	0.21	0/747
48	Bi	0.10	0/630	0.26	0/839
49	BI	0.12	0/1166	0.25	0/1559
50	BR	0.11	0/819	0.23	0/1098
51	BQ	0.11	0/1281	0.22	0/1689
52	BV	0.11	0/547	0.26	0/729
53	Bj	0.10	0/807	0.23	0/1070
54	BD	0.11	0/2069	0.25	0/2787
55	BF	0.11	0/1485	0.25	0/2003
56	BZ	0.11	0/759	0.25	0/1023
57	BP	0.11	0/984	0.24	0/1314
58	BM	0.12	0/1627	0.24	0/2170
59	BS	0.13	0/1275	0.28	0/1715
60	Bd	0.13	0/778	0.28	0/1036
61	BN	0.12	0/1483	0.25	0/1992
62	Bg	0.09	0/396	0.22	0/526
63	Bc	0.11	0/693	0.27	0/926
64	BJ	0.12	0/1080	0.25	0/1456
65	Bl	0.11	0/669	0.28	0/886
66	Bk	0.13	0/538	0.25	0/709
67	BA	0.12	0/1700	0.29	0/2288
All	All	0.16	4/182812 (0.0%)	0.32	2/268678 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	94	G	O3'-P	-9.21	1.47	1.61
1	1	96	U	C1'-N1	5.73	1.57	1.48
2	2	830	OMU	O3'-P	5.05	1.61	1.56
2	2	373	A2M	O3'-P	5.00	1.61	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2408	G	C4'-C3'-O3'	-8.62	96.46	109.40
1	1	1306	G	C2'-C3'-O3'	6.03	122.74	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	65181	0	32949	761	0
2	2	32291	0	16339	543	0
3	3	2703	0	1375	30	0
4	A	1900	0	1968	57	0
5	H	3074	0	3190	109	0
6	AA	1531	0	1623	54	0
7	AB	1571	0	1630	44	0
8	AC	449	0	435	18	0
9	AD	1452	0	1521	26	0
10	AE	1983	0	2058	47	0
11	AF	1808	0	1879	24	0
12	AG	977	0	1037	19	0
13	AH	1725	0	1780	56	0
14	AI	1034	0	1069	24	0
15	AJ	986	0	1070	19	0
16	AK	1073	0	1133	31	0
17	AL	809	0	859	26	0
18	AM	955	0	981	32	0
19	AN	1148	0	1248	12	0
20	AP	455	0	475	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	AQ	1305	0	1388	41	0
22	AR	893	0	912	13	0
23	AS	541	0	573	16	0
24	AU	1223	0	1263	25	0
25	AV	808	0	832	20	0
25	B6	790	0	806	11	0
26	AW	470	0	495	20	0
27	AX	516	0	544	15	0
28	AY	227	0	207	6	0
29	AZ	1541	0	1624	41	0
30	A0	343	0	407	3	0
31	A3	933	0	982	19	0
31	B4	933	0	982	26	0
31	BG	932	0	982	9	0
32	AT	1057	0	1131	35	0
33	AO	1116	0	1152	20	0
34	BB	1838	0	1903	21	0
35	BY	1235	0	1314	12	0
36	BO	1607	0	1638	22	0
37	BC	2870	0	3021	20	0
38	B5	614	0	671	13	0
38	BK	607	0	663	10	0
39	BL	1149	0	1218	20	0
40	Bf	435	0	494	6	0
41	BU	1011	0	1078	20	0
42	Bb	1095	0	1190	7	0
43	Be	503	0	533	9	0
44	BE	1485	0	1539	52	0
45	Ba	778	0	851	12	0
46	BT	696	0	758	7	0
47	BW	565	0	628	5	0
48	Bi	620	0	668	3	0
49	BI	1148	0	1237	14	0
50	BR	797	0	835	9	0
51	BQ	1265	0	1392	18	0
52	BV	532	0	523	6	0
53	Bj	789	0	842	2	0
54	BD	2026	0	2131	28	0
55	BF	1456	0	1514	22	0
56	BZ	749	0	796	14	0
57	BP	971	0	1039	6	0
58	BM	1588	0	1683	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	BS	1247	0	1280	12	0
60	Bd	759	0	825	8	0
61	BN	1452	0	1491	22	0
62	Bg	387	0	397	6	0
63	Bc	684	0	748	6	0
64	BJ	1066	0	1133	13	0
65	Bl	659	0	702	9	0
66	Bk	528	0	575	6	0
67	BA	1675	0	1787	59	0
68	1	164	0	0	0	0
68	2	65	0	0	0	0
68	3	1	0	0	0	0
68	AD	1	0	0	0	0
68	AK	1	0	0	0	0
68	AN	1	0	0	0	0
68	BB	2	0	0	0	0
68	BD	1	0	0	0	0
68	BM	1	0	0	0	0
68	BS	1	0	0	0	0
68	Bb	1	0	0	0	0
68	Bc	1	0	0	0	0
69	AC	2	0	0	0	0
69	AF	1	0	0	0	0
69	AP	1	0	0	0	0
69	AR	1	0	0	0	0
69	AW	1	0	0	0	0
69	BV	1	0	0	0	0
69	Bd	1	0	0	0	0
69	Be	1	0	0	0	0
69	Bg	1	0	0	0	0
69	Bi	1	0	0	0	0
69	Bj	1	0	0	0	0
69	Bk	1	0	0	0	0
All	All	173872	0	127996	2463	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (2463) 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)
1:1:117:G:O2'	1:1:118:U:OP1	1.67	1.12
1:1:2408:G:C8	1:1:2410:G:N7	2.16	1.12
1:1:100:G:N2	1:1:119:C:O2	1.82	1.12
1:1:2585:4AC:H5	1:1:2597:G:H1	1.18	1.01
1:1:2608:4AC:H5	1:1:2613:G:H1	1.21	1.00
1:1:102:C:N4	1:1:117:G:O6	1.97	0.97
1:1:2887:A:HO2'	64:BJ:2:ALA:N	1.60	0.97
21:AQ:41:ARG:HG3	21:AQ:82:LEU:HD11	1.47	0.96
2:2:82:C:O2	2:2:91:G:N2	2.05	0.89
1:1:2348:G:N2	1:1:2421:C:O2	2.05	0.89
2:2:631:G:H22	2:2:708:G:H1	1.17	0.88
33:AO:45:LEU:HD12	33:AO:49:MET:HE1	1.56	0.87
1:1:1306:G:H8	1:1:1306:G:H5''	1.40	0.85
55:BF:158:THR:HG21	55:BF:172:ILE:H	1.42	0.85
11:AF:131:TRP:HA	14:AI:97:PHE:HB3	1.60	0.84
2:2:680:OMG:H2'	2:2:681:G:C8	2.13	0.83
1:1:931:U:H3	1:1:1046:G:H1	1.25	0.83
15:AJ:81:ILE:HD11	15:AJ:102:GLU:HB3	1.59	0.83
1:1:438:U:O2'	1:1:440:G:N7	2.11	0.82
1:1:785:G:H5''	1:1:2259:U:H5''	1.62	0.82
2:2:803:G:N2	2:2:821:C:O2	2.11	0.82
5:H:10:MET:HE3	5:H:102:VAL:HG11	1.59	0.82
4:A:116:ARG:HE	19:AN:100:HIS:HB2	1.42	0.82
13:AH:30:ASP:OD2	13:AH:157:ARG:NH2	2.13	0.82
1:1:1303:A:C1'	1:1:1304:C:OP1	2.29	0.81
1:1:235:G:H1	1:1:242:C:H5	1.28	0.81
2:2:133:C:O2	2:2:236:G:N2	2.12	0.80
2:2:134:C:O2	2:2:235:G:N2	2.12	0.80
1:1:2408:G:H8	1:1:2410:G:N7	1.77	0.80
7:AB:43:LEU:HD21	7:AB:155:PRO:HB2	1.63	0.80
1:1:1303:A:H1'	1:1:1304:C:OP1	1.82	0.80
18:AM:53:ASP:OD1	18:AM:53:ASP:N	2.15	0.80
2:2:646:C:O2	2:2:678:G:N2	2.12	0.79
1:1:2166:U:O4	1:1:2170:G:N1	2.16	0.79
2:2:651:G:H21	18:AM:38:THR:HG21	1.49	0.78
1:1:710:C:O2	1:1:747:G:N2	2.13	0.78
9:AD:58:LEU:HD13	9:AD:70:ARG:HA	1.67	0.77
2:2:569:G:OP2	10:AE:191:LYS:NZ	2.17	0.77
2:2:714:G:O2'	21:AQ:55:ARG:NH1	2.18	0.77
5:H:234:MET:HE3	5:H:242:LEU:HD22	1.68	0.76
2:2:625:C:H2'	2:2:626:4AC:H6	1.67	0.76
2:2:1095:A:H2'	2:2:1096:G:C8	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:296:ASP:OD2	5:H:358:HIS:NE2	2.18	0.76
6:AA:112:THR:HG21	6:AA:155:PHE:HB2	1.68	0.75
12:AG:68:ASP:HA	12:AG:116:ILE:HA	1.66	0.75
2:2:707:U:O2'	21:AQ:118:SER:OG	2.03	0.75
7:AB:142:ASP:H	7:AB:145:ASN:HD22	1.33	0.75
3:3:2:G:N2	3:3:123:C:O2	2.15	0.75
67:BA:18:ALA:O	67:BA:21:ARG:NH1	2.20	0.75
2:2:624:A:H5''	21:AQ:98:LEU:HD21	1.68	0.74
9:AD:35:LEU:HD12	9:AD:41:LEU:HD23	1.69	0.74
1:1:2535:G:H22	1:1:2543:U:H3	1.35	0.74
67:BA:37:LEU:HB2	67:BA:201:GLN:HE21	1.52	0.74
2:2:96:C:H2'	2:2:97:A:C8	2.22	0.74
2:2:978:G:N2	2:2:998:C:O2	2.14	0.74
18:AM:92:LYS:HD3	18:AM:121:ILE:HG22	1.69	0.74
1:1:1713:G:H21	1:1:1787:A:H8	1.36	0.74
23:AS:25:THR:HG23	23:AS:27:ASP:H	1.51	0.74
5:H:200:GLY:HA2	67:BA:48:ARG:HH22	1.52	0.74
2:2:1099:C:O2	2:2:1114:G:N2	2.19	0.74
14:AI:96:ALA:HB3	14:AI:99:PHE:HB2	1.70	0.73
1:1:103:C:H2'	1:1:104:C:C6	2.23	0.73
2:2:660:G:H1'	5:H:379:ARG:HD3	1.71	0.73
1:1:1140:G:O2'	1:1:1143:A:N6	2.21	0.73
44:BE:34:VAL:HG22	44:BE:36:GLU:H	1.54	0.73
1:1:866:C:O2'	1:1:868:C:OP2	2.07	0.73
3:3:2:G:N1	3:3:123:C:N3	2.30	0.73
1:1:117:G:O2'	1:1:118:U:P	2.47	0.72
13:AH:17:VAL:HG21	13:AH:120:ILE:HD11	1.71	0.72
31:B4:83:LYS:HG2	31:B4:95:ALA:HB1	1.69	0.72
2:2:1491:U:H2'	2:2:1492:A:H8	1.53	0.72
13:AH:133:ARG:NH1	13:AH:208:GLU:OE2	2.22	0.72
5:H:338:VAL:HG11	16:AK:135:ARG:HB3	1.72	0.72
1:1:2408:G:C8	1:1:2410:G:C8	2.78	0.72
2:2:1379:G:H2'	2:2:1380:OMU:H6	1.70	0.72
1:1:2426:C:H2'	1:1:2427:G:H8	1.53	0.72
1:1:102:C:C4	1:1:103:C:C4	2.78	0.72
1:1:103:C:H2'	1:1:104:C:H6	1.55	0.71
44:BE:24:ARG:HH21	44:BE:146:PRO:HG3	1.55	0.71
53:Bj:6:GLN:HG2	53:Bj:94:VAL:HG11	1.72	0.71
17:AL:6:ILE:HG22	17:AL:98:ILE:HG12	1.72	0.71
5:H:214:MET:SD	5:H:216:LYS:NZ	2.63	0.71
10:AE:212:VAL:HA	10:AE:226:LEU:HA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:102:C:N4	1:1:103:C:N4	2.38	0.71
2:2:918:A:H2'	2:2:919:G:H8	1.55	0.71
1:1:792:A:H62	1:1:1509:C:H5	1.38	0.71
67:BA:38:LYS:O	67:BA:201:GLN:NE2	2.23	0.71
1:1:2698:G:OP1	62:Bg:19:ARG:NH1	2.24	0.71
2:2:652:G:N3	18:AM:41:ARG:NH2	2.38	0.71
1:1:117:G:HO2'	1:1:118:U:P	2.13	0.71
2:2:658:G:OP2	18:AM:24:ASN:ND2	2.23	0.71
11:AF:212:VAL:H	14:AI:70:ASN:HD21	1.38	0.71
2:2:663:A:H2'	2:2:664:U:H6	1.56	0.71
11:AF:33:ASP:OD2	11:AF:35:HIS:ND1	2.23	0.71
45:Ba:16:ARG:HA	45:Ba:19:LYS:HG3	1.73	0.71
7:AB:73:ARG:NH1	7:AB:119:ASP:OD2	2.24	0.70
25:AV:6:THR:OG1	25:AV:7:GLU:OE1	2.09	0.70
8:AC:32:CYS:HB2	8:AC:36:GLY:H	1.56	0.70
25:B6:51:THR:HG22	25:B6:71:TYR:HD1	1.56	0.70
1:1:2242:C:O2'	45:Ba:24:ARG:NH2	2.24	0.70
28:AY:25:CYS:HB3	31:A3:45:ARG:HH22	1.56	0.70
2:2:925:G:N7	33:AO:132:ARG:NH2	2.35	0.70
10:AE:132:MET:HE1	10:AE:152:LEU:HD21	1.74	0.70
1:1:1364:C:O2'	1:1:1365:G:O4'	2.07	0.70
2:2:918:A:H2'	2:2:919:G:C8	2.27	0.70
38:BK:45:ARG:NH2	38:BK:66:ALA:O	2.24	0.70
1:1:908:A:N3	54:BD:33:ARG:NH2	2.39	0.70
55:BF:10:GLU:HB3	55:BF:52:LYS:HD3	1.73	0.70
2:2:647:C:O2	2:2:677:G:N2	2.17	0.69
25:AV:72:TYR:OH	25:AV:82:GLU:OE1	2.09	0.69
1:1:2103:U:O2'	1:1:2104:A:N7	2.24	0.69
2:2:183:U:H2'	2:2:184:G:H8	1.57	0.69
2:2:211:A:H4'	2:2:212:G:OP1	1.92	0.69
2:2:456:C:H2'	2:2:457:G:H8	1.56	0.69
4:A:112:ALA:HB1	4:A:160:LEU:HD11	1.73	0.69
29:AZ:37:LYS:NZ	29:AZ:38:THR:O	2.25	0.69
50:BR:19:HIS:HD2	50:BR:21:ARG:H	1.39	0.69
2:2:627:G:H2'	2:2:628:G:C8	2.26	0.69
2:2:1012:G:H1	2:2:1184:4AC:H4	1.38	0.69
2:2:1183:C:N4	2:2:1184:4AC:O7	2.25	0.69
61:BN:56:GLN:HE21	61:BN:125:ARG:HE	1.40	0.69
1:1:1577:A:OP1	51:BQ:2:LYS:NZ	2.24	0.69
2:2:813:G:O2'	6:AA:177:LYS:O	2.06	0.69
31:B4:116:MET:HA	31:B4:119:ARG:HH12	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:6:VAL:HG13	5:H:10:MET:HE1	1.75	0.69
6:AA:54:LYS:HD3	6:AA:60:PHE:HA	1.75	0.69
16:AK:93:MET:SD	16:AK:93:MET:N	2.64	0.69
10:AE:129:ASN:HB3	10:AE:141:ASN:HD22	1.58	0.69
2:2:1177:OMU:HM22	2:2:1178:A:H5'	1.74	0.68
41:BU:5:SER:O	41:BU:11:GLN:NE2	2.27	0.68
1:1:653:G:N1	1:1:656:A:OP2	2.25	0.68
5:H:38:ILE:N	5:H:50:LEU:O	2.25	0.68
21:AQ:76:LEU:HG	21:AQ:81:ILE:HD11	1.74	0.68
44:BE:100:ASN:HB3	44:BE:181:VAL:HA	1.74	0.68
2:2:1300:C:H2'	2:2:1301:G:H8	1.59	0.68
10:AE:237:LYS:HG2	10:AE:238:PRO:HD2	1.75	0.68
2:2:141:G:OP1	2:2:212:G:N2	2.25	0.68
17:AL:93:ASP:OD1	17:AL:93:ASP:N	2.24	0.68
18:AM:39:ILE:HG23	18:AM:74:LYS:HD2	1.75	0.68
2:2:965:A:H5''	2:2:966:C:H5	1.58	0.68
1:1:1998:A:H2'	1:1:1999:C:C6	2.29	0.68
1:1:2311:A:H2'	1:1:2312:G:C8	2.29	0.68
2:2:75:G:H2'	2:2:76:G:C8	2.29	0.68
2:2:647:C:N3	2:2:677:G:N1	2.30	0.68
38:BK:36:THR:OG1	38:BK:68:ASP:OD1	2.12	0.68
1:1:102:C:C4	1:1:103:C:C5	2.81	0.67
1:1:2416:G:H1'	67:BA:208:LYS:HZ2	1.59	0.67
17:AL:82:MET:N	17:AL:82:MET:SD	2.67	0.67
1:1:117:G:C2	1:1:118:U:C6	2.83	0.67
1:1:2409:A:C8	5:H:194:GLN:HG3	2.30	0.67
67:BA:41:ASP:O	67:BA:47:ASN:ND2	2.25	0.67
36:BO:8:ARG:HG3	50:BR:23:ARG:HG3	1.76	0.67
66:Bk:3:ARG:HH21	66:Bk:5:LYS:HB2	1.58	0.67
4:A:205:GLU:OE2	4:A:234:LYS:NZ	2.27	0.67
17:AL:43:LYS:HD3	29:AZ:3:ILE:HD11	1.77	0.67
1:1:2498:A:H2	1:1:2503:U:H3	1.42	0.67
21:AQ:98:LEU:HD22	21:AQ:125:ILE:HD11	1.77	0.67
6:AA:70:GLN:O	6:AA:82:LYS:N	2.25	0.67
56:BZ:34:LEU:HD22	56:BZ:97:ALA:HB2	1.75	0.67
67:BA:65:ILE:HB	67:BA:82:LEU:HD11	1.75	0.67
67:BA:79:ARG:HH22	67:BA:145:LEU:H	1.42	0.67
10:AE:15:ALA:O	10:AE:23:ARG:NH2	2.27	0.67
5:H:262:LEU:HD11	5:H:266:ARG:HH21	1.59	0.66
10:AE:174:LEU:HD12	10:AE:175:GLU:HG2	1.77	0.66
27:AX:10:GLU:O	27:AX:30:ARG:N	2.18	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2408:G:N7	1:1:2410:G:N7	2.43	0.66
2:2:225:C:H2'	2:2:226:U:H6	1.61	0.66
1:1:418:A:H2'	1:1:419:G:C8	2.31	0.66
1:1:1075:U:OP1	50:BR:2:VAL:HG21	1.96	0.66
1:1:1306:G:H8	1:1:1306:G:C5'	2.07	0.66
44:BE:21:ARG:O	44:BE:145:ARG:NH1	2.29	0.66
5:H:131:LYS:HD2	5:H:133:GLU:H	1.59	0.66
1:1:210:C:H2'	1:1:211:4AC:H6	1.76	0.66
1:1:720:A:H2'	1:1:721:A:H8	1.60	0.66
1:1:793:G:OP2	39:BL:12:ARG:NH2	2.29	0.66
5:H:129:LYS:HD2	5:H:228:ARG:HH12	1.60	0.66
44:BE:30:ILE:HG22	44:BE:139:VAL:HG22	1.77	0.66
38:BK:21:LYS:O	38:BK:41:ASN:ND2	2.29	0.65
5:H:27:ILE:O	5:H:31:GLU:HG2	1.97	0.65
6:AA:26:ASP:OD1	6:AA:26:ASP:N	2.21	0.65
1:1:1331:C:H2'	1:1:1332:A:C8	2.30	0.65
2:2:849:G:OP2	19:AN:4:LYS:NZ	2.28	0.65
1:1:1787:A:OP1	60:Bd:30:LYS:NZ	2.26	0.65
24:AU:102:LEU:HD13	24:AU:119:ARG:HD2	1.79	0.65
38:B5:6:VAL:HG21	38:B5:64:ARG:HG3	1.79	0.65
49:BI:108:LYS:HD3	49:BI:109:ASP:H	1.61	0.65
1:1:764:A:O2'	63:Bc:17:GLN:NE2	2.29	0.65
1:1:1806:G:OP2	1:1:1806:G:N2	2.28	0.65
2:2:316:G:N1	9:AD:3:ASP:OD1	2.29	0.65
25:AV:36:VAL:HG21	25:AV:56:ILE:HD11	1.79	0.65
2:2:82:C:H2'	2:2:83:C:C6	2.31	0.65
2:2:692:G:OP1	2:2:824:G:N2	2.25	0.65
7:AB:182:ILE:HB	7:AB:187:GLU:HB3	1.78	0.65
1:1:894:A:H2'	1:1:895:A:C8	2.31	0.65
1:1:2385:C:H5'	5:H:154:ALA:HB2	1.79	0.65
50:BR:45:ILE:H	50:BR:59:HIS:HD2	1.44	0.65
21:AQ:70:ASP:OD1	21:AQ:70:ASP:N	2.27	0.65
1:1:2343:G:OP1	1:1:2343:G:H4'	1.97	0.65
2:2:258:U:O3'	15:AJ:10:ARG:NH2	2.30	0.65
1:1:1329:G:H2'	1:1:1330:C:H6	1.62	0.65
1:1:1942:G:OP1	64:BJ:86:ARG:NH1	2.31	0.65
15:AJ:33:SER:HB3	15:AJ:56:ARG:HD3	1.79	0.65
34:BB:5:LEU:H	34:BB:8:GLN:HE21	1.45	0.65
1:1:230:G:OP1	43:Be:21:ARG:NH1	2.30	0.64
6:AA:90:ARG:NH1	18:AM:119:THR:O	2.23	0.64
5:H:20:ASN:OD1	5:H:70:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:BA:11:ILE:HD13	67:BA:184:ILE:HD11	1.78	0.64
44:BE:65:ASN:HD22	44:BE:68:PHE:H	1.44	0.64
1:1:2337:C:H2'	1:1:2338:G:H8	1.63	0.64
2:2:646:C:N3	2:2:678:G:N1	2.33	0.64
2:2:1214:U:O4	13:AH:170:SER:OG	2.13	0.64
1:1:116:G:H2'	1:1:117:G:H8	1.62	0.64
5:H:259:ASP:N	5:H:259:ASP:OD1	2.30	0.64
32:AT:32:GLN:HG3	32:AT:71:ILE:HD12	1.79	0.64
2:2:703:4AC:O5'	2:2:703:4AC:H6	1.98	0.64
18:AM:85:ALA:H	18:AM:119:THR:HG22	1.62	0.64
34:BB:28:VAL:HG11	34:BB:72:ILE:HG13	1.80	0.64
1:1:2585:4AC:H5	1:1:2597:G:N1	2.03	0.64
7:AB:120:PRO:HB3	7:AB:127:MET:HE2	1.80	0.64
6:AA:117:LYS:HB2	6:AA:192:LEU:HB2	1.79	0.64
1:1:102:C:C2	1:1:103:C:C6	2.86	0.64
1:1:2368:G:OP2	67:BA:26:ASN:ND2	2.31	0.64
1:1:2608:4AC:H5	1:1:2613:G:N1	2.05	0.64
1:1:418:A:H2'	1:1:419:G:H8	1.62	0.64
1:1:2009:G:N2	1:1:2012:G:OP2	2.30	0.64
4:A:40:ILE:HG13	4:A:74:TYR:HD2	1.63	0.64
10:AE:175:GLU:OE2	10:AE:239:ARG:NH2	2.30	0.64
67:BA:126:LYS:HG3	67:BA:127:TYR:HD1	1.63	0.64
4:A:183:VAL:HG13	4:A:204:ILE:HD12	1.80	0.63
23:AS:47:ARG:NH1	23:AS:48:ASN:OD1	2.31	0.63
29:AZ:41:GLY:HA3	29:AZ:77:ASN:HB3	1.79	0.63
1:1:253:G:H2'	1:1:254:C:H6	1.63	0.63
2:2:1075:G:O2'	23:AS:6:GLN:NE2	2.25	0.63
15:AJ:57:LEU:HB2	15:AJ:118:GLY:HA2	1.81	0.63
1:1:2035:U:OP2	1:1:2040:A:N6	2.24	0.63
1:1:2701:A:N6	1:1:2713:G:O2'	2.31	0.63
2:2:1499:G:H2'	2:2:1500:A:C8	2.34	0.63
5:H:35:PRO:O	5:H:52:GLN:NE2	2.31	0.63
13:AH:38:ASN:HB3	13:AH:62:HIS:HA	1.80	0.63
31:A3:70:CYS:HA	31:A3:75:ILE:HD12	1.79	0.63
1:1:1301:A:O2'	1:1:1365:G:H2'	1.98	0.63
1:1:1303:A:H62	1:1:1366:A:N6	1.95	0.63
2:2:978:G:N1	2:2:998:C:N3	2.36	0.63
8:AC:55:CYS:HB3	8:AC:58:CYS:SG	2.39	0.63
1:1:763:C:H2'	1:1:764:A:C8	2.34	0.63
2:2:1042:G:N2	2:2:1045:A:OP2	2.28	0.63
4:A:138:ASP:O	4:A:146:GLN:NE2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:BA:62:ASP:HA	67:BA:153:LYS:HE2	1.80	0.63
2:2:1386:C:H2'	2:2:1387:A:C8	2.34	0.62
3:3:9:G:OP1	36:BO:24:ARG:NH1	2.32	0.62
1:1:1365:G:H4'	1:1:1366:A:OP1	1.98	0.62
2:2:219:G:H21	2:2:222:A:H8	1.47	0.62
13:AH:135:ASP:HB2	13:AH:152:ILE:HG13	1.80	0.62
18:AM:18:HIS:HB2	18:AM:29:HIS:HB3	1.82	0.62
1:1:1612:A:H2'	1:1:1613:A:C8	2.34	0.62
1:1:2108:G:N1	1:1:2130:A:OP2	2.31	0.62
2:2:82:C:N3	2:2:91:G:N1	2.38	0.62
2:2:872:A:H5''	30:A0:28:ARG:HH21	1.65	0.62
61:BN:97:ASN:HD22	61:BN:98:PRO:HD2	1.65	0.62
1:1:1309:G:H2'	1:1:1310:G:H4'	1.81	0.62
1:1:2362:C:H2'	1:1:2363:G:C8	2.34	0.62
2:2:484:G:H5''	2:2:496:G:H4'	1.80	0.62
2:2:1212:A:H2	2:2:1215:G:N3	1.96	0.62
67:BA:170:VAL:HG11	67:BA:184:ILE:HG22	1.80	0.62
1:1:31:G:H4'	45:Ba:14:PRO:HG3	1.81	0.62
13:AH:42:ARG:NH2	16:AK:102:TYR:O	2.27	0.62
13:AH:152:ILE:HG22	13:AH:157:ARG:HG2	1.79	0.62
15:AJ:87:ARG:HG3	15:AJ:88:GLN:HG2	1.81	0.62
25:AV:1:MET:HG2	25:AV:23:ILE:HD11	1.80	0.62
1:1:3007:A:H2	1:1:3009:A:H62	1.48	0.62
10:AE:206:PRO:HB3	22:AR:8:ARG:HD2	1.82	0.62
28:AY:31:MET:HG2	28:AY:32:ALA:N	2.14	0.62
1:1:67:C:OP2	1:1:68:U:O2'	2.16	0.62
3:3:10:G:O6	36:BO:12:ARG:NH1	2.32	0.62
7:AB:171:LEU:O	7:AB:175:ILE:HG22	2.00	0.62
13:AH:105:LYS:O	13:AH:109:LYS:NZ	2.32	0.62
17:AL:45:ILE:HD11	29:AZ:4:GLU:HG3	1.82	0.62
21:AQ:69:PRO:HD3	21:AQ:76:LEU:HD21	1.81	0.62
27:AX:61:GLU:OE1	27:AX:61:GLU:N	2.33	0.62
26:AW:48:GLU:HB3	26:AW:55:ILE:HB	1.81	0.62
14:AI:90:GLU:OE2	14:AI:113:HIS:NE2	2.33	0.62
2:2:1123:C:H2'	2:2:1124:U:C6	2.34	0.61
61:BN:105:ALA:O	61:BN:109:GLY:N	2.33	0.61
2:2:914:G:OP2	13:AH:74:SER:OG	2.18	0.61
31:A3:114:ILE:HD12	31:A3:117:LYS:HE3	1.83	0.61
44:BE:123:ILE:HD11	44:BE:126:VAL:HG13	1.82	0.61
56:BZ:61:TYR:OH	56:BZ:64:GLU:OE2	2.18	0.61
1:1:2878:G:OP2	1:1:2962:C:O2'	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:774:OMU:HM22	2:2:775:G:H5'	1.82	0.61
2:2:1224:A:H2'	2:2:1225:A:C8	2.35	0.61
2:2:1380:OMU:HM22	2:2:1381:C:H5'	1.81	0.61
9:AD:131:GLU:N	9:AD:154:TYR:O	2.32	0.61
55:BF:10:GLU:HG2	55:BF:54:VAL:HG22	1.82	0.61
1:1:2537:C:N4	44:BE:33:GLY:O	2.34	0.61
2:2:142:G:N2	2:2:174:C:O2	2.19	0.61
1:1:253:G:H2'	1:1:254:C:C6	2.35	0.61
2:2:1089:G:N2	2:2:1090:U:O4	2.25	0.61
13:AH:14:GLU:HG2	13:AH:16:LYS:HG3	1.83	0.61
1:1:1498:C:H2'	1:1:1499:G:H8	1.65	0.61
2:2:270:U:OP1	15:AJ:30:ARG:NH1	2.28	0.61
2:2:518:U:H2'	2:2:519:OMG:H8	1.65	0.61
2:2:791:G:OP2	21:AQ:9:ARG:NH2	2.34	0.61
33:AO:20:GLN:HE22	33:AO:22:ARG:HH21	1.47	0.61
34:BB:74:PRO:HD2	34:BB:77:LEU:HD22	1.82	0.61
17:AL:76:GLU:H	17:AL:76:GLU:CD	2.08	0.61
21:AQ:64:LYS:HB3	21:AQ:75:LYS:HD3	1.83	0.61
1:1:871:G:H2'	1:1:872:C:C6	2.36	0.61
1:1:1676:A:N1	1:1:1692:G:O2'	2.33	0.61
2:2:37:C:H2'	2:2:38:A:H8	1.66	0.60
2:2:783:A:OP1	2:2:1495:G:O2'	2.19	0.60
6:AA:69:PHE:HB3	6:AA:81:THR:HB	1.81	0.60
9:AD:109:VAL:HG23	9:AD:114:LEU:HB2	1.83	0.60
27:AX:10:GLU:N	27:AX:30:ARG:O	2.32	0.60
1:1:761:U:H2'	1:1:762:G:H8	1.65	0.60
1:1:54:G:H2'	1:1:55:U:H4'	1.81	0.60
1:1:806:G:OP1	54:BD:27:ARG:NH2	2.34	0.60
2:2:318:C:H2'	2:2:319:4AC:H6	1.83	0.60
6:AA:110:ILE:HD11	6:AA:147:TYR:HA	1.83	0.60
56:BZ:34:LEU:HD23	56:BZ:85:ILE:HG13	1.83	0.60
1:1:1308:G:N2	1:1:1362:G:N7	2.39	0.60
2:2:609:A:N7	14:AI:107:SER:HA	2.16	0.60
31:BG:29:THR:HG21	31:BG:106:LYS:HG3	1.83	0.60
2:2:97:A:H2'	2:2:98:C:H6	1.66	0.60
2:2:1076:A:H61	29:AZ:155:GLY:HA3	1.64	0.60
2:2:1350:U:H2'	2:2:1351:A:H8	1.66	0.60
44:BE:121:ILE:HG12	44:BE:134:ILE:HG23	1.83	0.60
67:BA:208:LYS:HB3	67:BA:214:ALA:HA	1.82	0.60
1:1:55:U:O2'	1:1:56:C:H5'	2.02	0.60
1:1:1283:A:H2'	1:1:1284:A:C8	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:AV:33:ARG:NH2	25:AV:53:ILE:O	2.35	0.60
39:BL:1:MET:HE3	54:BD:33:ARG:HD2	1.84	0.60
1:1:1278:C:OP1	1:1:1281:C:N4	2.35	0.60
1:1:2109:A:H2'	1:1:2110:A:C8	2.37	0.60
1:1:2823:C:H2'	1:1:2824:G:C8	2.37	0.60
1:1:2352:G:O6	5:H:194:GLN:NE2	2.35	0.60
13:AH:112:GLU:HB2	13:AH:119:PRO:HG3	1.83	0.60
14:AI:49:GLU:H	14:AI:64:GLN:HE21	1.50	0.60
18:AM:32:ASP:OD1	18:AM:34:THR:OG1	2.18	0.60
1:1:648:G:H21	59:BS:104:GLN:HE22	1.49	0.60
1:1:1331:C:H2'	1:1:1332:A:H8	1.65	0.60
2:2:973:A:O2'	31:A3:35:GLY:HA2	2.02	0.60
16:AK:103:ASP:HB3	16:AK:106:MET:HE3	1.83	0.60
2:2:636:4AC:O7	2:2:636:4AC:H5	2.02	0.60
2:2:641:G:H2'	2:2:642:U:C6	2.37	0.60
2:2:1286:G:OP2	32:AT:30:ALA:N	2.34	0.60
22:AR:84:ASP:HB3	22:AR:109:ALA:HB2	1.84	0.60
44:BE:32:ILE:HD12	44:BE:44:ALA:HB1	1.84	0.60
67:BA:206:TYR:HE1	67:BA:216:LYS:HD3	1.66	0.60
23:AS:22:ASN:OD1	23:AS:22:ASN:N	2.31	0.59
1:1:2362:C:H2'	1:1:2363:G:H8	1.67	0.59
2:2:1191:C:OP1	20:AP:9:ARG:NH2	2.35	0.59
39:BL:97:GLU:HB3	39:BL:102:ILE:HD13	1.84	0.59
1:1:1303:A:C8	1:1:1304:C:C5	2.90	0.59
2:2:1025:5MC:H2'	2:2:1026:G:H8	1.66	0.59
29:AZ:64:GLU:OE1	29:AZ:64:GLU:N	2.35	0.59
44:BE:40:ARG:HA	44:BE:43:LYS:HB2	1.85	0.59
1:1:107:G:C5'	1:1:107:G:C8	2.85	0.59
2:2:703:4AC:H2'	2:2:704:G:H8	1.67	0.59
2:2:985:C:OP1	32:AT:61:LYS:NZ	2.35	0.59
26:AW:36:ARG:HA	26:AW:49:PRO:HD3	1.84	0.59
1:1:772:U:H2'	1:1:773:C:C6	2.36	0.59
1:1:1329:G:H2'	1:1:1330:C:C6	2.36	0.59
3:3:98:G:H2'	3:3:99:G:C8	2.37	0.59
1:1:205:G:N7	40:Bf:34:ARG:NH2	2.50	0.59
1:1:2559:A:H2'	1:1:2560:G:C8	2.37	0.59
29:AZ:20:PHE:HD1	29:AZ:21:LEU:HD23	1.68	0.59
1:1:1303:A:O4'	1:1:1304:C:OP1	2.19	0.59
2:2:484:G:N2	19:AN:65:PRO:O	2.34	0.59
2:2:803:G:N1	2:2:821:C:N3	2.34	0.59
3:3:97:G:H2'	3:3:98:G:H8	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:451:4AC:H5''	41:BU:119:ARG:HG2	1.84	0.59
1:1:795:U:H2'	1:1:796:C:C6	2.38	0.59
1:1:908:A:H2'	1:1:909:C:C6	2.38	0.59
22:AR:86:VAL:HG23	22:AR:105:VAL:HG12	1.85	0.59
67:BA:35:VAL:HG13	67:BA:202:ILE:HD13	1.85	0.59
1:1:2001:4AC:OP2	51:BQ:76:ARG:NH1	2.36	0.59
2:2:28:G:H2'	2:2:29:C:C6	2.38	0.59
2:2:223:G:H2'	2:2:224:G:H8	1.68	0.59
2:2:483:G:H4'	2:2:485:C:C2	2.38	0.59
2:2:1261:A:H2	2:2:1327:G:H1'	1.67	0.59
21:AQ:57:GLN:NE2	26:AW:38:ARG:H	2.01	0.59
31:BG:39:THR:HG23	31:BG:100:ALA:HB2	1.85	0.59
1:1:1306:G:C5'	1:1:1306:G:C8	2.85	0.59
1:1:2426:C:H2'	1:1:2427:G:C8	2.37	0.59
2:2:1365:U:H2'	2:2:1366:G:C8	2.38	0.59
14:AI:60:VAL:HG11	26:AW:7:VAL:HG21	1.85	0.59
1:1:710:C:N3	1:1:747:G:N1	2.38	0.58
2:2:1104:C:HO2'	24:AU:2:ALA:N	2.00	0.58
2:2:247:G:OP1	22:AR:66:ARG:NH1	2.35	0.58
2:2:1455:G:H2'	2:2:1456:G:C8	2.39	0.58
9:AD:61:ALA:O	9:AD:70:ARG:NH2	2.36	0.58
67:BA:64:LYS:HB2	67:BA:107:TYR:HA	1.85	0.58
2:2:410:C:O2'	2:2:587:A:N3	2.34	0.58
2:2:477:G:H4'	2:2:478:C:H5''	1.85	0.58
2:2:1242:A:N3	2:2:1300:C:O2'	2.36	0.58
44:BE:57:ILE:HD12	44:BE:79:LYS:HG3	1.85	0.58
2:2:134:C:N3	2:2:235:G:N1	2.38	0.58
31:A3:22:ALA:HB1	31:A3:111:VAL:HG22	1.85	0.58
1:1:1303:A:C4'	1:1:1304:C:OP1	2.51	0.58
1:1:1653:U:OP2	51:BQ:42:ARG:NH2	2.37	0.58
31:A3:33:ARG:HH22	31:A3:42:ALA:HB2	1.68	0.58
32:AT:98:MET:HA	33:AO:112:ILE:HD11	1.84	0.58
1:1:90:C:H2'	1:1:91:4AC:H6	1.84	0.58
2:2:37:C:H2'	2:2:38:A:C8	2.38	0.58
2:2:89:G:H2'	2:2:90:G:O4'	2.04	0.58
32:AT:77:VAL:HA	32:AT:94:ILE:HG22	1.86	0.58
1:1:107:G:O5'	1:1:107:G:H8	1.87	0.58
2:2:498:A:H62	2:2:1180:G:H21	1.49	0.58
2:2:1345:G:O3'	16:AK:70:GLY:HA3	2.04	0.58
5:H:40:VAL:HG21	5:H:73:TYR:HB2	1.86	0.58
48:Bi:82:VAL:HG12	48:Bi:83:GLU:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:872:C:H2'	1:1:873:C:C6	2.39	0.58
11:AF:212:VAL:N	14:AI:70:ASN:HD21	2.02	0.58
13:AH:134:GLU:HA	13:AH:151:ASP:HA	1.85	0.58
29:AZ:169:ALA:HB3	29:AZ:176:ILE:HB	1.85	0.58
57:BP:22:SER:OG	57:BP:27:VAL:O	2.22	0.58
67:BA:68:ILE:HG12	67:BA:85:ILE:HD12	1.84	0.58
2:2:657:OMG:H2'	2:2:658:G:C8	2.39	0.58
1:1:1421:C:H2'	1:1:1422:A:C8	2.38	0.57
2:2:962:G:O2'	20:AP:7:ASN:OD1	2.14	0.57
2:2:1415:U:H2'	2:2:1416:C:C6	2.38	0.57
13:AH:160:VAL:HG12	13:AH:164:ASN:HD21	1.68	0.57
1:1:1905:G:N1	1:1:1908:A:OP2	2.33	0.57
2:2:1267:G:H2'	2:2:1268:C:H6	1.68	0.57
28:AY:42:ARG:NH1	28:AY:43:CYS:SG	2.77	0.57
51:BQ:86:THR:HG23	51:BQ:91:LYS:HG3	1.86	0.57
2:2:712:C:OP1	2:2:822:C:O2'	2.22	0.57
2:2:999:G:O2'	2:2:1000:G:H5'	2.03	0.57
3:3:36:C:HO2'	36:BO:142:TYR:HH	1.51	0.57
3:3:52:A:H5''	36:BO:170:GLY:H	1.68	0.57
23:AS:20:TYR:HB3	23:AS:23:GLU:HB2	1.86	0.57
32:AT:80:THR:HA	32:AT:93:GLU:HA	1.86	0.57
1:1:32:G:H2'	1:1:33:G:H8	1.69	0.57
1:1:116:G:H2'	1:1:117:G:C8	2.40	0.57
1:1:763:C:H2'	1:1:764:A:H8	1.69	0.57
2:2:1321:G:O6	16:AK:10:ARG:NH2	2.34	0.57
46:BT:75:SER:OG	46:BT:78:GLU:OE1	2.21	0.57
1:1:872:C:H2'	1:1:873:C:H6	1.70	0.57
37:BC:291:LYS:NZ	37:BC:300:GLU:OE2	2.31	0.57
54:BD:75:THR:O	54:BD:78:ARG:HG2	2.04	0.57
67:BA:93:ILE:HG13	67:BA:100:ALA:HB2	1.86	0.57
1:1:1710:C:H2'	1:1:1711:G:H8	1.70	0.57
1:1:2419:C:H2'	1:1:2420:A:H8	1.70	0.57
2:2:135:U:H2'	2:2:136:C:C6	2.39	0.57
2:2:146:A:H2'	2:2:147:U:C6	2.40	0.57
2:2:1123:C:H2'	2:2:1124:U:H6	1.69	0.57
2:2:1241:A:H2'	2:2:1242:A:C8	2.39	0.57
2:2:1328:C:H2'	2:2:1329:G:H8	1.68	0.57
4:A:166:VAL:HG23	4:A:231:ILE:HB	1.86	0.57
5:H:19:ILE:HG13	5:H:70:ARG:HH11	1.68	0.57
10:AE:48:ILE:HA	10:AE:52:TYR:HB2	1.86	0.57
31:A3:14:GLU:OE1	31:A3:117:LYS:NZ	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BY:83:GLU:OE1	35:BY:83:GLU:N	2.33	0.57
57:BP:36:ARG:NH1	57:BP:120:GLU:OE2	2.30	0.57
1:1:1317:G:H2'	1:1:1318:G:H8	1.69	0.57
1:1:2168:A:H2'	1:1:2169:A:C8	2.39	0.57
1:1:2887:A:O2'	64:BJ:2:ALA:N	2.35	0.57
10:AE:32:PRO:HD2	10:AE:39:MET:HE1	1.87	0.57
12:AG:112:ILE:HG23	12:AG:116:ILE:HD11	1.86	0.57
41:BU:28:ALA:HA	41:BU:45:PRO:HA	1.87	0.57
6:AA:132:THR:HA	6:AA:135:GLU:HB2	1.86	0.57
1:1:870:A:H4'	1:1:871:G:OP2	2.05	0.57
1:1:2990:G:H21	55:BF:149:GLN:HE22	1.51	0.57
2:2:343:U:H2'	2:2:344:C:H6	1.69	0.57
2:2:482:U:H2'	2:2:483:G:O4'	2.05	0.57
2:2:1441:U:H2'	2:2:1442:A:C8	2.40	0.57
21:AQ:22:PRO:HG3	21:AQ:65:LEU:HB3	1.86	0.57
35:BY:123:ARG:NH1	35:BY:155:LEU:O	2.37	0.57
37:BC:278:GLU:HG3	37:BC:325:PRO:HD3	1.87	0.57
2:2:1069:OMG:HM22	2:2:1070:A:H5'	1.85	0.56
8:AC:21:ILE:HG22	8:AC:43:CYS:HB3	1.87	0.56
9:AD:34:GLU:HB2	9:AD:118:MET:HG2	1.86	0.56
21:AQ:38:VAL:O	21:AQ:42:LYS:HG2	2.05	0.56
39:BL:47:TRP:CZ2	39:BL:51:ILE:HD11	2.40	0.56
41:BU:16:TYR:O	41:BU:23:ARG:NH2	2.38	0.56
44:BE:26:GLU:OE2	44:BE:83:ARG:NH2	2.35	0.56
25:B6:17:LYS:HB2	25:B6:71:TYR:HB3	1.86	0.56
67:BA:67:VAL:HG22	67:BA:111:ILE:HB	1.87	0.56
1:1:1734:G:H2'	1:1:1735:G:H8	1.70	0.56
1:1:2337:C:H2'	1:1:2338:G:C8	2.41	0.56
11:AF:160:PRO:HD2	11:AF:163:LEU:HD22	1.86	0.56
18:AM:81:ILE:HB	18:AM:115:VAL:HG12	1.88	0.56
53:Bj:1:MET:N	53:Bj:88:LYS:O	2.39	0.56
1:1:850:A:N6	39:BL:117:LYS:O	2.32	0.56
1:1:1116:G:H2'	1:1:1117:C:C6	2.40	0.56
1:1:1327:C:N4	1:1:1352:C:O3'	2.37	0.56
1:1:1685:A:N3	1:1:1755:4AC:O2'	2.36	0.56
2:2:1492:A:H2'	2:2:1493:C:C6	2.40	0.56
13:AH:72:MET:HA	13:AH:93:LEU:HB3	1.87	0.56
14:AI:36:GLU:OE2	14:AI:39:ARG:NH2	2.28	0.56
22:AR:83:GLY:O	22:AR:109:ALA:CB	2.54	0.56
27:AX:43:ARG:NH1	27:AX:62:ARG:O	2.38	0.56
44:BE:5:ILE:HB	44:BE:8:ARG:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:BQ:3:THR:HG22	51:BQ:5:LYS:HD3	1.88	0.56
67:BA:98:ARG:HD2	67:BA:102:LYS:HE3	1.88	0.56
1:1:100:G:O2'	1:1:101:U:H5'	2.05	0.56
1:1:264:G:OP1	1:1:403:G:O2'	2.23	0.56
1:1:1164:C:OP1	61:BN:19:ARG:NH1	2.37	0.56
2:2:121:U:H2'	2:2:122:C:C6	2.41	0.56
13:AH:90:HIS:H	13:AH:90:HIS:CD2	2.23	0.56
33:AO:110:ARG:HD2	33:AO:121:GLU:HG2	1.86	0.56
36:BO:34:ARG:NH1	36:BO:105:ASP:OD2	2.39	0.56
55:BF:120:ARG:NH1	55:BF:157:ALA:O	2.37	0.56
1:1:1842:A:H2'	1:1:1843:A:C8	2.40	0.56
1:1:2370:G:O2'	1:1:2374:A:N7	2.37	0.56
1:1:2650:G:H2'	1:1:2651:C:H6	1.70	0.56
2:2:212:G:H4'	2:2:213:G:H8	1.70	0.56
5:H:13:ARG:NH2	5:H:33:GLU:O	2.38	0.56
5:H:382:LYS:HB2	18:AM:52:ARG:HE	1.70	0.56
12:AG:101:GLU:OE2	12:AG:103:ARG:NH2	2.35	0.56
17:AL:24:LYS:NZ	17:AL:34:MET:SD	2.79	0.56
1:1:1842:A:H2'	1:1:1843:A:H8	1.70	0.56
2:2:716:U:OP1	21:AQ:16:ARG:NH2	2.38	0.56
5:H:37:LEU:HD22	5:H:112:VAL:HG21	1.86	0.56
20:AP:9:ARG:NH1	20:AP:27:TYR:OH	2.39	0.56
39:BL:86:ASP:OD1	39:BL:86:ASP:N	2.33	0.56
44:BE:104:ALA:O	44:BE:168:LYS:NZ	2.22	0.56
54:BD:142:LEU:HD23	54:BD:241:VAL:HG22	1.87	0.56
2:2:662:A:H2'	2:2:663:A:C8	2.40	0.56
5:H:256:THR:OG1	5:H:259:ASP:OD1	2.23	0.56
32:AT:75:GLU:OE1	32:AT:76:MET:N	2.39	0.56
1:1:908:A:H2'	1:1:909:C:H6	1.70	0.56
1:1:913:C:H2'	1:1:914:G:H8	1.71	0.56
10:AE:168:VAL:HG22	10:AE:169:PRO:HA	1.88	0.56
22:AR:83:GLY:O	22:AR:109:ALA:HB2	2.05	0.56
25:AV:10:GLU:OE2	25:AV:73:TYR:OH	2.17	0.56
40:Bf:9:LYS:NZ	40:Bf:51:GLU:OXT	2.39	0.56
55:BF:89:LYS:HG2	55:BF:176:GLU:HB3	1.88	0.56
1:1:16:A:N1	1:1:2287:4AC:O2'	2.38	0.56
1:1:1306:G:H2'	1:1:1307:C:O4'	2.06	0.56
21:AQ:99:ILE:HG22	21:AQ:157:VAL:HG12	1.88	0.56
1:1:382:C:H2'	1:1:383:C:H6	1.70	0.56
1:1:1943:G:O2'	1:1:2232:U:O4	2.18	0.56
2:2:1414:A:H2'	2:2:1415:U:C6	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:214:MET:O	5:H:216:LYS:NZ	2.33	0.56
18:AM:47:VAL:HG23	18:AM:48:VAL:HG23	1.88	0.56
26:AW:36:ARG:NH2	26:AW:48:GLU:OE1	2.39	0.56
1:1:1406:G:OP2	35:BY:127:ARG:NH2	2.37	0.55
1:1:2341:G:H5'	1:1:2342:C:OP2	2.06	0.55
2:2:893:G:H2'	2:2:894:G:C8	2.41	0.55
16:AK:99:PHE:HB3	16:AK:107:LEU:HD11	1.88	0.55
58:BM:141:LYS:NZ	66:Bk:11:ASP:OD2	2.38	0.55
1:1:762:G:H2'	1:1:763:C:C6	2.41	0.55
1:1:2305:C:H2'	1:1:2306:C:H6	1.71	0.55
2:2:632:A:OP1	6:AA:132:THR:HG21	2.06	0.55
13:AH:88:ARG:O	13:AH:92:SER:HB3	2.05	0.55
1:1:238:C:H4'	1:1:239:C:O5'	2.06	0.55
2:2:387:G:H2'	2:2:388:G:H8	1.71	0.55
5:H:306:ASP:N	5:H:306:ASP:OD1	2.40	0.55
56:BZ:28:LYS:HE3	56:BZ:52:TYR:CZ	2.42	0.55
1:1:209:G:O2'	47:BW:40:ASN:ND2	2.39	0.55
2:2:546:4AC:OP1	21:AQ:7:ARG:NH1	2.31	0.55
2:2:1434:U:H2'	2:2:1435:C:C6	2.41	0.55
6:AA:48:VAL:HG22	6:AA:70:GLN:HG2	1.88	0.55
1:1:2419:C:H2'	1:1:2420:A:C8	2.41	0.55
17:AL:92:GLU:HG2	29:AZ:36:LYS:HE3	1.87	0.55
29:AZ:37:LYS:HD2	29:AZ:42:THR:HB	1.88	0.55
34:BB:202:HIS:HD2	34:BB:204:PHE:H	1.52	0.55
37:BC:79:ARG:HH21	37:BC:167:GLN:HE22	1.55	0.55
1:1:600:G:H2'	54:BD:183:LYS:HE3	1.87	0.55
2:2:343:U:H2'	2:2:344:C:C6	2.40	0.55
5:H:74:LYS:HD3	5:H:75:PRO:HD2	1.89	0.55
17:AL:8:LEU:HB2	17:AL:71:ARG:HB2	1.88	0.55
18:AM:18:HIS:N	18:AM:29:HIS:O	2.38	0.55
18:AM:31:THR:HG22	18:AM:38:THR:HA	1.88	0.55
24:AU:26:ILE:O	24:AU:26:ILE:HG13	2.07	0.55
38:BK:45:ARG:NH1	65:Bl:1:MET:O	2.38	0.55
1:1:978:G:O2'	1:1:1014:G:H4'	2.07	0.55
2:2:196:G:H2'	2:2:196:G:N3	2.20	0.55
2:2:418:G:H4'	9:AD:170:MET:HE2	1.88	0.55
5:H:84:ASP:OD2	5:H:86:SER:OG	2.21	0.55
1:1:2386:C:OP2	5:H:157:ARG:NH2	2.39	0.55
2:2:183:U:H2'	2:2:184:G:C8	2.41	0.55
2:2:778:U:O2'	2:2:872:A:N1	2.37	0.55
2:2:894:G:O2'	2:2:1373:C:OP2	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1267:G:H2'	2:2:1268:C:C6	2.41	0.55
32:AT:117:ALA:HB3	32:AT:120:ILE:HB	1.89	0.55
56:BZ:40:ASN:HB2	56:BZ:66:THR:HA	1.88	0.55
1:1:567:A:H1'	1:1:2121:A:C2	2.41	0.55
1:1:705:A:H2'	1:1:706:G:C8	2.42	0.55
1:1:1742:A:H2'	1:1:1743:A:C8	2.42	0.55
1:1:2272:C:OP1	1:1:2686:G:O2'	2.21	0.55
1:1:2304:C:H2'	1:1:2305:C:C6	2.41	0.55
1:1:2311:A:H2'	1:1:2312:G:H8	1.69	0.55
2:2:135:U:O2	10:AE:147:ASN:ND2	2.34	0.55
15:AJ:82:GLU:HA	15:AJ:90:ALA:HB2	1.88	0.55
26:AW:18:VAL:HG12	26:AW:60:ILE:HA	1.89	0.55
1:1:102:C:N3	1:1:103:C:C5	2.74	0.55
1:1:595:A:O2'	54:BD:44:GLN:NE2	2.40	0.55
1:1:720:A:H2'	1:1:721:A:C8	2.42	0.55
1:1:1140:G:HO2'	1:1:1143:A:H62	1.53	0.55
2:2:546:4AC:P	21:AQ:7:ARG:HH12	2.30	0.55
1:1:281:G:OP2	1:1:281:G:N2	2.33	0.54
1:1:2823:C:H2'	1:1:2824:G:H8	1.72	0.54
2:2:24:U:H2'	2:2:25:C:C6	2.41	0.54
2:2:244:G:H2'	2:2:245:G:H8	1.72	0.54
5:H:63:ASP:OD2	5:H:65:THR:OG1	2.25	0.54
16:AK:86:LEU:O	16:AK:90:THR:HG22	2.07	0.54
37:BC:137:THR:OG1	37:BC:140:ASP:OD1	2.23	0.54
49:BI:56:ARG:HA	49:BI:65:PRO:HD2	1.88	0.54
1:1:32:G:H2'	1:1:33:G:C8	2.42	0.54
1:1:1306:G:H5''	1:1:1306:G:C8	2.30	0.54
1:1:2314:U:H2'	1:1:2315:U:C6	2.42	0.54
2:2:1441:U:H2'	2:2:1442:A:H8	1.72	0.54
7:AB:66:SER:HB3	7:AB:113:ASP:HB2	1.87	0.54
10:AE:68:GLU:HB2	10:AE:70:LYS:HG3	1.89	0.54
19:AN:61:GLU:HG3	19:AN:69:MET:HE1	1.90	0.54
38:B5:12:ILE:HG23	38:B5:48:MET:HE1	1.87	0.54
1:1:462:G:H21	1:1:485:A:H62	1.55	0.54
8:AC:55:CYS:SG	8:AC:57:LYS:N	2.78	0.54
34:BB:122:VAL:HG21	34:BB:129:ALA:HB2	1.89	0.54
1:1:795:U:H2'	1:1:796:C:H6	1.72	0.54
1:1:2050:U:H2'	1:1:2051:C:H6	1.73	0.54
2:2:709:G:OP1	21:AQ:101:ARG:NH2	2.40	0.54
5:H:113:ILE:HD11	5:H:118:LEU:HB2	1.90	0.54
6:AA:70:GLN:HG3	6:AA:84:LYS:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AC:56:PRO:HB2	8:AC:57:LYS:HE2	1.87	0.54
54:BD:49:ASP:HB3	54:BD:52:ALA:HB2	1.88	0.54
31:B4:116:MET:HA	31:B4:119:ARG:NH1	2.22	0.54
67:BA:36:ASN:HB2	67:BA:203:LYS:HE3	1.90	0.54
1:1:94:G:H3'	1:1:95:G:H5'	1.89	0.54
2:2:1301:G:H2'	2:2:1302:C:C6	2.42	0.54
3:3:124:C:H2'	3:3:125:A:H8	1.72	0.54
5:H:173:LEU:HD13	5:H:251:VAL:HG21	1.89	0.54
13:AH:81:VAL:HG21	13:AH:167:LEU:HD22	1.88	0.54
14:AI:97:PHE:HD1	14:AI:98:GLU:HG2	1.73	0.54
1:1:353:C:OP2	1:1:2628:C:O2'	2.19	0.54
1:1:1266:G:N2	65:Bl:43:SER:HB2	2.22	0.54
1:1:1715:U:H5	1:1:1824:A:N7	2.06	0.54
2:2:35:G:O2'	2:2:305:U:OP1	2.25	0.54
58:BM:157:ARG:HB2	58:BM:162:LEU:HB2	1.89	0.54
59:BS:60:PRO:HG2	59:BS:78:PHE:CZ	2.42	0.54
61:BN:44:GLU:OE1	61:BN:44:GLU:N	2.35	0.54
1:1:189:G:H22	1:1:224:A:H2	1.54	0.54
1:1:1048:4AC:O2'	43:Be:51:TRP:O	2.25	0.54
2:2:498:A:H62	2:2:1180:G:N2	2.05	0.54
2:2:724:U:H2'	2:2:725:G:O4'	2.08	0.54
7:AB:191:PRO:HG2	7:AB:194:GLU:HB2	1.88	0.54
10:AE:131:ARG:HE	10:AE:141:ASN:HD21	1.56	0.54
11:AF:22:LEU:HD11	11:AF:37:ILE:HG22	1.89	0.54
14:AI:44:TYR:HH	14:AI:112:SER:HG	1.53	0.54
39:BL:79:LYS:HB3	39:BL:116:GLY:HA3	1.89	0.54
50:BR:50:HIS:HA	50:BR:53:MET:HE2	1.89	0.54
31:BG:56:ASP:O	31:BG:83:LYS:NZ	2.41	0.54
1:1:2477:G:H2'	1:1:2478:C:H6	1.72	0.54
2:2:470:G:H2'	2:2:471:OMG:H8	1.72	0.54
11:AF:146:GLU:O	11:AF:207:ASN:ND2	2.34	0.54
12:AG:47:LEU:HA	12:AG:50:LEU:HD23	1.90	0.54
44:BE:40:ARG:HE	44:BE:135:PHE:HE1	1.54	0.54
1:1:1575:A:H2'	1:1:1576:C:C6	2.42	0.54
1:1:1874:G:O2'	40:Bf:3:ARG:O	2.26	0.54
13:AH:26:VAL:HG13	13:AH:39:LEU:HD13	1.90	0.54
13:AH:150:VAL:HG12	27:AX:44:ASN:HB2	1.89	0.54
65:Bl:63:GLU:OE1	65:Bl:63:GLU:N	2.38	0.54
1:1:896:G:H2'	1:1:897:C:H6	1.72	0.54
1:1:1756:G:OP1	60:Bd:77:ARG:NH1	2.31	0.54
1:1:2342:C:H3'	1:1:2343:G:H5''	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1099:C:H2'	2:2:1100:C:C6	2.43	0.54
2:2:1105:G:N2	24:AU:141:GLU:OE2	2.41	0.54
3:3:30:C:H5'	44:BE:149:ARG:HD3	1.89	0.54
5:H:38:ILE:HB	5:H:50:LEU:HB3	1.90	0.54
5:H:48:GLY:HA2	5:H:75:PRO:HA	1.90	0.54
5:H:119:LEU:HD12	5:H:231:VAL:HG21	1.90	0.54
17:AL:77:ALA:HA	17:AL:82:MET:SD	2.48	0.54
1:1:1841:A:H2'	1:1:1842:A:C8	2.43	0.53
1:1:2118:U:N3	1:1:2121:A:OP2	2.33	0.53
1:1:2955:U:OP1	37:BC:232:LYS:NZ	2.39	0.53
2:2:387:G:H2'	2:2:388:G:C8	2.43	0.53
2:2:1032:A:N1	2:2:1073:G:O2'	2.37	0.53
2:2:1261:A:C2	2:2:1327:G:H1'	2.42	0.53
3:3:98:G:H2'	3:3:99:G:H8	1.71	0.53
29:AZ:51:PRO:O	29:AZ:55:ILE:N	2.36	0.53
50:BR:45:ILE:H	50:BR:59:HIS:CD2	2.25	0.53
1:1:1303:A:C2	1:1:1368:G:H1'	2.43	0.53
1:1:1306:G:O2'	1:1:1307:C:OP1	2.23	0.53
1:1:2047:A:N6	1:1:2084:G:O2'	2.34	0.53
2:2:790:G:HO2'	14:AI:2:THR:N	2.06	0.53
13:AH:154:PRO:HA	13:AH:157:ARG:HG3	1.88	0.53
16:AK:43:PHE:HA	16:AK:46:LEU:HD22	1.90	0.53
17:AL:2:GLN:NE2	17:AL:77:ALA:O	2.41	0.53
67:BA:63:VAL:HG22	67:BA:153:LYS:HD2	1.90	0.53
1:1:360:A:H2'	1:1:361:A:C8	2.43	0.53
1:1:1064:C:H2'	1:1:1065:4AC:H6	1.90	0.53
4:A:60:SER:O	4:A:64:MET:HG2	2.09	0.53
5:H:152:ALA:O	5:H:156:MET:HG2	2.08	0.53
7:AB:53:LYS:O	7:AB:53:LYS:NZ	2.40	0.53
7:AB:58:PHE:HB2	8:AC:33:PRO:HA	1.90	0.53
17:AL:45:ILE:HG12	20:AP:34:HIS:CD2	2.43	0.53
27:AX:30:ARG:HG2	27:AX:40:VAL:HG12	1.91	0.53
29:AZ:38:THR:OG1	29:AZ:41:GLY:O	2.21	0.53
44:BE:145:ARG:NE	44:BE:164:HIS:O	2.39	0.53
1:1:1216:G:H21	1:1:2498:A:H62	1.56	0.53
1:1:1283:A:H2'	1:1:1284:A:H8	1.74	0.53
1:1:2281:G:OP1	49:BI:77:ARG:NH2	2.39	0.53
1:1:2858:U:H3	1:1:3007:A:H62	1.56	0.53
2:2:907:A:H2'	2:2:908:C:C6	2.42	0.53
5:H:267:MET:O	5:H:268:VAL:HG22	2.08	0.53
13:AH:133:ARG:HG3	13:AH:157:ARG:NH1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AS:39:THR:HB	23:AS:41:VAL:HG13	1.89	0.53
1:1:124:C:H2'	1:1:125:A:O5'	2.09	0.53
2:2:344:C:H2'	2:2:345:C:H6	1.72	0.53
2:2:424:C:O2'	2:2:426:G:O6	2.27	0.53
2:2:1231:G:H4'	2:2:1232:C:OP2	2.08	0.53
2:2:1384:U:H2'	2:2:1385:C:C6	2.44	0.53
2:2:646:C:H2'	2:2:647:C:C6	2.44	0.53
9:AD:155:ALA:HB3	9:AD:158:SER:HB2	1.91	0.53
21:AQ:139:LYS:HB3	21:AQ:141:LYS:HD3	1.90	0.53
1:1:52:G:N1	1:1:60:4AC:N3	2.43	0.53
1:1:102:C:C2	1:1:103:C:C5	2.97	0.53
1:1:762:G:H2'	1:1:763:C:H6	1.73	0.53
1:1:792:A:N1	1:1:1060:G:O2'	2.38	0.53
1:1:3014:C:H2'	1:1:3015:G:H8	1.74	0.53
1:1:3021:U:O2	1:1:3021:U:H2'	2.09	0.53
2:2:730:C:H2'	2:2:731:4AC:H6	1.90	0.53
14:AI:20:VAL:HG23	14:AI:22:LYS:HD3	1.91	0.53
21:AQ:82:LEU:HD13	21:AQ:87:LEU:HB2	1.91	0.53
24:AU:40:HIS:CE1	24:AU:41:LYS:HE2	2.44	0.53
56:BZ:22:GLU:OE1	56:BZ:25:ARG:NH2	2.37	0.53
57:BP:19:ARG:NH2	57:BP:38:GLU:OE1	2.34	0.53
1:1:776:G:H2'	1:1:2270:C:C5	2.43	0.53
1:1:1303:A:C8	1:1:1304:C:H5	2.26	0.53
1:1:1769:A:N1	1:1:1831:G:O2'	2.42	0.53
1:1:2326:U:H2'	1:1:2327:G:H8	1.73	0.53
2:2:190:C:H2'	2:2:191:U:C6	2.44	0.53
2:2:305:U:OP2	9:AD:8:ARG:NH2	2.42	0.53
10:AE:37:HIS:HB2	10:AE:42:SER:HB3	1.91	0.53
13:AH:43:LEU:N	16:AK:102:TYR:OH	2.39	0.53
22:AR:91:THR:OG1	22:AR:92:ARG:N	2.42	0.53
44:BE:43:LYS:HD3	44:BE:132:ILE:HA	1.91	0.53
44:BE:122:ASN:OD1	44:BE:122:ASN:N	2.40	0.53
54:BD:149:GLN:HA	54:BD:207:ILE:HB	1.91	0.53
1:1:434:A:H2'	1:1:435:C:C6	2.44	0.53
1:1:569:C:O2'	1:1:2119:A:N6	2.41	0.53
1:1:794:U:H2'	1:1:795:U:C6	2.44	0.53
1:1:2332:U:N3	1:1:2456:C:OP2	2.41	0.53
2:2:1386:C:H2'	2:2:1387:A:H8	1.74	0.53
2:2:1491:U:H2'	2:2:1492:A:C8	2.39	0.53
8:AC:42:ARG:HD3	8:AC:53:TYR:CD1	2.44	0.53
12:AG:77:ASP:OD1	12:AG:77:ASP:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:B4:93:GLU:H	31:B4:93:GLU:CD	2.16	0.53
1:1:1703:G:OP2	60:Bd:32:LYS:NZ	2.41	0.53
1:1:2535:G:N2	1:1:2543:U:H3	2.05	0.53
1:1:2723:C:H5'	1:1:2802:G:H5''	1.90	0.53
2:2:675:C:H2'	2:2:676:G:H8	1.74	0.53
2:2:975:G:H2'	2:2:1000:G:N2	2.23	0.53
2:2:1499:G:H2'	2:2:1500:A:H8	1.72	0.53
5:H:63:ASP:HB3	5:H:66:LYS:HE2	1.90	0.53
10:AE:105:ASN:N	10:AE:109:LYS:O	2.40	0.53
13:AH:212:GLU:OE1	27:AX:58:ARG:NH1	2.42	0.53
39:BL:86:ASP:HA	39:BL:89:LEU:HB2	1.91	0.53
31:BG:120:GLU:OE1	31:BG:120:GLU:N	2.43	0.53
31:B4:27:ARG:HG3	31:B4:90:ALA:HA	1.91	0.53
1:1:1049:G:OP1	43:Be:53:LYS:NZ	2.41	0.52
2:2:1141:A:H4'	2:2:1142:U:OP1	2.09	0.52
4:A:121:HIS:CD2	4:A:158:LEU:HD11	2.44	0.52
16:AK:90:THR:HG21	16:AK:95:LEU:HD23	1.91	0.52
1:1:889:U:H2'	1:1:890:G:C8	2.44	0.52
1:1:1146:C:H2'	1:1:1147:C:C6	2.44	0.52
1:1:2886:U:OP2	1:1:2887:A:O2'	2.28	0.52
2:2:525:U:H4'	2:2:526:A:H3'	1.91	0.52
2:2:1212:A:C8	2:2:1277:C:H1'	2.44	0.52
11:AF:66:LEU:HD12	11:AF:170:VAL:HG13	1.92	0.52
40:Bf:21:ARG:O	40:Bf:38:HIS:HE1	1.93	0.52
44:BE:27:LYS:HD3	44:BE:83:ARG:NH2	2.25	0.52
25:B6:51:THR:HG22	25:B6:71:TYR:CD1	2.41	0.52
1:1:371:G:OP1	66:Bk:43:TRP:NE1	2.36	0.52
1:1:594:G:OP2	41:BU:10:LYS:NZ	2.38	0.52
1:1:848:A:HO2'	1:1:887:G:HO2'	1.55	0.52
1:1:1366:A:H2'	1:1:1367:G:H4'	1.92	0.52
2:2:134:C:H2'	2:2:135:U:C6	2.45	0.52
15:AJ:78:ILE:HG22	15:AJ:79:ARG:HG2	1.92	0.52
44:BE:118:ASP:OD1	44:BE:118:ASP:N	2.33	0.52
46:BT:21:GLU:OE1	46:BT:21:GLU:N	2.41	0.52
1:1:952:U:H2'	1:1:953:G:O4'	2.09	0.52
2:2:41:G:H2'	2:2:42:C:C6	2.45	0.52
2:2:456:C:H2'	2:2:457:G:C8	2.42	0.52
2:2:1176:G:N2	20:AP:45:GLU:OE2	2.31	0.52
16:AK:34:GLU:OE1	16:AK:34:GLU:N	2.40	0.52
37:BC:293:VAL:HG22	37:BC:298:GLU:HG2	1.92	0.52
44:BE:28:VAL:HG22	44:BE:82:LEU:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:BA:151:LYS:O	67:BA:155:THR:OG1	2.22	0.52
1:1:133:G:H2'	1:1:134:C:C6	2.45	0.52
1:1:835:4AC:O2'	1:1:906:U:OP1	2.26	0.52
2:2:433:C:H2'	2:2:434:U:C6	2.45	0.52
2:2:484:G:N2	19:AN:67:SER:OG	2.30	0.52
5:H:145:PRO:HD3	5:H:168:ASP:HA	1.91	0.52
13:AH:135:ASP:OD2	27:AX:46:ARG:NH1	2.42	0.52
17:AL:45:ILE:HG12	20:AP:34:HIS:HD2	1.75	0.52
26:AW:50:THR:OG1	26:AW:53:LYS:O	2.27	0.52
1:1:1667:4AC:H2'	1:1:1668:G:H8	1.75	0.52
1:1:2305:C:H2'	1:1:2306:C:C6	2.45	0.52
2:2:465:G:H2'	2:2:466:G:C8	2.45	0.52
2:2:593:G:OP1	10:AE:20:TYR:OH	2.18	0.52
12:AG:38:ILE:HD12	12:AG:39:PRO:HD2	1.91	0.52
16:AK:100:ILE:HG22	16:AK:107:LEU:HD13	1.92	0.52
44:BE:56:PRO:HA	44:BE:80:VAL:HG22	1.90	0.52
1:1:757:G:O2'	1:1:1478:G:OP1	2.25	0.52
1:1:1687:C:H5''	60:Bd:64:PRO:HB3	1.91	0.52
2:2:373:A2M:HM'2	2:2:374:A:C5	2.45	0.52
5:H:56:ILE:HA	5:H:59:HIS:CE1	2.44	0.52
5:H:100:LEU:HG	5:H:101:PRO:HD2	1.92	0.52
6:AA:54:LYS:HB3	6:AA:63:GLY:HA2	1.91	0.52
7:AB:161:ARG:NH1	7:AB:197:MET:O	2.43	0.52
16:AK:76:GLU:O	16:AK:80:ILE:HG12	2.10	0.52
26:AW:17:ARG:HB2	26:AW:64:LEU:HD11	1.91	0.52
31:BG:36:THR:HB	58:BM:3:MET:HE3	1.91	0.52
1:1:371:G:O2'	66:Bk:23:CYS:SG	2.67	0.52
1:1:2893:A:C8	4:A:223:LYS:HD2	2.45	0.52
2:2:963:C:O2	2:2:1187:A:N6	2.43	0.52
5:H:147:ASP:O	5:H:210:LEU:N	2.42	0.52
5:H:297:ILE:HD13	5:H:361:ILE:HD11	1.90	0.52
21:AQ:29:THR:HG23	21:AQ:31:GLU:H	1.75	0.52
38:B5:76:GLU:OE1	38:B5:76:GLU:N	2.31	0.52
54:BD:226:GLY:H	54:BD:229:HIS:HD2	1.56	0.52
67:BA:42:LEU:O	67:BA:48:ARG:NE	2.43	0.52
1:1:299:A:H5''	39:BL:37:ALA:HB2	1.91	0.52
1:1:360:A:H2'	1:1:361:A:H8	1.74	0.52
8:AC:16:SER:OG	8:AC:46:CYS:SG	2.60	0.52
10:AE:87:ILE:HD12	10:AE:104:PRO:HG3	1.92	0.52
1:1:431:G:OP2	1:1:431:G:H8	1.93	0.52
1:1:2408:G:H3'	1:1:2408:G:OP2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2678:OMG:HM21	1:1:2680:A:H2'	1.92	0.52
2:2:145:G:H2'	2:2:146:A:C8	2.45	0.52
2:2:836:A:H5'	2:2:1043:U:C5	2.45	0.52
7:AB:188:PHE:CE2	7:AB:190:ILE:HB	2.45	0.52
28:AY:22:CYS:HB2	28:AY:25:CYS:HB2	1.92	0.52
43:Be:28:PHE:HA	43:Be:35:CYS:HA	1.91	0.52
67:BA:36:ASN:O	67:BA:202:ILE:HD12	2.10	0.52
1:1:3014:C:H2'	1:1:3015:G:C8	2.45	0.51
2:2:1215:G:H2'	2:2:1216:G:H8	1.75	0.51
2:2:1327:G:H8	2:2:1327:G:OP2	1.92	0.51
6:AA:153:LEU:HD21	6:AA:161:GLU:HG3	1.92	0.51
41:BU:7:GLN:HE21	41:BU:10:LYS:HD2	1.73	0.51
1:1:1006:G:H2'	1:1:1007:C:C6	2.45	0.51
1:1:2559:A:H2'	1:1:2560:G:H8	1.76	0.51
1:1:2988:A:N1	55:BF:74:HIS:HE1	2.08	0.51
2:2:920:C:H2'	2:2:921:G:H8	1.75	0.51
2:2:1434:U:H2'	2:2:1435:C:H6	1.75	0.51
45:Ba:1:MET:SD	45:Ba:1:MET:N	2.72	0.51
67:BA:102:LYS:O	67:BA:106:LYS:HG2	2.09	0.51
2:2:464:A:H4'	2:2:465:G:OP1	2.09	0.51
16:AK:106:MET:HG3	16:AK:107:LEU:HD12	1.91	0.51
33:AO:139:GLN:O	33:AO:140:THR:OG1	2.23	0.51
61:BN:127:LYS:H	61:BN:130:GLN:NE2	2.09	0.51
67:BA:27:PHE:O	67:BA:29:GLN:NE2	2.42	0.51
1:1:1035:G:H5'	1:1:1036:G:OP1	2.11	0.51
1:1:1306:G:C6	1:1:1307:C:C2	2.98	0.51
1:1:2384:U:HO2'	1:1:2385:C:H6	1.57	0.51
1:1:2416:G:H2'	1:1:2417:C:C6	2.45	0.51
2:2:212:G:H4'	2:2:213:G:C8	2.45	0.51
2:2:505:G:H2'	2:2:506:C:C6	2.45	0.51
2:2:1132:C:H5'	23:AS:49:ARG:HE	1.76	0.51
4:A:109:HIS:O	4:A:209:GLY:HA3	2.10	0.51
5:H:10:MET:SD	5:H:113:ILE:HB	2.50	0.51
6:AA:49:VAL:HG22	18:AM:34:THR:HG22	1.91	0.51
21:AQ:68:ASP:HB3	21:AQ:71:ASN:O	2.10	0.51
31:A3:66:LEU:HB3	31:A3:67:PRO:HD3	1.91	0.51
1:1:979:C:H2'	1:1:980:C:H6	1.75	0.51
1:1:2399:G:H2'	1:1:2400:C:H6	1.76	0.51
2:2:923:G:OP2	33:AO:130:ARG:NH2	2.43	0.51
2:2:1333:C:H3'	20:AP:32:ARG:HH12	1.76	0.51
4:A:48:TYR:CG	4:A:73:PRO:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B6:23:ILE:HG21	25:B6:31:PRO:HG3	1.92	0.51
59:BS:37:ARG:NH1	59:BS:38:GLU:OE2	2.42	0.51
61:BN:20:ARG:NH2	61:BN:27:PRO:O	2.31	0.51
2:2:797:G:H5''	7:AB:24:LYS:O	2.11	0.51
1:1:122:G:H2'	1:1:123:A:C8	2.45	0.51
1:1:893:A:N1	1:1:2603:A:O2'	2.40	0.51
1:1:1763:G:H2'	1:1:1764:C:C6	2.45	0.51
6:AA:53:LEU:HD12	6:AA:65:VAL:HG11	1.92	0.51
6:AA:102:THR:HG23	6:AA:129:ARG:HA	1.91	0.51
54:BD:112:LEU:HA	54:BD:115:MET:HE3	1.93	0.51
67:BA:40:ILE:HB	67:BA:201:GLN:HE22	1.74	0.51
1:1:115:G:N3	1:1:115:G:H2'	2.26	0.51
1:1:2535:G:H1	1:1:2543:U:H3	1.58	0.51
2:2:1238:C:P	24:AU:119:ARG:HH22	2.33	0.51
3:3:79:G:H1'	3:3:80:U:OP2	2.11	0.51
10:AE:33:ARG:HG3	10:AE:34:PRO:HD2	1.93	0.51
13:AH:109:LYS:O	13:AH:113:LYS:HG2	2.10	0.51
21:AQ:149:ASP:HB2	21:AQ:152:GLN:HB3	1.92	0.51
31:B4:40:THR:HA	31:B4:43:VAL:HG12	1.93	0.51
1:1:658:G:H5''	1:1:661:C:H1'	1.93	0.51
1:1:1324:A:O2'	1:1:1329:G:O6	2.27	0.51
1:1:2373:G:H8	1:1:2373:G:OP2	1.93	0.51
2:2:41:G:H2'	2:2:42:C:H6	1.75	0.51
2:2:1103:C:O2'	24:AU:130:ASP:OD2	2.26	0.51
6:AA:19:TRP:CZ3	6:AA:37:PRO:HB3	2.46	0.51
15:AJ:42:LYS:HB3	15:AJ:59:ALA:HB3	1.93	0.51
25:AV:3:ILE:HD13	25:AV:23:ILE:HB	1.93	0.51
36:BO:36:VAL:HG12	36:BO:105:ASP:HB3	1.93	0.51
51:BQ:105:GLU:OE2	51:BQ:139:TYR:OH	2.23	0.51
55:BF:92:VAL:HG22	55:BF:172:ILE:HG12	1.93	0.51
1:1:508:C:H2'	1:1:509:A:C8	2.46	0.51
1:1:1401:C:O2'	65:BI:42:GLY:O	2.27	0.51
1:1:1415:C:OP2	35:BY:118:ARG:NH2	2.43	0.51
1:1:1754:C:OP1	60:Bd:41:ARG:NH1	2.44	0.51
1:1:2473:U:H2'	1:1:2474:U:C6	2.46	0.51
2:2:930:A:N3	2:2:957:4AC:O2'	2.42	0.51
2:2:1100:C:H2'	2:2:1101:U:C6	2.46	0.51
10:AE:88:MET:N	10:AE:102:VAL:O	2.40	0.51
44:BE:129:ASP:HB3	44:BE:132:ILE:HG13	1.93	0.51
55:BF:55:ILE:HD11	55:BF:75:ILE:HD12	1.93	0.51
58:BM:41:ARG:HD3	58:BM:42:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:896:G:H2'	1:1:897:C:C6	2.46	0.50
1:1:1077:C:H5'	1:1:2662:A:O2'	2.11	0.50
1:1:1303:A:H2	1:1:1368:G:H1'	1.75	0.50
1:1:2142:A:HO2'	34:BB:215:THR:HG1	1.58	0.50
1:1:2406:A:H8	1:1:2406:A:O5'	1.93	0.50
2:2:223:G:H2'	2:2:224:G:C8	2.46	0.50
2:2:1415:U:H2'	2:2:1416:C:H6	1.73	0.50
7:AB:59:LEU:HD12	7:AB:171:LEU:HD11	1.92	0.50
26:AW:32:HIS:NE2	26:AW:53:LYS:HD3	2.26	0.50
62:Bg:8:GLU:OE1	62:Bg:44:ARG:NH2	2.36	0.50
1:1:1308:G:N2	1:1:1362:G:C8	2.75	0.50
1:1:1574:C:H2'	1:1:1575:A:C8	2.46	0.50
1:1:2066:A:H2'	1:1:2067:G:O4'	2.11	0.50
1:1:2255:A:H2'	1:1:2256:A:C8	2.46	0.50
2:2:1211:C:OP2	13:AH:91:ARG:NH2	2.43	0.50
3:3:122:G:H2'	3:3:123:C:H6	1.76	0.50
29:AZ:40:LEU:HD23	29:AZ:40:LEU:H	1.75	0.50
45:Ba:25:TRP:HA	45:Ba:64:GLU:HG2	1.92	0.50
61:BN:31:ILE:HB	61:BN:63:GLU:HG2	1.93	0.50
1:1:732:G:H2'	1:1:733:C:H6	1.76	0.50
1:1:1145:C:H2'	1:1:1146:C:C6	2.46	0.50
2:2:1125:G:O2'	2:2:1126:G:H8	1.93	0.50
2:2:1200:C:OP1	33:AO:119:ARG:NH2	2.45	0.50
2:2:1293:A:H3'	32:AT:31:ARG:HD3	1.93	0.50
2:2:1416:C:H2'	2:2:1417:U:H6	1.76	0.50
4:A:30:ARG:NE	4:A:34:GLU:OE2	2.43	0.50
4:A:191:LYS:HB3	4:A:203:LEU:HD23	1.92	0.50
25:AV:59:TYR:CE1	25:AV:66:LYS:HD3	2.47	0.50
1:1:769:C:O2'	42:Bb:27:GLU:OE2	2.29	0.50
1:1:864:G:H2'	1:1:865:C:O4'	2.12	0.50
1:1:1019:C:H2'	1:1:1020:G:H8	1.76	0.50
1:1:1755:4AC:O7	1:1:1755:4AC:H5	2.12	0.50
1:1:2719:G:H2'	1:1:2720:A:H8	1.76	0.50
10:AE:2:ALA:HB2	10:AE:7:LYS:HG3	1.93	0.50
10:AE:218:GLU:CD	10:AE:218:GLU:H	2.19	0.50
44:BE:67:ASP:OD1	44:BE:67:ASP:N	2.36	0.50
38:BK:38:ALA:HB1	38:BK:72:LYS:HB2	1.94	0.50
66:Bk:4:LEU:HD13	66:Bk:37:VAL:HG13	1.93	0.50
1:1:107:G:N2	1:1:112:A:N7	2.60	0.50
1:1:285:A:H5''	43:Be:55:TRP:HZ3	1.76	0.50
1:1:895:A:H2'	1:1:896:G:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1015:A:H5'	34:BB:176:GLY:HA2	1.94	0.50
1:1:1317:G:H2'	1:1:1318:G:C8	2.47	0.50
1:1:2065:A:H2'	1:1:2066:A:C8	2.47	0.50
2:2:101:G:N2	2:2:388:G:O3'	2.44	0.50
2:2:636:4AC:HM73	2:2:703:4AC:HM71	1.92	0.50
2:2:1083:C:H1'	2:2:1153:A:C4	2.47	0.50
5:H:371:LYS:O	5:H:375:GLU:HG2	2.11	0.50
8:AC:17:CYS:HB3	8:AC:46:CYS:SG	2.51	0.50
31:B4:8:LYS:H	31:B4:79:TYR:HE2	1.58	0.50
1:1:703:U:H3'	1:1:704:G:H5'	1.92	0.50
1:1:801:C:H2'	1:1:802:4AC:H6	1.94	0.50
1:1:1258:A:OP2	49:BI:89:ARG:NH2	2.44	0.50
2:2:977:A:C5	2:2:978:G:H1'	2.47	0.50
5:H:52:GLN:HA	5:H:55:ILE:HD12	1.93	0.50
12:AG:39:PRO:HG2	12:AG:42:GLU:HB2	1.93	0.50
18:AM:27:ILE:O	18:AM:27:ILE:HG13	2.10	0.50
20:AP:22:ILE:HG13	20:AP:37:MET:O	2.11	0.50
44:BE:120:HIS:HD1	44:BE:135:PHE:H	1.59	0.50
1:1:1330:C:H2'	1:1:1331:C:H6	1.76	0.50
1:1:1393:G:H5'	49:BI:78:THR:HG23	1.92	0.50
1:1:2427:G:H2'	1:1:2428:C:C6	2.47	0.50
2:2:891:U:H2'	2:2:892:U:C6	2.47	0.50
18:AM:29:HIS:ND1	18:AM:41:ARG:HB3	2.27	0.50
19:AN:133:SER:HB3	19:AN:136:GLU:HG2	1.94	0.50
41:BU:37:GLU:O	41:BU:40:LYS:NZ	2.45	0.50
1:1:124:C:C2'	1:1:125:A:O5'	2.60	0.50
1:1:271:A:H2'	1:1:272:G:H4'	1.93	0.50
1:1:279:A:H2'	1:1:280:G:H8	1.76	0.50
1:1:332:A:H5''	1:1:333:A:C8	2.47	0.50
1:1:2645:U:H2'	1:1:2646:G:H8	1.76	0.50
2:2:94:G:H2'	2:2:95:C:C6	2.46	0.50
2:2:636:4AC:H5''	2:2:636:4AC:H6	1.94	0.50
2:2:1329:G:H2'	2:2:1330:C:C6	2.47	0.50
4:A:22:ILE:HD12	4:A:44:LEU:HD21	1.93	0.50
5:H:140:VAL:HG13	5:H:253:GLY:HA2	1.93	0.50
5:H:241:GLY:HA2	5:H:256:THR:HG22	1.94	0.50
38:B5:9:ILE:HG12	38:B5:23:VAL:HG12	1.92	0.50
44:BE:115:PHE:O	44:BE:139:VAL:N	2.41	0.50
61:BN:56:GLN:NE2	61:BN:125:ARG:HH21	2.10	0.50
1:1:382:C:H2'	1:1:383:C:C6	2.47	0.50
1:1:617:G:N2	1:1:620:A:OP2	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2302:A:H2	1:1:2735:C:H42	1.59	0.50
2:2:913:OMG:OP1	13:AH:73:ARG:HB2	2.11	0.50
2:2:1122:U:H2'	2:2:1123:C:O4'	2.12	0.50
2:2:1463:G:H5''	5:H:358:HIS:CE1	2.46	0.50
13:AH:132:PRO:HG2	13:AH:152:ILE:HD12	1.94	0.50
34:BB:75:GLU:HG3	48:Bi:65:GLY:HA2	1.94	0.50
58:BM:43:THR:OG1	58:BM:129:GLU:OE2	2.30	0.50
1:1:118:U:H2'	1:1:118:U:O2	2.11	0.49
1:1:659:A:OP2	59:BS:4:ARG:NH1	2.41	0.49
1:1:1011:C:H2'	1:1:1012:G:O4'	2.12	0.49
13:AH:203:LYS:HG3	13:AH:207:ILE:HD13	1.94	0.49
41:BU:87:ASN:OD1	41:BU:89:THR:OG1	2.30	0.49
1:1:1993:G:N2	1:1:1995:G:H3'	2.26	0.49
2:2:303:4AC:OP1	2:2:576:U:O2'	2.24	0.49
2:2:1086:C:H2'	2:2:1087:C:C6	2.47	0.49
2:2:1200:C:P	33:AO:119:ARG:HH22	2.34	0.49
6:AA:19:TRP:HZ3	6:AA:37:PRO:HB3	1.76	0.49
9:AD:126:VAL:HG12	9:AD:127:HIS:HD2	1.77	0.49
10:AE:179:PHE:CZ	10:AE:227:LYS:HG3	2.47	0.49
11:AF:31:ILE:HD12	11:AF:36:GLU:HB3	1.93	0.49
31:A3:114:ILE:HA	31:A3:117:LYS:HE3	1.94	0.49
44:BE:52:THR:HA	44:BE:90:MET:HE1	1.95	0.49
1:1:492:C:H2'	1:1:493:G:O4'	2.12	0.49
2:2:233:G:H2'	2:2:234:A:C8	2.47	0.49
5:H:19:ILE:HD13	5:H:47:LYS:NZ	2.27	0.49
20:AP:5:ASP:HA	20:AP:8:LYS:HG2	1.94	0.49
24:AU:26:ILE:HD13	24:AU:55:VAL:HG11	1.93	0.49
27:AX:26:GLN:OE1	27:AX:42:ARG:NH1	2.44	0.49
31:A3:15:LEU:HG	31:A3:114:ILE:HD11	1.93	0.49
54:BD:5:VAL:N	54:BD:14:ASP:O	2.40	0.49
1:1:2524:G:H2'	1:1:2525:G:H8	1.78	0.49
1:1:2847:U:H2'	1:1:2848:C:H6	1.77	0.49
2:2:1099:C:H2'	2:2:1100:C:H6	1.77	0.49
2:2:1282:C:H5''	33:AO:126:VAL:HG22	1.95	0.49
2:2:1339:C:H2'	2:2:1340:G:H8	1.78	0.49
5:H:234:MET:N	5:H:234:MET:SD	2.84	0.49
7:AB:158:ASN:OD1	7:AB:158:ASN:N	2.45	0.49
12:AG:24:PRO:O	12:AG:28:LYS:NZ	2.43	0.49
13:AH:6:SER:HB3	24:AU:143:ILE:HD11	1.93	0.49
61:BN:83:HIS:HD2	61:BN:136:ARG:HE	1.59	0.49
1:1:1698:A:H2'	1:1:1699:G:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:418:G:H2'	2:2:419:U:C6	2.47	0.49
2:2:663:A:H2'	2:2:664:U:C6	2.43	0.49
2:2:717:C:H2'	2:2:718:4AC:H6	1.94	0.49
5:H:42:ASP:HB2	5:H:47:LYS:HE3	1.95	0.49
16:AK:25:ARG:N	16:AK:61:ASP:OD1	2.45	0.49
19:AN:44:LEU:HG	19:AN:50:ALA:HB2	1.95	0.49
61:BN:29:PRO:HA	61:BN:59:GLN:HE22	1.77	0.49
1:1:107:G:C8	1:1:107:G:H5''	2.48	0.49
1:1:465:A:OP2	41:BU:60:LYS:NZ	2.45	0.49
1:1:1071:A:H4'	1:1:1087:G:N2	2.28	0.49
1:1:1173:C:H2'	1:1:1174:A:H8	1.77	0.49
1:1:2277:C:H2'	1:1:2278:A:C8	2.48	0.49
1:1:2455:A:H4'	1:1:2456:C:O5'	2.12	0.49
2:2:97:A:H2'	2:2:98:C:C6	2.45	0.49
2:2:850:C:H2'	2:2:851:4AC:H6	1.95	0.49
2:2:866:G:H2'	2:2:867:C:H6	1.77	0.49
4:A:204:ILE:HG12	4:A:206:ILE:HG23	1.95	0.49
5:H:171:GLY:HA3	5:H:250:LYS:HE2	1.93	0.49
29:AZ:186:ASP:OD1	29:AZ:186:ASP:N	2.27	0.49
36:BO:30:SER:HB2	36:BO:32:LYS:HE3	1.95	0.49
1:1:21:C:H2'	1:1:22:4AC:H6	1.94	0.49
1:1:866:C:H4'	1:1:867:U:OP1	2.13	0.49
1:1:1330:C:H2'	1:1:1331:C:C6	2.48	0.49
1:1:2393:G:C2	1:1:2394:G:N7	2.81	0.49
1:1:2635:G:O2'	1:1:2636:C:O5'	2.26	0.49
2:2:951:C:O2	20:AP:12:ARG:NE	2.46	0.49
3:3:124:C:C2	3:3:125:A:C8	3.01	0.49
44:BE:28:VAL:HG13	44:BE:87:ALA:HB1	1.94	0.49
59:BS:120:HIS:HB2	59:BS:145:HIS:HB2	1.95	0.49
1:1:728:C:OP1	38:BK:47:ARG:NH2	2.42	0.49
1:1:2047:A:H61	1:1:2084:G:HO2'	1.57	0.49
1:1:2249:4AC:OP1	59:BS:70:GLN:NE2	2.46	0.49
1:1:2401:C:C2	1:1:2402:G:C8	3.01	0.49
1:1:2986:U:H1'	1:1:2987:A:H5''	1.94	0.49
2:2:1321:G:C8	16:AK:112:ARG:HB3	2.48	0.49
2:2:1373:C:O2	2:2:1471:A:N6	2.46	0.49
67:BA:185:GLU:HA	67:BA:188:LEU:HB3	1.94	0.49
1:1:56:C:H5''	1:1:57:A:OP1	2.13	0.49
1:1:521:G:H4'	1:1:522:A:N7	2.27	0.49
1:1:845:C:H2'	1:1:846:C:C6	2.48	0.49
1:1:871:G:H2'	1:1:872:C:H6	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1577:A:H5'	51:BQ:2:LYS:NZ	2.27	0.49
1:1:2347:G:H1	1:1:2422:U:H3	1.61	0.49
2:2:109:C:H2'	2:2:110:U:C6	2.47	0.49
2:2:429:A:H2'	2:2:430:C:H6	1.77	0.49
2:2:477:G:H5''	2:2:478:C:OP1	2.13	0.49
2:2:1185:G:H5'	2:2:1187:A:H1'	1.94	0.49
14:AI:97:PHE:CD1	14:AI:98:GLU:HG2	2.48	0.49
36:BO:88:LEU:HD12	36:BO:127:ALA:HB2	1.95	0.49
56:BZ:30:GLY:HA2	56:BZ:58:ILE:HD11	1.94	0.49
1:1:1067:C:H2'	1:1:1068:4AC:H6	1.95	0.49
2:2:703:4AC:H2'	2:2:704:G:C8	2.47	0.49
2:2:1417:U:H2'	2:2:1418:C:C6	2.48	0.49
5:H:53:ASP:O	5:H:57:ARG:HG2	2.13	0.49
44:BE:60:LYS:HA	44:BE:75:PRO:HA	1.93	0.49
54:BD:146:ASP:O	54:BD:149:GLN:HG2	2.11	0.49
64:BJ:85:GLN:HA	64:BJ:102:ASN:HD22	1.77	0.49
1:1:773:C:H5'	39:BL:22:LYS:HE2	1.94	0.48
1:1:1210:U:H4'	61:BN:8:ILE:HG23	1.95	0.48
1:1:2564:A:H5''	36:BO:22:ARG:NH2	2.28	0.48
2:2:147:U:H2'	2:2:148:A:H8	1.78	0.48
2:2:196:G:H3'	2:2:197:G:H5'	1.94	0.48
2:2:268:G:H2'	2:2:269:G:C8	2.48	0.48
2:2:451:A:C4	2:2:452:G:C8	3.00	0.48
2:2:695:A:H2'	2:2:696:A:C8	2.47	0.48
3:3:97:G:H2'	3:3:98:G:C8	2.48	0.48
4:A:170:LYS:HB3	4:A:227:GLN:HB2	1.94	0.48
9:AD:105:LEU:O	9:AD:109:VAL:HG12	2.13	0.48
35:BY:94:GLU:OE1	35:BY:94:GLU:N	2.42	0.48
37:BC:188:SER:HB3	37:BC:191:GLU:HB2	1.95	0.48
1:1:279:A:H2'	1:1:280:G:C8	2.48	0.48
1:1:1306:G:HO2'	1:1:1307:C:P	2.35	0.48
1:1:1939:G:O2'	1:1:2919:G:H4'	2.12	0.48
2:2:1105:G:N3	24:AU:138:LYS:HE2	2.29	0.48
2:2:1150:A:H3'	2:2:1151:G:H8	1.78	0.48
2:2:1435:C:H2'	2:2:1436:G:O4'	2.13	0.48
3:3:124:C:H2'	3:3:125:A:C8	2.48	0.48
4:A:12:ARG:HG2	4:A:21:GLU:HG2	1.95	0.48
55:BF:143:ASP:HB3	55:BF:146:ALA:HB3	1.94	0.48
67:BA:40:ILE:HB	67:BA:201:GLN:NE2	2.28	0.48
1:1:435:C:H2'	1:1:436:C:H6	1.77	0.48
1:1:2148:G:O2'	4:A:16:HIS:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:233:G:H2'	2:2:234:A:H8	1.78	0.48
2:2:484:G:C8	2:2:496:G:O4'	2.67	0.48
6:AA:22:ILE:HD11	6:AA:36:THR:HG23	1.95	0.48
7:AB:193:GLU:CD	7:AB:193:GLU:H	2.20	0.48
13:AH:190:LEU:HB3	13:AH:198:SER:HB3	1.93	0.48
14:AI:55:ASP:N	14:AI:55:ASP:OD1	2.44	0.48
24:AU:130:ASP:O	24:AU:134:THR:HG23	2.13	0.48
51:BQ:15:LEU:HD13	51:BQ:52:LYS:HB2	1.95	0.48
1:1:1259:A:N6	63:Bc:14:LYS:HB2	2.27	0.48
2:2:83:C:H2'	2:2:84:C:C6	2.48	0.48
2:2:110:U:H2'	2:2:111:C:C6	2.49	0.48
2:2:518:U:H2'	2:2:519:OMG:C8	2.47	0.48
2:2:908:C:H2'	2:2:909:A:H8	1.78	0.48
2:2:1100:C:H2'	2:2:1101:U:H6	1.78	0.48
6:AA:14:TRP:CZ2	18:AM:74:LYS:HB3	2.48	0.48
6:AA:84:LYS:O	6:AA:191:VAL:HG22	2.13	0.48
9:AD:109:VAL:HG13	9:AD:121:ALA:HB1	1.96	0.48
10:AE:202:ILE:HG13	10:AE:213:VAL:HG23	1.94	0.48
15:AJ:104:GLU:H	15:AJ:104:GLU:CD	2.20	0.48
58:BM:76:TRP:CD1	58:BM:76:TRP:H	2.29	0.48
1:1:1631:C:C2	1:1:1632:G:C8	3.02	0.48
2:2:643:A:O2'	18:AM:122:PRO:HB3	2.14	0.48
2:2:653:U:H1'	2:2:654:A:C8	2.48	0.48
2:2:943:G:OP2	16:AK:130:ARG:NH2	2.44	0.48
2:2:1071:G:H2'	2:2:1072:C:H6	1.79	0.48
5:H:382:LYS:NZ	18:AM:52:ARG:HG3	2.29	0.48
6:AA:112:THR:HG23	6:AA:114:ASP:H	1.78	0.48
14:AI:56:GLY:N	21:AQ:18:PRO:HB3	2.29	0.48
32:AT:95:LYS:H	32:AT:98:MET:HG3	1.78	0.48
37:BC:17:ARG:HB2	37:BC:233:ARG:NH2	2.29	0.48
44:BE:103:LYS:HA	44:BE:184:VAL:HG22	1.95	0.48
67:BA:21:ARG:HH22	67:BA:209:THR:H	1.60	0.48
1:1:1203:G:H2'	1:1:1204:G:H8	1.78	0.48
1:1:2522:U:H2'	1:1:2523:C:C6	2.49	0.48
1:1:2558:A:H2'	1:1:2559:A:C8	2.48	0.48
2:2:1302:C:C2	2:2:1303:G:C8	3.02	0.48
10:AE:199:ILE:HD12	10:AE:213:VAL:HG21	1.95	0.48
17:AL:10:SER:HB3	17:AL:94:VAL:HA	1.95	0.48
44:BE:108:ASP:OD2	44:BE:112:ASN:HB2	2.13	0.48
63:Bc:8:LEU:HD11	63:Bc:25:LYS:HB2	1.96	0.48
63:Bc:41:ARG:HE	63:Bc:87:ILE:C	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:117:G:N3	1:1:118:U:C6	2.82	0.48
1:1:703:U:O4	31:B4:83:LYS:NZ	2.38	0.48
1:1:715:A:H2'	1:1:716:A:C8	2.48	0.48
1:1:1698:A:H2'	1:1:1699:G:C8	2.48	0.48
1:1:2944:C:O2'	1:1:2946:C:OP2	2.18	0.48
2:2:200:C:OP1	10:AE:134:LYS:HD3	2.14	0.48
2:2:908:C:C2	2:2:909:A:C8	3.02	0.48
2:2:1202:5MC:H2'	2:2:1203:G:C8	2.48	0.48
2:2:1287:G:H2'	2:2:1288:C:H6	1.78	0.48
2:2:1388:C:H2'	2:2:1389:C:C6	2.48	0.48
2:2:1416:C:H2'	2:2:1417:U:C6	2.48	0.48
16:AK:103:ASP:O	16:AK:106:MET:HG2	2.14	0.48
17:AL:18:GLU:O	17:AL:22:GLN:HG2	2.13	0.48
21:AQ:91:ILE:HG13	21:AQ:96:MET:HG2	1.96	0.48
22:AR:105:VAL:HG21	22:AR:108:ARG:HH11	1.79	0.48
23:AS:6:GLN:HB2	23:AS:9:ILE:HG12	1.96	0.48
37:BC:184:ILE:HG13	37:BC:196:ILE:HD11	1.95	0.48
41:BU:31:LEU:HD23	41:BU:102:ILE:HB	1.95	0.48
1:1:102:C:N3	1:1:103:C:C4	2.81	0.48
1:1:213:U:O4	41:BU:47:ARG:NH2	2.47	0.48
1:1:535:U:H2'	1:1:536:C:C6	2.49	0.48
1:1:683:A:O2'	1:1:769:C:H5''	2.14	0.48
1:1:855:C:H2'	1:1:856:G:O4'	2.13	0.48
2:2:541:G:N2	2:2:851:4AC:O2	2.38	0.48
2:2:594:G:O2'	9:AD:65:GLN:NE2	2.44	0.48
2:2:920:C:H5''	33:AO:135:PHE:CZ	2.48	0.48
2:2:1312:G:OP1	13:AH:80:LYS:NZ	2.37	0.48
2:2:1502:C:O5'	2:2:1502:C:H6	1.97	0.48
4:A:168:ALA:HB3	4:A:229:LYS:HB3	1.95	0.48
23:AS:15:GLU:HA	23:AS:18:ASN:ND2	2.28	0.48
50:BR:19:HIS:CD2	50:BR:21:ARG:H	2.27	0.48
65:BL:9:SER:OG	65:BL:56:GLU:OE1	2.32	0.48
1:1:53:G:H2'	1:1:54:G:O4'	2.14	0.48
1:1:98:C:H6	1:1:98:C:H5''	1.79	0.48
1:1:761:U:H2'	1:1:762:G:C8	2.48	0.48
1:1:1110:G:N3	1:1:2499:A:H2'	2.29	0.48
1:1:1780:4AC:O7	1:1:1780:4AC:H5	2.13	0.48
2:2:736:G:H2'	2:2:737:C:H6	1.77	0.48
2:2:800:U:H2'	2:2:801:C:C6	2.48	0.48
2:2:1035:U:H2'	2:2:1036:C:C6	2.49	0.48
2:2:1172:G:H2'	2:2:1173:U:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1303:G:H5''	33:AO:32:GLY:H	1.78	0.48
3:3:93:G:H2'	3:3:94:A:C8	2.49	0.48
23:AS:18:ASN:OD1	23:AS:19:LYS:N	2.47	0.48
37:BC:17:ARG:HB2	37:BC:233:ARG:HH21	1.78	0.48
25:B6:41:VAL:HG21	25:B6:48:PRO:HG3	1.95	0.48
64:BJ:16:ARG:NH1	64:BJ:60:ASP:OD1	2.43	0.48
1:1:796:C:H2'	1:1:797:G:H8	1.78	0.48
1:1:1058:U:O2'	1:1:2300:A:N1	2.46	0.48
1:1:1574:C:H2'	1:1:1575:A:H8	1.79	0.48
1:1:1591:A:H2'	1:1:1593:C:C5	2.49	0.48
1:1:2050:U:H2'	1:1:2051:C:C6	2.49	0.48
1:1:2130:A:H2'	1:1:2131:A:C8	2.49	0.48
2:2:1215:G:H2'	2:2:1216:G:C8	2.49	0.48
2:2:1223:C:O2'	16:AK:69:GLY:O	2.30	0.48
2:2:1446:U:H2'	2:2:1447:C:C6	2.49	0.48
35:BY:91:MET:HB2	35:BY:95:GLU:HG3	1.95	0.48
38:B5:18:ALA:HB3	60:Bd:67:PRO:HG2	1.96	0.48
54:BD:251:LYS:HE3	54:BD:251:LYS:HB2	1.78	0.48
59:BS:20:ALA:HB1	59:BS:97:ASN:HD22	1.79	0.48
1:1:635:G:O2'	1:1:659:A:N1	2.39	0.47
2:2:189:A:O2'	10:AE:132:MET:HE2	2.15	0.47
2:2:344:C:H2'	2:2:345:C:C6	2.48	0.47
2:2:1349:A:H2'	2:2:1350:U:O4'	2.14	0.47
2:2:1492:A:H2'	2:2:1493:C:H6	1.79	0.47
3:3:121:G:H2'	3:3:122:G:H8	1.79	0.47
12:AG:3:THR:OG1	12:AG:20:GLU:OE2	2.26	0.47
13:AH:111:ILE:HD11	13:AH:122:VAL:HB	1.95	0.47
67:BA:79:ARG:NH1	67:BA:144:ASN:OD1	2.47	0.47
1:1:1019:C:H2'	1:1:1020:G:C8	2.49	0.47
2:2:157:A:H2'	2:2:158:A:O4'	2.14	0.47
2:2:861:G:O2'	2:2:877:G:O6	2.31	0.47
2:2:1354:U:H2'	2:2:1355:C:C6	2.48	0.47
25:AV:46:LEU:HB2	25:AV:71:TYR:CE1	2.50	0.47
27:AX:32:LEU:O	27:AX:37:LYS:HG3	2.14	0.47
35:BY:60:ASN:H	35:BY:148:ASN:HD21	1.62	0.47
1:1:848:A:O2'	1:1:887:G:O2'	2.23	0.47
1:1:1300:U:H5''	1:1:1301:A:OP2	2.14	0.47
1:1:2363:G:H5''	67:BA:157:ARG:HH12	1.78	0.47
1:1:2408:G:N3	1:1:2408:G:C2'	2.77	0.47
2:2:429:A:H2'	2:2:430:C:C6	2.49	0.47
2:2:1086:C:H2'	2:2:1087:C:H6	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1388:C:H2'	2:2:1389:C:H6	1.78	0.47
7:AB:60:ALA:HA	7:AB:175:ILE:HD12	1.96	0.47
1:1:102:C:C4	1:1:103:C:N4	2.81	0.47
1:1:1227:G:H5'	42:Bb:55:LYS:HB2	1.95	0.47
1:1:2535:G:H5'	1:1:2536:U:OP2	2.14	0.47
1:1:2611:A:H2'	1:1:2612:A:C8	2.50	0.47
2:2:327:G:O2'	2:2:1437:A:H4'	2.14	0.47
2:2:1339:C:H2'	2:2:1340:G:C8	2.49	0.47
2:2:1402:A:H2'	2:2:1403:G:C8	2.49	0.47
2:2:1402:A:H2'	2:2:1403:G:H8	1.79	0.47
10:AE:152:LEU:HD22	10:AE:152:LEU:HA	1.65	0.47
44:BE:24:ARG:NH2	44:BE:146:PRO:HG3	2.28	0.47
44:BE:116:GLY:HA2	44:BE:138:ASP:HA	1.97	0.47
44:BE:148:PHE:HA	44:BE:160:ILE:HD11	1.96	0.47
1:1:102:C:OP2	1:1:102:C:H6	1.96	0.47
1:1:1687:C:OP2	60:Bd:66:ARG:NE	2.36	0.47
1:1:2130:A:H2'	1:1:2131:A:H8	1.79	0.47
1:1:2523:C:H2'	1:1:2524:G:H8	1.80	0.47
1:1:2645:U:H2'	1:1:2646:G:C8	2.48	0.47
2:2:656:G:H2'	2:2:657:OMG:O4'	2.15	0.47
2:2:934:OMG:C2	2:2:935:G:C8	3.02	0.47
2:2:1066:A:H4'	2:2:1067:A:O5'	2.14	0.47
2:2:1368:A:N1	2:2:1469:6MZ:O2'	2.42	0.47
5:H:338:VAL:HG22	5:H:343:VAL:HG23	1.96	0.47
6:AA:45:LEU:HD23	6:AA:71:VAL:HG12	1.96	0.47
16:AK:22:GLY:HA3	16:AK:61:ASP:CG	2.40	0.47
22:AR:87:LEU:HB2	22:AR:106:LEU:HD21	1.96	0.47
29:AZ:76:GLU:OE1	29:AZ:76:GLU:N	2.46	0.47
31:B4:86:LEU:HD11	31:B4:99:VAL:HG12	1.95	0.47
31:B4:101:ILE:HD11	31:B4:104:PRO:HA	1.95	0.47
67:BA:68:ILE:HG23	67:BA:85:ILE:HB	1.95	0.47
1:1:493:G:H5'	41:BU:1:MET:HG2	1.94	0.47
1:1:704:G:H8	1:1:704:G:OP2	1.98	0.47
1:1:1311:G:H4'	1:1:1340:A:H2	1.79	0.47
1:1:1625:A:H2'	1:1:1626:C:C6	2.50	0.47
1:1:1914:A:OP1	51:BQ:56:LYS:NZ	2.48	0.47
1:1:2537:C:OP2	1:1:2538:A:O2'	2.30	0.47
1:1:2712:C:H2'	1:1:2713:G:O4'	2.15	0.47
1:1:2924:C:H2'	1:1:2925:4AC:H6	1.96	0.47
2:2:541:G:O2'	2:2:788:G:H5'	2.14	0.47
2:2:1035:U:H2'	2:2:1036:C:H6	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Bi:6:LYS:HD3	48:Bi:23:ARG:NH2	2.29	0.47
31:B4:4:PRO:HG2	31:B4:7:VAL:HG23	1.97	0.47
67:BA:187:VAL:O	67:BA:191:ILE:HG12	2.14	0.47
1:1:293:G:H5''	58:BM:73:ARG:HH21	1.79	0.47
1:1:631:A:N3	41:BU:93:TYR:OH	2.40	0.47
1:1:1250:A:H2'	1:1:1251:A:C8	2.49	0.47
1:1:1413:C:H2'	1:1:1414:C:H6	1.80	0.47
1:1:1689:C:N4	60:Bd:65:GLU:OE1	2.32	0.47
1:1:2259:U:O2	42:Bb:30:ARG:NH2	2.47	0.47
1:1:2693:C:H2'	1:1:2694:U:C6	2.50	0.47
2:2:567:C:H2'	2:2:568:U:O4'	2.15	0.47
2:2:629:G:O2'	2:2:803:G:OP1	2.32	0.47
2:2:642:U:C2	2:2:643:A:C8	3.02	0.47
2:2:907:A:H2'	2:2:908:C:H6	1.79	0.47
2:2:1201:A:H4'	33:AO:139:GLN:HB2	1.97	0.47
4:A:164:MET:HE1	4:A:205:GLU:HG3	1.95	0.47
6:AA:52:THR:HG22	6:AA:54:LYS:H	1.77	0.47
6:AA:109:ASN:ND2	6:AA:119:ARG:HE	2.12	0.47
7:AB:24:LYS:HA	7:AB:143:THR:HG22	1.95	0.47
11:AF:63:GLN:HB3	11:AF:89:VAL:HG12	1.96	0.47
15:AJ:41:ASP:OD1	15:AJ:61:ALA:N	2.34	0.47
20:AP:12:ARG:HG2	20:AP:14:PHE:O	2.14	0.47
21:AQ:96:MET:HE1	21:AQ:157:VAL:HA	1.96	0.47
23:AS:9:ILE:HD11	23:AS:46:ILE:HG23	1.96	0.47
24:AU:34:PHE:HE1	33:AO:42:VAL:HG23	1.79	0.47
34:BB:61:VAL:HG11	34:BB:83:ILE:HD11	1.96	0.47
54:BD:33:ARG:NH1	54:BD:109:GLU:OE2	2.48	0.47
54:BD:201:VAL:HG11	54:BD:207:ILE:HG21	1.96	0.47
55:BF:110:ILE:HB	55:BF:120:ARG:HB2	1.97	0.47
31:B4:6:TYR:HB3	31:B4:60:GLU:OE2	2.15	0.47
67:BA:132:ASN:O	67:BA:133:LYS:HD2	2.14	0.47
1:1:1309:G:H2'	1:1:1310:G:C4'	2.45	0.47
1:1:1324:A:H4'	1:1:1325:A:H5''	1.97	0.47
1:1:1790:C:H2'	1:1:1791:G:H8	1.80	0.47
1:1:2360:G:H2'	1:1:2361:G:H8	1.79	0.47
2:2:227:C:H2'	2:2:228:C:C6	2.50	0.47
2:2:1287:G:P	32:AT:33:ARG:HH21	2.38	0.47
2:2:1409:G:H2'	2:2:1410:C:H6	1.80	0.47
4:A:68:PHE:HB3	4:A:79:ILE:HD12	1.97	0.47
5:H:313:ILE:HD11	16:AK:135:ARG:HH21	1.79	0.47
6:AA:127:ALA:HB2	6:AA:182:LYS:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AC:58:CYS:SG	8:AC:60:TRP:HB3	2.55	0.47
32:AT:3:ARG:HA	32:AT:3:ARG:HE	1.80	0.47
37:BC:38:MET:HE3	37:BC:182:TYR:CG	2.50	0.47
38:B5:50:ILE:HA	38:B5:50:ILE:HD13	1.80	0.47
1:1:117:G:C5	1:1:118:U:C5	3.02	0.47
1:1:450:C:H2'	1:1:451:4AC:H6	1.97	0.47
1:1:1308:G:C2'	1:1:1309:G:H5'	2.44	0.47
4:A:76:VAL:O	4:A:80:ILE:HG13	2.15	0.47
4:A:100:LYS:NZ	4:A:141:LYS:O	2.43	0.47
11:AF:167:ILE:O	11:AF:172:LYS:NZ	2.34	0.47
13:AH:98:VAL:O	13:AH:102:GLU:HG2	2.15	0.47
49:BI:57:THR:H	49:BI:64:GLY:HA3	1.80	0.47
54:BD:19:PRO:HB2	54:BD:21:VAL:HG12	1.97	0.47
59:BS:63:LEU:HD12	59:BS:70:GLN:HG2	1.96	0.47
1:1:953:G:N2	1:1:975:G:O2'	2.48	0.47
1:1:1253:G:H2'	1:1:1254:C:C6	2.50	0.47
1:1:2725:U:H2'	1:1:2726:G:O4'	2.14	0.47
2:2:394:4AC:H2'	2:2:395:G:C8	2.50	0.47
2:2:625:C:H2'	2:2:626:4AC:C6	2.43	0.47
2:2:717:C:H4'	21:AQ:47:THR:HG22	1.97	0.47
2:2:908:C:H1'	2:2:1356:C:H42	1.80	0.47
2:2:1210:A:H2'	2:2:1211:C:C6	2.50	0.47
4:A:109:HIS:ND1	4:A:121:HIS:O	2.40	0.47
5:H:250:LYS:NZ	5:H:251:VAL:O	2.47	0.47
7:AB:176:LEU:HD22	7:AB:181:GLU:HG3	1.97	0.47
13:AH:68:ILE:HG12	13:AH:104:VAL:HG21	1.96	0.47
16:AK:119:PRO:O	16:AK:120:ASN:HB2	2.15	0.47
26:AW:39:CYS:N	26:AW:44:ALA:O	2.48	0.47
27:AX:26:GLN:NE2	27:AX:65:ARG:O	2.39	0.47
30:A0:31:LYS:HE3	30:A0:31:LYS:HB2	1.73	0.47
34:BB:122:VAL:HG13	34:BB:127:THR:HG22	1.96	0.47
42:Bb:103:ALA:HB3	42:Bb:106:VAL:HG23	1.97	0.47
43:Be:56:LYS:HB3	43:Be:62:HIS:HB3	1.95	0.47
67:BA:50:LYS:HG2	67:BA:159:GLN:OE1	2.15	0.47
1:1:150:G:N3	1:1:604:G:O2'	2.49	0.46
1:1:809:A:N7	1:1:903:G:O2'	2.41	0.46
1:1:1481:G:N2	1:1:1484:A:OP2	2.40	0.46
1:1:1666:C:H2'	1:1:1667:4AC:H6	1.97	0.46
1:1:2504:A:H2'	1:1:2505:U:C6	2.49	0.46
2:2:483:G:H4'	2:2:485:C:N3	2.30	0.46
2:2:1134:G:C2	2:2:1135:C:C6	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:64:MET:CE	4:A:76:VAL:HG11	2.45	0.46
4:A:64:MET:HE3	4:A:76:VAL:HG11	1.96	0.46
17:AL:40:LEU:HB2	17:AL:70:LYS:HB2	1.96	0.46
23:AS:25:THR:HG22	23:AS:30:HIS:CD2	2.49	0.46
29:AZ:79:GLN:OE1	29:AZ:79:GLN:N	2.48	0.46
32:AT:84:HIS:CD2	32:AT:86:GLY:H	2.32	0.46
31:B4:34:LYS:HD2	31:B4:92:ILE:HD11	1.97	0.46
67:BA:87:SER:HA	67:BA:90:LEU:HD12	1.97	0.46
1:1:377:C:O2'	1:1:422:C:H5''	2.15	0.46
1:1:1307:C:OP1	1:1:2982:C:O2'	2.31	0.46
1:1:1847:C:H2'	1:1:1848:U:C6	2.49	0.46
1:1:3004:4AC:H2'	1:1:3005:G:O4'	2.15	0.46
2:2:385:G:H2'	2:2:386:C:C6	2.49	0.46
2:2:746:C:H2'	2:2:747:G:C8	2.49	0.46
2:2:1200:C:H5'	32:AT:113:VAL:CG1	2.45	0.46
16:AK:49:LEU:HD13	16:AK:86:LEU:HD11	1.97	0.46
29:AZ:20:PHE:O	29:AZ:24:GLU:HG2	2.15	0.46
29:AZ:87:ASN:HB2	29:AZ:90:LEU:HB2	1.97	0.46
32:AT:43:GLU:HB3	32:AT:67:CYS:SG	2.55	0.46
34:BB:41:LEU:HB2	34:BB:85:ILE:HG23	1.97	0.46
61:BN:99:MET:HG3	61:BN:101:THR:HG23	1.97	0.46
31:B4:90:ALA:O	31:B4:92:ILE:HG12	2.15	0.46
1:1:120:A:H5''	1:1:120:A:C8	2.49	0.46
1:1:727:G:N2	1:1:730:A:OP2	2.45	0.46
1:1:733:C:H2'	1:1:734:G:H8	1.81	0.46
1:1:1568:G:OP2	40:Bf:3:ARG:NH2	2.40	0.46
1:1:1997:A:OP1	51:BQ:71:LYS:NZ	2.48	0.46
1:1:2361:G:OP1	1:1:2410:G:N2	2.29	0.46
1:1:2623:G:H5''	1:1:2624:C:H5'	1.97	0.46
2:2:483:G:N1	2:2:499:A:OP2	2.37	0.46
2:2:1274:G:H1'	2:2:1277:C:N4	2.30	0.46
4:A:142:ASP:O	4:A:146:GLN:HG2	2.15	0.46
5:H:373:GLU:OE2	5:H:376:ARG:NH2	2.49	0.46
12:AG:113:SER:O	12:AG:116:ILE:HG12	2.16	0.46
15:AJ:34:ASN:HB3	15:AJ:94:ILE:HD13	1.96	0.46
31:B4:35:GLY:O	31:B4:39:THR:HB	2.15	0.46
1:1:429:A:H1'	1:1:431:G:N7	2.30	0.46
1:1:814:A:H2'	1:1:815:A:C8	2.50	0.46
1:1:894:A:H2'	1:1:895:A:H8	1.77	0.46
1:1:1211:A:H2'	1:1:1212:A:C8	2.50	0.46
1:1:1421:C:H2'	1:1:1422:A:H8	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2144:OMG:HM22	1:1:2145:G:H5'	1.97	0.46
1:1:2522:U:OP1	1:1:2614:G:O2'	2.34	0.46
2:2:1101:U:H2'	2:2:1102:C:C6	2.51	0.46
2:2:1389:C:H2'	2:2:1390:C:H6	1.80	0.46
10:AE:207:MET:HE1	22:AR:30:HIS:HA	1.98	0.46
44:BE:34:VAL:HG11	44:BE:41:LEU:HD23	1.98	0.46
50:BR:89:HIS:HD2	50:BR:91:VAL:H	1.63	0.46
56:BZ:36:ILE:HD12	56:BZ:83:LEU:HD11	1.97	0.46
1:1:29:U:H2'	1:1:30:G:H8	1.81	0.46
1:1:107:G:H21	1:1:112:A:H62	1.64	0.46
1:1:197:G:P	41:BU:118:ARG:HH22	2.38	0.46
1:1:349:G:N2	1:1:357:4AC:O2	2.37	0.46
1:1:789:OMG:HM22	1:1:790:G:H5'	1.98	0.46
1:1:1145:C:H2'	1:1:1146:C:H6	1.81	0.46
1:1:2888:G:OP2	64:BJ:3:LYS:NZ	2.39	0.46
2:2:427:G:H2'	2:2:428:C:C6	2.50	0.46
2:2:618:C:OP1	21:AQ:75:LYS:HG2	2.15	0.46
5:H:123:VAL:O	5:H:228:ARG:NH2	2.49	0.46
6:AA:109:ASN:HD21	6:AA:119:ARG:HE	1.64	0.46
21:AQ:57:GLN:NE2	26:AW:38:ARG:O	2.47	0.46
44:BE:43:LYS:HG2	44:BE:132:ILE:HG22	1.97	0.46
46:BT:4:TYR:CE1	47:BW:19:ARG:HD2	2.50	0.46
54:BD:138:PRO:HA	25:B6:13:LEU:HD21	1.97	0.46
59:BS:14:PRO:O	59:BS:105:LYS:HD3	2.15	0.46
1:1:2380:G:C6	1:1:2392:G:C6	3.04	0.46
1:1:2408:G:N7	1:1:2410:G:C8	2.82	0.46
2:2:255:A:C2	2:2:291:A:C5	3.04	0.46
2:2:1344:G:C2	2:2:1345:G:C8	3.04	0.46
2:2:1503:A:H2'	2:2:1504:C:C6	2.50	0.46
5:H:39:LEU:HD21	5:H:101:PRO:HB3	1.98	0.46
11:AF:20:THR:O	11:AF:24:MET:HG2	2.16	0.46
12:AG:76:PRO:C	12:AG:110:ASN:HD21	2.24	0.46
29:AZ:87:ASN:OD1	29:AZ:87:ASN:N	2.47	0.46
38:B5:23:VAL:HG21	38:B5:71:VAL:HG21	1.97	0.46
41:BU:96:HIS:HD2	41:BU:98:SER:H	1.62	0.46
1:1:51:A:H5''	1:1:52:G:OP2	2.16	0.46
1:1:120:A:C8	1:1:120:A:C5'	2.98	0.46
1:1:134:C:H2'	1:1:135:C:C6	2.51	0.46
1:1:659:A:H5''	1:1:660:G:H3'	1.97	0.46
2:2:148:A:C4	2:2:149:A:C8	3.03	0.46
6:AA:102:THR:HG21	6:AA:130:ILE:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AC:35:CYS:HB3	8:AC:58:CYS:HB3	1.97	0.46
11:AF:3:GLN:HA	11:AF:6:LYS:HE3	1.98	0.46
17:AL:64:TRP:HB3	20:AP:52:PHE:HB3	1.97	0.46
37:BC:159:GLU:OE2	37:BC:161:ARG:NE	2.37	0.46
2:2:972:G:H4'	2:2:973:A:OP1	2.16	0.46
2:2:1343:C:H2'	2:2:1344:G:C8	2.50	0.46
2:2:1362:C:H2'	2:2:1363:C:C6	2.51	0.46
5:H:23:LEU:HD12	5:H:64:PRO:HA	1.98	0.46
5:H:382:LYS:HB2	18:AM:52:ARG:HB2	1.98	0.46
10:AE:57:LYS:HE3	10:AE:57:LYS:HB3	1.64	0.46
13:AH:38:ASN:H	13:AH:63:ILE:HG23	1.81	0.46
21:AQ:94:ASP:OD1	21:AQ:95:LEU:N	2.48	0.46
44:BE:43:LYS:HA	44:BE:132:ILE:HG22	1.98	0.46
1:1:889:U:H2'	1:1:890:G:H8	1.79	0.46
1:1:946:G:H2'	1:1:947:C:C6	2.51	0.46
1:1:1998:A:H2'	1:1:1999:C:H6	1.78	0.46
8:AC:29:HIS:HA	8:AC:40:ILE:O	2.16	0.46
29:AZ:61:ARG:N	29:AZ:64:GLU:OE1	2.48	0.46
31:B4:18:LYS:HG2	31:B4:110:LEU:HD11	1.98	0.46
1:1:42:U:H4'	1:1:43:A:H5'	1.97	0.46
1:1:163:A:H5''	1:1:165:G:O4'	2.15	0.46
1:1:705:A:H2'	1:1:706:G:H8	1.79	0.46
1:1:796:C:H2'	1:1:797:G:C8	2.51	0.46
2:2:1236:C:H2'	2:2:1237:C:H6	1.81	0.46
6:AA:53:LEU:HD13	6:AA:62:LYS:HB3	1.98	0.46
6:AA:114:ASP:HB2	6:AA:155:PHE:H	1.81	0.46
10:AE:57:LYS:HD2	10:AE:58:THR:HB	1.98	0.46
13:AH:206:GLU:HG2	13:AH:207:ILE:HD12	1.98	0.46
29:AZ:77:ASN:N	29:AZ:78:PRO:HD3	2.31	0.46
55:BF:125:LEU:HD12	55:BF:146:ALA:HA	1.98	0.46
1:1:117:G:C6	1:1:118:U:C5	3.04	0.45
1:1:1296:G:N3	61:BN:178:SER:HB3	2.31	0.45
1:1:1392:G:OP1	49:BI:52:ARG:NH2	2.49	0.45
1:1:2058:A:H2'	1:1:2059:G:H8	1.81	0.45
1:1:2524:G:H2'	1:1:2525:G:C8	2.52	0.45
1:1:2604:G:H2'	1:1:2605:C:C6	2.51	0.45
2:2:398:A:H3'	2:2:399:C:C6	2.51	0.45
2:2:416:C:H5''	9:AD:119:ARG:HG3	1.98	0.45
2:2:641:G:OP1	6:AA:119:ARG:NH1	2.49	0.45
2:2:729:G:H2'	2:2:730:C:C6	2.51	0.45
4:A:166:VAL:HG22	4:A:232:GLU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:5:GLN:HE21	5:H:7:GLN:HG2	1.80	0.45
5:H:16:LYS:HD2	5:H:41:PHE:CZ	2.51	0.45
9:AD:54:ARG:O	9:AD:58:LEU:HG	2.17	0.45
33:AO:119:ARG:HG2	33:AO:126:VAL:HG12	1.98	0.45
39:BL:107:GLN:OE1	39:BL:107:GLN:N	2.46	0.45
61:BN:21:GLU:OE1	61:BN:21:GLU:N	2.35	0.45
1:1:1598:G:H5''	46:BT:13:THR:HG22	1.98	0.45
1:1:1681:C:OP2	38:B5:42:LYS:NZ	2.30	0.45
1:1:1775:A:C2	56:BZ:81:ALA:HB2	2.51	0.45
1:1:2081:G:OP1	34:BB:202:HIS:HE1	2.00	0.45
2:2:94:G:H2'	2:2:95:C:H6	1.81	0.45
2:2:946:G:OP2	20:AP:29:PRO:HG3	2.16	0.45
2:2:1482:A:H2'	2:2:1483:G:C8	2.51	0.45
3:3:71:U:H2'	3:3:72:C:C6	2.51	0.45
5:H:239:ILE:HG13	5:H:241:GLY:H	1.80	0.45
10:AE:131:ARG:NE	10:AE:141:ASN:HD21	2.14	0.45
18:AM:13:LYS:HB2	18:AM:76:ILE:HD12	1.97	0.45
19:AN:43:PRO:O	19:AN:80:ASN:ND2	2.50	0.45
38:B5:54:GLU:OE1	56:BZ:52:TYR:OH	2.28	0.45
1:1:877:U:H2'	1:1:878:G:O4'	2.16	0.45
1:1:1303:A:N9	1:1:1304:C:C5	2.84	0.45
2:2:531:U:OP2	19:AN:5:LYS:NZ	2.49	0.45
2:2:1346:C:H2'	2:2:1347:G:O4'	2.16	0.45
5:H:46:TYR:OH	5:H:76:ALA:O	2.30	0.45
5:H:208:MET:HE1	5:H:213:ALA:HB3	1.97	0.45
13:AH:115:THR:HG23	13:AH:117:LYS:HB2	1.98	0.45
27:AX:36:ASP:OD2	27:AX:60:THR:OG1	2.30	0.45
36:BO:52:ASP:HB3	36:BO:55:GLY:O	2.16	0.45
54:BD:19:PRO:HG3	54:BD:251:LYS:HE2	1.98	0.45
59:BS:116:HIS:HB3	59:BS:149:VAL:HB	1.99	0.45
1:1:254:C:H2'	1:1:255:C:C6	2.51	0.45
1:1:1177:G:H2'	1:1:1178:C:H6	1.81	0.45
1:1:1733:A:C2	1:1:1734:G:H1'	2.51	0.45
1:1:1806:G:H2'	1:1:1807:U:H5''	1.98	0.45
1:1:2607:C:H2'	1:1:2608:4AC:O2	2.16	0.45
2:2:29:C:H2'	2:2:30:C:C6	2.51	0.45
2:2:353:A:H3'	2:2:354:C:H6	1.82	0.45
2:2:566:C:H2'	2:2:567:C:H6	1.81	0.45
2:2:1150:A:H3'	2:2:1151:G:C8	2.51	0.45
5:H:5:GLN:HG3	5:H:7:GLN:HG3	1.99	0.45
5:H:23:LEU:HB2	5:H:64:PRO:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:11:LYS:HE3	6:AA:11:LYS:H	1.81	0.45
7:AB:43:LEU:HD23	7:AB:44:ASP:N	2.31	0.45
10:AE:88:MET:HE3	10:AE:88:MET:HB3	1.66	0.45
32:AT:15:GLN:O	32:AT:19:MET:HG3	2.16	0.45
50:BR:43:ILE:HD11	50:BR:77:VAL:HG11	1.99	0.45
1:1:113:G:H2'	1:1:114:G:H8	1.80	0.45
1:1:2599:G:H2'	1:1:2600:U:C6	2.52	0.45
2:2:225:C:H2'	2:2:226:U:C6	2.44	0.45
2:2:1085:C:H2'	2:2:1086:C:H6	1.81	0.45
5:H:269:GLU:OE1	5:H:269:GLU:N	2.50	0.45
7:AB:111:GLU:OE2	11:AF:43:GLN:NE2	2.43	0.45
14:AI:55:ASP:HB3	26:AW:8:ILE:HG13	1.99	0.45
24:AU:146:GLU:OE1	24:AU:146:GLU:N	2.47	0.45
25:AV:7:GLU:OE1	25:AV:20:TYR:HB2	2.17	0.45
55:BF:139:VAL:HG12	55:BF:147:VAL:HG13	1.98	0.45
1:1:144:G:H2'	1:1:145:G:C8	2.52	0.45
1:1:310:U:H2'	1:1:311:A:H8	1.82	0.45
1:1:540:U:O2'	1:1:542:G:N7	2.40	0.45
1:1:552:G:OP2	58:BM:68:ARG:NH2	2.42	0.45
1:1:2265:U:H2'	1:1:2266:G:C8	2.50	0.45
1:1:2304:C:H2'	1:1:2305:C:H6	1.81	0.45
2:2:24:U:H2'	2:2:25:C:H6	1.80	0.45
2:2:1123:C:C2	2:2:1124:U:C5	3.05	0.45
4:A:141:LYS:HD2	4:A:141:LYS:HA	1.68	0.45
10:AE:45:LEU:N	10:AE:83:PHE:O	2.49	0.45
13:AH:70:LYS:HG3	13:AH:162:LEU:HB3	1.99	0.45
17:AL:62:ASP:OD2	20:AP:44:ARG:NH1	2.45	0.45
24:AU:40:HIS:HA	24:AU:81:LYS:HB2	1.98	0.45
27:AX:42:ARG:NH1	27:AX:66:GLU:HA	2.31	0.45
32:AT:95:LYS:HG2	32:AT:96:PRO:HD2	1.98	0.45
37:BC:194:ASN:O	37:BC:198:GLU:HG2	2.16	0.45
61:BN:30:LYS:H	61:BN:59:GLN:NE2	2.14	0.45
1:1:431:G:H2'	1:1:432:A:C8	2.52	0.45
1:1:2046:C:H2'	1:1:2047:A:C8	2.52	0.45
1:1:2197:G:H3'	1:1:2198:5MC:HM53	1.99	0.45
2:2:815:G:H2'	2:2:816:C:H6	1.81	0.45
2:2:1020:A:C2	2:2:1180:G:C4	3.05	0.45
2:2:1132:C:O2'	23:AS:52:GLY:HA3	2.17	0.45
2:2:1482:A:H2'	2:2:1483:G:H8	1.82	0.45
3:3:70:A:H2'	3:3:71:U:O4'	2.17	0.45
13:AH:28:VAL:HG21	13:AH:37:ILE:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:AT:98:MET:HG2	33:AO:112:ILE:HG13	1.97	0.45
54:BD:21:VAL:HG23	54:BD:115:MET:HG2	1.97	0.45
1:1:727:G:N7	38:BK:17:ARG:NH2	2.64	0.45
1:1:1161:A:H2'	1:1:1164:C:C5	2.51	0.45
1:1:2477:G:H2'	1:1:2478:C:C6	2.50	0.45
1:1:2931:U:H2'	1:1:2932:C:C6	2.52	0.45
2:2:168:A:H2'	2:2:169:A:C8	2.51	0.45
2:2:1052:C:H2'	2:2:1053:A:H8	1.82	0.45
4:A:143:ALA:O	4:A:147:VAL:HG23	2.17	0.45
7:AB:61:ARG:NH2	8:AC:32:CYS:O	2.50	0.45
15:AJ:101:ILE:O	15:AJ:108:ALA:N	2.44	0.45
16:AK:49:LEU:HD22	16:AK:82:ILE:HD12	1.99	0.45
17:AL:26:ILE:HD12	17:AL:88:ILE:HD12	1.98	0.45
25:AV:25:HIS:ND1	25:AV:25:HIS:O	2.50	0.45
35:BY:91:MET:HE1	35:BY:99:LYS:HD2	1.99	0.45
1:1:1471:A:H5''	42:Bb:105:THR:HG22	1.99	0.45
2:2:142:G:N1	2:2:174:C:N3	2.37	0.45
2:2:1083:C:H2'	2:2:1084:C:H6	1.82	0.45
4:A:24:VAL:HG11	4:A:29:ALA:HB2	1.99	0.45
5:H:50:LEU:HD22	5:H:54:LEU:HB3	1.98	0.45
6:AA:117:LYS:HD2	6:AA:193:GLY:HA3	1.97	0.45
7:AB:82:LYS:O	7:AB:86:VAL:HG12	2.17	0.45
17:AL:95:THR:HG21	29:AZ:6:TYR:CE2	2.51	0.45
20:AP:36:LEU:HD22	20:AP:38:LEU:HD12	1.99	0.45
26:AW:53:LYS:HE3	26:AW:53:LYS:HB2	1.82	0.45
29:AZ:25:LEU:HB2	29:AZ:30:TYR:HB2	1.98	0.45
31:A3:49:LYS:HD3	31:A3:103:GLU:H	1.81	0.45
49:BI:72:ASP:OD1	49:BI:72:ASP:N	2.47	0.45
1:1:133:G:H2'	1:1:134:C:H6	1.81	0.45
1:1:2360:G:H2'	1:1:2361:G:C8	2.52	0.45
1:1:2372:C:H3'	1:1:2373:G:H5'	1.99	0.45
2:2:609:A:H2'	2:2:610:C:C6	2.52	0.45
2:2:975:G:N7	31:A3:37:ASN:HB3	2.32	0.45
6:AA:11:LYS:H	6:AA:11:LYS:CE	2.30	0.45
6:AA:16:LEU:HD23	6:AA:16:LEU:HA	1.86	0.45
17:AL:21:ASN:O	17:AL:25:GLN:HG2	2.17	0.45
44:BE:32:ILE:HD11	44:BE:78:VAL:HB	1.99	0.45
44:BE:93:ARG:HB3	44:BE:124:PRO:HD2	1.99	0.45
45:Ba:4:LYS:HE2	45:Ba:4:LYS:HB3	1.87	0.45
45:Ba:21:ILE:HG13	45:Ba:22:VAL:HG13	1.99	0.45
1:1:1933:C:H2'	1:1:1934:4AC:H6	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2102:G:H2'	1:1:2103:U:O4'	2.17	0.44
1:1:2153:A:O2'	2:2:1463:G:O2'	2.34	0.44
1:1:2405:C:OP1	67:BA:102:LYS:NZ	2.38	0.44
1:1:2596:C:H2'	1:1:2597:G:C8	2.51	0.44
2:2:82:C:H2'	2:2:83:C:C5	2.52	0.44
2:2:203:A:H2'	2:2:204:G:C8	2.52	0.44
2:2:966:C:H2'	2:2:967:G:H8	1.82	0.44
2:2:1095:A:H2'	2:2:1096:G:H8	1.80	0.44
2:2:1288:C:OP2	32:AT:34:ARG:NH1	2.48	0.44
2:2:1378:C:H2'	2:2:1379:G:C8	2.52	0.44
6:AA:57:THR:HG22	6:AA:58:GLY:H	1.81	0.44
6:AA:121:MET:N	6:AA:121:MET:SD	2.90	0.44
13:AH:3:LYS:H	13:AH:3:LYS:HD2	1.83	0.44
41:BU:37:GLU:H	41:BU:37:GLU:HG3	1.67	0.44
44:BE:32:ILE:HG12	44:BE:78:VAL:O	2.16	0.44
1:1:192:C:OP1	47:BW:7:ARG:NH2	2.50	0.44
1:1:857:C:OP2	1:1:878:G:N1	2.30	0.44
1:1:2310:G:H2'	1:1:2311:A:C8	2.52	0.44
1:1:2346:G:C2	1:1:2347:G:C8	3.05	0.44
1:1:2650:G:H2'	1:1:2651:C:C6	2.51	0.44
1:1:2990:G:H21	55:BF:149:GLN:NE2	2.15	0.44
2:2:711:A:H4'	2:2:823:G:O2'	2.17	0.44
2:2:1112:A:H2'	2:2:1113:G:H8	1.82	0.44
4:A:41:GLU:HA	4:A:74:TYR:HE2	1.83	0.44
5:H:323:GLU:H	5:H:323:GLU:HG2	1.62	0.44
12:AG:96:PRO:O	12:AG:97:LYS:HG2	2.17	0.44
26:AW:5:ARG:NH2	26:AW:6:ASN:HB3	2.32	0.44
34:BB:202:HIS:CD2	34:BB:204:PHE:H	2.33	0.44
49:BI:29:VAL:HG22	49:BI:98:LYS:HB2	1.99	0.44
1:1:68:U:H4'	1:1:69:U:O5'	2.17	0.44
1:1:1306:G:N1	1:1:1307:C:C2	2.85	0.44
1:1:1710:C:H2'	1:1:1711:G:C8	2.51	0.44
1:1:1878:4AC:O7	1:1:1878:4AC:H5	2.16	0.44
1:1:2392:G:C4	1:1:2393:G:C8	3.06	0.44
1:1:2471:A:H2'	1:1:2472:G:C8	2.52	0.44
1:1:2610:A:H4'	36:BO:134:SER:HB2	2.00	0.44
1:1:2706:C:N4	62:Bg:47:ARG:O	2.49	0.44
2:2:1112:A:H2'	2:2:1113:G:C8	2.52	0.44
2:2:1360:C:H2'	2:2:1361:U:H6	1.82	0.44
2:2:1409:G:H2'	2:2:1410:C:C6	2.53	0.44
3:3:57:A:O2'	44:BE:164:HIS:HD2	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:52:GLN:H	5:H:52:GLN:CD	2.25	0.44
7:AB:197:MET:HE3	7:AB:197:MET:HB2	1.87	0.44
10:AE:43:ILE:HB	10:AE:110:LEU:HD12	2.00	0.44
10:AE:203:LYS:O	10:AE:211:ASP:HB2	2.18	0.44
13:AH:80:LYS:HG3	13:AH:85:PHE:CE1	2.51	0.44
13:AH:135:ASP:O	13:AH:150:VAL:N	2.46	0.44
41:BU:106:ASN:O	41:BU:112:ARG:NH1	2.43	0.44
1:1:960:C:H2'	1:1:961:U:H6	1.82	0.44
1:1:1111:G:O2'	1:1:1168:G:O6	2.33	0.44
1:1:1606:G:O2'	1:1:1640:A:N3	2.45	0.44
1:1:1806:G:O2'	1:1:1808:U:OP1	2.22	0.44
1:1:2372:C:H4'	1:1:2373:G:OP2	2.17	0.44
1:1:2391:C:H2'	1:1:2392:G:H8	1.82	0.44
1:1:2916:C:H4'	52:BV:18:THR:HG22	1.99	0.44
2:2:148:A:C5	2:2:149:A:C8	3.06	0.44
2:2:593:G:H5'	10:AE:107:ILE:HD13	1.99	0.44
2:2:646:C:H2'	2:2:647:C:H6	1.83	0.44
55:BF:32:LYS:NZ	55:BF:83:THR:O	2.50	0.44
67:BA:103:LEU:HD12	67:BA:107:TYR:CE2	2.52	0.44
1:1:120:A:C5'	1:1:120:A:H8	2.31	0.44
1:1:1171:C:H2'	1:1:1172:C:C6	2.53	0.44
1:1:2390:U:H2'	1:1:2391:C:C6	2.53	0.44
1:1:2705:C:C2	1:1:2706:C:O2	2.70	0.44
2:2:579:C:H2'	2:2:580:A:C8	2.53	0.44
2:2:805:C:OP1	26:AW:53:LYS:N	2.45	0.44
2:2:1076:A:N6	29:AZ:155:GLY:HA3	2.31	0.44
2:2:1104:C:O2'	24:AU:2:ALA:N	2.51	0.44
3:3:45:A:O3'	44:BE:152:ARG:NH2	2.49	0.44
3:3:85:C:H2'	3:3:86:C:C6	2.53	0.44
6:AA:86:MET:HG3	6:AA:189:ILE:H	1.83	0.44
11:AF:131:TRP:NE1	14:AI:97:PHE:HA	2.33	0.44
31:A3:56:ASP:OD2	31:A3:83:LYS:HB2	2.17	0.44
36:BO:48:ILE:HG21	36:BO:99:ILE:HD13	2.00	0.44
55:BF:91:LYS:HD3	62:Bg:6:GLU:HG2	1.99	0.44
1:1:30:G:H21	45:Ba:42:HIS:HE1	1.65	0.44
1:1:651:G:O6	59:BS:2:GLY:N	2.51	0.44
1:1:1266:G:H21	65:Bl:43:SER:HB2	1.81	0.44
1:1:2370:G:N2	1:1:2374:A:N1	2.58	0.44
1:1:2870:G:O2'	1:1:3005:G:N2	2.29	0.44
2:2:98:C:H2'	2:2:99:C:H6	1.83	0.44
2:2:509:C:H2'	2:2:510:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1196:G:OP1	32:AT:109:THR:HG21	2.18	0.44
2:2:1505:5MC:H2'	2:2:1506:U:C6	2.52	0.44
4:A:72:ASP:O	4:A:76:VAL:HG23	2.18	0.44
25:AV:92:ILE:HG22	25:AV:93:ILE:HG23	1.99	0.44
1:1:775:U:O2'	1:1:1234:A:N1	2.45	0.44
1:1:2055:G:N7	34:BB:145:SER:OG	2.48	0.44
1:1:2394:G:C6	1:1:2395:U:C4	3.05	0.44
1:1:2719:G:H2'	1:1:2720:A:C8	2.52	0.44
1:1:2792:C:H2'	1:1:2793:A:C8	2.53	0.44
2:2:27:U:H2'	2:2:28:G:O4'	2.18	0.44
2:2:484:G:C5'	2:2:496:G:H4'	2.46	0.44
2:2:836:A:H5'	2:2:1043:U:H5	1.80	0.44
2:2:879:A:H2'	2:2:880:A:C8	2.53	0.44
2:2:1261:A:H2'	2:2:1262:A:C8	2.52	0.44
2:2:1398:G:H2'	2:2:1399:C:H6	1.82	0.44
5:H:131:LYS:HE3	5:H:131:LYS:HB3	1.49	0.44
6:AA:153:LEU:HG	6:AA:157:ASP:HB3	1.98	0.44
13:AH:111:ILE:O	13:AH:115:THR:HG22	2.18	0.44
31:A3:20:LEU:HD23	31:A3:20:LEU:HA	1.82	0.44
38:B5:49:ASN:OD1	38:B5:50:ILE:N	2.50	0.44
44:BE:137:MET:HE2	44:BE:137:MET:HB2	1.93	0.44
25:B6:4:LYS:HE2	25:B6:4:LYS:HB3	1.75	0.44
31:B4:50:LEU:HD11	31:B4:114:ILE:HD11	1.99	0.44
67:BA:32:GLU:HA	67:BA:169:PRO:HA	2.00	0.44
1:1:1617:4AC:H2'	1:1:1618:G:H8	1.83	0.44
2:2:200:C:H2'	2:2:201:C:H6	1.81	0.44
2:2:393:C:H2'	2:2:394:4AC:H6	2.00	0.44
2:2:1125:G:O4'	17:AL:39:PRO:HB2	2.18	0.44
2:2:1281:U:H2'	2:2:1282:C:C6	2.53	0.44
2:2:1427:G:O2'	12:AG:77:ASP:OD2	2.30	0.44
4:A:20:PHE:HB3	4:A:49:VAL:HG11	1.99	0.44
5:H:330:LEU:HB2	5:H:351:TRP:CZ3	2.53	0.44
25:AV:39:LYS:HE2	25:AV:39:LYS:HB3	1.85	0.44
29:AZ:100:ALA:O	29:AZ:104:GLU:HG2	2.17	0.44
31:A3:13:LYS:O	31:A3:17:GLU:HG2	2.18	0.44
32:AT:61:LYS:HB2	32:AT:62:PRO:HD2	1.98	0.44
35:BY:3:LYS:HA	35:BY:3:LYS:HD3	1.82	0.44
37:BC:284:ILE:HD11	37:BC:321:ALA:HB2	1.99	0.44
51:BQ:24:ILE:HG23	51:BQ:32:VAL:HG21	2.00	0.44
64:BJ:106:ILE:HG22	64:BJ:114:ARG:HD3	2.00	0.44
1:1:95:G:C6	1:1:125:A:C2	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:102:C:OP2	1:1:102:C:C6	2.71	0.44
1:1:112:A:H3'	1:1:113:G:H8	1.83	0.44
1:1:198:A:C2	1:1:216:A:C5	3.05	0.44
1:1:1306:G:O2'	1:1:1307:C:P	2.75	0.44
1:1:1729:G:N1	1:1:1732:G:OP2	2.51	0.44
1:1:2287:4AC:H2'	1:1:2288:G:H8	1.82	0.44
1:1:2799:G:H2'	1:1:2800:G:C8	2.52	0.44
2:2:269:G:H5'	15:AJ:32:PRO:HA	1.98	0.44
2:2:455:C:O2'	25:AV:29:PRO:HD3	2.17	0.44
2:2:511:4AC:H2'	2:2:512:G:O4'	2.18	0.44
2:2:662:A:H2'	2:2:663:A:H8	1.83	0.44
2:2:1217:G:H2'	2:2:1218:C:C6	2.53	0.44
5:H:262:LEU:HB3	5:H:263:PRO:HD3	1.99	0.44
13:AH:23:THR:O	13:AH:23:THR:OG1	2.36	0.44
51:BQ:142:LEU:HD13	51:BQ:148:LEU:HD21	1.99	0.44
64:BJ:116:THR:C	64:BJ:136:ILE:HD11	2.43	0.44
1:1:77:C:H4'	37:BC:311:GLY:HA2	2.00	0.43
1:1:447:A:O2'	1:1:448:A:O4'	2.35	0.43
1:1:1549:C:H2'	1:1:1550:4AC:H6	1.99	0.43
1:1:2517:U:H4'	1:1:2518:A:O4'	2.18	0.43
1:1:2881:G:H2'	1:1:2882:C:C6	2.53	0.43
2:2:465:G:H2'	2:2:466:G:H8	1.81	0.43
2:2:724:U:OP1	2:2:789:C:O2'	2.35	0.43
2:2:1271:U:H1'	2:2:1272:C:H5	1.83	0.43
2:2:1329:G:H2'	2:2:1330:C:H6	1.82	0.43
4:A:112:ALA:HB2	4:A:162:ILE:HG22	1.99	0.43
7:AB:73:ARG:O	7:AB:77:GLN:HG3	2.18	0.43
14:AI:80:PRO:HD3	14:AI:124:ARG:NH1	2.33	0.43
29:AZ:69:LEU:HA	29:AZ:73:PHE:HD2	1.82	0.43
52:BV:23:VAL:HG11	64:BJ:141:VAL:HG21	2.00	0.43
55:BF:11:ILE:HB	55:BF:53:VAL:HG13	1.99	0.43
56:BZ:55:LEU:HD23	56:BZ:55:LEU:HA	1.86	0.43
57:BP:10:ASN:HD22	57:BP:13:ARG:HH12	1.66	0.43
1:1:99:U:O4	1:1:120:A:N1	2.51	0.43
1:1:618:U:O2'	43:Be:17:HIS:HD2	2.01	0.43
1:1:1739:G:O2'	1:1:1816:U:O2'	2.17	0.43
1:1:2058:A:H2'	1:1:2059:G:C8	2.53	0.43
1:1:2599:G:H2'	1:1:2600:U:H6	1.83	0.43
2:2:191:U:H2'	2:2:192:G:O4'	2.18	0.43
2:2:453:C:C2	2:2:454:U:C5	3.06	0.43
2:2:1131:A:C2	2:2:1155:G:C4	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1237:C:OP1	24:AU:119:ARG:NH1	2.50	0.43
2:2:1287:G:H2'	2:2:1288:C:C6	2.52	0.43
3:3:28:C:H2'	3:3:29:A:O4'	2.18	0.43
4:A:138:ASP:HB3	4:A:146:GLN:HE22	1.83	0.43
5:H:242:LEU:HD21	5:H:255:LEU:HD12	2.00	0.43
7:AB:166:LEU:O	7:AB:170:ILE:HG22	2.18	0.43
15:AJ:63:ALA:HB2	15:AJ:77:ILE:HD11	2.01	0.43
16:AK:47:GLU:HB3	16:AK:48:PRO:HD3	2.00	0.43
26:AW:19:LYS:HE2	26:AW:19:LYS:HB2	1.88	0.43
32:AT:4:LYS:HD3	32:AT:5:GLU:H	1.83	0.43
38:B5:38:ALA:HB1	38:B5:72:LYS:HB2	2.00	0.43
46:BT:11:VAL:HB	46:BT:27:THR:HG23	2.00	0.43
31:BG:118:VAL:HA	31:BG:121:LEU:HD23	2.00	0.43
64:BJ:9:THR:HG21	64:BJ:111:GLY:HA3	2.00	0.43
1:1:45:G:H2'	1:1:46:C:C6	2.53	0.43
1:1:84:A:OP1	45:Ba:2:PRO:HD2	2.18	0.43
1:1:772:U:O2'	39:BL:22:LYS:NZ	2.39	0.43
1:1:992:C:H3'	1:1:993:U:H4'	2.00	0.43
1:1:993:U:OP2	1:1:1951:C:O2'	2.34	0.43
1:1:1480:C:H5'	42:Bb:76:PRO:HD3	2.00	0.43
1:1:1734:G:H2'	1:1:1735:G:C8	2.52	0.43
1:1:1806:G:H1'	1:1:1809:A:C8	2.54	0.43
1:1:2044:C:H5'	34:BB:196:LYS:HE2	2.00	0.43
1:1:2498:A:N3	1:1:2498:A:H2'	2.34	0.43
2:2:1052:C:H2'	2:2:1053:A:C8	2.53	0.43
4:A:125:ARG:HE	4:A:158:LEU:HD13	1.82	0.43
6:AA:155:PHE:O	6:AA:159:VAL:HG12	2.18	0.43
11:AF:131:TRP:CD1	14:AI:97:PHE:HA	2.52	0.43
21:AQ:25:TRP:CD2	26:AW:64:LEU:HD23	2.53	0.43
24:AU:2:ALA:HB3	24:AU:134:THR:HG22	2.01	0.43
38:B5:4:ILE:HG22	38:B5:4:ILE:O	2.17	0.43
43:Be:48:LYS:HE2	43:Be:55:TRP:CE3	2.54	0.43
44:BE:48:LEU:HD21	44:BE:80:VAL:HG23	1.99	0.43
55:BF:41:TRP:CG	55:BF:67:ILE:HG21	2.52	0.43
1:1:295:A:H2'	1:1:296:U:C6	2.53	0.43
1:1:465:A:C4	1:1:467:G:C8	3.07	0.43
1:1:614:A:H2'	1:1:615:OMC:O4'	2.18	0.43
1:1:671:G:H2'	1:1:672:G:C8	2.53	0.43
1:1:1207:G:OP1	61:BN:15:PRO:HG3	2.17	0.43
1:1:1660:C:O2'	46:BT:23:GLU:OE1	2.36	0.43
1:1:2686:G:C4	1:1:2687:A:C8	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:504:G:H2'	2:2:505:G:H8	1.84	0.43
2:2:836:A:H2'	2:2:837:G:C8	2.54	0.43
2:2:854:C:O2'	2:2:855:U:H5'	2.18	0.43
5:H:163:ARG:CZ	5:H:241:GLY:HA3	2.49	0.43
5:H:209:LYS:HD3	5:H:209:LYS:HA	1.83	0.43
5:H:260:LEU:O	5:H:263:PRO:HD2	2.18	0.43
6:AA:123:MET:HB2	6:AA:187:ARG:HG3	2.01	0.43
10:AE:181:LYS:HG2	10:AE:200:VAL:O	2.19	0.43
21:AQ:25:TRP:CG	26:AW:64:LEU:HD23	2.54	0.43
26:AW:27:GLN:HE22	26:AW:40:ASN:H	1.67	0.43
32:AT:73:LEU:O	32:AT:76:MET:HG2	2.18	0.43
32:AT:125:SER:HB3	32:AT:128:PHE:O	2.17	0.43
31:B4:27:ARG:HH11	31:B4:91:GLY:N	2.17	0.43
67:BA:23:LYS:HG2	67:BA:24:PRO:HD2	2.00	0.43
67:BA:108:ASP:OD1	67:BA:108:ASP:N	2.52	0.43
1:1:750:G:H2'	1:1:751:G:C8	2.53	0.43
1:1:939:G:H2'	1:1:940:C:C6	2.53	0.43
1:1:1298:C:H2'	1:1:1299:U:C6	2.54	0.43
1:1:2169:A:H2'	1:1:2170:G:O4'	2.19	0.43
1:1:2970:A:H2'	1:1:2971:A:C8	2.53	0.43
2:2:77:G:H2'	2:2:78:G:H8	1.84	0.43
2:2:264:G:H2'	2:2:265:U:C6	2.53	0.43
2:2:716:U:H5'	21:AQ:55:ARG:HD3	1.99	0.43
4:A:110:ARG:O	4:A:207:PRO:HB2	2.18	0.43
5:H:136:MET:HE1	5:H:253:GLY:HA3	2.00	0.43
7:AB:87:THR:HG23	7:AB:89:ALA:H	1.84	0.43
14:AI:102:LEU:HB2	14:AI:113:HIS:HB3	2.01	0.43
16:AK:80:ILE:HD12	16:AK:106:MET:HA	2.00	0.43
21:AQ:15:LYS:HB2	21:AQ:15:LYS:HE3	1.81	0.43
23:AS:31:ASN:ND2	23:AS:55:THR:OG1	2.52	0.43
54:BD:27:ARG:NH1	54:BD:30:LEU:HD13	2.34	0.43
61:BN:4:ARG:NH2	61:BN:9:ASP:OD1	2.51	0.43
1:1:99:U:H3	1:1:120:A:H2	1.66	0.43
1:1:107:G:C8	1:1:107:G:O5'	2.71	0.43
1:1:1366:A:C8	1:1:1367:G:H4'	2.53	0.43
1:1:1706:G:H2'	1:1:1707:C:C6	2.54	0.43
1:1:2697:G:H2'	1:1:2698:G:H8	1.84	0.43
2:2:128:C:H2'	2:2:129:OMC:C6	2.53	0.43
2:2:453:C:H2'	2:2:454:U:C6	2.54	0.43
2:2:645:C:H2'	2:2:646:C:C6	2.53	0.43
2:2:653:U:O4	2:2:670:A:H1'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:773:OMC:HM22	2:2:774:OMU:O4'	2.18	0.43
2:2:934:OMG:HM22	2:2:935:G:H5'	2.01	0.43
2:2:1291:C:H2'	2:2:1292:A:C8	2.54	0.43
6:AA:23:TYR:HB2	6:AA:80:TYR:HD1	1.83	0.43
10:AE:126:ARG:HG2	10:AE:143:HIS:HB3	2.01	0.43
11:AF:218:ILE:HG23	11:AF:223:ILE:HB	2.01	0.43
25:AV:37:LYS:HB2	25:AV:53:ILE:HD11	2.01	0.43
25:B6:9:LYS:HB3	25:B6:18:GLU:HB2	2.00	0.43
57:BP:15:ILE:HD13	57:BP:38:GLU:HG3	2.00	0.43
58:BM:126:LYS:HG2	58:BM:128:PHE:CE2	2.54	0.43
1:1:114:G:N3	1:1:115:G:C8	2.86	0.43
1:1:203:C:OP2	1:1:204:A:O2'	2.31	0.43
1:1:272:G:C4	1:1:273:C:C5	3.06	0.43
1:1:636:C:H1'	1:1:651:G:N2	2.34	0.43
1:1:1760:A:N1	1:1:1773:C:O2'	2.49	0.43
1:1:2153:A:HO2'	2:2:1463:G:HO2'	1.65	0.43
1:1:2910:C:H4'	37:BC:11:SER:HB2	1.99	0.43
2:2:502:C:C2	2:2:503:C:C5	3.07	0.43
2:2:678:G:H2'	2:2:679:G:C8	2.53	0.43
2:2:919:G:H2'	2:2:920:C:C6	2.54	0.43
2:2:1167:G:OP2	29:AZ:131:ARG:NH2	2.52	0.43
2:2:1262:A:N3	2:2:1326:C:O2'	2.45	0.43
4:A:89:THR:HG22	4:A:91:GLN:HG2	2.00	0.43
5:H:168:ASP:OD1	5:H:172:LYS:N	2.52	0.43
32:AT:68:ARG:HB3	32:AT:104:GLY:HA3	2.01	0.43
38:B5:69:GLU:OE1	38:B5:69:GLU:N	2.50	0.43
39:BL:44:LYS:HG3	39:BL:47:TRP:CB	2.48	0.43
67:BA:80:LEU:HD21	67:BA:146:GLU:HG2	2.00	0.43
1:1:29:U:H2'	1:1:30:G:C8	2.54	0.43
1:1:117:G:N2	1:1:118:U:H1'	2.34	0.43
1:1:529:G:OP2	58:BM:44:ARG:NH1	2.51	0.43
1:1:1616:C:H2'	1:1:1617:4AC:H6	2.01	0.43
1:1:2109:A:H2'	1:1:2110:A:H8	1.82	0.43
1:1:2366:A:N1	1:1:2402:G:O2'	2.41	0.43
2:2:80:G:N1	2:2:94:G:C6	2.87	0.43
2:2:153:C:O2'	12:AG:18:GLN:HB2	2.19	0.43
2:2:1201:A:H5'	2:2:1202:5MC:OP2	2.18	0.43
4:A:43:ILE:HG21	4:A:81:LEU:HD11	2.01	0.43
5:H:314:ILE:HG23	5:H:337:VAL:HG22	2.01	0.43
9:AD:173:LYS:HB2	9:AD:173:LYS:HE3	1.78	0.43
12:AG:61:MET:HB2	12:AG:121:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AG:110:ASN:HD22	12:AG:110:ASN:HA	1.64	0.43
13:AH:108:PHE:HD1	13:AH:108:PHE:HA	1.71	0.43
13:AH:164:ASN:OD1	13:AH:203:LYS:HD2	2.19	0.43
17:AL:37:PRO:HA	17:AL:73:ILE:HG13	2.01	0.43
28:AY:22:CYS:SG	28:AY:29:VAL:HG21	2.59	0.43
36:BO:34:ARG:O	36:BO:48:ILE:HA	2.19	0.43
36:BO:47:GLN:HG2	36:BO:61:SER:HB2	2.01	0.43
1:1:2098:G:H2'	1:1:2099:C:H6	1.84	0.43
2:2:70:U:H2'	2:2:71:C:C6	2.53	0.43
2:2:84:C:H2'	2:2:85:U:O4'	2.19	0.43
2:2:702:C:H2'	2:2:703:4AC:C6	2.49	0.43
2:2:1000:G:H8	2:2:1000:G:OP2	2.01	0.43
2:2:1147:4AC:O7	2:2:1147:4AC:H5	2.18	0.43
4:A:172:PRO:HG3	4:A:225:ASN:HB2	2.01	0.43
4:A:178:ARG:HG3	4:A:221:LEU:HD22	2.01	0.43
5:H:197:GLU:HB3	5:H:198:LEU:H	1.62	0.43
7:AB:182:ILE:HD13	7:AB:188:PHE:HB3	2.00	0.43
11:AF:67:ASP:HB2	11:AF:194:THR:HG21	2.01	0.43
24:AU:40:HIS:H	24:AU:40:HIS:CD2	2.37	0.43
67:BA:89:GLU:O	67:BA:93:ILE:N	2.51	0.43
1:1:380:A:C2	1:1:409:U:C2	3.07	0.43
1:1:1232:A:N1	1:1:2267:G:O2'	2.45	0.43
1:1:1662:4AC:O7	1:1:1662:4AC:H5	2.18	0.43
1:1:2010:C:N3	1:1:2947:C:O2'	2.41	0.43
1:1:2408:G:N3	1:1:2408:G:O2'	2.42	0.43
1:1:2782:G:H2'	1:1:2783:G:C8	2.54	0.43
1:1:2804:A:OP2	1:1:2804:A:H8	2.01	0.43
1:1:3022:C:O2	1:1:3022:C:O2'	2.25	0.43
2:2:170:U:H4'	2:2:171:C:OP2	2.16	0.43
2:2:345:C:C2	2:2:346:A:C8	3.07	0.43
2:2:422:C:N4	2:2:424:C:H1'	2.33	0.43
2:2:806:G:OP1	26:AW:53:LYS:NZ	2.52	0.43
2:2:949:A:N6	2:2:1198:U:O5'	2.52	0.43
2:2:1157:G:H4'	2:2:1158:G:OP2	2.19	0.43
2:2:1429:U:P	12:AG:82:ARG:HH22	2.41	0.43
4:A:13:LEU:O	4:A:13:LEU:HD13	2.19	0.43
4:A:32:PHE:HB2	4:A:43:ILE:HD11	1.99	0.43
8:AC:54:LYS:HA	8:AC:61:GLU:HA	2.01	0.43
19:AN:40:LYS:HE3	19:AN:40:LYS:HB2	1.94	0.43
29:AZ:192:GLU:H	29:AZ:192:GLU:HG2	1.49	0.43
36:BO:68:ILE:HD11	36:BO:77:CYS:SG	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:BU:20:LEU:HD23	41:BU:23:ARG:HD2	2.01	0.43
44:BE:11:ILE:HD11	44:BE:170:GLU:CD	2.44	0.43
56:BZ:90:GLU:H	56:BZ:90:GLU:HG3	1.64	0.43
62:Bg:29:GLU:OE1	62:Bg:29:GLU:N	2.42	0.43
1:1:42:U:C4	52:BV:51:LYS:HB2	2.54	0.42
1:1:102:C:N3	1:1:117:G:N1	2.37	0.42
1:1:473:C:H2'	1:1:474:C:C6	2.54	0.42
1:1:846:C:O2'	1:1:889:U:OP1	2.37	0.42
1:1:1133:A:O2'	1:1:1134:G:H5'	2.19	0.42
1:1:1422:A:H2'	1:1:1423:C:C6	2.54	0.42
1:1:1667:4AC:H2'	1:1:1668:G:C8	2.51	0.42
1:1:1697:G:H2'	1:1:1698:A:H8	1.83	0.42
1:1:1731:U:H4'	1:1:1732:G:O5'	2.18	0.42
2:2:98:C:H2'	2:2:99:C:C6	2.54	0.42
2:2:243:C:H2'	2:2:244:G:H8	1.83	0.42
2:2:816:C:H5''	6:AA:128:ARG:HH11	1.83	0.42
2:2:1237:C:OP2	24:AU:70:ILE:HG12	2.18	0.42
5:H:374:LEU:HD13	5:H:374:LEU:HA	1.84	0.42
22:AR:73:HIS:O	22:AR:102:VAL:HG12	2.19	0.42
37:BC:260:ARG:HB2	49:BI:59:THR:HG21	2.01	0.42
40:Bf:3:ARG:NH1	40:Bf:4:ASN:O	2.52	0.42
1:1:50:A:O2'	1:1:62:A:N6	2.48	0.42
1:1:58:A:C5	1:1:59:C:H1'	2.54	0.42
1:1:1783:G:H2'	1:1:1784:U:C6	2.55	0.42
2:2:146:A:H2'	2:2:147:U:H6	1.84	0.42
2:2:199:C:C2	2:2:200:C:C5	3.07	0.42
2:2:657:OMG:HM22	2:2:658:G:O4'	2.19	0.42
2:2:788:G:H2'	2:2:789:C:C6	2.53	0.42
2:2:817:U:H2'	2:2:818:C:C6	2.54	0.42
2:2:879:A:H2'	2:2:880:A:H8	1.84	0.42
5:H:220:THR:HB	5:H:245:VAL:HG22	2.00	0.42
6:AA:90:ARG:NH2	18:AM:119:THR:OG1	2.43	0.42
8:AC:54:LYS:HB2	8:AC:54:LYS:HE3	1.75	0.42
11:AF:57:VAL:HG22	11:AF:89:VAL:HB	2.01	0.42
15:AJ:39:GLU:OE1	15:AJ:39:GLU:N	2.43	0.42
19:AN:73:VAL:HG11	19:AN:97:ILE:HG21	2.01	0.42
21:AQ:84:LYS:HA	21:AQ:84:LYS:HD2	1.68	0.42
58:BM:151:LEU:HD11	66:Bk:26:VAL:HG11	2.01	0.42
67:BA:32:GLU:HG2	67:BA:208:LYS:HG3	2.01	0.42
67:BA:97:PRO:O	67:BA:101:ARG:HB2	2.19	0.42
1:1:2128:U:H2'	1:1:2129:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2551:A:H2'	1:1:2551:A:N3	2.34	0.42
1:1:2584:C:H2'	1:1:2585:4AC:O2	2.20	0.42
2:2:1085:C:H2'	2:2:1086:C:C6	2.55	0.42
2:2:1192:C:H2'	2:2:1193:C:H6	1.84	0.42
2:2:1236:C:H2'	2:2:1237:C:C6	2.54	0.42
2:2:1287:G:C4	2:2:1288:C:C5	3.08	0.42
2:2:1300:C:H2'	2:2:1301:G:C8	2.47	0.42
29:AZ:170:LEU:HD13	29:AZ:175:VAL:HG12	2.00	0.42
34:BB:124:ALA:O	34:BB:127:THR:HB	2.18	0.42
37:BC:91:LEU:HD23	37:BC:91:LEU:HA	1.89	0.42
51:BQ:2:LYS:HE2	51:BQ:2:LYS:HB2	1.77	0.42
52:BV:5:ASN:HB2	52:BV:14:PHE:CZ	2.55	0.42
1:1:406:A:H5''	1:1:408:G:O4'	2.19	0.42
1:1:925:A:OP2	1:1:925:A:H8	2.02	0.42
1:1:1566:C:OP2	1:1:1879:G:N2	2.44	0.42
1:1:2691:G:H21	61:BN:101:THR:HB	1.85	0.42
1:1:2871:A:H2'	1:1:2872:G:O4'	2.19	0.42
2:2:332:U:H2'	2:2:333:G:O4'	2.19	0.42
2:2:1232:C:H2'	2:2:1233:4AC:H6	2.01	0.42
2:2:1358:U:C4	2:2:1359:G:N7	2.87	0.42
3:3:121:G:H2'	3:3:122:G:C8	2.55	0.42
7:AB:70:VAL:HG12	7:AB:92:ILE:HB	2.01	0.42
11:AF:9:ALA:HB2	11:AF:55:PRO:HB3	2.01	0.42
14:AI:28:LYS:HB3	14:AI:29:PRO:HD3	2.00	0.42
18:AM:134:GLY:O	18:AM:136:ARG:HD3	2.19	0.42
21:AQ:66:PHE:HB2	21:AQ:76:LEU:HD23	2.00	0.42
29:AZ:62:ILE:HD12	29:AZ:80:ILE:HG21	2.01	0.42
31:A3:9:PHE:CE2	31:A3:122:MET:HE2	2.54	0.42
32:AT:59:TYR:CZ	32:AT:61:LYS:HG3	2.54	0.42
32:AT:98:MET:HG2	33:AO:112:ILE:CG1	2.49	0.42
36:BO:92:TYR:HE2	36:BO:193:ILE:HD13	1.85	0.42
67:BA:74:ALA:O	67:BA:78:ARG:HG3	2.19	0.42
1:1:68:U:O2'	52:BV:51:LYS:NZ	2.53	0.42
1:1:103:C:C2	1:1:117:G:C2	3.08	0.42
1:1:793:G:P	39:BL:12:ARG:HH22	2.41	0.42
1:1:1653:U:P	51:BQ:42:ARG:HH22	2.42	0.42
1:1:2184:U:OP2	4:A:89:THR:HG23	2.19	0.42
2:2:1384:U:H2'	2:2:1385:C:H6	1.81	0.42
6:AA:112:THR:HG23	6:AA:114:ASP:N	2.34	0.42
6:AA:194:GLU:H	6:AA:194:GLU:HG3	1.50	0.42
7:AB:72:VAL:HG13	7:AB:123:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AB:117:ILE:O	7:AB:139:ALA:HA	2.20	0.42
13:AH:117:LYS:HD2	13:AH:117:LYS:HA	1.89	0.42
21:AQ:109:LEU:HD11	21:AQ:119:MET:HA	2.01	0.42
24:AU:141:GLU:HB2	24:AU:148:LYS:HD2	2.00	0.42
29:AZ:35:ILE:O	29:AZ:36:LYS:HD2	2.20	0.42
29:AZ:38:THR:HB	29:AZ:39:PRO:HD2	2.01	0.42
49:BI:6:ALA:HA	49:BI:9:LEU:HD12	2.00	0.42
31:B4:12:PRO:HG2	31:B4:15:LEU:HB3	2.01	0.42
1:1:549:G:H2'	1:1:550:G:H8	1.85	0.42
1:1:673:C:H2'	1:1:674:G:H8	1.85	0.42
1:1:2077:U:H2'	1:1:2078:G:C8	2.54	0.42
1:1:2981:G:H5''	1:1:2982:C:H5	1.84	0.42
2:2:53:4AC:O7	2:2:53:4AC:H5	2.18	0.42
2:2:801:C:H2'	2:2:802:G:H8	1.84	0.42
2:2:1199:A:H2'	2:2:1200:C:C6	2.55	0.42
5:H:136:MET:HE2	5:H:136:MET:HB2	1.94	0.42
13:AH:58:LYS:NZ	13:AH:159:ASP:OD2	2.49	0.42
25:AV:45:ASP:OD1	25:AV:45:ASP:N	2.50	0.42
29:AZ:108:HIS:NE2	29:AZ:110:ARG:HG3	2.33	0.42
55:BF:111:GLU:HG2	55:BF:119:PRO:HB3	2.01	0.42
25:B6:46:LEU:HG	25:B6:71:TYR:CD1	2.54	0.42
65:BI:29:LYS:HE2	65:BI:29:LYS:HB3	1.90	0.42
67:BA:79:ARG:HH12	67:BA:144:ASN:HA	1.84	0.42
1:1:787:C:H2'	1:1:788:A:C8	2.55	0.42
1:1:2042:A:H1'	1:1:2179:A:N6	2.33	0.42
1:1:2398:A:H3'	1:1:2398:A:N3	2.35	0.42
2:2:749:A:H4'	2:2:1483:G:O2'	2.19	0.42
2:2:926:G:H2'	2:2:927:U:C6	2.55	0.42
2:2:1089:G:C4'	17:AL:38:ILE:HD11	2.49	0.42
2:2:1225:A:H2'	2:2:1226:U:C6	2.53	0.42
7:AB:36:ARG:HD2	7:AB:42:VAL:HG23	2.02	0.42
7:AB:107:LYS:HG2	7:AB:108:ASN:N	2.35	0.42
9:AD:111:LYS:HA	9:AD:111:LYS:HD2	1.77	0.42
11:AF:21:LYS:O	11:AF:25:LEU:HG	2.19	0.42
11:AF:22:LEU:HD21	11:AF:37:ILE:HB	2.01	0.42
32:AT:34:ARG:O	32:AT:38:ARG:HG3	2.19	0.42
43:Be:55:TRP:CD1	43:Be:55:TRP:H	2.37	0.42
56:BZ:34:LEU:HD13	56:BZ:97:ALA:HB1	2.00	0.42
67:BA:138:VAL:HB	67:BA:142:MET:HE2	2.01	0.42
1:1:208:A:H2'	1:1:209:G:O4'	2.20	0.42
1:1:1161:A:H2'	1:1:1164:C:H5	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1379:C:H2'	1:1:1380:G:O4'	2.19	0.42
1:1:1617:4AC:O7	1:1:1617:4AC:H5	2.20	0.42
2:2:402:G:C2	2:2:403:G:C8	3.07	0.42
2:2:415:G:H21	9:AD:123:GLN:NE2	2.18	0.42
2:2:566:C:H2'	2:2:567:C:C6	2.55	0.42
2:2:728:G:H2'	2:2:729:G:H8	1.84	0.42
2:2:866:G:H2'	2:2:867:C:C6	2.55	0.42
2:2:1238:C:OP1	24:AU:119:ARG:NH2	2.53	0.42
3:3:45:A:C4	3:3:46:A:C8	3.08	0.42
4:A:30:ARG:O	4:A:34:GLU:HG3	2.20	0.42
5:H:243:VAL:HA	5:H:254:ILE:HD13	2.00	0.42
5:H:383:ARG:O	5:H:384:PHE:HB3	2.18	0.42
7:AB:170:ILE:HD13	7:AB:173:ARG:HH21	1.84	0.42
9:AD:151:THR:O	9:AD:153:THR:HG22	2.20	0.42
16:AK:4:ILE:HD13	16:AK:88:GLU:HG3	2.01	0.42
22:AR:34:PHE:O	22:AR:87:LEU:HD12	2.20	0.42
34:BB:103:PRO:HA	34:BB:134:ARG:NH1	2.33	0.42
36:BO:155:MET:O	36:BO:159:GLN:HG2	2.20	0.42
45:Ba:33:LYS:HE3	45:Ba:33:LYS:HB2	1.88	0.42
54:BD:132:HIS:HD1	54:BD:169:ASP:CG	2.27	0.42
31:B4:34:LYS:HE3	31:B4:34:LYS:HB2	1.87	0.42
31:B4:52:ILE:O	31:B4:98:SER:HA	2.20	0.42
1:1:431:G:H2'	1:1:432:A:H8	1.85	0.42
1:1:1327:C:H42	1:1:1353:A:P	2.42	0.42
1:1:1333:U:O2'	1:1:1343:A:OP1	2.34	0.42
1:1:1847:C:OP1	1:1:1862:U:H5	2.01	0.42
1:1:2287:4AC:H2'	1:1:2288:G:C8	2.55	0.42
1:1:2291:G:H3'	1:1:2810:G:H5''	2.00	0.42
1:1:2331:U:H1'	58:BM:123:GLY:HA3	2.01	0.42
1:1:2827:G:N2	1:1:2830:A:OP2	2.42	0.42
2:2:135:U:H2'	2:2:136:C:H6	1.84	0.42
2:2:273:C:H2'	2:2:274:G:O4'	2.20	0.42
2:2:609:A:H2'	2:2:610:C:H6	1.83	0.42
2:2:835:A:H2'	2:2:836:A:C8	2.55	0.42
2:2:1283:G:N2	33:AO:80:ASN:O	2.52	0.42
2:2:1361:U:H2'	2:2:1362:C:H6	1.84	0.42
5:H:6:VAL:HG22	5:H:10:MET:SD	2.60	0.42
5:H:153:LEU:HD23	5:H:153:LEU:HA	1.87	0.42
5:H:273:ARG:HB2	32:AT:132:LYS:C	2.45	0.42
7:AB:90:ARG:HH22	7:AB:108:ASN:HD21	1.66	0.42
7:AB:103:ASN:O	7:AB:106:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AB:165:ALA:HB3	7:AB:196:GLU:HG3	2.02	0.42
28:AY:31:MET:HG2	28:AY:32:ALA:H	1.85	0.42
29:AZ:61:ARG:O	29:AZ:65:LEU:N	2.35	0.42
35:BY:86:LYS:HE3	35:BY:86:LYS:HB3	1.87	0.42
39:BL:36:MET:HE3	39:BL:39:THR:HG21	2.01	0.42
51:BQ:60:ARG:HG2	51:BQ:63:ALA:HB3	2.00	0.42
64:BJ:117:GLU:HG2	64:BJ:118:ILE:N	2.35	0.42
1:1:960:C:H2'	1:1:961:U:C6	2.55	0.42
1:1:1093:C:H2'	1:1:1094:C:H6	1.84	0.42
1:1:1115:A:H2'	1:1:1116:G:C8	2.55	0.42
1:1:1306:G:N1	1:1:1307:C:O2	2.53	0.42
1:1:1524:G:N7	59:BS:28:SER:OG	2.47	0.42
1:1:1777:A:H2'	1:1:1778:A:H8	1.84	0.42
2:2:479:4AC:O7	2:2:479:4AC:H5	2.20	0.42
2:2:849:G:H2'	2:2:850:C:C6	2.55	0.42
2:2:955:A:H5'	2:2:956:C:OP2	2.19	0.42
2:2:1389:C:H2'	2:2:1390:C:C6	2.55	0.42
4:A:68:PHE:CD1	4:A:79:ILE:HG21	2.55	0.42
6:AA:112:THR:HA	6:AA:150:ALA:HB1	2.01	0.42
10:AE:3:ARG:HG3	10:AE:4:LYS:HG2	2.01	0.42
17:AL:53:PRO:HA	20:AP:41:HIS:HD2	1.84	0.42
19:AN:98:ASP:OD1	19:AN:99:GLU:N	2.51	0.42
21:AQ:3:ARG:HG2	21:AQ:8:LYS:O	2.20	0.42
24:AU:41:LYS:H	24:AU:41:LYS:HG2	1.73	0.42
29:AZ:22:GLU:OE1	29:AZ:93:LYS:NZ	2.39	0.42
29:AZ:62:ILE:HD13	29:AZ:62:ILE:HA	1.85	0.42
32:AT:82:TYR:CE2	32:AT:91:PRO:HB3	2.55	0.42
1:1:144:G:H2'	1:1:145:G:H8	1.84	0.41
1:1:151:C:H2'	1:1:152:U:C6	2.55	0.41
1:1:458:4AC:O7	1:1:458:4AC:H5	2.20	0.41
1:1:696:A:H2'	1:1:697:A:C8	2.55	0.41
1:1:1992:U:H2'	1:1:1993:G:O4'	2.19	0.41
1:1:2587:U:OP2	1:1:2588:A:O2'	2.30	0.41
2:2:109:C:H2'	2:2:110:U:H6	1.85	0.41
2:2:861:G:C8	30:A0:2:LYS:HB2	2.54	0.41
2:2:975:G:C6	2:2:1000:G:C5	3.07	0.41
10:AE:217:ASP:OD1	10:AE:221:GLU:N	2.53	0.41
18:AM:49:LYS:HB2	18:AM:49:LYS:HE2	1.87	0.41
18:AM:58:TYR:HA	18:AM:61:MET:HE2	2.01	0.41
23:AS:56:LYS:O	23:AS:60:MET:HG3	2.20	0.41
24:AU:21:LYS:HA	24:AU:52:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A3:9:PHE:HE2	31:A3:122:MET:HE2	1.85	0.41
34:BB:112:GLU:OE2	34:BB:156:ARG:NH2	2.42	0.41
39:BL:16:THR:HG21	39:BL:20:GLY:O	2.20	0.41
57:BP:3:ARG:NH2	57:BP:38:GLU:O	2.51	0.41
58:BM:167:LYS:HG2	58:BM:172:LEU:HD12	2.01	0.41
31:B4:31:LYS:H	31:B4:103:GLU:HB3	1.85	0.41
31:B4:73:LYS:C	31:B4:74:GLU:HG3	2.45	0.41
1:1:906:U:H2'	1:1:907:C:C6	2.55	0.41
1:1:961:U:H2'	1:1:962:C:C6	2.55	0.41
1:1:1173:C:H2'	1:1:1174:A:C8	2.56	0.41
1:1:1733:A:H2'	1:1:1734:G:O4'	2.20	0.41
1:1:2052:C:OP1	34:BB:238:ARG:NH2	2.51	0.41
1:1:2746:U:H2'	1:1:2747:C:C6	2.55	0.41
1:1:2847:U:H2'	1:1:2848:C:C6	2.54	0.41
2:2:176:A:H2'	2:2:177:U:C6	2.55	0.41
2:2:505:G:H2'	2:2:506:C:H6	1.84	0.41
2:2:562:A:C2	2:2:563:G:C8	3.09	0.41
2:2:645:C:H2'	2:2:646:C:H6	1.85	0.41
2:2:658:G:H2'	2:2:659:U:C6	2.55	0.41
2:2:1215:G:C2	2:2:1216:G:C5	3.08	0.41
2:2:1306:A:H2'	2:2:1307:A:C8	2.54	0.41
2:2:1491:U:OP1	18:AM:136:ARG:NH2	2.50	0.41
6:AA:18:GLN:HE21	6:AA:18:GLN:HB2	1.69	0.41
7:AB:43:LEU:HD23	7:AB:44:ASP:H	1.85	0.41
10:AE:64:LYS:NZ	25:AV:80:TYR:O	2.48	0.41
12:AG:69:LYS:HG3	12:AG:115:GLU:O	2.20	0.41
25:AV:7:GLU:OE1	25:AV:7:GLU:N	2.52	0.41
39:BL:40:GLY:HA2	39:BL:44:LYS:HD2	2.02	0.41
63:Bc:26:PRO:HB2	63:Bc:29:VAL:CG1	2.50	0.41
1:1:633:A:N3	1:1:635:G:H5''	2.35	0.41
1:1:676:C:H2'	1:1:677:G:O4'	2.19	0.41
1:1:1303:A:H1'	1:1:1304:C:P	2.60	0.41
1:1:2881:G:H2'	1:1:2882:C:H6	1.86	0.41
2:2:135:U:H1'	10:AE:146:THR:HA	2.01	0.41
2:2:202:C:C2	2:2:203:A:C8	3.08	0.41
2:2:557:C:C2	2:2:616:G:C2	3.09	0.41
2:2:801:C:H2'	2:2:802:G:C8	2.55	0.41
2:2:930:A:C5	32:AT:87:LYS:HD2	2.55	0.41
2:2:1091:U:O2	2:2:1254:A:H5'	2.19	0.41
2:2:1479:4AC:O7	2:2:1479:4AC:H5	2.20	0.41
8:AC:33:PRO:HD2	8:AC:60:TRP:CZ3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AQ:122:LEU:O	21:AQ:126:GLU:HB2	2.20	0.41
27:AX:67:ILE:HD13	27:AX:67:ILE:HA	1.91	0.41
54:BD:35:VAL:HG13	54:BD:228:GLU:HG3	2.03	0.41
61:BN:12:VAL:HG12	61:BN:56:GLN:HG3	2.00	0.41
67:BA:184:ILE:O	67:BA:188:LEU:N	2.42	0.41
1:1:843:A:H2'	1:1:844:A:C8	2.55	0.41
1:1:1697:G:H2'	1:1:1698:A:C8	2.55	0.41
1:1:1809:A:C5	1:1:1810:G:H1'	2.55	0.41
1:1:2302:A:H2'	1:1:2303:C:H5'	2.02	0.41
1:1:2543:U:O2'	44:BE:31:ASN:ND2	2.52	0.41
1:1:2992:4AC:CM7	1:1:2992:4AC:H5	2.49	0.41
2:2:199:C:H2'	2:2:200:C:H6	1.86	0.41
2:2:244:G:C2	2:2:245:G:C5	3.09	0.41
2:2:1107:U:H6	2:2:1107:U:H2'	1.58	0.41
2:2:1286:G:OP2	32:AT:29:PRO:HA	2.21	0.41
2:2:1381:C:C2	2:2:1382:A:C8	3.08	0.41
8:AC:57:LYS:HA	8:AC:57:LYS:HD3	1.89	0.41
9:AD:168:ARG:O	9:AD:172:GLU:HG2	2.20	0.41
24:AU:110:PHE:HD1	24:AU:110:PHE:HA	1.69	0.41
25:AV:74:ASP:HB3	25:AV:77:ARG:HB2	2.03	0.41
31:A3:6:TYR:O	31:A3:8:LYS:NZ	2.52	0.41
31:A3:86:LEU:HD12	31:A3:87:GLY:N	2.36	0.41
39:BL:44:LYS:HG3	39:BL:47:TRP:HB2	2.02	0.41
67:BA:142:MET:HE3	67:BA:142:MET:HB3	1.79	0.41
1:1:1180:G:H21	35:BY:25:MET:HE2	1.84	0.41
1:1:1310:G:H21	1:1:1340:A:H1'	1.86	0.41
1:1:2287:4AC:O7	1:1:2287:4AC:H5	2.20	0.41
1:1:2399:G:H2'	1:1:2400:C:C6	2.56	0.41
1:1:2810:G:H2'	1:1:2811:C:H6	1.85	0.41
2:2:90:G:H8	2:2:90:G:OP2	2.02	0.41
2:2:119:C:H2'	2:2:120:G:H8	1.86	0.41
2:2:478:C:H2'	2:2:479:4AC:H6	2.03	0.41
2:2:1360:C:C2	2:2:1361:U:C5	3.08	0.41
4:A:164:MET:HE3	4:A:164:MET:HB2	1.92	0.41
5:H:7:GLN:HA	5:H:10:MET:HE2	2.02	0.41
5:H:198:LEU:HD23	5:H:198:LEU:HA	1.89	0.41
7:AB:64:PRO:HG3	7:AB:179:ARG:CZ	2.50	0.41
18:AM:27:ILE:HD11	18:AM:29:HIS:HB2	2.01	0.41
29:AZ:17:ILE:HG22	29:AZ:73:PHE:CG	2.56	0.41
61:BN:96:GLU:HB2	61:BN:120:ILE:HD13	2.02	0.41
31:B4:3:LYS:N	31:B4:4:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:B4:66:LEU:HD12	31:B4:66:LEU:HA	1.93	0.41
1:1:796:C:H5''	54:BD:100:ILE:HG12	2.03	0.41
1:1:1646:A:H1'	1:1:1667:4AC:H1'	2.02	0.41
1:1:1699:G:H2'	1:1:1700:G:H8	1.85	0.41
1:1:1765:4AC:H4'	1:1:1778:A:H4'	2.03	0.41
1:1:1934:4AC:H5	1:1:1934:4AC:O7	2.21	0.41
2:2:17:4AC:O7	2:2:17:4AC:H5	2.21	0.41
2:2:417:C:H2'	2:2:418:G:H8	1.86	0.41
2:2:1385:C:H2'	2:2:1386:C:C6	2.56	0.41
5:H:141:ILE:HG12	5:H:159:HIS:CD2	2.56	0.41
14:AI:104:VAL:HG22	14:AI:125:LEU:HD23	2.03	0.41
16:AK:121:ARG:HG3	16:AK:130:ARG:N	2.35	0.41
17:AL:33:ARG:N	17:AL:76:GLU:OE2	2.53	0.41
18:AM:26:THR:HG21	18:AM:60:ALA:HB2	2.02	0.41
24:AU:20:LEU:HD12	24:AU:20:LEU:HA	1.83	0.41
27:AX:36:ASP:HB3	27:AX:39:ARG:HD3	2.03	0.41
36:BO:54:LYS:HE3	36:BO:54:LYS:HB2	1.66	0.41
31:B4:6:TYR:OH	31:B4:55:GLU:HG3	2.20	0.41
67:BA:15:VAL:HG22	67:BA:207:VAL:HG11	2.02	0.41
1:1:392:A:O2'	1:1:393:C:H5''	2.20	0.41
1:1:532:C:H2'	1:1:533:4AC:H6	2.03	0.41
1:1:922:4AC:O7	1:1:922:4AC:H5	2.21	0.41
1:1:1048:4AC:O7	1:1:1048:4AC:H5	2.20	0.41
1:1:1065:4AC:O7	1:1:1065:4AC:H5	2.21	0.41
1:1:1086:G:H2'	1:1:1087:G:H8	1.86	0.41
1:1:1578:G:C6	1:1:1579:G:N7	2.88	0.41
1:1:1867:4AC:O7	1:1:1867:4AC:H5	2.21	0.41
1:1:2342:C:C4	1:1:2343:G:C8	3.08	0.41
1:1:2919:G:H2'	1:1:2920:U:C6	2.56	0.41
2:2:83:C:H6	2:2:83:C:O5'	2.03	0.41
2:2:91:G:H2'	2:2:92:A:C8	2.56	0.41
2:2:668:A:P	2:2:670:A:H5'	2.60	0.41
2:2:671:A:C4	2:2:672:U:C6	3.09	0.41
2:2:1243:A:O2'	2:2:1299:C:O2'	2.33	0.41
3:3:32:4AC:O7	3:3:32:4AC:H5	2.20	0.41
16:AK:11:LYS:O	16:AK:12:THR:OG1	2.36	0.41
20:AP:50:LEU:HB2	20:AP:52:PHE:HD1	1.86	0.41
29:AZ:161:LEU:HD13	29:AZ:187:ALA:HB1	2.02	0.41
33:AO:54:LEU:HD12	33:AO:54:LEU:HA	1.84	0.41
36:BO:181:LEU:N	36:BO:182:PRO:HD2	2.36	0.41
44:BE:134:ILE:H	44:BE:134:ILE:HG12	1.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Ba:5:PRO:HG2	45:Ba:78:GLU:OE2	2.21	0.41
38:BK:27:ILE:O	65:Bl:26:ARG:NH1	2.42	0.41
58:BM:47:ARG:HA	58:BM:47:ARG:HD2	1.87	0.41
1:1:203:C:H3'	1:1:204:A:H2'	2.01	0.41
1:1:802:4AC:O7	1:1:802:4AC:H5	2.21	0.41
1:1:1393:G:OP2	49:BI:52:ARG:NH2	2.47	0.41
1:1:1413:C:H2'	1:1:1414:C:C6	2.56	0.41
1:1:1460:4AC:H5	1:1:1460:4AC:O7	2.21	0.41
1:1:1545:A:H1'	1:1:1547:U:OP2	2.21	0.41
1:1:1550:4AC:O7	1:1:1550:4AC:H5	2.20	0.41
1:1:2329:4AC:O7	1:1:2329:4AC:H5	2.20	0.41
1:1:2373:G:N3	1:1:2398:A:N6	2.68	0.41
2:2:212:G:H2'	2:2:212:G:N3	2.36	0.41
2:2:244:G:H2'	2:2:245:G:C8	2.53	0.41
2:2:563:G:H21	14:AI:124:ARG:NH2	2.19	0.41
2:2:1414:A:H2'	2:2:1415:U:H6	1.84	0.41
2:2:1476:A:H2'	2:2:1477:G:C8	2.56	0.41
4:A:219:ASN:O	4:A:223:LYS:N	2.53	0.41
7:AB:32:ILE:HD12	7:AB:143:THR:HG23	2.01	0.41
7:AB:101:MET:HB2	7:AB:129:GLU:HG2	2.03	0.41
9:AD:165:HIS:CE1	9:AD:167:GLU:HB2	2.56	0.41
13:AH:18:MET:HB3	13:AH:20:ARG:HH11	1.85	0.41
15:AJ:31:GLU:H	15:AJ:31:GLU:CD	2.29	0.41
22:AR:15:LYS:HD3	22:AR:24:HIS:CD2	2.56	0.41
32:AT:97:GLU:CD	33:AO:111:ARG:HH21	2.28	0.41
45:Ba:47:GLU:HB2	45:Ba:88:ILE:HD12	2.02	0.41
51:BQ:140:MET:O	51:BQ:144:GLU:HG2	2.21	0.41
54:BD:29:ASP:OD1	54:BD:29:ASP:N	2.54	0.41
1:1:103:C:O2'	1:1:104:C:H5'	2.21	0.41
1:1:117:G:C4	1:1:118:U:C6	3.09	0.41
1:1:120:A:H2'	1:1:121:G:C8	2.56	0.41
1:1:254:C:H2'	1:1:255:C:H6	1.84	0.41
1:1:455:G:O3'	1:1:456:U:H4'	2.21	0.41
1:1:568:U:H2'	1:1:569:C:C6	2.56	0.41
1:1:791:G:H5''	1:1:792:A:OP1	2.21	0.41
1:1:806:G:H2'	1:1:807:C:C6	2.56	0.41
1:1:857:C:H2'	1:1:858:A:H8	1.86	0.41
1:1:974:G:OP1	51:BQ:92:LYS:NZ	2.48	0.41
1:1:1363:U:H2'	1:1:1364:C:C4	2.56	0.41
1:1:1487:U:H2'	1:1:1488:C:C6	2.56	0.41
1:1:1632:G:H2'	1:1:1633:C:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1742:A:H2'	1:1:1743:A:H8	1.84	0.41
1:1:1897:C:C2	1:1:1898:C:C5	3.09	0.41
1:1:2531:G:H2'	1:1:2532:C:C6	2.56	0.41
2:2:200:C:P	10:AE:134:LYS:HD3	2.60	0.41
2:2:946:G:C8	20:AP:40:ARG:HD3	2.55	0.41
2:2:1130:G:N7	23:AS:44:LYS:NZ	2.65	0.41
2:2:1312:G:H1'	5:H:268:VAL:HG21	2.03	0.41
2:2:1360:C:H2'	2:2:1361:U:C6	2.56	0.41
3:3:94:A:C5	3:3:95:G:H1'	2.56	0.41
4:A:15:VAL:HG22	4:A:16:HIS:ND1	2.36	0.41
4:A:22:ILE:HG22	4:A:49:VAL:HA	2.02	0.41
5:H:26:ALA:O	5:H:29:ILE:HG22	2.20	0.41
5:H:90:LYS:HB2	5:H:265:SER:HB2	2.03	0.41
5:H:165:PRO:HG3	5:H:254:ILE:HD11	2.02	0.41
5:H:332:GLN:OE1	5:H:347:ARG:HD2	2.21	0.41
6:AA:18:GLN:NE2	6:AA:77:GLN:OE1	2.54	0.41
6:AA:98:ARG:CZ	6:AA:98:ARG:HB3	2.50	0.41
7:AB:191:PRO:HB2	7:AB:193:GLU:HG2	2.02	0.41
8:AC:32:CYS:SG	8:AC:55:CYS:HB2	2.60	0.41
9:AD:43:LYS:HB3	9:AD:43:LYS:HE2	1.85	0.41
9:AD:98:GLU:H	9:AD:98:GLU:HG2	1.56	0.41
13:AH:164:ASN:CG	13:AH:203:LYS:HD2	2.46	0.41
21:AQ:39:LYS:HG3	21:AQ:40:LEU:N	2.34	0.41
21:AQ:115:ASP:CG	21:AQ:118:SER:HB2	2.46	0.41
34:BB:149:LYS:HD3	34:BB:151:PHE:CZ	2.55	0.41
35:BY:149:ASP:N	35:BY:149:ASP:OD1	2.52	0.41
44:BE:43:LYS:HD3	44:BE:133:GLY:H	1.86	0.41
31:BG:110:LEU:HD23	31:BG:110:LEU:HA	1.91	0.41
25:B6:13:LEU:HD12	25:B6:13:LEU:HA	1.77	0.41
58:BM:73:ARG:HD2	58:BM:90:TYR:CD1	2.56	0.41
64:BJ:95:MET:HB3	64:BJ:95:MET:HE2	1.84	0.41
67:BA:49:PHE:CG	67:BA:194:LYS:HG2	2.55	0.41
67:BA:91:GLU:OE1	67:BA:123:TYR:OH	2.31	0.41
1:1:217:A:C2	41:BU:20:LEU:HB3	2.56	0.41
1:1:243:4AC:O7	1:1:243:4AC:H5	2.21	0.41
1:1:298:G:H4'	39:BL:34:ARG:HD3	2.02	0.41
1:1:770:C:H2'	1:1:771:G:H8	1.86	0.41
1:1:846:C:H2'	1:1:847:G:O4'	2.21	0.41
1:1:1767:U:O2'	1:1:1769:A:N7	2.52	0.41
1:1:2363:G:H2'	1:1:2364:G:C8	2.56	0.41
1:1:2421:C:H2'	1:1:2422:U:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2548:4AC:O7	1:1:2548:4AC:H5	2.21	0.41
1:1:2593:A:H4'	39:BL:51:ILE:HG22	2.02	0.41
1:1:2718:4AC:O7	1:1:2718:4AC:H5	2.21	0.41
1:1:2865:4AC:O7	1:1:2865:4AC:H5	2.21	0.41
4:A:4:SER:HB3	4:A:7:LYS:HB2	2.03	0.41
4:A:21:GLU:HB2	4:A:53:ALA:HB2	2.02	0.41
6:AA:11:LYS:O	6:AA:15:LYS:HE3	2.21	0.41
29:AZ:37:LYS:HA	29:AZ:42:THR:HA	2.03	0.41
37:BC:356:SER:OG	52:BV:15:GLU:OE2	2.26	0.41
42:Bb:29:TRP:CD1	42:Bb:29:TRP:H	2.39	0.41
44:BE:131:GLU:OE1	44:BE:132:ILE:HG23	2.21	0.41
44:BE:184:VAL:HG23	44:BE:186:GLU:H	1.86	0.41
47:BW:5:GLU:H	47:BW:5:GLU:HG2	1.67	0.41
49:BI:98:LYS:HD3	49:BI:98:LYS:HA	1.90	0.41
38:BK:77:LYS:HE3	38:BK:77:LYS:HB3	1.94	0.41
31:BG:28:ASP:OD1	31:BG:28:ASP:N	2.53	0.41
54:BD:27:ARG:NH1	54:BD:29:ASP:OD2	2.54	0.41
55:BF:44:VAL:HG22	55:BF:57:LYS:HB2	2.02	0.41
62:Bg:30:LYS:HB3	62:Bg:37:LYS:HG3	2.03	0.41
65:Bl:8:VAL:HG22	65:Bl:57:ILE:HG23	2.03	0.41
67:BA:105:LYS:HG2	67:BA:131:ARG:HH12	1.86	0.41
1:1:451:4AC:O7	1:1:451:4AC:H5	2.21	0.40
1:1:1395:U:OP2	49:BI:39:THR:OG1	2.32	0.40
1:1:2268:C:H2'	1:1:2269:G:O4'	2.21	0.40
2:2:36:C:H2'	2:2:37:C:H6	1.86	0.40
2:2:204:G:O2'	15:AJ:64:ASN:ND2	2.54	0.40
2:2:636:4AC:HM73	2:2:703:4AC:CM7	2.51	0.40
2:2:764:C:H2'	2:2:765:G:H8	1.86	0.40
2:2:815:G:H2'	2:2:816:C:C6	2.56	0.40
2:2:895:C:H2'	2:2:896:G:H8	1.86	0.40
2:2:1283:G:H2'	2:2:1284:C:C6	2.56	0.40
2:2:1375:G:H2'	2:2:1376:OMC:O4'	2.20	0.40
3:3:114:C:H6	3:3:114:C:H2'	1.73	0.40
5:H:79:VAL:HG13	5:H:102:VAL:HG13	2.03	0.40
5:H:386:GLU:HG2	18:AM:23:TYR:CZ	2.55	0.40
6:AA:113:LYS:HE3	6:AA:154:ASN:HD22	1.85	0.40
11:AF:170:VAL:HG21	11:AF:194:THR:HG23	2.02	0.40
13:AH:70:LYS:O	13:AH:73:ARG:HD3	2.21	0.40
36:BO:87:GLY:HA2	36:BO:90:ILE:HG22	2.03	0.40
41:BU:4:ASN:OD1	41:BU:4:ASN:N	2.53	0.40
54:BD:9:ASN:HD22	54:BD:9:ASN:N	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:BZ:34:LEU:HD12	56:BZ:35:ILE:N	2.35	0.40
61:BN:44:GLU:OE1	61:BN:138:ASN:HA	2.21	0.40
1:1:422:C:H2'	1:1:423:C:H6	1.86	0.40
1:1:1030:U:OP2	34:BB:9:ARG:HD2	2.22	0.40
1:1:1154:C:H2'	1:1:1155:C:C6	2.56	0.40
1:1:1932:C:H2'	1:1:1933:C:H6	1.86	0.40
1:1:2363:G:H2'	1:1:2364:G:H8	1.86	0.40
1:1:2545:4AC:O7	1:1:2545:4AC:H5	2.20	0.40
1:1:2684:C:C2	1:1:2685:A:C8	3.09	0.40
1:1:2821:A:H2'	1:1:2822:C:H6	1.86	0.40
2:2:239:G:H2'	2:2:240:G:O4'	2.21	0.40
2:2:892:U:H2'	2:2:893:G:O4'	2.20	0.40
2:2:1097:U:H2'	2:2:1098:C:H6	1.86	0.40
2:2:1101:U:H2'	2:2:1102:C:H6	1.86	0.40
4:A:99:GLU:O	4:A:103:GLN:HG3	2.20	0.40
4:A:165:LYS:NZ	4:A:211:GLU:OE1	2.47	0.40
5:H:7:GLN:HA	5:H:10:MET:CE	2.50	0.40
10:AE:42:SER:HA	10:AE:86:GLY:HA2	2.02	0.40
15:AJ:37:VAL:HB	15:AJ:93:ASN:ND2	2.36	0.40
25:AV:96:LYS:H	25:AV:96:LYS:HG3	1.72	0.40
36:BO:36:VAL:HG22	36:BO:47:GLN:HB2	2.04	0.40
31:BG:31:LYS:HE3	31:BG:31:LYS:HB3	1.90	0.40
64:BJ:56:ALA:HB1	64:BJ:60:ASP:HB2	2.03	0.40
1:1:40:U:H2'	1:1:41:G:O4'	2.22	0.40
1:1:787:C:H2'	1:1:788:A:H8	1.84	0.40
1:1:1146:C:H2'	1:1:1147:C:H6	1.86	0.40
1:1:1594:4AC:O7	1:1:1594:4AC:H5	2.22	0.40
1:1:2276:C:C2	1:1:2277:C:C5	3.09	0.40
1:1:2339:C:C2	1:1:2340:G:C8	3.09	0.40
1:1:2447:A:H2'	1:1:2448:A:C8	2.55	0.40
2:2:546:4AC:O7	2:2:546:4AC:H5	2.21	0.40
2:2:759:A:O2'	2:2:761:A:N7	2.46	0.40
2:2:1028:4AC:O7	2:2:1028:4AC:H5	2.21	0.40
2:2:1398:G:H2'	2:2:1399:C:C6	2.57	0.40
5:H:52:GLN:O	5:H:56:ILE:HG13	2.22	0.40
5:H:185:ARG:CZ	5:H:204:PRO:HD2	2.51	0.40
9:AD:30:MET:HE1	9:AD:37:ASN:C	2.46	0.40
9:AD:70:ARG:HG3	9:AD:89:LEU:HD22	2.03	0.40
10:AE:110:LEU:HD23	10:AE:110:LEU:HA	1.89	0.40
16:AK:105:THR:HA	16:AK:108:VAL:HG22	2.03	0.40
47:BW:38:LEU:HD23	47:BW:38:LEU:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:141:G:O2'	1:1:142:A:OP2	2.36	0.40
1:1:728:C:H5''	38:BK:46:ARG:NH2	2.36	0.40
1:1:2027:4AC:O7	1:1:2027:4AC:H5	2.21	0.40
1:1:2570:4AC:O7	1:1:2570:4AC:H5	2.21	0.40
1:1:2699:C:H2'	1:1:2700:G:O4'	2.21	0.40
11:AF:70:LEU:HD13	11:AF:81:VAL:HG13	2.04	0.40
13:AH:23:THR:OG1	13:AH:39:LEU:HB3	2.20	0.40
32:AT:14:GLU:CD	32:AT:14:GLU:H	2.29	0.40
32:AT:19:MET:HB3	32:AT:23:GLU:HG3	2.03	0.40
37:BC:150:ASP:O	37:BC:154:GLU:HG2	2.22	0.40
51:BQ:139:TYR:O	51:BQ:143:GLU:HG2	2.21	0.40
25:B6:21:PHE:CE2	25:B6:23:ILE:HD11	2.56	0.40
63:Bc:10:TYR:CD1	63:Bc:19:THR:HA	2.56	0.40
1:1:94:G:H3'	1:1:95:G:C5'	2.51	0.40
1:1:113:G:H2'	1:1:114:G:C8	2.56	0.40
1:1:285:A:H2'	1:1:286:A:C8	2.56	0.40
1:1:394:G:H2'	1:1:395:A:C8	2.56	0.40
1:1:663:U:H4'	1:1:1493:G:H4'	2.02	0.40
1:1:1763:G:H2'	1:1:1764:C:H6	1.83	0.40
1:1:2062:4AC:O7	1:1:2062:4AC:H5	2.22	0.40
1:1:2136:4AC:H5	1:1:2136:4AC:O7	2.22	0.40
1:1:2249:4AC:O7	1:1:2249:4AC:H5	2.21	0.40
1:1:2456:C:H2'	1:1:2457:A:O4'	2.21	0.40
1:1:2596:C:H2'	1:1:2597:G:H8	1.87	0.40
2:2:330:A:H2'	2:2:331:C:C6	2.56	0.40
3:3:71:U:H2'	3:3:72:C:H6	1.85	0.40
4:A:223:LYS:HD3	4:A:223:LYS:HA	1.84	0.40
5:H:185:ARG:NH1	5:H:204:PRO:HD2	2.36	0.40
5:H:197:GLU:OE1	5:H:199:ALA:N	2.53	0.40
7:AB:23:GLN:HB2	7:AB:144:GLU:CB	2.52	0.40
7:AB:198:LYS:HE2	7:AB:198:LYS:HB2	1.68	0.40
12:AG:7:VAL:O	12:AG:121:VAL:HG12	2.22	0.40
13:AH:105:LYS:HE2	13:AH:105:LYS:HB3	1.78	0.40
13:AH:173:CYS:HB3	13:AH:183:ALA:HB2	2.04	0.40
18:AM:76:ILE:HG23	18:AM:110:LEU:HD21	2.03	0.40
29:AZ:17:ILE:HD12	29:AZ:33:LEU:HD21	2.03	0.40
29:AZ:42:THR:O	29:AZ:78:PRO:HA	2.22	0.40
46:BT:80:ALA:O	46:BT:85:LEU:HB2	2.21	0.40
54:BD:27:ARG:HB3	54:BD:30:LEU:HB2	2.04	0.40
55:BF:88:TYR:HB2	55:BF:139:VAL:HB	2.04	0.40
55:BF:155:GLU:O	55:BF:158:THR:HG22	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:BA:21:ARG:NH2	67:BA:213:PRO:O	2.31	0.40
67:BA:132:ASN:HA	67:BA:134:MET:HE2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	233/236 (99%)	227 (97%)	6 (3%)	0	100	100
5	H	384/392 (98%)	371 (97%)	12 (3%)	1 (0%)	36	46
6	AA	186/199 (94%)	185 (100%)	1 (0%)	0	100	100
7	AB	194/202 (96%)	192 (99%)	2 (1%)	0	100	100
8	AC	55/63 (87%)	53 (96%)	2 (4%)	0	100	100
9	AD	171/180 (95%)	167 (98%)	4 (2%)	0	100	100
10	AE	240/243 (99%)	234 (98%)	6 (2%)	0	100	100
11	AF	227/236 (96%)	221 (97%)	6 (3%)	0	100	100
12	AG	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
13	AH	212/215 (99%)	210 (99%)	2 (1%)	0	100	100
14	AI	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
15	AJ	123/127 (97%)	122 (99%)	1 (1%)	0	100	100
16	AK	133/135 (98%)	131 (98%)	1 (1%)	1 (1%)	16	20
17	AL	98/102 (96%)	97 (99%)	1 (1%)	0	100	100
18	AM	125/137 (91%)	120 (96%)	4 (3%)	1 (1%)	16	20
19	AN	144/147 (98%)	144 (100%)	0	0	100	100
20	AP	53/56 (95%)	53 (100%)	0	0	100	100
21	AQ	155/158 (98%)	154 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	AR	106/113 (94%)	104 (98%)	2 (2%)	0	100	100
23	AS	62/67 (92%)	62 (100%)	0	0	100	100
24	AU	147/150 (98%)	145 (99%)	2 (1%)	0	100	100
25	AV	94/99 (95%)	94 (100%)	0	0	100	100
25	B6	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
26	AW	59/65 (91%)	58 (98%)	1 (2%)	0	100	100
27	AX	63/71 (89%)	62 (98%)	1 (2%)	0	100	100
28	AY	27/51 (53%)	22 (82%)	5 (18%)	0	100	100
29	AZ	194/210 (92%)	190 (98%)	3 (2%)	1 (0%)	24	31
30	A0	34/37 (92%)	34 (100%)	0	0	100	100
31	A3	120/123 (98%)	111 (92%)	9 (8%)	0	100	100
31	B4	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
31	BG	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
32	AT	128/132 (97%)	126 (98%)	2 (2%)	0	100	100
33	AO	136/148 (92%)	132 (97%)	4 (3%)	0	100	100
34	BB	236/239 (99%)	229 (97%)	6 (2%)	1 (0%)	30	38
35	BY	152/155 (98%)	151 (99%)	1 (1%)	0	100	100
36	BO	196/203 (97%)	195 (100%)	1 (0%)	0	100	100
37	BC	358/361 (99%)	350 (98%)	8 (2%)	0	100	100
38	B5	79/82 (96%)	77 (98%)	2 (2%)	0	100	100
38	BK	78/82 (95%)	76 (97%)	2 (3%)	0	100	100
39	BL	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
40	Bf	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
41	BU	119/121 (98%)	119 (100%)	0	0	100	100
42	Bb	127/130 (98%)	127 (100%)	0	0	100	100
43	Be	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
44	BE	183/188 (97%)	180 (98%)	3 (2%)	0	100	100
45	Ba	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
46	BT	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
47	BW	66/68 (97%)	66 (100%)	0	0	100	100
48	Bi	80/83 (96%)	76 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	BI	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
50	BR	94/97 (97%)	94 (100%)	0	0	100	100
51	BQ	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
52	BV	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
53	Bj	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
54	BD	253/255 (99%)	250 (99%)	3 (1%)	0	100	100
55	BF	181/184 (98%)	181 (100%)	0	0	100	100
56	BZ	96/99 (97%)	95 (99%)	1 (1%)	0	100	100
57	BP	118/120 (98%)	118 (100%)	0	0	100	100
58	BM	191/194 (98%)	189 (99%)	2 (1%)	0	100	100
59	BS	152/155 (98%)	149 (98%)	3 (2%)	0	100	100
60	Bd	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
61	BN	176/181 (97%)	172 (98%)	4 (2%)	0	100	100
62	Bg	46/51 (90%)	46 (100%)	0	0	100	100
63	Bc	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
64	BJ	138/141 (98%)	138 (100%)	0	0	100	100
65	Bl	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
66	Bk	61/65 (94%)	61 (100%)	0	0	100	100
67	BA	213/219 (97%)	207 (97%)	6 (3%)	0	100	100
All	All	8995/9316 (97%)	8834 (98%)	156 (2%)	5 (0%)	49	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	H	268	VAL
16	AK	120	ASN
29	AZ	61	ARG
18	AM	124	ASP
34	BB	122	VAL

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	A	201/202 (100%)	185 (92%)	16 (8%)	11	15
5	H	332/338 (98%)	303 (91%)	29 (9%)	9	12
6	AA	160/167 (96%)	123 (77%)	37 (23%)	1	1
7	AB	168/173 (97%)	135 (80%)	33 (20%)	1	1
8	AC	50/55 (91%)	46 (92%)	4 (8%)	11	15
9	AD	156/160 (98%)	149 (96%)	7 (4%)	24	37
10	AE	213/214 (100%)	186 (87%)	27 (13%)	4	5
11	AF	192/198 (97%)	184 (96%)	8 (4%)	26	40
12	AG	107/108 (99%)	104 (97%)	3 (3%)	38	56
13	AH	183/184 (100%)	161 (88%)	22 (12%)	5	5
14	AI	106/107 (99%)	102 (96%)	4 (4%)	29	44
15	AJ	101/103 (98%)	96 (95%)	5 (5%)	22	33
16	AK	111/111 (100%)	98 (88%)	13 (12%)	5	6
17	AL	89/91 (98%)	75 (84%)	14 (16%)	2	2
18	AM	94/104 (90%)	81 (86%)	13 (14%)	3	4
19	AN	120/121 (99%)	116 (97%)	4 (3%)	33	50
20	AP	45/46 (98%)	44 (98%)	1 (2%)	45	65
21	AQ	142/143 (99%)	122 (86%)	20 (14%)	3	3
22	AR	97/102 (95%)	86 (89%)	11 (11%)	5	7
23	AS	58/61 (95%)	52 (90%)	6 (10%)	7	8
24	AU	126/127 (99%)	105 (83%)	21 (17%)	2	2
25	AV	88/90 (98%)	74 (84%)	14 (16%)	2	2
25	B6	86/90 (96%)	83 (96%)	3 (4%)	32	48
26	AW	53/56 (95%)	43 (81%)	10 (19%)	1	1
27	AX	55/60 (92%)	42 (76%)	13 (24%)	1	1
28	AY	22/42 (52%)	22 (100%)	0	100	100
29	AZ	155/168 (92%)	136 (88%)	19 (12%)	4	5
30	A0	34/35 (97%)	34 (100%)	0	100	100
31	A3	98/99 (99%)	96 (98%)	2 (2%)	48	67
31	B4	98/99 (99%)	89 (91%)	9 (9%)	8	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	BG	98/99 (99%)	97 (99%)	1 (1%)	68	82
32	AT	113/114 (99%)	93 (82%)	20 (18%)	2	2
33	AO	115/123 (94%)	97 (84%)	18 (16%)	2	2
34	BB	188/189 (100%)	186 (99%)	2 (1%)	65	81
35	BY	132/133 (99%)	131 (99%)	1 (1%)	73	86
36	BO	167/170 (98%)	162 (97%)	5 (3%)	36	53
37	BC	306/307 (100%)	304 (99%)	2 (1%)	76	87
38	B5	65/66 (98%)	60 (92%)	5 (8%)	12	16
38	BK	64/66 (97%)	62 (97%)	2 (3%)	35	52
39	BL	118/118 (100%)	115 (98%)	3 (2%)	42	60
40	Bf	46/47 (98%)	46 (100%)	0	100	100
41	BU	109/109 (100%)	109 (100%)	0	100	100
42	Bb	117/118 (99%)	116 (99%)	1 (1%)	70	84
43	Be	52/53 (98%)	51 (98%)	1 (2%)	50	69
44	BE	158/160 (99%)	139 (88%)	19 (12%)	5	5
45	Ba	84/84 (100%)	84 (100%)	0	100	100
46	BT	77/77 (100%)	75 (97%)	2 (3%)	40	59
47	BW	63/63 (100%)	61 (97%)	2 (3%)	34	51
48	Bi	61/62 (98%)	61 (100%)	0	100	100
49	BI	122/122 (100%)	122 (100%)	0	100	100
50	BR	86/87 (99%)	84 (98%)	2 (2%)	44	63
51	BQ	132/133 (99%)	129 (98%)	3 (2%)	44	63
52	BV	54/58 (93%)	54 (100%)	0	100	100
53	Bj	83/84 (99%)	81 (98%)	2 (2%)	43	62
54	BD	212/212 (100%)	206 (97%)	6 (3%)	38	56
55	BF	156/157 (99%)	154 (99%)	2 (1%)	61	77
56	BZ	79/80 (99%)	75 (95%)	4 (5%)	21	32
57	BP	102/102 (100%)	99 (97%)	3 (3%)	37	55
58	BM	160/161 (99%)	160 (100%)	0	100	100
59	BS	130/131 (99%)	129 (99%)	1 (1%)	73	86
60	Bd	82/82 (100%)	81 (99%)	1 (1%)	63	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
61	BN	149/151 (99%)	149 (100%)	0	100	100
62	Bg	37/39 (95%)	37 (100%)	0	100	100
63	Bc	74/74 (100%)	73 (99%)	1 (1%)	59	76
64	BJ	108/109 (99%)	107 (99%)	1 (1%)	70	84
65	Bl	72/72 (100%)	70 (97%)	2 (3%)	38	56
66	Bk	55/57 (96%)	55 (100%)	0	100	100
67	BA	182/186 (98%)	176 (97%)	6 (3%)	33	50
All	All	7748/7909 (98%)	7262 (94%)	486 (6%)	18	23

All (486) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ILE
4	A	13	LEU
4	A	50	PHE
4	A	62	LYS
4	A	70	THR
4	A	95	GLU
4	A	99	GLU
4	A	116	ARG
4	A	121	HIS
4	A	136	ARG
4	A	160	LEU
4	A	164	MET
4	A	171	ILE
4	A	176	VAL
4	A	184	ARG
4	A	188	ARG
5	H	92	LEU
5	H	100	LEU
5	H	118	LEU
5	H	119	LEU
5	H	120	GLU
5	H	123	VAL
5	H	149	VAL
5	H	161	ILE
5	H	166	VAL
5	H	214	MET
5	H	215	ILE
5	H	234	MET

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Mol	Chain	Res	Type
5	H	242	LEU
5	H	258	LYS
5	H	259	ASP
5	H	260	LEU
5	H	268	VAL
5	H	323	GLU
5	H	343	VAL
5	H	350	THR
5	H	359	ASP
5	H	369	LEU
5	H	374	LEU
5	H	378	ILE
5	H	379	ARG
5	H	382	LYS
5	H	383	ARG
5	H	384	PHE
5	H	385	ILE
6	AA	11	LYS
6	AA	13	LYS
6	AA	18	GLN
6	AA	26	ASP
6	AA	27	PHE
6	AA	31	VAL
6	AA	32	GLU
6	AA	35	LEU
6	AA	40	ASP
6	AA	51	VAL
6	AA	53	LEU
6	AA	54	LYS
6	AA	55	ASP
6	AA	57	THR
6	AA	60	PHE
6	AA	70	GLN
6	AA	74	VAL
6	AA	82	LYS
6	AA	94	ARG
6	AA	96	LEU
6	AA	97	VAL
6	AA	98	ARG
6	AA	99	ARG
6	AA	117	LYS
6	AA	118	LEU

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Mol	Chain	Res	Type
6	AA	120	VAL
6	AA	132	THR
6	AA	134	GLN
6	AA	135	GLU
6	AA	138	ILE
6	AA	140	LYS
6	AA	154	ASN
6	AA	170	GLU
6	AA	181	LEU
6	AA	182	LYS
6	AA	194	GLU
6	AA	196	GLU
7	AB	9	LEU
7	AB	19	ILE
7	AB	21	THR
7	AB	23	GLN
7	AB	24	LYS
7	AB	25	THR
7	AB	35	VAL
7	AB	36	ARG
7	AB	43	LEU
7	AB	46	ARG
7	AB	49	ASP
7	AB	54	VAL
7	AB	61	ARG
7	AB	74	LEU
7	AB	80	VAL
7	AB	85	GLU
7	AB	86	VAL
7	AB	114	VAL
7	AB	146	LEU
7	AB	147	LEU
7	AB	156	THR
7	AB	158	ASN
7	AB	164	LEU
7	AB	167	ILE
7	AB	171	LEU
7	AB	175	ILE
7	AB	178	ASN
7	AB	181	GLU
7	AB	185	ARG
7	AB	188	PHE

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Mol	Chain	Res	Type
7	AB	193	GLU
7	AB	196	GLU
7	AB	197	MET
8	AC	10	GLU
8	AC	21	ILE
8	AC	48	LEU
8	AC	61	GLU
9	AD	83	LEU
9	AD	93	LEU
9	AD	98	GLU
9	AD	138	ARG
9	AD	153	THR
9	AD	156	ARG
9	AD	169	MET
10	AE	20	TYR
10	AE	68	GLU
10	AE	73	VAL
10	AE	76	ARG
10	AE	85	VAL
10	AE	88	MET
10	AE	95	GLU
10	AE	106	ARG
10	AE	111	ILE
10	AE	122	ILE
10	AE	126	ARG
10	AE	131	ARG
10	AE	152	LEU
10	AE	156	ASP
10	AE	161	SER
10	AE	166	MET
10	AE	168	VAL
10	AE	174	LEU
10	AE	177	LEU
10	AE	180	GLU
10	AE	188	THR
10	AE	196	LYS
10	AE	203	LYS
10	AE	216	GLU
10	AE	219	GLU
10	AE	226	LEU
10	AE	228	GLU
11	AF	4	GLU

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Mol	Chain	Res	Type
11	AF	7	GLU
11	AF	16	TRP
11	AF	57	VAL
11	AF	66	LEU
11	AF	122	ILE
11	AF	217	MET
11	AF	229	MET
12	AG	33	ARG
12	AG	59	VAL
12	AG	77	ASP
13	AH	11	ILE
13	AH	14	GLU
13	AH	18	MET
13	AH	23	THR
13	AH	27	GLU
13	AH	40	GLU
13	AH	44	LEU
13	AH	67	LEU
13	AH	88	ARG
13	AH	93	LEU
13	AH	105	LYS
13	AH	108	PHE
13	AH	111	ILE
13	AH	113	LYS
13	AH	136	THR
13	AH	140	MET
13	AH	155	MET
13	AH	177	LYS
13	AH	203	LYS
13	AH	206	GLU
13	AH	208	GLU
13	AH	212	GLU
14	AI	4	LEU
14	AI	62	ARG
14	AI	69	ILE
14	AI	119	LYS
15	AJ	78	ILE
15	AJ	96	THR
15	AJ	102	GLU
15	AJ	117	ASP
15	AJ	124	LEU
16	AK	7	THR

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Mol	Chain	Res	Type
16	AK	18	VAL
16	AK	46	LEU
16	AK	49	LEU
16	AK	66	VAL
16	AK	67	GLN
16	AK	93	MET
16	AK	100	ILE
16	AK	104	ARG
16	AK	112	ARG
16	AK	114	THR
16	AK	124	LYS
16	AK	135	ARG
17	AL	23	ILE
17	AL	33	ARG
17	AL	34	MET
17	AL	66	LEU
17	AL	74	ASP
17	AL	75	ILE
17	AL	76	GLU
17	AL	82	MET
17	AL	85	ILE
17	AL	87	ARG
17	AL	88	ILE
17	AL	93	ASP
17	AL	98	ILE
17	AL	99	GLU
18	AM	13	LYS
18	AM	27	ILE
18	AM	30	ILE
18	AM	48	VAL
18	AM	53	ASP
18	AM	61	MET
18	AM	83	VAL
18	AM	90	LYS
18	AM	93	THR
18	AM	102	ILE
18	AM	117	ASP
18	AM	121	ILE
18	AM	124	ASP
19	AN	58	ILE
19	AN	67	SER
19	AN	76	GLN

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Mol	Chain	Res	Type
19	AN	100	HIS
20	AP	46	VAL
21	AQ	16	ARG
21	AQ	27	GLU
21	AQ	29	THR
21	AQ	33	ILE
21	AQ	34	GLU
21	AQ	35	ASN
21	AQ	39	LYS
21	AQ	40	LEU
21	AQ	41	ARG
21	AQ	60	ILE
21	AQ	65	LEU
21	AQ	70	ASP
21	AQ	76	LEU
21	AQ	84	LYS
21	AQ	95	LEU
21	AQ	118	SER
21	AQ	131	ARG
21	AQ	134	LYS
21	AQ	138	ARG
21	AQ	157	VAL
22	AR	4	ASP
22	AR	14	GLU
22	AR	27	LEU
22	AR	29	ILE
22	AR	38	VAL
22	AR	45	LYS
22	AR	49	VAL
22	AR	86	VAL
22	AR	94	LEU
22	AR	102	VAL
22	AR	103	VAL
23	AS	22	ASN
23	AS	37	GLU
23	AS	39	THR
23	AS	41	VAL
23	AS	43	SER
23	AS	62	GLU
24	AU	20	LEU
24	AU	22	GLU
24	AU	25	GLU

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Mol	Chain	Res	Type
24	AU	26	ILE
24	AU	30	GLU
24	AU	34	PHE
24	AU	35	VAL
24	AU	42	GLU
24	AU	44	LEU
24	AU	58	ILE
24	AU	68	VAL
24	AU	80	ARG
24	AU	88	GLU
24	AU	97	ILE
24	AU	100	LYS
24	AU	110	PHE
24	AU	112	GLU
24	AU	117	LYS
24	AU	129	LEU
24	AU	140	LEU
24	AU	143	ILE
25	AV	1	MET
25	AV	2	GLU
25	AV	12	LYS
25	AV	23	ILE
25	AV	30	THR
25	AV	34	LYS
25	AV	40	LEU
25	AV	45	ASP
25	AV	46	LEU
25	AV	76	ASP
25	AV	77	ARG
25	AV	79	LEU
25	AV	87	LEU
25	AV	96	LYS
26	AW	5	ARG
26	AW	7	VAL
26	AW	12	ARG
26	AW	16	LEU
26	AW	26	GLU
26	AW	29	VAL
26	AW	46	LEU
26	AW	57	ARG
26	AW	60	ILE
26	AW	63	VAL

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Mol	Chain	Res	Type
27	AX	5	GLU
27	AX	11	VAL
27	AX	12	ILE
27	AX	13	GLU
27	AX	28	LYS
27	AX	30	ARG
27	AX	32	LEU
27	AX	33	GLU
27	AX	40	VAL
27	AX	51	VAL
27	AX	57	LEU
27	AX	59	GLU
27	AX	62	ARG
29	AZ	10	GLU
29	AZ	17	ILE
29	AZ	23	LYS
29	AZ	40	LEU
29	AZ	44	VAL
29	AZ	50	ASN
29	AZ	80	ILE
29	AZ	87	ASN
29	AZ	90	LEU
29	AZ	94	VAL
29	AZ	117	MET
29	AZ	136	LEU
29	AZ	150	TYR
29	AZ	151	LEU
29	AZ	159	GLU
29	AZ	162	VAL
29	AZ	186	ASP
29	AZ	188	ARG
29	AZ	192	GLU
31	A3	58	ASP
31	A3	69	LEU
32	AT	9	ARG
32	AT	14	GLU
32	AT	16	LEU
32	AT	37	LYS
32	AT	43	GLU
32	AT	47	LEU
32	AT	48	LEU
32	AT	56	LYS

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Mol	Chain	Res	Type
32	AT	60	ASN
32	AT	68	ARG
32	AT	73	LEU
32	AT	75	GLU
32	AT	90	VAL
32	AT	92	VAL
32	AT	109	THR
32	AT	113	VAL
32	AT	115	HIS
32	AT	124	ARG
32	AT	129	VAL
32	AT	131	VAL
33	AO	10	VAL
33	AO	15	LEU
33	AO	31	VAL
33	AO	33	ILE
33	AO	40	CYS
33	AO	42	VAL
33	AO	57	GLU
33	AO	61	LYS
33	AO	64	GLU
33	AO	66	LEU
33	AO	67	GLN
33	AO	86	GLU
33	AO	100	MET
33	AO	112	ILE
33	AO	119	ARG
33	AO	126	VAL
33	AO	136	ARG
33	AO	139	GLN
34	BB	85	ILE
34	BB	127	THR
35	BY	104	GLU
36	BO	112	VAL
36	BO	137	ILE
36	BO	172	LEU
36	BO	179	GLU
36	BO	181	LEU
37	BC	56	ASP
37	BC	170	VAL
38	B5	23	VAL
38	B5	33	VAL

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Mol	Chain	Res	Type
38	B5	50	ILE
38	B5	60	ILE
38	B5	71	VAL
39	BL	69	VAL
39	BL	86	ASP
39	BL	115	THR
42	Bb	91	GLU
43	Be	14	THR
44	BE	3	ILE
44	BE	28	VAL
44	BE	32	ILE
44	BE	34	VAL
44	BE	57	ILE
44	BE	62	LYS
44	BE	63	LYS
44	BE	67	ASP
44	BE	71	ARG
44	BE	72	ARG
44	BE	118	ASP
44	BE	122	ASN
44	BE	123	ILE
44	BE	132	ILE
44	BE	134	ILE
44	BE	137	MET
44	BE	142	THR
44	BE	173	VAL
44	BE	184	VAL
46	BT	12	ILE
46	BT	75	SER
47	BW	56	THR
47	BW	63	ARG
50	BR	3	GLN
50	BR	77	VAL
38	BK	62	ILE
38	BK	70	GLU
51	BQ	56	LYS
51	BQ	71	LYS
51	BQ	111	GLU
53	Bj	28	ARG
53	Bj	90	GLU
31	BG	121	LEU
54	BD	9	ASN

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Mol	Chain	Res	Type
54	BD	27	ARG
54	BD	78	ARG
54	BD	92	THR
54	BD	222	VAL
54	BD	249	ARG
55	BF	26	VAL
55	BF	53	VAL
56	BZ	34	LEU
56	BZ	79	VAL
56	BZ	91	SER
56	BZ	96	LEU
25	B6	13	LEU
25	B6	46	LEU
25	B6	51	THR
57	BP	7	THR
57	BP	16	ARG
57	BP	69	LEU
59	BS	155	ARG
60	Bd	89	MET
63	Bc	29	VAL
64	BJ	63	VAL
65	Bl	59	GLU
65	Bl	75	LEU
31	B4	14	GLU
31	B4	20	LEU
31	B4	29	THR
31	B4	39	THR
31	B4	56	ASP
31	B4	62	ILE
31	B4	69	LEU
31	B4	78	ILE
31	B4	108	ARG
67	BA	8	ARG
67	BA	37	LEU
67	BA	57	HIS
67	BA	99	GLN
67	BA	158	ILE
67	BA	202	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (167) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	111	HIS
5	H	159	HIS
5	H	194	GLN
5	H	370	GLN
6	AA	18	GLN
6	AA	77	GLN
6	AA	78	ASN
6	AA	109	ASN
6	AA	154	ASN
7	AB	11	GLN
7	AB	108	ASN
7	AB	125	GLN
7	AB	145	ASN
8	AC	34	ASN
9	AD	65	GLN
9	AD	72	GLN
9	AD	120	GLN
9	AD	135	GLN
10	AE	67	ASN
10	AE	121	ASN
10	AE	141	ASN
10	AE	143	HIS
11	AF	58	ASN
11	AF	120	ASN
11	AF	196	ASN
12	AG	18	GLN
12	AG	37	GLN
12	AG	110	ASN
13	AH	38	ASN
13	AH	69	ASN
13	AH	90	HIS
13	AH	164	ASN
13	AH	193	ASN
14	AI	9	ASN
14	AI	64	GLN
14	AI	70	ASN
15	AJ	52	ASN
15	AJ	64	ASN
15	AJ	121	ASN
16	AK	74	GLN
20	AP	26	GLN
20	AP	34	HIS
21	AQ	5	HIS

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Mol	Chain	Res	Type
21	AQ	57	GLN
21	AQ	117	HIS
22	AR	74	ASN
22	AR	79	ASN
23	AS	30	HIS
24	AU	40	HIS
25	AV	11	ASN
26	AW	27	GLN
28	AY	34	HIS
29	AZ	77	ASN
29	AZ	95	GLN
30	A0	29	GLN
31	A3	65	HIS
32	AT	15	GLN
32	AT	60	ASN
32	AT	66	HIS
32	AT	84	HIS
32	AT	101	HIS
32	AT	114	GLN
32	AT	115	HIS
33	AO	20	GLN
33	AO	139	GLN
34	BB	8	GLN
34	BB	50	HIS
34	BB	202	HIS
34	BB	229	HIS
35	BY	14	ASN
35	BY	48	GLN
35	BY	98	GLN
35	BY	148	ASN
36	BO	42	ASN
36	BO	43	HIS
36	BO	44	HIS
36	BO	76	HIS
36	BO	109	HIS
37	BC	5	HIS
37	BC	88	GLN
37	BC	167	GLN
37	BC	241	HIS
37	BC	257	HIS
37	BC	270	GLN
37	BC	274	HIS

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Mol	Chain	Res	Type
37	BC	309	HIS
37	BC	348	GLN
39	BL	57	HIS
39	BL	84	ASN
40	Bf	19	GLN
40	Bf	20	ASN
40	Bf	38	HIS
41	BU	7	GLN
41	BU	96	HIS
42	Bb	26	GLN
42	Bb	104	HIS
42	Bb	119	GLN
43	Be	17	HIS
44	BE	31	ASN
44	BE	65	ASN
44	BE	110	HIS
44	BE	164	HIS
45	Ba	42	HIS
47	BW	40	ASN
48	Bi	55	GLN
49	BI	51	GLN
49	BI	119	HIS
50	BR	3	GLN
50	BR	19	HIS
50	BR	33	GLN
50	BR	42	HIS
50	BR	59	HIS
50	BR	89	HIS
50	BR	96	GLN
38	BK	31	ASN
51	BQ	58	GLN
51	BQ	67	HIS
51	BQ	75	HIS
51	BQ	112	GLN
52	BV	57	GLN
53	Bj	37	GLN
54	BD	9	ASN
54	BD	44	GLN
54	BD	213	ASN
54	BD	214	HIS
54	BD	229	HIS
54	BD	235	HIS

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Mol	Chain	Res	Type
55	BF	24	ASN
55	BF	74	HIS
55	BF	149	GLN
56	BZ	21	ASN
25	B6	11	ASN
25	B6	54	GLN
57	BP	10	ASN
57	BP	23	ASN
57	BP	43	GLN
57	BP	110	ASN
58	BM	25	GLN
58	BM	87	GLN
58	BM	97	GLN
58	BM	154	HIS
58	BM	174	ASN
58	BM	189	ASN
59	BS	45	ASN
59	BS	70	GLN
59	BS	97	ASN
59	BS	104	GLN
60	Bd	35	HIS
60	Bd	44	ASN
60	Bd	70	HIS
61	BN	38	ASN
61	BN	56	GLN
61	BN	59	GLN
61	BN	70	ASN
61	BN	81	ASN
61	BN	83	HIS
61	BN	97	ASN
61	BN	130	GLN
61	BN	179	GLN
63	Bc	17	GLN
63	Bc	18	HIS
63	Bc	28	ASN
64	BJ	47	HIS
64	BJ	102	ASN
31	B4	65	HIS
67	BA	162	ASN
67	BA	201	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3016/3018 (99%)	442 (14%)	20 (0%)
2	2	1495/1512 (98%)	209 (13%)	20 (1%)
3	3	125/128 (97%)	13 (10%)	1 (0%)
All	All	4636/4658 (99%)	664 (14%)	41 (0%)

All (664) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	12	G
1	1	28	A
1	1	39	A
1	1	51	A
1	1	52	G
1	1	55	U
1	1	57	A
1	1	58	A
1	1	59	C
1	1	69	U
1	1	75	G
1	1	81	C
1	1	82	C
1	1	85	A
1	1	88	G
1	1	94	G
1	1	95	G
1	1	98	C
1	1	99	U
1	1	100	G
1	1	101	U
1	1	102	C
1	1	104	C
1	1	105	C
1	1	107	G
1	1	115	G
1	1	116	G
1	1	118	U
1	1	120	A
1	1	121	G
1	1	122	G
1	1	123	A
1	1	125	A
1	1	127	U
1	1	148	C

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Mol	Chain	Res	Type
1	1	154	G
1	1	160	C
1	1	163	A
1	1	178	A
1	1	185	A
1	1	188	A
1	1	189	G
1	1	199	G
1	1	205	G
1	1	231	A
1	1	232	A
1	1	233	U
1	1	238	C
1	1	239	C
1	1	240	U
1	1	241	C
1	1	244	G
1	1	245	C
1	1	247	G
1	1	248	C
1	1	249	U
1	1	250	U
1	1	251	A
1	1	252	U
1	1	253	G
1	1	254	C
1	1	268	A
1	1	269	U
1	1	270	A
1	1	272	G
1	1	273	C
1	1	275	C
1	1	285	A
1	1	300	A
1	1	303	A
1	1	319	G
1	1	320	A
1	1	326	A
1	1	332	A
1	1	333	A
1	1	337	A
1	1	352	G

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Mol	Chain	Res	Type
1	1	370	G
1	1	393	C
1	1	408	G
1	1	416	G
1	1	417	U
1	1	422	C
1	1	424	C
1	1	429	A
1	1	430	U
1	1	431	G
1	1	433	G
1	1	438	U
1	1	439	C
1	1	447	A
1	1	448	A
1	1	449	G
1	1	456	U
1	1	466	C
1	1	472	G
1	1	484	G
1	1	485	A
1	1	493	G
1	1	501	A
1	1	507	G
1	1	516	C
1	1	517	G
1	1	522	A
1	1	523	C
1	1	529	G
1	1	544	U
1	1	545	A
1	1	553	G
1	1	560	G
1	1	565	G
1	1	575	C
1	1	611	A
1	1	621	G
1	1	635	G
1	1	657	A
1	1	661	C
1	1	683	A
1	1	684	G

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Mol	Chain	Res	Type
1	1	685	G
1	1	689	C
1	1	696	A
1	1	699	G
1	1	704	G
1	1	731	C
1	1	738	G
1	1	746	G
1	1	769	C
1	1	781	A
1	1	785	G
1	1	792	A
1	1	809	A
1	1	849	C
1	1	851	U
1	1	852	G
1	1	865	C
1	1	866	C
1	1	867	U
1	1	870	A
1	1	871	G
1	1	893	A
1	1	917	A
1	1	924	A
1	1	925	A
1	1	935	U
1	1	963	A
1	1	965	C
1	1	967	G
1	1	970	G
1	1	975	G
1	1	979	C
1	1	983	C
1	1	993	U
1	1	998	U
1	1	1015	A
1	1	1026	G
1	1	1027	G
1	1	1033	A
1	1	1035	G
1	1	1036	G
1	1	1043	G

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Mol	Chain	Res	Type
1	1	1053	A
1	1	1056	G
1	1	1063	C
1	1	1073	C
1	1	1079	G
1	1	1096	G
1	1	1101	A
1	1	1111	G
1	1	1118	A
1	1	1129	G
1	1	1131	G
1	1	1132	C
1	1	1133	A
1	1	1134	G
1	1	1140	G
1	1	1141	A
1	1	1143	A
1	1	1144	G
1	1	1148	C
1	1	1149	C
1	1	1159	U
1	1	1162	A
1	1	1164	C
1	1	1199	G
1	1	1200	G
1	1	1225	G
1	1	1231	A
1	1	1234	A
1	1	1235	A
1	1	1240	G
1	1	1241	A
1	1	1252	G
1	1	1261	G
1	1	1262	U
1	1	1263	G
1	1	1272	G
1	1	1281	C
1	1	1282	A
1	1	1288	U
1	1	1289	G
1	1	1297	C
1	1	1301	A

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Mol	Chain	Res	Type
1	1	1302	G
1	1	1303	A
1	1	1304	C
1	1	1305	A
1	1	1306	G
1	1	1307	C
1	1	1309	G
1	1	1310	G
1	1	1316	A
1	1	1317	G
1	1	1322	A
1	1	1325	A
1	1	1326	G
1	1	1339	A
1	1	1343	A
1	1	1344	G
1	1	1345	U
1	1	1346	G
1	1	1353	A
1	1	1359	C
1	1	1362	G
1	1	1363	U
1	1	1364	C
1	1	1365	G
1	1	1366	A
1	1	1367	G
1	1	1371	C
1	1	1387	G
1	1	1389	C
1	1	1393	G
1	1	1397	A
1	1	1411	G
1	1	1433	G
1	1	1443	C
1	1	1470	G
1	1	1514	C
1	1	1533	U
1	1	1560	A
1	1	1561	G
1	1	1577	A
1	1	1578	G
1	1	1580	C

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Mol	Chain	Res	Type
1	1	1601	U
1	1	1630	G
1	1	1639	A
1	1	1641	A
1	1	1645	A
1	1	1648	C
1	1	1657	A
1	1	1678	G
1	1	1685	A
1	1	1687	C
1	1	1692	G
1	1	1705	C
1	1	1714	G
1	1	1730	A
1	1	1731	U
1	1	1732	G
1	1	1748	A
1	1	1759	G
1	1	1761	G
1	1	1763	G
1	1	1782	G
1	1	1787	A
1	1	1788	A
1	1	1796	U
1	1	1799	C
1	1	1805	C
1	1	1808	U
1	1	1809	A
1	1	1810	G
1	1	1830	G
1	1	1840	A
1	1	1856	U
1	1	1857	U
1	1	1883	A
1	1	1890	C
1	1	1891	A
1	1	1895	G
1	1	1896	C
1	1	1901	G
1	1	1908	A
1	1	1920	U
1	1	1921	G

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Mol	Chain	Res	Type
1	1	1922	U
1	1	1923	C
1	1	1928	G
1	1	1929	A
1	1	1950	G
1	1	1972	G
1	1	1976	A
1	1	1987	G
1	1	1996	U
1	1	1997	A
1	1	2020	G
1	1	2029	A
1	1	2042	A
1	1	2056	C
1	1	2085	A
1	1	2095	A
1	1	2119	A
1	1	2142	A
1	1	2147	OMG
1	1	2154	A
1	1	2155	C
1	1	2156	U
1	1	2157	A
1	1	2167	U
1	1	2168	A
1	1	2170	G
1	1	2171	G
1	1	2177	A
1	1	2178	A
1	1	2179	A
1	1	2181	U
1	1	2196	U
1	1	2206	C
1	1	2208	U
1	1	2211	A
1	1	2212	U
1	1	2213	G
1	1	2232	U
1	1	2233	G
1	1	2234	U
1	1	2253	G
1	1	2267	G

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Mol	Chain	Res	Type
1	1	2270	C
1	1	2271	G
1	1	2272	C
1	1	2273	A
1	1	2276	C
1	1	2292	G
1	1	2295	A
1	1	2300	A
1	1	2301	G
1	1	2303	C
1	1	2309	G
1	1	2310	G
1	1	2333	G
1	1	2342	C
1	1	2343	G
1	1	2344	G
1	1	2348	G
1	1	2351	C
1	1	2352	G
1	1	2353	C
1	1	2370	G
1	1	2372	C
1	1	2373	G
1	1	2384	U
1	1	2388	G
1	1	2389	G
1	1	2393	G
1	1	2397	G
1	1	2398	A
1	1	2399	G
1	1	2406	A
1	1	2407	U
1	1	2408	G
1	1	2409	A
1	1	2412	C
1	1	2416	G
1	1	2426	C
1	1	2430	G
1	1	2431	C
1	1	2438	A
1	1	2446	A
1	1	2455	A

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Mol	Chain	Res	Type
1	1	2456	C
1	1	2468	G
1	1	2469	G
1	1	2488	A
1	1	2497	A
1	1	2498	A
1	1	2499	A
1	1	2510	G
1	1	2514	C
1	1	2518	A
1	1	2519	A
1	1	2536	U
1	1	2539	G
1	1	2540	G
1	1	2550	U
1	1	2551	A
1	1	2553	A
1	1	2556	G
1	1	2566	A
1	1	2574	C
1	1	2576	G
1	1	2588	A
1	1	2592	G
1	1	2617	G
1	1	2619	C
1	1	2636	C
1	1	2659	G
1	1	2664	A
1	1	2666	A
1	1	2673	C
1	1	2677	G
1	1	2680	A
1	1	2691	G
1	1	2706	C
1	1	2710	A
1	1	2723	C
1	1	2730	C
1	1	2733	5MC
1	1	2734	G
1	1	2735	C
1	1	2750	A
1	1	2761	G

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Mol	Chain	Res	Type
1	1	2766	A
1	1	2798	A
1	1	2799	G
1	1	2805	C
1	1	2810	G
1	1	2814	G
1	1	2831	G
1	1	2834	A
1	1	2835	G
1	1	2845	U
1	1	2846	A
1	1	2847	U
1	1	2861	U
1	1	2877	A
1	1	2878	G
1	1	2896	G
1	1	2906	G
1	1	2922	U
1	1	2945	G
1	1	2956	A
1	1	2957	C
1	1	2964	G
1	1	2978	A
1	1	2981	G
1	1	2987	A
1	1	2995	A
1	1	2996	G
1	1	3006	A
1	1	3021	U
2	2	45	U
2	2	52	C
2	2	54	G
2	2	57	U
2	2	59	A
2	2	72	A
2	2	76	G
2	2	80	G
2	2	81	U
2	2	82	C
2	2	86	U
2	2	88	U
2	2	89	G

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Mol	Chain	Res	Type
2	2	90	G
2	2	112	A
2	2	115	A
2	2	117	C
2	2	126	A
2	2	128	C
2	2	154	G
2	2	171	C
2	2	196	G
2	2	197	G
2	2	211	A
2	2	212	G
2	2	213	G
2	2	219	G
2	2	222	A
2	2	223	G
2	2	225	C
2	2	227	C
2	2	229	G
2	2	254	U
2	2	256	G
2	2	260	G
2	2	275	G
2	2	276	C
2	2	284	G
2	2	290	G
2	2	298	C
2	2	315	A
2	2	337	C
2	2	338	A
2	2	353	A
2	2	354	C
2	2	355	G
2	2	358	G
2	2	360	G
2	2	361	C
2	2	363	G
2	2	371	G
2	2	376	C
2	2	381	C
2	2	406	A
2	2	415	G

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Mol	Chain	Res	Type
2	2	420	G
2	2	424	C
2	2	426	G
2	2	436	U
2	2	437	U
2	2	461	A
2	2	465	G
2	2	474	A
2	2	477	G
2	2	478	C
2	2	484	G
2	2	485	C
2	2	493	G
2	2	497	U
2	2	498	A
2	2	499	A
2	2	500	U
2	2	513	A
2	2	530	U
2	2	533	G
2	2	539	A
2	2	542	C
2	2	543	G
2	2	562	A
2	2	571	C
2	2	600	G
2	2	620	U
2	2	632	A
2	2	636	4AC
2	2	637	G
2	2	640	G
2	2	642	U
2	2	654	A
2	2	670	A
2	2	677	G
2	2	681	G
2	2	684	C
2	2	689	G
2	2	690	U
2	2	691	G
2	2	701	C
2	2	715	G

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Mol	Chain	Res	Type
2	2	722	G
2	2	744	A
2	2	751	4AC
2	2	760	U
2	2	761	A
2	2	782	A
2	2	784	G
2	2	787	OMU
2	2	788	G
2	2	795	A
2	2	843	A
2	2	845	G
2	2	861	G
2	2	873	OMG
2	2	885	A
2	2	893	G
2	2	897	G
2	2	905	C
2	2	906	U
2	2	932	U
2	2	934	OMG
2	2	941	A
2	2	943	G
2	2	946	G
2	2	947	G
2	2	949	A
2	2	966	C
2	2	968	G
2	2	973	A
2	2	974	U
2	2	975	G
2	2	977	A
2	2	988	A
2	2	990	G
2	2	991	G
2	2	996	G
2	2	999	G
2	2	1000	G
2	2	1001	A
2	2	1003	G
2	2	1004	C
2	2	1005	G

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Mol	Chain	Res	Type
2	2	1030	U
2	2	1059	G
2	2	1060	U
2	2	1066	A
2	2	1104	C
2	2	1107	U
2	2	1110	G
2	2	1112	A
2	2	1132	C
2	2	1133	U
2	2	1134	G
2	2	1141	A
2	2	1142	U
2	2	1143	A
2	2	1149	G
2	2	1156	G
2	2	1157	G
2	2	1158	G
2	2	1170	A
2	2	1171	G
2	2	1176	G
2	2	1186	A
2	2	1187	A
2	2	1196	G
2	2	1201	A
2	2	1212	A
2	2	1215	G
2	2	1222	A
2	2	1230	U
2	2	1231	G
2	2	1232	C
2	2	1254	A
2	2	1274	G
2	2	1276	U
2	2	1279	G
2	2	1293	A
2	2	1294	C
2	2	1297	G
2	2	1310	U
2	2	1327	G
2	2	1338	U
2	2	1344	G

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Mol	Chain	Res	Type
2	2	1353	G
2	2	1357	C
2	2	1371	C
2	2	1393	G
2	2	1397	G
2	2	1398	G
2	2	1400	C
2	2	1401	U
2	2	1420	U
2	2	1421	U
2	2	1422	C
2	2	1424	G
2	2	1427	G
2	2	1437	A
2	2	1456	G
2	2	1461	A
2	2	1466	G
2	2	1468	A
2	2	1471	A
2	2	1475	U
2	2	1486	G
2	2	1488	MA6
2	2	1498	5MC
2	2	1499	G
2	2	1503	A
2	2	1504	C
2	2	1505	5MC
2	2	1508	C
3	3	5	C
3	3	9	G
3	3	25	C
3	3	30	C
3	3	56	U
3	3	57	A
3	3	58	A
3	3	79	G
3	3	80	U
3	3	89	C
3	3	95	G
3	3	96	G
3	3	115	G

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	68	U
1	1	117	G
1	1	120	A
1	1	122	G
1	1	238	C
1	1	656	A
1	1	866	C
1	1	870	A
1	1	992	C
1	1	1035	G
1	1	1303	A
1	1	1306	G
1	1	1363	U
1	1	1364	C
1	1	1365	G
1	1	1731	U
1	1	2397	G
1	1	2455	A
1	1	2733	5MC
1	1	2986	U
2	2	170	U
2	2	211	A
2	2	212	G
2	2	283	A
2	2	464	A
2	2	498	A
2	2	499	A
2	2	653	U
2	2	669	U
2	2	676	G
2	2	680	OMG
2	2	812	C
2	2	842	U
2	2	972	G
2	2	1119	C
2	2	1141	A
2	2	1155	G
2	2	1157	G
2	2	1231	G
2	2	1460	G
3	3	79	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	5MC	2	535	2	18,22,23	0.94	2 (11%)	26,32,35	1.14	2 (7%)
1	5MC	1	2162	1	18,22,23	0.95	2 (11%)	26,32,35	1.11	2 (7%)
2	OMU	2	64	2	19,22,23	1.24	3 (15%)	26,31,34	1.75	5 (19%)
1	4AC	1	1885	1	21,24,25	1.02	2 (9%)	29,34,37	1.32	4 (13%)
2	OMU	2	774	2	19,22,23	1.26	3 (15%)	26,31,34	1.77	4 (15%)
1	4AC	1	341	1	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
2	4AC	2	590	2	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	OMU	1	2784	1	19,22,23	1.20	3 (15%)	26,31,34	1.71	5 (19%)
1	OMG	1	2138	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	4AC	1	922	1	21,24,25	1.04	2 (9%)	29,34,37	1.39	4 (13%)
1	4AC	1	2287	1	21,24,25	1.01	2 (9%)	29,34,37	1.37	4 (13%)
2	OMU	2	1177	2	19,22,23	1.22	3 (15%)	26,31,34	1.71	4 (15%)
1	4AC	1	2585	1	21,24,25	1.06	2 (9%)	29,34,37	1.72	6 (20%)
1	4AC	1	1068	1	21,24,25	1.03	2 (9%)	29,34,37	1.34	4 (13%)
2	4AC	2	868	2	21,24,25	1.04	2 (9%)	29,34,37	1.33	5 (17%)
2	4AC	2	1233	2	21,24,25	1.01	2 (9%)	29,34,37	1.39	4 (13%)
2	MA6	2	1487	2	23,26,27	1.47	4 (17%)	34,38,41	2.11	10 (29%)
1	4AC	1	1594	68,1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
2	6MZ	2	1469	68,2	22,25,26	1.50	4 (18%)	30,36,39	2.19	10 (33%)
2	4AC	2	319	2	21,24,25	1.03	2 (9%)	29,34,37	1.33	4 (13%)
2	4AC	2	1479	2	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
1	5MC	1	2203	1	18,22,23	0.95	2 (11%)	26,32,35	1.11	2 (7%)
2	4AC	2	303	2	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
2	4AC	2	718	2	21,24,25	1.01	2 (9%)	29,34,37	1.39	4 (13%)
2	4AC	2	286	2	21,24,25	1.03	2 (9%)	29,34,37	1.39	4 (13%)
2	UR3	2	1467	2	19,22,23	0.95	0	26,32,35	1.44	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	4AC	2	1028	2	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	2062	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	2083	1	21,24,25	1.04	2 (9%)	29,34,37	1.27	4 (13%)
1	4AC	1	2865	1	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
2	4AC	2	17	2	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	1554	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	641	1	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	1962	1	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
1	5MC	1	2733	1	18,22,23	0.97	2 (11%)	26,32,35	1.28	3 (11%)
1	4AC	1	1755	1	21,24,25	1.04	2 (9%)	29,34,37	1.56	4 (13%)
1	4AC	1	2642	1	21,24,25	1.02	2 (9%)	29,34,37	1.31	4 (13%)
2	OMC	2	846	2	19,22,23	0.81	0	26,31,34	0.79	0
1	4AC	1	2925	1	21,24,25	1.04	2 (9%)	29,34,37	1.33	5 (17%)
1	4AC	1	1878	1	21,24,25	1.01	2 (9%)	29,34,37	1.51	4 (13%)
1	4AC	1	1065	1	21,24,25	1.02	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	2136	1	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
2	OMG	2	1069	2	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
2	OMU	2	787	2	19,22,23	1.23	3 (15%)	26,31,34	1.84	5 (19%)
1	4AC	1	1557	1	21,24,25	1.01	2 (9%)	29,34,37	1.31	4 (13%)
2	OMG	2	471	2	23,26,27	1.21	3 (13%)	33,38,41	1.90	6 (18%)
1	4AC	1	2966	1	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	22	1	21,24,25	1.04	2 (9%)	29,34,37	1.32	5 (17%)
1	4AC	1	451	1	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	2329	1	21,24,25	1.03	2 (9%)	29,34,37	1.36	4 (13%)
1	5MC	1	2163	1	18,22,23	0.95	2 (11%)	26,32,35	1.10	2 (7%)
1	4AC	1	229	1	21,24,25	1.04	2 (9%)	29,34,37	1.32	4 (13%)
2	4AC	2	511	2	21,24,25	1.03	2 (9%)	29,34,37	1.39	4 (13%)
1	4AC	1	243	1	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
2	A2M	2	373	2	22,25,26	1.46	4 (18%)	31,36,39	2.05	8 (25%)
1	4AC	1	1934	1	21,24,25	1.01	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	1695	1	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
1	5MC	1	2183	1	18,22,23	0.95	2 (11%)	26,32,35	1.12	2 (7%)
1	4AC	1	533	1	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
2	OMC	2	129	2	19,22,23	0.81	0	26,31,34	0.81	0
1	4AC	1	2027	1	21,24,25	1.03	2 (9%)	29,34,37	1.34	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	1	2992	1	21,24,25	1.04	2 (9%)	29,34,37	0.87	2 (6%)
2	4AC	2	731	2	21,24,25	1.02	2 (9%)	29,34,37	1.40	4 (13%)
2	OMC	2	773	2	19,22,23	0.84	0	26,31,34	0.94	1 (3%)
1	OMG	1	328	1	23,26,27	1.21	3 (13%)	33,38,41	1.95	7 (21%)
1	OMG	1	789	1	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
1	4AC	1	694	1	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
2	LHH	2	1041	2	22,25,26	0.34	0	29,35,38	0.49	1 (3%)
2	OMC	2	1040	2	19,22,23	1.17	2 (10%)	26,31,34	0.92	1 (3%)
2	LHH	2	250	2	22,25,26	0.31	0	29,35,38	0.47	0
1	4AC	1	1765	1	21,24,25	1.04	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	1	1938	1	21,24,25	1.03	2 (9%)	29,34,37	1.33	4 (13%)
1	OMG	1	2147	1	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
1	OMG	1	2144	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	4AC	1	802	1	21,24,25	1.00	2 (9%)	29,34,37	1.38	4 (13%)
2	5MC	2	875	2	18,22,23	0.96	2 (11%)	26,32,35	1.17	3 (11%)
1	5MC	1	2093	1	18,22,23	0.95	2 (11%)	26,32,35	1.11	2 (7%)
1	4AC	1	1048	1	21,24,25	1.03	2 (9%)	29,34,37	1.39	4 (13%)
2	4AC	2	703	2	21,24,25	0.98	2 (9%)	29,34,37	2.22	2 (6%)
2	4AC	2	626	2	21,24,25	1.02	2 (9%)	29,34,37	1.42	4 (13%)
2	4AC	2	1184	2	21,24,25	1.06	2 (9%)	29,34,37	1.59	3 (10%)
2	5MC	2	1374	2	18,22,23	0.97	2 (11%)	26,32,35	1.14	3 (11%)
1	OMG	1	2678	1	23,26,27	1.20	3 (13%)	33,38,41	1.96	6 (18%)
1	4AC	1	2249	1	21,24,25	1.04	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	1293	1	21,24,25	1.02	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	2545	1	21,24,25	1.02	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	2937	68,1	21,24,25	1.03	2 (9%)	29,34,37	1.56	4 (13%)
2	OMG	2	519	2	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
1	4AC	1	2608	1	21,24,25	1.05	2 (9%)	29,34,37	1.73	5 (17%)
1	4AC	1	2960	1	21,24,25	1.02	2 (9%)	29,34,37	1.29	4 (13%)
3	4AC	3	32	3	21,24,25	1.02	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	1667	1	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	1460	1	21,24,25	1.02	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	1621	1	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
2	4AC	2	851	2	21,24,25	1.04	2 (9%)	29,34,37	1.30	5 (17%)
1	4AC	1	835	1	21,24,25	1.03	2 (9%)	29,34,37	1.34	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	1	1550	1	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	1	3004	1	21,24,25	1.03	2 (9%)	29,34,37	1.30	4 (13%)
1	4AC	1	2908	1	21,24,25	1.03	2 (9%)	29,34,37	1.30	4 (13%)
2	B8H	2	938	2	19,22,23	0.80	1 (5%)	22,32,35	0.85	0
1	A2M	1	1055	1	22,25,26	1.47	4 (18%)	31,36,39	2.07	8 (25%)
1	4AC	1	60	1	21,24,25	1.04	2 (9%)	29,34,37	1.36	4 (13%)
1	OMG	1	923	68,1	23,26,27	1.19	3 (13%)	33,38,41	1.95	7 (21%)
2	OMU	2	20	2	19,22,23	1.22	2 (10%)	26,31,34	1.77	5 (19%)
1	4AC	1	2001	1	21,24,25	1.03	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	829	1	21,24,25	1.02	2 (9%)	29,34,37	1.32	4 (13%)
2	4AC	2	839	2	21,24,25	1.02	2 (9%)	29,34,37	1.37	4 (13%)
2	OMU	2	830	2	19,22,23	1.25	3 (15%)	26,31,34	1.74	5 (19%)
2	OMU	2	1380	2	19,22,23	1.26	4 (21%)	26,31,34	1.71	5 (19%)
2	4AC	2	379	2	21,24,25	1.01	2 (9%)	29,34,37	1.39	4 (13%)
2	OMG	2	873	2	23,26,27	1.20	3 (13%)	33,38,41	1.97	6 (18%)
2	MA6	2	1488	2	23,26,27	1.48	4 (17%)	34,38,41	2.13	9 (26%)
1	4AC	1	1873	1	21,24,25	1.02	2 (9%)	29,34,37	1.31	4 (13%)
2	OMG	2	680	2	23,26,27	1.24	3 (13%)	33,38,41	2.08	6 (18%)
1	4AC	1	91	1	21,24,25	1.03	2 (9%)	29,34,37	1.44	4 (13%)
2	5MC	2	1496	2	18,22,23	0.93	2 (11%)	26,32,35	1.09	2 (7%)
1	4AC	1	161	1	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
2	5MC	2	1505	2	18,22,23	0.97	2 (11%)	26,32,35	1.13	2 (7%)
2	4AC	2	1239	2	21,24,25	1.03	2 (9%)	29,34,37	1.36	4 (13%)
2	4AC	2	848	2	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
2	4AC	2	957	2	21,24,25	1.03	2 (9%)	29,34,37	1.36	4 (13%)
2	OMG	2	657	2	23,26,27	1.27	3 (13%)	33,38,41	2.01	6 (18%)
2	4AC	2	828	2	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
2	5MC	2	1202	2	18,22,23	0.93	1 (5%)	26,32,35	1.01	2 (7%)
1	4AC	1	357	1	21,24,25	1.01	2 (9%)	29,34,37	1.36	4 (13%)
2	OMG	2	934	2	23,26,27	1.22	3 (13%)	33,38,41	1.97	6 (18%)
2	4AC	2	751	2	21,24,25	1.02	2 (9%)	29,34,37	1.32	4 (13%)
1	4AC	1	1780	1	21,24,25	1.02	1 (4%)	29,34,37	1.55	4 (13%)
2	4AC	2	1147	2	21,24,25	1.00	2 (9%)	29,34,37	1.46	4 (13%)
2	4AC	2	394	2	21,24,25	1.05	2 (9%)	29,34,37	1.55	4 (13%)
2	OMG	2	467	2	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	1	1867	1	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
2	4AC	2	479	2	21,24,25	1.02	2 (9%)	29,34,37	1.43	4 (13%)
1	4AC	1	1222	68,1	21,24,25	1.02	2 (9%)	29,34,37	1.32	4 (13%)
2	4AC	2	636	2	21,24,25	1.05	2 (9%)	29,34,37	2.16	6 (20%)
2	5MC	2	1498	2	18,22,23	0.93	2 (11%)	26,32,35	1.41	5 (19%)
2	OMC	2	1376	2	19,22,23	0.81	0	26,31,34	0.79	0
1	4AC	1	981	1	21,24,25	1.01	2 (9%)	29,34,37	1.28	4 (13%)
1	4AC	1	314	1	21,24,25	1.03	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	1243	1	21,24,25	1.03	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	1	1662	1	21,24,25	1.01	2 (9%)	29,34,37	1.38	4 (13%)
1	5MC	1	2198	1	18,22,23	0.94	2 (11%)	26,32,35	1.13	2 (7%)
1	4AC	1	2548	1	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	2570	1	21,24,25	1.01	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	1	1617	1	21,24,25	1.01	2 (9%)	29,34,37	1.36	4 (13%)
2	4AC	2	546	2	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	2495	1	21,24,25	1.03	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	2718	1	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	211	1	21,24,25	1.03	2 (9%)	29,34,37	1.33	4 (13%)
2	4AC	2	53	2	21,24,25	1.00	2 (9%)	29,34,37	1.43	4 (13%)
1	4AC	1	136	1	21,24,25	1.01	2 (9%)	29,34,37	1.32	4 (13%)
1	LHH	1	616	1	22,25,26	0.30	0	29,35,38	0.46	0
2	OMG	2	913	2	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
2	5MC	2	1025	2	18,22,23	0.95	2 (11%)	26,32,35	1.15	3 (11%)
1	A2M	1	2173	1	22,25,26	1.44	4 (18%)	31,36,39	2.10	10 (32%)
1	OMC	1	615	1	19,22,23	0.82	0	26,31,34	0.95	1 (3%)
1	4AC	1	458	1	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
2	5MC	2	693	2	18,22,23	0.95	2 (11%)	26,32,35	1.12	2 (7%)
1	OMC	1	1948	1	19,22,23	0.81	0	26,31,34	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5MC	2	535	2	-	0/7/25/26	0/2/2/2
1	5MC	1	2162	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMU	2	64	2	-	0/9/27/28	0/2/2/2
1	4AC	1	1885	1	-	0/11/29/30	0/2/2/2
2	OMU	2	774	2	-	0/9/27/28	0/2/2/2
1	4AC	1	341	1	-	0/11/29/30	0/2/2/2
2	4AC	2	590	2	-	0/11/29/30	0/2/2/2
1	OMU	1	2784	1	-	0/9/27/28	0/2/2/2
1	OMG	1	2138	1	-	0/9/27/28	0/3/3/3
1	4AC	1	922	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2287	1	-	0/11/29/30	0/2/2/2
2	OMU	2	1177	2	-	1/9/27/28	0/2/2/2
1	4AC	1	2585	1	-	3/11/29/30	0/2/2/2
1	4AC	1	1068	1	-	0/11/29/30	0/2/2/2
2	4AC	2	868	2	-	0/11/29/30	0/2/2/2
2	4AC	2	1233	2	-	0/11/29/30	0/2/2/2
2	MA6	2	1487	2	-	0/11/29/30	0/3/3/3
1	4AC	1	1594	68,1	-	0/11/29/30	0/2/2/2
2	6MZ	2	1469	68,2	-	0/9/27/28	0/3/3/3
2	4AC	2	319	2	-	0/11/29/30	0/2/2/2
2	4AC	2	1479	2	-	0/11/29/30	0/2/2/2
1	5MC	1	2203	1	-	0/7/25/26	0/2/2/2
2	4AC	2	303	2	-	0/11/29/30	0/2/2/2
2	4AC	2	718	2	-	0/11/29/30	0/2/2/2
2	4AC	2	286	2	-	0/11/29/30	0/2/2/2
2	UR3	2	1467	2	-	0/7/25/26	0/2/2/2
2	4AC	2	1028	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2062	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2083	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2865	1	-	0/11/29/30	0/2/2/2
2	4AC	2	17	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1554	1	-	0/11/29/30	0/2/2/2
1	4AC	1	641	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1962	1	-	0/11/29/30	0/2/2/2
1	5MC	1	2733	1	-	4/7/25/26	0/2/2/2
1	4AC	1	1755	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2642	1	-	0/11/29/30	0/2/2/2
2	OMC	2	846	2	-	0/9/27/28	0/2/2/2
1	4AC	1	2925	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1878	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1065	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2136	1	-	0/11/29/30	0/2/2/2
2	OMG	2	1069	2	-	1/9/27/28	0/3/3/3
2	OMU	2	787	2	-	6/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	1	1557	1	-	0/11/29/30	0/2/2/2
2	OMG	2	471	2	-	0/9/27/28	0/3/3/3
1	4AC	1	2966	1	-	0/11/29/30	0/2/2/2
1	4AC	1	22	1	-	0/11/29/30	0/2/2/2
1	4AC	1	451	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2329	1	-	0/11/29/30	0/2/2/2
1	5MC	1	2163	1	-	0/7/25/26	0/2/2/2
1	4AC	1	229	1	-	0/11/29/30	0/2/2/2
2	4AC	2	511	2	-	0/11/29/30	0/2/2/2
1	4AC	1	243	1	-	0/11/29/30	0/2/2/2
2	A2M	2	373	2	-	0/9/27/28	0/3/3/3
1	4AC	1	1934	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1695	1	-	0/11/29/30	0/2/2/2
1	5MC	1	2183	1	-	0/7/25/26	0/2/2/2
1	4AC	1	533	1	-	0/11/29/30	0/2/2/2
2	OMC	2	129	2	-	0/9/27/28	0/2/2/2
1	4AC	1	2027	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2992	1	-	2/11/29/30	0/2/2/2
2	4AC	2	731	2	-	0/11/29/30	0/2/2/2
2	OMC	2	773	2	-	0/9/27/28	0/2/2/2
1	OMG	1	328	1	-	0/9/27/28	0/3/3/3
1	OMG	1	789	1	-	2/9/27/28	0/3/3/3
1	4AC	1	694	1	-	0/11/29/30	0/2/2/2
2	LHH	2	1041	2	-	0/13/31/32	0/2/2/2
2	OMC	2	1040	2	-	0/9/27/28	0/2/2/2
2	LHH	2	250	2	-	1/13/31/32	0/2/2/2
1	4AC	1	1765	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1938	1	-	0/11/29/30	0/2/2/2
1	OMG	1	2147	1	-	3/9/27/28	0/3/3/3
1	OMG	1	2144	1	-	1/9/27/28	0/3/3/3
1	4AC	1	802	1	-	0/11/29/30	0/2/2/2
2	5MC	2	875	2	-	0/7/25/26	0/2/2/2
1	5MC	1	2093	1	-	0/7/25/26	0/2/2/2
1	4AC	1	1048	1	-	0/11/29/30	0/2/2/2
2	4AC	2	703	2	-	3/11/29/30	0/2/2/2
2	4AC	2	626	2	-	0/11/29/30	0/2/2/2
2	4AC	2	1184	2	-	0/11/29/30	0/2/2/2
2	5MC	2	1374	2	-	2/7/25/26	0/2/2/2
1	OMG	1	2678	1	-	1/9/27/28	0/3/3/3
1	4AC	1	2249	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1293	1	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	1	2545	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2937	68,1	-	1/11/29/30	0/2/2/2
2	OMG	2	519	2	-	0/9/27/28	0/3/3/3
1	4AC	1	2608	1	-	3/11/29/30	0/2/2/2
1	4AC	1	2960	1	-	0/11/29/30	0/2/2/2
3	4AC	3	32	3	-	0/11/29/30	0/2/2/2
1	4AC	1	1667	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1460	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1621	1	-	0/11/29/30	0/2/2/2
2	4AC	2	851	2	-	0/11/29/30	0/2/2/2
1	4AC	1	835	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1550	1	-	0/11/29/30	0/2/2/2
1	4AC	1	3004	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2908	1	-	0/11/29/30	0/2/2/2
2	B8H	2	938	2	-	0/7/25/26	0/2/2/2
1	A2M	1	1055	1	-	1/9/27/28	0/3/3/3
1	4AC	1	60	1	-	0/11/29/30	0/2/2/2
1	OMG	1	923	68,1	-	2/9/27/28	0/3/3/3
2	OMU	2	20	2	-	6/9/27/28	0/2/2/2
1	4AC	1	2001	1	-	0/11/29/30	0/2/2/2
1	4AC	1	829	1	-	0/11/29/30	0/2/2/2
2	4AC	2	839	2	-	0/11/29/30	0/2/2/2
2	OMU	2	830	2	-	0/9/27/28	0/2/2/2
2	OMU	2	1380	2	-	2/9/27/28	0/2/2/2
2	4AC	2	379	2	-	0/11/29/30	0/2/2/2
2	OMG	2	873	2	-	1/9/27/28	0/3/3/3
2	MA6	2	1488	2	-	1/11/29/30	0/3/3/3
1	4AC	1	1873	1	-	0/11/29/30	0/2/2/2
2	OMG	2	680	2	-	1/9/27/28	0/3/3/3
1	4AC	1	91	1	-	0/11/29/30	0/2/2/2
2	5MC	2	1496	2	-	0/7/25/26	0/2/2/2
1	4AC	1	161	1	-	0/11/29/30	0/2/2/2
2	5MC	2	1505	2	-	2/7/25/26	0/2/2/2
2	4AC	2	1239	2	-	0/11/29/30	0/2/2/2
2	4AC	2	848	2	-	0/11/29/30	0/2/2/2
2	4AC	2	957	2	-	0/11/29/30	0/2/2/2
2	OMG	2	657	2	-	0/9/27/28	0/3/3/3
2	4AC	2	828	2	-	0/11/29/30	0/2/2/2
2	5MC	2	1202	2	-	1/7/25/26	0/2/2/2
1	4AC	1	357	1	-	0/11/29/30	0/2/2/2
2	OMG	2	934	2	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4AC	2	751	2	-	2/11/29/30	0/2/2/2
1	4AC	1	1780	1	-	0/11/29/30	0/2/2/2
2	4AC	2	1147	2	-	0/11/29/30	0/2/2/2
2	4AC	2	394	2	-	0/11/29/30	0/2/2/2
2	OMG	2	467	2	-	0/9/27/28	0/3/3/3
1	4AC	1	1867	1	-	0/11/29/30	0/2/2/2
2	4AC	2	479	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1222	68,1	-	0/11/29/30	0/2/2/2
2	4AC	2	636	2	-	2/11/29/30	0/2/2/2
2	5MC	2	1498	2	-	5/7/25/26	0/2/2/2
2	OMC	2	1376	2	-	1/9/27/28	0/2/2/2
1	4AC	1	981	1	-	0/11/29/30	0/2/2/2
1	4AC	1	314	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1243	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1662	1	-	0/11/29/30	0/2/2/2
1	5MC	1	2198	1	-	0/7/25/26	0/2/2/2
1	4AC	1	2548	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2570	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1617	1	-	0/11/29/30	0/2/2/2
2	4AC	2	546	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2495	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2718	1	-	0/11/29/30	0/2/2/2
1	4AC	1	211	1	-	0/11/29/30	0/2/2/2
2	4AC	2	53	2	-	0/11/29/30	0/2/2/2
1	4AC	1	136	1	-	0/11/29/30	0/2/2/2
1	LHH	1	616	1	-	0/13/31/32	0/2/2/2
2	OMG	2	913	2	-	1/9/27/28	0/3/3/3
2	5MC	2	1025	2	-	0/7/25/26	0/2/2/2
1	A2M	1	2173	1	-	0/9/27/28	0/3/3/3
1	OMC	1	615	1	-	1/9/27/28	0/2/2/2
1	4AC	1	458	1	-	0/11/29/30	0/2/2/2
2	5MC	2	693	2	-	0/7/25/26	0/2/2/2
1	OMC	1	1948	1	-	0/9/27/28	0/2/2/2

All (331) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1469	6MZ	C5-C4	4.66	1.47	1.39
2	2	1488	MA6	C5-C4	4.60	1.47	1.39
2	2	1487	MA6	C5-C4	4.54	1.47	1.39
1	1	1055	A2M	C5-C4	4.44	1.47	1.39
2	2	373	A2M	C5-C4	4.44	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2173	A2M	C5-C4	4.33	1.47	1.39
2	2	657	OMG	C5-C4	3.30	1.48	1.38
2	2	394	4AC	C5-C4	3.25	1.47	1.40
2	2	680	OMG	C5-C4	3.13	1.47	1.38
1	1	2992	4AC	C5-C4	3.10	1.47	1.40
1	1	2147	OMG	C5-C4	3.09	1.47	1.38
1	1	2138	OMG	C5-C4	3.07	1.47	1.38
2	2	471	OMG	C5-C4	3.06	1.47	1.38
2	2	519	OMG	C5-C4	3.03	1.47	1.38
2	2	1069	OMG	C5-C4	3.03	1.47	1.38
1	1	1765	4AC	C5-C4	3.02	1.47	1.40
2	2	873	OMG	C5-C4	3.02	1.47	1.38
2	2	934	OMG	C5-C4	3.02	1.47	1.38
1	1	2083	4AC	C5-C4	3.01	1.47	1.40
1	1	1695	4AC	C5-C4	3.01	1.47	1.40
1	1	2733	5MC	C6-C5	3.01	1.39	1.34
2	2	1028	4AC	C5-C4	3.00	1.47	1.40
2	2	467	OMG	C5-C4	3.00	1.47	1.38
1	1	829	4AC	C5-C4	3.00	1.47	1.40
1	1	2144	OMG	C5-C4	2.99	1.47	1.38
1	1	229	4AC	C5-C4	2.99	1.47	1.40
1	1	1867	4AC	C5-C4	2.99	1.47	1.40
1	1	2908	4AC	C5-C4	2.99	1.47	1.40
1	1	2001	4AC	C5-C4	2.99	1.47	1.40
2	2	851	4AC	C5-C4	2.98	1.47	1.40
1	1	328	OMG	C5-C4	2.98	1.47	1.38
1	1	1938	4AC	C5-C4	2.98	1.47	1.40
1	1	3004	4AC	C5-C4	2.98	1.47	1.40
1	1	2136	4AC	C5-C4	2.98	1.47	1.40
1	1	2495	4AC	C5-C4	2.98	1.47	1.40
1	1	2548	4AC	C5-C4	2.98	1.47	1.40
1	1	2329	4AC	C5-C4	2.97	1.47	1.40
1	1	533	4AC	C5-C4	2.97	1.47	1.40
1	1	314	4AC	C5-C4	2.97	1.47	1.40
1	1	2960	4AC	C5-C4	2.97	1.47	1.40
1	1	211	4AC	C5-C4	2.97	1.47	1.40
2	2	590	4AC	C5-C4	2.96	1.47	1.40
1	1	1962	4AC	C5-C4	2.96	1.47	1.40
1	1	2925	4AC	C5-C4	2.96	1.47	1.40
1	1	641	4AC	C5-C4	2.96	1.47	1.40
1	1	243	4AC	C5-C4	2.96	1.47	1.40
1	1	22	4AC	C5-C4	2.95	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1621	4AC	C5-C4	2.95	1.47	1.40
1	1	922	4AC	C5-C4	2.95	1.47	1.40
2	2	848	4AC	C5-C4	2.95	1.47	1.40
1	1	835	4AC	C5-C4	2.95	1.47	1.40
1	1	1667	4AC	C5-C4	2.95	1.47	1.40
2	2	17	4AC	C5-C4	2.95	1.47	1.40
1	1	2027	4AC	C5-C4	2.95	1.47	1.40
1	1	2865	4AC	C5-C4	2.95	1.47	1.40
1	1	694	4AC	C5-C4	2.94	1.47	1.40
1	1	1243	4AC	C5-C4	2.94	1.47	1.40
2	2	868	4AC	C5-C4	2.94	1.47	1.40
1	1	2642	4AC	C5-C4	2.94	1.47	1.40
1	1	2570	4AC	C5-C4	2.94	1.47	1.40
1	1	341	4AC	C5-C4	2.94	1.47	1.40
1	1	2966	4AC	C5-C4	2.94	1.47	1.40
1	1	2249	4AC	C5-C4	2.94	1.47	1.40
1	1	789	OMG	C5-C4	2.94	1.46	1.38
2	2	546	4AC	C5-C4	2.94	1.47	1.40
1	1	161	4AC	C5-C4	2.93	1.47	1.40
1	1	458	4AC	C5-C4	2.93	1.47	1.40
1	1	60	4AC	C5-C4	2.93	1.47	1.40
1	1	136	4AC	C5-C4	2.93	1.47	1.40
1	1	2718	4AC	C5-C4	2.93	1.47	1.40
2	2	913	OMG	C5-C4	2.93	1.46	1.38
3	3	32	4AC	C5-C4	2.93	1.47	1.40
1	1	1222	4AC	C5-C4	2.93	1.47	1.40
1	1	2678	OMG	C5-C4	2.93	1.46	1.38
1	1	1873	4AC	C5-C4	2.92	1.47	1.40
2	2	303	4AC	C5-C4	2.92	1.47	1.40
1	1	451	4AC	C5-C4	2.92	1.47	1.40
2	2	1479	4AC	C5-C4	2.92	1.47	1.40
1	1	2545	4AC	C5-C4	2.92	1.47	1.40
1	1	923	OMG	C5-C4	2.91	1.46	1.38
1	1	1617	4AC	C5-C4	2.91	1.47	1.40
1	1	1048	4AC	C5-C4	2.90	1.47	1.40
1	1	1460	4AC	C5-C4	2.90	1.47	1.40
1	1	2062	4AC	C5-C4	2.90	1.47	1.40
1	1	1554	4AC	C5-C4	2.89	1.47	1.40
2	2	1184	4AC	C5-C4	2.89	1.47	1.40
2	2	319	4AC	C5-C4	2.89	1.47	1.40
1	1	1068	4AC	C5-C4	2.89	1.47	1.40
1	1	1065	4AC	C5-C4	2.89	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1550	4AC	C5-C4	2.89	1.47	1.40
1	1	1594	4AC	C5-C4	2.89	1.47	1.40
2	2	751	4AC	C5-C4	2.89	1.47	1.40
2	2	511	4AC	C5-C4	2.88	1.47	1.40
1	1	1557	4AC	C5-C4	2.88	1.47	1.40
2	2	286	4AC	C5-C4	2.88	1.47	1.40
1	1	981	4AC	C5-C4	2.88	1.47	1.40
1	1	1662	4AC	C5-C4	2.87	1.47	1.40
1	1	1885	4AC	C5-C4	2.87	1.47	1.40
2	2	1239	4AC	C5-C4	2.87	1.47	1.40
1	1	2937	4AC	C5-C4	2.87	1.47	1.40
1	1	357	4AC	C5-C4	2.86	1.47	1.40
2	2	957	4AC	C5-C4	2.85	1.46	1.40
1	1	1934	4AC	C5-C4	2.85	1.46	1.40
2	2	1233	4AC	C5-C4	2.84	1.46	1.40
2	2	828	4AC	C5-C4	2.83	1.46	1.40
1	1	1293	4AC	C5-C4	2.83	1.46	1.40
1	1	2287	4AC	C5-C4	2.83	1.46	1.40
2	2	479	4AC	C5-C4	2.82	1.46	1.40
2	2	718	4AC	C5-C4	2.82	1.46	1.40
2	2	1202	5MC	C6-C5	2.81	1.39	1.34
2	2	657	OMG	C6-N1	-2.81	1.33	1.38
1	1	802	4AC	C5-C4	2.81	1.46	1.40
2	2	1469	6MZ	C5-C6	2.80	1.49	1.41
2	2	839	4AC	C5-C4	2.80	1.46	1.40
2	2	53	4AC	C5-C4	2.80	1.46	1.40
1	1	1755	4AC	C5-C4	2.78	1.46	1.40
2	2	1487	MA6	C5-C6	2.78	1.48	1.41
1	1	1878	4AC	C5-C4	2.78	1.46	1.40
2	2	379	4AC	C5-C4	2.76	1.46	1.40
2	2	1147	4AC	C5-C4	2.75	1.46	1.40
1	1	1780	4AC	C5-C4	2.75	1.46	1.40
2	2	787	OMU	C4-N3	-2.75	1.33	1.38
2	2	1488	MA6	C5-C6	2.74	1.48	1.41
1	1	328	OMG	C6-N1	-2.73	1.33	1.38
1	1	91	4AC	C5-C4	2.73	1.46	1.40
1	1	2203	5MC	C6-C5	2.72	1.39	1.34
2	2	471	OMG	C6-N1	-2.72	1.33	1.38
1	1	2163	5MC	C6-C5	2.72	1.39	1.34
2	2	774	OMU	C4-N3	-2.71	1.33	1.38
2	2	626	4AC	C5-C4	2.71	1.46	1.40
2	2	20	OMU	C4-N3	-2.71	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2162	5MC	C6-C5	2.70	1.39	1.34
2	2	731	4AC	C5-C4	2.70	1.46	1.40
2	2	1380	OMU	C4-N3	-2.70	1.33	1.38
2	2	1025	5MC	C6-C5	2.69	1.39	1.34
1	1	2093	5MC	C6-C5	2.68	1.39	1.34
1	1	2585	4AC	C5-C4	2.68	1.46	1.40
2	2	934	OMG	C6-N1	-2.67	1.33	1.38
2	2	1505	5MC	C6-C5	2.67	1.39	1.34
1	1	2183	5MC	C6-C5	2.66	1.39	1.34
2	2	873	OMG	C6-N1	-2.66	1.33	1.38
2	2	830	OMU	C4-N3	-2.66	1.33	1.38
2	2	373	A2M	C5-C6	2.66	1.48	1.41
1	1	2608	4AC	C5-C4	2.65	1.46	1.40
2	2	535	5MC	C6-C5	2.64	1.38	1.34
1	1	2173	A2M	C5-C6	2.64	1.48	1.41
1	1	1055	A2M	C5-C6	2.63	1.48	1.41
2	2	875	5MC	C6-C5	2.62	1.38	1.34
1	1	2678	OMG	C6-N1	-2.62	1.34	1.38
2	2	693	5MC	C6-C5	2.61	1.38	1.34
1	1	2198	5MC	C6-C5	2.60	1.38	1.34
2	2	1177	OMU	C4-N3	-2.60	1.33	1.38
1	1	2138	OMG	C6-N1	-2.60	1.34	1.38
1	1	2784	OMU	C4-N3	-2.60	1.33	1.38
2	2	1374	5MC	C6-C5	2.60	1.38	1.34
1	1	789	OMG	C6-N1	-2.60	1.34	1.38
1	1	2144	OMG	C6-N1	-2.59	1.34	1.38
2	2	64	OMU	C4-N3	-2.58	1.33	1.38
2	2	1069	OMG	C6-N1	-2.57	1.34	1.38
1	1	923	OMG	C6-N1	-2.56	1.34	1.38
2	2	519	OMG	C6-N1	-2.55	1.34	1.38
2	2	1374	5MC	C6-N1	-2.55	1.33	1.38
2	2	1496	5MC	C6-N1	-2.55	1.33	1.38
2	2	467	OMG	C6-N1	-2.55	1.34	1.38
2	2	680	OMG	C6-N1	-2.54	1.34	1.38
1	1	2147	OMG	C6-N1	-2.53	1.34	1.38
2	2	787	OMU	C2-N3	-2.53	1.33	1.38
2	2	913	OMG	C6-N1	-2.51	1.34	1.38
1	1	2585	4AC	C4-N3	-2.51	1.28	1.32
2	2	657	OMG	C5-N7	-2.49	1.34	1.39
2	2	703	4AC	C5-C4	2.47	1.46	1.40
2	2	1184	4AC	C4-N3	-2.47	1.28	1.32
2	2	1498	5MC	C6-C5	2.47	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1505	5MC	C6-N1	-2.46	1.33	1.38
2	2	1496	5MC	C6-C5	2.42	1.38	1.34
1	1	2608	4AC	C4-N3	-2.42	1.28	1.32
1	1	229	4AC	C4-N3	-2.42	1.28	1.32
2	2	875	5MC	C6-N1	-2.40	1.33	1.38
1	1	22	4AC	C4-N3	-2.38	1.28	1.32
2	2	751	4AC	C4-N3	-2.38	1.28	1.32
2	2	286	4AC	C4-N3	-2.37	1.28	1.32
2	2	839	4AC	C4-N3	-2.37	1.28	1.32
2	2	535	5MC	C6-N1	-2.37	1.34	1.38
1	1	2093	5MC	C6-N1	-2.36	1.34	1.38
2	2	731	4AC	C4-N3	-2.36	1.28	1.32
2	2	851	4AC	C4-N3	-2.35	1.28	1.32
1	1	2198	5MC	C6-N1	-2.35	1.34	1.38
2	2	693	5MC	C6-N1	-2.34	1.34	1.38
1	1	1055	A2M	C8-N7	2.34	1.36	1.31
1	1	2173	A2M	C8-N7	2.33	1.36	1.31
2	2	828	4AC	C4-N3	-2.33	1.28	1.32
2	2	511	4AC	C4-N3	-2.33	1.28	1.32
2	2	373	A2M	C8-N7	2.33	1.36	1.31
1	1	2183	5MC	C6-N1	-2.33	1.34	1.38
2	2	20	OMU	C2-N3	-2.33	1.33	1.38
1	1	2203	5MC	C6-N1	-2.33	1.34	1.38
1	1	2083	4AC	C4-N3	-2.32	1.28	1.32
1	1	2784	OMU	C2-N3	-2.31	1.33	1.38
2	2	1025	5MC	C6-N1	-2.31	1.34	1.38
2	2	1498	5MC	C6-N1	-2.31	1.34	1.38
2	2	957	4AC	C4-N3	-2.31	1.28	1.32
2	2	938	B8H	C2-N1	2.31	1.42	1.38
1	1	2925	4AC	C4-N3	-2.30	1.28	1.32
1	1	981	4AC	C4-N3	-2.30	1.28	1.32
1	1	1885	4AC	C4-N3	-2.30	1.28	1.32
1	1	1243	4AC	C4-N3	-2.30	1.28	1.32
1	1	1055	A2M	C5-N7	-2.29	1.34	1.39
2	2	471	OMG	C5-N7	-2.29	1.34	1.39
2	2	319	4AC	C4-N3	-2.29	1.28	1.32
1	1	3004	4AC	C4-N3	-2.29	1.28	1.32
2	2	868	4AC	C4-N3	-2.29	1.28	1.32
1	1	328	OMG	C5-N7	-2.29	1.34	1.39
1	1	2163	5MC	C6-N1	-2.29	1.34	1.38
1	1	1873	4AC	C4-N3	-2.28	1.28	1.32
1	1	1048	4AC	C4-N3	-2.28	1.28	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	934	OMG	C5-N7	-2.28	1.34	1.39
2	2	64	OMU	C2-N3	-2.27	1.33	1.38
2	2	1488	MA6	C5-N7	-2.27	1.34	1.39
1	1	2162	5MC	C6-N1	-2.27	1.34	1.38
2	2	626	4AC	C4-N3	-2.27	1.28	1.32
1	1	2495	4AC	C4-N3	-2.27	1.28	1.32
2	2	636	4AC	C5-C4	2.26	1.45	1.40
2	2	373	A2M	C5-N7	-2.26	1.34	1.39
2	2	519	OMG	C5-N7	-2.26	1.34	1.39
1	1	2249	4AC	C4-N3	-2.26	1.28	1.32
1	1	1557	4AC	C4-N3	-2.26	1.28	1.32
2	2	1469	6MZ	C8-N7	2.26	1.35	1.31
1	1	835	4AC	C4-N3	-2.26	1.28	1.32
1	1	91	4AC	C4-N3	-2.26	1.28	1.32
1	1	2147	OMG	C5-N7	-2.25	1.34	1.39
2	2	1040	OMC	C5-C4	-2.25	1.37	1.42
1	1	922	4AC	C4-N3	-2.25	1.28	1.32
1	1	2678	OMG	C5-N7	-2.25	1.34	1.39
1	1	1068	4AC	C4-N3	-2.25	1.28	1.32
1	1	1621	4AC	C4-N3	-2.25	1.28	1.32
2	2	830	OMU	C2-N3	-2.25	1.34	1.38
1	1	1460	4AC	C4-N3	-2.24	1.28	1.32
1	1	1594	4AC	C4-N3	-2.24	1.28	1.32
2	2	1239	4AC	C4-N3	-2.24	1.28	1.32
1	1	1938	4AC	C4-N3	-2.24	1.28	1.32
2	2	590	4AC	C4-N3	-2.23	1.28	1.32
1	1	789	OMG	C5-N7	-2.23	1.34	1.39
1	1	2173	A2M	C5-N7	-2.23	1.34	1.39
1	1	314	4AC	C4-N3	-2.23	1.28	1.32
1	1	641	4AC	C4-N3	-2.23	1.28	1.32
2	2	680	OMG	C5-N7	-2.23	1.34	1.39
2	2	1069	OMG	C5-N7	-2.23	1.34	1.39
1	1	2144	OMG	C5-N7	-2.22	1.34	1.39
1	1	923	OMG	C5-N7	-2.22	1.34	1.39
1	1	1765	4AC	C4-N3	-2.22	1.28	1.32
2	2	1177	OMU	C2-N3	-2.22	1.34	1.38
1	1	1934	4AC	C4-N3	-2.21	1.29	1.32
1	1	2062	4AC	C4-N3	-2.21	1.29	1.32
1	1	2908	4AC	C4-N3	-2.21	1.29	1.32
1	1	2960	4AC	C4-N3	-2.21	1.29	1.32
1	1	1293	4AC	C4-N3	-2.21	1.29	1.32
1	1	694	4AC	C4-N3	-2.21	1.29	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	774	OMU	C2-N3	-2.21	1.34	1.38
1	1	2027	4AC	C4-N3	-2.21	1.29	1.32
2	2	379	4AC	C4-N3	-2.21	1.29	1.32
1	1	357	4AC	C4-N3	-2.21	1.29	1.32
1	1	829	4AC	C4-N3	-2.21	1.29	1.32
2	2	873	OMG	C5-N7	-2.21	1.34	1.39
2	2	467	OMG	C5-N7	-2.20	1.34	1.39
2	2	64	OMU	C5-C4	-2.20	1.38	1.43
1	1	1554	4AC	C4-N3	-2.19	1.29	1.32
1	1	161	4AC	C4-N3	-2.19	1.29	1.32
1	1	2138	OMG	C5-N7	-2.19	1.34	1.39
2	2	1380	OMU	C2-N3	-2.18	1.34	1.38
1	1	1222	4AC	C4-N3	-2.18	1.29	1.32
1	1	2642	4AC	C4-N3	-2.18	1.29	1.32
2	2	303	4AC	C4-N3	-2.18	1.29	1.32
1	1	1878	4AC	C4-N3	-2.18	1.29	1.32
2	2	1040	OMC	C6-N1	-2.18	1.32	1.38
1	1	211	4AC	C4-N3	-2.18	1.29	1.32
2	2	1487	MA6	C5-N7	-2.18	1.34	1.39
1	1	533	4AC	C4-N3	-2.17	1.29	1.32
2	2	913	OMG	C5-N7	-2.17	1.34	1.39
2	2	830	OMU	C5-C4	-2.17	1.38	1.43
1	1	1667	4AC	C4-N3	-2.17	1.29	1.32
2	2	1028	4AC	C4-N3	-2.17	1.29	1.32
1	1	2136	4AC	C4-N3	-2.17	1.29	1.32
1	1	1867	4AC	C4-N3	-2.17	1.29	1.32
2	2	636	4AC	C2-N3	2.16	1.40	1.36
1	1	451	4AC	C4-N3	-2.16	1.29	1.32
1	1	2865	4AC	C4-N3	-2.16	1.29	1.32
1	1	2966	4AC	C4-N3	-2.16	1.29	1.32
2	2	848	4AC	C4-N3	-2.16	1.29	1.32
1	1	2733	5MC	C6-N1	-2.15	1.34	1.38
1	1	2718	4AC	C4-N3	-2.15	1.29	1.32
1	1	2548	4AC	C4-N3	-2.15	1.29	1.32
1	1	136	4AC	C4-N3	-2.15	1.29	1.32
2	2	17	4AC	C4-N3	-2.15	1.29	1.32
2	2	1469	6MZ	C5-N7	-2.15	1.35	1.39
1	1	2992	4AC	C4-N3	-2.15	1.29	1.32
1	1	341	4AC	C4-N3	-2.15	1.29	1.32
2	2	1233	4AC	C4-N3	-2.14	1.29	1.32
1	1	2287	4AC	C4-N3	-2.14	1.29	1.32
1	1	1065	4AC	C4-N3	-2.14	1.29	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1962	4AC	C4-N3	-2.14	1.29	1.32
1	1	2001	4AC	C4-N3	-2.14	1.29	1.32
1	1	2329	4AC	C4-N3	-2.14	1.29	1.32
2	2	1479	4AC	C4-N3	-2.13	1.29	1.32
2	2	718	4AC	C4-N3	-2.13	1.29	1.32
1	1	1617	4AC	C4-N3	-2.13	1.29	1.32
2	2	1488	MA6	C8-N7	2.13	1.35	1.31
1	1	1662	4AC	C4-N3	-2.13	1.29	1.32
1	1	243	4AC	C4-N3	-2.12	1.29	1.32
2	2	479	4AC	C4-N3	-2.11	1.29	1.32
2	2	53	4AC	C4-N3	-2.11	1.29	1.32
2	2	546	4AC	C4-N3	-2.11	1.29	1.32
1	1	1550	4AC	C4-N3	-2.10	1.29	1.32
1	1	458	4AC	C4-N3	-2.10	1.29	1.32
1	1	2570	4AC	C4-N3	-2.10	1.29	1.32
2	2	1380	OMU	C5-C4	-2.09	1.39	1.43
2	2	1487	MA6	C8-N7	2.09	1.35	1.31
1	1	2545	4AC	C4-N3	-2.08	1.29	1.32
1	1	2937	4AC	C4-N3	-2.08	1.29	1.32
1	1	802	4AC	C4-N3	-2.08	1.29	1.32
1	1	60	4AC	C4-N3	-2.08	1.29	1.32
1	1	1695	4AC	C4-N3	-2.07	1.29	1.32
3	3	32	4AC	C4-N3	-2.06	1.29	1.32
2	2	1380	OMU	C2-N1	2.06	1.41	1.38
2	2	1177	OMU	C5-C4	-2.05	1.39	1.43
2	2	703	4AC	C2-N3	2.05	1.40	1.36
2	2	787	OMU	C5-C4	-2.05	1.39	1.43
2	2	774	OMU	C5-C4	-2.05	1.39	1.43
1	1	1755	4AC	C4-N3	-2.04	1.29	1.32
2	2	394	4AC	C4-N3	-2.04	1.29	1.32
2	2	1147	4AC	C4-N3	-2.01	1.29	1.32
1	1	2784	OMU	C5-C4	-2.01	1.39	1.43

All (643) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	703	4AC	N4-C4-N3	8.33	127.82	113.85
2	2	703	4AC	C5-C4-N4	-7.74	109.48	122.92
2	2	657	OMG	C5-C4-N3	-6.66	117.66	128.46
2	2	680	OMG	C5-C4-N3	-6.57	117.81	128.46
1	1	1055	A2M	C5-C4-N3	-6.38	118.42	126.75
2	2	873	OMG	C5-C4-N3	-6.30	118.24	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	373	A2M	C5-C4-N3	-6.24	118.61	126.75
2	2	519	OMG	C5-C4-N3	-6.20	118.40	128.46
1	1	2147	OMG	C5-C4-N3	-6.18	118.43	128.46
1	1	2678	OMG	C5-C4-N3	-6.16	118.46	128.46
2	2	1488	MA6	C5-C4-N3	-6.15	118.72	126.75
1	1	2144	OMG	C5-C4-N3	-6.15	118.49	128.46
2	2	471	OMG	C5-C4-N3	-6.14	118.50	128.46
1	1	2138	OMG	C5-C4-N3	-6.14	118.50	128.46
1	1	2173	A2M	C5-C4-N3	-6.13	118.75	126.75
2	2	934	OMG	C5-C4-N3	-6.12	118.53	128.46
1	1	328	OMG	C5-C4-N3	-6.10	118.56	128.46
2	2	1069	OMG	C5-C4-N3	-6.08	118.59	128.46
2	2	467	OMG	C5-C4-N3	-6.06	118.62	128.46
2	2	394	4AC	O7-C7-N4	6.04	131.60	121.82
1	1	789	OMG	C5-C4-N3	-5.99	118.74	128.46
1	1	923	OMG	C5-C4-N3	-5.93	118.84	128.46
2	2	1487	MA6	C5-C4-N3	-5.90	119.06	126.75
2	2	1469	6MZ	C5-C4-N3	-5.87	119.09	126.75
2	2	1467	UR3	C4-N3-C2	-5.86	119.05	124.56
2	2	913	OMG	C5-C4-N3	-5.72	119.18	128.46
2	2	636	4AC	N4-C4-N3	5.68	123.39	113.85
2	2	636	4AC	O7-C7-N4	5.58	130.85	121.82
2	2	636	4AC	C5-C4-N4	-5.44	113.46	122.92
2	2	1184	4AC	CM7-C7-N4	-5.26	106.20	115.29
2	2	1184	4AC	O7-C7-N4	5.16	130.17	121.82
2	2	657	OMG	N9-C4-N3	5.09	136.15	125.94
2	2	680	OMG	C2-N3-C4	5.04	121.28	112.30
2	2	873	OMG	C2-N3-C4	5.00	121.21	112.30
1	1	1780	4AC	O7-C7-N4	4.97	129.87	121.82
1	1	2678	OMG	C2-N3-C4	4.94	121.09	112.30
1	1	2144	OMG	C2-N3-C4	4.91	121.05	112.30
2	2	467	OMG	C2-N3-C4	4.89	121.02	112.30
1	1	923	OMG	C2-N3-C4	4.89	121.02	112.30
1	1	789	OMG	C2-N3-C4	4.89	121.01	112.30
2	2	934	OMG	C2-N3-C4	4.89	121.01	112.30
1	1	2138	OMG	C2-N3-C4	4.88	121.00	112.30
1	1	1878	4AC	O7-C7-N4	4.88	129.72	121.82
1	1	2147	OMG	C2-N3-C4	4.88	120.99	112.30
2	2	519	OMG	C2-N3-C4	4.87	120.98	112.30
2	2	787	OMU	C4-N3-C2	-4.87	120.15	126.58
2	2	1069	OMG	C2-N3-C4	4.87	120.98	112.30
1	1	1055	A2M	N3-C4-N9	4.85	135.08	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1755	4AC	O7-C7-N4	4.85	129.66	121.82
1	1	91	4AC	O7-C7-N4	4.84	129.66	121.82
2	2	657	OMG	C2-N3-C4	4.84	120.92	112.30
2	2	839	4AC	O7-C7-N4	4.83	129.63	121.82
2	2	373	A2M	N3-C4-N9	4.82	135.02	127.08
1	1	328	OMG	C2-N3-C4	4.80	120.85	112.30
1	1	2937	4AC	C5-C4-N4	-4.79	114.60	122.92
2	2	913	OMG	C2-N3-C4	4.79	120.84	112.30
2	2	479	4AC	O7-C7-N4	4.79	129.56	121.82
2	2	731	4AC	O7-C7-N4	4.78	129.55	121.82
2	2	680	OMG	N9-C4-N3	4.76	135.51	125.94
2	2	471	OMG	C2-N3-C4	4.76	120.77	112.30
2	2	1233	4AC	O7-C7-N4	4.75	129.51	121.82
2	2	828	4AC	O7-C7-N4	4.75	129.51	121.82
2	2	1147	4AC	O7-C7-N4	4.74	129.49	121.82
2	2	20	OMU	C4-N3-C2	-4.74	120.33	126.58
2	2	286	4AC	O7-C7-N4	4.73	129.47	121.82
2	2	873	OMG	N9-C4-N3	4.72	135.42	125.94
1	1	2173	A2M	N3-C4-N9	4.71	134.85	127.08
2	2	626	4AC	O7-C7-N4	4.71	129.45	121.82
1	1	2147	OMG	N9-C4-N3	4.71	135.39	125.94
1	1	2608	4AC	N4-C4-N3	4.70	121.74	113.85
2	2	379	4AC	O7-C7-N4	4.70	129.42	121.82
2	2	718	4AC	O7-C7-N4	4.69	129.41	121.82
2	2	511	4AC	O7-C7-N4	4.68	129.39	121.82
2	2	957	4AC	O7-C7-N4	4.64	129.32	121.82
1	1	1293	4AC	O7-C7-N4	4.63	129.32	121.82
1	1	2937	4AC	N4-C4-N3	4.63	121.62	113.85
1	1	2678	OMG	N9-C4-N3	4.63	135.23	125.94
2	2	53	4AC	O7-C7-N4	4.62	129.29	121.82
2	2	519	OMG	N9-C4-N3	4.62	135.22	125.94
2	2	471	OMG	N9-C4-N3	4.60	135.18	125.94
2	2	1239	4AC	O7-C7-N4	4.60	129.26	121.82
1	1	2138	OMG	N9-C4-N3	4.59	135.16	125.94
1	1	2144	OMG	N9-C4-N3	4.59	135.15	125.94
2	2	1488	MA6	N3-C4-N9	4.59	134.64	127.08
2	2	774	OMU	N3-C2-N1	4.59	120.98	114.89
2	2	774	OMU	C4-N3-C2	-4.57	120.55	126.58
1	1	2608	4AC	C5-C4-N4	-4.56	115.00	122.92
1	1	328	OMG	N9-C4-N3	4.55	135.07	125.94
2	2	1177	OMU	C4-N3-C2	-4.50	120.64	126.58
1	1	1934	4AC	O7-C7-N4	4.50	129.10	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2784	OMU	C4-N3-C2	-4.50	120.65	126.58
1	1	2545	4AC	O7-C7-N4	4.50	129.09	121.82
1	1	2585	4AC	N4-C4-N3	4.49	121.39	113.85
2	2	1069	OMG	N9-C4-N3	4.49	134.96	125.94
1	1	1065	4AC	O7-C7-N4	4.48	129.08	121.82
1	1	1460	4AC	O7-C7-N4	4.48	129.07	121.82
1	1	1554	4AC	O7-C7-N4	4.48	129.07	121.82
1	1	789	OMG	N9-C4-N3	4.48	134.93	125.94
1	1	1243	4AC	O7-C7-N4	4.46	129.04	121.82
1	1	923	OMG	N9-C4-N3	4.46	134.89	125.94
3	3	32	4AC	O7-C7-N4	4.45	129.03	121.82
2	2	1487	MA6	C2-N1-C6	4.45	122.27	111.75
2	2	590	4AC	O7-C7-N4	4.45	129.02	121.82
2	2	934	OMG	N9-C4-N3	4.45	134.87	125.94
1	1	1048	4AC	O7-C7-N4	4.45	129.01	121.82
1	1	2136	4AC	O7-C7-N4	4.44	129.01	121.82
2	2	787	OMU	N3-C2-N1	4.44	120.79	114.89
1	1	533	4AC	O7-C7-N4	4.44	129.01	121.82
2	2	17	4AC	O7-C7-N4	4.44	129.01	121.82
1	1	1662	4AC	O7-C7-N4	4.44	129.01	121.82
2	2	751	4AC	O7-C7-N4	4.44	129.01	121.82
2	2	830	OMU	C4-N3-C2	-4.44	120.72	126.58
1	1	458	4AC	O7-C7-N4	4.44	129.00	121.82
2	2	64	OMU	C4-N3-C2	-4.44	120.73	126.58
2	2	467	OMG	N9-C4-N3	4.44	134.84	125.94
1	1	1962	4AC	O7-C7-N4	4.43	129.00	121.82
1	1	1617	4AC	O7-C7-N4	4.43	128.99	121.82
2	2	303	4AC	O7-C7-N4	4.43	128.99	121.82
1	1	341	4AC	O7-C7-N4	4.42	128.98	121.82
2	2	1487	MA6	N3-C4-N9	4.42	134.36	127.08
1	1	2249	4AC	O7-C7-N4	4.42	128.97	121.82
2	2	1028	4AC	O7-C7-N4	4.42	128.97	121.82
1	1	2570	4AC	O7-C7-N4	4.41	128.96	121.82
1	1	1765	4AC	O7-C7-N4	4.41	128.96	121.82
1	1	1873	4AC	O7-C7-N4	4.41	128.96	121.82
1	1	1550	4AC	O7-C7-N4	4.41	128.95	121.82
1	1	243	4AC	O7-C7-N4	4.41	128.95	121.82
1	1	1867	4AC	O7-C7-N4	4.40	128.94	121.82
1	1	314	4AC	O7-C7-N4	4.40	128.93	121.82
1	1	922	4AC	O7-C7-N4	4.39	128.93	121.82
1	1	2548	4AC	O7-C7-N4	4.39	128.93	121.82
2	2	1488	MA6	C2-N1-C6	4.39	122.12	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2062	4AC	O7-C7-N4	4.39	128.92	121.82
1	1	1938	4AC	O7-C7-N4	4.39	128.92	121.82
1	1	2287	4AC	O7-C7-N4	4.39	128.92	121.82
1	1	1222	4AC	O7-C7-N4	4.39	128.92	121.82
1	1	451	4AC	O7-C7-N4	4.39	128.92	121.82
1	1	229	4AC	O7-C7-N4	4.39	128.92	121.82
1	1	1594	4AC	O7-C7-N4	4.38	128.91	121.82
1	1	2718	4AC	O7-C7-N4	4.38	128.91	121.82
1	1	2966	4AC	O7-C7-N4	4.38	128.91	121.82
1	1	802	4AC	O7-C7-N4	4.38	128.91	121.82
1	1	1667	4AC	O7-C7-N4	4.38	128.91	121.82
1	1	1695	4AC	O7-C7-N4	4.38	128.90	121.82
2	2	1469	6MZ	C6-C5-N7	4.37	137.12	132.39
2	2	1479	4AC	O7-C7-N4	4.37	128.90	121.82
1	1	641	4AC	O7-C7-N4	4.37	128.89	121.82
1	1	1068	4AC	O7-C7-N4	4.37	128.88	121.82
1	1	1621	4AC	O7-C7-N4	4.37	128.88	121.82
1	1	2329	4AC	O7-C7-N4	4.37	128.88	121.82
1	1	694	4AC	O7-C7-N4	4.36	128.88	121.82
2	2	546	4AC	O7-C7-N4	4.36	128.87	121.82
1	1	357	4AC	O7-C7-N4	4.36	128.87	121.82
1	1	60	4AC	O7-C7-N4	4.35	128.86	121.82
1	1	835	4AC	O7-C7-N4	4.35	128.86	121.82
2	2	848	4AC	O7-C7-N4	4.35	128.86	121.82
1	1	161	4AC	O7-C7-N4	4.34	128.85	121.82
1	1	2865	4AC	O7-C7-N4	4.34	128.85	121.82
1	1	211	4AC	O7-C7-N4	4.34	128.84	121.82
1	1	1557	4AC	O7-C7-N4	4.34	128.84	121.82
1	1	1885	4AC	O7-C7-N4	4.33	128.83	121.82
1	1	136	4AC	O7-C7-N4	4.33	128.83	121.82
1	1	3004	4AC	O7-C7-N4	4.33	128.82	121.82
2	2	20	OMU	N3-C2-N1	4.33	120.64	114.89
1	1	2495	4AC	O7-C7-N4	4.32	128.81	121.82
1	1	829	4AC	O7-C7-N4	4.32	128.81	121.82
2	2	1380	OMU	C4-N3-C2	-4.32	120.89	126.58
1	1	2027	4AC	O7-C7-N4	4.30	128.78	121.82
2	2	319	4AC	O7-C7-N4	4.30	128.78	121.82
1	1	2908	4AC	O7-C7-N4	4.30	128.77	121.82
1	1	2001	4AC	O7-C7-N4	4.30	128.77	121.82
2	2	1469	6MZ	N3-C4-N9	4.29	134.15	127.08
1	1	2925	4AC	O7-C7-N4	4.28	128.75	121.82
1	1	2960	4AC	O7-C7-N4	4.28	128.74	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2642	4AC	O7-C7-N4	4.27	128.73	121.82
1	1	2585	4AC	C5-C4-N4	-4.26	115.51	122.92
2	2	830	OMU	N3-C2-N1	4.23	120.50	114.89
1	1	22	4AC	O7-C7-N4	4.22	128.65	121.82
1	1	981	4AC	O7-C7-N4	4.22	128.64	121.82
2	2	868	4AC	O7-C7-N4	4.19	128.60	121.82
1	1	2784	OMU	N3-C2-N1	4.17	120.42	114.89
1	1	2083	4AC	O7-C7-N4	4.17	128.56	121.82
2	2	1380	OMU	N3-C2-N1	4.16	120.42	114.89
2	2	851	4AC	O7-C7-N4	4.14	128.51	121.82
2	2	913	OMG	N9-C4-N3	4.12	134.22	125.94
2	2	1177	OMU	N3-C2-N1	4.05	120.26	114.89
2	2	64	OMU	N3-C2-N1	3.94	120.12	114.89
2	2	1469	6MZ	C4-C5-N7	-3.92	105.84	110.62
2	2	1488	MA6	C2-N3-C4	3.91	120.99	111.75
1	1	1055	A2M	C2-N3-C4	3.89	120.93	111.75
2	2	1487	MA6	C4-C5-N7	-3.88	105.89	110.62
1	1	2173	A2M	C2-N3-C4	3.88	120.92	111.75
2	2	1488	MA6	C4-C5-N7	-3.83	105.95	110.62
2	2	1487	MA6	C2-N3-C4	3.82	120.78	111.75
2	2	1469	6MZ	C2-N3-C4	3.80	120.74	111.75
2	2	373	A2M	C2-N3-C4	3.79	120.71	111.75
1	1	1755	4AC	C5-C4-N4	-3.78	116.36	122.92
2	2	787	OMU	C5-C4-N3	3.76	120.47	114.84
2	2	636	4AC	C1'-N1-C2	3.75	126.78	118.42
1	1	1755	4AC	N4-C4-N3	3.73	120.12	113.85
2	2	64	OMU	C5-C4-N3	3.73	120.41	114.84
1	1	1780	4AC	C5-C4-N4	-3.68	116.53	122.92
2	2	1177	OMU	C5-C4-N3	3.66	120.31	114.84
2	2	20	OMU	C5-C4-N3	3.65	120.30	114.84
1	1	1780	4AC	N4-C4-N3	3.63	119.95	113.85
1	1	2733	5MC	C5-C6-N1	-3.63	119.61	123.34
1	1	2784	OMU	C5-C4-N3	3.61	120.24	114.84
2	2	535	5MC	C5-C6-N1	-3.58	119.66	123.34
2	2	1025	5MC	C5-C6-N1	-3.56	119.68	123.34
1	1	2203	5MC	C5-C6-N1	-3.55	119.68	123.34
2	2	1505	5MC	C5-C6-N1	-3.55	119.69	123.34
1	1	2183	5MC	C5-C6-N1	-3.55	119.69	123.34
2	2	1147	4AC	N4-C4-N3	3.54	119.80	113.85
2	2	394	4AC	CM7-C7-N4	-3.54	109.18	115.29
2	2	913	OMG	C6-C5-N7	3.53	136.81	130.25
1	1	2093	5MC	C5-C6-N1	-3.52	119.72	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	875	5MC	C5-C6-N1	-3.48	119.76	123.34
1	1	2162	5MC	C5-C6-N1	-3.46	119.78	123.34
1	1	2163	5MC	C5-C6-N1	-3.45	119.78	123.34
2	2	1380	OMU	C5-C4-N3	3.45	120.00	114.84
2	2	830	OMU	C5-C4-N3	3.45	120.00	114.84
2	2	693	5MC	C5-C6-N1	-3.45	119.79	123.34
1	1	2198	5MC	C5-C6-N1	-3.45	119.79	123.34
1	1	1878	4AC	C5-C4-N4	-3.44	116.94	122.92
2	2	774	OMU	C5-C4-N3	3.44	119.99	114.84
1	1	2937	4AC	O7-C7-N4	3.43	127.37	121.82
1	1	2585	4AC	O7-C7-N4	3.42	127.35	121.82
2	2	53	4AC	N4-C4-N3	3.41	119.57	113.85
1	1	2608	4AC	O7-C7-N4	3.34	127.23	121.82
1	1	1055	A2M	C4-C5-N7	-3.33	106.56	110.62
2	2	64	OMU	O4-C4-C5	-3.33	119.30	125.16
1	1	2173	A2M	C4-C5-N7	-3.30	106.60	110.62
1	1	923	OMG	C6-C5-N7	3.30	136.38	130.25
2	2	467	OMG	C6-C5-N7	3.30	136.38	130.25
1	1	1878	4AC	N4-C4-N3	3.29	119.37	113.85
2	2	934	OMG	C6-C5-N7	3.28	136.35	130.25
2	2	1469	6MZ	N1-C2-N3	-3.28	123.47	128.60
2	2	286	4AC	CM7-C7-N4	-3.26	109.65	115.29
1	1	789	OMG	C6-C5-N7	3.26	136.31	130.25
2	2	839	4AC	CM7-C7-N4	-3.25	109.67	115.29
2	2	1374	5MC	C5-C6-N1	-3.25	120.00	123.34
2	2	373	A2M	C4-C5-N7	-3.24	106.67	110.62
1	1	1878	4AC	CM7-C7-N4	-3.24	109.69	115.29
1	1	2585	4AC	O2-C2-N3	-3.24	117.07	122.33
2	2	828	4AC	CM7-C7-N4	-3.23	109.70	115.29
2	2	1147	4AC	C5-C4-N4	-3.22	117.33	122.92
2	2	1069	OMG	C6-C5-N7	3.21	136.22	130.25
2	2	1487	MA6	N1-C2-N3	-3.20	123.59	128.60
2	2	1488	MA6	N1-C2-N3	-3.19	123.61	128.60
2	2	1498	5MC	O2-C2-N3	-3.18	117.16	122.33
1	1	2173	A2M	N3-C2-N1	-3.17	123.64	128.60
1	1	328	OMG	C6-C5-N7	3.15	136.11	130.25
1	1	2138	OMG	C6-C5-N7	3.15	136.11	130.25
1	1	1065	4AC	N4-C4-N3	3.14	119.12	113.85
1	1	1550	4AC	N4-C4-N3	3.14	119.12	113.85
1	1	1662	4AC	N4-C4-N3	3.14	119.12	113.85
2	2	1469	6MZ	C5-N7-C8	3.14	107.97	103.51
1	1	802	4AC	N4-C4-N3	3.13	119.11	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	32	4AC	N4-C4-N3	3.13	119.10	113.85
2	2	479	4AC	C5-C4-N4	-3.13	117.49	122.92
2	2	479	4AC	N4-C4-N3	3.12	119.09	113.85
1	1	2144	OMG	C6-C5-N7	3.11	136.04	130.25
2	2	53	4AC	C5-C4-N4	-3.11	117.52	122.92
2	2	479	4AC	CM7-C7-N4	-3.11	109.92	115.29
1	1	2287	4AC	N4-C4-N3	3.10	119.06	113.85
1	1	2678	OMG	C6-C5-N7	3.09	136.00	130.25
1	1	1243	4AC	CM7-C7-N4	-3.09	109.95	115.29
2	2	680	OMG	C6-C5-N7	3.09	135.99	130.25
1	1	2329	4AC	N4-C4-N3	3.08	119.03	113.85
2	2	546	4AC	N4-C4-N3	3.07	119.01	113.85
2	2	519	OMG	C6-C5-N7	3.07	135.96	130.25
1	1	2545	4AC	N4-C4-N3	3.07	119.01	113.85
1	1	1662	4AC	C5-C4-N4	-3.07	117.59	122.92
2	2	957	4AC	CM7-C7-N4	-3.07	109.99	115.29
1	1	60	4AC	N4-C4-N3	3.07	119.00	113.85
2	2	873	OMG	C6-C5-N7	3.06	135.94	130.25
2	2	1479	4AC	N4-C4-N3	3.06	118.99	113.85
1	1	229	4AC	CM7-C7-N4	-3.06	110.00	115.29
2	2	1496	5MC	C5-C6-N1	-3.06	120.19	123.34
2	2	1487	MA6	C5-N7-C8	3.05	107.84	103.51
2	2	787	OMU	O4-C4-C5	-3.04	119.81	125.16
2	2	626	4AC	CM7-C7-N4	-3.03	110.05	115.29
2	2	1233	4AC	CM7-C7-N4	-3.03	110.05	115.29
2	2	1177	OMU	O4-C4-C5	-3.03	119.83	125.16
1	1	1055	A2M	N3-C2-N1	-3.03	123.86	128.60
1	1	2784	OMU	O4-C4-C5	-3.03	119.83	125.16
1	1	1617	4AC	N4-C4-N3	3.03	118.93	113.85
1	1	458	4AC	N4-C4-N3	3.02	118.92	113.85
1	1	1293	4AC	CM7-C7-N4	-3.01	110.08	115.29
1	1	91	4AC	N4-C4-N3	3.01	118.91	113.85
2	2	718	4AC	CM7-C7-N4	-3.01	110.09	115.29
2	2	1488	MA6	C5-N7-C8	3.01	107.78	103.51
2	2	511	4AC	CM7-C7-N4	-3.01	110.09	115.29
1	1	2001	4AC	N4-C4-N3	3.01	118.90	113.85
2	2	731	4AC	CM7-C7-N4	-3.00	110.10	115.29
2	2	1202	5MC	C5-C6-N1	-3.00	120.25	123.34
1	1	1550	4AC	C5-C4-N4	-2.99	117.73	122.92
1	1	533	4AC	N4-C4-N3	2.99	118.87	113.85
1	1	2608	4AC	O2-C2-N3	-2.99	117.47	122.33
2	2	1233	4AC	C5-C4-N4	-2.99	117.73	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1885	4AC	CM7-C7-N4	-2.98	110.13	115.29
2	2	590	4AC	CM7-C7-N4	-2.98	110.13	115.29
1	1	2287	4AC	C5-C4-N4	-2.98	117.74	122.92
1	1	2027	4AC	N4-C4-N3	2.98	118.85	113.85
1	1	357	4AC	N4-C4-N3	2.98	118.85	113.85
2	2	373	A2M	N3-C2-N1	-2.98	123.95	128.60
3	3	32	4AC	C5-C4-N4	-2.97	117.75	122.92
1	1	1873	4AC	CM7-C7-N4	-2.97	110.15	115.29
2	2	379	4AC	CM7-C7-N4	-2.97	110.15	115.29
1	1	2718	4AC	N4-C4-N3	2.97	118.84	113.85
2	2	471	OMG	C6-C5-N7	2.97	135.78	130.25
1	1	243	4AC	N4-C4-N3	2.97	118.84	113.85
1	1	1934	4AC	N4-C4-N3	2.97	118.83	113.85
1	1	922	4AC	N4-C4-N3	2.97	118.83	113.85
1	1	60	4AC	C5-C4-N4	-2.96	117.78	122.92
2	2	626	4AC	N4-C4-N3	2.95	118.81	113.85
1	1	1460	4AC	N4-C4-N3	2.95	118.80	113.85
1	1	1554	4AC	CM7-C7-N4	-2.95	110.20	115.29
1	1	2147	OMG	C6-C5-N7	2.95	135.73	130.25
1	1	1065	4AC	C5-C4-N4	-2.95	117.80	122.92
1	1	2136	4AC	CM7-C7-N4	-2.94	110.20	115.29
1	1	2545	4AC	C5-C4-N4	-2.94	117.81	122.92
2	2	17	4AC	CM7-C7-N4	-2.94	110.21	115.29
2	2	1233	4AC	N4-C4-N3	2.94	118.78	113.85
2	2	1498	5MC	C1'-N1-C6	-2.94	116.24	121.12
2	2	1028	4AC	N4-C4-N3	2.94	118.78	113.85
1	1	2062	4AC	N4-C4-N3	2.93	118.78	113.85
1	1	641	4AC	CM7-C7-N4	-2.93	110.22	115.29
1	1	1934	4AC	C5-C4-N4	-2.93	117.83	122.92
2	2	774	OMU	O4-C4-C5	-2.93	120.01	125.16
1	1	2966	4AC	CM7-C7-N4	-2.93	110.23	115.29
2	2	751	4AC	CM7-C7-N4	-2.93	110.23	115.29
2	2	830	OMU	O4-C4-C5	-2.93	120.01	125.16
2	2	1380	OMU	O4-C4-C5	-2.93	120.01	125.16
1	1	1617	4AC	C5-C4-N4	-2.92	117.84	122.92
1	1	2495	4AC	CM7-C7-N4	-2.92	110.24	115.29
2	2	1239	4AC	CM7-C7-N4	-2.92	110.24	115.29
1	1	1621	4AC	CM7-C7-N4	-2.92	110.25	115.29
2	2	848	4AC	N4-C4-N3	2.92	118.75	113.85
1	1	2570	4AC	N4-C4-N3	2.91	118.75	113.85
1	1	341	4AC	N4-C4-N3	2.91	118.74	113.85
2	2	303	4AC	N4-C4-N3	2.91	118.74	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	91	4AC	CM7-C7-N4	-2.91	110.26	115.29
1	1	1867	4AC	CM7-C7-N4	-2.91	110.27	115.29
2	2	636	4AC	C1'-N1-C6	-2.91	114.50	120.84
1	1	22	4AC	CM7-C7-N4	-2.90	110.27	115.29
1	1	802	4AC	C5-C4-N4	-2.90	117.88	122.92
1	1	829	4AC	CM7-C7-N4	-2.90	110.28	115.29
1	1	981	4AC	CM7-C7-N4	-2.90	110.28	115.29
1	1	211	4AC	CM7-C7-N4	-2.90	110.28	115.29
1	1	1765	4AC	CM7-C7-N4	-2.90	110.28	115.29
1	1	1222	4AC	N4-C4-N3	2.90	118.71	113.85
1	1	1460	4AC	CM7-C7-N4	-2.89	110.29	115.29
2	2	379	4AC	N4-C4-N3	2.89	118.71	113.85
1	1	2545	4AC	CM7-C7-N4	-2.89	110.29	115.29
1	1	451	4AC	N4-C4-N3	2.89	118.70	113.85
2	2	848	4AC	CM7-C7-N4	-2.89	110.29	115.29
1	1	2865	4AC	CM7-C7-N4	-2.89	110.30	115.29
1	1	1934	4AC	CM7-C7-N4	-2.89	110.30	115.29
2	2	731	4AC	N4-C4-N3	2.89	118.70	113.85
1	1	2249	4AC	CM7-C7-N4	-2.89	110.30	115.29
1	1	2083	4AC	CM7-C7-N4	-2.88	110.31	115.29
1	1	2329	4AC	C5-C4-N4	-2.88	117.92	122.92
1	1	314	4AC	N4-C4-N3	2.88	118.68	113.85
1	1	1048	4AC	N4-C4-N3	2.88	118.68	113.85
1	1	1048	4AC	CM7-C7-N4	-2.88	110.32	115.29
2	2	636	4AC	CM7-C7-N4	-2.88	110.32	115.29
1	1	1594	4AC	N4-C4-N3	2.88	118.68	113.85
1	1	1460	4AC	C5-C4-N4	-2.88	117.92	122.92
1	1	2548	4AC	CM7-C7-N4	-2.88	110.32	115.29
1	1	91	4AC	C5-C4-N4	-2.87	117.93	122.92
1	1	458	4AC	C5-C4-N4	-2.87	117.93	122.92
1	1	1938	4AC	CM7-C7-N4	-2.87	110.33	115.29
1	1	161	4AC	CM7-C7-N4	-2.87	110.34	115.29
1	1	243	4AC	C5-C4-N4	-2.87	117.94	122.92
3	3	32	4AC	CM7-C7-N4	-2.86	110.34	115.29
1	1	1667	4AC	N4-C4-N3	2.86	118.65	113.85
1	1	2865	4AC	N4-C4-N3	2.86	118.65	113.85
1	1	1048	4AC	C5-C4-N4	-2.86	117.95	122.92
1	1	2966	4AC	N4-C4-N3	2.86	118.65	113.85
1	1	1962	4AC	N4-C4-N3	2.86	118.65	113.85
2	2	1479	4AC	C5-C4-N4	-2.85	117.96	122.92
1	1	2570	4AC	CM7-C7-N4	-2.85	110.36	115.29
1	1	243	4AC	CM7-C7-N4	-2.85	110.36	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1068	4AC	CM7-C7-N4	-2.85	110.36	115.29
2	2	1028	4AC	CM7-C7-N4	-2.85	110.36	115.29
2	2	1028	4AC	C5-C4-N4	-2.85	117.97	122.92
2	2	303	4AC	CM7-C7-N4	-2.85	110.37	115.29
1	1	1293	4AC	N4-C4-N3	2.85	118.63	113.85
2	2	394	4AC	N4-C4-N3	2.85	118.63	113.85
1	1	1962	4AC	CM7-C7-N4	-2.84	110.38	115.29
1	1	694	4AC	CM7-C7-N4	-2.84	110.38	115.29
1	1	1695	4AC	CM7-C7-N4	-2.84	110.38	115.29
2	2	20	OMU	O4-C4-C5	-2.84	120.17	125.16
1	1	2548	4AC	N4-C4-N3	2.84	118.62	113.85
1	1	533	4AC	C5-C4-N4	-2.84	117.99	122.92
1	1	835	4AC	CM7-C7-N4	-2.84	110.39	115.29
1	1	2062	4AC	CM7-C7-N4	-2.84	110.39	115.29
1	1	922	4AC	C5-C4-N4	-2.84	117.99	122.92
2	2	303	4AC	C5-C4-N4	-2.84	117.99	122.92
1	1	341	4AC	CM7-C7-N4	-2.83	110.39	115.29
2	2	848	4AC	C5-C4-N4	-2.83	118.00	122.92
1	1	451	4AC	CM7-C7-N4	-2.83	110.39	115.29
1	1	1695	4AC	N4-C4-N3	2.83	118.61	113.85
1	1	2718	4AC	C5-C4-N4	-2.83	118.00	122.92
2	2	546	4AC	C5-C4-N4	-2.83	118.01	122.92
2	2	379	4AC	C5-C4-N4	-2.82	118.01	122.92
2	2	17	4AC	N4-C4-N3	2.82	118.59	113.85
1	1	357	4AC	CM7-C7-N4	-2.82	110.41	115.29
1	1	1554	4AC	N4-C4-N3	2.82	118.59	113.85
1	1	2136	4AC	N4-C4-N3	2.82	118.59	113.85
1	1	802	4AC	CM7-C7-N4	-2.82	110.42	115.29
1	1	1667	4AC	CM7-C7-N4	-2.82	110.42	115.29
1	1	694	4AC	N4-C4-N3	2.82	118.58	113.85
1	1	1594	4AC	CM7-C7-N4	-2.82	110.42	115.29
2	2	718	4AC	N4-C4-N3	2.82	118.58	113.85
1	1	1867	4AC	N4-C4-N3	2.81	118.57	113.85
1	1	1780	4AC	CM7-C7-N4	-2.81	110.43	115.29
1	1	2027	4AC	C5-C4-N4	-2.81	118.04	122.92
1	1	2570	4AC	C5-C4-N4	-2.81	118.05	122.92
1	1	3004	4AC	CM7-C7-N4	-2.80	110.45	115.29
1	1	2642	4AC	N4-C4-N3	2.80	118.56	113.85
2	2	626	4AC	C5-C4-N4	-2.80	118.05	122.92
2	2	718	4AC	C5-C4-N4	-2.80	118.05	122.92
2	2	680	OMG	C4-C5-N7	-2.80	106.29	110.72
1	1	136	4AC	CM7-C7-N4	-2.80	110.45	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2249	4AC	N4-C4-N3	2.79	118.54	113.85
1	1	2718	4AC	CM7-C7-N4	-2.79	110.47	115.29
1	1	451	4AC	C5-C4-N4	-2.79	118.08	122.92
1	1	2908	4AC	CM7-C7-N4	-2.79	110.47	115.29
1	1	1867	4AC	C5-C4-N4	-2.78	118.08	122.92
1	1	1068	4AC	N4-C4-N3	2.78	118.52	113.85
1	1	1617	4AC	CM7-C7-N4	-2.78	110.48	115.29
1	1	458	4AC	CM7-C7-N4	-2.78	110.48	115.29
1	1	2966	4AC	C5-C4-N4	-2.78	118.09	122.92
1	1	211	4AC	N4-C4-N3	2.78	118.52	113.85
1	1	1594	4AC	C5-C4-N4	-2.78	118.09	122.92
1	1	2925	4AC	CM7-C7-N4	-2.78	110.49	115.29
1	1	2548	4AC	C5-C4-N4	-2.78	118.10	122.92
2	2	319	4AC	CM7-C7-N4	-2.77	110.50	115.29
2	2	17	4AC	C5-C4-N4	-2.77	118.10	122.92
1	1	2062	4AC	C5-C4-N4	-2.77	118.11	122.92
1	1	2173	A2M	C5-N7-C8	2.77	107.44	103.51
1	1	2865	4AC	C5-C4-N4	-2.77	118.11	122.92
1	1	1065	4AC	CM7-C7-N4	-2.76	110.51	115.29
1	1	2908	4AC	N4-C4-N3	2.76	118.49	113.85
1	1	1667	4AC	C5-C4-N4	-2.76	118.12	122.92
1	1	1765	4AC	N4-C4-N3	2.76	118.49	113.85
1	1	357	4AC	C5-C4-N4	-2.76	118.13	122.92
1	1	136	4AC	N4-C4-N3	2.76	118.48	113.85
1	1	161	4AC	N4-C4-N3	2.76	118.48	113.85
1	1	1554	4AC	C5-C4-N4	-2.76	118.13	122.92
1	1	2001	4AC	C5-C4-N4	-2.76	118.13	122.92
2	2	868	4AC	CM7-C7-N4	-2.76	110.53	115.29
1	1	341	4AC	C5-C4-N4	-2.75	118.14	122.92
1	1	1557	4AC	CM7-C7-N4	-2.75	110.53	115.29
1	1	922	4AC	CM7-C7-N4	-2.75	110.53	115.29
2	2	731	4AC	C5-C4-N4	-2.75	118.14	122.92
1	1	641	4AC	N4-C4-N3	2.75	118.47	113.85
1	1	1222	4AC	C5-C4-N4	-2.75	118.14	122.92
1	1	1662	4AC	CM7-C7-N4	-2.75	110.54	115.29
2	2	851	4AC	CM7-C7-N4	-2.75	110.54	115.29
1	1	1962	4AC	C5-C4-N4	-2.75	118.15	122.92
1	1	2136	4AC	C5-C4-N4	-2.75	118.15	122.92
1	1	1055	A2M	C5-N7-C8	2.74	107.40	103.51
1	1	1695	4AC	C5-C4-N4	-2.74	118.16	122.92
1	1	314	4AC	CM7-C7-N4	-2.74	110.56	115.29
2	2	590	4AC	N4-C4-N3	2.73	118.44	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2249	4AC	C5-C4-N4	-2.73	118.17	122.92
1	1	2585	4AC	C1'-N1-C2	2.73	124.52	118.42
1	1	1243	4AC	C5-C4-N4	-2.73	118.17	122.92
1	1	1293	4AC	C5-C4-N4	-2.73	118.18	122.92
1	1	694	4AC	C5-C4-N4	-2.73	118.18	122.92
1	1	1222	4AC	CM7-C7-N4	-2.72	110.58	115.29
1	1	2287	4AC	CM7-C7-N4	-2.72	110.59	115.29
2	2	868	4AC	N4-C4-N3	2.72	118.42	113.85
1	1	533	4AC	CM7-C7-N4	-2.72	110.60	115.29
1	1	1765	4AC	C5-C4-N4	-2.72	118.20	122.92
2	2	319	4AC	N4-C4-N3	2.71	118.41	113.85
1	1	1557	4AC	N4-C4-N3	2.71	118.41	113.85
2	2	1239	4AC	N4-C4-N3	2.71	118.41	113.85
1	1	835	4AC	N4-C4-N3	2.71	118.40	113.85
1	1	1550	4AC	CM7-C7-N4	-2.71	110.61	115.29
1	1	2960	4AC	N4-C4-N3	2.71	118.40	113.85
1	1	1938	4AC	N4-C4-N3	2.70	118.39	113.85
1	1	314	4AC	C5-C4-N4	-2.70	118.22	122.92
1	1	2173	A2M	C2'-C1'-N9	-2.70	108.98	113.53
1	1	2960	4AC	CM7-C7-N4	-2.70	110.62	115.29
2	2	1479	4AC	CM7-C7-N4	-2.69	110.64	115.29
1	1	60	4AC	CM7-C7-N4	-2.68	110.65	115.29
2	2	467	OMG	C4-C5-N7	-2.68	106.48	110.72
1	1	2027	4AC	CM7-C7-N4	-2.68	110.66	115.29
1	1	1621	4AC	N4-C4-N3	2.68	118.35	113.85
2	2	373	A2M	C5-N7-C8	2.68	107.31	103.51
1	1	641	4AC	C5-C4-N4	-2.67	118.29	122.92
2	2	546	4AC	CM7-C7-N4	-2.67	110.68	115.29
2	2	1498	5MC	C5-C4-N3	-2.67	118.80	121.67
1	1	2329	4AC	CM7-C7-N4	-2.66	110.69	115.29
1	1	2642	4AC	CM7-C7-N4	-2.66	110.69	115.29
2	2	913	OMG	C4-C5-N7	-2.66	106.52	110.72
1	1	161	4AC	C5-C4-N4	-2.66	118.30	122.92
2	2	1147	4AC	CM7-C7-N4	-2.66	110.70	115.29
1	1	1243	4AC	N4-C4-N3	2.65	118.31	113.85
2	2	934	OMG	C4-C5-N7	-2.65	106.52	110.72
2	2	957	4AC	N4-C4-N3	2.65	118.30	113.85
1	1	1621	4AC	C5-C4-N4	-2.65	118.32	122.92
2	2	1069	OMG	C4-C5-N7	-2.64	106.54	110.72
2	2	519	OMG	C4-C5-N7	-2.64	106.54	110.72
1	1	2642	4AC	C5-C4-N4	-2.64	118.33	122.92
2	2	511	4AC	C5-C4-N4	-2.64	118.33	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2908	4AC	C5-C4-N4	-2.64	118.34	122.92
1	1	1068	4AC	C5-C4-N4	-2.63	118.34	122.92
1	1	981	4AC	N4-C4-N3	2.63	118.27	113.85
2	2	751	4AC	N4-C4-N3	2.63	118.26	113.85
1	1	2733	5MC	C5-C4-N3	-2.63	118.84	121.67
2	2	53	4AC	CM7-C7-N4	-2.63	110.75	115.29
2	2	511	4AC	N4-C4-N3	2.63	118.26	113.85
2	2	286	4AC	C5-C4-N4	-2.62	118.37	122.92
2	2	957	4AC	C5-C4-N4	-2.62	118.37	122.92
1	1	2925	4AC	N4-C4-N3	2.62	118.25	113.85
2	2	590	4AC	C5-C4-N4	-2.61	118.39	122.92
1	1	789	OMG	C4-C5-N7	-2.60	106.60	110.72
1	1	2608	4AC	C1'-N1-C2	2.60	124.23	118.42
1	1	2495	4AC	N4-C4-N3	2.60	118.22	113.85
1	1	2138	OMG	C4-C5-N7	-2.59	106.61	110.72
1	1	211	4AC	C5-C4-N4	-2.59	118.41	122.92
1	1	981	4AC	C5-C4-N4	-2.59	118.42	122.92
1	1	1557	4AC	C5-C4-N4	-2.59	118.42	122.92
2	2	875	5MC	C5-C4-N3	-2.59	118.88	121.67
1	1	1938	4AC	C5-C4-N4	-2.58	118.43	122.92
2	2	873	OMG	C4-C5-N7	-2.58	106.64	110.72
2	2	1239	4AC	C5-C4-N4	-2.58	118.44	122.92
2	2	1374	5MC	C5-C4-N3	-2.58	118.89	121.67
1	1	2495	4AC	C5-C4-N4	-2.58	118.44	122.92
1	1	1885	4AC	N4-C4-N3	2.58	118.18	113.85
1	1	835	4AC	C5-C4-N4	-2.57	118.45	122.92
1	1	3004	4AC	N4-C4-N3	2.57	118.17	113.85
1	1	1873	4AC	N4-C4-N3	2.57	118.17	113.85
1	1	136	4AC	C5-C4-N4	-2.56	118.47	122.92
2	2	319	4AC	C5-C4-N4	-2.56	118.47	122.92
1	1	829	4AC	N4-C4-N3	2.56	118.15	113.85
1	1	1873	4AC	C5-C4-N4	-2.56	118.47	122.92
2	2	1202	5MC	C5-C4-N3	-2.56	118.91	121.67
2	2	286	4AC	N4-C4-N3	2.56	118.15	113.85
1	1	2960	4AC	C5-C4-N4	-2.56	118.48	122.92
1	1	1755	4AC	CM7-C7-N4	-2.55	110.88	115.29
1	1	2144	OMG	C4-C5-N7	-2.55	106.68	110.72
1	1	328	OMG	C4-C5-N7	-2.54	106.69	110.72
1	1	923	OMG	C4-C5-N7	-2.54	106.70	110.72
1	1	1885	4AC	C5-C4-N4	-2.53	118.52	122.92
2	2	1025	5MC	C5-C4-N3	-2.53	118.94	121.67
1	1	2678	OMG	C4-C5-N7	-2.53	106.72	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2183	5MC	C5-C4-N3	-2.53	118.95	121.67
2	2	657	OMG	C6-C5-N7	2.52	134.93	130.25
1	1	3004	4AC	C5-C4-N4	-2.52	118.55	122.92
2	2	839	4AC	C5-C4-N4	-2.52	118.55	122.92
2	2	1487	MA6	C4-N9-C8	2.52	108.45	105.73
1	1	2173	A2M	C4-N9-C8	2.51	108.45	105.73
1	1	2925	4AC	C5-C4-N4	-2.50	118.58	122.92
1	1	829	4AC	C5-C4-N4	-2.50	118.58	122.92
1	1	2093	5MC	C5-C4-N3	-2.50	118.98	121.67
2	2	1505	5MC	C5-C4-N3	-2.50	118.98	121.67
1	1	2001	4AC	CM7-C7-N4	-2.48	111.00	115.29
1	1	2162	5MC	C5-C4-N3	-2.48	118.99	121.67
1	1	2147	OMG	C4-C5-N7	-2.48	106.80	110.72
1	1	2198	5MC	C5-C4-N3	-2.47	119.00	121.67
1	1	2203	5MC	C5-C4-N3	-2.47	119.01	121.67
2	2	1496	5MC	C5-C4-N3	-2.47	119.01	121.67
2	2	839	4AC	N4-C4-N3	2.47	117.99	113.85
2	2	1498	5MC	C1'-N1-C2	2.46	123.91	118.42
1	1	2163	5MC	C5-C4-N3	-2.46	119.02	121.67
2	2	693	5MC	C5-C4-N3	-2.46	119.02	121.67
2	2	1498	5MC	C5-C6-N1	-2.45	120.82	123.34
2	2	535	5MC	C5-C4-N3	-2.45	119.03	121.67
2	2	20	OMU	O2-C2-N1	-2.44	119.54	122.79
2	2	828	4AC	C5-C4-N4	-2.44	118.68	122.92
1	1	615	OMC	O2-C2-N3	-2.41	118.41	122.33
2	2	828	4AC	N4-C4-N3	2.41	117.89	113.85
2	2	471	OMG	C4-C5-N7	-2.40	106.92	110.72
1	1	229	4AC	N4-C4-N3	2.40	117.88	113.85
1	1	22	4AC	N4-C4-N3	2.40	117.87	113.85
1	1	2992	4AC	CM7-C7-N4	2.39	119.43	115.29
2	2	1469	6MZ	C4-N9-C8	2.39	108.32	105.73
2	2	868	4AC	C5-C4-N4	-2.38	118.78	122.92
2	2	373	A2M	C4-N9-C8	2.35	108.28	105.73
2	2	851	4AC	N4-C4-N3	2.34	117.78	113.85
2	2	64	OMU	C1'-N1-C2	2.33	121.80	117.57
1	1	2083	4AC	N4-C4-N3	2.32	117.75	113.85
1	1	229	4AC	C5-C4-N4	-2.31	118.90	122.92
1	1	22	4AC	C5-C4-N4	-2.31	118.91	122.92
2	2	657	OMG	C4-C5-N7	-2.31	107.07	110.72
1	1	2733	5MC	O2-C2-N3	-2.29	118.61	122.33
1	1	2678	OMG	O6-C6-C5	-2.28	120.55	126.60
2	2	751	4AC	C5-C4-N4	-2.28	118.96	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2173	A2M	C6-C5-N7	2.28	136.27	132.02
2	2	1040	OMC	O2'-C2'-C1'	-2.28	104.64	109.08
1	1	2784	OMU	O2-C2-N1	-2.27	119.77	122.79
1	1	328	OMG	O6-C6-C5	-2.27	120.58	126.60
1	1	2937	4AC	CM7-C7-N4	-2.27	111.37	115.29
2	2	471	OMG	O6-C6-C5	-2.26	120.59	126.60
1	1	2083	4AC	C5-C4-N4	-2.26	118.99	122.92
2	2	830	OMU	C1'-N1-C2	2.24	121.63	117.57
1	1	1055	A2M	C4-N9-C8	2.24	108.15	105.73
2	2	851	4AC	C5-C4-N4	-2.23	119.04	122.92
2	2	1487	MA6	C6-C5-N7	2.23	137.03	133.28
2	2	1469	6MZ	C2-N1-C6	2.23	122.74	115.25
2	2	787	OMU	O2-C2-N1	-2.22	119.84	122.79
1	1	923	OMG	O6-C6-C5	-2.21	120.73	126.60
2	2	875	5MC	O2-C2-N3	-2.21	118.74	122.33
2	2	1488	MA6	C4-N9-C8	2.21	108.12	105.73
2	2	1184	4AC	O2-C2-N3	-2.19	118.78	122.33
2	2	773	OMC	O2-C2-N3	-2.17	118.80	122.33
2	2	1380	OMU	C1'-N1-C2	2.16	121.48	117.57
2	2	1487	MA6	N1-C6-N6	2.15	119.43	117.08
1	1	2147	OMG	O6-C6-C5	-2.14	120.92	126.60
1	1	789	OMG	O6-C6-C5	-2.14	120.92	126.60
2	2	934	OMG	O6-C6-C5	-2.14	120.93	126.60
2	2	913	OMG	O6-C6-C5	-2.14	120.94	126.60
2	2	519	OMG	O6-C6-C5	-2.13	120.96	126.60
2	2	868	4AC	O2-C2-N3	-2.12	118.88	122.33
1	1	2144	OMG	O6-C6-C5	-2.12	120.97	126.60
2	2	1025	5MC	O2-C2-N3	-2.12	118.88	122.33
2	2	873	OMG	O6-C6-C5	-2.12	120.97	126.60
2	2	851	4AC	O2-C2-N3	-2.11	118.89	122.33
2	2	467	OMG	O6-C6-C5	-2.11	121.01	126.60
1	1	2138	OMG	O6-C6-C5	-2.11	121.02	126.60
2	2	1488	MA6	C6-C5-N7	2.11	136.82	133.28
2	2	657	OMG	O6-C6-C5	-2.10	121.02	126.60
1	1	1055	A2M	C6-C5-N7	2.10	135.94	132.02
2	2	373	A2M	C6-C5-N7	2.08	135.90	132.02
2	2	1469	6MZ	N9-C8-N7	-2.05	111.11	113.91
1	1	2173	A2M	N9-C8-N7	-2.04	111.12	113.91
2	2	1069	OMG	O6-C6-C5	-2.04	121.19	126.60
2	2	680	OMG	O3'-C3'-C4'	2.03	116.93	111.05
1	1	2585	4AC	CM7-C7-N4	-2.03	111.78	115.29
1	1	2992	4AC	O7-C7-CM7	-2.03	118.30	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1374	5MC	O2-C2-N3	-2.02	119.05	122.33
2	2	1041	LHH	C2'-C3'-C4'	-2.01	97.62	101.99
1	1	2925	4AC	O2-C2-N3	-2.01	119.06	122.33
1	1	22	4AC	O2-C2-N3	-2.01	119.06	122.33
1	1	328	OMG	C5-C6-N1	2.01	118.29	113.19
2	2	394	4AC	C5-C4-N4	-2.01	119.43	122.92
1	1	923	OMG	C5-C6-N1	2.00	118.27	113.19

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	2147	OMG	C3'-C4'-C5'-O5'
1	1	2585	4AC	O4'-C1'-N1-C2
1	1	2585	4AC	O4'-C1'-N1-C6
1	1	2608	4AC	O4'-C1'-N1-C2
1	1	2608	4AC	O4'-C1'-N1-C6
2	2	680	OMG	C1'-C2'-O2'-CM2
2	2	787	OMU	O4'-C4'-C5'-O5'
2	2	934	OMG	O4'-C4'-C5'-O5'
2	2	1505	5MC	O4'-C4'-C5'-O5'
2	2	636	4AC	C3'-C4'-C5'-O5'
2	2	787	OMU	C3'-C4'-C5'-O5'
2	2	934	OMG	C3'-C4'-C5'-O5'
2	2	1505	5MC	C3'-C4'-C5'-O5'
1	1	2147	OMG	O4'-C4'-C5'-O5'
1	1	789	OMG	C3'-C4'-C5'-O5'
2	2	20	OMU	C2'-C1'-N1-C6
2	2	751	4AC	O4'-C4'-C5'-O5'
2	2	1374	5MC	O4'-C4'-C5'-O5'
2	2	636	4AC	O4'-C4'-C5'-O5'
1	1	789	OMG	O4'-C4'-C5'-O5'
2	2	751	4AC	C3'-C4'-C5'-O5'
1	1	2992	4AC	O7-C7-N4-C4
1	1	2992	4AC	CM7-C7-N4-C4
2	2	703	4AC	O7-C7-N4-C4
2	2	703	4AC	CM7-C7-N4-C4
1	1	2733	5MC	C2'-C1'-N1-C6
2	2	20	OMU	O4'-C4'-C5'-O5'
1	1	923	OMG	C1'-C2'-O2'-CM2
1	1	1055	A2M	C3'-C2'-O2'-CM'
2	2	913	OMG	C3'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
2	2	1177	OMU	C3'-C2'-O2'-CM2
2	2	20	OMU	O4'-C1'-N1-C6
1	1	2585	4AC	N3-C4-N4-C7
1	1	2608	4AC	N3-C4-N4-C7
1	1	2937	4AC	N3-C4-N4-C7
2	2	703	4AC	N3-C4-N4-C7
2	2	873	OMG	C4'-C5'-O5'-P
2	2	1374	5MC	C3'-C4'-C5'-O5'
1	1	2733	5MC	O4'-C1'-N1-C6
2	2	1488	MA6	C4'-C5'-O5'-P
2	2	787	OMU	C2'-C1'-N1-C6
1	1	2147	OMG	C3'-C2'-O2'-CM2
2	2	1498	5MC	C2'-C1'-N1-C6
2	2	1498	5MC	O4'-C1'-N1-C6
2	2	20	OMU	C2'-C1'-N1-C2
2	2	20	OMU	C3'-C4'-C5'-O5'
1	1	2733	5MC	O4'-C1'-N1-C2
2	2	20	OMU	O4'-C1'-N1-C2
1	1	923	OMG	C3'-C2'-O2'-CM2
1	1	2144	OMG	C3'-C2'-O2'-CM2
2	2	1069	OMG	C3'-C2'-O2'-CM2
2	2	787	OMU	O4'-C1'-N1-C6
2	2	1376	OMC	O4'-C4'-C5'-O5'
2	2	787	OMU	O4'-C1'-N1-C2
2	2	1202	5MC	O4'-C4'-C5'-O5'
2	2	250	LHH	C1'-C2'-O2'-C1
2	2	1380	OMU	C1'-C2'-O2'-CM2
2	2	1498	5MC	O4'-C1'-N1-C2
1	1	2733	5MC	C2'-C1'-N1-C2
2	2	1498	5MC	C2'-C1'-N1-C2
1	1	615	OMC	C2'-C1'-N1-C2
2	2	787	OMU	C2'-C1'-N1-C2
1	1	2678	OMG	C3'-C2'-O2'-CM2
2	2	1380	OMU	C3'-C2'-O2'-CM2
2	2	1498	5MC	O4'-C4'-C5'-O5'

There are no ring outliers.

88 monomers are involved in 128 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	774	OMU	2	0
1	1	922	4AC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	2287	4AC	4	0
2	2	1177	OMU	1	0
1	1	2585	4AC	3	0
1	1	1068	4AC	1	0
2	2	1233	4AC	1	0
1	1	1594	4AC	1	0
2	2	1469	6MZ	1	0
2	2	319	4AC	1	0
2	2	1479	4AC	1	0
2	2	303	4AC	1	0
2	2	718	4AC	1	0
2	2	1028	4AC	1	0
1	1	2062	4AC	1	0
1	1	2865	4AC	1	0
2	2	17	4AC	1	0
1	1	1755	4AC	2	0
1	1	2925	4AC	1	0
1	1	1878	4AC	1	0
1	1	1065	4AC	2	0
1	1	2136	4AC	1	0
2	2	1069	OMG	1	0
2	2	471	OMG	1	0
1	1	22	4AC	1	0
1	1	451	4AC	3	0
1	1	2329	4AC	1	0
2	2	511	4AC	1	0
1	1	243	4AC	1	0
2	2	373	A2M	1	0
1	1	1934	4AC	2	0
1	1	533	4AC	1	0
2	2	129	OMC	1	0
1	1	2027	4AC	1	0
1	1	2992	4AC	1	0
2	2	731	4AC	1	0
2	2	773	OMC	1	0
1	1	789	OMG	1	0
1	1	1765	4AC	1	0
1	1	2144	OMG	1	0
1	1	802	4AC	2	0
1	1	1048	4AC	2	0
2	2	703	4AC	6	0
2	2	626	4AC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	1184	4AC	2	0
1	1	2678	OMG	1	0
1	1	2249	4AC	2	0
1	1	2545	4AC	1	0
2	2	519	OMG	2	0
1	1	2608	4AC	3	0
3	3	32	4AC	1	0
1	1	1667	4AC	4	0
1	1	1460	4AC	1	0
2	2	851	4AC	2	0
1	1	835	4AC	1	0
1	1	1550	4AC	2	0
1	1	3004	4AC	1	0
1	1	60	4AC	1	0
1	1	2001	4AC	1	0
2	2	1380	OMU	2	0
2	2	680	OMG	1	0
1	1	91	4AC	1	0
2	2	1505	5MC	1	0
2	2	957	4AC	1	0
2	2	657	OMG	3	0
2	2	1202	5MC	2	0
1	1	357	4AC	1	0
2	2	934	OMG	2	0
1	1	1780	4AC	1	0
2	2	1147	4AC	1	0
2	2	394	4AC	2	0
1	1	1867	4AC	1	0
2	2	479	4AC	2	0
2	2	636	4AC	4	0
2	2	1376	OMC	1	0
1	1	1662	4AC	1	0
1	1	2198	5MC	1	0
1	1	2548	4AC	1	0
1	1	2570	4AC	1	0
1	1	1617	4AC	3	0
2	2	546	4AC	3	0
1	1	2718	4AC	1	0
1	1	211	4AC	1	0
2	2	53	4AC	1	0
2	2	913	OMG	1	0
2	2	1025	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	615	OMC	1	0
1	1	458	4AC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 253 ligands modelled in this entry, 253 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	107:G	O3'	112:A	P	12.79

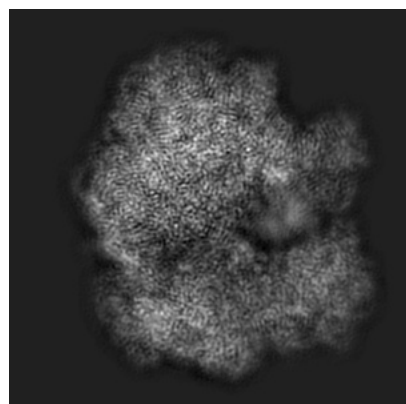
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55136. These allow visual inspection of the internal detail of the map and identification of artifacts.

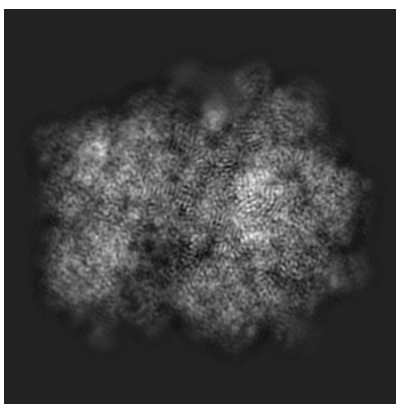
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

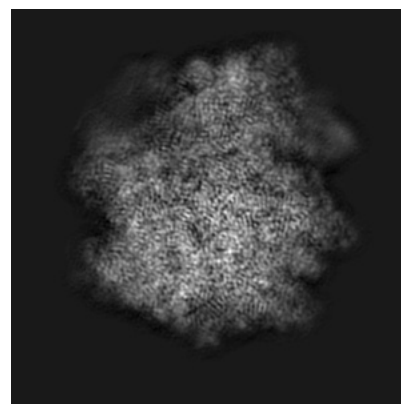
6.1.1 Primary map



X

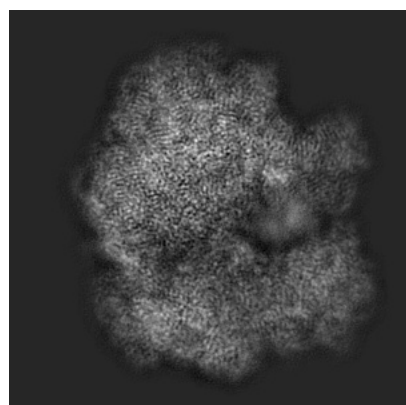


Y

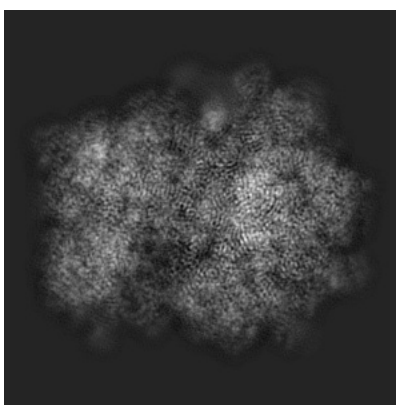


Z

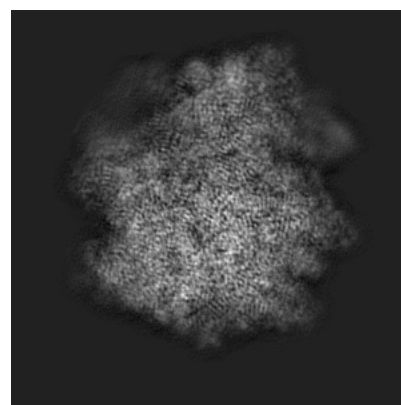
6.1.2 Raw map



X



Y

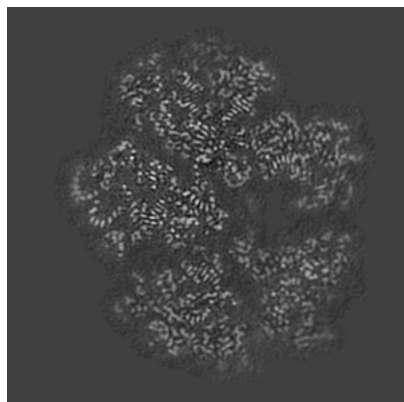


Z

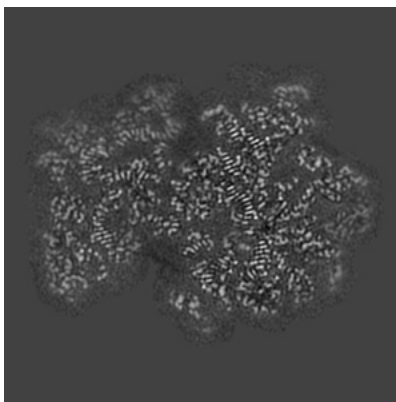
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

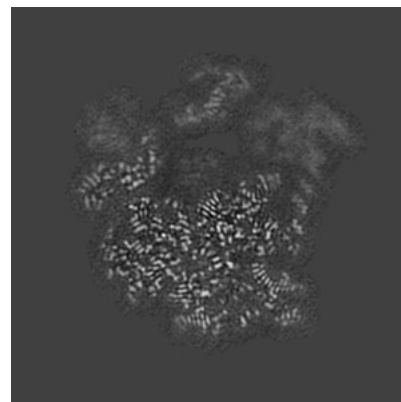
6.2.1 Primary map



X Index: 180

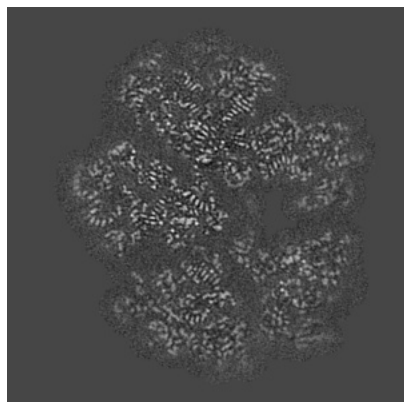


Y Index: 180

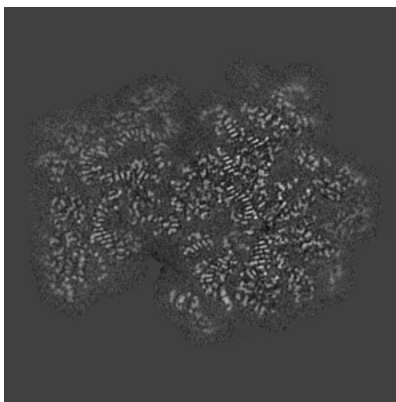


Z Index: 180

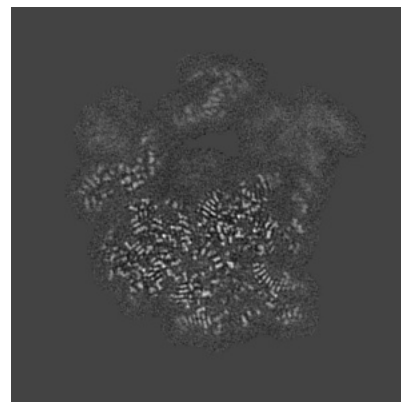
6.2.2 Raw map



X Index: 180



Y Index: 180

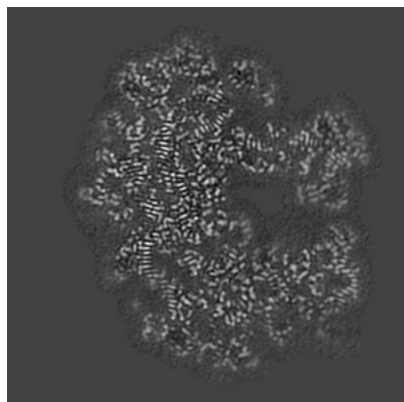


Z Index: 180

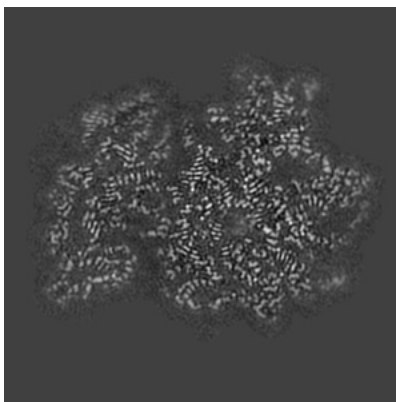
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

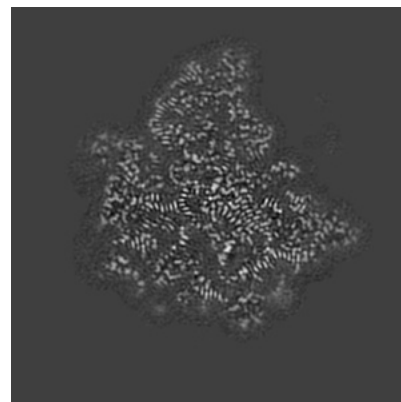
6.3.1 Primary map



X Index: 196

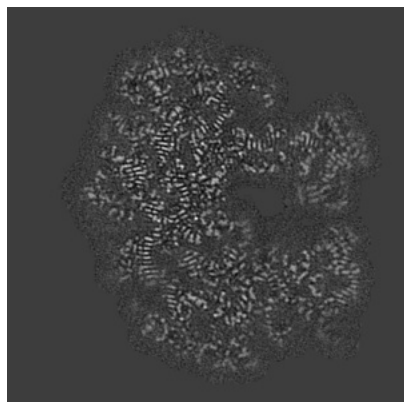


Y Index: 170

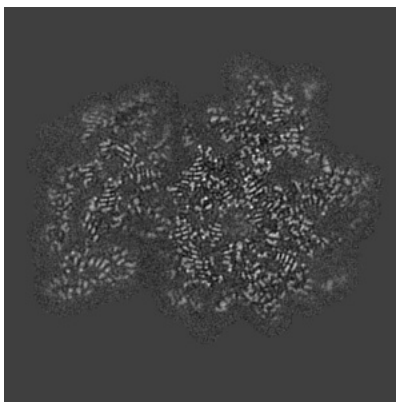


Z Index: 232

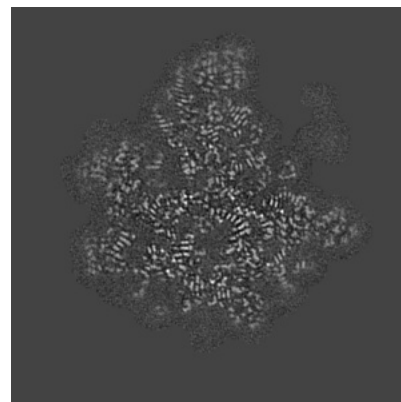
6.3.2 Raw map



X Index: 195



Y Index: 171

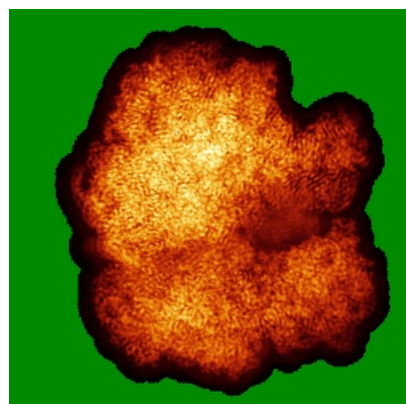


Z Index: 224

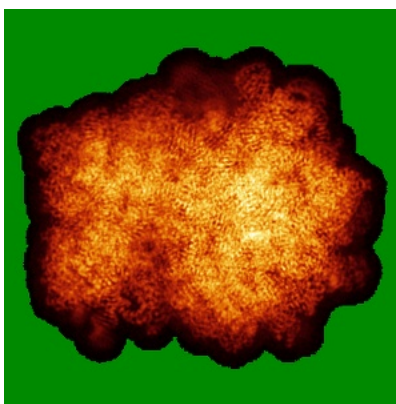
The images above show the largest variance slices of the map in three orthogonal directions.

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

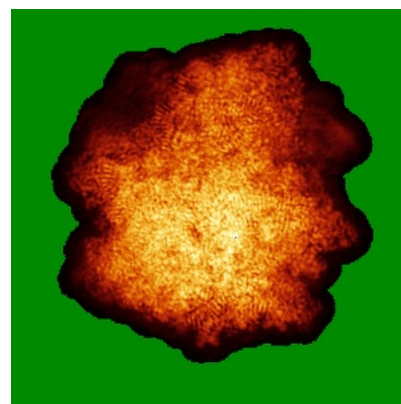
6.4.1 Primary map



X

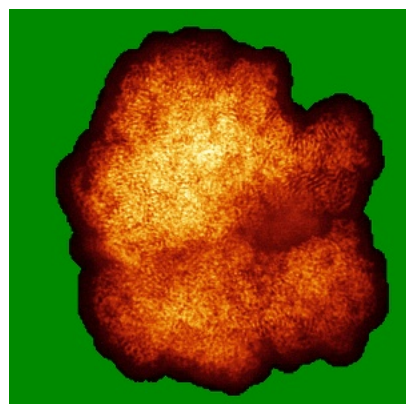


Y

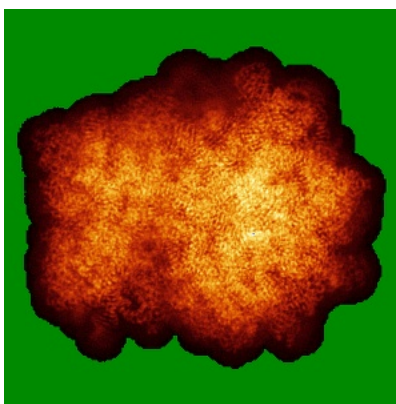


Z

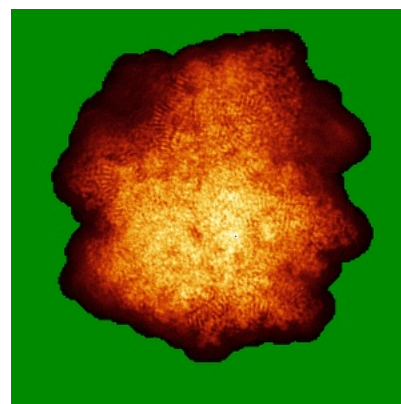
6.4.2 Raw map



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](#)

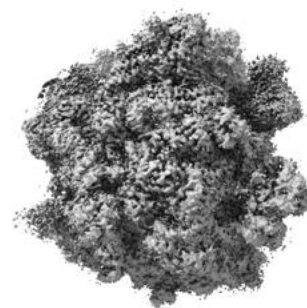
6.5.1 Primary map



X



Y



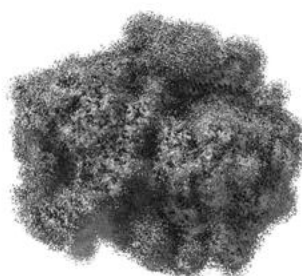
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

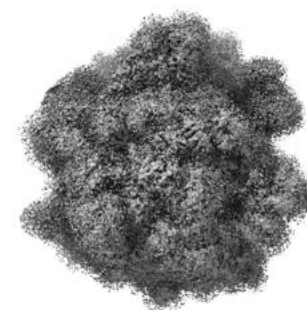
6.5.2 Raw map



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.

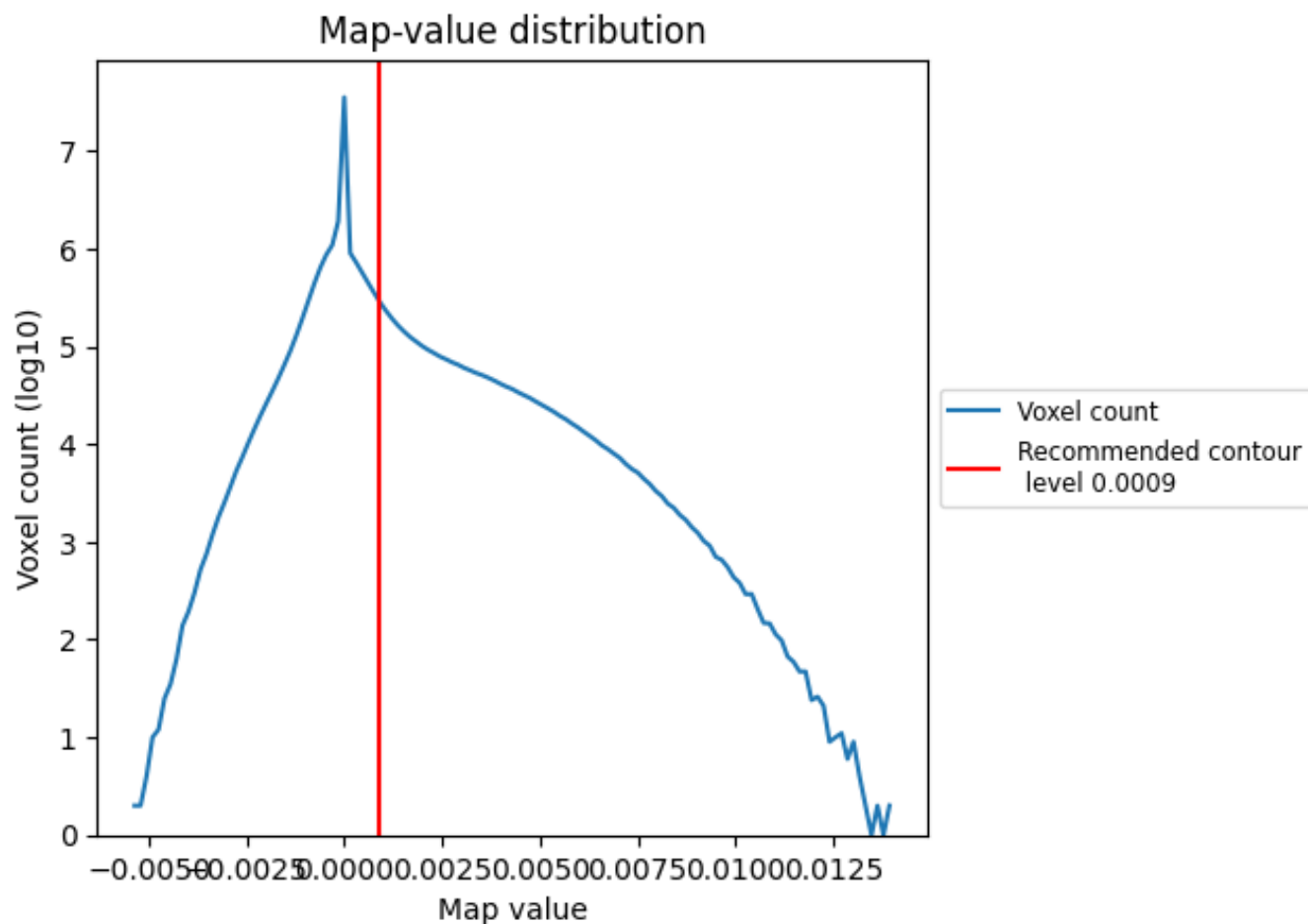
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

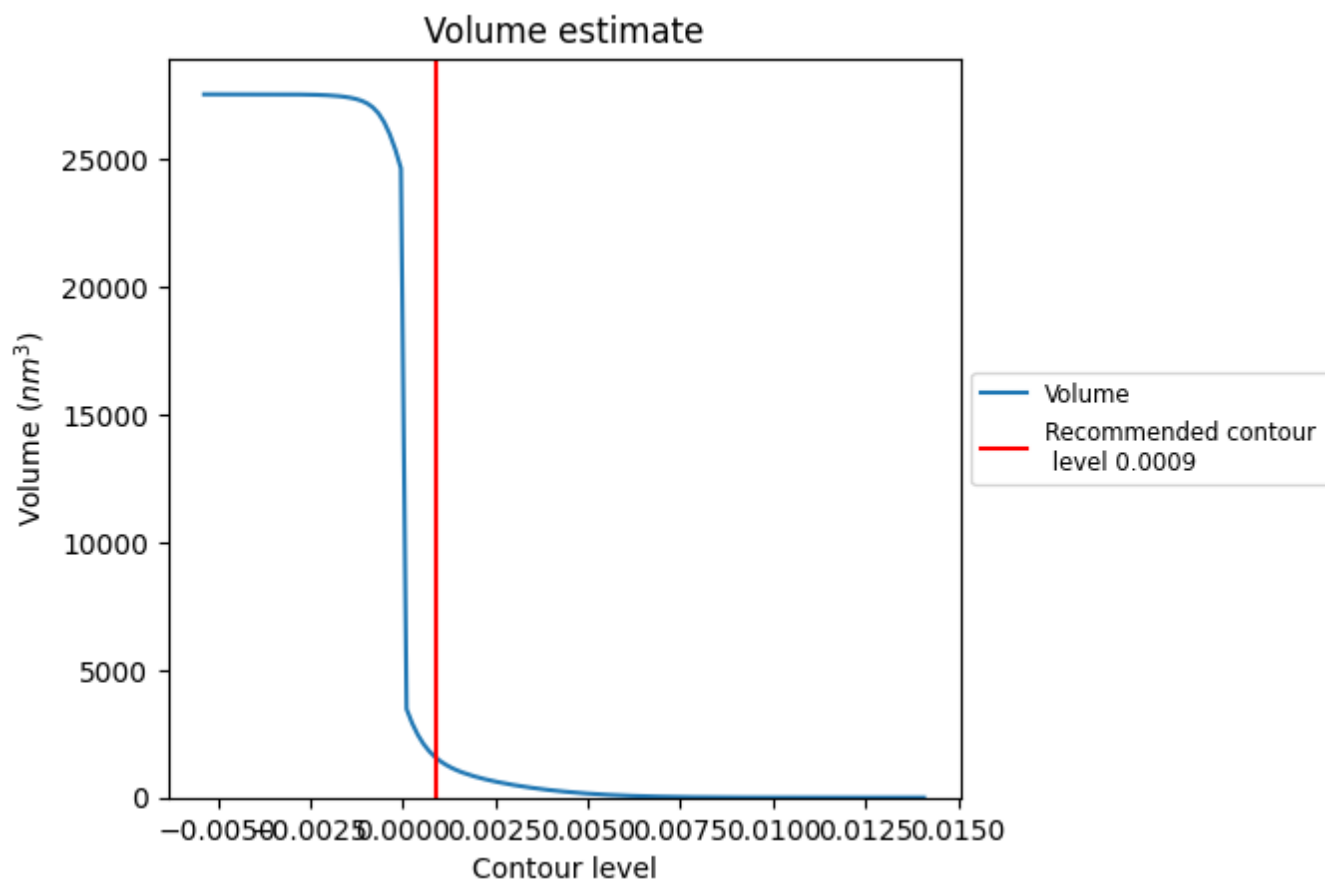
This section contains the results of statistical analysis of the map.

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.

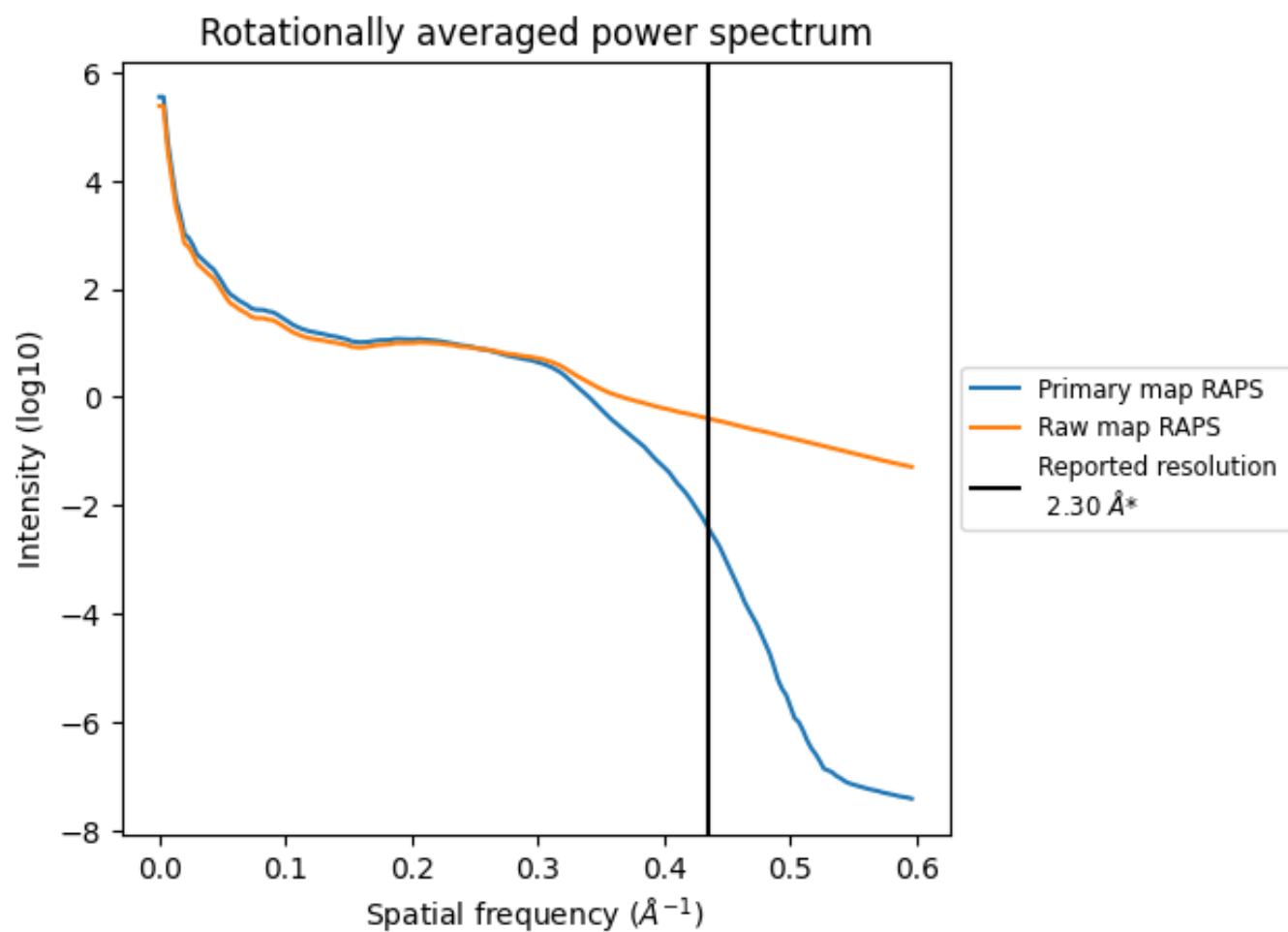
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1563 nm^3 ; this corresponds to an approximate mass of 1412 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 ⓘ

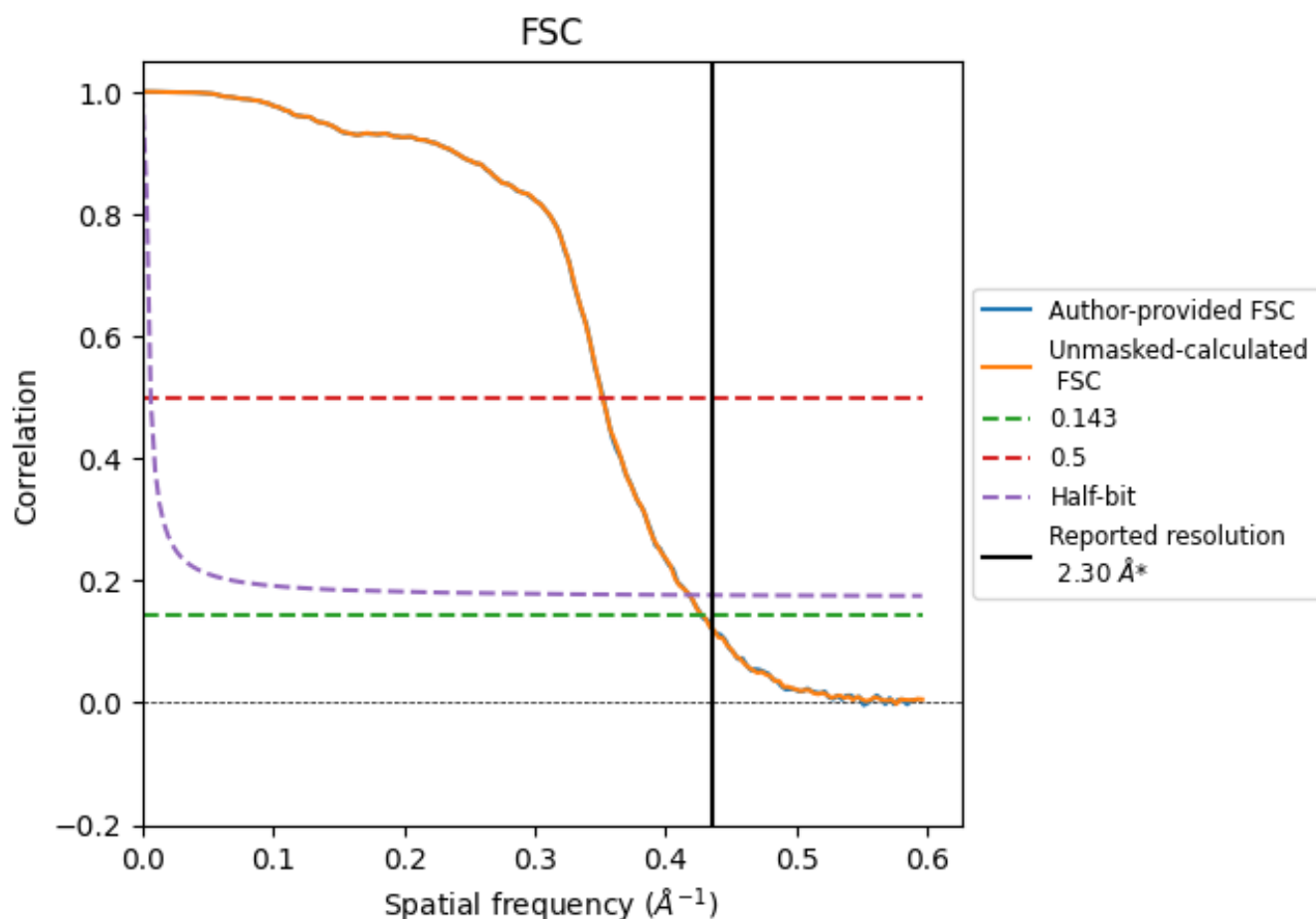


*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

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 $0.435 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

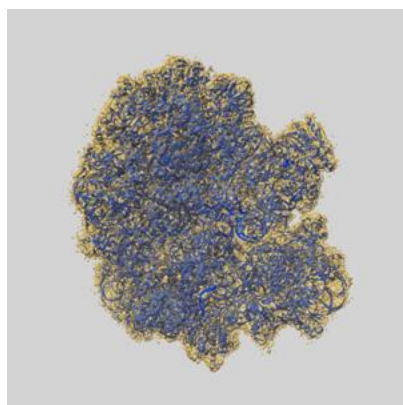
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.34	2.84	2.39
Unmasked-calculated*	2.34	2.84	2.39

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

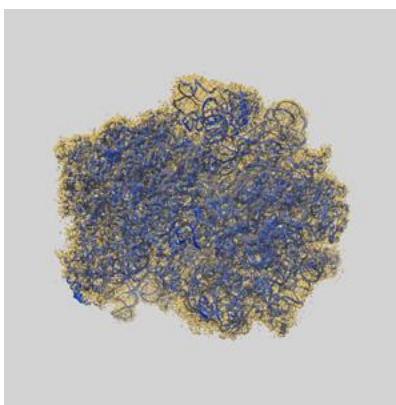
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55136 and PDB model 9SRB. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

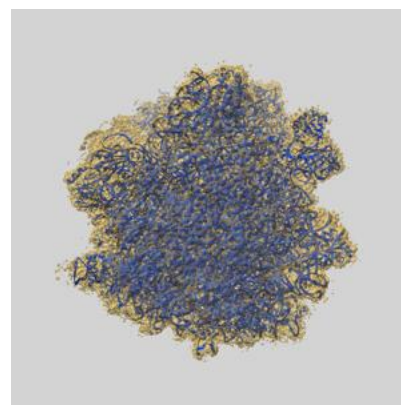
9.1 Map-model overlay [i](#)



X



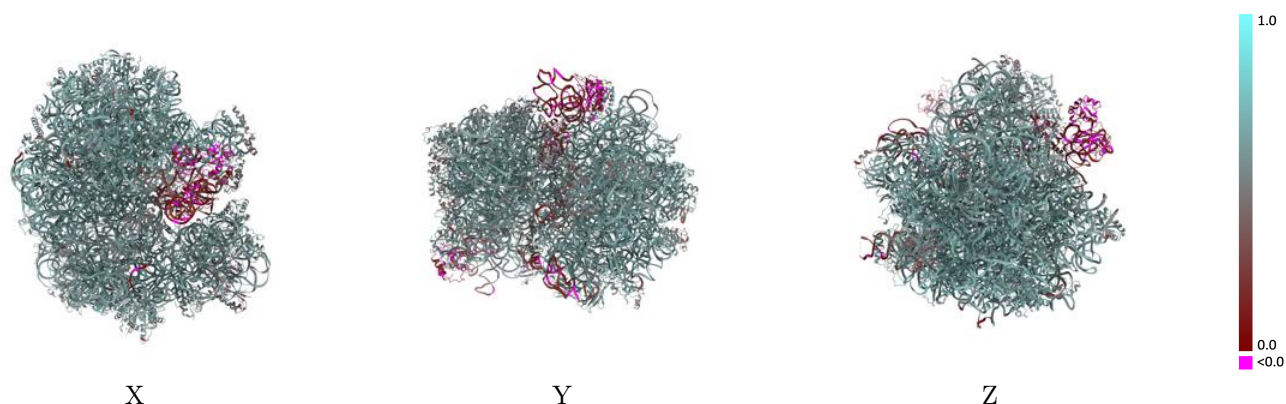
Y



Z

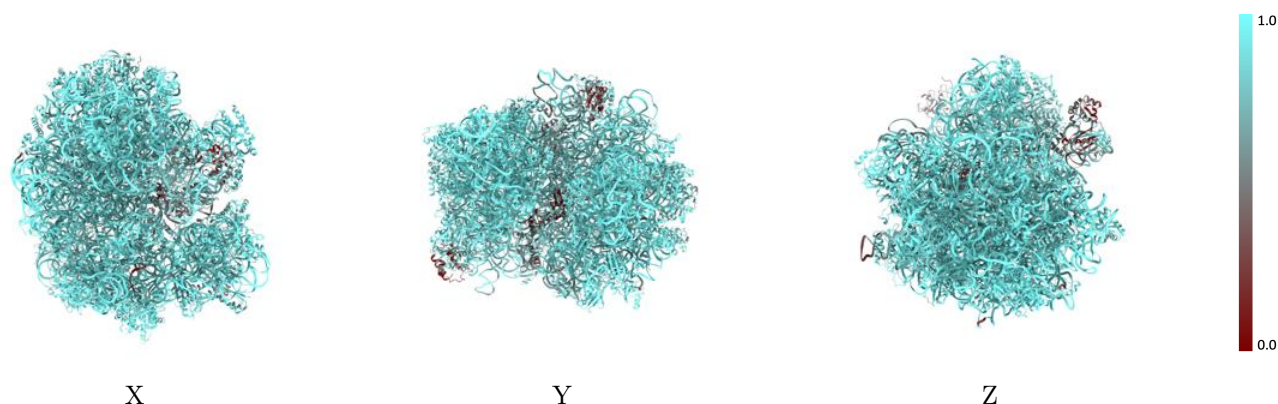
The images above show the 3D surface view of the map at the recommended contour level 0.0009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



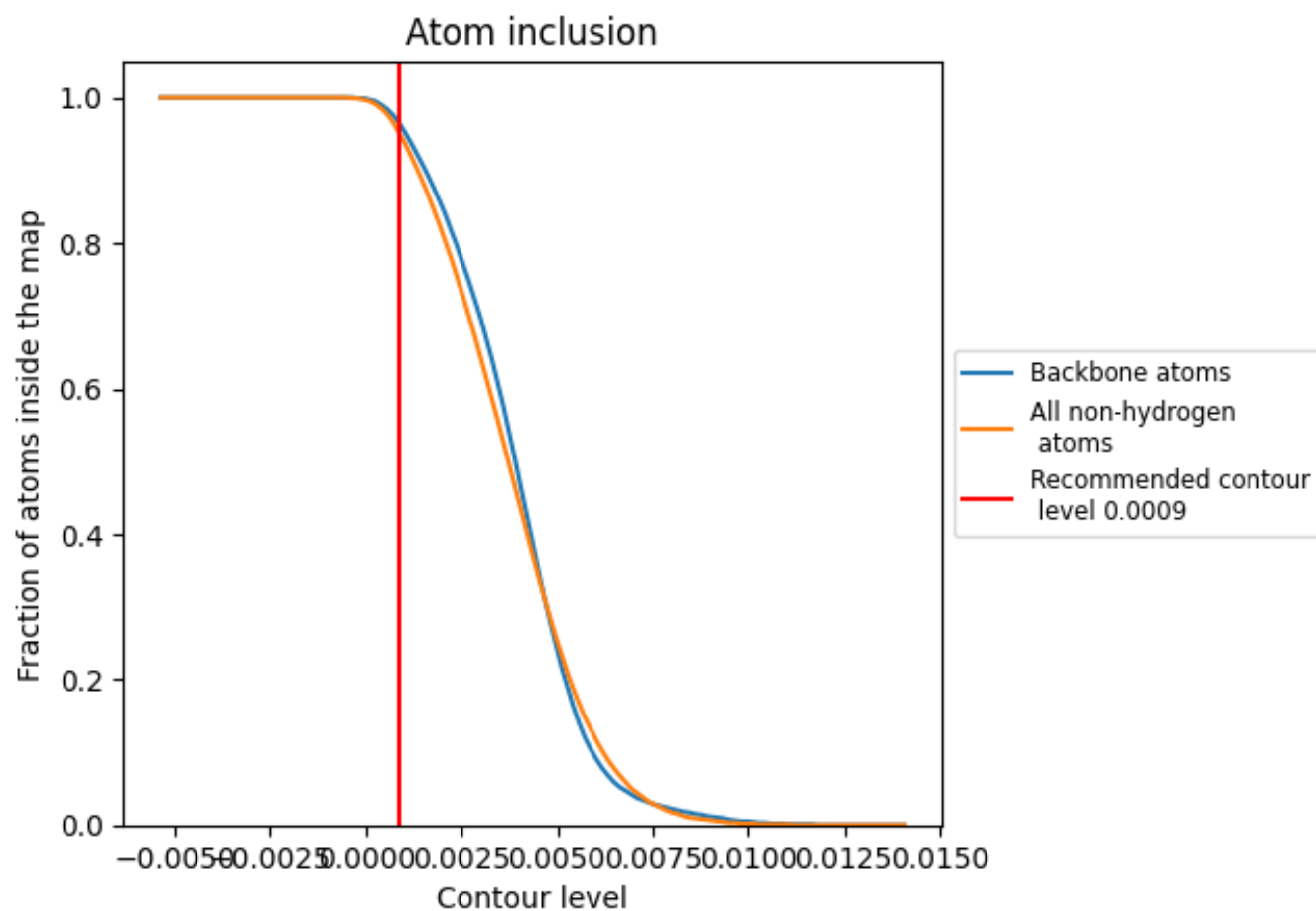
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0009).

9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.0009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9490	 0.5840
1	 0.9750	 0.6010
2	 0.9880	 0.6010
3	 0.9980	 0.6030
A	 0.3810	 0.4020
A0	 0.9500	 0.6260
A3	 0.3100	 0.1270
AA	 0.8820	 0.5190
AB	 0.9620	 0.5690
AC	 0.9500	 0.5650
AD	 0.9590	 0.5870
AE	 0.9760	 0.5950
AF	 0.9700	 0.5980
AG	 0.9250	 0.5570
AH	 0.9530	 0.5770
AI	 0.9850	 0.6250
AJ	 0.9590	 0.6080
AK	 0.9590	 0.5750
AL	 0.8780	 0.5100
AM	 0.9070	 0.5590
AN	 0.9480	 0.5950
AO	 0.9440	 0.5750
AP	 0.9520	 0.5860
AQ	 0.9380	 0.5720
AR	 0.9630	 0.6110
AS	 0.9660	 0.5390
AT	 0.9260	 0.5590
AU	 0.9710	 0.5810
AV	 0.9420	 0.5670
AW	 0.9520	 0.5400
AX	 0.9490	 0.5740
AY	 0.3810	 0.1070
AZ	 0.9140	 0.5370
B4	 0.8290	 0.4190
B5	 0.9820	 0.5940



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Continued from previous page...

Chain	Atom inclusion	Q-score
B6	 0.7840	 0.5600
BA	 0.4530	 0.0690
BB	 0.9750	 0.6470
BC	 0.9750	 0.6440
BD	 0.9850	 0.6360
BE	 0.9040	 0.5040
BF	 0.9690	 0.5960
BG	 0.9600	 0.5830
BI	 0.9750	 0.6440
BJ	 0.9620	 0.6480
BK	 0.9680	 0.5620
BL	 0.9570	 0.6090
BM	 0.9920	 0.6560
BN	 0.9540	 0.6090
BO	 0.9610	 0.5600
BP	 0.9820	 0.6390
BQ	 0.9770	 0.6350
BR	 0.9820	 0.6400
BS	 0.9870	 0.6420
BT	 0.9810	 0.6220
BU	 0.9750	 0.6220
BV	 0.9820	 0.6410
BW	 0.9100	 0.5680
BY	 0.9850	 0.6340
BZ	 0.9460	 0.5690
Ba	 0.9630	 0.6100
Bb	 0.9800	 0.6450
Bc	 0.9750	 0.6410
Bd	 0.9770	 0.6280
Be	 0.9920	 0.6560
Bf	 0.9980	 0.6530
Bg	 0.9890	 0.6190
Bi	 0.9700	 0.6410
Bj	 0.9590	 0.6230
Bk	 0.9670	 0.6060
Bl	 0.9810	 0.5890
H	 0.6550	 0.3180