



Full wwPDB EM Validation Report ⓘ

Aug 3, 2026 – 01:02 pm BST

PDB ID : 9SRA / pdb_00009sra
EMDB ID : EMD-55135
Title : Cryo-EM structure of P. abyssi HibA:ribosome with an SD:antiSD duplex
Authors : Madru, C.M.; Bourgeois, G.B.; Mechulam, Y.M.; Schmitt, E.S.
Deposited on : 2025-09-24
Resolution : 2.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

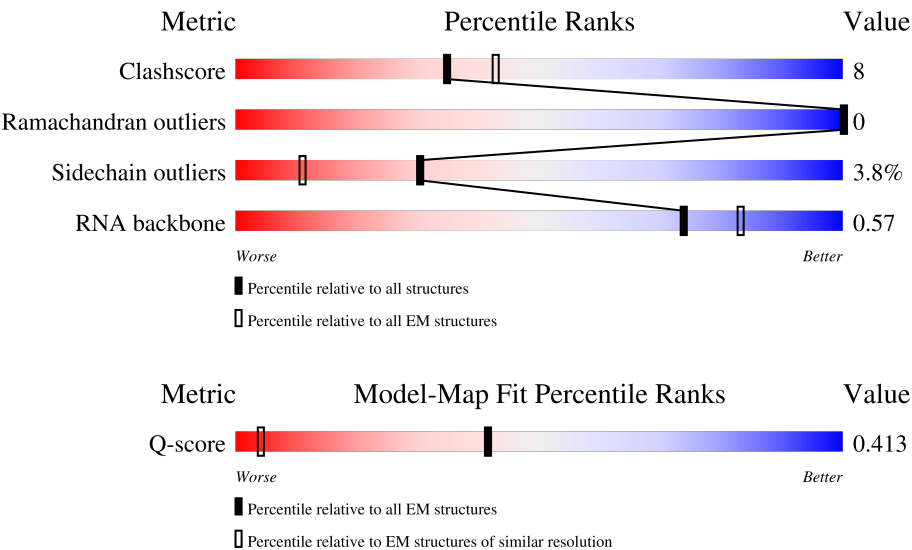
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal 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 i

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

The reported resolution of this entry is 2.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	3018	
2	2	1512	
3	3	128	

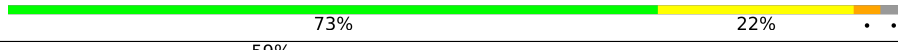
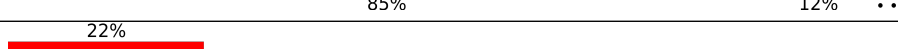
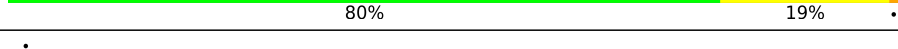
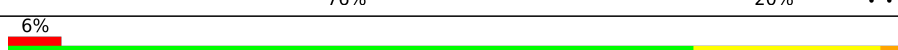
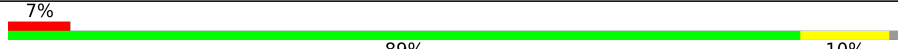
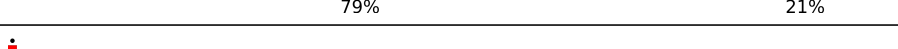
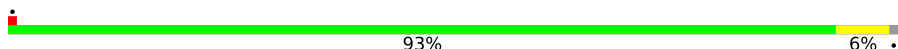
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Mol	Chain	Length	Quality of chain
4	H	392	 66% 76% 20% . .
5	AA	199	 70% 23% . 6%
6	AB	202	 83% 14% .
7	AC	63	 71% 19% 10%
8	AD	180	 85% 11% .
9	AE	243	 79% 20%
10	AF	236	 83% 14% .
11	AG	125	 72% 26% ..
12	AH	215	 76% 20% .
13	AI	130	 85% 14% ..
14	AJ	127	 87% 9% . .
15	AK	135	 84% 16%
16	AL	102	 74% 22% . .
17	AM	137	 82% 10% . 7%
18	AN	147	 84% 15% .
19	AP	56	 62% 34% . .
20	AQ	158	 85% 13% ..
21	AR	113	 78% 16% . 5%
22	AS	67	 70% 25% .
23	AU	150	 81% 17% ..
24	AV	99	 85% 12% .
24	B6	99	 61% 64% 28% . 5%
25	AW	65	 82% 12% 6%
26	AX	71	 75% 11% 6% 8%
27	AY	51	 63% 61% 35% .

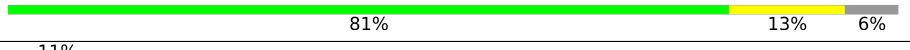
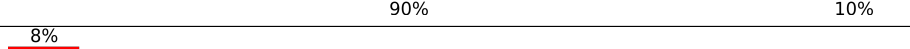
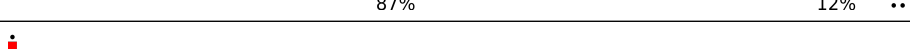
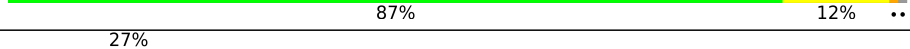
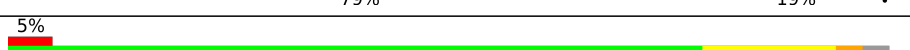
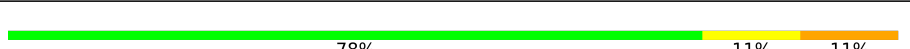
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Mol	Chain	Length	Quality of chain
28	AZ	210	
29	A0	37	
30	A3	123	
30	B4	123	
30	BG	123	
31	AT	132	
32	AO	148	
33	BB	239	
34	BY	155	
35	BO	203	
36	BC	361	
37	B5	82	
37	BK	82	
38	BL	147	
39	Bf	51	
40	BU	121	
41	Bb	130	
42	Be	62	
43	BE	188	
44	Ba	94	
45	BT	86	
46	BW	68	
47	Bi	83	
48	BI	142	
49	BR	97	

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Mol	Chain	Length	Quality of chain
50	BQ	151	
51	BV	67	
52	Bj	94	
53	BD	255	
54	BF	184	
55	BZ	99	
56	BP	120	
57	BM	194	
58	BS	155	
59	Bd	91	
60	BN	181	
61	Bg	51	
62	Bc	87	
63	BJ	141	
64	Bl	77	
65	Bk	65	
66	sd	9	

2 Entry composition

There are 68 unique types of molecules in this entry. The entry contains 170684 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	1497	Total	C	N	O	P	0	0
			32311	14417	5959	10438	1497		

- 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 Dehydrogenase.

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

- Molecule 5 is a protein called 30S ribosomal protein S3Ae.

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

- Molecule 6 is a protein called 30S ribosomal protein S2.

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

- Molecule 7 is a protein called Zn-ribbon RNA-binding protein involved in translation.

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

- Molecule 8 is a protein called 30S ribosomal protein S4.

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

- Molecule 9 is a protein called 30S ribosomal protein S4e.

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

- Molecule 10 is a protein called 30S ribosomal protein S5.

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

- Molecule 11 is a protein called 30S ribosomal protein S6e.

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

- Molecule 12 is a protein called 30S ribosomal protein S7.

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

- Molecule 13 is a protein called 30S ribosomal protein S8.

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

- Molecule 14 is a protein called 30S ribosomal protein S8e.

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

- Molecule 15 is a protein called 30S ribosomal protein S9.

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

- Molecule 16 is a protein called 30S ribosomal protein S10.

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

- Molecule 17 is a protein called 30S ribosomal protein S11.

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

- Molecule 18 is a protein called 30S ribosomal protein S12.

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

- Molecule 19 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 20 is a protein called 30S ribosomal protein S15.

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

- Molecule 21 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AR	107	Total	C	N	O	S	0	0
			884	562	172	147	3		

- Molecule 22 is a protein called 30S ribosomal protein S17e.

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

- Molecule 23 is a protein called 30S ribosomal protein S19e.

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

- Molecule 24 is a protein called 30S ribosomal protein S24e.

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

- Molecule 25 is a protein called 30S ribosomal protein S27e.

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

- Molecule 26 is a protein called 30S ribosomal protein S28e.

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

- Molecule 27 is a protein called 30S ribosomal protein S27ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AY	49	Total	C	N	O	S	0	0
			400	257	76	62	5		

- Molecule 28 is a protein called 30S ribosomal protein S3.

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

- Molecule 29 is a protein called eS32.

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

- Molecule 30 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 31 is a protein called 30S ribosomal protein S19.

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

- Molecule 32 is a protein called 30S ribosomal protein S13.

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 37 is a protein called Large ribosomal subunit protein eL14.

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

- Molecule 38 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 39 is a protein called Large ribosomal subunit protein eL39.

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

- Molecule 40 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 41 is a protein called Large ribosomal subunit protein eL32.

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

- Molecule 42 is a protein called Large ribosomal subunit protein eL37.

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

- Molecule 43 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 44 is a protein called Large ribosomal subunit protein eL31.

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 46 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 47 is a protein called Large ribosomal subunit protein eL43.

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

- Molecule 48 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 49 is a protein called Large ribosomal subunit protein eL21.

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

- Molecule 50 is a protein called Large ribosomal subunit protein eL19.

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

- Molecule 51 is a protein called Large ribosomal subunit protein eL24.

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

- Molecule 52 is a protein called Large ribosomal subunit protein eL42.

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

- Molecule 53 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 54 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 55 is a protein called Large ribosomal subunit protein eL30.

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

- Molecule 56 is a protein called Large ribosomal subunit protein eL18.

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

- Molecule 57 is a protein called Large ribosomal subunit protein eL15.

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

- Molecule 58 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 59 is a protein called Large ribosomal subunit protein eL34.

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

- Molecule 60 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 61 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 62 is a protein called Large ribosomal subunit protein eL33.

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

- Molecule 63 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 64 is a protein called Large ribosomal subunit protein eL20.

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

- Molecule 65 is a protein called C2H2-type domain-containing protein.

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

- Molecule 66 is a RNA chain called antiSD-RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	sd	9	Total	C	N	O	P	0	0
			199	88	39	63	9		

- Molecule 67 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
67	1	166	Total	Mg	0
			166	166	
67	2	69	Total	Mg	0
			69	69	
67	3	1	Total	Mg	0
			1	1	
67	AK	1	Total	Mg	0
			1	1	
67	AN	1	Total	Mg	0
			1	1	
67	BB	2	Total	Mg	0
			2	2	
67	Bb	1	Total	Mg	0
			1	1	
67	BD	1	Total	Mg	0
			1	1	
67	BM	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
67	BS	1	Total	Mg	0
			1	1	

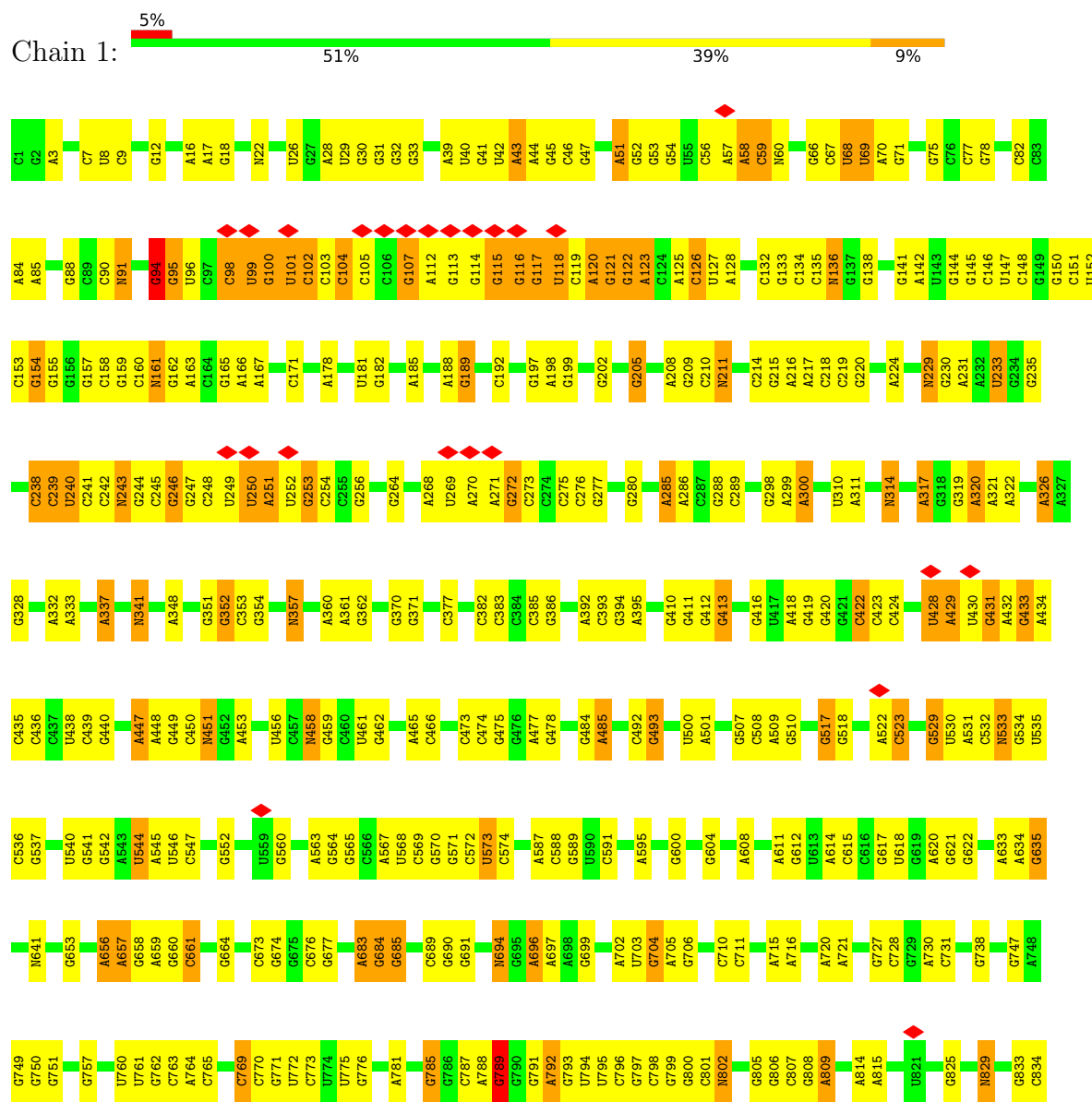
- Molecule 68 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

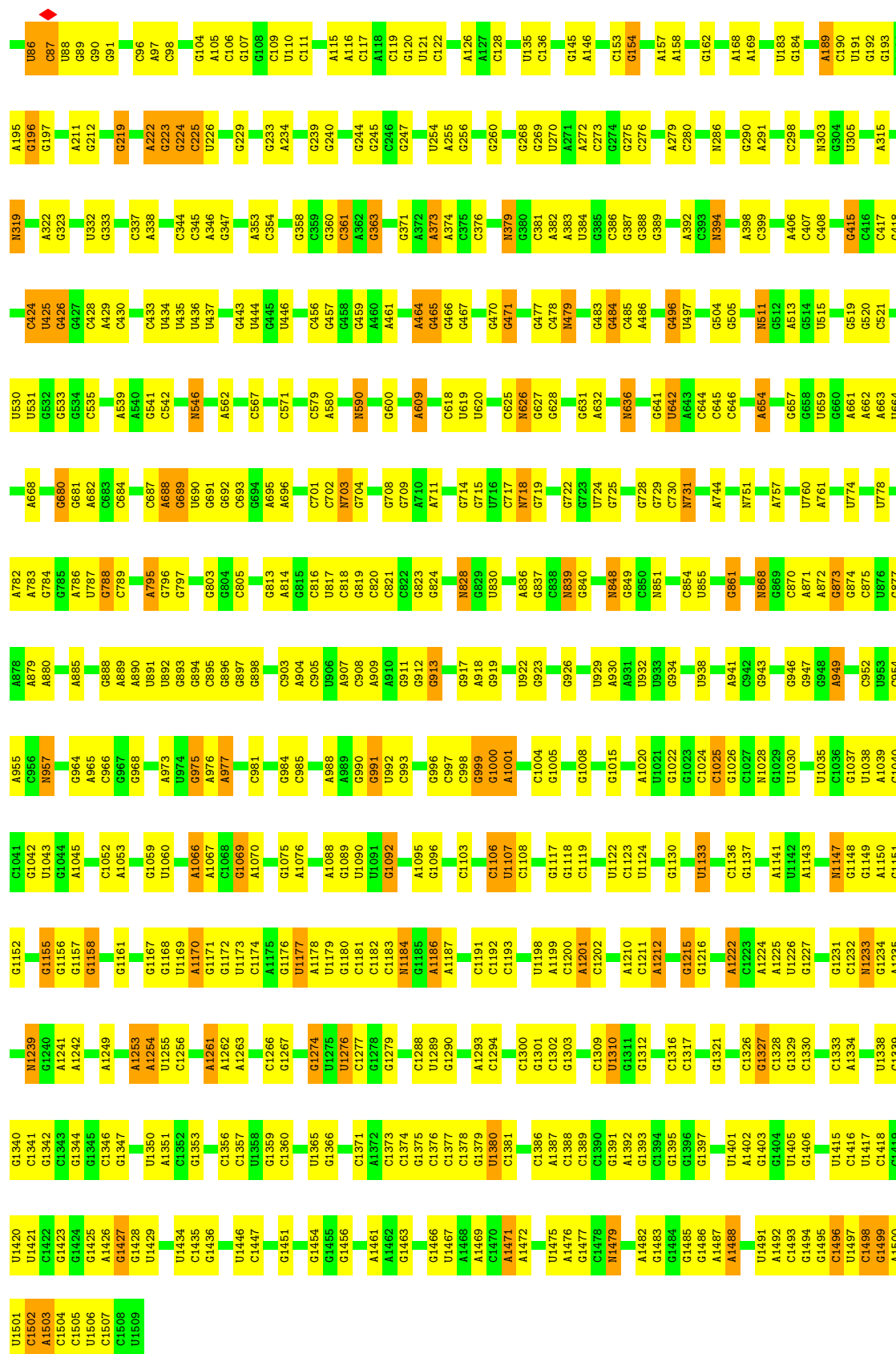
3 Residue-property plots

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

• Molecule 1: rRNA 23S

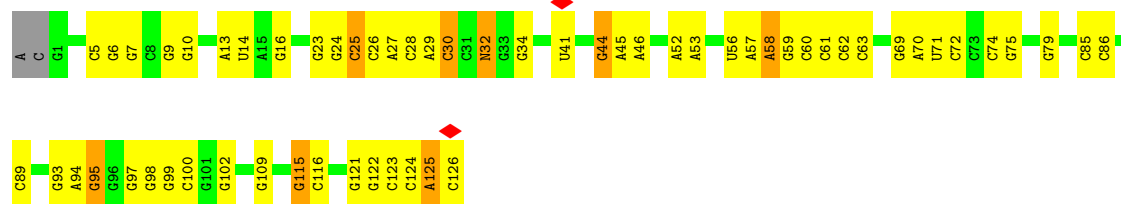


G1943	A1854	G1769	A1582	U1482	G1392	G1323	A1251	C1153	G1078	U993	A919	N835
G1950	A1855	A1780	U1583	A1484	G1393	A1324	G1252	C1154	G1079	U998	C920	G841
C1951	U1856	G1761	C1587	A1485	C1394	A1325	G1253	C1155	A1081		C921	N922
A1952	U1857	U1762	C1588	C1489	U1395	G1326	C1254	U1159	A1084	G1006	A824	A844
A1954	C1858	G1763	U1589	G1490	C1396	C1327	C1255	U1161	U1085	G1007	A924	C845
	U1862	N1765	C1590	C1498	A1397	A1328	C1256	A1162	G1086	C1011	A925	C846
N1962			A1591	G1499	C1401	G1329	A1259	A1163	G1087	G1012	A926	G847
G1972	A1685	A1769	G1592	C1498	G1402	C1330	U1260	G1168	C1093	U1013	G929	A848
	C1686	U1770	C1593	G1499	G1406	C1331	U1261	A1169	G1094	G1014	G930	C849
A1976	C1687		N1594	C1508	C1407	C1332	U1262	G1170	C1095	A1015	U931	A850
G1979	G1688	G1692	G1598	C1509	C1411	U1333	G1263	A1171	G1096	C1019	A834	U851
U1979	N1695		G1599	C1514	G1415	C1334	C1265	C1171	A1101	G1020	U935	C855
G1980	G1696	U1781	U1600	C1515		G1335	G1266	C1172	G1102	U1026	G936	G856
	G1697	G1783	U1601	G1517	C1415		U1269	G1173	G1103	G1027	U937	C857
G1983	A1698	U1784	G1606		G1420	U1337	U1272	C1174	C1104	G1031	G939	A858
	G1699			G1520	C1421	U1338	G1278	G1179	G1105	A1032	C940	G864
U1986	G1700		A1612	G1524	C1422	A1339	U1279	G1180	G1106	A1033	C941	C865
G1987	A1788		A1613	U1525	G1423	U1340	C1280	G1186	U1107	A1034	G946	C866
C1988	G1789		G1614	A1526	G1424	A1341	C1281	U1187	G1108	G1035	C947	U867
	C1790		G1615	U1533	G1425	A1342	A1282	A1188	G1109	G1036	G948	C868
U1992	G1705	G1706	N1617		A1426	A1343	A1283	U1189	G1110	G1037	G949	G869
G1993	C1707		G1618	G1540	A1430	G1344	A1284	A1198	G1111	U1038	G950	A870
C1994	C1708		C1619	U1541	U1431	U1345	G1285	G1199	A1115	A1039	G951	C871
U1995	G1709		G1620	U1544	U1432	A1346	A1288	G1200	G1116	A1040	U952	C872
U1996	C1710		N1621	A1545	G1433	G1347	U1289	G1201	G1117	U1041	G953	U877
A1997	G1711			U1546	G1434	U1348	G1290	U1202	C1118	C1042	A954	G878
A1998	G1712		A1625	U1547	U1435	U1349	U1291	G1203	G1119	G1043	A955	A879
C1999	G1713		C1626	U1548	U1436	U1349	U1292	G1204	U1120		A956	G880
C2000	G1714			U1549	C1437	A1350	N1293	G1205	G1046	U1048	U957	G887
N2001	U1715		G1630	N1550	U1438	A1351	G1294	G1206	A1122		C959	G888
A2004	U1716		G1631	G1551	G1440	C1352	G1295	G1207	U1123	A1053	C960	U889
G2005	G1726		G1632	A1552		A1353	U1299	G1208	U1124	U1054	C961	G890
	C1727		G1633	C1553	G1443	G1354	U1300	G1209	G1125	A1055	C962	C891
G2009			A1639	N1554	G1444	C1355	A1301	U1210	G1129	U1056	A963	A892
G2012	A1730		A1640	C1555	G1445	U1356	G1302	A1211	U1130	G1057	A964	A893
	U1731		A1641	C1556		C1357	A1303	A1212	G1131	C1058	C965	A894
G2020	G1732			N1557	G1449	U1358	G1304	G1216	G1132	U1059	A966	A895
A1914	A1733		A1645	G1558	G1450	C1359	A1305		A1133	G1060	U973	G896
U1920	G1734		A1646	G1559	C1451	U1360	G1306	G1221	G1134		G974	C897
G2028	G1735		A1647	U1560	G1452	C1361	C1307	G1222	G1135	C1063	G975	U806
A2029	C1736		C1648	G1561		G1362	G1308	A1224	G1136	N1065	A976	C907
C2030			G1649		U1457	U1363	G1309	G1225	G1137	G1066	G977	A908
U2031	G1739		G1650	A1567	G1458	C1364	G1310		G1138	C1067	C978	C909
				G1568	C1459	U1365	G1311	A1231	C1139	U1068	C979	G910
U2035	A1742		U1653	G1569	N1460	C1366	G1314	A1234	A1141	A1071	C980	C913
A2040	A1743		A1654	G1570	G1461	U1367	U1315		A1142	U1072	G981	G914
A2041	A1748		U1655	C1574	G1462	G1367	A1316	G1240	A1143	G1073	G982	
A2042	U1749		A1657	C1575	G1469		G1317	A1241	G1144	U1074	U984	
A2043	A1750		G1661	C1576	G1470	C1370	C1318	G1242	C1145	A1074	U990	
C2044	A1751		N1662	U1577	G1478	C1371	C1319	C1243	C1146	U1075	G991	A917
A2045	G1752		U1663	G1578	C1479	G1372	C1320	N1243	C1147	C1076	C992	G918
C2046	U1755		U1664	C1580	G1481	G1374	U1321	A1250	C1148	C1077		
A2047	G1756			A1581		G1380	A1322					
						G1386						
						G1387						
						A1388						
						C1389						
						G1390						
						G1391						



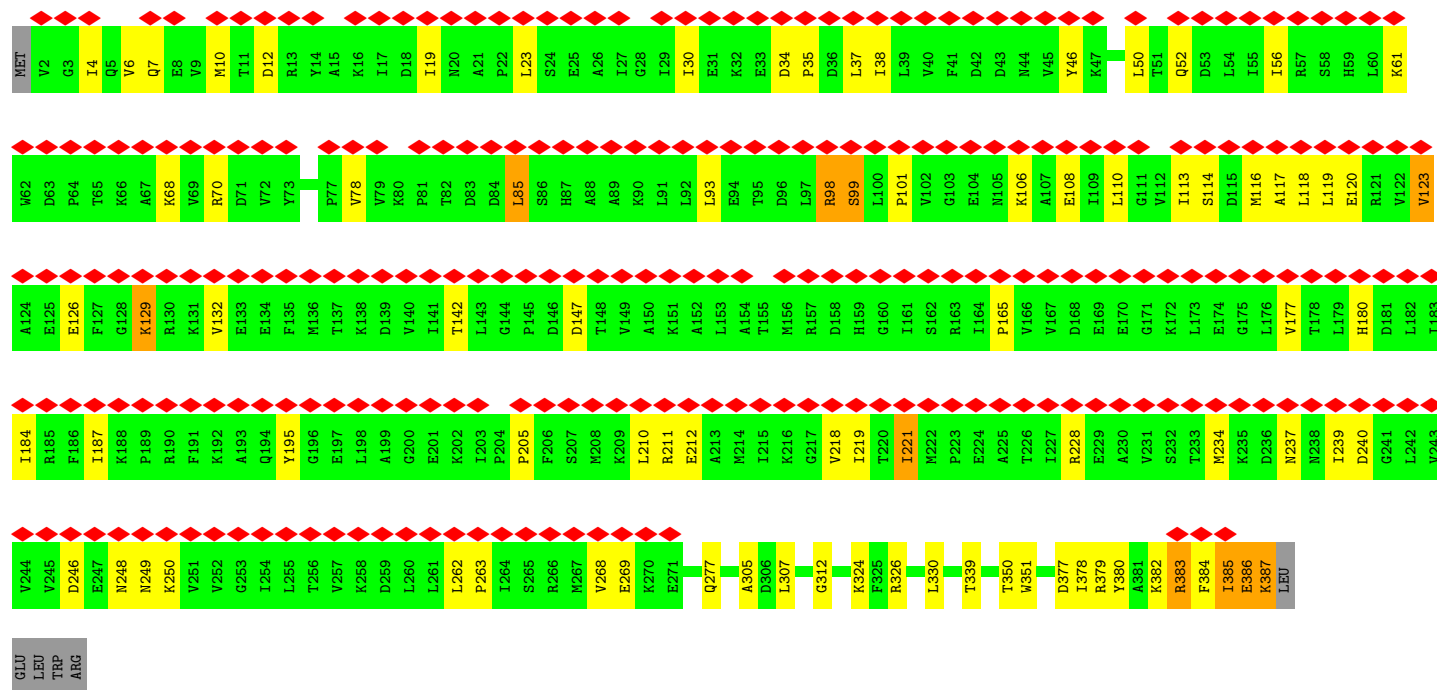
• Molecule 3: rRNA 5S

Chain 3: 



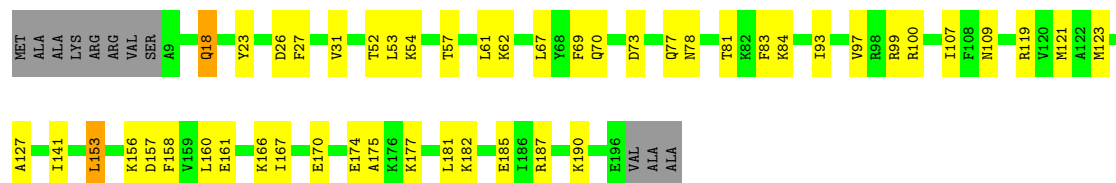
• Molecule 4: Dehydrogenase

Chain H: 



• Molecule 5: 30S ribosomal protein S3Ae

Chain AA: 

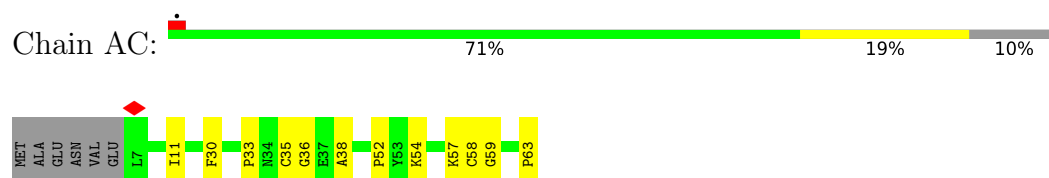


• Molecule 6: 30S ribosomal protein S2

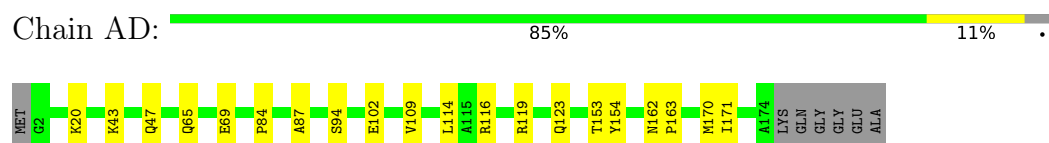
Chain AB: 



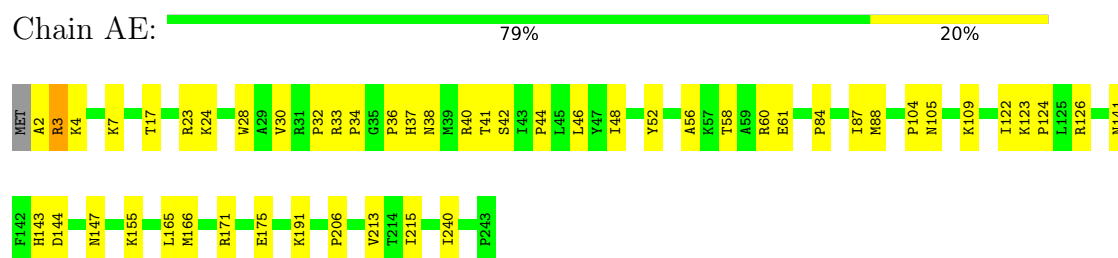
- Molecule 7: Zn-ribbon RNA-binding protein involved in translation



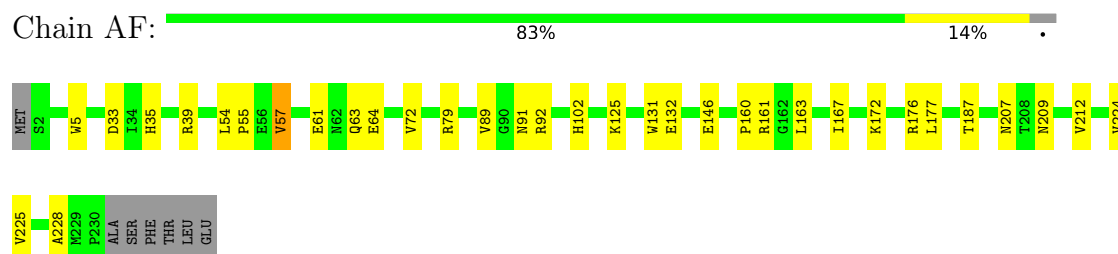
- Molecule 8: 30S ribosomal protein S4



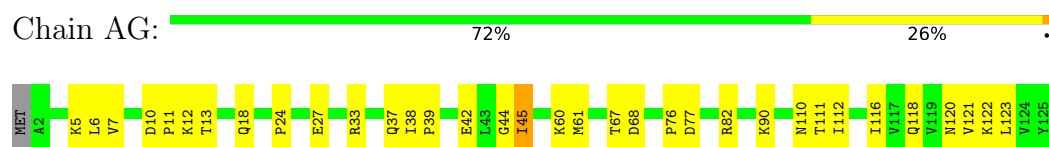
- Molecule 9: 30S ribosomal protein S4e



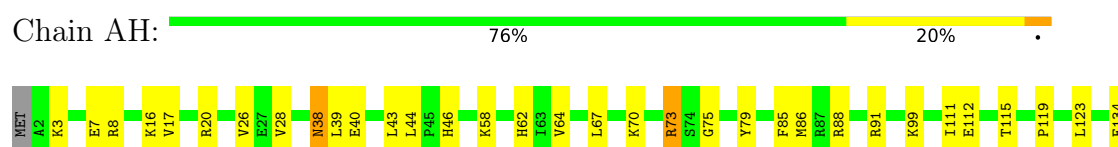
- Molecule 10: 30S ribosomal protein S5



- Molecule 11: 30S ribosomal protein S6e



- Molecule 12: 30S ribosomal protein S7





- Molecule 13: 30S ribosomal protein S8

Chain AI: 85% 14% ..



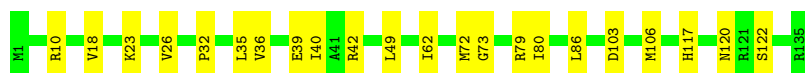
- Molecule 14: 30S ribosomal protein S8e

Chain AJ: 87% 9% ..



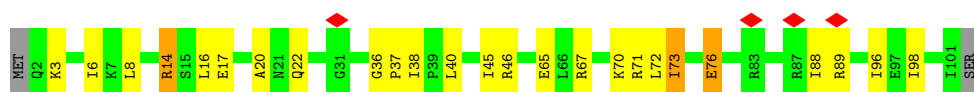
- Molecule 15: 30S ribosomal protein S9

Chain AK: 84% 16%



- Molecule 16: 30S ribosomal protein S10

Chain AL: 74% 22% ..



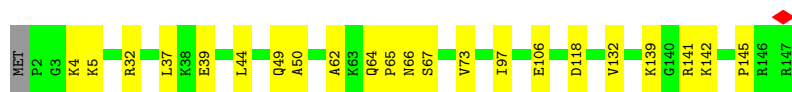
- Molecule 17: 30S ribosomal protein S11

Chain AM: 82% 10% 7%



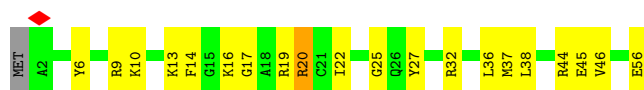
- Molecule 18: 30S ribosomal protein S12

Chain AN: 84% 15%



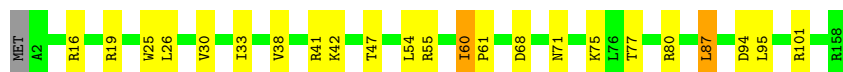
- Molecule 19: 30S ribosomal protein S14 type Z

Chain AP: 62% 34%



- Molecule 20: 30S ribosomal protein S15

Chain AQ: 85% 13% ..



- Molecule 21: 30S ribosomal protein S17

Chain AR: 78% 16% • 5%



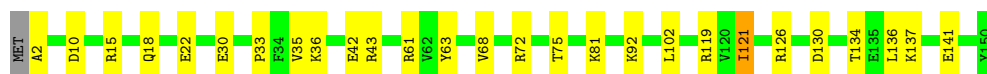
- Molecule 22: 30S ribosomal protein S17e

Chain AS: 70% 25% •



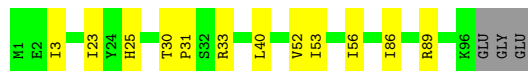
- Molecule 23: 30S ribosomal protein S19e

Chain AU: 81% 17% ..



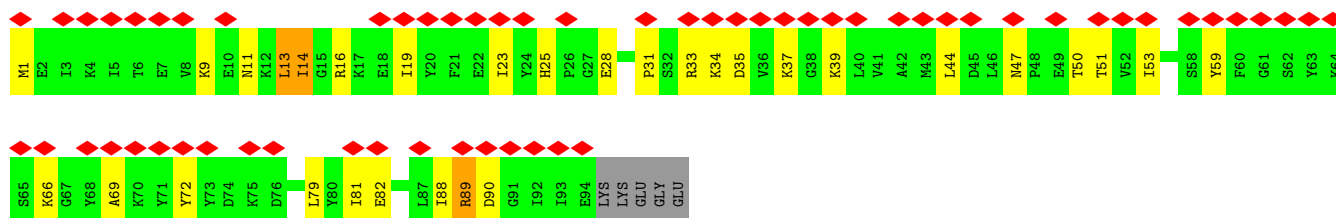
- Molecule 24: 30S ribosomal protein S24e

Chain AV: 85% 12% •



- Molecule 24: 30S ribosomal protein S24e

Chain B6: 61% 64% 28% • 5%



- Molecule 25: 30S ribosomal protein S27e

Chain AW: 



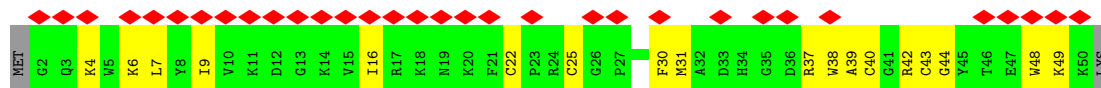
- Molecule 26: 30S ribosomal protein S28e

Chain AX: 



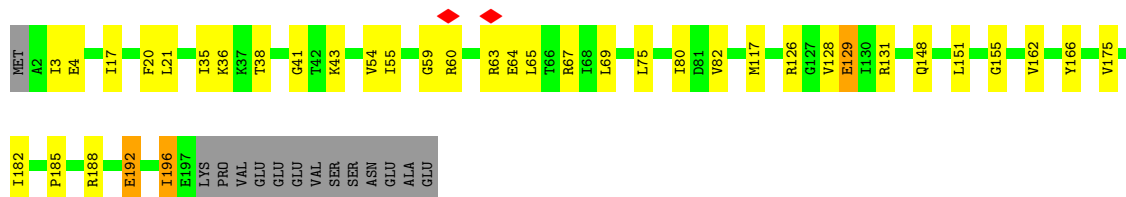
- Molecule 27: 30S ribosomal protein S27ae

Chain AY: 



- Molecule 28: 30S ribosomal protein S3

Chain AZ: 



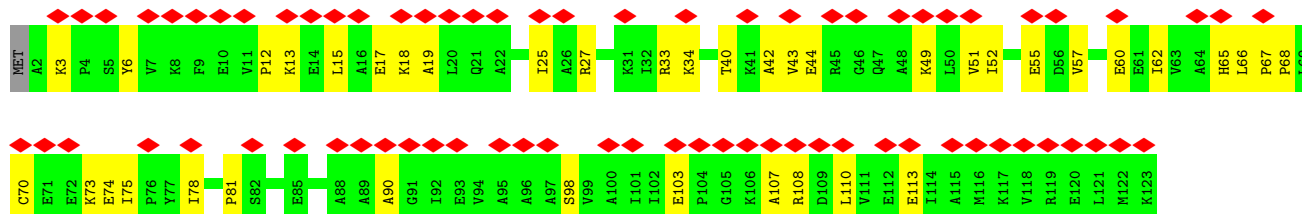
- Molecule 29: eS32

Chain A0: 

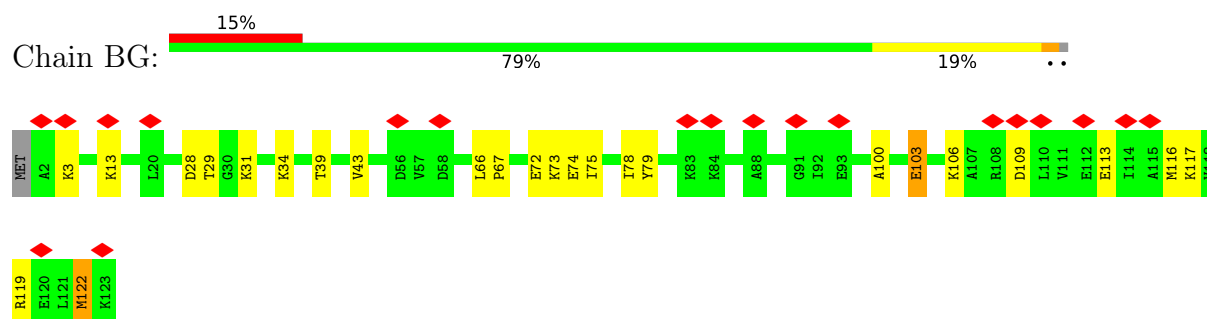


- Molecule 30: 50S ribosomal protein L7Ae

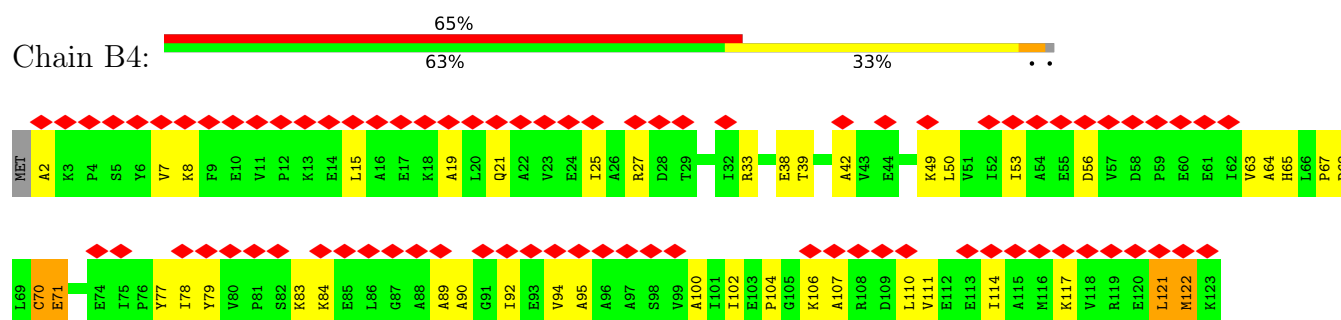
Chain A3: 



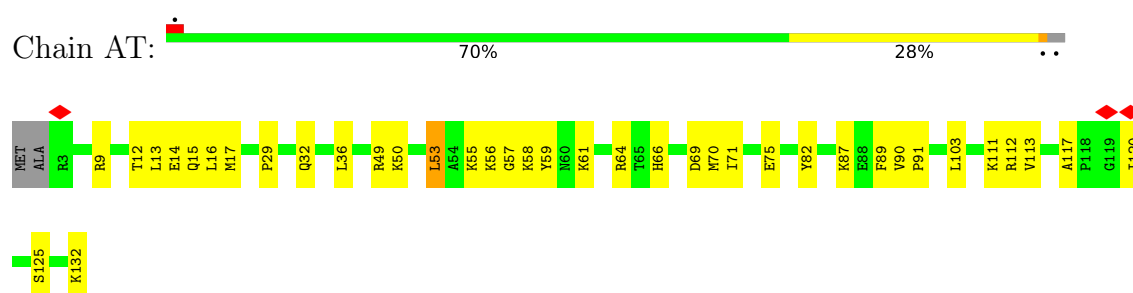
- Molecule 30: 50S ribosomal protein L7Ae



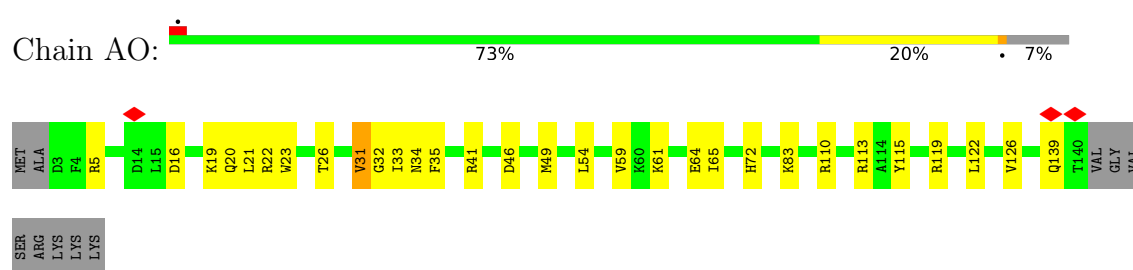
- Molecule 30: 50S ribosomal protein L7Ae



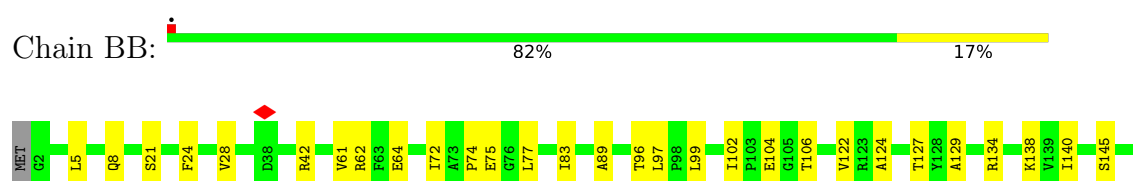
- Molecule 31: 30S ribosomal protein S19



- Molecule 32: 30S ribosomal protein S13

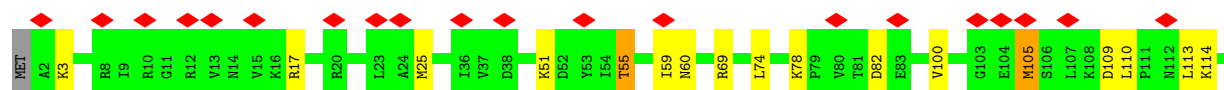
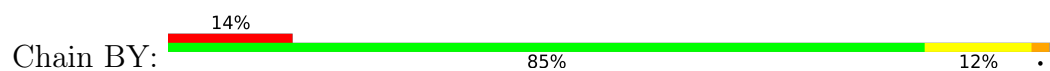


- Molecule 33: Large ribosomal subunit protein uL2

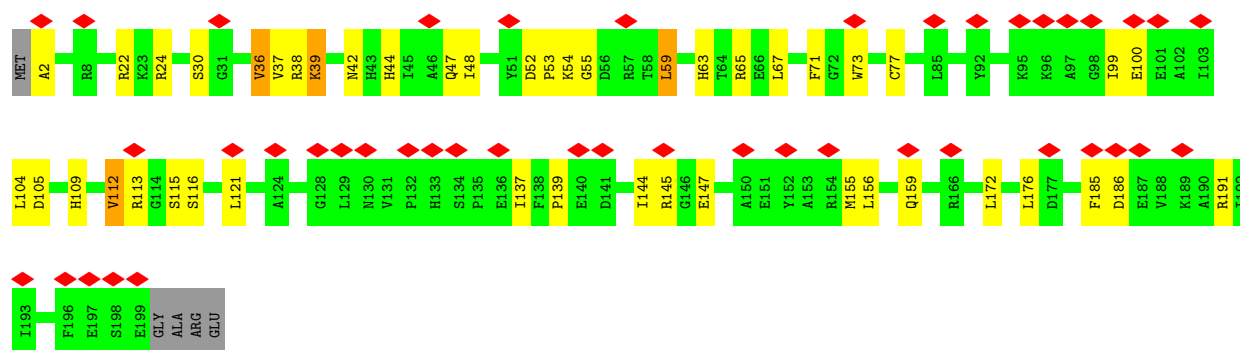
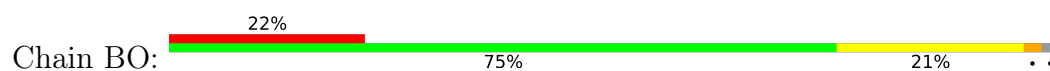




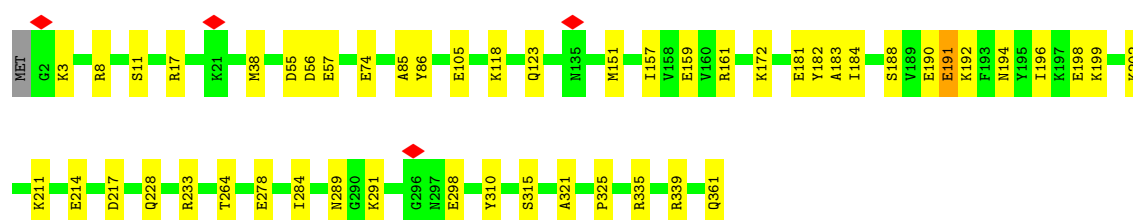
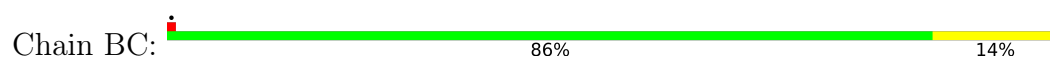
- Molecule 34: Large ribosomal subunit protein uL30



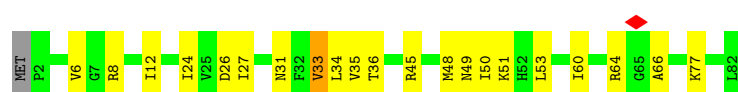
- Molecule 35: Large ribosomal subunit protein uL18



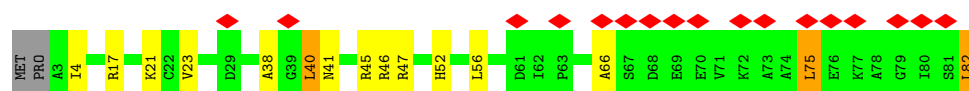
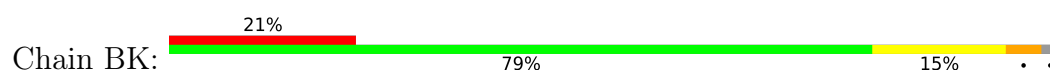
- Molecule 36: Large ribosomal subunit protein uL3



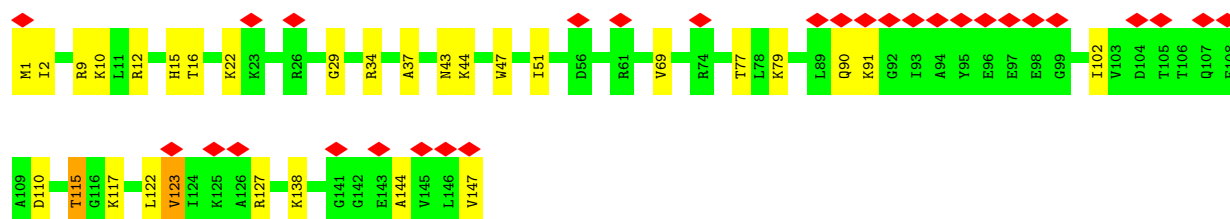
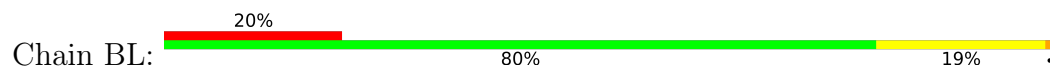
- Molecule 37: Large ribosomal subunit protein eL14



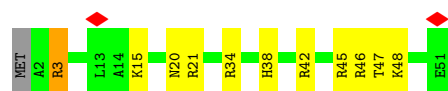
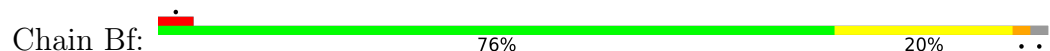
- Molecule 37: Large ribosomal subunit protein eL14



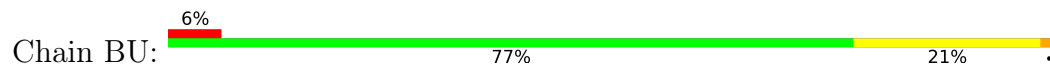
- Molecule 38: Large ribosomal subunit protein uL15



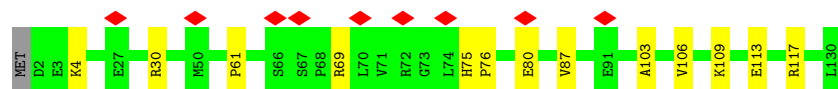
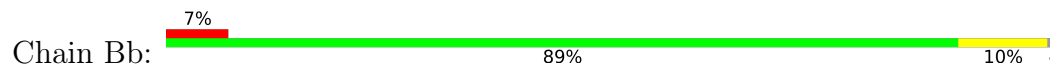
- Molecule 39: Large ribosomal subunit protein eL39



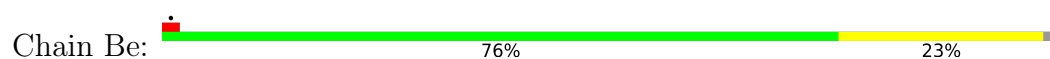
- Molecule 40: Large ribosomal subunit protein uL24



- Molecule 41: Large ribosomal subunit protein eL32

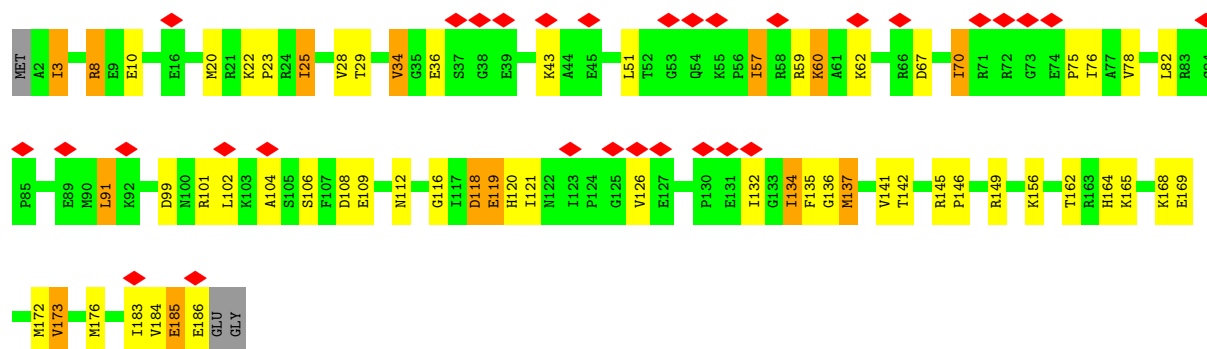


- Molecule 42: Large ribosomal subunit protein eL37

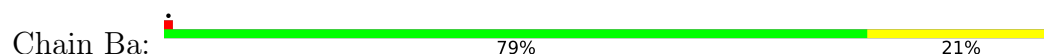


- Molecule 43: Large ribosomal subunit protein uL5

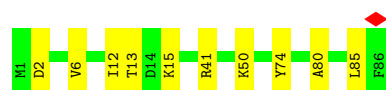




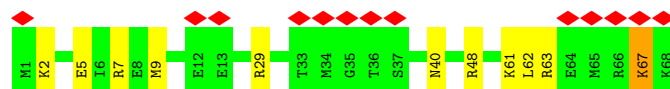
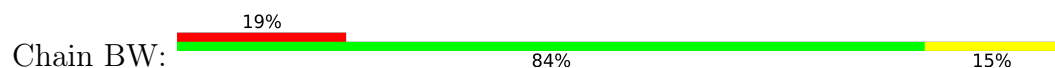
- Molecule 44: Large ribosomal subunit protein eL31



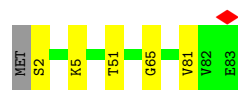
- Molecule 45: Large ribosomal subunit protein uL23



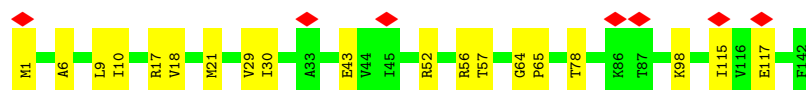
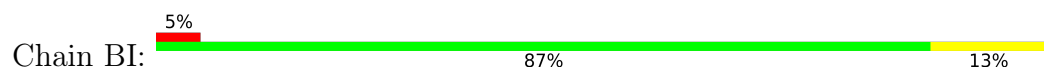
- Molecule 46: Large ribosomal subunit protein uL29



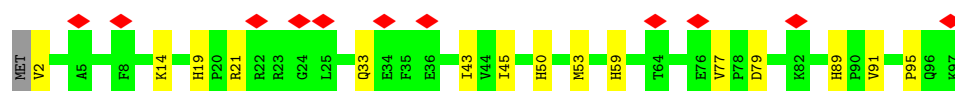
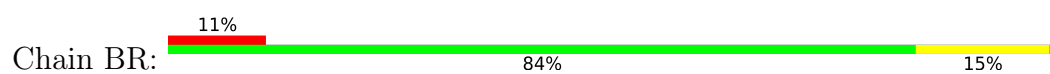
- Molecule 47: Large ribosomal subunit protein eL43



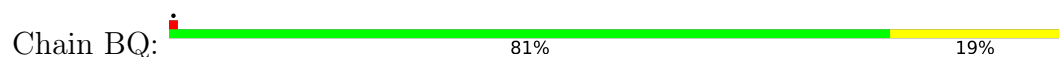
- Molecule 48: Large ribosomal subunit protein uL13



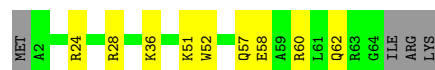
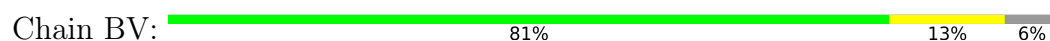
- Molecule 49: Large ribosomal subunit protein eL21



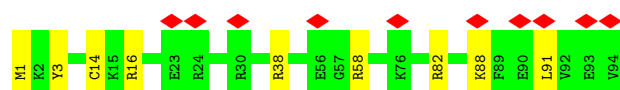
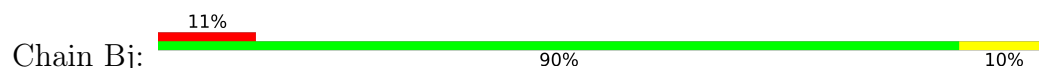
- Molecule 50: Large ribosomal subunit protein eL19



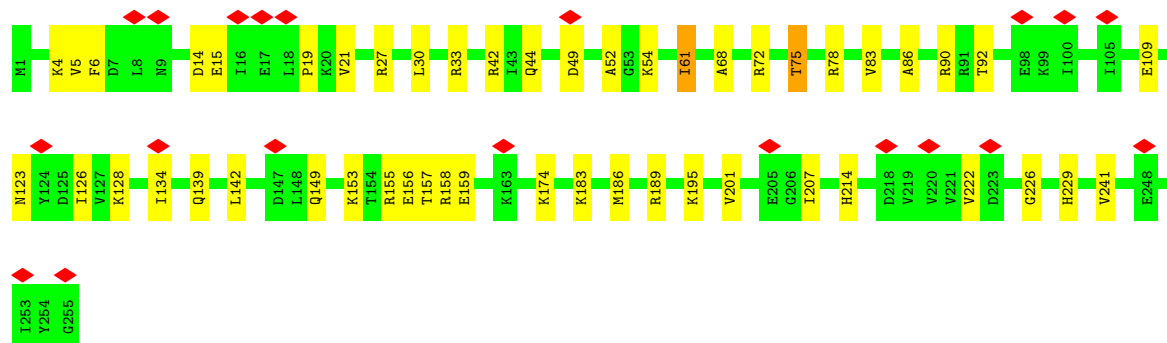
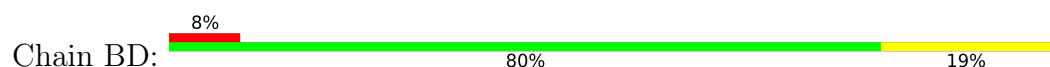
- Molecule 51: Large ribosomal subunit protein eL24



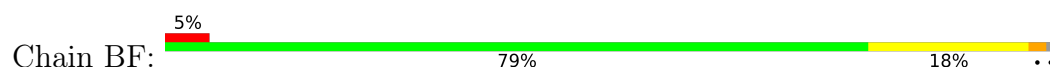
- Molecule 52: Large ribosomal subunit protein eL42



- Molecule 53: Large ribosomal subunit protein uL4

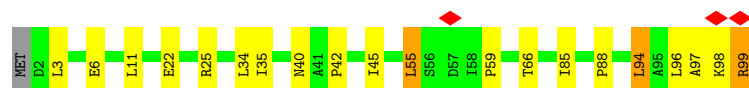
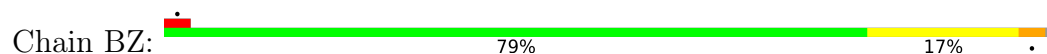


- Molecule 54: Large ribosomal subunit protein uL6

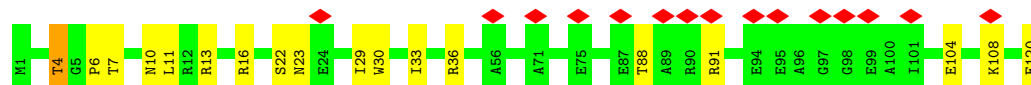
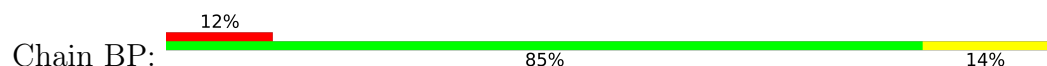




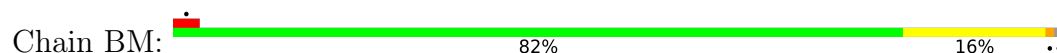
- Molecule 55: Large ribosomal subunit protein eL30



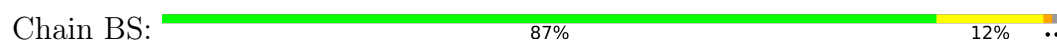
- Molecule 56: Large ribosomal subunit protein eL18



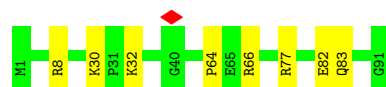
- Molecule 57: Large ribosomal subunit protein eL15



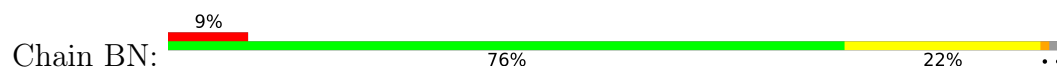
- Molecule 58: Large ribosomal subunit protein uL22

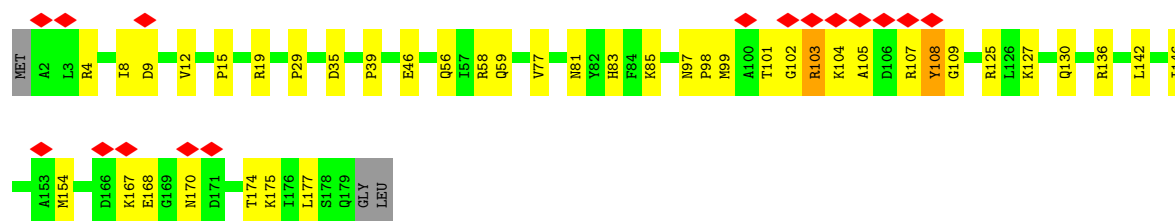


- Molecule 59: Large ribosomal subunit protein eL34

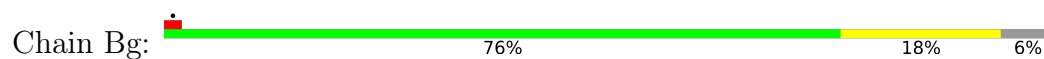


- Molecule 60: Large ribosomal subunit protein uL16

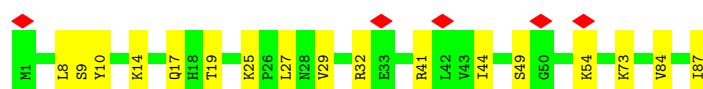
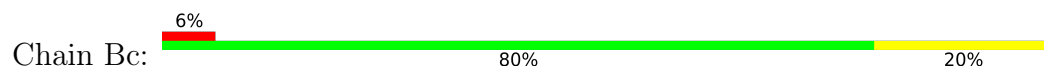




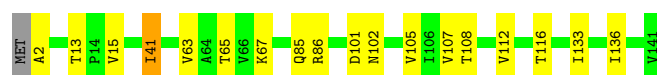
- Molecule 61: Large ribosomal subunit protein eL40



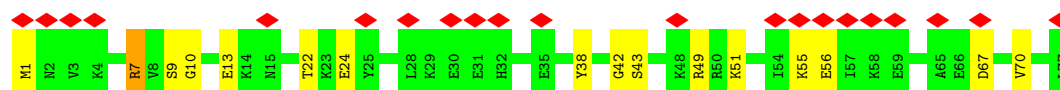
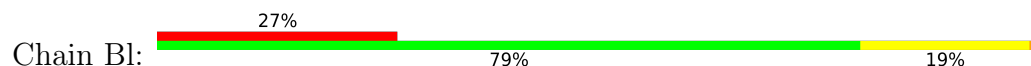
- Molecule 62: Large ribosomal subunit protein eL33



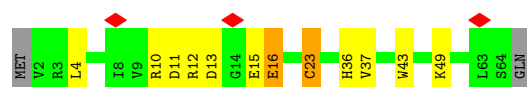
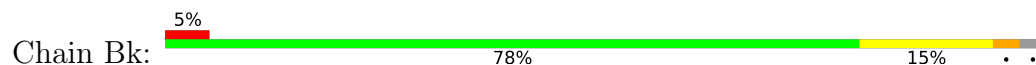
- Molecule 63: Large ribosomal subunit protein uL14



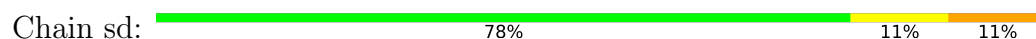
- Molecule 64: Large ribosomal subunit protein eL20



- Molecule 65: C2H2-type domain-containing protein



- Molecule 66: antiSD-RNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	182000	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	0.891	Depositor
Minimum map value	-0.355	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	302.04, 302.04, 302.04	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: 5MC, A2M, UR3, OMG, ZN, OMU, 4AC, MG, 6MZ, OMC, LHH, MA6, B8H

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	0.14	3/70601 (0.0%)	0.32	0/110066
2	2	0.18	0/34457	0.30	2/53715 (0.0%)
3	3	0.16	0/2995	0.34	0/4669
4	H	0.31	1/3120 (0.0%)	0.49	3/4209 (0.1%)
5	AA	0.13	0/1557	0.28	0/2087
6	AB	0.12	0/1602	0.26	0/2165
7	AC	0.11	0/463	0.27	0/628
8	AD	0.12	0/1476	0.23	0/1980
9	AE	0.13	0/2032	0.29	0/2742
10	AF	0.12	0/1838	0.25	0/2478
11	AG	0.12	0/993	0.29	0/1329
12	AH	0.21	0/1762	0.37	0/2366
13	AI	0.13	0/1055	0.25	0/1415
14	AJ	0.13	0/995	0.24	0/1327
15	AK	0.12	0/1089	0.26	0/1459
16	AL	0.11	0/817	0.28	0/1097
17	AM	0.14	0/973	0.28	0/1311
18	AN	0.12	0/1165	0.27	0/1547
19	AP	0.13	0/465	0.32	0/613
20	AQ	0.13	0/1333	0.26	0/1791
21	AR	0.13	0/907	0.27	0/1225
22	AS	0.12	0/548	0.28	0/725
23	AU	0.11	0/1253	0.26	0/1689
24	AV	0.11	0/826	0.24	0/1108
24	B6	0.15	0/808	0.35	0/1086
25	AW	0.12	0/476	0.27	0/641
26	AX	0.10	0/518	0.23	0/694
27	AY	0.09	0/412	0.25	0/549
28	AZ	0.10	0/1563	0.24	0/2099
29	A0	0.15	0/349	0.37	0/451
30	A3	0.11	0/945	0.31	0/1274
30	B4	0.17	0/945	0.36	0/1274

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	BG	0.18	0/944	0.33	0/1274
31	AT	0.14	0/1077	0.29	0/1439
32	AO	0.10	0/1135	0.28	0/1526
33	BB	0.12	0/1882	0.31	0/2538
34	BY	0.10	0/1254	0.26	0/1677
35	BO	0.17	0/1645	0.33	0/2209
36	BC	0.11	0/2933	0.30	0/3943
37	B5	0.14	0/619	0.30	0/830
37	BK	0.11	0/611	0.32	0/819
38	BL	0.13	0/1167	0.32	0/1552
39	Bf	0.11	0/443	0.26	0/589
40	BU	0.31	0/1027	0.45	1/1368 (0.1%)
41	Bb	0.10	0/1120	0.27	0/1494
42	Be	0.09	0/514	0.29	0/676
43	BE	0.21	0/1509	0.40	0/2022
44	Ba	0.10	0/793	0.28	0/1064
45	BT	0.11	0/705	0.28	0/945
46	BW	0.13	0/566	0.28	0/747
47	Bi	0.11	0/630	0.32	0/839
48	BI	0.08	0/1166	0.25	0/1559
49	BR	0.10	0/819	0.27	0/1098
50	BQ	0.09	0/1281	0.25	0/1689
51	BV	0.09	0/547	0.34	0/729
52	Bj	0.11	0/807	0.26	0/1070
53	BD	0.13	0/2069	0.31	0/2787
54	BF	0.15	0/1485	0.30	0/2003
55	BZ	0.14	0/759	0.32	0/1023
56	BP	0.09	0/984	0.25	0/1314
57	BM	0.11	0/1627	0.26	0/2170
58	BS	0.13	0/1275	0.32	0/1715
59	Bd	0.10	0/778	0.27	0/1036
60	BN	0.12	0/1483	0.30	0/1992
61	Bg	0.11	0/396	0.25	0/526
62	Bc	0.11	0/693	0.30	0/926
63	BJ	0.12	0/1080	0.30	0/1456
64	Bl	0.14	0/669	0.29	0/886
65	Bk	0.14	0/538	0.28	0/709
66	sd	0.24	0/223	0.49	0/347
All	All	0.15	4/179591 (0.0%)	0.31	6/264395 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	377	ASP	C-N	14.46	1.54	1.33
1	1	94	G	O3'-P	-10.51	1.45	1.61
1	1	96	U	C1'-N1	5.73	1.57	1.48
1	1	2173	A2M	O3'-P	5.03	1.61	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	377	ASP	CA-C-N	-15.23	101.77	123.10
4	H	377	ASP	C-N-CA	-15.23	101.77	123.10
4	H	383	ARG	N-CA-C	6.30	120.58	113.01
40	BU	115	ILE	CB-CA-C	-5.83	104.27	112.14
2	2	1499	G	C2'-C3'-O3'	-5.44	105.54	113.70
2	2	1500	A	C1'-C2'-O2'	-5.18	100.62	108.40

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	32950	1072	0
2	2	32311	0	16352	422	0
3	3	2703	0	1375	44	0
4	H	3074	0	3190	85	0
5	AA	1531	0	1623	28	0
6	AB	1571	0	1630	19	0
7	AC	449	0	435	8	0
8	AD	1452	0	1521	10	0
9	AE	1983	0	2060	28	0
10	AF	1808	0	1879	27	0
11	AG	977	0	1037	21	0
12	AH	1725	0	1780	35	0
13	AI	1034	0	1069	15	0
14	AJ	986	0	1070	9	0
15	AK	1073	0	1133	15	0
16	AL	809	0	859	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	AM	955	0	981	26	0
18	AN	1148	0	1248	14	0
19	AP	455	0	475	18	0
20	AQ	1305	0	1388	18	0
21	AR	884	0	906	11	0
22	AS	541	0	573	10	0
23	AU	1223	0	1263	18	0
24	AV	808	0	832	9	0
24	B6	790	0	806	16	0
25	AW	470	0	495	7	0
26	AX	516	0	544	9	0
27	AY	400	0	401	8	0
28	AZ	1541	0	1624	20	0
29	A0	343	0	407	7	0
30	A3	933	0	982	25	0
30	B4	933	0	982	30	0
30	BG	932	0	982	9	0
31	AT	1057	0	1131	26	0
32	AO	1116	0	1152	20	0
33	BB	1838	0	1903	30	0
34	BY	1235	0	1314	15	0
35	BO	1607	0	1638	30	0
36	BC	2870	0	3020	30	0
37	B5	614	0	671	13	0
37	BK	607	0	663	10	0
38	BL	1149	0	1218	23	0
39	Bf	435	0	494	9	0
40	BU	1011	0	1078	26	0
41	Bb	1095	0	1190	8	0
42	Be	503	0	533	12	0
43	BE	1485	0	1539	41	0
44	Ba	778	0	851	14	0
45	BT	696	0	758	7	0
46	BW	565	0	628	6	0
47	Bi	620	0	668	3	0
48	BI	1148	0	1237	15	0
49	BR	797	0	835	12	0
50	BQ	1265	0	1392	26	0
51	BV	532	0	523	6	0
52	Bj	789	0	842	7	0
53	BD	2026	0	2131	34	0
54	BF	1456	0	1514	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	BZ	749	0	796	14	0
56	BP	971	0	1039	10	0
57	BM	1588	0	1683	20	0
58	BS	1247	0	1280	10	0
59	Bd	759	0	825	6	0
60	BN	1452	0	1491	29	0
61	Bg	387	0	397	6	0
62	Bc	684	0	748	10	0
63	BJ	1066	0	1133	11	0
64	Bl	659	0	702	12	0
65	Bk	528	0	575	9	0
66	sd	199	0	98	7	0
67	1	166	0	0	0	0
67	2	69	0	0	0	0
67	3	1	0	0	0	0
67	AK	1	0	0	0	0
67	AN	1	0	0	0	0
67	BB	2	0	0	0	0
67	BD	1	0	0	0	0
67	BM	1	0	0	0	0
67	BS	1	0	0	0	0
67	Bb	1	0	0	0	0
68	AC	2	0	0	0	0
68	AF	1	0	0	0	0
68	AP	1	0	0	0	0
68	AR	1	0	0	0	0
68	AW	1	0	0	0	0
68	BV	1	0	0	0	0
68	Bd	1	0	0	0	0
68	Be	1	0	0	0	0
68	Bg	1	0	0	0	0
68	Bi	1	0	0	0	0
68	Bj	1	0	0	0	0
68	Bk	1	0	0	0	0
All	All	170684	0	124542	2351	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 (2351) 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)
1:1:107:G:N2	1:1:112:A:N7	1.85	1.20
1:1:107:G:N2	1:1:112:A:C8	2.14	1.15
1:1:117:G:O2'	1:1:118:U:OP1	1.67	1.12
1:1:100:G:N2	1:1:119:C:O2	1.82	1.12
1:1:2887:A:HO2'	63:BJ:2:ALA:N	1.50	1.07
1:1:2585:4AC:H5	1:1:2597:G:H1	1.17	1.03
1:1:2608:4AC:H5	1:1:2613:G:H1	1.23	1.02
2:2:977:A:H62	2:2:999:G:N2	1.57	1.01
4:H:382:LYS:HD3	17:AM:52:ARG:CD	1.91	1.00
2:2:977:A:N6	2:2:999:G:H21	1.60	0.98
1:1:102:C:N4	1:1:117:G:O6	1.97	0.97
1:1:2001:4AC:OP2	50:BQ:76:ARG:NH1	1.98	0.95
1:1:3:A:H8	1:1:2863:G:H21	1.10	0.92
4:H:382:LYS:HD3	17:AM:52:ARG:HD2	1.53	0.88
35:BO:145:ARG:NH2	35:BO:186:ASP:OD2	2.07	0.86
4:H:382:LYS:HB2	17:AM:52:ARG:HB2	1.58	0.86
2:2:717:C:OP2	20:AQ:16:ARG:NH2	2.10	0.84
4:H:382:LYS:CD	17:AM:52:ARG:HD2	2.05	0.84
1:1:931:U:H3	1:1:1046:G:H1	1.25	0.84
4:H:384:PHE:HE2	26:AX:65:ARG:HH22	1.24	0.83
4:H:383:ARG:HD2	17:AM:24:ASN:HD22	1.43	0.82
4:H:382:LYS:HD3	17:AM:52:ARG:HD3	1.62	0.82
5:AA:127:ALA:HB2	5:AA:182:LYS:HB2	1.60	0.82
6:AB:52:LEU:HD13	6:AB:170:ILE:HD11	1.61	0.81
4:H:382:LYS:CB	17:AM:52:ARG:HB2	2.11	0.80
65:Bk:23:CYS:SG	65:Bk:36:HIS:HE1	2.04	0.80
2:2:659:U:O4	4:H:383:ARG:HD3	1.83	0.78
12:AH:190:LEU:HB3	12:AH:198:SER:HB2	1.66	0.78
1:1:235:G:H1	1:1:242:C:H5	1.29	0.78
1:1:1146:C:H2'	1:1:1147:C:C6	2.19	0.78
2:2:636:4AC:HM73	2:2:703:4AC:HM73	1.65	0.77
26:AX:33:GLU:HA	26:AX:37:LYS:HE2	1.66	0.77
1:1:300:A:OP2	38:BL:43:ASN:ND2	2.17	0.77
1:1:2346:G:N2	1:1:2423:C:O2	2.11	0.77
1:1:1569:G:N7	39:Bf:3:ARG:NH2	2.31	0.77
2:2:631:G:H22	2:2:708:G:H1	1.30	0.77
1:1:418:A:H2'	1:1:419:G:C8	2.20	0.76
2:2:918:A:H2'	2:2:919:G:H8	1.51	0.76
1:1:1713:G:H21	1:1:1787:A:H8	1.32	0.75
1:1:1842:A:H2'	1:1:1843:A:H8	1.52	0.75
33:BB:5:LEU:H	33:BB:8:GLN:HE21	1.34	0.75
1:1:2963:A:O2'	1:1:2964:G:O4'	2.03	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BQ:126:ARG:HH11	50:BQ:131:GLN:HE22	1.33	0.75
37:B5:6:VAL:HG21	37:B5:64:ARG:HG3	1.69	0.75
2:2:96:C:H2'	2:2:97:A:C8	2.21	0.75
2:2:415:G:H21	8:AD:123:GLN:HE22	1.34	0.75
2:2:977:A:H62	2:2:999:G:H21	0.83	0.75
36:BC:188:SER:HB2	36:BC:191:GLU:HB2	1.68	0.75
1:1:2035:U:OP2	1:1:2040:A:N6	2.20	0.74
1:1:761:U:H2'	1:1:762:G:H8	1.52	0.74
4:H:384:PHE:CE2	26:AX:65:ARG:NH2	2.55	0.74
16:AL:38:ILE:HB	16:AL:72:LEU:HB3	1.70	0.74
2:2:714:G:O2'	20:AQ:55:ARG:NH1	2.21	0.74
2:2:154:G:H21	11:AG:118:GLN:HE22	1.34	0.74
4:H:19:ILE:HG12	4:H:70:ARG:HD2	1.69	0.74
1:1:894:A:H2'	1:1:895:A:C8	2.23	0.73
1:1:103:C:H2'	1:1:104:C:C6	2.23	0.73
1:1:1756:G:OP1	59:Bd:77:ARG:NH1	2.19	0.73
64:Bl:10:GLY:HA2	64:Bl:55:LYS:HG2	1.70	0.73
1:1:418:A:H2'	1:1:419:G:H8	1.52	0.73
1:1:793:G:OP2	38:BL:12:ARG:NH2	2.19	0.73
10:AF:212:VAL:H	13:AI:70:ASN:HD21	1.36	0.73
37:BK:45:ARG:NH2	37:BK:66:ALA:O	2.22	0.73
1:1:3021:U:H3'	1:1:3021:U:OP2	1.87	0.73
1:1:788:A:H2'	1:1:789:OMG:H8	1.53	0.73
2:2:627:G:H2'	2:2:628:G:C8	2.24	0.73
6:AB:56:GLY:HA3	6:AB:174:GLU:HG3	1.71	0.73
48:BI:17:ARG:NH1	48:BI:117:GLU:OE2	2.20	0.73
1:1:1283:A:H2'	1:1:1284:A:H8	1.54	0.73
1:1:1667:4AC:H2'	1:1:1668:G:H8	1.53	0.73
1:1:3014:C:H2'	1:1:3015:G:H8	1.54	0.73
35:BO:113:ARG:HG3	35:BO:137:ILE:HA	1.71	0.72
1:1:117:G:O2'	1:1:118:U:P	2.47	0.72
1:1:2559:A:H2'	1:1:2560:G:C8	2.24	0.72
13:AI:96:ALA:HB3	13:AI:99:PHE:HB2	1.69	0.72
2:2:428:C:H2'	2:2:429:A:H8	1.54	0.72
1:1:2310:G:H2'	1:1:2311:A:H8	1.53	0.72
4:H:380:TYR:HD1	12:AH:146:TYR:HA	1.54	0.72
2:2:918:A:H2'	2:2:919:G:C8	2.24	0.72
2:2:965:A:H5''	2:2:966:C:H5	1.55	0.72
3:3:74:C:O2	3:3:109:G:N2	2.17	0.72
2:2:1201:A:H4'	32:AO:139:GLN:HA	1.71	0.72
1:1:102:C:C4	1:1:103:C:C4	2.78	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1177:OMU:HM22	2:2:1178:A:H5'	1.70	0.72
1:1:103:C:H2'	1:1:104:C:H6	1.55	0.71
2:2:1379:G:H2'	2:2:1380:OMU:H6	1.72	0.71
54:BF:139:VAL:HG12	54:BF:147:VAL:HG13	1.72	0.71
30:B4:83:LYS:HG2	30:B4:95:ALA:HB1	1.72	0.71
2:2:1022:G:H22	2:2:1177:OMU:HN3	1.38	0.71
1:1:102:C:N4	1:1:103:C:N4	2.38	0.71
1:1:205:G:N7	39:Bf:34:ARG:NH2	2.38	0.71
1:1:112:A:H3'	1:1:113:G:C8	2.26	0.71
1:1:117:G:HO2'	1:1:118:U:P	2.13	0.71
1:1:653:G:N1	1:1:656:A:OP2	2.24	0.71
53:BD:123:ASN:HD22	53:BD:126:ILE:H	1.39	0.70
1:1:1905:G:N1	1:1:1908:A:OP2	2.23	0.70
38:BL:1:MET:HE1	53:BD:30:LEU:HD12	1.71	0.70
24:B6:23:ILE:HG21	24:B6:31:PRO:HG3	1.74	0.70
49:BR:19:HIS:HD2	49:BR:21:ARG:H	1.37	0.70
1:1:1710:C:H2'	1:1:1711:G:H8	1.57	0.69
1:1:2701:A:N6	1:1:2713:G:O2'	2.24	0.69
2:2:687:C:OP2	2:2:688:A:O2'	2.09	0.69
4:H:312:GLY:HA3	4:H:339:THR:HG22	1.74	0.69
1:1:1283:A:H2'	1:1:1284:A:C8	2.27	0.69
53:BD:49:ASP:HB3	53:BD:52:ALA:HB2	1.74	0.69
4:H:384:PHE:HE2	26:AX:65:ARG:NH2	1.90	0.69
13:AI:51:GLU:OE2	13:AI:62:ARG:NH2	2.26	0.69
2:2:680:OMG:H2'	2:2:681:G:C8	2.28	0.68
1:1:32:G:H2'	1:1:33:G:H8	1.58	0.68
1:1:792:A:H62	1:1:1509:C:H5	1.42	0.68
1:1:2346:G:N1	1:1:2423:C:N3	2.29	0.68
1:1:2823:C:H2'	1:1:2824:G:H8	1.58	0.68
4:H:378:ILE:HG13	4:H:378:ILE:O	1.93	0.68
48:BI:29:VAL:HG22	48:BI:98:LYS:HB2	1.74	0.68
1:1:67:C:OP2	1:1:68:U:O2'	2.12	0.68
1:1:600:G:H2'	53:BD:183:LYS:HE3	1.74	0.68
1:1:2827:G:N2	1:1:2830:A:OP2	2.25	0.68
57:BM:157:ARG:HB2	57:BM:162:LEU:HB2	1.75	0.68
1:1:1653:U:OP2	50:BQ:42:ARG:NH2	2.26	0.68
3:3:97:G:H2'	3:3:98:G:H8	1.58	0.68
4:H:387:LYS:C	4:H:387:LYS:HD3	2.19	0.68
1:1:2135:C:H2'	1:1:2136:4AC:H6	1.75	0.68
2:2:952:C:O2	19:AP:17:GLY:N	2.26	0.68
40:BU:119:ARG:HG2	40:BU:119:ARG:NH2	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1842:A:H2'	1:1:1843:A:C8	2.28	0.67
1:1:2341:G:O2'	1:1:2342:C:O4'	2.11	0.67
1:1:102:C:C4	1:1:103:C:C5	2.81	0.67
2:2:778:U:O2'	2:2:872:A:N1	2.27	0.67
1:1:889:U:H2'	1:1:890:G:H8	1.59	0.67
1:1:2706:C:N4	61:Bg:47:ARG:O	2.27	0.67
1:1:113:G:H2'	1:1:114:G:H8	1.59	0.67
1:1:117:G:C2	1:1:118:U:C6	2.83	0.67
1:1:230:G:OP1	42:Be:21:ARG:NH1	2.28	0.67
1:1:1806:G:OP2	1:1:1806:G:N2	2.19	0.67
2:2:386:C:H2'	2:2:387:G:H8	1.58	0.67
2:2:985:C:OP1	31:AT:61:LYS:NZ	2.26	0.67
60:BN:97:ASN:HD22	60:BN:98:PRO:HD2	1.58	0.67
30:BG:116:MET:SD	30:BG:119:ARG:NH2	2.67	0.67
55:BZ:98:LYS:O	55:BZ:99:ARG:NH1	2.28	0.67
1:1:850:A:N6	38:BL:117:LYS:O	2.24	0.67
1:1:2311:A:H2'	1:1:2312:G:C8	2.29	0.67
2:2:975:G:N2	2:2:1000:G:O2'	2.27	0.67
4:H:383:ARG:HG2	17:AM:55:PRO:HG3	1.76	0.67
1:1:144:G:H2'	1:1:145:G:H8	1.60	0.66
2:2:1130:G:N7	22:AS:44:LYS:NZ	2.42	0.66
61:Bg:32:ARG:HG3	61:Bg:33:LYS:HD2	1.78	0.66
3:3:98:G:H2'	3:3:99:G:H8	1.61	0.66
1:1:2990:G:H21	54:BF:149:GLN:HE22	1.44	0.66
1:1:125:A:H2'	1:1:126:C:C6	2.31	0.66
1:1:2559:A:H2'	1:1:2560:G:H8	1.61	0.66
43:BE:104:ALA:O	43:BE:168:LYS:NZ	2.29	0.66
1:1:763:C:H2'	1:1:764:A:H8	1.61	0.66
1:1:1841:A:H2'	1:1:1842:A:C8	2.31	0.66
16:AL:8:LEU:HB2	16:AL:71:ARG:HB2	1.78	0.66
1:1:1137:G:H2'	1:1:1138:G:C8	2.31	0.65
1:1:2823:C:H2'	1:1:2824:G:C8	2.31	0.65
4:H:378:ILE:HB	12:AH:145:ARG:HH12	1.61	0.65
21:AR:43:PRO:HB2	21:AR:46:THR:HB	1.77	0.65
1:1:1031:G:H1	33:BB:201:ASN:HD21	1.45	0.65
1:1:1146:C:H2'	1:1:1147:C:H6	1.60	0.65
1:1:2310:G:H2'	1:1:2311:A:C8	2.31	0.65
9:AE:58:THR:HG22	9:AE:60:ARG:H	1.61	0.65
1:1:162:G:H21	1:1:163:A:H62	1.44	0.65
1:1:1250:A:H2'	1:1:1251:A:H8	1.62	0.65
2:2:813:G:O2'	5:AA:177:LYS:O	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:BJ:13:THR:HG22	63:BJ:15:VAL:H	1.62	0.65
1:1:806:G:OP1	53:BD:27:ARG:NH2	2.29	0.65
2:2:567:C:OP1	13:AI:84:ARG:NH2	2.27	0.65
1:1:2109:A:H2'	1:1:2110:A:C8	2.31	0.65
2:2:1350:U:H2'	2:2:1351:A:H8	1.61	0.65
5:AA:123:MET:HE3	5:AA:187:ARG:HD3	1.78	0.65
1:1:617:G:N2	1:1:620:A:OP2	2.26	0.65
1:1:848:A:O2'	1:1:887:G:O2'	2.15	0.65
1:1:2388:G:H2'	1:1:2389:G:C8	2.32	0.65
2:2:435:U:O2'	2:2:437:U:O4	2.14	0.65
1:1:763:C:H2'	1:1:764:A:C8	2.32	0.65
1:1:1676:A:N1	1:1:1692:G:O2'	2.29	0.65
3:3:25:C:O2	3:3:123:C:O2'	2.15	0.65
26:AX:18:THR:HG21	26:AX:67:ILE:HG12	1.77	0.65
2:2:912:G:OP1	12:AH:73:ARG:NH2	2.30	0.64
53:BD:226:GLY:H	53:BD:229:HIS:HD2	1.45	0.64
1:1:764:A:O2'	62:Bc:17:GLN:NE2	2.28	0.64
2:2:1075:G:N3	22:AS:6:GLN:NE2	2.45	0.64
1:1:1415:C:OP2	34:BY:118:ARG:NH2	2.28	0.64
1:1:1612:A:H2'	1:1:1613:A:C8	2.32	0.64
1:1:2471:A:H2'	1:1:2472:G:C8	2.33	0.64
3:3:74:C:N3	3:3:109:G:N1	2.37	0.64
30:B4:39:THR:HG23	30:B4:100:ALA:HB2	1.79	0.64
1:1:116:G:H2'	1:1:117:G:H8	1.62	0.64
1:1:2951:C:O2'	36:BC:361:GLN:O	2.13	0.64
2:2:1022:G:HO2'	28:AZ:166:TYR:HH	1.42	0.64
43:BE:60:LYS:HA	43:BE:75:PRO:HA	1.80	0.64
2:2:1106:C:H4'	2:2:1107:U:OP1	1.96	0.64
3:3:98:G:H2'	3:3:99:G:C8	2.33	0.64
1:1:1250:A:H2'	1:1:1251:A:C8	2.32	0.64
1:1:1489:C:H2'	1:1:1490:G:H8	1.62	0.64
28:AZ:36:LYS:HB2	28:AZ:43:LYS:HB3	1.80	0.64
1:1:785:G:H5''	1:1:2259:U:H5''	1.78	0.64
4:H:382:LYS:N	4:H:382:LYS:HD2	2.12	0.64
1:1:102:C:C2	1:1:103:C:C6	2.86	0.64
1:1:2887:A:O2'	63:BJ:2:ALA:N	2.27	0.64
12:AH:88:ARG:HB3	12:AH:91:ARG:HG3	1.80	0.64
22:AS:39:THR:HG22	22:AS:41:VAL:H	1.62	0.63
60:BN:105:ALA:O	60:BN:109:GLY:N	2.31	0.63
2:2:496:G:N2	4:H:324:LYS:O	2.30	0.63
24:AV:33:ARG:NH2	24:AV:53:ILE:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B6:25:HIS:HB2	24:B6:28:GLU:HB2	1.81	0.63
1:1:352:G:H5'	1:1:353:C:H5''	1.81	0.63
1:1:360:A:H2'	1:1:361:A:C8	2.33	0.63
1:1:2524:G:H2'	1:1:2525:G:H8	1.63	0.63
4:H:382:LYS:HB2	17:AM:52:ARG:CB	2.28	0.63
1:1:144:G:H2'	1:1:145:G:C8	2.34	0.63
1:1:458:4AC:H2'	1:1:459:G:H8	1.63	0.63
1:1:1173:C:H2'	1:1:1174:A:H8	1.63	0.63
1:1:1826:C:OP1	59:Bd:8:ARG:NH2	2.28	0.63
2:2:1380:OMU:HM22	2:2:1381:C:H5'	1.80	0.63
15:AK:117:HIS:ND1	15:AK:122:SER:O	2.30	0.63
40:BU:119:ARG:HG2	40:BU:119:ARG:HH21	1.63	0.63
1:1:1440:G:OP1	34:BY:114:LYS:NZ	2.24	0.63
2:2:1176:G:N2	19:AP:45:GLU:OE2	2.31	0.63
30:B4:84:LYS:HD2	30:B4:95:ALA:HB2	1.80	0.63
1:1:788:A:H2'	1:1:789:OMG:C8	2.34	0.63
2:2:1042:G:N2	2:2:1045:A:OP2	2.26	0.63
1:1:1421:C:H2'	1:1:1422:A:H8	1.63	0.63
1:1:112:A:H3'	1:1:113:G:H8	1.63	0.63
2:2:75:G:H2'	2:2:76:G:C8	2.34	0.63
5:AA:93:ILE:HG23	5:AA:123:MET:HE1	1.81	0.63
1:1:2608:4AC:H5	1:1:2613:G:N1	2.05	0.62
1:1:1310:G:O2'	1:1:1339:A:N6	2.31	0.62
60:BN:56:GLN:HE21	60:BN:125:ARG:HE	1.45	0.62
2:2:183:U:H2'	2:2:184:G:H8	1.64	0.62
58:BS:116:HIS:HB3	58:BS:149:VAL:HB	1.81	0.62
1:1:32:G:H2'	1:1:33:G:C8	2.34	0.62
27:AY:37:ARG:HH21	27:AY:39:ALA:HA	1.63	0.62
1:1:567:A:H1'	1:1:2121:A:C2	2.34	0.62
1:1:1006:G:H2'	1:1:1007:C:C6	2.35	0.62
1:1:834:C:H2'	1:1:835:4AC:H6	1.80	0.62
1:1:1421:C:H2'	1:1:1422:A:C8	2.34	0.62
3:3:9:G:OP1	35:BO:24:ARG:NH1	2.32	0.62
1:1:94:G:H3'	1:1:95:G:H5'	1.81	0.62
15:AK:26:VAL:HG13	15:AK:62:ILE:HB	1.82	0.62
30:B4:92:ILE:HG22	30:B4:94:VAL:H	1.64	0.62
21:AR:74:ASN:HD21	21:AR:80:ALA:H	1.48	0.62
2:2:908:C:H2'	2:2:909:A:H8	1.64	0.62
43:BE:118:ASP:OD1	43:BE:118:ASP:N	2.33	0.62
1:1:2377:C:H42	1:1:2394:G:H1	1.48	0.62
1:1:493:G:H5'	40:BU:1:MET:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:833:G:H2'	1:1:834:C:H6	1.65	0.61
1:1:869:G:O2'	1:1:870:A:O5'	2.15	0.61
1:1:889:U:H2'	1:1:890:G:C8	2.34	0.61
1:1:908:A:N3	53:BD:33:ARG:NH2	2.48	0.61
20:AQ:54:LEU:HD23	20:AQ:60:ILE:HD11	1.81	0.61
1:1:2706:C:OP2	1:1:2707:C:N4	2.24	0.61
4:H:7:GLN:HA	4:H:10:MET:HG2	1.82	0.61
2:2:1025:5MC:H2'	2:2:1026:G:H8	1.65	0.61
23:AU:42:GLU:HG3	23:AU:43:ARG:HG3	1.82	0.61
2:2:1212:A:H2	2:2:1215:G:N3	1.99	0.61
23:AU:137:LYS:NZ	23:AU:141:GLU:OE2	2.31	0.61
1:1:705:A:H2'	1:1:706:G:C8	2.36	0.61
1:1:1371:C:H2'	1:1:1372:G:H8	1.66	0.61
2:2:121:U:H2'	2:2:122:C:C6	2.35	0.61
2:2:1215:G:OP1	12:AH:99:LYS:NZ	2.32	0.61
4:H:378:ILE:HB	12:AH:145:ARG:NH1	2.14	0.61
15:AK:79:ARG:NH2	15:AK:103:ASP:OD2	2.34	0.61
24:AV:23:ILE:HG21	24:AV:31:PRO:HG2	1.82	0.61
1:1:360:A:H2'	1:1:361:A:H8	1.65	0.61
4:H:56:ILE:HD12	4:H:184:ILE:HD11	1.82	0.61
1:1:3014:C:H2'	1:1:3015:G:C8	2.36	0.61
2:2:1503:A:H2'	2:2:1504:C:H6	1.66	0.61
4:H:246:ASP:OD1	4:H:250:LYS:N	2.34	0.61
1:1:569:C:O2'	1:1:2119:A:N6	2.34	0.61
1:1:691:G:OP1	62:Bc:49:SER:OG	2.17	0.61
2:2:386:C:H2'	2:2:387:G:C8	2.36	0.61
2:2:1089:G:N2	2:2:1090:U:O4	2.32	0.60
33:BB:74:PRO:HD2	33:BB:77:LEU:HD22	1.82	0.60
1:1:2431:C:H2'	1:1:2432:G:C8	2.37	0.60
2:2:1149:G:H2'	2:2:1150:A:H8	1.65	0.60
2:2:1310:U:O4	12:AH:91:ARG:NH2	2.33	0.60
4:H:383:ARG:NH1	17:AM:24:ASN:ND2	2.49	0.60
40:BU:120:ALA:O	40:BU:121:GLY:OXT	2.19	0.60
49:BR:89:HIS:HD2	49:BR:91:VAL:H	1.48	0.60
1:1:2878:G:OP2	1:1:2962:C:O2'	2.18	0.60
11:AG:10:ASP:HB3	11:AG:123:LEU:HD12	1.83	0.60
30:A3:18:LYS:NZ	30:A3:113:GLU:OE1	2.33	0.60
35:BO:145:ARG:HH21	35:BO:186:ASP:CG	2.06	0.60
12:AH:70:LYS:HG3	12:AH:162:LEU:HB3	1.83	0.60
1:1:113:G:H2'	1:1:114:G:C8	2.36	0.60
2:2:1088:A:H4'	16:AL:36:GLY:HA3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A3:33:ARG:HH22	30:A3:42:ALA:HB2	1.65	0.60
40:BU:119:ARG:HH21	40:BU:119:ARG:CG	2.14	0.60
49:BR:19:HIS:CD2	49:BR:21:ARG:H	2.18	0.60
1:1:1209:G:N2	1:1:1212:A:OP2	2.25	0.60
2:2:1290:G:N1	2:2:1293:A:OP2	2.34	0.60
3:3:7:G:O2'	35:BO:47:GLN:NE2	2.34	0.60
38:BL:2:ILE:HG13	56:BP:4:THR:HG21	1.84	0.60
1:1:2449:G:H2'	1:1:2450:G:H8	1.67	0.60
2:2:893:G:H2'	2:2:894:G:C8	2.37	0.60
2:2:579:C:H2'	2:2:580:A:H8	1.67	0.60
12:AH:7:GLU:OE2	12:AH:20:ARG:NH2	2.30	0.60
2:2:681:G:H2'	2:2:682:A:H8	1.67	0.59
5:AA:109:ASN:HD21	5:AA:119:ARG:HE	1.49	0.59
1:1:1301:A:H4'	1:1:1302:G:H5'	1.82	0.59
2:2:1401:U:H2'	2:2:1402:A:H8	1.67	0.59
49:BR:43:ILE:HD11	49:BR:77:VAL:HG11	1.84	0.59
2:2:24:U:H2'	2:2:25:C:C6	2.36	0.59
2:2:1227:G:H5'	16:AL:46:ARG:HH22	1.68	0.59
53:BD:27:ARG:HB3	53:BD:30:LEU:HB2	1.84	0.59
1:1:1943:G:O2'	1:1:2232:U:O4	2.16	0.59
57:BM:29:LYS:NZ	57:BM:33:GLU:OE2	2.28	0.59
66:sd:12:A:H2'	66:sd:12:A:N3	2.17	0.59
1:1:394:G:H2'	1:1:395:A:H8	1.68	0.59
1:1:913:C:H2'	1:1:914:G:H8	1.67	0.59
1:1:1266:G:N2	64:Bl:43:SER:HB2	2.18	0.59
1:1:2105:U:H2'	1:1:2106:G:H8	1.68	0.59
32:AO:5:ARG:NH2	32:AO:54:LEU:O	2.33	0.59
43:BE:145:ARG:HD2	43:BE:164:HIS:CD2	2.38	0.59
62:Bc:8:LEU:HD11	62:Bc:25:LYS:HB2	1.84	0.59
30:B4:121:LEU:HD12	30:B4:122:MET:SD	2.43	0.59
1:1:537:G:H5'	57:BM:89:LYS:HE3	1.85	0.59
1:1:1667:4AC:H2'	1:1:1668:G:C8	2.37	0.59
1:1:929:G:H2'	1:1:930:G:C8	2.38	0.59
1:1:1019:C:H2'	1:1:1020:G:H8	1.68	0.59
1:1:2635:G:O2'	1:1:2636:C:O5'	2.21	0.59
37:B5:31:ASN:HD21	55:BZ:25:ARG:HH11	1.49	0.59
48:BI:1:MET:HE1	48:BI:29:VAL:HG23	1.84	0.59
1:1:1115:A:H2'	1:1:1116:G:C8	2.37	0.59
1:1:1763:G:H2'	1:1:1764:C:C6	2.37	0.59
2:2:195:A:O2'	2:2:197:G:N7	2.34	0.59
4:H:142:THR:HG22	4:H:165:PRO:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:163:A:H2	1:1:233:U:H3	1.50	0.59
1:1:1116:G:H2'	1:1:1117:C:C6	2.37	0.59
27:AY:42:ARG:NH1	27:AY:43:CYS:SG	2.76	0.59
43:BE:70:ILE:HG13	43:BE:76:ILE:HG21	1.85	0.58
3:3:16:G:HO2'	35:BO:2:ALA:N	2.01	0.58
7:AC:54:LYS:NZ	7:AC:59:GLY:O	2.36	0.58
30:A3:27:ARG:HD2	30:A3:90:ALA:HA	1.84	0.58
1:1:2523:C:H2'	1:1:2524:G:H8	1.67	0.58
1:1:189:G:H22	1:1:224:A:H2	1.52	0.58
1:1:573:U:H2'	1:1:574:C:H6	1.68	0.58
3:3:97:G:H2'	3:3:98:G:C8	2.38	0.58
33:BB:225:ARG:NH1	33:BB:225:ARG:O	2.37	0.58
55:BZ:88:PRO:HG3	55:BZ:94:LEU:HD13	1.84	0.58
1:1:835:4AC:O2'	1:1:906:U:OP1	2.21	0.58
1:1:993:U:OP2	1:1:1951:C:O2'	2.15	0.58
1:1:1810:G:OP2	50:BQ:43:ARG:NH1	2.37	0.58
54:BF:55:ILE:HD11	54:BF:75:ILE:HD12	1.84	0.58
1:1:2430:G:H3'	1:1:2431:C:H6	1.67	0.58
2:2:1302:C:OP1	32:AO:34:ASN:ND2	2.33	0.58
2:2:1503:A:H2'	2:2:1504:C:C6	2.38	0.58
11:AG:12:LYS:HG2	11:AG:13:THR:HG23	1.85	0.58
1:1:978:G:O2'	1:1:1014:G:H4'	2.02	0.58
1:1:1742:A:H2'	1:1:1743:A:C8	2.38	0.58
1:1:2311:A:H2'	1:1:2312:G:H8	1.67	0.58
6:AB:169:TRP:HE3	6:AB:170:ILE:HG22	1.68	0.58
1:1:796:C:H2'	1:1:797:G:H8	1.66	0.58
2:2:1261:A:H2'	2:2:1262:A:C8	2.39	0.58
54:BF:45:LYS:HE3	54:BF:47:PHE:HE2	1.68	0.58
1:1:197:G:O6	40:BU:111:ARG:NH1	2.36	0.58
1:1:394:G:H2'	1:1:395:A:C8	2.39	0.58
1:1:2130:A:H2'	1:1:2131:A:C8	2.39	0.58
23:AU:15:ARG:HG3	23:AU:136:LEU:HD12	1.85	0.58
27:AY:6:LYS:HG3	27:AY:7:LEU:HG	1.84	0.58
1:1:1498:C:H2'	1:1:1499:G:H8	1.68	0.58
2:2:695:A:H2'	2:2:696:A:C8	2.38	0.58
2:2:1365:U:H2'	2:2:1366:G:C8	2.39	0.58
35:BO:139:PRO:HG2	35:BO:144:ILE:HD11	1.86	0.58
36:BC:278:GLU:HG3	36:BC:325:PRO:HD3	1.86	0.58
1:1:1075:U:OP1	49:BR:2:VAL:HG21	2.04	0.57
1:1:2963:A:H5'	36:BC:339:ARG:HH21	1.68	0.57
2:2:1378:C:H2'	2:2:1379:G:C8	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:AY:9:ILE:HG23	27:AY:16:ILE:HG23	1.85	0.57
36:BC:74:GLU:OE1	36:BC:310:TYR:OH	2.17	0.57
1:1:371:G:O2'	65:Bk:23:CYS:SG	2.56	0.57
1:1:2050:U:H2'	1:1:2051:C:H6	1.68	0.57
1:1:2585:4AC:H5	1:1:2597:G:N1	2.03	0.57
20:AQ:77:THR:HB	20:AQ:80:ARG:HD2	1.86	0.57
1:1:1601:U:O4	45:BT:15:LYS:NZ	2.27	0.57
4:H:387:LYS:HB2	66:sd:12:A:H4'	1.86	0.57
9:AE:37:HIS:HB2	9:AE:42:SER:HB3	1.86	0.57
30:BG:39:THR:HG23	30:BG:100:ALA:HB2	1.87	0.57
60:BN:12:VAL:HG12	60:BN:56:GLN:HG3	1.85	0.57
30:B4:49:LYS:HB2	30:B4:50:LEU:HD12	1.85	0.57
1:1:116:G:H2'	1:1:117:G:C8	2.40	0.57
14:AJ:42:LYS:HB3	14:AJ:59:ALA:HB3	1.87	0.57
1:1:787:C:H2'	1:1:788:A:H8	1.69	0.57
1:1:696:A:H2'	1:1:697:A:C8	2.40	0.57
1:1:1317:G:H2'	1:1:1318:G:C8	2.40	0.57
1:1:1551:G:H2'	1:1:1552:A:C8	2.40	0.57
2:2:1224:A:H2'	2:2:1225:A:C8	2.40	0.57
56:BP:10:ASN:HD22	56:BP:13:ARG:HH12	1.52	0.57
1:1:2343:G:H2'	1:1:2344:G:H8	1.69	0.57
2:2:861:G:O2'	2:2:877:G:O6	2.20	0.57
2:2:1095:A:H2'	2:2:1096:G:C8	2.40	0.57
1:1:371:G:OP1	65:Bk:43:TRP:NE1	2.30	0.57
1:1:2314:U:H2'	1:1:2315:U:C6	2.40	0.57
1:1:2565:A:OP1	35:BO:22:ARG:NH2	2.38	0.57
2:2:976:A:N6	2:2:1001:A:O4'	2.38	0.57
20:AQ:19:ARG:NH2	25:AW:65:GLU:OE2	2.36	0.57
43:BE:99:ASP:OD1	43:BE:101:ARG:HD3	2.04	0.57
1:1:2963:A:H2'	1:1:2963:A:N3	2.19	0.57
1:1:2986:U:H1'	1:1:2987:A:H5''	1.86	0.57
5:AA:70:GLN:HG3	5:AA:84:LYS:HD2	1.86	0.57
6:AB:81:LYS:HG3	6:AB:93:PRO:HG3	1.85	0.57
41:Bb:103:ALA:HB3	41:Bb:106:VAL:HG23	1.87	0.57
1:1:84:A:OP1	44:Ba:2:PRO:HD2	2.05	0.57
1:1:351:G:OP2	1:1:353:C:N4	2.36	0.57
1:1:728:C:H5'	37:BK:47:ARG:HB3	1.86	0.57
1:1:870:A:H4'	1:1:871:G:OP2	2.04	0.57
1:1:1371:C:H2'	1:1:1372:G:C8	2.39	0.57
1:1:3001:C:H2'	1:1:3002:C:H6	1.70	0.57
2:2:1401:U:H2'	2:2:1402:A:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AJ:33:SER:HB3	14:AJ:56:ARG:HD3	1.86	0.57
53:BD:153:LYS:HB2	53:BD:156:GLU:HG3	1.86	0.57
1:1:26:U:O2	36:BC:123:GLN:NE2	2.38	0.56
1:1:1617:4AC:H2'	1:1:1618:G:H8	1.69	0.56
1:1:1877:C:O2'	1:1:1883:A:N1	2.38	0.56
1:1:2265:U:H2'	1:1:2266:G:C8	2.40	0.56
1:1:2326:U:H2'	1:1:2327:G:H8	1.70	0.56
1:1:192:C:OP1	46:BW:7:ARG:NH2	2.39	0.56
1:1:563:A:H2'	1:1:564:G:C8	2.39	0.56
1:1:1734:G:H2'	1:1:1735:G:H8	1.70	0.56
1:1:1998:A:H2'	1:1:1999:C:C6	2.40	0.56
1:1:2287:4AC:H2'	1:1:2288:G:H8	1.71	0.56
1:1:2388:G:H2'	1:1:2389:G:H8	1.68	0.56
1:1:2524:G:H2'	1:1:2525:G:C8	2.40	0.56
2:2:485:C:H2'	2:2:486:A:O4'	2.05	0.56
2:2:1328:C:H2'	2:2:1329:G:H8	1.70	0.56
9:AE:87:ILE:HD12	9:AE:104:PRO:HD3	1.87	0.56
9:AE:206:PRO:HB3	21:AR:8:ARG:HD3	1.87	0.56
16:AL:14:ARG:NH2	16:AL:17:GLU:OE1	2.38	0.56
19:AP:19:ARG:HD2	19:AP:32:ARG:HD3	1.87	0.56
31:AT:12:THR:HG22	31:AT:14:GLU:H	1.70	0.56
31:AT:82:TYR:HB3	31:AT:89:PHE:HB3	1.87	0.56
33:BB:202:HIS:HD2	33:BB:204:PHE:H	1.53	0.56
35:BO:155:MET:O	35:BO:159:GLN:HG2	2.05	0.56
1:1:85:A:OP1	44:Ba:44:LYS:NZ	2.34	0.56
1:1:595:A:O2'	53:BD:44:GLN:NE2	2.39	0.56
1:1:1953:A:H2'	1:1:1954:A:H8	1.70	0.56
1:1:2426:C:H2'	1:1:2427:G:H8	1.69	0.56
3:3:41:U:H3'	43:BE:57:ILE:HD11	1.86	0.56
35:BO:44:HIS:HE1	35:BO:116:SER:HB3	1.69	0.56
37:B5:31:ASN:HD21	55:BZ:25:ARG:NH1	2.02	0.56
65:Bk:10:ARG:NH1	65:Bk:16:GLU:OE1	2.38	0.56
1:1:100:G:O2'	1:1:101:U:H5'	2.05	0.56
1:1:794:U:H2'	1:1:795:U:C6	2.41	0.56
1:1:1006:G:H2'	1:1:1007:C:H6	1.71	0.56
1:1:2117:G:H2'	1:1:2118:U:C6	2.41	0.56
15:AK:36:VAL:O	15:AK:42:ARG:NH1	2.39	0.56
20:AQ:25:TRP:CD2	25:AW:64:LEU:HD21	2.41	0.56
1:1:1606:G:O2'	1:1:1640:A:N3	2.33	0.56
1:1:2058:A:H2'	1:1:2059:G:H8	1.70	0.56
1:1:2532:C:H2'	1:1:2533:G:H8	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B5:26:ASP:HB2	37:B5:34:LEU:HB3	1.87	0.56
50:BQ:60:ARG:HG2	50:BQ:63:ALA:HB3	1.87	0.56
1:1:1141:A:H5''	1:1:1142:A:C8	2.39	0.56
1:1:1314:G:H2'	1:1:1315:U:C5	2.40	0.56
2:2:504:G:H2'	2:2:505:G:H8	1.70	0.56
2:2:709:G:OP1	20:AQ:101:ARG:NH2	2.39	0.56
32:AO:64:GLU:OE1	32:AO:64:GLU:N	2.36	0.56
40:BU:28:ALA:HA	40:BU:45:PRO:HA	1.88	0.56
1:1:1874:G:O2'	39:Bf:3:ARG:O	2.24	0.56
11:AG:39:PRO:HG2	11:AG:42:GLU:HB3	1.87	0.56
13:AI:55:ASP:OD1	13:AI:55:ASP:N	2.39	0.56
34:BY:74:LEU:HB2	34:BY:78:LYS:HB2	1.86	0.56
1:1:300:A:H5''	38:BL:37:ALA:HB1	1.88	0.56
1:1:529:G:OP2	57:BM:44:ARG:NH1	2.39	0.56
9:AE:33:ARG:HG3	9:AE:34:PRO:HD2	1.86	0.56
48:BI:56:ARG:HA	48:BI:65:PRO:HD2	1.88	0.56
1:1:451:4AC:OP1	40:BU:118:ARG:NH1	2.38	0.56
1:1:2558:A:H2'	1:1:2559:A:C8	2.41	0.56
2:2:37:C:H2'	2:2:38:A:H8	1.71	0.56
3:3:27:A:OP1	35:BO:65:ARG:NH2	2.31	0.56
4:H:383:ARG:HH11	17:AM:24:ASN:ND2	2.04	0.56
18:AN:73:VAL:HG11	18:AN:97:ILE:HG21	1.87	0.56
1:1:16:A:N1	1:1:2287:4AC:O2'	2.37	0.55
1:1:720:A:H2'	1:1:721:A:H8	1.71	0.55
1:1:2539:G:H2'	1:1:2539:G:N3	2.20	0.55
2:2:1415:U:H2'	2:2:1416:C:C6	2.41	0.55
4:H:119:LEU:O	4:H:123:VAL:HB	2.07	0.55
9:AE:105:ASN:N	9:AE:109:LYS:O	2.38	0.55
23:AU:121:ILE:HD11	23:AU:126:ARG:HH21	1.72	0.55
1:1:1110:G:N3	1:1:2499:A:H2'	2.21	0.55
1:1:2376:G:H1	1:1:2395:U:H3	1.54	0.55
2:2:1266:C:H2'	2:2:1267:G:H8	1.71	0.55
2:2:1309:C:O2'	12:AH:175:ARG:NH1	2.39	0.55
3:3:115:G:H2'	3:3:116:C:C6	2.41	0.55
9:AE:126:ARG:H	9:AE:143:HIS:HD2	1.53	0.55
1:1:107:G:N2	1:1:112:A:H8	1.93	0.55
1:1:772:U:H2'	1:1:773:C:C6	2.41	0.55
1:1:814:A:H2'	1:1:815:A:C8	2.42	0.55
1:1:1342:G:N2	1:1:1345:U:O4	2.40	0.55
2:2:484:G:N2	18:AN:65:PRO:O	2.39	0.55
2:2:757:A:C8	4:H:307:LEU:HD11	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1392:A:N6	2:2:1451:G:O2'	2.39	0.55
5:AA:26:ASP:OD1	5:AA:26:ASP:N	2.37	0.55
28:AZ:60:ARG:HH21	28:AZ:63:ARG:HD2	1.71	0.55
1:1:434:A:H2'	1:1:435:C:C6	2.41	0.55
1:1:508:C:H2'	1:1:509:A:C8	2.41	0.55
1:1:957:U:O2'	1:1:1770:U:OP1	2.23	0.55
1:1:1071:A:H4'	1:1:1087:G:N2	2.22	0.55
21:AR:105:VAL:HG11	21:AR:108:ARG:HD2	1.88	0.55
1:1:1574:C:H2'	1:1:1575:A:H8	1.71	0.55
2:2:1491:U:H2'	2:2:1492:A:H8	1.71	0.55
33:BB:104:GLU:OE2	33:BB:134:ARG:N	2.36	0.55
34:BY:59:ILE:HA	34:BY:148:ASN:HD21	1.71	0.55
34:BY:60:ASN:H	34:BY:148:ASN:HD21	1.54	0.55
57:BM:136:HIS:ND1	65:Bk:13:ASP:OD1	2.32	0.55
1:1:133:G:H2'	1:1:134:C:C6	2.42	0.55
1:1:2709:U:C4	61:Bg:18:LEU:HD13	2.42	0.55
2:2:879:A:H2'	2:2:880:A:C8	2.42	0.55
23:AU:33:PRO:HB3	32:AO:41:ARG:HD3	1.88	0.55
2:2:659:U:C5	4:H:383:ARG:NE	2.75	0.55
1:1:1393:G:OP2	48:BI:52:ARG:NH2	2.31	0.55
1:1:2077:U:H2'	1:1:2078:G:H8	1.72	0.55
2:2:444:U:O2'	24:AV:56:ILE:O	2.24	0.55
31:AT:117:ALA:HB3	31:AT:120:ILE:HB	1.89	0.55
1:1:102:C:N3	1:1:103:C:C5	2.74	0.55
1:1:705:A:H2'	1:1:706:G:H8	1.70	0.55
15:AK:32:PRO:HG2	15:AK:35:LEU:HD12	1.89	0.55
16:AL:37:PRO:HA	16:AL:73:ILE:HG23	1.89	0.55
31:AT:9:ARG:NH1	32:AO:83:LYS:O	2.40	0.55
57:BM:111:LEU:HB2	57:BM:132:MET:HE2	1.88	0.55
1:1:1324:A:O2'	1:1:1329:G:O6	2.23	0.54
1:1:1739:G:HO2'	1:1:1816:U:HO2'	1.44	0.54
1:1:2531:G:H2'	1:1:2532:C:C6	2.42	0.54
2:2:1174:C:O2'	2:2:1179:U:O4	2.25	0.54
7:AC:35:CYS:SG	7:AC:36:GLY:N	2.80	0.54
1:1:217:A:C2	40:BU:20:LEU:HB3	2.42	0.54
1:1:238:C:H4'	1:1:239:C:O5'	2.06	0.54
1:1:1124:U:H2'	1:1:1125:G:C8	2.41	0.54
1:1:2087:G:H2'	1:1:2088:C:C6	2.42	0.54
1:1:2536:U:C2	43:BE:136:GLY:HA3	2.42	0.54
28:AZ:69:LEU:HD23	28:AZ:75:LEU:HD12	1.90	0.54
42:Be:28:PHE:HA	42:Be:35:CYS:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:BI:18:VAL:HG21	48:BI:30:ILE:HD11	1.88	0.54
1:1:770:C:H2'	1:1:771:G:H8	1.72	0.54
1:1:1393:G:H5'	48:BI:78:THR:HG23	1.88	0.54
55:BZ:34:LEU:HB3	55:BZ:85:ILE:HB	1.88	0.54
1:1:1331:C:H2'	1:1:1332:A:C8	2.43	0.54
1:1:2009:G:N2	1:1:2012:G:OP2	2.32	0.54
2:2:1300:C:OP1	23:AU:81:LYS:NZ	2.39	0.54
43:BE:162:THR:HA	43:BE:165:LYS:HG3	1.89	0.54
44:Ba:16:ARG:HA	44:Ba:19:LYS:HG3	1.89	0.54
49:BR:45:ILE:H	49:BR:59:HIS:HD2	1.54	0.54
1:1:1111:G:O2'	1:1:1168:G:O6	2.25	0.54
1:1:2419:C:H2'	1:1:2420:A:H8	1.72	0.54
2:2:1022:G:O2'	28:AZ:166:TYR:OH	2.22	0.54
10:AF:167:ILE:O	10:AF:172:LYS:NZ	2.30	0.54
18:AN:66:ASN:HD22	18:AN:118:ASP:HB3	1.72	0.54
28:AZ:38:THR:OG1	28:AZ:41:GLY:O	2.23	0.54
1:1:1015:A:H5'	33:BB:176:GLY:HA2	1.90	0.54
1:1:1576:C:H2'	1:1:1578:G:H5''	1.90	0.54
1:1:2917:U:H2'	1:1:2918:G:H8	1.73	0.54
2:2:189:A:O3'	9:AE:155:LYS:NZ	2.38	0.54
2:2:879:A:H2'	2:2:880:A:H8	1.72	0.54
4:H:123:VAL:HG13	4:H:228:ARG:HG3	1.88	0.54
12:AH:44:LEU:HD11	15:AK:40:ILE:HG13	1.90	0.54
32:AO:20:GLN:HE22	32:AO:22:ARG:HH21	1.54	0.54
33:BB:99:LEU:HD23	33:BB:102:ILE:HD12	1.90	0.54
49:BR:33:GLN:HE22	49:BR:95:PRO:HD3	1.73	0.54
53:BD:5:VAL:N	53:BD:14:ASP:O	2.28	0.54
1:1:1703:G:OP2	59:Bd:32:LYS:NZ	2.40	0.54
1:1:2265:U:H2'	1:1:2266:G:H8	1.73	0.54
1:1:2304:C:H2'	1:1:2305:C:C6	2.43	0.54
2:2:908:C:C2	2:2:909:A:C8	2.96	0.54
2:2:1215:G:H2'	2:2:1216:G:H8	1.72	0.54
2:2:1416:C:H2'	2:2:1417:U:C6	2.43	0.54
43:BE:119:GLU:HG3	43:BE:134:ILE:HG12	1.89	0.54
1:1:253:G:H2'	1:1:254:C:C6	2.43	0.54
1:1:385:C:H2'	1:1:386:G:H8	1.73	0.54
1:1:1326:G:N2	1:1:1344:G:O2'	2.41	0.54
1:1:2545:4AC:H2'	1:1:2546:G:C8	2.43	0.54
8:AD:109:VAL:HG13	8:AD:114:LEU:HB2	1.89	0.54
22:AS:38:LEU:HA	28:AZ:196:ILE:HD11	1.89	0.54
35:BO:63:HIS:HD2	35:BO:65:ARG:H	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BC:86:TYR:HB2	36:BC:159:GLU:HB3	1.90	0.54
60:BN:99:MET:HG3	60:BN:101:THR:HG23	1.90	0.54
1:1:841:G:N2	1:1:844:A:OP2	2.31	0.54
1:1:1019:C:H2'	1:1:1020:G:C8	2.43	0.54
1:1:1574:C:H2'	1:1:1575:A:C8	2.43	0.54
1:1:2449:G:H2'	1:1:2450:G:C8	2.43	0.54
2:2:1482:A:H2'	2:2:1483:G:C8	2.42	0.54
18:AN:139:LYS:HG2	18:AN:141:ARG:HH21	1.73	0.54
28:AZ:55:ILE:HG22	28:AZ:59:GLY:H	1.72	0.54
1:1:1294:G:OP1	64:Bl:22:THR:N	2.40	0.53
1:1:1687:C:OP2	59:Bd:66:ARG:NE	2.27	0.53
1:1:2531:G:H2'	1:1:2532:C:H6	1.73	0.53
2:2:681:G:H2'	2:2:682:A:C8	2.43	0.53
2:2:1222:A:OP2	23:AU:61:ARG:NH1	2.26	0.53
30:B4:2:ALA:HA	30:B4:7:VAL:HG11	1.90	0.53
1:1:757:G:O2'	1:1:1478:G:OP1	2.21	0.53
1:1:2623:G:H5''	1:1:2624:C:H5'	1.90	0.53
1:1:3020:U:OP2	1:1:3022:C:H5'	2.09	0.53
2:2:717:C:H4'	20:AQ:47:THR:HG22	1.90	0.53
28:AZ:117:MET:HE2	28:AZ:148:GLN:HG2	1.90	0.53
33:BB:61:VAL:HG11	33:BB:83:ILE:HD11	1.89	0.53
43:BE:43:LYS:HD3	43:BE:132:ILE:HA	1.90	0.53
1:1:795:U:H2'	1:1:796:C:C6	2.44	0.53
1:1:921:C:H2'	1:1:922:4AC:H6	1.89	0.53
1:1:1392:G:OP1	48:BI:52:ARG:NH2	2.41	0.53
4:H:99:SER:HB3	4:H:114:SER:HA	1.90	0.53
1:1:42:U:C4	51:BV:51:LYS:HB2	2.43	0.53
1:1:382:C:H2'	1:1:383:C:H6	1.71	0.53
1:1:535:U:H2'	1:1:536:C:C6	2.44	0.53
1:1:796:C:H2'	1:1:797:G:C8	2.43	0.53
1:1:1742:A:H2'	1:1:1743:A:H8	1.72	0.53
1:1:2130:A:H2'	1:1:2131:A:H8	1.72	0.53
2:2:609:A:N7	13:AI:107:SER:HA	2.24	0.53
2:2:992:U:H2'	2:2:993:C:C6	2.43	0.53
2:2:1169:U:H5''	2:2:1170:A:OP2	2.09	0.53
4:H:386:GLU:OE1	4:H:386:GLU:HA	2.08	0.53
1:1:622:G:N3	53:BD:75:THR:HG21	2.23	0.53
2:2:96:C:H2'	2:2:97:A:H8	1.73	0.53
2:2:1416:C:H2'	2:2:1417:U:H6	1.74	0.53
11:AG:37:GLN:HB3	11:AG:60:LYS:HE3	1.91	0.53
33:BB:122:VAL:HG13	33:BB:127:THR:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:475:G:O6	53:BD:158:ARG:NH1	2.40	0.53
1:1:939:G:H2'	1:1:940:C:C6	2.44	0.53
1:1:1598:G:H5''	45:BT:13:THR:HG22	1.91	0.53
1:1:2045:A:H2'	1:1:2046:C:C6	2.43	0.53
1:1:2162:5MC:H2'	1:1:2163:5MC:H6	1.72	0.53
1:1:2445:G:N2	1:1:2448:A:OP2	2.31	0.53
1:1:2498:A:H2	1:1:2503:U:H3	1.57	0.53
2:2:1133:U:H5''	22:AS:3:LYS:HD3	1.90	0.53
3:3:6:G:H2'	3:3:7:G:H8	1.74	0.53
31:AT:12:THR:HB	31:AT:15:GLN:HG3	1.89	0.53
1:1:102:C:C2	1:1:103:C:C5	2.97	0.53
1:1:720:A:OP1	62:Bc:32:ARG:NH2	2.41	0.53
1:1:1303:A:HO2'	1:1:1304:C:P	2.31	0.53
1:1:2799:G:H2'	1:1:2800:G:C8	2.42	0.53
2:2:1037:G:H2'	2:2:1038:U:C6	2.43	0.53
2:2:1434:U:H2'	2:2:1435:C:C6	2.44	0.53
4:H:6:VAL:HG13	4:H:113:ILE:HD12	1.90	0.53
6:AB:70:VAL:HG12	6:AB:92:ILE:HB	1.90	0.53
9:AE:124:PRO:HG2	9:AE:240:ILE:HD13	1.90	0.53
60:BN:29:PRO:HA	60:BN:59:GLN:HE22	1.74	0.53
1:1:1401:C:O2'	64:Bl:42:GLY:O	2.27	0.53
1:1:1575:A:H2'	1:1:1576:C:C6	2.43	0.53
1:1:2077:U:H2'	1:1:2078:G:C8	2.44	0.53
2:2:1329:G:H2'	2:2:1330:C:C6	2.44	0.53
35:BO:71:PHE:O	35:BO:191:ARG:NH2	2.42	0.53
61:Bg:36:TYR:CE2	61:Bg:38:ARG:HB2	2.43	0.53
1:1:382:C:H2'	1:1:383:C:C6	2.43	0.53
1:1:2426:C:H2'	1:1:2427:G:C8	2.44	0.53
1:1:2678:OMG:HM21	1:1:2680:A:H2'	1.90	0.53
2:2:28:G:H2'	2:2:29:C:C6	2.44	0.53
2:2:373:A2M:O5'	2:2:373:A2M:H8	2.09	0.53
2:2:1215:G:H2'	2:2:1216:G:C8	2.44	0.53
2:2:1501:U:H2'	2:2:1502:C:C6	2.44	0.53
9:AE:32:PRO:HB3	9:AE:44:PRO:HG3	1.89	0.53
23:AU:63:TYR:HE2	23:AU:126:ARG:HG3	1.72	0.53
30:A3:66:LEU:HB3	30:A3:67:PRO:HD3	1.91	0.53
1:1:1153:C:H2'	1:1:1154:C:C6	2.44	0.53
1:1:2652:C:H2'	1:1:2653:A:H8	1.73	0.53
2:2:579:C:H2'	2:2:580:A:C8	2.44	0.53
33:BB:42:ARG:HB3	33:BB:64:GLU:HG3	1.91	0.53
53:BD:201:VAL:HG11	53:BD:207:ILE:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:BS:45:ASN:ND2	58:BS:110:ASP:OD1	2.42	0.53
1:1:77:C:H2'	1:1:78:G:H8	1.74	0.52
1:1:773:C:H5'	38:BL:22:LYS:HE2	1.90	0.52
1:1:960:C:H2'	1:1:961:U:C6	2.43	0.52
1:1:1481:G:N2	1:1:1484:A:OP2	2.34	0.52
1:1:2197:G:H3'	1:1:2198:5MC:HM53	1.91	0.52
1:1:2536:U:O2	43:BE:136:GLY:HA3	2.08	0.52
2:2:1117:G:H2'	2:2:1118:G:H8	1.73	0.52
13:AI:90:GLU:OE2	13:AI:113:HIS:NE2	2.36	0.52
28:AZ:54:VAL:HG11	28:AZ:82:VAL:HG21	1.90	0.52
24:B6:37:LYS:HE3	24:B6:51:THR:HB	1.90	0.52
1:1:1979:G:H2'	1:1:1980:G:H8	1.75	0.52
1:1:2471:A:H2'	1:1:2472:G:H8	1.72	0.52
3:3:45:A:C4	3:3:46:A:C8	2.97	0.52
30:A3:12:PRO:HG2	30:A3:15:LEU:HD22	1.92	0.52
48:BI:57:THR:H	48:BI:64:GLY:HA3	1.74	0.52
66:sd:11:G:H5''	66:sd:11:G:C8	2.45	0.52
1:1:955:A:OP2	47:Bi:2:SER:N	2.42	0.52
1:1:1303:A:O2'	1:1:1304:C:O5'	2.19	0.52
1:1:2255:A:H2'	1:1:2256:A:C8	2.44	0.52
2:2:1193:C:HO2'	31:AT:66:HIS:HD1	1.58	0.52
1:1:197:G:OP1	40:BU:25:LYS:NZ	2.42	0.52
16:AL:6:ILE:HD12	16:AL:98:ILE:HG12	1.92	0.52
24:B6:81:ILE:HG23	24:B6:82:GLU:HG2	1.91	0.52
1:1:897:C:H2'	1:1:898:G:H8	1.75	0.52
1:1:1011:C:H2'	1:1:1012:G:O4'	2.09	0.52
1:1:1210:U:H4'	60:BN:8:ILE:HG23	1.90	0.52
1:1:1449:G:H2'	1:1:1450:G:H8	1.75	0.52
1:1:1550:4AC:OP1	50:BQ:8:ARG:NH1	2.43	0.52
1:1:1687:C:H5''	59:Bd:64:PRO:HB3	1.92	0.52
2:2:446:U:OP2	24:AV:89:ARG:NH2	2.43	0.52
9:AE:2:ALA:HB2	9:AE:7:LYS:HG3	1.92	0.52
12:AH:111:ILE:O	12:AH:115:THR:HG22	2.10	0.52
14:AJ:83:ASN:HD21	14:AJ:96:THR:HB	1.73	0.52
16:AL:65:GLU:OE2	16:AL:67:ARG:NE	2.38	0.52
41:Bb:87:VAL:HG13	41:Bb:117:ARG:HG2	1.91	0.52
65:Bk:4:LEU:HD13	65:Bk:37:VAL:HG13	1.92	0.52
1:1:792:A:N1	1:1:1060:G:O2'	2.37	0.52
5:AA:161:GLU:HB3	5:AA:167:ILE:HG13	1.90	0.52
51:BV:24:ARG:HE	51:BV:28:ARG:NH2	2.08	0.52
55:BZ:34:LEU:HD23	55:BZ:85:ILE:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2382:C:H2'	1:1:2383:C:C6	2.45	0.52
1:1:2523:C:H2'	1:1:2524:G:C8	2.45	0.52
2:2:1266:C:OP1	12:AH:3:LYS:NZ	2.43	0.52
10:AF:125:LYS:HG2	10:AF:225:VAL:HG22	1.91	0.52
53:BD:19:PRO:HB2	53:BD:21:VAL:HG12	1.92	0.52
55:BZ:22:GLU:OE1	55:BZ:25:ARG:NH2	2.42	0.52
1:1:429:A:H1'	1:1:431:G:C8	2.45	0.52
1:1:959:C:H5''	50:BQ:125:ILE:HG23	1.92	0.52
1:1:1715:U:H5	1:1:1824:A:N7	2.08	0.52
1:1:2944:C:O2'	1:1:2946:C:OP2	2.16	0.52
10:AF:146:GLU:O	10:AF:207:ASN:ND2	2.35	0.52
24:AV:25:HIS:ND1	24:AV:25:HIS:O	2.43	0.52
30:A3:70:CYS:HA	30:A3:75:ILE:HD12	1.92	0.52
34:BY:69:ARG:NH1	34:BY:82:ASP:OD2	2.39	0.52
1:1:1115:A:H2'	1:1:1116:G:H8	1.72	0.52
1:1:2001:4AC:P	50:BQ:76:ARG:HH12	2.32	0.52
2:2:418:G:H4'	8:AD:170:MET:HE2	1.92	0.52
2:2:836:A:H5'	2:2:1043:U:C5	2.45	0.52
4:H:383:ARG:HG2	17:AM:55:PRO:CG	2.39	0.52
5:AA:109:ASN:ND2	5:AA:119:ARG:HE	2.08	0.52
35:BO:59:LEU:HD23	35:BO:99:ILE:HD11	1.90	0.52
2:2:1402:A:H2'	2:2:1403:G:H8	1.75	0.52
43:BE:120:HIS:HD2	43:BE:135:PHE:H	1.58	0.52
66:sd:11:G:H3'	66:sd:12:A:H8	1.74	0.52
1:1:1303:A:O2'	1:1:1304:C:H6	1.93	0.51
1:1:1648:C:H2'	1:1:1649:G:H8	1.74	0.51
1:1:2712:C:H2'	1:1:2713:G:O4'	2.10	0.51
2:2:145:G:H2'	2:2:146:A:C8	2.45	0.51
2:2:465:G:H2'	2:2:466:G:C8	2.44	0.51
2:2:907:A:H2'	2:2:908:C:C6	2.45	0.51
43:BE:34:VAL:HG22	43:BE:36:GLU:H	1.74	0.51
44:Ba:21:ILE:HG13	44:Ba:22:VAL:HG13	1.92	0.51
1:1:1265:C:H2'	1:1:1266:G:H8	1.75	0.51
2:2:797:G:H5''	6:AB:24:LYS:O	2.10	0.51
3:3:124:C:H2'	3:3:125:A:C8	2.45	0.51
11:AG:112:ILE:HA	11:AG:116:ILE:HD12	1.93	0.51
20:AQ:25:TRP:CE2	25:AW:64:LEU:HD21	2.45	0.51
1:1:450:C:H2'	1:1:451:4AC:H6	1.91	0.51
1:1:462:G:H21	1:1:485:A:H62	1.58	0.51
1:1:569:C:H2'	1:1:570:G:C8	2.46	0.51
1:1:775:U:O2'	1:1:1234:A:N1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2606:C:H2'	1:1:2607:C:H6	1.75	0.51
2:2:1024:C:O3'	19:AP:44:ARG:NH2	2.43	0.51
5:AA:166:LYS:O	5:AA:170:GLU:HG2	2.11	0.51
1:1:2065:A:H2'	1:1:2066:A:C8	2.46	0.51
1:1:2504:A:H2'	1:1:2505:U:C6	2.45	0.51
1:1:2810:G:H2'	1:1:2811:C:H6	1.76	0.51
3:3:62:C:H2'	3:3:63:C:H6	1.76	0.51
5:AA:18:GLN:HB2	5:AA:77:GLN:HE22	1.74	0.51
1:1:158:C:H2'	1:1:159:G:C8	2.45	0.51
1:1:1489:C:H2'	1:1:1490:G:C8	2.45	0.51
24:AV:3:ILE:HG12	24:AV:23:ILE:HG12	1.92	0.51
29:A0:9:LYS:O	29:A0:13:ARG:NH1	2.36	0.51
60:BN:46:GLU:HG3	60:BN:136:ARG:HG2	1.92	0.51
1:1:934:A:N1	1:1:1038:C:H1'	2.25	0.51
2:2:37:C:H2'	2:2:38:A:C8	2.45	0.51
2:2:1346:C:OP1	15:AK:73:GLY:N	2.42	0.51
2:2:1373:C:O2	2:2:1471:A:N6	2.44	0.51
5:AA:23:TYR:HE2	5:AA:78:ASN:HB3	1.76	0.51
36:BC:194:ASN:O	36:BC:198:GLU:HG2	2.11	0.51
38:BL:1:MET:HE2	53:BD:33:ARG:HD2	1.92	0.51
62:Bc:41:ARG:HE	62:Bc:87:ILE:C	2.19	0.51
1:1:122:G:H2'	1:1:123:A:C8	2.45	0.51
1:1:2109:A:H2'	1:1:2110:A:H8	1.76	0.51
2:2:1069:OMG:HM22	2:2:1070:A:H5'	1.91	0.51
30:B4:56:ASP:OD1	30:B4:56:ASP:N	2.44	0.51
1:1:115:G:N3	1:1:115:G:H2'	2.26	0.51
2:2:470:G:H2'	2:2:471:OMG:H8	1.76	0.51
2:2:703:4AC:H2'	2:2:704:G:H8	1.76	0.51
2:2:1321:G:O6	15:AK:10:ARG:NH2	2.33	0.51
4:H:211:ARG:NH1	4:H:212:GLU:OE2	2.44	0.51
30:A3:57:VAL:HG11	30:A3:62:ILE:HD11	1.92	0.51
43:BE:169:GLU:O	43:BE:173:VAL:HG12	2.10	0.51
1:1:132:C:H2'	1:1:133:G:H8	1.76	0.51
1:1:761:U:H2'	1:1:762:G:C8	2.40	0.51
1:1:1086:G:H2'	1:1:1087:G:H8	1.76	0.51
1:1:2764:G:N2	1:1:2896:G:O2'	2.44	0.51
2:2:1076:A:H61	28:AZ:155:GLY:HA3	1.76	0.51
16:AL:22:GLN:HE22	16:AL:88:ILE:HG12	1.76	0.51
1:1:1055:A2M:HM'2	1:1:1057:C:C6	2.45	0.51
2:2:1267:G:OP1	12:AH:3:LYS:HB2	2.11	0.51
3:3:58:A:C5	3:3:59:G:C8	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AL:17:GLU:HA	16:AL:20:ALA:HB3	1.93	0.51
21:AR:17:ASP:OD1	21:AR:17:ASP:N	2.42	0.51
33:BB:138:LYS:HE2	33:BB:140:ILE:HD11	1.92	0.51
1:1:163:A:H5''	1:1:165:G:O4'	2.11	0.50
1:1:1067:C:H2'	1:1:1068:4AC:H6	1.92	0.50
1:1:1317:G:H2'	1:1:1318:G:H8	1.75	0.50
1:1:2268:C:H2'	1:1:2269:G:O4'	2.11	0.50
1:1:2305:C:H2'	1:1:2306:C:H6	1.76	0.50
1:1:3022:C:O2	1:1:3022:C:H2'	2.11	0.50
2:2:373:A2M:HM'2	2:2:374:A:C5	2.46	0.50
2:2:1310:U:O2'	12:AH:85:PHE:O	2.22	0.50
3:3:28:C:H2'	3:3:29:A:O4'	2.10	0.50
9:AE:36:PRO:HD2	9:AE:84:PRO:HG2	1.92	0.50
36:BC:161:ARG:HG2	36:BC:183:ALA:HA	1.92	0.50
1:1:573:U:H2'	1:1:574:C:C6	2.46	0.50
1:1:658:G:H5''	1:1:661:C:H1'	1.92	0.50
1:1:1524:G:N7	58:BS:28:SER:OG	2.37	0.50
1:1:1551:G:H2'	1:1:1552:A:H8	1.76	0.50
31:AT:17:MET:HE1	31:AT:55:LYS:HE3	1.92	0.50
36:BC:190:GLU:O	36:BC:194:ASN:ND2	2.45	0.50
40:BU:27:MET:HE2	40:BU:69:VAL:HG13	1.93	0.50
54:BF:4:ASP:OD1	54:BF:5:ALA:N	2.43	0.50
57:BM:76:TRP:CD1	57:BM:76:TRP:H	2.29	0.50
62:Bc:44:ILE:HG13	62:Bc:54:LYS:HG2	1.92	0.50
30:B4:64:ALA:O	30:B4:67:PRO:HD2	2.10	0.50
1:1:94:G:H3'	1:1:95:G:C5'	2.41	0.50
1:1:762:G:H2'	1:1:763:C:C6	2.46	0.50
2:2:1052:C:H2'	2:2:1053:A:H8	1.76	0.50
2:2:1103:C:O2'	23:AU:130:ASP:OD2	2.22	0.50
3:3:70:A:H2'	3:3:71:U:O4'	2.11	0.50
4:H:382:LYS:CG	17:AM:52:ARG:HD2	2.41	0.50
10:AF:92:ARG:HH21	10:AF:176:ARG:HD3	1.76	0.50
30:A3:52:ILE:HG12	30:A3:78:ILE:HD11	1.94	0.50
30:A3:107:ALA:H	30:A3:108:ARG:HE	1.57	0.50
1:1:809:A:N7	1:1:903:G:O2'	2.35	0.50
2:2:1429:U:OP1	11:AG:82:ARG:NH2	2.44	0.50
4:H:126:GLU:OE2	4:H:129:LYS:NZ	2.45	0.50
20:AQ:60:ILE:HG13	20:AQ:60:ILE:O	2.10	0.50
31:AT:32:GLN:OE1	31:AT:32:GLN:N	2.44	0.50
35:BO:44:HIS:CE1	35:BO:116:SER:HB3	2.45	0.50
43:BE:28:VAL:HG12	43:BE:141:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:540:U:O2'	1:1:542:G:N7	2.44	0.50
1:1:787:C:H2'	1:1:788:A:C8	2.46	0.50
1:1:2249:4AC:H2'	1:1:2250:G:H8	1.77	0.50
1:1:2532:C:H2'	1:1:2533:G:C8	2.47	0.50
2:2:1045:A:OP1	10:AF:102:HIS:NE2	2.39	0.50
4:H:384:PHE:CZ	26:AX:65:ARG:NH2	2.80	0.50
13:AI:28:LYS:HB3	13:AI:29:PRO:HD3	1.94	0.50
13:AI:104:VAL:HG22	13:AI:125:LEU:HD23	1.93	0.50
34:BY:148:ASN:O	34:BY:152:GLU:HG2	2.12	0.50
36:BC:289:ASN:HA	36:BC:315:SER:HA	1.92	0.50
37:B5:36:THR:HB	37:B5:45:ARG:HG3	1.92	0.50
1:1:544:U:P	52:Bj:38:ARG:HH21	2.35	0.50
1:1:1077:C:H5'	1:1:2662:A:O2'	2.11	0.50
1:1:1203:G:H2'	1:1:1204:G:H8	1.76	0.50
2:2:1435:C:H2'	2:2:1436:G:O4'	2.11	0.50
4:H:30:ILE:HG12	4:H:38:ILE:HD11	1.94	0.50
4:H:383:ARG:NH1	17:AM:24:ASN:HD21	2.09	0.50
1:1:216:A:C6	1:1:217:A:C5	3.00	0.50
1:1:1581:A:C4	1:1:1582:A:C8	2.99	0.50
1:1:2645:U:H2'	1:1:2646:G:H8	1.76	0.50
9:AE:126:ARG:H	9:AE:143:HIS:CD2	2.29	0.50
21:AR:27:LEU:HD21	21:AR:91:THR:HG21	1.94	0.50
1:1:31:G:H4'	44:Ba:14:PRO:HG3	1.93	0.50
1:1:150:G:N3	1:1:604:G:O2'	2.44	0.50
1:1:208:A:H2'	1:1:209:G:O4'	2.11	0.50
1:1:447:A:N7	1:1:500:U:O2'	2.42	0.50
1:1:2004:A:H2'	1:1:2005:G:C8	2.47	0.50
1:1:2153:A:O2'	2:2:1463:G:O2'	2.29	0.50
1:1:2675:U:H2'	1:1:2676:G:H8	1.77	0.50
2:2:135:U:H2'	2:2:136:C:C6	2.46	0.50
2:2:1491:U:H2'	2:2:1492:A:C8	2.47	0.50
9:AE:141:ASN:ND2	9:AE:147:ASN:OD1	2.41	0.50
12:AH:17:VAL:HG11	12:AH:64:VAL:HG21	1.93	0.50
33:BB:202:HIS:CD2	33:BB:204:PHE:H	2.29	0.50
57:BM:152:LYS:HG3	65:Bk:12:ARG:HA	1.94	0.50
1:1:147:U:OP2	53:BD:186:MET:HG2	2.11	0.50
1:1:215:G:N1	40:BU:111:ARG:HG3	2.27	0.50
1:1:1285:G:H5''	60:BN:154:MET:HE1	1.94	0.50
1:1:1406:G:OP2	34:BY:127:ARG:NH2	2.40	0.50
1:1:2058:A:H2'	1:1:2059:G:C8	2.47	0.50
2:2:992:U:H2'	2:2:993:C:H6	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B4:117:LYS:O	30:B4:121:LEU:HD23	2.12	0.50
1:1:118:U:H2'	1:1:118:U:O2	2.11	0.49
1:1:2675:U:H2'	1:1:2676:G:C8	2.47	0.49
1:1:2719:G:H2'	1:1:2720:A:H8	1.76	0.49
2:2:483:G:H4'	2:2:485:C:C2	2.47	0.49
53:BD:142:LEU:HD23	53:BD:241:VAL:HG22	1.93	0.49
1:1:66:G:H2'	1:1:67:C:C6	2.47	0.49
1:1:1425:G:H2'	1:1:1426:A:H8	1.78	0.49
1:1:1769:A:N1	1:1:1831:G:O2'	2.38	0.49
1:1:2164:U:H2'	1:1:2165:C:C6	2.46	0.49
1:1:2808:G:O2'	1:1:2811:C:OP2	2.21	0.49
10:AF:61:GLU:O	10:AF:92:ARG:NH1	2.39	0.49
23:AU:2:ALA:HB3	23:AU:134:THR:HG22	1.93	0.49
36:BC:217:ASP:HB2	36:BC:335:ARG:HG3	1.94	0.49
54:BF:10:GLU:HG2	54:BF:54:VAL:HG22	1.94	0.49
1:1:435:C:H2'	1:1:436:C:H6	1.77	0.49
1:1:959:C:H2'	1:1:960:C:H6	1.77	0.49
1:1:1940:A:H61	1:1:2237:C:H42	1.61	0.49
2:2:162:G:O2'	11:AG:120:ASN:ND2	2.46	0.49
2:2:1425:G:H2'	2:2:1426:A:C8	2.47	0.49
4:H:4:ILE:HB	4:H:85:LEU:HD22	1.93	0.49
8:AD:116:ARG:HG3	8:AD:171:ILE:HA	1.93	0.49
9:AE:87:ILE:HG22	9:AE:88:MET:HG2	1.94	0.49
33:BB:74:PRO:HG2	33:BB:77:LEU:HB2	1.94	0.49
1:1:107:G:C2	1:1:112:A:N7	2.75	0.49
1:1:909:C:H2'	1:1:910:G:H8	1.76	0.49
1:1:952:U:H2'	1:1:953:G:O4'	2.12	0.49
58:BS:46:ASP:OD1	58:BS:49:ARG:NH2	2.45	0.49
1:1:209:G:O2'	46:BW:40:ASN:ND2	2.45	0.49
1:1:458:4AC:H2'	1:1:459:G:C8	2.44	0.49
1:1:1164:C:H5''	60:BN:19:ARG:HH12	1.77	0.49
1:1:1327:C:N4	1:1:1352:C:O3'	2.43	0.49
1:1:1625:A:H2'	1:1:1626:C:C6	2.47	0.49
2:2:484:G:H1'	18:AN:67:SER:OG	2.13	0.49
2:2:1212:A:C8	2:2:1277:C:H1'	2.48	0.49
3:3:6:G:H2'	3:3:7:G:C8	2.48	0.49
38:BL:47:TRP:CZ2	38:BL:51:ILE:HD11	2.47	0.49
58:BS:63:LEU:HD11	58:BS:82:ARG:HB2	1.94	0.49
1:1:189:G:H2'	1:1:189:G:N3	2.27	0.49
1:1:453:A:N1	1:1:477:A:O2'	2.40	0.49
1:1:1153:C:H2'	1:1:1154:C:H6	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2314:U:H2'	1:1:2315:U:H6	1.77	0.49
2:2:225:C:H2'	2:2:226:U:H6	1.77	0.49
2:2:654:A:O2'	2:2:668:A:N6	2.44	0.49
2:2:988:A:OP1	31:AT:50:LYS:NZ	2.42	0.49
2:2:1482:A:H2'	2:2:1483:G:H8	1.77	0.49
6:AB:136:PRO:HG3	7:AC:30:PHE:HB3	1.95	0.49
1:1:475:G:H4'	1:1:477:A:N7	2.27	0.49
1:1:568:U:H2'	1:1:569:C:C6	2.47	0.49
1:1:1084:A:H62	1:1:1198:A:H2	1.59	0.49
1:1:1953:A:H2'	1:1:1954:A:C8	2.47	0.49
2:2:157:A:H2'	2:2:158:A:O4'	2.13	0.49
2:2:464:A:H4'	2:2:465:G:OP1	2.11	0.49
2:2:531:U:OP2	18:AN:5:LYS:NZ	2.45	0.49
2:2:922:U:H2'	2:2:923:G:C8	2.48	0.49
2:2:1088:A:O2'	16:AL:37:PRO:O	2.29	0.49
2:2:1507:C:OP1	5:AA:100:ARG:NH2	2.46	0.49
6:AB:61:ARG:NH2	7:AC:33:PRO:O	2.45	0.49
40:BU:106:ASN:O	40:BU:112:ARG:NH1	2.38	0.49
1:1:635:G:O2'	1:1:659:A:N1	2.41	0.49
1:1:770:C:H2'	1:1:771:G:C8	2.48	0.49
1:1:2044:C:H5'	33:BB:196:LYS:HE2	1.94	0.49
1:1:2153:A:HO2'	2:2:1463:G:HO2'	1.61	0.49
1:1:2259:U:O2	41:Bb:30:ARG:NH2	2.44	0.49
1:1:2394:G:H2'	1:1:2395:U:H6	1.78	0.49
1:1:2910:C:H4'	36:BC:11:SER:HB2	1.94	0.49
2:2:724:U:OP1	2:2:789:C:O2'	2.30	0.49
57:BM:101:GLU:OE2	57:BM:116:SER:OG	2.28	0.49
60:BN:39:PRO:O	60:BN:136:ARG:NH2	2.45	0.49
1:1:250:U:H4'	1:1:251:A:OP1	2.12	0.49
1:1:299:A:H5''	38:BL:37:ALA:HB2	1.95	0.49
1:1:1993:G:N2	1:1:1995:G:H3'	2.28	0.49
1:1:2066:A:H2'	1:1:2067:G:O4'	2.13	0.49
2:2:345:C:H2'	2:2:346:A:H8	1.77	0.49
2:2:1316:C:H2'	2:2:1317:C:C6	2.48	0.49
2:2:1386:C:H2'	2:2:1387:A:C8	2.48	0.49
2:2:1402:A:H2'	2:2:1403:G:C8	2.48	0.49
30:A3:49:LYS:HD3	30:A3:103:GLU:H	1.78	0.49
50:BQ:15:LEU:HD13	50:BQ:52:LYS:HB2	1.94	0.49
24:B6:47:ASN:HB3	24:B6:50:THR:HG22	1.95	0.49
1:1:428:U:O2	1:1:428:U:H2'	2.12	0.49
1:1:728:C:O2'	37:BK:52:HIS:ND1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:949:A:N6	2:2:1198:U:O5'	2.46	0.49
6:AB:166:LEU:O	6:AB:170:ILE:HG23	2.13	0.49
8:AD:65:GLN:O	8:AD:69:GLU:HG2	2.13	0.49
36:BC:17:ARG:HB2	36:BC:233:ARG:NH2	2.27	0.49
37:BK:21:LYS:O	37:BK:41:ASN:ND2	2.35	0.49
58:BS:72:HIS:HA	58:BS:79:GLY:O	2.11	0.49
1:1:544:U:OP1	52:Bj:38:ARG:NH2	2.45	0.48
1:1:959:C:H2'	1:1:960:C:C6	2.48	0.48
1:1:1649:G:H2'	1:1:1650:G:H8	1.78	0.48
2:2:42:C:OP1	18:AN:142:LYS:NZ	2.39	0.48
2:2:224:G:HO2'	2:2:225:C:H6	1.60	0.48
2:2:398:A:H3'	2:2:399:C:H6	1.78	0.48
2:2:929:U:H5''	31:AT:111:LYS:HD3	1.95	0.48
2:2:1300:C:H2'	2:2:1301:G:H8	1.78	0.48
2:2:1401:U:OP1	14:AJ:16:ARG:NH2	2.46	0.48
2:2:1476:A:H2'	2:2:1477:G:C8	2.47	0.48
2:2:1485:G:N1	2:2:1488:MA6:OP2	2.45	0.48
4:H:219:ILE:HG13	4:H:237:ASN:HD22	1.78	0.48
57:BM:31:ARG:NH1	57:BM:122:ASP:OD2	2.45	0.48
58:BS:20:ALA:HB1	58:BS:97:ASN:HD22	1.77	0.48
1:1:1211:A:H2'	1:1:1212:A:C8	2.48	0.48
1:1:1462:G:H5'	53:BD:195:LYS:HG2	1.95	0.48
1:1:2456:C:H2'	1:1:2457:A:O4'	2.13	0.48
2:2:964:G:H22	2:2:1186:A:P	2.36	0.48
13:AI:66:LEU:HB2	13:AI:68:LYS:HG3	1.95	0.48
16:AL:8:LEU:HB3	16:AL:16:LEU:HD22	1.95	0.48
42:Be:18:ILE:HG12	42:Be:30:VAL:HG22	1.95	0.48
49:BR:45:ILE:H	49:BR:59:HIS:CD2	2.30	0.48
60:BN:127:LYS:H	60:BN:130:GLN:NE2	2.10	0.48
1:1:134:C:H2'	1:1:135:C:C6	2.48	0.48
1:1:1897:C:C2	1:1:1898:C:C5	3.02	0.48
1:1:2740:G:HO2'	1:1:2786:U:HO2'	1.61	0.48
1:1:2929:U:H2'	1:1:2930:G:H8	1.78	0.48
2:2:168:A:H2'	2:2:169:A:C8	2.48	0.48
2:2:346:A:H2'	2:2:347:G:C8	2.48	0.48
2:2:724:U:H2'	2:2:725:G:O4'	2.12	0.48
10:AF:57:VAL:HG22	10:AF:89:VAL:HB	1.96	0.48
17:AM:43:SER:H	17:AM:46:MET:HG3	1.78	0.48
27:AY:4:LYS:HE3	27:AY:30:PHE:HE2	1.78	0.48
30:A3:3:LYS:HG2	30:A3:6:TYR:HB2	1.94	0.48
33:BB:106:THR:HA	47:Bi:81:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:BN:102:GLY:H	60:BN:105:ALA:HB2	1.77	0.48
1:1:1567:A:O2'	42:Be:12:ASN:O	2.28	0.48
2:2:917:G:C2	2:2:918:A:C8	3.01	0.48
37:BK:45:ARG:NH1	64:Bl:1:MET:O	2.43	0.48
24:B6:59:TYR:CE1	24:B6:66:LYS:HD3	2.49	0.48
1:1:1179:C:C2	1:1:1180:G:C8	3.02	0.48
28:AZ:128:VAL:HG23	28:AZ:182:ILE:HG12	1.96	0.48
30:BG:43:VAL:HG13	30:BG:75:ILE:HD12	1.95	0.48
62:Bc:10:TYR:CD1	62:Bc:19:THR:HA	2.49	0.48
1:1:563:A:H2'	1:1:564:G:H8	1.78	0.48
1:1:833:G:H2'	1:1:834:C:C6	2.45	0.48
1:1:1373:G:H2'	1:1:1374:G:H8	1.79	0.48
1:1:1697:G:H2'	1:1:1698:A:H8	1.78	0.48
1:1:2607:C:H2'	1:1:2608:4AC:O2	2.13	0.48
1:1:2643:G:C2	1:1:2644:G:C8	3.02	0.48
2:2:270:U:OP2	14:AJ:56:ARG:NH2	2.40	0.48
2:2:1183:C:H2'	2:2:1184:4AC:H6	1.95	0.48
2:2:1266:C:H2'	2:2:1267:G:C8	2.49	0.48
2:2:1415:U:H2'	2:2:1416:C:H6	1.78	0.48
10:AF:160:PRO:HD2	10:AF:163:LEU:HD22	1.96	0.48
11:AG:24:PRO:O	11:AG:27:GLU:HG2	2.14	0.48
11:AG:76:PRO:C	11:AG:110:ASN:HD21	2.21	0.48
36:BC:8:ARG:HH12	36:BC:264:THR:HB	1.79	0.48
43:BE:185:GLU:HG2	43:BE:186:GLU:HG2	1.94	0.48
45:BT:80:ALA:HA	45:BT:85:LEU:HD22	1.95	0.48
1:1:117:G:N3	1:1:118:U:C6	2.82	0.48
1:1:492:C:H2'	1:1:493:G:O4'	2.13	0.48
1:1:546:U:H2'	1:1:547:C:C6	2.49	0.48
1:1:801:C:H2'	1:1:802:4AC:H6	1.96	0.48
2:2:382:A:C2	2:2:383:A:C8	3.02	0.48
2:2:478:C:H2'	2:2:479:4AC:H6	1.95	0.48
9:AE:123:LYS:NZ	9:AE:144:ASP:OD2	2.47	0.48
11:AG:33:ARG:NH1	11:AG:111:THR:OG1	2.47	0.48
29:A0:29:GLN:O	29:A0:33:GLU:HG2	2.14	0.48
33:BB:122:VAL:HG21	33:BB:129:ALA:HB2	1.95	0.48
54:BF:92:VAL:HG22	54:BF:172:ILE:HG12	1.95	0.48
24:B6:13:LEU:HD22	24:B6:14:ILE:HG23	1.96	0.48
1:1:102:C:N3	1:1:103:C:C4	2.81	0.48
1:1:1253:G:H2'	1:1:1254:C:C6	2.48	0.48
1:1:1649:G:H2'	1:1:1650:G:C8	2.49	0.48
1:1:1756:G:H5'	37:B5:51:LYS:HE2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:644:C:H2'	2:2:645:C:C6	2.49	0.48
21:AR:38:VAL:HG22	21:AR:82:VAL:HA	1.95	0.48
45:BT:50:LYS:HG2	45:BT:74:TYR:CE2	2.48	0.48
1:1:98:C:H6	1:1:98:C:H5''	1.79	0.48
1:1:240:U:OP1	42:Be:21:ARG:HD3	2.14	0.48
1:1:1763:G:H2'	1:1:1764:C:H6	1.77	0.48
1:1:1939:G:O2'	1:1:2919:G:H4'	2.13	0.48
1:1:2799:G:H2'	1:1:2800:G:H8	1.79	0.48
2:2:625:C:H2'	2:2:626:4AC:H6	1.96	0.48
2:2:1225:A:H2'	2:2:1226:U:C6	2.49	0.48
2:2:1288:C:H2'	2:2:1289:U:C6	2.49	0.48
18:AN:39:GLU:OE1	18:AN:39:GLU:N	2.43	0.48
31:AT:13:LEU:HA	31:AT:16:LEU:HD12	1.95	0.48
32:AO:54:LEU:HD23	32:AO:59:VAL:HG22	1.95	0.48
44:Ba:78:GLU:HB3	44:Ba:85:LYS:HD2	1.95	0.48
52:Bj:1:MET:N	52:Bj:88:LYS:O	2.47	0.48
53:BD:61:ILE:HD11	53:BD:68:ALA:O	2.14	0.48
24:B6:53:ILE:HD13	24:B6:69:ALA:HB2	1.95	0.48
1:1:749:G:C2	1:1:750:G:C8	3.02	0.48
1:1:871:G:H2'	1:1:872:C:H6	1.79	0.48
1:1:908:A:H2'	1:1:909:C:C6	2.49	0.48
1:1:960:C:H2'	1:1:961:U:H6	1.78	0.48
1:1:1094:C:H2'	1:1:1095:G:C8	2.48	0.48
1:1:1120:U:C2	1:1:1121:G:C8	3.02	0.48
1:1:1552:A:O2'	44:Ba:56:GLU:OE2	2.30	0.48
1:1:1577:A:H62	50:BQ:36:ILE:HG21	1.79	0.48
1:1:1653:U:P	50:BQ:42:ARG:HH22	2.37	0.48
1:1:2254:A:H2	58:BS:131:ARG:HH22	1.62	0.48
2:2:891:U:H2'	2:2:892:U:C6	2.49	0.48
2:2:1210:A:H2'	2:2:1211:C:C6	2.48	0.48
2:2:1415:U:H4'	51:BV:62:GLN:O	2.13	0.48
10:AF:5:TRP:HB3	10:AF:55:PRO:HB2	1.95	0.48
36:BC:284:ILE:HD11	36:BC:321:ALA:HB2	1.96	0.48
36:BC:291:LYS:HB3	36:BC:298:GLU:CD	2.39	0.48
48:BI:1:MET:HE2	48:BI:1:MET:HB2	1.69	0.48
1:1:1171:C:H2'	1:1:1172:C:C6	2.49	0.47
1:1:1305:A:C6	1:1:1306:G:C6	3.01	0.47
1:1:1889:A:OP1	39:Bf:46:ARG:NH2	2.45	0.47
2:2:190:C:H2'	2:2:191:U:C6	2.49	0.47
2:2:219:G:H21	2:2:222:A:H8	1.61	0.47
2:2:730:C:H2'	2:2:731:4AC:H6	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:795:A:H2'	2:2:796:G:O4'	2.14	0.47
2:2:1501:U:H2'	2:2:1502:C:H6	1.79	0.47
3:3:74:C:H2'	3:3:75:G:H8	1.78	0.47
5:AA:175:ALA:HB3	5:AA:181:LEU:HD11	1.95	0.47
7:AC:38:ALA:HB2	7:AC:57:LYS:HG2	1.96	0.47
9:AE:165:LEU:HD23	9:AE:175:GLU:HB3	1.94	0.47
36:BC:184:ILE:HG13	36:BC:196:ILE:HD11	1.96	0.47
1:1:219:C:H2'	1:1:220:G:H8	1.79	0.47
1:1:285:A:OP2	42:Be:48:LYS:NZ	2.47	0.47
1:1:1173:C:H2'	1:1:1174:A:C8	2.47	0.47
1:1:1551:G:H5'	50:BQ:24:ILE:O	2.14	0.47
1:1:1733:A:H2'	1:1:1734:G:O4'	2.14	0.47
1:1:1987:G:N7	50:BQ:74:ARG:NH2	2.59	0.47
1:1:2098:G:H2'	1:1:2099:C:H6	1.80	0.47
2:2:641:G:H2'	2:2:642:U:C6	2.50	0.47
2:2:783:A:OP1	2:2:1495:G:O2'	2.27	0.47
2:2:816:C:H2'	2:2:817:U:H6	1.80	0.47
9:AE:3:ARG:HG3	9:AE:4:LYS:HG2	1.96	0.47
43:BE:28:VAL:HG11	43:BE:91:LEU:HG	1.96	0.47
50:BQ:36:ILE:HG13	50:BQ:37:THR:HG23	1.96	0.47
55:BZ:34:LEU:HD13	55:BZ:97:ALA:HB2	1.96	0.47
30:B4:19:ALA:HB2	30:B4:78:ILE:HD13	1.95	0.47
1:1:58:A:C5	1:1:59:C:H1'	2.49	0.47
1:1:163:A:H2	1:1:233:U:N3	2.12	0.47
1:1:412:G:O2'	1:1:413:G:H5'	2.13	0.47
1:1:1749:U:H2'	1:1:1750:A:H8	1.78	0.47
1:1:1853:G:H2'	1:1:1854:A:H8	1.79	0.47
1:1:1909:A:H2'	1:1:1910:G:C8	2.49	0.47
1:1:1933:C:H2'	1:1:1934:4AC:H6	1.95	0.47
1:1:2336:A:H2'	1:1:2337:C:C6	2.50	0.47
1:1:2469:G:H5'	33:BB:225:ARG:HG2	1.95	0.47
1:1:2611:A:H2'	1:1:2612:A:C8	2.49	0.47
1:1:2723:C:H5'	1:1:2802:G:H5''	1.95	0.47
1:1:2767:G:C2	1:1:2768:G:C8	3.02	0.47
3:3:62:C:H2'	3:3:63:C:C6	2.49	0.47
16:AL:45:ILE:HD11	28:AZ:4:GLU:HB3	1.96	0.47
34:BY:55:THR:HG21	34:BY:143:ARG:HH21	1.78	0.47
35:BO:73:TRP:HZ3	35:BO:185:PHE:HA	1.79	0.47
37:B5:27:ILE:HA	37:B5:33:VAL:HG22	1.97	0.47
1:1:102:C:C4	1:1:103:C:N4	2.81	0.47
1:1:113:G:C4	1:1:114:G:C8	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:845:C:H2'	1:1:846:C:C6	2.49	0.47
1:1:1102:G:C8	34:BY:25:MET:HE1	2.50	0.47
1:1:1133:A:H5'	1:1:2540:G:O4'	2.14	0.47
1:1:1699:G:H2'	1:1:1700:G:H8	1.78	0.47
1:1:1755:4AC:O7	1:1:1755:4AC:H5	2.15	0.47
1:1:2536:U:H5''	43:BE:116:GLY:HA3	1.95	0.47
1:1:2931:U:H2'	1:1:2932:C:C6	2.49	0.47
2:2:233:G:H2'	2:2:234:A:H8	1.79	0.47
2:2:270:U:P	14:AJ:56:ARG:HH22	2.37	0.47
2:2:663:A:H2'	2:2:664:U:H6	1.79	0.47
2:2:1262:A:H2'	2:2:1263:A:C8	2.50	0.47
12:AH:112:GLU:HB2	12:AH:119:PRO:HG3	1.96	0.47
34:BY:110:LEU:HD23	34:BY:113:LEU:HD22	1.96	0.47
37:B5:12:ILE:HG12	37:B5:48:MET:HE1	1.96	0.47
46:BW:29:ARG:NH2	46:BW:48:ARG:HD3	2.29	0.47
1:1:18:G:H8	1:1:2855:G:H4'	1.78	0.47
1:1:102:C:OP2	1:1:102:C:H6	1.96	0.47
1:1:411:G:C6	1:1:412:G:C5	3.03	0.47
1:1:895:A:H2'	1:1:896:G:O4'	2.14	0.47
1:1:1324:A:H4'	1:1:1325:A:H5''	1.95	0.47
1:1:1698:A:H2'	1:1:1699:G:C8	2.50	0.47
1:1:2533:G:O2'	43:BE:109:GLU:OE1	2.27	0.47
2:2:839:4AC:H2'	2:2:840:G:O4'	2.15	0.47
4:H:147:ASP:HB2	4:H:210:LEU:HD12	1.96	0.47
4:H:382:LYS:HG2	17:AM:52:ARG:HD2	1.96	0.47
5:AA:53:LEU:HD23	5:AA:62:LYS:HB3	1.97	0.47
7:AC:52:PRO:HA	7:AC:63:PRO:HD3	1.97	0.47
35:BO:42:ASN:O	35:BO:77:CYS:HB2	2.14	0.47
38:BL:44:LYS:HG3	38:BL:47:TRP:CG	2.49	0.47
40:BU:41:ILE:CG2	40:BU:119:ARG:HB3	2.43	0.47
1:1:1697:G:H2'	1:1:1698:A:C8	2.49	0.47
1:1:2482:G:H2'	1:1:2483:G:H8	1.79	0.47
1:1:2686:G:C4	1:1:2687:A:C8	3.02	0.47
2:2:659:U:C4	4:H:383:ARG:NE	2.82	0.47
2:2:1191:C:H2'	2:2:1192:C:H6	1.80	0.47
7:AC:35:CYS:HB3	7:AC:58:CYS:SG	2.55	0.47
1:1:197:G:P	40:BU:118:ARG:HH22	2.37	0.47
1:1:572:C:H2'	1:1:573:U:C6	2.49	0.47
1:1:676:C:H2'	1:1:677:G:O4'	2.14	0.47
1:1:1216:G:H21	1:1:2498:A:H62	1.63	0.47
1:1:1386:G:O6	1:1:2264:C:O2'	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2004:A:H2'	1:1:2005:G:H8	1.79	0.47
1:1:2373:G:N2	1:1:2397:G:N3	2.62	0.47
1:1:2431:C:H2'	1:1:2432:G:H8	1.77	0.47
1:1:2473:U:H2'	1:1:2474:U:C6	2.50	0.47
1:1:2488:A:C4	1:1:2506:C:H5'	2.49	0.47
2:2:955:A:O2'	2:2:1015:G:OP2	2.29	0.47
2:2:965:A:H5''	2:2:966:C:C5	2.43	0.47
4:H:387:LYS:C	4:H:387:LYS:CD	2.85	0.47
5:AA:69:PHE:HB3	5:AA:81:THR:HB	1.96	0.47
7:AC:11:ILE:HG23	10:AF:39:ARG:HD3	1.97	0.47
29:A0:29:GLN:NE2	29:A0:33:GLU:OE2	2.43	0.47
35:BO:36:VAL:HG22	35:BO:47:GLN:HB2	1.96	0.47
40:BU:4:ASN:N	40:BU:4:ASN:OD1	2.47	0.47
57:BM:167:LYS:HG2	57:BM:172:LEU:HD12	1.96	0.47
1:1:151:C:H2'	1:1:152:U:C6	2.50	0.47
1:1:1170:A:H5''	3:3:102:G:O2'	2.15	0.47
1:1:2688:G:C6	1:1:2689:U:C4	3.03	0.47
1:1:2782:G:H2'	1:1:2783:G:C8	2.49	0.47
2:2:196:G:H2'	2:2:196:G:N3	2.30	0.47
2:2:384:U:O2'	9:AE:28:TRP:O	2.31	0.47
2:2:1136:C:H2'	2:2:1137:G:H8	1.80	0.47
6:AB:142:ASP:H	6:AB:145:ASN:HD22	1.63	0.47
54:BF:75:ILE:HA	54:BF:78:MET:HE3	1.97	0.47
1:1:117:G:C5	1:1:118:U:C5	3.02	0.47
1:1:523:C:O2	1:1:523:C:H2'	2.13	0.47
1:1:2060:C:OP1	33:BB:226:LYS:NZ	2.48	0.47
2:2:29:C:H2'	2:2:30:C:C6	2.50	0.47
2:2:1038:U:C2	2:2:1039:A:C8	3.03	0.47
10:AF:72:VAL:HG13	10:AF:79:ARG:HB3	1.97	0.47
11:AG:61:MET:HG2	11:AG:121:VAL:HG22	1.97	0.47
52:Bj:14:CYS:O	52:Bj:16:ARG:HD3	2.15	0.47
1:1:171:C:P	39:Bf:15:LYS:HD3	2.55	0.47
1:1:683:A:O2'	1:1:769:C:H5''	2.14	0.47
1:1:1269:U:OP1	1:1:1290:U:O2'	2.30	0.47
1:1:2645:U:H2'	1:1:2646:G:C8	2.50	0.47
1:1:2919:G:H2'	1:1:2920:U:C6	2.50	0.47
2:2:425:U:H3'	2:2:426:G:C8	2.50	0.47
11:AG:68:ASP:HA	11:AG:116:ILE:HA	1.95	0.47
22:AS:30:HIS:O	22:AS:34:LYS:HG2	2.15	0.47
53:BD:75:THR:O	53:BD:78:ARG:HG2	2.15	0.47
60:BN:56:GLN:NE2	60:BN:125:ARG:HH21	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:90:C:H2'	1:1:91:4AC:H6	1.96	0.46
1:1:715:A:H2'	1:1:716:A:C8	2.50	0.46
1:1:992:C:H3'	1:1:993:U:H4'	1.96	0.46
1:1:1336:U:H2'	1:1:1337:U:C6	2.50	0.46
1:1:1698:A:H2'	1:1:1699:G:H8	1.79	0.46
1:1:1783:G:H2'	1:1:1784:U:C6	2.50	0.46
1:1:2272:C:OP1	1:1:2686:G:O2'	2.30	0.46
1:1:2358:U:H3	1:1:2388:G:H1'	1.80	0.46
1:1:2913:C:H5'	36:BC:325:PRO:HA	1.97	0.46
2:2:122:C:OP1	2:2:571:C:O2'	2.25	0.46
2:2:191:U:H2'	2:2:192:G:O4'	2.14	0.46
2:2:465:G:H2'	2:2:466:G:H8	1.78	0.46
2:2:1425:G:H2'	2:2:1426:A:H8	1.80	0.46
11:AG:12:LYS:HD3	11:AG:12:LYS:H	1.80	0.46
21:AR:22:PRO:HD3	21:AR:101:VAL:HG21	1.96	0.46
22:AS:23:GLU:OE2	22:AS:34:LYS:HE2	2.15	0.46
35:BO:52:ASP:HB3	35:BO:55:GLY:O	2.14	0.46
43:BE:25:ILE:HG13	43:BE:25:ILE:O	2.14	0.46
52:Bj:3:TYR:HB3	52:Bj:91:LEU:HD23	1.96	0.46
1:1:776:G:H2'	1:1:2270:C:C5	2.50	0.46
1:1:855:C:H2'	1:1:856:G:O4'	2.14	0.46
1:1:953:G:H1'	1:1:976:A:N6	2.30	0.46
1:1:1142:A:H4'	1:1:1143:A:C8	2.50	0.46
1:1:1437:C:H2'	1:1:1438:G:H8	1.80	0.46
1:1:1591:A:H2'	1:1:1593:C:C5	2.50	0.46
1:1:2162:5MC:H2'	1:1:2163:5MC:C6	2.50	0.46
1:1:2881:G:H2'	1:1:2882:C:C6	2.50	0.46
2:2:233:G:H2'	2:2:234:A:C8	2.50	0.46
2:2:541:G:O2'	2:2:788:G:H5'	2.15	0.46
2:2:688:A:H4'	2:2:689:G:O5'	2.13	0.46
5:AA:67:LEU:HD12	5:AA:83:PHE:HE1	1.79	0.46
30:B4:33:ARG:HB3	30:B4:38:GLU:HG3	1.97	0.46
1:1:120:A:H5''	1:1:120:A:C8	2.49	0.46
1:1:825:G:H4'	53:BD:42:ARG:HB3	1.97	0.46
1:1:1362:G:O2'	1:1:1363:U:H5'	2.16	0.46
1:1:1549:C:H2'	1:1:1550:4AC:H6	1.97	0.46
1:1:1570:G:OP2	1:1:1570:G:N2	2.44	0.46
1:1:2353:C:H42	1:1:2359:A:H62	1.63	0.46
1:1:2545:4AC:O7	1:1:2545:4AC:H5	2.14	0.46
1:1:2889:U:H2'	1:1:2890:A:H8	1.79	0.46
2:2:1066:A:H4'	2:2:1067:A:O5'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1123:C:H2'	2:2:1124:U:C6	2.50	0.46
11:AG:61:MET:HE2	11:AG:61:MET:HB3	1.82	0.46
18:AN:132:VAL:HG21	18:AN:145:PRO:HD3	1.96	0.46
23:AU:30:GLU:H	23:AU:30:GLU:HG3	1.61	0.46
44:Ba:25:TRP:CZ2	44:Ba:26:LYS:HD3	2.51	0.46
1:1:864:G:H2'	1:1:865:C:O4'	2.15	0.46
1:1:892:G:N2	1:1:894:A:H3'	2.31	0.46
1:1:917:A:H2'	1:1:919:A:H62	1.80	0.46
1:1:1425:G:H2'	1:1:1426:A:C8	2.51	0.46
1:1:2242:C:O2'	44:Ba:24:ARG:NH2	2.48	0.46
1:1:2547:C:H2'	1:1:2548:4AC:H6	1.98	0.46
2:2:888:G:H2'	2:2:889:A:C8	2.51	0.46
2:2:1241:A:H2'	2:2:1242:A:C8	2.50	0.46
6:AB:24:LYS:HB3	6:AB:24:LYS:HE3	1.71	0.46
6:AB:133:ILE:HG13	6:AB:135:ILE:HG23	1.96	0.46
44:Ba:1:MET:H2	44:Ba:2:PRO:HD3	1.79	0.46
1:1:29:U:H2'	1:1:30:G:H8	1.81	0.46
1:1:352:G:H5''	1:1:354:G:N7	2.30	0.46
1:1:1085:U:C4	1:1:1086:G:N7	2.84	0.46
1:1:1363:U:O2'	1:1:1364:C:OP1	2.33	0.46
1:1:2612:A:O3'	35:BO:30:SER:HB3	2.16	0.46
1:1:2655:G:OP2	52:Bj:82:ARG:NH1	2.49	0.46
2:2:729:G:H2'	2:2:730:C:C6	2.51	0.46
2:2:836:A:H2'	2:2:837:G:C8	2.50	0.46
2:2:1180:G:H2'	2:2:1181:C:H6	1.80	0.46
28:AZ:64:GLU:CD	28:AZ:67:ARG:HH22	2.23	0.46
32:AO:22:ARG:HD2	32:AO:33:ILE:HD11	1.97	0.46
38:BL:44:LYS:HG3	38:BL:47:TRP:CB	2.45	0.46
50:BQ:56:LYS:O	50:BQ:56:LYS:HG2	2.14	0.46
1:1:42:U:H4'	1:1:43:A:H5'	1.97	0.46
1:1:215:G:C2	40:BU:111:ARG:HG3	2.50	0.46
1:1:673:C:H2'	1:1:674:G:H8	1.81	0.46
1:1:974:G:OP1	50:BQ:92:LYS:NZ	2.35	0.46
1:1:1422:A:H2'	1:1:1423:C:C6	2.51	0.46
1:1:1618:G:H2'	1:1:1619:C:H6	1.81	0.46
1:1:1710:C:H2'	1:1:1711:G:C8	2.44	0.46
1:1:2108:G:N1	1:1:2130:A:OP2	2.49	0.46
1:1:2788:C:C2	1:1:2789:A:C8	3.04	0.46
2:2:244:G:H2'	2:2:245:G:C8	2.51	0.46
3:3:125:A:H2'	3:3:126:C:C6	2.51	0.46
4:H:387:LYS:CA	66:sd:12:A:H4'	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AF:63:GLN:HG2	10:AF:89:VAL:HG12	1.98	0.46
14:AJ:76:ARG:HE	14:AJ:76:ARG:HB3	1.64	0.46
1:1:120:A:C8	1:1:120:A:C5'	2.98	0.46
1:1:288:G:C4	1:1:317:A:N1	2.84	0.46
1:1:634:A:H5''	40:BU:91:VAL:HG21	1.97	0.46
1:1:1780:4AC:O7	1:1:1780:4AC:H5	2.15	0.46
2:2:24:U:H2'	2:2:25:C:H6	1.76	0.46
2:2:711:A:H4'	2:2:823:G:O2'	2.16	0.46
2:2:805:C:H5''	25:AW:53:LYS:HG3	1.97	0.46
4:H:50:LEU:HD12	4:H:50:LEU:HA	1.85	0.46
5:AA:107:ILE:HG12	5:AA:121:MET:HG3	1.98	0.46
5:AA:153:LEU:HG	5:AA:157:ASP:HB3	1.96	0.46
56:BP:88:THR:HG23	56:BP:91:ARG:HH21	1.81	0.46
30:B4:121:LEU:HG	30:B4:122:MET:H	1.81	0.46
1:1:431:G:H2'	1:1:432:A:H8	1.80	0.46
1:1:2356:C:H42	1:1:2411:A:H61	1.62	0.46
2:2:27:U:H2'	2:2:28:G:O4'	2.16	0.46
2:2:1427:G:H2'	2:2:1428:G:H8	1.81	0.46
20:AQ:33:ILE:HD11	20:AQ:60:ILE:HG21	1.97	0.46
53:BD:149:GLN:HA	53:BD:207:ILE:HB	1.98	0.46
55:BZ:42:PRO:HG2	55:BZ:45:ILE:HD12	1.98	0.46
63:BJ:107:VAL:HG12	63:BJ:108:THR:O	2.15	0.46
1:1:45:G:H2'	1:1:46:C:C6	2.51	0.46
1:1:107:G:C2	1:1:113:G:C6	3.04	0.46
1:1:271:A:H2'	1:1:272:G:H4'	1.97	0.46
1:1:1285:G:C6	1:1:1380:G:N2	2.84	0.46
1:1:1302:G:H8	1:1:1365:G:C2	2.34	0.46
1:1:1303:A:H1'	1:1:1304:C:H5'	1.98	0.46
2:2:1180:G:H2'	2:2:1181:C:C6	2.51	0.46
3:3:30:C:H5'	43:BE:149:ARG:HD3	1.98	0.46
37:B5:45:ARG:NH2	37:B5:66:ALA:O	2.43	0.46
53:BD:4:LYS:HA	53:BD:15:GLU:HA	1.97	0.46
1:1:181:U:H1'	1:1:202:G:N2	2.31	0.46
1:1:567:A:H2'	1:1:568:U:C6	2.51	0.46
1:1:1086:G:C4	1:1:1087:G:C8	3.04	0.46
1:1:1320:U:H2'	1:1:1321:U:O4'	2.16	0.46
1:1:1788:A:C4	1:1:1789:G:C8	3.03	0.46
1:1:1858:C:H2'	1:1:1859:C:H6	1.80	0.46
2:2:903:C:H2'	2:2:904:A:C8	2.51	0.46
2:2:998:C:H2'	2:2:999:G:C8	2.51	0.46
2:2:1326:C:H2'	2:2:1327:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AD:94:SER:HG	10:AF:161:ARG:HH21	1.59	0.46
31:AT:32:GLN:HG3	31:AT:71:ILE:HD12	1.98	0.46
48:BI:6:ALA:HA	48:BI:9:LEU:HD12	1.97	0.46
37:BK:23:VAL:HG23	37:BK:82:LEU:HD21	1.98	0.46
63:BJ:86:ARG:HE	63:BJ:101:ASP:HA	1.81	0.46
30:B4:27:ARG:NH2	30:B4:89:ALA:O	2.38	0.46
1:1:91:4AC:O7	1:1:91:4AC:H5	2.15	0.45
1:1:117:G:C6	1:1:118:U:C5	3.04	0.45
1:1:880:G:H22	1:1:1096:G:P	2.39	0.45
1:1:2193:A:C6	63:BJ:41:ILE:HG13	2.51	0.45
1:1:2482:G:C4	1:1:2483:G:C8	3.04	0.45
1:1:2970:A:H2'	1:1:2971:A:C8	2.51	0.45
2:2:109:C:H2'	2:2:110:U:C6	2.51	0.45
2:2:1339:C:H2'	2:2:1340:G:C8	2.51	0.45
2:2:1502:C:H2'	2:2:1503:A:C8	2.51	0.45
3:3:121:G:H2'	3:3:122:G:H8	1.80	0.45
4:H:113:ILE:HD11	4:H:118:LEU:HD12	1.98	0.45
10:AF:33:ASP:OD2	10:AF:35:HIS:ND1	2.27	0.45
16:AL:40:LEU:HB2	16:AL:70:LYS:HB2	1.99	0.45
32:AO:61:LYS:HE2	32:AO:65:ILE:HD11	1.98	0.45
30:BG:122:MET:HE3	30:BG:122:MET:HB2	1.80	0.45
56:BP:29:ILE:O	56:BP:33:ILE:HG12	2.16	0.45
30:B4:65:HIS:O	30:B4:68:PRO:HG2	2.17	0.45
1:1:1161:A:H2'	1:1:1164:C:C5	2.51	0.45
1:1:1787:A:H1'	1:1:1828:C:H1'	1.97	0.45
2:2:456:C:H2'	2:2:457:G:H8	1.81	0.45
2:2:896:G:C2	2:2:898:G:C8	3.04	0.45
6:AB:86:VAL:HG13	6:AB:87:THR:HG23	1.98	0.45
10:AF:224:VAL:HG11	10:AF:228:ALA:HA	1.98	0.45
14:AJ:21:ARG:NH2	14:AJ:27:GLU:OE2	2.47	0.45
1:1:2375:A:H3'	1:1:2376:G:C8	2.51	0.45
2:2:183:U:H2'	2:2:184:G:C8	2.49	0.45
2:2:1375:G:H2'	2:2:1376:OMC:O4'	2.16	0.45
31:AT:82:TYR:CE1	31:AT:91:PRO:HB3	2.52	0.45
43:BE:185:GLU:HG2	43:BE:186:GLU:N	2.31	0.45
51:BV:57:GLN:HA	51:BV:60:ARG:HG2	1.98	0.45
1:1:909:C:H2'	1:1:910:G:C8	2.51	0.45
1:1:1710:C:H4'	50:BQ:92:LYS:HE2	1.97	0.45
1:1:2416:G:H2'	1:1:2417:C:C6	2.52	0.45
2:2:244:G:H2'	2:2:245:G:H8	1.82	0.45
2:2:425:U:H3'	2:2:426:G:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:618:C:OP1	20:AQ:75:LYS:HG2	2.16	0.45
2:2:889:A:H2'	2:2:890:A:C8	2.52	0.45
2:2:991:G:H2'	2:2:992:U:C6	2.51	0.45
2:2:1182:C:H2'	2:2:1183:C:H6	1.82	0.45
2:2:1346:C:H2'	2:2:1347:G:O4'	2.16	0.45
4:H:383:ARG:CZ	4:H:383:ARG:HB2	2.44	0.45
4:H:384:PHE:O	4:H:384:PHE:CD1	2.69	0.45
12:AH:38:ASN:HB3	12:AH:62:HIS:HA	1.99	0.45
53:BD:83:VAL:HG23	53:BD:86:ALA:HB2	1.99	0.45
1:1:377:C:O2'	1:1:422:C:H5''	2.17	0.45
1:1:1093:C:H2'	1:1:1094:C:H6	1.80	0.45
1:1:1761:G:O4'	1:1:1763:G:H1'	2.16	0.45
1:1:2353:C:N4	1:1:2359:A:H62	2.14	0.45
1:1:2693:C:H2'	1:1:2694:U:C6	2.52	0.45
2:2:911:G:H2'	2:2:912:G:C8	2.52	0.45
2:2:1254:A:O2'	2:2:1255:U:H5'	2.16	0.45
10:AF:39:ARG:HH22	10:AF:209:ASN:ND2	2.14	0.45
10:AF:132:GLU:HG3	10:AF:160:PRO:HG3	1.98	0.45
15:AK:49:LEU:HD23	15:AK:86:LEU:HD11	1.99	0.45
17:AM:52:ARG:O	17:AM:55:PRO:HD2	2.17	0.45
20:AQ:38:VAL:O	20:AQ:42:LYS:HG2	2.16	0.45
55:BZ:34:LEU:HD12	55:BZ:35:ILE:N	2.32	0.45
55:BZ:59:PRO:HB2	55:BZ:97:ALA:HB1	1.99	0.45
30:B4:21:GLN:O	30:B4:25:ILE:HG12	2.16	0.45
1:1:552:G:OP2	57:BM:68:ARG:NH2	2.43	0.45
1:1:587:A:C6	1:1:588:C:C4	3.04	0.45
1:1:684:G:H4'	1:1:685:G:C8	2.51	0.45
1:1:1558:G:N2	1:1:1914:A:N7	2.64	0.45
1:1:2187:U:H2'	1:1:2188:C:C6	2.52	0.45
1:1:2304:C:H2'	1:1:2305:C:H6	1.82	0.45
1:1:2341:G:N2	1:1:2429:C:N3	2.65	0.45
1:1:2456:C:C2	1:1:2457:A:C8	3.04	0.45
1:1:2475:U:H5''	1:1:2476:G:H5'	1.99	0.45
2:2:389:G:N2	2:2:392:A:OP2	2.44	0.45
2:2:1405:U:H2'	2:2:1406:G:O4'	2.16	0.45
11:AG:11:PRO:HG3	11:AG:122:LYS:HE3	1.99	0.45
24:AV:40:LEU:HD23	24:AV:40:LEU:HA	1.85	0.45
1:1:70:A:H2'	1:1:71:G:C8	2.51	0.45
1:1:310:U:H2'	1:1:311:A:H8	1.81	0.45
1:1:431:G:P	1:1:431:G:H8	2.39	0.45
1:1:1434:G:H2'	1:1:1435:U:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1449:G:H2'	1:1:1450:G:C8	2.51	0.45
1:1:2721:G:N3	1:1:2723:C:N4	2.60	0.45
1:1:2804:A:O5'	1:1:2806:G:H4'	2.17	0.45
2:2:35:G:O2'	2:2:305:U:OP1	2.34	0.45
2:2:322:A:H2'	2:2:323:G:C8	2.52	0.45
3:3:23:G:N2	3:3:61:C:C2	2.84	0.45
13:AI:115:GLU:HA	13:AI:118:GLU:HG2	1.99	0.45
21:AR:60:TYR:O	21:AR:61:GLU:HG2	2.15	0.45
39:Bf:20:ASN:ND2	39:Bf:42:ARG:H	2.14	0.45
54:BF:89:LYS:HB3	54:BF:138:ILE:HD13	1.99	0.45
54:BF:158:THR:HG21	54:BF:171:GLY:HA2	1.99	0.45
61:Bg:15:TYR:O	61:Bg:24:ASN:N	2.46	0.45
30:B4:42:ALA:HB1	30:B4:102:ILE:HD11	1.98	0.45
1:1:710:C:H2'	1:1:711:C:H6	1.81	0.45
1:1:871:G:H2'	1:1:872:C:C6	2.51	0.45
1:1:1086:G:H1'	1:1:2592:G:C8	2.51	0.45
1:1:2717:C:P	60:BN:58:ARG:HH21	2.39	0.45
1:1:2725:U:H2'	1:1:2726:G:O4'	2.16	0.45
1:1:2871:A:H2'	1:1:2872:G:O4'	2.17	0.45
1:1:2929:U:H2'	1:1:2930:G:C8	2.51	0.45
2:2:892:U:H2'	2:2:893:G:O4'	2.17	0.45
2:2:930:A:C5	31:AT:87:LYS:HD2	2.51	0.45
2:2:1037:G:C5	2:2:1038:U:C4	3.05	0.45
6:AB:158:ASN:OD1	6:AB:159:LYS:NZ	2.47	0.45
9:AE:30:VAL:HG21	9:AE:46:LEU:HD23	1.98	0.45
17:AM:39:ILE:HG23	17:AM:74:LYS:HD2	1.99	0.45
28:AZ:20:PHE:HD1	28:AZ:21:LEU:HD12	1.82	0.45
30:A3:107:ALA:H	30:A3:108:ARG:HH21	1.65	0.45
36:BC:199:LYS:HA	36:BC:202:LYS:HD3	1.99	0.45
39:Bf:21:ARG:O	39:Bf:38:HIS:HE1	2.00	0.45
43:BE:3:ILE:HG21	43:BE:185:GLU:HB3	1.97	0.45
50:BQ:93:GLU:CD	50:BQ:93:GLU:H	2.25	0.45
55:BZ:40:ASN:HB2	55:BZ:66:THR:HA	1.98	0.45
1:1:959:C:H5''	50:BQ:125:ILE:CG2	2.47	0.45
1:1:1206:G:H2'	1:1:1207:G:H8	1.82	0.45
1:1:2169:A:H2'	1:1:2170:G:O4'	2.17	0.45
1:1:2326:U:H2'	1:1:2327:G:C8	2.48	0.45
2:2:153:C:O2'	11:AG:18:GLN:HB2	2.17	0.45
2:2:662:A:H2'	2:2:663:A:C8	2.52	0.45
2:2:1446:U:H2'	2:2:1447:C:C6	2.51	0.45
4:H:221:ILE:HD13	4:H:221:ILE:HA	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AH:46:HIS:HD2	15:AK:40:ILE:HD11	1.81	0.45
17:AM:32:ASP:OD1	17:AM:34:THR:OG1	2.33	0.45
19:AP:20:ARG:HD3	19:AP:27:TYR:CZ	2.51	0.45
30:A3:18:LYS:NZ	30:A3:110:LEU:O	2.49	0.45
32:AO:46:ASP:O	32:AO:49:MET:HG2	2.17	0.45
33:BB:75:GLU:HG3	47:Bi:65:GLY:HA2	1.98	0.45
43:BE:120:HIS:O	43:BE:126:VAL:HG11	2.16	0.45
60:BN:35:ASP:OD1	60:BN:85:LYS:HD3	2.17	0.45
1:1:51:A:HO2'	1:1:2005:G:HO2'	1.63	0.45
1:1:385:C:H2'	1:1:386:G:C8	2.51	0.45
1:1:750:G:H2'	1:1:751:G:C8	2.52	0.45
1:1:1096:G:N2	1:1:1186:G:H1'	2.32	0.45
1:1:1779:C:H2'	1:1:1780:4AC:H6	1.98	0.45
1:1:1806:G:C8	1:1:1809:A:C8	3.05	0.45
1:1:2001:4AC:O7	1:1:2001:4AC:H5	2.16	0.45
1:1:2341:G:O2'	1:1:2342:C:O5'	2.34	0.45
1:1:2484:C:H2'	1:1:2485:G:O4'	2.16	0.45
2:2:106:C:H2'	2:2:107:G:O4'	2.17	0.45
2:2:120:G:H2'	2:2:121:U:C6	2.52	0.45
2:2:428:C:H2'	2:2:429:A:C8	2.43	0.45
2:2:913:OMG:OP1	12:AH:73:ARG:HB2	2.16	0.45
2:2:1212:A:H5'	12:AH:175:ARG:HG2	1.98	0.45
12:AH:8:ARG:HH22	23:AU:10:ASP:CG	2.25	0.45
27:AY:22:CYS:HB2	27:AY:25:CYS:HB2	1.99	0.45
35:BO:112:VAL:HG22	35:BO:115:SER:HB3	1.99	0.45
36:BC:211:LYS:O	36:BC:214:GLU:HG2	2.17	0.45
60:BN:142:LEU:O	60:BN:146:ILE:HG12	2.17	0.45
30:B4:104:PRO:HB3	30:B4:111:VAL:HG11	1.99	0.45
30:B4:107:ALA:HB1	30:B4:110:LEU:HB2	1.99	0.45
1:1:43:A:H2'	1:1:44:A:C8	2.51	0.44
1:1:46:C:H2'	1:1:47:G:H8	1.83	0.44
1:1:704:G:H8	1:1:704:G:OP2	2.00	0.44
1:1:1259:A:N6	62:Bc:14:LYS:HB2	2.31	0.44
1:1:1371:C:H4'	60:BN:177:LEU:HB3	1.99	0.44
1:1:2087:G:H2'	1:1:2088:C:H6	1.81	0.44
1:1:2678:OMG:N3	1:1:2733:5MC:HM52	2.32	0.44
2:2:661:A:H4'	17:AM:52:ARG:HH11	1.82	0.44
2:2:922:U:H2'	2:2:923:G:H8	1.82	0.44
12:AH:75:GLY:O	12:AH:86:MET:HB2	2.17	0.44
28:AZ:129:GLU:HB2	28:AZ:151:LEU:HD22	1.99	0.44
35:BO:104:LEU:HD22	35:BO:121:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BL:102:ILE:HG23	38:BL:123:VAL:HG22	1.99	0.44
24:B6:1:MET:O	24:B6:39:LYS:NZ	2.43	0.44
60:BN:83:HIS:HD2	60:BN:136:ARG:HE	1.65	0.44
1:1:146:C:O2'	1:1:147:U:H5'	2.17	0.44
1:1:534:G:H2'	1:1:535:U:C6	2.52	0.44
1:1:1068:4AC:O7	1:1:1068:4AC:H5	2.17	0.44
1:1:2164:U:H2'	1:1:2165:C:H6	1.83	0.44
1:1:2804:A:OP2	1:1:2804:A:H8	2.00	0.44
2:2:417:C:H2'	2:2:418:G:H8	1.81	0.44
2:2:504:G:H2'	2:2:505:G:C8	2.51	0.44
3:3:13:A:N1	3:3:69:G:O2'	2.50	0.44
5:AA:27:PHE:CD1	5:AA:156:LYS:HD2	2.52	0.44
10:AF:39:ARG:HH22	10:AF:209:ASN:HD22	1.66	0.44
15:AK:80:ILE:HG22	15:AK:106:MET:HA	1.99	0.44
22:AS:17:PHE:CE1	22:AS:58:VAL:HG12	2.53	0.44
43:BE:120:HIS:CD2	43:BE:134:ILE:HA	2.52	0.44
1:1:361:A:C4	1:1:362:G:C8	3.05	0.44
1:1:1073:C:C2	1:1:1074:A:N7	2.85	0.44
1:1:1436:C:OP2	41:Bb:69:ARG:NH2	2.49	0.44
1:1:1648:C:H2'	1:1:1649:G:C8	2.52	0.44
1:1:2480:G:O2'	1:1:2728:U:OP1	2.20	0.44
1:1:2796:A:C8	1:1:2881:G:H5'	2.53	0.44
2:2:344:C:H2'	2:2:345:C:C6	2.53	0.44
2:2:684:C:O2'	2:2:701:C:O4'	2.29	0.44
2:2:877:G:N7	29:A0:2:LYS:NZ	2.60	0.44
2:2:1152:G:N2	2:2:1155:G:OP2	2.49	0.44
6:AB:169:TRP:CE3	6:AB:170:ILE:HG22	2.49	0.44
23:AU:63:TYR:CE2	23:AU:126:ARG:HG3	2.52	0.44
30:A3:43:VAL:HG21	30:A3:66:LEU:HD11	2.00	0.44
24:B6:88:ILE:HD11	56:BP:108:LYS:HD2	2.00	0.44
30:B4:15:LEU:HD13	30:B4:117:LYS:HD2	1.99	0.44
1:1:157:G:H2'	1:1:158:C:C6	2.53	0.44
1:1:1402:G:O2'	64:Bl:49:ARG:NE	2.46	0.44
1:1:1909:A:H2'	1:1:1910:G:H8	1.82	0.44
1:1:2394:G:H2'	1:1:2395:U:C6	2.53	0.44
2:2:1341:C:OP1	15:AK:120:ASN:N	2.48	0.44
9:AE:166:MET:SD	9:AE:171:ARG:HG3	2.57	0.44
35:BO:63:HIS:CD2	35:BO:65:ARG:H	2.35	0.44
50:BQ:123:LEU:HD11	50:BQ:142:LEU:HD21	2.00	0.44
56:BP:6:PRO:HB3	56:BP:11:LEU:HD23	1.99	0.44
60:BN:97:ASN:HD22	60:BN:98:PRO:CD	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B4:70:CYS:SG	30:B4:71:GLU:N	2.91	0.44
1:1:120:A:C5'	1:1:120:A:H8	2.31	0.44
1:1:431:G:H2'	1:1:432:A:C8	2.53	0.44
1:1:433:G:H2'	1:1:434:A:C8	2.53	0.44
1:1:973:U:H2'	1:1:974:G:C8	2.53	0.44
1:1:1431:U:O2	56:BP:7:THR:HG23	2.17	0.44
1:1:2047:A:N6	1:1:2084:G:O2'	2.44	0.44
1:1:2393:G:H2'	1:1:2394:G:C8	2.53	0.44
1:1:2858:U:H3	1:1:3007:A:H62	1.66	0.44
2:2:193:G:H22	21:AR:29:ILE:HG13	1.82	0.44
4:H:34:ASP:N	4:H:35:PRO:HD3	2.32	0.44
5:AA:141:ILE:HD13	5:AA:174:GLU:HG3	1.99	0.44
38:BL:91:LYS:HD3	38:BL:91:LYS:HA	1.82	0.44
43:BE:102:LEU:O	43:BE:183:ILE:HA	2.18	0.44
43:BE:108:ASP:OD2	43:BE:112:ASN:HB2	2.17	0.44
58:BS:29:PRO:HG3	58:BS:144:THR:HG22	1.99	0.44
64:BL:67:ASP:HB3	64:BL:70:VAL:HG22	1.99	0.44
1:1:298:G:H4'	38:BL:34:ARG:HD3	1.98	0.44
1:1:517:G:H2'	1:1:518:G:H8	1.83	0.44
1:1:727:G:N2	1:1:730:A:OP2	2.38	0.44
1:1:1254:C:H2'	1:1:1261:G:C8	2.52	0.44
1:1:1616:C:H2'	1:1:1617:4AC:H6	1.99	0.44
1:1:1739:G:O2'	1:1:1816:U:O2'	2.21	0.44
1:1:2664:A:O2'	1:1:2665:A:H2'	2.18	0.44
1:1:2698:G:OP1	61:Bg:19:ARG:NH1	2.41	0.44
2:2:692:G:OP1	2:2:824:G:N2	2.36	0.44
2:2:703:4AC:O7	2:2:703:4AC:H5	2.17	0.44
2:2:1301:G:H2'	2:2:1302:C:C6	2.53	0.44
4:H:387:LYS:CD	4:H:387:LYS:N	2.80	0.44
12:AH:58:LYS:NZ	12:AH:159:ASP:OD2	2.48	0.44
1:1:40:U:H2'	1:1:41:G:O4'	2.18	0.44
1:1:141:G:O2'	1:1:142:A:OP2	2.33	0.44
1:1:953:G:N2	1:1:975:G:O2'	2.49	0.44
1:1:1065:4AC:H2'	1:1:1066:G:H8	1.82	0.44
1:1:1084:A:N6	1:1:1198:A:H2	2.16	0.44
1:1:1222:4AC:O7	1:1:1222:4AC:H5	2.17	0.44
1:1:1878:4AC:O7	1:1:1878:4AC:H5	2.16	0.44
1:1:2046:C:O2'	33:BB:175:ALA:HB2	2.17	0.44
2:2:1417:U:H2'	2:2:1418:C:C6	2.53	0.44
32:AO:23:TRP:O	32:AO:26:THR:OG1	2.31	0.44
43:BE:10:GLU:H	43:BE:10:GLU:HG2	1.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:BG:113:GLU:O	30:BG:117:LYS:HG2	2.17	0.44
55:BZ:55:LEU:HD12	55:BZ:55:LEU:HA	1.84	0.44
1:1:9:C:O2	1:1:85:A:O2'	2.34	0.44
1:1:285:A:H2'	1:1:286:A:C8	2.51	0.44
1:1:614:A:H2'	1:1:615:OMC:O4'	2.18	0.44
1:1:1426:A:OP1	56:BP:23:ASN:ND2	2.47	0.44
1:1:2056:C:O4'	1:1:2058:A:C8	2.71	0.44
1:1:2267:G:H2'	1:1:2268:C:C6	2.52	0.44
2:2:105:A:H5'	2:2:106:C:C5	2.53	0.44
2:2:1420:U:O2'	2:2:1423:G:O6	2.31	0.44
3:3:34:G:C2	3:3:44:G:C6	3.05	0.44
10:AF:54:LEU:HD21	10:AF:91:ASN:HB3	1.99	0.44
34:BY:3:LYS:HA	34:BY:3:LYS:HD3	1.77	0.44
40:BU:41:ILE:HG22	40:BU:119:ARG:HB3	1.99	0.44
46:BW:67:LYS:HE3	46:BW:67:LYS:HB3	1.65	0.44
1:1:102:C:OP2	1:1:102:C:C6	2.71	0.44
1:1:433:G:H2'	1:1:434:A:H8	1.83	0.44
1:1:589:G:C4	1:1:591:C:N4	2.86	0.44
1:1:802:4AC:H5	1:1:802:4AC:O7	2.18	0.44
1:1:1144:G:O2'	1:1:1145:C:H5''	2.18	0.44
1:1:1171:C:H2'	1:1:1172:C:H6	1.82	0.44
1:1:1187:A:H2'	1:1:1188:U:C6	2.53	0.44
1:1:1575:A:H2'	1:1:1576:C:H6	1.82	0.44
1:1:1979:G:H2'	1:1:1980:G:C8	2.52	0.44
1:1:2975:C:OP1	54:BF:177:LYS:NZ	2.46	0.44
4:H:98:ARG:NE	4:H:240:ASP:OD2	2.47	0.44
5:AA:52:THR:HG22	5:AA:54:LYS:H	1.83	0.44
8:AD:153:THR:OG1	8:AD:154:TYR:N	2.51	0.44
11:AG:44:GLY:O	11:AG:45:ILE:HG13	2.17	0.44
33:BB:89:ALA:O	33:BB:97:LEU:HD21	2.18	0.44
57:BM:43:THR:OG1	57:BM:129:GLU:OE2	2.28	0.44
1:1:132:C:H2'	1:1:133:G:C8	2.53	0.43
1:1:1084:A:H2'	1:1:1085:U:C6	2.52	0.43
1:1:1508:G:N7	38:BL:9:ARG:NH2	2.66	0.43
1:1:1516:U:H2'	1:1:1517:G:H8	1.83	0.43
1:1:1699:G:H2'	1:1:1700:G:C8	2.53	0.43
1:1:2393:G:H2'	1:1:2394:G:H8	1.83	0.43
1:1:2589:A:O2'	49:BR:79:ASP:OD2	2.35	0.43
1:1:2907:C:H2'	1:1:2908:4AC:H6	2.00	0.43
2:2:424:C:H4'	2:2:425:U:C5	2.53	0.43
12:AH:26:VAL:HB	12:AH:39:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A3:13:LYS:O	30:A3:17:GLU:HG2	2.18	0.43
42:Be:29:ASN:N	42:Be:34:TYR:O	2.48	0.43
30:BG:31:LYS:H	30:BG:103:GLU:HB3	1.82	0.43
60:BN:107:ARG:NH1	60:BN:108:TYR:OH	2.50	0.43
30:B4:8:LYS:H	30:B4:79:TYR:HE2	1.65	0.43
1:1:99:U:O4	1:1:120:A:N1	2.51	0.43
1:1:1983:G:C8	1:1:2012:G:C5	3.06	0.43
1:1:2287:4AC:O7	1:1:2287:4AC:H5	2.18	0.43
1:1:2698:G:H2'	1:1:2699:C:C6	2.52	0.43
1:1:2725:U:H4'	60:BN:103:ARG:HG2	2.01	0.43
1:1:2816:U:H2'	1:1:2817:U:H2'	2.00	0.43
2:2:479:4AC:O7	2:2:479:4AC:H5	2.19	0.43
2:2:820:C:C2	2:2:821:C:C5	3.06	0.43
2:2:893:G:H2'	2:2:894:G:H8	1.82	0.43
2:2:1052:C:H2'	2:2:1053:A:C8	2.52	0.43
4:H:116:MET:HE1	4:H:234:MET:HE3	2.00	0.43
14:AJ:63:ALA:HB2	14:AJ:77:ILE:HD11	2.01	0.43
27:AY:40:CYS:HB3	27:AY:44:GLY:H	1.84	0.43
29:A0:20:LYS:HE2	29:A0:24:ARG:NH2	2.33	0.43
30:A3:3:LYS:HD2	30:A3:60:GLU:HG2	2.00	0.43
36:BC:291:LYS:HB3	36:BC:298:GLU:OE2	2.18	0.43
46:BW:2:LYS:HB2	46:BW:5:GLU:OE1	2.17	0.43
63:BJ:116:THR:C	63:BJ:136:ILE:HD11	2.44	0.43
1:1:210:C:H2'	1:1:211:4AC:H6	1.99	0.43
1:1:877:U:H2'	1:1:878:G:O4'	2.18	0.43
1:1:1299:U:H4'	1:1:1303:A:H5''	2.00	0.43
1:1:1791:G:C6	1:1:1792:C:C4	3.06	0.43
1:1:2031:U:O4	1:1:2045:A:H2	2.01	0.43
1:1:2522:U:H2'	1:1:2523:C:C6	2.53	0.43
1:1:2653:A:H2'	1:1:2654:G:H8	1.83	0.43
1:1:2779:G:H22	1:1:2793:A:H2	1.65	0.43
1:1:2971:A:H2'	1:1:2972:G:O4'	2.18	0.43
2:2:68:A:C8	2:2:104:G:O2'	2.69	0.43
2:2:272:A:H2'	2:2:273:C:C6	2.53	0.43
2:2:433:C:H2'	2:2:434:U:C6	2.53	0.43
2:2:836:A:H5'	2:2:1043:U:H5	1.80	0.43
2:2:1161:G:O2'	19:AP:56:GLU:OXT	2.30	0.43
2:2:1479:4AC:O7	2:2:1479:4AC:H5	2.17	0.43
6:AB:142:ASP:H	6:AB:145:ASN:ND2	2.16	0.43
10:AF:61:GLU:H	10:AF:61:GLU:CD	2.27	0.43
28:AZ:65:LEU:HD23	28:AZ:80:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BC:55:ASP:C	36:BC:57:GLU:H	2.26	0.43
43:BE:137:MET:HE3	43:BE:137:MET:HB2	1.94	0.43
57:BM:126:LYS:HG2	57:BM:128:PHE:CE2	2.53	0.43
63:BJ:65:THR:HG23	63:BJ:67:LYS:HE3	1.99	0.43
63:BJ:85:GLN:HA	63:BJ:102:ASN:HD22	1.83	0.43
1:1:29:U:H2'	1:1:30:G:C8	2.53	0.43
1:1:217:A:C8	1:1:218:C:C5	3.07	0.43
1:1:320:A:C4	1:1:321:A:C8	3.06	0.43
1:1:1058:U:O2'	1:1:2300:A:N1	2.50	0.43
1:1:1253:G:H2'	1:1:1254:C:H6	1.82	0.43
1:1:1278:C:OP1	1:1:1281:C:N4	2.51	0.43
1:1:2495:4AC:OP1	49:BR:14:LYS:NZ	2.44	0.43
2:2:119:C:H2'	2:2:120:G:H8	1.82	0.43
2:2:361:C:H4'	2:2:363:G:OP1	2.18	0.43
2:2:636:4AC:O7	2:2:636:4AC:H5	2.17	0.43
2:2:1184:4AC:O7	2:2:1184:4AC:H5	2.17	0.43
2:2:1356:C:H4'	12:AH:140:MET:HE3	2.01	0.43
10:AF:131:TRP:HA	13:AI:97:PHE:HB3	2.00	0.43
12:AH:212:GLU:HG3	12:AH:215:ARG:NH1	2.33	0.43
32:AO:65:ILE:HG12	32:AO:72:HIS:HD2	1.81	0.43
36:BC:161:ARG:HD2	36:BC:181:GLU:OE2	2.19	0.43
1:1:216:A:C4	1:1:217:A:C8	3.06	0.43
1:1:435:C:H5'	65:Bk:4:LEU:HB2	2.00	0.43
1:1:533:4AC:O7	1:1:533:4AC:H5	2.18	0.43
1:1:728:C:H5''	37:BK:46:ARG:NH2	2.34	0.43
1:1:799:G:H2'	1:1:800:G:H8	1.82	0.43
1:1:922:4AC:O7	1:1:922:4AC:H5	2.19	0.43
1:1:1430:A:H4'	1:1:1431:U:H5'	1.99	0.43
1:1:1853:G:C2	1:1:1854:A:C5	3.06	0.43
1:1:2336:A:H2'	1:1:2337:C:H6	1.84	0.43
1:1:2455:A:H1'	1:1:2456:C:OP2	2.19	0.43
2:2:46:G:H2'	2:2:47:G:H8	1.82	0.43
2:2:628:G:N2	2:2:803:G:H4'	2.33	0.43
2:2:839:4AC:O7	2:2:839:4AC:H5	2.18	0.43
3:3:97:G:C2	3:3:98:G:C5	3.07	0.43
8:AD:162:ASN:HD22	8:AD:163:PRO:HD2	1.84	0.43
10:AF:64:GLU:HG2	10:AF:177:LEU:HD11	2.00	0.43
23:AU:75:THR:OG1	23:AU:92:LYS:NZ	2.37	0.43
23:AU:102:LEU:HD13	23:AU:119:ARG:HD3	1.99	0.43
28:AZ:188:ARG:HG3	28:AZ:192:GLU:HG3	1.99	0.43
24:B6:33:ARG:CZ	24:B6:89:ARG:HD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:99:U:H3	1:1:120:A:H2	1.66	0.43
1:1:134:C:H2'	1:1:135:C:H6	1.84	0.43
1:1:211:4AC:H5	1:1:211:4AC:O7	2.18	0.43
1:1:1154:C:H2'	1:1:1155:C:C6	2.53	0.43
1:1:1243:4AC:O7	1:1:1243:4AC:H5	2.19	0.43
1:1:1265:C:H2'	1:1:1266:G:C8	2.53	0.43
1:1:1617:4AC:H2'	1:1:1618:G:C8	2.53	0.43
1:1:1882:A:H1'	39:Bf:45:ARG:HH22	1.83	0.43
1:1:1901:G:C6	1:1:1914:A:C5	3.06	0.43
1:1:2081:G:OP1	33:BB:202:HIS:HE1	2.02	0.43
1:1:2200:G:C4	1:1:2201:A:C8	3.06	0.43
2:2:46:G:H2'	2:2:47:G:C8	2.53	0.43
2:2:332:U:H2'	2:2:333:G:O4'	2.18	0.43
2:2:379:4AC:O7	2:2:379:4AC:H5	2.19	0.43
2:2:484:G:O2'	4:H:324:LYS:O	2.32	0.43
2:2:819:G:H2'	2:2:820:C:H6	1.84	0.43
2:2:1231:G:N2	19:AP:13:LYS:O	2.50	0.43
2:2:1346:C:H5''	15:AK:72:MET:HB2	2.01	0.43
3:3:52:A:H62	35:BO:42:ASN:HD21	1.65	0.43
3:3:98:G:H5''	64:Bl:51:LYS:HE3	2.00	0.43
3:3:100:C:O2	34:BY:51:LYS:HE3	2.18	0.43
4:H:177:VAL:HG21	4:H:210:LEU:HD22	2.01	0.43
4:H:380:TYR:CD1	12:AH:146:TYR:HA	2.44	0.43
30:A3:52:ILE:O	30:A3:98:SER:HA	2.19	0.43
36:BC:85:ALA:HB1	36:BC:157:ILE:HD12	2.01	0.43
38:BL:110:ASP:OD1	38:BL:127:ARG:NH1	2.51	0.43
38:BL:138:LYS:HE3	38:BL:144:ALA:H	1.82	0.43
24:B6:14:ILE:H	24:B6:14:ILE:HG12	1.57	0.43
60:BN:168:GLU:HG2	60:BN:170:ASN:HD22	1.83	0.43
30:B4:8:LYS:HE2	30:B4:8:LYS:HB2	1.88	0.43
1:1:114:G:N3	1:1:115:G:C8	2.86	0.43
1:1:127:U:H2'	1:1:128:A:H8	1.83	0.43
1:1:166:A:H2'	1:1:167:A:C8	2.54	0.43
1:1:937:U:H2'	1:1:938:A:H8	1.83	0.43
1:1:1048:4AC:O2'	42:Be:51:TRP:O	2.31	0.43
1:1:1661:C:H2'	1:1:1662:4AC:H6	2.01	0.43
1:1:2071:U:O4'	1:1:2073:G:C8	2.71	0.43
1:1:2448:A:H2'	1:1:2449:G:O4'	2.18	0.43
1:1:2498:A:N3	1:1:2498:A:H2'	2.34	0.43
1:1:2534:G:O3'	43:BE:106:SER:HA	2.18	0.43
2:2:818:C:H2'	2:2:819:G:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1117:G:H2'	2:2:1118:G:C8	2.53	0.43
4:H:219:ILE:HG13	4:H:237:ASN:ND2	2.33	0.43
4:H:249:ASN:O	4:H:249:ASN:ND2	2.48	0.43
54:BF:45:LYS:HE2	54:BF:56:TYR:CD2	2.54	0.43
1:1:117:G:N2	1:1:118:U:H1'	2.34	0.43
1:1:720:A:H2'	1:1:721:A:C8	2.52	0.43
1:1:760:U:H2'	1:1:761:U:C6	2.54	0.43
1:1:762:G:H2'	1:1:763:C:H6	1.83	0.43
1:1:1516:U:OP1	53:BD:72:ARG:NH2	2.52	0.43
1:1:1594:4AC:O7	1:1:1594:4AC:H5	2.19	0.43
1:1:1615:C:H2'	1:1:1616:C:H6	1.84	0.43
1:1:1646:A:H1'	1:1:1667:4AC:H1'	2.01	0.43
1:1:2216:G:H2'	1:1:2217:U:O4'	2.19	0.43
1:1:2545:4AC:H2'	1:1:2546:G:H8	1.83	0.43
1:1:2908:4AC:O7	1:1:2908:4AC:H5	2.18	0.43
2:2:255:A:C2	2:2:291:A:C5	3.06	0.43
2:2:443:G:O2'	24:AV:30:THR:O	2.35	0.43
2:2:854:C:O2'	2:2:855:U:H5'	2.19	0.43
2:2:1234:G:O2'	2:2:1249:A:N6	2.52	0.43
4:H:117:ALA:O	4:H:120:GLU:HG3	2.18	0.43
5:AA:121:MET:O	5:AA:187:ARG:N	2.50	0.43
16:AL:3:LYS:HA	16:AL:76:GLU:HA	2.01	0.43
20:AQ:41:ARG:HG2	20:AQ:87:LEU:HD12	2.01	0.43
26:AX:4:ASP:HB3	26:AX:5:GLU:H	1.57	0.43
34:BY:100:VAL:HA	34:BY:105:MET:O	2.19	0.43
34:BY:105:MET:HB2	34:BY:109:ASP:OD2	2.19	0.43
36:BC:151:MET:HG2	36:BC:157:ILE:HG12	2.00	0.43
54:BF:90:LEU:HB2	54:BF:137:ILE:HB	2.00	0.43
24:B6:19:ILE:HD13	24:B6:44:LEU:HD12	2.00	0.43
57:BM:20:GLY:O	57:BM:24:LYS:HG2	2.19	0.43
57:BM:64:VAL:HG21	57:BM:104:ALA:HB2	1.99	0.43
1:1:40:U:OP1	51:BV:36:LYS:HD2	2.19	0.43
1:1:151:C:H2'	1:1:152:U:H6	1.84	0.43
1:1:243:4AC:O7	1:1:243:4AC:H5	2.19	0.43
1:1:276:C:H2'	1:1:277:G:H8	1.82	0.43
1:1:659:A:H5''	1:1:660:G:H3'	2.00	0.43
1:1:1048:4AC:O7	1:1:1048:4AC:H5	2.18	0.43
1:1:1135:G:H2'	1:1:1136:G:C8	2.53	0.43
1:1:1479:C:H2'	1:1:1480:C:H6	1.84	0.43
1:1:1662:4AC:O7	1:1:1662:4AC:H5	2.19	0.43
1:1:1715:U:H2'	1:1:1716:A:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2490:G:C8	1:1:2661:C:C4	3.06	0.43
1:1:2650:G:H2'	1:1:2651:C:H6	1.84	0.43
1:1:2724:U:H2'	1:1:2725:U:O4'	2.19	0.43
2:2:954:C:H4'	2:2:955:A:O4'	2.19	0.43
2:2:1329:G:H2'	2:2:1330:C:H6	1.83	0.43
3:3:74:C:H2'	3:3:75:G:C8	2.54	0.43
19:AP:36:LEU:HD22	19:AP:38:LEU:HD12	2.01	0.43
31:AT:29:PRO:HG2	31:AT:32:GLN:OE1	2.19	0.43
37:B5:8:ARG:HB3	37:B5:24:ILE:HD13	2.01	0.43
30:BG:29:THR:HG21	30:BG:106:LYS:HG3	2.01	0.43
53:BD:33:ARG:NH1	53:BD:109:GLU:OE2	2.52	0.43
60:BN:77:VAL:HG12	60:BN:81:ASN:HB2	1.99	0.43
30:B4:50:LEU:HD23	30:B4:114:ILE:HD11	2.01	0.43
1:1:31:G:C4	1:1:32:G:C8	3.07	0.43
1:1:321:A:H2'	1:1:322:A:H8	1.83	0.43
1:1:805:G:H2'	1:1:806:G:H8	1.84	0.43
1:1:893:A:N1	1:1:2603:A:O2'	2.49	0.43
1:1:1460:4AC:H2'	1:1:1461:G:H8	1.84	0.43
1:1:1582:A:C5	1:1:1583:U:C5	3.07	0.43
1:1:1631:C:C2	1:1:1632:G:C8	3.06	0.43
1:1:2052:C:OP1	33:BB:238:ARG:NH2	2.52	0.43
1:1:2053:C:OP1	33:BB:233:ARG:NH1	2.49	0.43
1:1:2249:4AC:O7	1:1:2249:4AC:H5	2.19	0.43
1:1:2463:A:H2'	1:1:2464:G:C8	2.53	0.43
1:1:2544:C:OP2	43:BE:62:LYS:NZ	2.48	0.43
2:2:247:G:OP1	21:AR:66:ARG:NH1	2.46	0.43
2:2:659:U:C4	4:H:383:ARG:HD3	2.52	0.43
2:2:1426:A:H4'	11:AG:90:LYS:HG2	2.01	0.43
4:H:330:LEU:HB2	4:H:351:TRP:CZ3	2.54	0.43
11:AG:5:LYS:HG2	11:AG:18:GLN:HE21	1.84	0.43
16:AL:6:ILE:HB	16:AL:73:ILE:HD12	2.00	0.43
20:AQ:68:ASP:HB3	20:AQ:71:ASN:O	2.19	0.43
35:BO:38:ARG:HA	35:BO:109:HIS:HE1	1.83	0.43
30:B4:106:LYS:HE3	30:B4:106:LYS:HB3	1.91	0.43
1:1:102:C:N3	1:1:117:G:N1	2.37	0.42
1:1:785:G:C2	1:1:1520:G:C5	3.07	0.42
1:1:1065:4AC:O7	1:1:1065:4AC:H5	2.19	0.42
1:1:2517:U:H4'	1:1:2518:A:O4'	2.19	0.42
1:1:2593:A:H4'	38:BL:51:ILE:HG22	2.01	0.42
1:1:2698:G:H2'	1:1:2699:C:H6	1.83	0.42
1:1:2866:G:H2'	1:1:2867:C:C6	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2881:G:H2'	1:1:2882:C:H6	1.84	0.42
10:AF:61:GLU:C	10:AF:92:ARG:HH12	2.26	0.42
17:AM:52:ARG:H	17:AM:52:ARG:HG2	1.53	0.42
20:AQ:26:LEU:HD11	20:AQ:60:ILE:HG22	2.01	0.42
26:AX:59:GLU:OE2	26:AX:62:ARG:HD2	2.19	0.42
32:AO:115:TYR:O	32:AO:119:ARG:HG2	2.18	0.42
41:Bb:4:LYS:HE2	41:Bb:4:LYS:HB3	1.81	0.42
49:BR:50:HIS:HA	49:BR:53:MET:HE3	2.00	0.42
64:Bl:9:SER:OG	64:Bl:56:GLU:OE1	2.37	0.42
1:1:321:A:H2'	1:1:322:A:C8	2.53	0.42
1:1:461:U:H2'	1:1:462:G:O4'	2.19	0.42
1:1:568:U:H2'	1:1:569:C:H6	1.84	0.42
1:1:1200:G:C2	1:1:1201:G:C8	3.08	0.42
1:1:1207:G:OP1	60:BN:15:PRO:HG3	2.19	0.42
1:1:1764:C:H2'	1:1:1765:4AC:H6	2.00	0.42
1:1:2050:U:H2'	1:1:2051:C:C6	2.50	0.42
2:2:97:A:H2'	2:2:98:C:H6	1.84	0.42
4:H:38:ILE:HB	4:H:50:LEU:HB3	2.00	0.42
9:AE:38:ASN:HD21	9:AE:41:THR:HG23	1.83	0.42
18:AN:44:LEU:HG	18:AN:50:ALA:HB2	2.02	0.42
40:BU:65:LYS:HE2	40:BU:65:LYS:HB3	1.91	0.42
49:BR:89:HIS:CD2	49:BR:91:VAL:H	2.33	0.42
1:1:451:4AC:O7	1:1:451:4AC:H5	2.19	0.42
1:1:727:G:N7	37:BK:17:ARG:NH2	2.66	0.42
1:1:1222:4AC:H2'	1:1:1223:G:O4'	2.19	0.42
1:1:1795:A:C8	1:1:1797:G:C8	3.08	0.42
1:1:2128:U:H2'	1:1:2129:G:O4'	2.19	0.42
1:1:2960:4AC:H2'	1:1:2961:G:H8	1.84	0.42
1:1:3007:A:H2	1:1:3009:A:H62	1.67	0.42
2:2:110:U:H2'	2:2:111:C:C6	2.53	0.42
2:2:1289:U:H2'	2:2:1290:G:O4'	2.19	0.42
3:3:71:U:H2'	3:3:72:C:C6	2.54	0.42
25:AW:36:ARG:HA	25:AW:49:PRO:HD3	2.01	0.42
32:AO:31:VAL:HG23	32:AO:35:PHE:HB3	2.00	0.42
37:B5:26:ASP:OD1	37:B5:64:ARG:HG2	2.18	0.42
40:BU:50:ASP:OD2	40:BU:112:ARG:NH2	2.43	0.42
40:BU:83:LEU:HD12	40:BU:83:LEU:HA	1.91	0.42
48:BI:17:ARG:O	48:BI:21:MET:HG3	2.19	0.42
24:B6:34:LYS:HG3	24:B6:35:ASP:N	2.34	0.42
1:1:136:4AC:O7	1:1:136:4AC:H5	2.20	0.42
1:1:229:4AC:H2'	1:1:230:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:536:C:H2'	1:1:537:G:H8	1.84	0.42
1:1:620:A:N1	1:1:1046:G:O2'	2.49	0.42
1:1:703:U:H3'	1:1:704:G:H5'	2.00	0.42
1:1:990:U:H2'	1:1:991:G:C8	2.55	0.42
1:1:1284:A:H2	1:1:2698:G:O4'	2.03	0.42
1:1:1387:G:H4'	1:1:1388:A:H5'	2.01	0.42
1:1:1460:4AC:OP1	53:BD:189:ARG:NE	2.34	0.42
1:1:1587:C:H2'	1:1:1588:G:O4'	2.19	0.42
1:1:2301:G:N7	1:1:2733:5MC:H1'	2.34	0.42
2:2:429:A:H2'	2:2:430:C:H6	1.85	0.42
2:2:873:OMG:HM22	2:2:874:G:O4'	2.20	0.42
2:2:1147:4AC:O7	2:2:1147:4AC:H5	2.19	0.42
2:2:1156:G:H4'	2:2:1158:G:H5''	2.00	0.42
2:2:1274:G:H1'	2:2:1277:C:N4	2.34	0.42
2:2:1376:OMC:HM22	2:2:1377:C:H5'	2.01	0.42
3:3:94:A:C5	3:3:95:G:H1'	2.54	0.42
8:AD:43:LYS:O	8:AD:47:GLN:HG3	2.20	0.42
10:AF:131:TRP:NE1	13:AI:97:PHE:HA	2.34	0.42
12:AH:140:MET:HE2	12:AH:145:ARG:NE	2.34	0.42
18:AN:49:GLN:HG2	18:AN:106:GLU:HG2	2.00	0.42
28:AZ:126:ARG:HG3	28:AZ:185:PRO:HA	2.01	0.42
31:AT:17:MET:HE3	31:AT:75:GLU:HA	2.02	0.42
33:BB:209:HIS:O	33:BB:209:HIS:ND1	2.53	0.42
64:BI:7:ARG:NH1	64:BI:24:GLU:OE2	2.52	0.42
30:B4:90:ALA:O	30:B4:92:ILE:HG12	2.19	0.42
66:sd:12:A:P	66:sd:12:A:O4'	2.78	0.42
1:1:7:C:H2'	1:1:8:U:O4'	2.20	0.42
1:1:103:C:C2	1:1:117:G:C2	3.08	0.42
1:1:1617:4AC:O7	1:1:1617:4AC:H5	2.20	0.42
1:1:2405:C:H2'	1:1:2406:A:C8	2.54	0.42
1:1:2630:C:H2'	1:1:2631:C:H6	1.85	0.42
1:1:2687:A:H2'	1:1:2688:G:H8	1.84	0.42
1:1:2824:G:H2'	1:1:2825:U:C6	2.53	0.42
1:1:2833:C:H5''	4:H:195:TYR:CE1	2.54	0.42
2:2:23:A:N1	2:2:890:A:H2	2.18	0.42
2:2:903:C:H2'	2:2:904:A:H8	1.85	0.42
2:2:907:A:H2'	2:2:908:C:H6	1.85	0.42
4:H:52:GLN:O	4:H:56:ILE:HG12	2.19	0.42
4:H:382:LYS:CG	17:AM:52:ARG:HB2	2.48	0.42
32:AO:54:LEU:HD12	32:AO:54:LEU:HA	1.87	0.42
48:BI:115:ILE:HG22	48:BI:117:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:18:G:C8	1:1:2855:G:H4'	2.55	0.42
1:1:133:G:H2'	1:1:134:C:H6	1.82	0.42
1:1:154:G:C5	1:1:155:G:C8	3.07	0.42
1:1:288:G:H2'	1:1:289:C:H6	1.83	0.42
1:1:341:4AC:O7	1:1:341:4AC:H5	2.20	0.42
1:1:573:U:C2	1:1:574:C:C5	3.07	0.42
1:1:1035:G:H5'	1:1:1036:G:OP1	2.19	0.42
1:1:1120:U:H2'	1:1:1121:G:O4'	2.19	0.42
1:1:1206:G:H2'	1:1:1207:G:C8	2.55	0.42
1:1:1479:C:H2'	1:1:1480:C:C6	2.54	0.42
1:1:1598:G:O2'	1:1:1655:A:N1	2.43	0.42
1:1:1709:U:H2'	1:1:1710:C:C6	2.55	0.42
1:1:1932:C:H2'	1:1:1933:C:H6	1.85	0.42
1:1:2462:U:H2'	1:1:2463:A:H8	1.84	0.42
1:1:2718:4AC:O7	1:1:2718:4AC:H5	2.18	0.42
1:1:2786:U:H2'	1:1:2787:U:C6	2.55	0.42
2:2:268:G:H2'	2:2:269:G:C8	2.55	0.42
2:2:645:C:H2'	2:2:646:C:H6	1.84	0.42
2:2:702:C:H2'	2:2:703:4AC:H6	2.01	0.42
2:2:1235:A:H4'	23:AU:72:ARG:HH12	1.84	0.42
2:2:1276:U:OP1	32:AO:19:LYS:NZ	2.52	0.42
2:2:1334:A:H8	19:AP:14:PHE:HB2	1.84	0.42
4:H:78:VAL:HG12	4:H:101:PRO:HG2	2.01	0.42
4:H:205:PRO:HA	60:BN:107:ARG:HH12	1.84	0.42
30:A3:73:LYS:HG2	30:A3:74:GLU:N	2.35	0.42
35:BO:36:VAL:HG12	35:BO:105:ASP:HB3	2.00	0.42
35:BO:145:ARG:NH1	35:BO:147:GLU:OE2	2.49	0.42
43:BE:57:ILE:HA	43:BE:57:ILE:HD13	1.82	0.42
53:BD:54:LYS:NZ	53:BD:90:ARG:HD2	2.35	0.42
54:BF:88:TYR:HB2	54:BF:139:VAL:HB	2.02	0.42
64:Bl:38:TYR:HB3	64:Bl:49:ARG:HG2	2.00	0.42
65:Bk:11:ASP:OD1	65:Bk:15:GLU:N	2.43	0.42
1:1:938:A:H2'	1:1:939:G:H8	1.83	0.42
1:1:1077:C:H4'	38:BL:44:LYS:HB2	2.01	0.42
1:1:1283:A:C2	1:1:1284:A:C5	3.07	0.42
1:1:1685:A:N3	1:1:1755:4AC:O2'	2.42	0.42
1:1:2925:4AC:H2'	1:1:2926:G:H8	1.85	0.42
2:2:1200:C:H5'	31:AT:113:VAL:HB	2.01	0.42
2:2:1342:G:OP2	15:AK:122:SER:OG	2.34	0.42
2:2:1493:C:H2'	2:2:1494:G:C8	2.55	0.42
12:AH:73:ARG:HH22	12:AH:163:ARG:HG3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:AX:60:THR:O	26:AX:60:THR:OG1	2.34	0.42
31:AT:69:ASP:OD1	31:AT:69:ASP:N	2.51	0.42
43:BE:20:MET:O	43:BE:146:PRO:HD2	2.19	0.42
24:B6:72:TYR:CE2	24:B6:81:ILE:HG21	2.55	0.42
1:1:198:A:C2	1:1:216:A:C5	3.07	0.42
1:1:478:G:N2	53:BD:174:LYS:HD2	2.33	0.42
1:1:571:G:H2'	1:1:572:C:O4'	2.20	0.42
1:1:1460:4AC:O7	1:1:1460:4AC:H5	2.19	0.42
1:1:1706:G:H2'	1:1:1707:C:C6	2.55	0.42
1:1:2098:G:H2'	1:1:2099:C:C6	2.54	0.42
1:1:2596:C:H2'	1:1:2597:G:C8	2.54	0.42
2:2:51:U:O4	9:AE:24:LYS:NZ	2.52	0.42
2:2:65:G:H2'	2:2:66:C:C6	2.55	0.42
4:H:326:ARG:NH2	18:AN:62:ALA:O	2.50	0.42
9:AE:56:ALA:HB1	9:AE:61:GLU:HG3	2.02	0.42
18:AN:32:ARG:HG2	18:AN:37:LEU:HD12	2.02	0.42
19:AP:20:ARG:NH1	19:AP:25:GLY:O	2.53	0.42
43:BE:120:HIS:HD2	43:BE:134:ILE:HA	1.85	0.42
56:BP:22:SER:HB2	56:BP:30:TRP:HB2	2.02	0.42
60:BN:175:LYS:H	60:BN:175:LYS:HD2	1.85	0.42
30:B4:83:LYS:HE2	30:B4:83:LYS:HB3	1.85	0.42
1:1:84:A:P	44:Ba:2:PRO:HD2	2.60	0.42
1:1:2596:C:H2'	1:1:2597:G:H8	1.84	0.42
1:1:2925:4AC:O7	1:1:2925:4AC:H5	2.20	0.42
2:2:319:4AC:O7	2:2:319:4AC:H5	2.20	0.42
2:2:788:G:H2'	2:2:789:C:C6	2.55	0.42
2:2:870:C:H2'	2:2:871:A:C8	2.55	0.42
2:2:957:4AC:O7	2:2:957:4AC:H5	2.20	0.42
25:AW:32:HIS:NE2	25:AW:53:LYS:HG2	2.35	0.42
27:AY:38:TRP:CD1	27:AY:49:LYS:HD2	2.54	0.42
30:A3:65:HIS:C	30:A3:68:PRO:HD2	2.45	0.42
32:AO:110:ARG:O	32:AO:113:ARG:HD2	2.20	0.42
33:BB:124:ALA:O	33:BB:127:THR:HB	2.20	0.42
40:BU:34:GLU:O	40:BU:37:GLU:HG3	2.19	0.42
43:BE:169:GLU:O	43:BE:172:MET:HG2	2.20	0.42
44:Ba:81:ARG:HG2	44:Ba:86:VAL:HG11	2.02	0.42
57:BM:121:GLU:OE1	57:BM:126:LYS:HD3	2.20	0.42
62:Bc:9:SER:OG	62:Bc:10:TYR:O	2.37	0.42
30:B4:53:ILE:HG23	30:B4:63:VAL:HG21	2.02	0.42
1:1:656:A:H4'	1:1:657:A:O5'	2.19	0.42
1:1:797:G:H2'	1:1:798:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1202:U:C2	1:1:1203:G:C8	3.08	0.42
1:1:1318:G:H2'	1:1:1319:C:H6	1.84	0.42
1:1:1663:G:H2'	1:1:1664:U:C6	2.55	0.42
1:1:1668:G:H2'	1:1:1669:C:C6	2.55	0.42
1:1:1677:G:N3	1:1:1692:G:H1'	2.34	0.42
1:1:1790:C:H2'	1:1:1791:G:H8	1.85	0.42
1:1:2350:G:H5'	1:1:2387:G:H22	1.84	0.42
1:1:2457:A:C4	1:1:2458:G:C8	3.07	0.42
1:1:2642:4AC:H2'	1:1:2643:G:H8	1.84	0.42
2:2:459:G:O2'	2:2:461:A:H1'	2.20	0.42
2:2:718:4AC:H2'	2:2:719:G:O4'	2.20	0.42
2:2:1391:G:N2	2:2:1451:G:H2'	2.35	0.42
9:AE:48:ILE:HA	9:AE:52:TYR:HB2	2.02	0.42
12:AH:40:GLU:OE1	12:AH:40:GLU:N	2.53	0.42
29:A0:36:LEU:HD13	29:A0:36:LEU:H	1.85	0.42
30:A3:40:THR:O	30:A3:44:GLU:HB2	2.20	0.42
32:AO:16:ASP:HB3	32:AO:19:LYS:HD3	2.01	0.42
1:1:161:4AC:O7	1:1:161:4AC:H5	2.20	0.41
1:1:357:4AC:O7	1:1:357:4AC:H5	2.19	0.41
1:1:868:C:H5''	1:1:869:G:C2	2.55	0.41
1:1:951:G:H2'	1:1:952:U:C6	2.55	0.41
1:1:1086:G:N3	1:1:1087:G:C8	2.88	0.41
1:1:1899:C:O2'	1:1:1900:U:H5'	2.20	0.41
1:1:2055:G:N7	33:BB:145:SER:OG	2.45	0.41
1:1:2341:G:H4'	1:1:2342:C:OP1	2.20	0.41
1:1:2465:G:H2'	1:1:2466:U:C6	2.55	0.41
1:1:2485:G:C4	1:1:2486:G:C8	3.08	0.41
2:2:619:U:O4	2:2:719:G:O2'	2.30	0.41
2:2:868:4AC:O7	2:2:868:4AC:H5	2.20	0.41
2:2:1122:U:H2'	2:2:1123:C:O4'	2.20	0.41
2:2:1334:A:C8	19:AP:14:PHE:HB2	2.55	0.41
2:2:1359:G:H2'	2:2:1360:C:H6	1.85	0.41
3:3:10:G:H4'	35:BO:53:PRO:O	2.20	0.41
4:H:305:ALA:HB2	31:AT:132:LYS:HE3	2.01	0.41
19:AP:22:ILE:H	19:AP:22:ILE:HG13	1.64	0.41
25:AW:17:ARG:HG2	25:AW:61:LEU:HD22	2.01	0.41
55:BZ:98:LYS:C	55:BZ:99:ARG:HD2	2.45	0.41
1:1:612:G:N7	42:Be:62:HIS:NE2	2.65	0.41
1:1:946:G:H2'	1:1:947:C:C6	2.55	0.41
1:1:1225:G:C6	1:1:1240:G:C5	3.08	0.41
1:1:1266:G:H21	64:Bl:43:SER:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1600:U:N3	1:1:1876:A:C8	2.88	0.41
1:1:1621:4AC:O7	1:1:1621:4AC:H5	2.20	0.41
1:1:2322:A:C4	1:1:2323:G:C8	3.08	0.41
1:1:2329:4AC:O7	1:1:2329:4AC:H5	2.19	0.41
1:1:2391:C:H2'	1:1:2392:G:H8	1.85	0.41
1:1:2588:A:N6	1:1:2595:G:O6	2.53	0.41
1:1:2850:A:H2'	1:1:2851:C:C6	2.56	0.41
1:1:2865:4AC:O7	1:1:2865:4AC:H5	2.20	0.41
1:1:2922:U:H6	1:1:2944:C:H5'	1.84	0.41
1:1:3004:4AC:H2'	1:1:3005:G:O4'	2.19	0.41
2:2:53:4AC:O7	2:2:53:4AC:H5	2.20	0.41
2:2:86:U:H5'	2:2:87:C:OP2	2.20	0.41
2:2:816:C:H2'	2:2:817:U:C6	2.55	0.41
2:2:828:4AC:O7	2:2:828:4AC:H5	2.20	0.41
2:2:895:C:H2'	2:2:896:G:H8	1.85	0.41
2:2:1212:A:N7	2:2:1277:C:H1'	2.35	0.41
2:2:1479:4AC:O7	29:A0:15:ARG:NH2	2.51	0.41
4:H:382:LYS:CE	17:AM:52:ARG:HD2	2.49	0.41
6:AB:191:PRO:HB2	6:AB:193:GLU:HG3	2.01	0.41
9:AE:17:THR:HA	9:AE:23:ARG:NH2	2.35	0.41
30:A3:19:ALA:HB1	30:A3:78:ILE:HD13	2.02	0.41
45:BT:12:ILE:CD1	45:BT:85:LEU:HG	2.50	0.41
1:1:509:A:H2'	1:1:510:G:C8	2.55	0.41
1:1:618:U:O2'	42:Be:17:HIS:HD2	2.02	0.41
1:1:791:G:H2'	1:1:1509:C:N4	2.35	0.41
1:1:948:A:H2'	1:1:949:G:O4'	2.21	0.41
1:1:1283:A:N3	1:1:2718:4AC:O2'	2.49	0.41
1:1:1706:G:H2'	1:1:1707:C:H6	1.84	0.41
1:1:2000:C:O2'	1:1:2001:4AC:H5'	2.20	0.41
1:1:2110:A:H2'	1:1:2111:G:O4'	2.19	0.41
1:1:2643:G:C2	1:1:2644:G:N7	2.88	0.41
1:1:2960:4AC:O7	1:1:2960:4AC:H5	2.20	0.41
1:1:2990:G:H21	54:BF:149:GLN:NE2	2.13	0.41
2:2:695:A:H2'	2:2:696:A:H8	1.82	0.41
2:2:1095:A:H4'	15:AK:18:VAL:HG21	2.02	0.41
17:AM:12:GLU:OE1	17:AM:12:GLU:N	2.46	0.41
36:BC:38:MET:HE3	36:BC:182:TYR:CG	2.55	0.41
54:BF:155:GLU:HG3	54:BF:174:ILE:HG13	2.00	0.41
58:BS:14:PRO:O	58:BS:105:LYS:HD3	2.20	0.41
1:1:419:G:C4	1:1:420:G:C8	3.08	0.41
1:1:894:A:C2	1:1:2603:A:H1'	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1255:C:C2	1:1:1256:C:C5	3.09	0.41
1:1:1618:G:H2'	1:1:1619:C:C6	2.54	0.41
1:1:1877:C:H2'	1:1:1878:4AC:H6	2.02	0.41
1:1:2062:4AC:O7	1:1:2062:4AC:H5	2.19	0.41
1:1:2082:C:H2'	1:1:2083:4AC:H6	2.02	0.41
1:1:2083:4AC:O7	1:1:2083:4AC:H5	2.20	0.41
1:1:2105:U:H2'	1:1:2106:G:C8	2.51	0.41
1:1:2136:4AC:O7	1:1:2136:4AC:H5	2.20	0.41
1:1:2977:G:O6	1:1:2985:C:H5''	2.20	0.41
2:2:849:G:OP2	18:AN:4:LYS:NZ	2.46	0.41
2:2:1191:C:H1'	19:AP:6:TYR:O	2.20	0.41
2:2:1231:G:N2	19:AP:13:LYS:HG2	2.35	0.41
3:3:93:G:H2'	3:3:94:A:C8	2.56	0.41
10:AF:131:TRP:CE2	13:AI:97:PHE:HA	2.55	0.41
22:AS:6:GLN:HB3	22:AS:9:ILE:HG12	2.01	0.41
38:BL:77:THR:HB	38:BL:115:THR:HG23	2.01	0.41
40:BU:33:LYS:HB3	40:BU:33:LYS:HE2	1.75	0.41
53:BD:155:ARG:O	53:BD:159:GLU:HG2	2.19	0.41
1:1:141:G:N2	1:1:664:G:H1'	2.35	0.41
1:1:181:U:C2	1:1:182:G:C8	3.08	0.41
1:1:1144:G:HO2'	1:1:1145:C:H5''	1.85	0.41
1:1:1482:U:O2'	41:Bb:61:PRO:HB3	2.19	0.41
1:1:1516:U:H2'	1:1:1517:G:C8	2.55	0.41
1:1:1545:A:H1'	1:1:1547:U:OP2	2.21	0.41
1:1:2131:A:H2'	1:1:2132:G:O4'	2.20	0.41
1:1:2305:C:H2'	1:1:2306:C:C6	2.55	0.41
1:1:2949:G:H2'	1:1:2950:G:O4'	2.21	0.41
1:1:3001:C:H2'	1:1:3002:C:C6	2.51	0.41
2:2:1141:A:O2'	2:2:1143:A:N7	2.47	0.41
2:2:1168:G:H2'	2:2:1169:U:O4'	2.20	0.41
59:Bd:30:LYS:HE2	59:Bd:30:LYS:HB2	1.84	0.41
1:1:113:G:H8	1:1:113:G:O5'	2.03	0.41
1:1:246:G:C6	1:1:256:G:C6	3.09	0.41
1:1:348:A:H2	1:1:541:G:C2	2.39	0.41
1:1:1348:G:N1	1:1:1349:U:O4	2.54	0.41
1:1:1355:C:H2'	1:1:1356:U:O4'	2.20	0.41
1:1:1554:4AC:O7	1:1:1554:4AC:H5	2.20	0.41
1:1:1580:C:C5	1:1:1589:U:H5''	2.55	0.41
1:1:1695:4AC:O7	1:1:1695:4AC:H5	2.21	0.41
1:1:1713:G:N2	1:1:1787:A:H8	2.08	0.41
1:1:1853:G:H2'	1:1:1854:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1992:U:H2'	1:1:1993:G:O4'	2.20	0.41
1:1:2086:C:H2'	1:1:2087:G:H8	1.85	0.41
1:1:2546:G:H2'	1:1:2547:C:C6	2.56	0.41
2:2:1233:4AC:O7	2:2:1233:4AC:H5	2.19	0.41
2:2:1239:4AC:O7	2:2:1239:4AC:H5	2.20	0.41
3:3:14:U:OP2	3:3:70:A:O2'	2.38	0.41
20:AQ:60:ILE:HD12	20:AQ:61:PRO:O	2.21	0.41
30:A3:55:GLU:O	30:A3:55:GLU:HG2	2.19	0.41
42:Be:48:LYS:HE2	42:Be:55:TRP:CE3	2.55	0.41
45:BT:2:ASP:O	45:BT:6:VAL:HG23	2.21	0.41
50:BQ:21:ARG:NH1	50:BQ:55:VAL:HG23	2.36	0.41
54:BF:170:ASP:OD1	54:BF:170:ASP:N	2.53	0.41
1:1:288:G:H2'	1:1:289:C:C6	2.55	0.41
1:1:694:4AC:O7	1:1:694:4AC:H5	2.20	0.41
1:1:1293:4AC:O7	1:1:1293:4AC:H5	2.20	0.41
1:1:1327:C:H42	1:1:1353:A:P	2.43	0.41
1:1:1406:G:H2'	1:1:1407:C:O4'	2.21	0.41
1:1:1540:G:H2'	1:1:1541:U:C6	2.55	0.41
1:1:1765:4AC:O7	1:1:1765:4AC:H5	2.20	0.41
1:1:1847:C:H2'	1:1:1848:U:C6	2.54	0.41
1:1:1867:4AC:O7	1:1:1867:4AC:H5	2.21	0.41
1:1:2287:4AC:H2'	1:1:2288:G:C8	2.51	0.41
1:1:2992:4AC:CM7	1:1:2992:4AC:H5	2.50	0.41
2:2:383:A:C6	2:2:384:U:C4	3.08	0.41
2:2:645:C:H2'	2:2:646:C:C6	2.56	0.41
2:2:731:4AC:O7	2:2:731:4AC:H5	2.20	0.41
2:2:1182:C:H2'	2:2:1183:C:C6	2.56	0.41
2:2:1350:U:H2'	2:2:1351:A:C8	2.49	0.41
4:H:180:HIS:O	4:H:184:ILE:HG12	2.21	0.41
30:A3:51:VAL:HG11	30:A3:66:LEU:HD21	2.02	0.41
31:AT:59:TYR:HE1	31:AT:61:LYS:HE2	1.85	0.41
53:BD:128:LYS:HB2	53:BD:134:ILE:HD11	2.02	0.41
54:BF:165:ARG:O	54:BF:169:GLN:HG2	2.21	0.41
1:1:285:A:H2'	1:1:286:A:H8	1.86	0.41
1:1:1667:4AC:O7	1:1:1667:4AC:H5	2.20	0.41
1:1:2042:A:H1'	1:1:2179:A:N6	2.35	0.41
1:1:2330:G:C6	1:1:2460:G:C6	3.09	0.41
2:2:407:C:H2'	2:2:408:C:H6	1.86	0.41
2:2:626:4AC:O7	2:2:626:4AC:H5	2.19	0.41
2:2:848:4AC:O7	2:2:848:4AC:H5	2.21	0.41
2:2:1118:G:H2'	2:2:1119:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1303:G:H5''	32:AO:32:GLY:H	1.85	0.41
3:3:32:4AC:O7	3:3:32:4AC:H5	2.20	0.41
4:H:46:TYR:HD2	4:H:106:LYS:HG2	1.86	0.41
30:A3:55:GLU:OE2	30:A3:81:PRO:HA	2.20	0.41
31:AT:56:LYS:HG3	31:AT:58:LYS:HD3	2.03	0.41
31:AT:64:ARG:HB3	31:AT:82:TYR:HB2	2.02	0.41
33:BB:28:VAL:HG11	33:BB:72:ILE:HG12	2.02	0.41
36:BC:105:GLU:OE2	36:BC:118:LYS:HG3	2.21	0.41
41:Bb:75:HIS:CG	41:Bb:76:PRO:HD2	2.55	0.41
48:BI:43:GLU:H	48:BI:43:GLU:CD	2.28	0.41
37:BK:38:ALA:HB3	37:BK:40:LEU:HD23	2.03	0.41
50:BQ:71:LYS:HE3	50:BQ:71:LYS:HB2	1.88	0.41
53:BD:6:PHE:HE1	53:BD:139:GLN:HG2	1.85	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
1:1:435:C:C2	1:1:436:C:C5	3.09	0.41
1:1:458:4AC:O7	1:1:458:4AC:H5	2.20	0.41
1:1:475:G:H4'	1:1:477:A:C8	2.56	0.41
1:1:530:U:H2'	1:1:531:A:H8	1.86	0.41
1:1:532:C:H2'	1:1:533:4AC:H6	2.02	0.41
1:1:702:A:C6	30:B4:92:ILE:HD12	2.56	0.41
1:1:814:A:H2'	1:1:815:A:H8	1.86	0.41
1:1:857:C:H2'	1:1:858:A:H8	1.86	0.41
1:1:935:U:C4	42:Be:15:PRO:HA	2.56	0.41
1:1:940:C:H2'	1:1:941:C:H6	1.86	0.41
1:1:961:U:H2'	1:1:962:C:H6	1.86	0.41
1:1:981:4AC:O7	1:1:981:4AC:H5	2.19	0.41
1:1:984:U:H4'	1:1:1909:A:H5'	2.03	0.41
1:1:1457:U:H2'	1:1:1458:G:H8	1.86	0.41
1:1:1525:U:O2	1:1:1526:A:C8	2.74	0.41
1:1:1577:A:N3	1:1:1577:A:H2'	2.35	0.41
1:1:1726:G:H2'	1:1:1727:C:H6	1.86	0.41
1:1:1736:C:O3'	50:BQ:57:GLY:HA3	2.21	0.41
1:1:1755:4AC:HM73	1:1:1780:4AC:HM73	2.03	0.41
1:1:2058:A:C4	1:1:2059:G:C8	3.09	0.41
1:1:2182:C:C4	1:1:2206:C:O4'	2.74	0.41
1:1:2477:G:H2'	1:1:2478:C:H6	1.85	0.41
1:1:2593:A:H2	1:1:2662:A:H61	1.67	0.41
1:1:2606:C:H2'	1:1:2607:C:C6	2.54	0.41
1:1:2719:G:H2'	1:1:2720:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2776:G:H4'	1:1:2876:A:C2	2.56	0.41
2:2:394:4AC:H5	2:2:394:4AC:O7	2.21	0.41
2:2:520:G:H2'	2:2:521:C:C6	2.56	0.41
2:2:644:C:H2'	2:2:645:C:H6	1.85	0.41
2:2:973:A:C5	30:A3:34:LYS:HE3	2.55	0.41
2:2:976:A:H2	2:2:1000:G:N3	2.18	0.41
2:2:1253:A:H1'	2:2:1256:C:N4	2.36	0.41
2:2:1333:C:OP1	19:AP:19:ARG:NH2	2.53	0.41
2:2:1388:C:H2'	2:2:1389:C:H6	1.85	0.41
2:2:1496:5MC:H2'	2:2:1497:U:C6	2.56	0.41
2:2:1506:U:H4'	5:AA:99:ARG:NH2	2.35	0.41
3:3:62:C:C2	3:3:63:C:C5	3.09	0.41
3:3:85:C:H2'	3:3:86:C:C6	2.56	0.41
4:H:246:ASP:CG	4:H:248:ASN:H	2.29	0.41
5:AA:153:LEU:HD21	5:AA:161:GLU:HG3	2.03	0.41
12:AH:73:ARG:NH2	12:AH:163:ARG:HG3	2.34	0.41
22:AS:57:LEU:HD23	22:AS:57:LEU:HA	1.95	0.41
23:AU:121:ILE:H	23:AU:121:ILE:HG13	1.62	0.41
31:AT:70:MET:O	31:AT:103:LEU:N	2.50	0.41
35:BO:39:LYS:H	35:BO:109:HIS:CE1	2.39	0.41
37:B5:49:ASN:OD1	37:B5:50:ILE:N	2.54	0.41
38:BL:15:HIS:CD2	38:BL:16:THR:HG23	2.56	0.41
40:BU:16:TYR:O	40:BU:23:ARG:NH2	2.54	0.41
44:Ba:28:ALA:HB3	44:Ba:29:PRO:HD3	2.03	0.41
44:Ba:85:LYS:HA	44:Ba:85:LYS:HD3	1.76	0.41
50:BQ:104:LYS:HB2	50:BQ:104:LYS:HE3	1.84	0.41
54:BF:7:VAL:HB	54:BF:60:PRO:HG3	2.02	0.41
56:BP:36:ARG:NH1	56:BP:120:GLU:OE2	2.39	0.41
60:BN:4:ARG:NH2	60:BN:9:ASP:OD1	2.52	0.41
1:1:152:U:H2'	1:1:153:C:C6	2.55	0.41
1:1:314:4AC:H5	1:1:314:4AC:O7	2.21	0.41
1:1:869:G:H2'	1:1:871:G:C8	2.56	0.41
1:1:1056:G:H5'	38:BL:29:GLY:HA3	2.02	0.41
1:1:1852:G:H2'	1:1:1853:G:H8	1.86	0.41
1:1:1986:U:H2'	1:1:1987:G:O4'	2.21	0.41
1:1:2163:5MC:H2'	1:1:2164:U:C6	2.56	0.41
1:1:2653:A:H2'	1:1:2654:G:C8	2.55	0.41
2:2:64:OMU:HM22	2:2:65:G:O4'	2.21	0.41
2:2:279:A:H2'	2:2:280:C:C6	2.56	0.41
2:2:1167:G:OP2	28:AZ:131:ARG:NH2	2.54	0.41
4:H:385:ILE:CD1	4:H:385:ILE:H	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:153:LEU:HD23	5:AA:158:PHE:HA	2.03	0.41
12:AH:140:MET:HA	12:AH:144:ILE:O	2.21	0.41
31:AT:53:LEU:O	31:AT:57:GLY:N	2.54	0.41
43:BE:8:ARG:HD3	43:BE:173:VAL:HG23	2.02	0.41
43:BE:120:HIS:CD2	43:BE:135:PHE:H	2.36	0.41
43:BE:173:VAL:HA	43:BE:176:MET:HG2	2.02	0.41
24:B6:34:LYS:HE3	24:B6:34:LYS:HB2	1.82	0.41
1:1:410:G:C4	1:1:411:G:C8	3.10	0.40
1:1:473:C:H2'	1:1:474:C:C6	2.56	0.40
1:1:633:A:H4'	1:1:634:A:OP1	2.21	0.40
1:1:764:A:H2'	1:1:765:C:C6	2.55	0.40
1:1:807:C:H2'	1:1:808:G:O4'	2.22	0.40
1:1:906:U:H2'	1:1:907:C:C6	2.54	0.40
1:1:924:A:N3	1:1:2675:U:O2'	2.44	0.40
1:1:966:A:H1'	2:2:728:G:O2'	2.21	0.40
1:1:1934:4AC:O7	1:1:1934:4AC:H5	2.20	0.40
1:1:2027:4AC:O7	1:1:2027:4AC:H5	2.20	0.40
1:1:2572:G:H2'	1:1:2573:C:C6	2.56	0.40
1:1:2725:U:C2	1:1:2726:G:C8	3.10	0.40
1:1:3004:4AC:O7	1:1:3004:4AC:H5	2.21	0.40
2:2:926:G:O2'	31:AT:125:SER:OG	2.35	0.40
2:2:991:G:H2'	2:2:992:U:H6	1.86	0.40
2:2:1365:U:H2'	2:2:1366:G:H8	1.86	0.40
3:3:75:G:C6	3:3:109:G:C6	3.09	0.40
10:AF:212:VAL:N	13:AI:70:ASN:HD21	2.12	0.40
16:AL:38:ILE:HD13	16:AL:38:ILE:HA	1.80	0.40
46:BW:9:MET:O	46:BW:61:LYS:HE2	2.22	0.40
30:BG:66:LEU:HB2	30:BG:67:PRO:HD3	2.03	0.40
60:BN:104:LYS:HD3	60:BN:104:LYS:HA	1.92	0.40
1:1:69:U:C4	51:BV:52:TRP:HA	2.56	0.40
1:1:152:U:H2'	1:1:153:C:H6	1.85	0.40
1:1:229:4AC:O7	1:1:229:4AC:H5	2.21	0.40
1:1:434:A:H2'	1:1:435:C:H6	1.84	0.40
1:1:569:C:H2'	1:1:570:G:H8	1.86	0.40
1:1:829:4AC:O7	1:1:829:4AC:H5	2.22	0.40
1:1:843:A:H2'	1:1:844:A:C8	2.56	0.40
1:1:1107:U:C4	1:1:1108:G:N7	2.89	0.40
1:1:1255:C:H1'	1:1:1262:U:N3	2.36	0.40
1:1:1395:U:OP1	48:BI:10:ILE:HD13	2.21	0.40
1:1:1734:G:H2'	1:1:1735:G:C8	2.54	0.40
1:1:1822:C:H2'	1:1:1823:G:O4'	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1847:C:OP1	1:1:1862:U:H5	2.03	0.40
1:1:1931:A:H4'	36:BC:228:GLN:HA	2.03	0.40
1:1:2227:C:H2'	1:1:2228:C:H6	1.86	0.40
1:1:2294:A:OP1	1:1:2295:A:O2'	2.34	0.40
1:1:2447:A:H2'	1:1:2448:A:C8	2.55	0.40
1:1:2834:A:H2'	4:H:195:TYR:CE2	2.56	0.40
1:1:2880:U:H2'	1:1:2881:G:C8	2.57	0.40
2:2:105:A:H5'	2:2:106:C:H5	1.86	0.40
2:2:407:C:H2'	2:2:408:C:C6	2.56	0.40
2:2:1356:C:H2'	2:2:1357:C:H6	1.87	0.40
2:2:1434:U:H2'	2:2:1435:C:H6	1.82	0.40
9:AE:38:ASN:HD22	9:AE:40:ARG:H	1.69	0.40
33:BB:21:SER:HA	33:BB:24:PHE:CD2	2.56	0.40
43:BE:22:LYS:HA	43:BE:23:PRO:HD3	1.95	0.40
50:BQ:3:THR:HG22	50:BQ:5:LYS:HG3	2.03	0.40
50:BQ:60:ARG:O	50:BQ:64:ARG:HG3	2.22	0.40
57:BM:41:ARG:HA	57:BM:41:ARG:HD3	1.89	0.40
63:BJ:133:ILE:HA	63:BJ:136:ILE:HG22	2.03	0.40
1:1:17:A:C2	1:1:2287:4AC:H1'	2.56	0.40
1:1:326:A:N1	1:1:337:A:H5''	2.36	0.40
1:1:422:C:H2'	1:1:423:C:H6	1.85	0.40
1:1:690:G:OP1	62:Bc:73:LYS:NZ	2.52	0.40
1:1:791:G:H5''	1:1:792:A:OP1	2.20	0.40
1:1:1420:G:H2'	1:1:1421:C:C6	2.56	0.40
1:1:1525:U:H2'	1:1:1526:A:H8	1.86	0.40
1:1:1556:C:H2'	1:1:1557:4AC:H6	2.03	0.40
1:1:2171:G:N2	1:1:2209:G:H2'	2.36	0.40
1:1:2764:G:O2'	1:1:2890:A:N1	2.53	0.40
2:2:52:C:H2'	2:2:53:4AC:H6	2.04	0.40
2:2:225:C:C2	2:2:226:U:C6	3.09	0.40
2:2:511:4AC:O2'	2:2:515:U:OP1	2.38	0.40
4:H:262:LEU:HB3	4:H:263:PRO:HD3	2.02	0.40
4:H:385:ILE:HG23	17:AM:23:TYR:HB3	2.02	0.40
4:H:387:LYS:CB	66:sd:12:A:H4'	2.51	0.40
17:AM:65:ARG:HG3	17:AM:66:ARG:N	2.34	0.40
19:AP:22:ILE:HG13	19:AP:37:MET:O	2.22	0.40
24:AV:86:ILE:HD12	24:AV:86:ILE:HA	1.94	0.40
36:BC:184:ILE:O	36:BC:192:LYS:HE3	2.22	0.40
37:BK:75:LEU:HD11	37:BK:82:LEU:HD13	2.04	0.40
1:1:166:A:H2'	1:1:167:A:H8	1.86	0.40
1:1:422:C:H2'	1:1:423:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:465:A:OP2	40:BU:60:LYS:NZ	2.52	0.40
1:1:710:C:H2'	1:1:711:C:C6	2.55	0.40
1:1:961:U:H2'	1:1:962:C:C6	2.57	0.40
1:1:1071:A:H4'	1:1:1087:G:H22	1.86	0.40
1:1:1104:C:H2'	1:1:1105:G:H8	1.87	0.40
1:1:1751:A:H2'	1:1:1752:G:O4'	2.22	0.40
1:1:1809:A:C5	1:1:1810:G:H1'	2.56	0.40
1:1:1938:4AC:H5	1:1:1938:4AC:O7	2.22	0.40
1:1:2331:U:H1'	57:BM:123:GLY:HA3	2.04	0.40
1:1:2548:4AC:O7	1:1:2548:4AC:H5	2.22	0.40
1:1:2657:A:H4'	52:Bj:58:ARG:HG2	2.04	0.40
1:1:2772:C:H2'	1:1:2773:A:O4'	2.22	0.40
2:2:223:G:H2'	2:2:224:G:C8	2.57	0.40
2:2:546:4AC:O7	2:2:546:4AC:H5	2.21	0.40
2:2:590:4AC:O7	2:2:590:4AC:H5	2.21	0.40
2:2:1020:A:C2	2:2:1180:G:C4	3.09	0.40
2:2:1066:A:H62	6:AB:128:LYS:NZ	2.18	0.40
2:2:1092:G:H5'	2:2:1254:A:O2'	2.21	0.40
2:2:1172:G:H2'	2:2:1173:U:C6	2.56	0.40
2:2:1333:C:OP1	19:AP:16:LYS:HE3	2.21	0.40
4:H:387:LYS:N	4:H:387:LYS:HD2	2.36	0.40
6:AB:51:ARG:HD3	6:AB:51:ARG:HA	1.86	0.40
9:AE:213:VAL:HG23	9:AE:215:ILE:HD11	2.02	0.40
12:AH:16:LYS:O	12:AH:43:LEU:HA	2.22	0.40
20:AQ:94:ASP:OD1	20:AQ:95:LEU:N	2.54	0.40
23:AU:35:VAL:HG22	23:AU:36:LYS:O	2.21	0.40
35:BO:156:LEU:HD23	35:BO:156:LEU:HA	1.87	0.40
39:Bf:48:LYS:HA	39:Bf:48:LYS:HD3	1.89	0.40
43:BE:8:ARG:HD3	43:BE:173:VAL:CG2	2.52	0.40
54:BF:90:LEU:HD22	54:BF:174:ILE:HA	2.04	0.40
63:BJ:105:VAL:O	63:BJ:107:VAL:HG23	2.22	0.40
30:B4:49:LYS:HG3	30:B4:104:PRO:HD3	2.04	0.40
1:1:1064:C:H2'	1:1:1065:4AC:H6	2.04	0.40
1:1:1066:G:C6	1:1:1452:G:C6	3.10	0.40
1:1:1241:A:C6	1:1:1445:G:H1'	2.57	0.40
1:1:1469:A:C4	41:Bb:109:LYS:HB2	2.56	0.40
1:1:1726:G:H2'	1:1:1727:C:C6	2.55	0.40
1:1:2748:C:H2'	1:1:2749:C:C6	2.57	0.40
1:1:2922:U:C6	1:1:2944:C:H5'	2.57	0.40
2:2:239:G:H2'	2:2:240:G:O4'	2.21	0.40
2:2:387:G:H2'	2:2:388:G:H8	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:429:A:H2'	2:2:430:C:C6	2.56	0.40
2:2:1151:G:H2'	2:2:1152:G:O4'	2.21	0.40
2:2:1225:A:H2'	2:2:1226:U:H6	1.86	0.40
5:AA:54:LYS:HB2	5:AA:54:LYS:HE2	1.94	0.40
5:AA:61:LEU:HD23	5:AA:61:LEU:HA	1.86	0.40
8:AD:84:PRO:HD2	8:AD:87:ALA:HB2	2.03	0.40
11:AG:67:THR:OG1	11:AG:118:GLN:NE2	2.54	0.40
19:AP:20:ARG:HD3	19:AP:27:TYR:CE1	2.57	0.40
37:B5:35:VAL:HG11	37:B5:53:LEU:HD11	2.04	0.40
45:BT:12:ILE:HG22	45:BT:12:ILE:O	2.22	0.40
30:BG:78:ILE:HG12	30:BG:79:TYR:H	1.87	0.40
53:BD:157:THR:OG1	53:BD:214:HIS:HE1	2.05	0.40
57:BM:73:ARG:HD2	57:BM:90:TYR:CD1	2.57	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	H	384/392 (98%)	382 (100%)	2 (0%)	0	100	100
5	AA	186/199 (94%)	181 (97%)	5 (3%)	0	100	100
6	AB	194/202 (96%)	193 (100%)	1 (0%)	0	100	100
7	AC	55/63 (87%)	53 (96%)	2 (4%)	0	100	100
8	AD	171/180 (95%)	169 (99%)	2 (1%)	0	100	100
9	AE	240/243 (99%)	236 (98%)	4 (2%)	0	100	100
10	AF	227/236 (96%)	222 (98%)	5 (2%)	0	100	100
11	AG	122/125 (98%)	117 (96%)	5 (4%)	0	100	100
12	AH	212/215 (99%)	210 (99%)	2 (1%)	0	100	100
13	AI	127/130 (98%)	125 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	AJ	123/127 (97%)	122 (99%)	1 (1%)	0	100	100
15	AK	133/135 (98%)	129 (97%)	4 (3%)	0	100	100
16	AL	98/102 (96%)	97 (99%)	1 (1%)	0	100	100
17	AM	125/137 (91%)	122 (98%)	3 (2%)	0	100	100
18	AN	144/147 (98%)	143 (99%)	1 (1%)	0	100	100
19	AP	53/56 (95%)	53 (100%)	0	0	100	100
20	AQ	155/158 (98%)	152 (98%)	3 (2%)	0	100	100
21	AR	105/113 (93%)	101 (96%)	4 (4%)	0	100	100
22	AS	62/67 (92%)	58 (94%)	4 (6%)	0	100	100
23	AU	147/150 (98%)	147 (100%)	0	0	100	100
24	AV	94/99 (95%)	92 (98%)	2 (2%)	0	100	100
24	B6	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
25	AW	59/65 (91%)	58 (98%)	1 (2%)	0	100	100
26	AX	63/71 (89%)	63 (100%)	0	0	100	100
27	AY	47/51 (92%)	41 (87%)	6 (13%)	0	100	100
28	AZ	194/210 (92%)	182 (94%)	12 (6%)	0	100	100
29	A0	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
30	A3	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
30	B4	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
30	BG	120/123 (98%)	120 (100%)	0	0	100	100
31	AT	128/132 (97%)	127 (99%)	1 (1%)	0	100	100
32	AO	136/148 (92%)	128 (94%)	8 (6%)	0	100	100
33	BB	236/239 (99%)	230 (98%)	6 (2%)	0	100	100
34	BY	152/155 (98%)	152 (100%)	0	0	100	100
35	BO	196/203 (97%)	195 (100%)	1 (0%)	0	100	100
36	BC	358/361 (99%)	349 (98%)	9 (2%)	0	100	100
37	B5	79/82 (96%)	79 (100%)	0	0	100	100
37	BK	78/82 (95%)	75 (96%)	3 (4%)	0	100	100
38	BL	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
39	Bf	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
40	BU	119/121 (98%)	118 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	Bb	127/130 (98%)	127 (100%)	0	0	100	100
42	Be	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
43	BE	183/188 (97%)	183 (100%)	0	0	100	100
44	Ba	92/94 (98%)	92 (100%)	0	0	100	100
45	BT	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
46	BW	66/68 (97%)	66 (100%)	0	0	100	100
47	Bi	80/83 (96%)	77 (96%)	3 (4%)	0	100	100
48	BI	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
49	BR	94/97 (97%)	94 (100%)	0	0	100	100
50	BQ	148/151 (98%)	148 (100%)	0	0	100	100
51	BV	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
52	Bj	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
53	BD	253/255 (99%)	248 (98%)	5 (2%)	0	100	100
54	BF	181/184 (98%)	180 (99%)	1 (1%)	0	100	100
55	BZ	96/99 (97%)	95 (99%)	1 (1%)	0	100	100
56	BP	118/120 (98%)	118 (100%)	0	0	100	100
57	BM	191/194 (98%)	188 (98%)	3 (2%)	0	100	100
58	BS	152/155 (98%)	151 (99%)	1 (1%)	0	100	100
59	Bd	89/91 (98%)	89 (100%)	0	0	100	100
60	BN	176/181 (97%)	169 (96%)	7 (4%)	0	100	100
61	Bg	46/51 (90%)	46 (100%)	0	0	100	100
62	Bc	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
63	BJ	138/141 (98%)	138 (100%)	0	0	100	100
64	Bl	75/77 (97%)	75 (100%)	0	0	100	100
65	Bk	61/65 (94%)	60 (98%)	1 (2%)	0	100	100
All	All	8568/8861 (97%)	8416 (98%)	152 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	332/338 (98%)	306 (92%)	26 (8%)	11	13
5	AA	160/167 (96%)	151 (94%)	9 (6%)	19	24
6	AB	168/173 (97%)	163 (97%)	5 (3%)	36	49
7	AC	50/55 (91%)	50 (100%)	0	100	100
8	AD	156/160 (98%)	153 (98%)	3 (2%)	50	66
9	AE	213/214 (100%)	210 (99%)	3 (1%)	59	75
10	AF	192/198 (97%)	190 (99%)	2 (1%)	68	81
11	AG	107/108 (99%)	102 (95%)	5 (5%)	23	31
12	AH	183/184 (100%)	166 (91%)	17 (9%)	8	9
13	AI	106/107 (99%)	105 (99%)	1 (1%)	70	84
14	AJ	101/103 (98%)	97 (96%)	4 (4%)	28	38
15	AK	111/111 (100%)	109 (98%)	2 (2%)	51	68
16	AL	89/91 (98%)	84 (94%)	5 (6%)	19	24
17	AM	94/104 (90%)	91 (97%)	3 (3%)	34	47
18	AN	120/121 (99%)	119 (99%)	1 (1%)	73	85
19	AP	45/46 (98%)	41 (91%)	4 (9%)	9	10
20	AQ	142/143 (99%)	139 (98%)	3 (2%)	47	63
21	AR	96/102 (94%)	94 (98%)	2 (2%)	47	63
22	AS	58/61 (95%)	54 (93%)	4 (7%)	14	16
23	AU	126/127 (99%)	122 (97%)	4 (3%)	34	47
24	AV	88/90 (98%)	87 (99%)	1 (1%)	65	79
24	B6	86/90 (96%)	78 (91%)	8 (9%)	8	9
25	AW	53/56 (95%)	53 (100%)	0	100	100
26	AX	55/60 (92%)	49 (89%)	6 (11%)	6	6
27	AY	40/42 (95%)	38 (95%)	2 (5%)	22	28
28	AZ	155/168 (92%)	147 (95%)	8 (5%)	21	26
29	A0	34/35 (97%)	33 (97%)	1 (3%)	37	51
30	A3	98/99 (99%)	97 (99%)	1 (1%)	68	81
30	B4	98/99 (99%)	93 (95%)	5 (5%)	21	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BG	98/99 (99%)	88 (90%)	10 (10%)	7	7
31	AT	113/114 (99%)	108 (96%)	5 (4%)	25	34
32	AO	115/123 (94%)	111 (96%)	4 (4%)	32	43
33	BB	188/189 (100%)	185 (98%)	3 (2%)	55	71
34	BY	132/133 (99%)	128 (97%)	4 (3%)	36	49
35	BO	167/170 (98%)	156 (93%)	11 (7%)	15	18
36	BC	306/307 (100%)	302 (99%)	4 (1%)	61	76
37	B5	65/66 (98%)	62 (95%)	3 (5%)	24	32
37	BK	64/66 (97%)	59 (92%)	5 (8%)	11	13
38	BL	118/118 (100%)	110 (93%)	8 (7%)	14	17
39	Bf	46/47 (98%)	44 (96%)	2 (4%)	26	35
40	BU	109/109 (100%)	105 (96%)	4 (4%)	30	41
41	Bb	117/118 (99%)	115 (98%)	2 (2%)	53	69
42	Be	52/53 (98%)	52 (100%)	0	100	100
43	BE	158/160 (99%)	134 (85%)	24 (15%)	3	2
44	Ba	84/84 (100%)	82 (98%)	2 (2%)	43	58
45	BT	77/77 (100%)	76 (99%)	1 (1%)	61	76
46	BW	63/63 (100%)	60 (95%)	3 (5%)	23	30
47	Bi	61/62 (98%)	59 (97%)	2 (3%)	33	45
48	BI	122/122 (100%)	122 (100%)	0	100	100
49	BR	86/87 (99%)	86 (100%)	0	100	100
50	BQ	132/133 (99%)	132 (100%)	0	100	100
51	BV	54/58 (93%)	53 (98%)	1 (2%)	50	66
52	Bj	83/84 (99%)	83 (100%)	0	100	100
53	BD	212/212 (100%)	208 (98%)	4 (2%)	50	66
54	BF	156/157 (99%)	145 (93%)	11 (7%)	13	16
55	BZ	79/80 (99%)	72 (91%)	7 (9%)	9	10
56	BP	102/102 (100%)	99 (97%)	3 (3%)	37	51
57	BM	160/161 (99%)	157 (98%)	3 (2%)	50	66
58	BS	130/131 (99%)	128 (98%)	2 (2%)	57	73
59	Bd	82/82 (100%)	80 (98%)	2 (2%)	43	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
60	BN	149/151 (99%)	145 (97%)	4 (3%)	39	53
61	Bg	37/39 (95%)	37 (100%)	0	100	100
62	Bc	74/74 (100%)	71 (96%)	3 (4%)	27	37
63	BJ	108/109 (99%)	105 (97%)	3 (3%)	38	52
64	Bl	72/72 (100%)	70 (97%)	2 (3%)	38	52
65	Bk	55/57 (96%)	52 (94%)	3 (6%)	19	24
All	All	7382/7521 (98%)	7102 (96%)	280 (4%)	30	40

All (280) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	12	ASP
4	H	23	LEU
4	H	37	LEU
4	H	61	LYS
4	H	68	LYS
4	H	85	LEU
4	H	93	LEU
4	H	98	ARG
4	H	99	SER
4	H	108	GLU
4	H	110	LEU
4	H	123	VAL
4	H	129	LYS
4	H	132	VAL
4	H	187	ILE
4	H	218	VAL
4	H	221	ILE
4	H	239	ILE
4	H	268	VAL
4	H	269	GLU
4	H	277	GLN
4	H	350	THR
4	H	379	ARG
4	H	385	ILE
4	H	386	GLU
4	H	387	LYS
5	AA	18	GLN
5	AA	31	VAL
5	AA	57	THR

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Mol	Chain	Res	Type
5	AA	73	ASP
5	AA	97	VAL
5	AA	153	LEU
5	AA	160	LEU
5	AA	185	GLU
5	AA	190	LYS
6	AB	4	GLU
6	AB	9	LEU
6	AB	32	ILE
6	AB	74	LEU
6	AB	170	ILE
8	AD	20	LYS
8	AD	102	GLU
8	AD	119	ARG
9	AE	3	ARG
9	AE	122	ILE
9	AE	191	LYS
10	AF	57	VAL
10	AF	187	THR
11	AG	6	LEU
11	AG	7	VAL
11	AG	38	ILE
11	AG	45	ILE
11	AG	77	ASP
12	AH	28	VAL
12	AH	38	ASN
12	AH	67	LEU
12	AH	73	ARG
12	AH	79	TYR
12	AH	123	LEU
12	AH	134	GLU
12	AH	136	THR
12	AH	140	MET
12	AH	144	ILE
12	AH	145	ARG
12	AH	146	TYR
12	AH	151	ASP
12	AH	172	LYS
12	AH	176	THR
12	AH	190	LEU
12	AH	197	LYS
13	AI	55	ASP

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Mol	Chain	Res	Type
14	AJ	18	VAL
14	AJ	42	LYS
14	AJ	88	GLN
14	AJ	96	THR
15	AK	23	LYS
15	AK	39	GLU
16	AL	14	ARG
16	AL	73	ILE
16	AL	76	GLU
16	AL	89	ARG
16	AL	96	ILE
17	AM	12	GLU
17	AM	30	ILE
17	AM	38	THR
18	AN	64	GLN
19	AP	9	ARG
19	AP	10	LYS
19	AP	20	ARG
19	AP	46	VAL
20	AQ	30	VAL
20	AQ	60	ILE
20	AQ	87	LEU
21	AR	38	VAL
21	AR	48	THR
22	AS	14	ARG
22	AS	60	MET
22	AS	61	LYS
22	AS	62	GLU
23	AU	18	GLN
23	AU	22	GLU
23	AU	68	VAL
23	AU	121	ILE
24	AV	52	VAL
26	AX	40	VAL
26	AX	49	VAL
26	AX	59	GLU
26	AX	60	THR
26	AX	65	ARG
26	AX	67	ILE
27	AY	31	MET
27	AY	48	TRP
28	AZ	3	ILE

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Mol	Chain	Res	Type
28	AZ	17	ILE
28	AZ	35	ILE
28	AZ	129	GLU
28	AZ	162	VAL
28	AZ	175	VAL
28	AZ	192	GLU
28	AZ	196	ILE
29	A0	36	LEU
30	A3	25	ILE
31	AT	36	LEU
31	AT	49	ARG
31	AT	53	LEU
31	AT	90	VAL
31	AT	112	ARG
32	AO	21	LEU
32	AO	31	VAL
32	AO	122	LEU
32	AO	126	VAL
33	BB	62	ARG
33	BB	96	THR
33	BB	239	LYS
34	BY	17	ARG
34	BY	55	THR
34	BY	105	MET
34	BY	127	ARG
35	BO	36	VAL
35	BO	37	VAL
35	BO	39	LYS
35	BO	48	ILE
35	BO	54	LYS
35	BO	59	LEU
35	BO	67	LEU
35	BO	100	GLU
35	BO	112	VAL
35	BO	172	LEU
35	BO	176	LEU
36	BC	3	LYS
36	BC	56	ASP
36	BC	172	LYS
36	BC	191	GLU
37	B5	33	VAL
37	B5	60	ILE

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Mol	Chain	Res	Type
37	B5	77	LYS
38	BL	10	LYS
38	BL	69	VAL
38	BL	79	LYS
38	BL	90	GLN
38	BL	115	THR
38	BL	122	LEU
38	BL	123	VAL
38	BL	147	VAL
39	Bf	3	ARG
39	Bf	47	THR
40	BU	1	MET
40	BU	68	GLU
40	BU	83	LEU
40	BU	119	ARG
41	Bb	80	GLU
41	Bb	113	GLU
43	BE	3	ILE
43	BE	8	ARG
43	BE	25	ILE
43	BE	29	THR
43	BE	34	VAL
43	BE	51	LEU
43	BE	57	ILE
43	BE	59	ARG
43	BE	60	LYS
43	BE	67	ASP
43	BE	70	ILE
43	BE	78	VAL
43	BE	82	LEU
43	BE	91	LEU
43	BE	118	ASP
43	BE	119	GLU
43	BE	121	ILE
43	BE	134	ILE
43	BE	137	MET
43	BE	142	THR
43	BE	156	LYS
43	BE	173	VAL
43	BE	184	VAL
43	BE	185	GLU
44	Ba	3	ILE

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Mol	Chain	Res	Type
44	Ba	7	GLU
45	BT	41	ARG
46	BW	62	LEU
46	BW	63	ARG
46	BW	67	LYS
47	Bi	5	LYS
47	Bi	51	THR
37	BK	4	ILE
37	BK	40	LEU
37	BK	56	LEU
37	BK	75	LEU
37	BK	82	LEU
51	BV	58	GLU
30	BG	3	LYS
30	BG	13	LYS
30	BG	28	ASP
30	BG	34	LYS
30	BG	72	GLU
30	BG	73	LYS
30	BG	74	GLU
30	BG	103	GLU
30	BG	109	ASP
30	BG	122	MET
53	BD	61	ILE
53	BD	75	THR
53	BD	92	THR
53	BD	222	VAL
54	BF	26	VAL
54	BF	38	GLU
54	BF	84	GLU
54	BF	89	LYS
54	BF	90	LEU
54	BF	91	LYS
54	BF	129	THR
54	BF	136	GLU
54	BF	155	GLU
54	BF	158	THR
54	BF	183	THR
55	BZ	3	LEU
55	BZ	6	GLU
55	BZ	11	LEU
55	BZ	55	LEU

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Mol	Chain	Res	Type
55	BZ	94	LEU
55	BZ	96	LEU
55	BZ	99	ARG
24	B6	9	LYS
24	B6	11	ASN
24	B6	13	LEU
24	B6	14	ILE
24	B6	16	ARG
24	B6	79	LEU
24	B6	89	ARG
24	B6	90	ASP
56	BP	4	THR
56	BP	16	ARG
56	BP	104	GLU
57	BM	3	MET
57	BM	5	LYS
57	BM	76	TRP
58	BS	144	THR
58	BS	155	ARG
59	Bd	82	GLU
59	Bd	83	GLN
60	BN	103	ARG
60	BN	108	TYR
60	BN	167	LYS
60	BN	174	THR
62	Bc	27	LEU
62	Bc	29	VAL
62	Bc	84	VAL
63	BJ	41	ILE
63	BJ	63	VAL
63	BJ	112	VAL
64	Bl	7	ARG
64	Bl	13	GLU
30	B4	70	CYS
30	B4	71	GLU
30	B4	77	TYR
30	B4	121	LEU
30	B4	122	MET
65	Bk	16	GLU
65	Bk	23	CYS
65	Bk	49	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (166)

such sidechains are listed below:

Mol	Chain	Res	Type
4	H	52	GLN
4	H	237	ASN
4	H	238	ASN
5	AA	77	GLN
5	AA	109	ASN
6	AB	11	GLN
6	AB	108	ASN
6	AB	145	ASN
8	AD	47	GLN
8	AD	50	ASN
8	AD	65	GLN
8	AD	72	GLN
8	AD	123	GLN
8	AD	162	ASN
9	AE	38	ASN
9	AE	139	GLN
9	AE	143	HIS
10	AF	58	ASN
10	AF	115	ASN
10	AF	120	ASN
10	AF	196	ASN
10	AF	209	ASN
11	AG	18	GLN
11	AG	110	ASN
11	AG	118	GLN
11	AG	120	ASN
12	AH	48	HIS
12	AH	55	HIS
12	AH	147	HIS
12	AH	193	ASN
13	AI	9	ASN
13	AI	16	ASN
13	AI	64	GLN
13	AI	70	ASN
14	AJ	40	GLN
14	AJ	52	ASN
14	AJ	64	ASN
14	AJ	83	ASN
14	AJ	121	ASN
15	AK	5	GLN
15	AK	67	GLN
16	AL	22	GLN

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Mol	Chain	Res	Type
17	AM	24	ASN
17	AM	99	GLN
18	AN	64	GLN
18	AN	66	ASN
18	AN	76	GLN
19	AP	26	GLN
20	AQ	71	ASN
20	AQ	123	GLN
21	AR	55	HIS
21	AR	74	ASN
22	AS	18	ASN
23	AU	18	GLN
23	AU	47	GLN
26	AX	26	GLN
28	AZ	77	ASN
30	A3	65	HIS
31	AT	15	GLN
31	AT	84	HIS
31	AT	114	GLN
32	AO	18	ASN
32	AO	20	GLN
32	AO	67	GLN
33	BB	8	GLN
33	BB	201	ASN
33	BB	202	HIS
33	BB	229	HIS
34	BY	14	ASN
34	BY	77	ASN
34	BY	148	ASN
35	BO	20	ASN
35	BO	42	ASN
35	BO	44	HIS
35	BO	47	GLN
35	BO	63	HIS
35	BO	76	HIS
35	BO	109	HIS
36	BC	143	GLN
36	BC	167	GLN
36	BC	194	ASN
36	BC	257	HIS
36	BC	270	GLN
36	BC	274	HIS

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Mol	Chain	Res	Type
36	BC	309	HIS
37	B5	31	ASN
38	BL	15	HIS
38	BL	43	ASN
38	BL	84	ASN
38	BL	90	GLN
39	Bf	19	GLN
39	Bf	20	ASN
39	Bf	38	HIS
40	BU	7	GLN
40	BU	17	ASN
40	BU	106	ASN
41	Bb	26	GLN
42	Be	17	HIS
43	BE	65	ASN
43	BE	120	HIS
43	BE	164	HIS
44	Ba	42	HIS
44	Ba	46	GLN
45	BT	37	GLN
46	BW	24	GLN
46	BW	40	ASN
48	BI	41	ASN
48	BI	51	GLN
48	BI	111	GLN
48	BI	119	HIS
49	BR	6	HIS
49	BR	19	HIS
49	BR	33	GLN
49	BR	42	HIS
49	BR	59	HIS
49	BR	89	HIS
49	BR	96	GLN
37	BK	31	ASN
50	BQ	58	GLN
50	BQ	75	HIS
50	BQ	131	GLN
50	BQ	136	HIS
52	Bj	37	GLN
53	BD	44	GLN
53	BD	93	HIS
53	BD	123	ASN

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Mol	Chain	Res	Type
53	BD	213	ASN
53	BD	214	HIS
53	BD	229	HIS
53	BD	235	HIS
54	BF	74	HIS
54	BF	112	ASN
54	BF	149	GLN
54	BF	156	GLN
55	BZ	21	ASN
24	B6	11	ASN
56	BP	10	ASN
56	BP	23	ASN
56	BP	110	ASN
57	BM	87	GLN
57	BM	97	GLN
57	BM	110	ASN
57	BM	154	HIS
57	BM	174	ASN
57	BM	189	ASN
58	BS	70	GLN
58	BS	97	ASN
59	Bd	35	HIS
60	BN	38	ASN
60	BN	56	GLN
60	BN	59	GLN
60	BN	60	ASN
60	BN	70	ASN
60	BN	76	ASN
60	BN	81	ASN
60	BN	83	HIS
60	BN	97	ASN
60	BN	130	GLN
60	BN	170	ASN
62	Bc	17	GLN
62	Bc	18	HIS
62	Bc	28	ASN
62	Bc	30	ASN
63	BJ	47	HIS
63	BJ	102	ASN
64	Bl	15	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3016/3018 (99%)	472 (15%)	25 (0%)
2	2	1496/1512 (98%)	165 (11%)	3 (0%)
3	3	125/128 (97%)	16 (12%)	0
66	sd	8/9 (88%)	1 (12%)	0
All	All	4645/4667 (99%)	654 (14%)	28 (0%)

All (654) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	12	G
1	1	28	A
1	1	39	A
1	1	43	A
1	1	51	A
1	1	52	G
1	1	53	G
1	1	54	G
1	1	56	C
1	1	57	A
1	1	58	A
1	1	59	C
1	1	69	U
1	1	75	G
1	1	82	C
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	126	C

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Mol	Chain	Res	Type
1	1	138	G
1	1	148	C
1	1	154	G
1	1	160	C
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	214	C
1	1	231	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	246	G
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	264	G
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	280	G
1	1	285	A
1	1	300	A
1	1	317	A
1	1	319	G
1	1	320	A
1	1	326	A
1	1	332	A

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Mol	Chain	Res	Type
1	1	333	A
1	1	337	A
1	1	352	G
1	1	370	G
1	1	392	A
1	1	393	C
1	1	413	G
1	1	416	G
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	440	G
1	1	447	A
1	1	448	A
1	1	449	G
1	1	456	U
1	1	466	C
1	1	484	G
1	1	485	A
1	1	493	G
1	1	501	A
1	1	507	G
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	560	G
1	1	565	G
1	1	573	U
1	1	608	A
1	1	611	A
1	1	621	G
1	1	635	G
1	1	657	A
1	1	661	C

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Mol	Chain	Res	Type
1	1	683	A
1	1	684	G
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	747	G
1	1	769	C
1	1	781	A
1	1	785	G
1	1	789	OMG
1	1	792	A
1	1	809	A
1	1	849	C
1	1	851	U
1	1	865	C
1	1	866	C
1	1	867	U
1	1	868	C
1	1	869	G
1	1	870	A
1	1	871	G
1	1	893	A
1	1	917	A
1	1	925	A
1	1	926	A
1	1	935	U
1	1	963	A
1	1	965	C
1	1	975	G
1	1	979	C
1	1	983	C
1	1	993	U
1	1	998	U
1	1	1026	G
1	1	1027	G
1	1	1033	A
1	1	1035	G
1	1	1036	G

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Mol	Chain	Res	Type
1	1	1040	A
1	1	1042	C
1	1	1043	G
1	1	1053	A
1	1	1056	G
1	1	1063	C
1	1	1073	C
1	1	1079	G
1	1	1081	A
1	1	1096	G
1	1	1101	A
1	1	1111	G
1	1	1118	A
1	1	1122	A
1	1	1129	G
1	1	1131	G
1	1	1132	C
1	1	1133	A
1	1	1135	G
1	1	1136	G
1	1	1140	G
1	1	1141	A
1	1	1145	C
1	1	1147	C
1	1	1148	C
1	1	1159	U
1	1	1162	A
1	1	1164	C
1	1	1199	G
1	1	1200	G
1	1	1221	C
1	1	1225	G
1	1	1231	A
1	1	1234	A
1	1	1240	G
1	1	1241	A
1	1	1252	G
1	1	1259	A
1	1	1261	G
1	1	1262	U
1	1	1263	G
1	1	1272	G

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Mol	Chain	Res	Type
1	1	1280	C
1	1	1281	C
1	1	1282	A
1	1	1288	U
1	1	1295	G
1	1	1300	U
1	1	1301	A
1	1	1303	A
1	1	1304	C
1	1	1305	A
1	1	1306	G
1	1	1307	C
1	1	1308	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	1352	C
1	1	1353	A
1	1	1359	C
1	1	1361	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	1370	C
1	1	1371	C
1	1	1372	G
1	1	1387	G
1	1	1389	C
1	1	1390	G
1	1	1397	A
1	1	1411	G

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Mol	Chain	Res	Type
1	1	1431	U
1	1	1433	G
1	1	1443	C
1	1	1470	G
1	1	1514	C
1	1	1520	G
1	1	1533	U
1	1	1560	A
1	1	1561	G
1	1	1577	A
1	1	1578	G
1	1	1580	C
1	1	1601	U
1	1	1630	G
1	1	1633	C
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	1805	C
1	1	1806	G
1	1	1807	U
1	1	1808	U
1	1	1809	A
1	1	1810	G
1	1	1830	G

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Mol	Chain	Res	Type
1	1	1840	A
1	1	1856	U
1	1	1857	U
1	1	1862	U
1	1	1883	A
1	1	1890	C
1	1	1891	A
1	1	1895	G
1	1	1896	C
1	1	1908	A
1	1	1920	U
1	1	1921	G
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	1988	C
1	1	1996	U
1	1	1997	A
1	1	2020	G
1	1	2029	A
1	1	2056	C
1	1	2085	A
1	1	2103	U
1	1	2119	A
1	1	2135	C
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	2170	G
1	1	2171	G
1	1	2178	A
1	1	2179	A
1	1	2181	U
1	1	2196	U

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Mol	Chain	Res	Type
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	2267	G
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	2299	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	2339	C
1	1	2340	G
1	1	2341	G
1	1	2342	C
1	1	2345	G
1	1	2347	G
1	1	2348	G
1	1	2350	G
1	1	2351	C
1	1	2352	G
1	1	2353	C
1	1	2354	A
1	1	2355	G
1	1	2356	C
1	1	2357	G
1	1	2358	U
1	1	2362	C
1	1	2363	G
1	1	2366	A
1	1	2368	G
1	1	2372	C

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Mol	Chain	Res	Type
1	1	2373	G
1	1	2376	G
1	1	2385	C
1	1	2386	C
1	1	2387	G
1	1	2388	G
1	1	2397	G
1	1	2398	A
1	1	2403	U
1	1	2405	C
1	1	2406	A
1	1	2410	G
1	1	2411	A
1	1	2418	C
1	1	2420	A
1	1	2425	U
1	1	2430	G
1	1	2431	C
1	1	2432	G
1	1	2438	A
1	1	2446	A
1	1	2455	A
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	2550	U
1	1	2551	A
1	1	2553	A
1	1	2556	G
1	1	2566	A
1	1	2567	A
1	1	2571	G

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Mol	Chain	Res	Type
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	2626	A
1	1	2636	C
1	1	2659	G
1	1	2664	A
1	1	2665	A
1	1	2666	A
1	1	2673	C
1	1	2677	G
1	1	2680	A
1	1	2691	G
1	1	2696	G
1	1	2700	G
1	1	2705	C
1	1	2706	C
1	1	2707	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
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	2817	U
1	1	2818	U
1	1	2831	G
1	1	2834	A
1	1	2845	U
1	1	2846	A
1	1	2853	G

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Mol	Chain	Res	Type
1	1	2861	U
1	1	2877	A
1	1	2878	G
1	1	2885	U
1	1	2896	G
1	1	2906	G
1	1	2922	U
1	1	2944	C
1	1	2945	G
1	1	2963	A
1	1	2964	G
1	1	2978	A
1	1	2987	A
1	1	2995	A
1	1	2996	G
1	1	3006	A
1	1	3021	U
1	1	3022	C
2	2	45	U
2	2	52	C
2	2	54	G
2	2	57	U
2	2	59	A
2	2	66	C
2	2	72	A
2	2	76	G
2	2	86	U
2	2	87	C
2	2	88	U
2	2	89	G
2	2	90	G
2	2	91	G
2	2	115	A
2	2	116	A
2	2	117	C
2	2	126	A
2	2	128	C
2	2	154	G
2	2	189	A
2	2	196	G
2	2	211	A
2	2	212	G

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Mol	Chain	Res	Type
2	2	219	G
2	2	222	A
2	2	223	G
2	2	224	G
2	2	225	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	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	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
2	2	424	C
2	2	425	U
2	2	426	G
2	2	436	U
2	2	465	G
2	2	477	G
2	2	484	G
2	2	496	G
2	2	497	U
2	2	513	A
2	2	530	U
2	2	533	G
2	2	539	A
2	2	542	C
2	2	562	A

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Mol	Chain	Res	Type
2	2	600	G
2	2	609	A
2	2	620	U
2	2	632	A
2	2	642	U
2	2	654	A
2	2	689	G
2	2	690	U
2	2	691	G
2	2	715	G
2	2	722	G
2	2	744	A
2	2	760	U
2	2	761	A
2	2	782	A
2	2	784	G
2	2	786	A
2	2	788	G
2	2	795	A
2	2	814	A
2	2	861	G
2	2	885	A
2	2	897	G
2	2	905	C
2	2	932	U
2	2	941	A
2	2	943	G
2	2	946	G
2	2	947	G
2	2	949	A
2	2	968	G
2	2	975	G
2	2	977	A
2	2	981	C
2	2	984	G
2	2	990	G
2	2	991	G
2	2	996	G
2	2	997	C
2	2	999	G
2	2	1000	G
2	2	1001	A

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Mol	Chain	Res	Type
2	2	1004	C
2	2	1005	G
2	2	1008	G
2	2	1030	U
2	2	1035	U
2	2	1059	G
2	2	1060	U
2	2	1066	A
2	2	1092	G
2	2	1107	U
2	2	1108	C
2	2	1133	U
2	2	1148	G
2	2	1155	G
2	2	1157	G
2	2	1158	G
2	2	1170	A
2	2	1171	G
2	2	1186	A
2	2	1187	A
2	2	1199	A
2	2	1201	A
2	2	1212	A
2	2	1215	G
2	2	1222	A
2	2	1232	C
2	2	1253	A
2	2	1254	A
2	2	1261	A
2	2	1274	G
2	2	1276	U
2	2	1279	G
2	2	1294	C
2	2	1310	U
2	2	1312	G
2	2	1327	G
2	2	1338	U
2	2	1344	G
2	2	1353	G
2	2	1371	C
2	2	1393	G
2	2	1395	G

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Mol	Chain	Res	Type
2	2	1397	G
2	2	1421	U
2	2	1427	G
2	2	1454	G
2	2	1456	G
2	2	1461	A
2	2	1466	G
2	2	1471	A
2	2	1472	A
2	2	1475	U
2	2	1486	G
2	2	1498	5MC
2	2	1499	G
2	2	1502	C
2	2	1503	A
3	3	5	C
3	3	24	G
3	3	25	C
3	3	26	C
3	3	30	C
3	3	44	G
3	3	53	A
3	3	56	U
3	3	57	A
3	3	58	A
3	3	60	C
3	3	79	G
3	3	89	C
3	3	95	G
3	3	115	G
3	3	125	A
66	sd	12	A

All (28) 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	250	U

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Mol	Chain	Res	Type
1	1	428	U
1	1	656	A
1	1	866	C
1	1	867	U
1	1	869	G
1	1	870	A
1	1	992	C
1	1	1035	G
1	1	1288	U
1	1	1303	A
1	1	1363	U
1	1	1364	C
1	1	1731	U
1	1	2341	G
1	1	2367	G
1	1	2455	A
1	1	2733	5MC
1	1	2986	U
1	1	3021	U
2	2	464	A
2	2	688	A
2	2	1106	C

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	6MZ	2	1469	67,2	22,25,26	1.48	4 (18%)	30,36,39	2.22	10 (33%)
1	4AC	1	1557	1	21,24,25	1.03	2 (9%)	29,34,37	1.34	4 (13%)
2	4AC	2	379	2	21,24,25	1.01	2 (9%)	29,34,37	1.39	4 (13%)
1	4AC	1	2027	1	21,24,25	1.03	2 (9%)	29,34,37	1.38	4 (13%)
2	OMG	2	657	2	23,26,27	1.23	3 (13%)	33,38,41	1.97	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	1	229	1	21,24,25	1.04	2 (9%)	29,34,37	1.40	4 (13%)
2	4AC	2	751	2	21,24,25	1.03	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	694	1	21,24,25	1.02	1 (4%)	29,34,37	1.37	4 (13%)
1	4AC	1	357	1	21,24,25	1.03	2 (9%)	29,34,37	1.39	4 (13%)
2	4AC	2	731	2	21,24,25	1.02	2 (9%)	29,34,37	1.38	4 (13%)
2	UR3	2	1467	2	19,22,23	0.97	0	26,32,35	1.47	2 (7%)
1	4AC	1	2585	1	21,24,25	1.05	2 (9%)	29,34,37	1.79	6 (20%)
2	OMG	2	680	2	23,26,27	1.21	3 (13%)	33,38,41	1.96	6 (18%)
2	4AC	2	1479	2	21,24,25	1.00	2 (9%)	29,34,37	1.43	4 (13%)
1	4AC	1	981	1	21,24,25	1.01	2 (9%)	29,34,37	1.41	4 (13%)
1	4AC	1	1765	1	21,24,25	1.04	2 (9%)	29,34,37	1.38	4 (13%)
2	4AC	2	839	2	21,24,25	1.03	2 (9%)	29,34,37	1.53	5 (17%)
2	OMG	2	519	2	23,26,27	1.19	3 (13%)	33,38,41	1.96	6 (18%)
2	5MC	2	1202	2	18,22,23	0.98	2 (11%)	26,32,35	1.25	3 (11%)
2	4AC	2	848	2	21,24,25	1.01	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	922	1	21,24,25	1.03	2 (9%)	29,34,37	1.49	4 (13%)
1	4AC	1	2495	1	21,24,25	1.04	2 (9%)	29,34,37	1.37	4 (13%)
1	OMU	1	2784	1	19,22,23	1.18	2 (10%)	26,31,34	1.70	5 (19%)
1	4AC	1	1755	1	21,24,25	1.01	1 (4%)	29,34,37	1.67	4 (13%)
2	OMG	2	471	2	23,26,27	1.22	3 (13%)	33,38,41	1.94	6 (18%)
2	5MC	2	1505	66,2	18,22,23	0.98	2 (11%)	26,32,35	1.17	3 (11%)
2	5MC	2	535	2	18,22,23	0.93	2 (11%)	26,32,35	1.15	2 (7%)
1	4AC	1	1621	1	21,24,25	1.03	1 (4%)	29,34,37	1.40	4 (13%)
1	4AC	1	1293	1	21,24,25	1.04	2 (9%)	29,34,37	1.35	4 (13%)
2	5MC	2	1025	2	18,22,23	0.95	2 (11%)	26,32,35	1.11	2 (7%)
2	4AC	2	718	2	21,24,25	1.00	2 (9%)	29,34,37	1.39	4 (13%)
1	5MC	1	2733	1	18,22,23	0.98	1 (5%)	26,32,35	1.34	4 (15%)
1	4AC	1	136	1	21,24,25	1.03	1 (4%)	29,34,37	1.40	4 (13%)
1	4AC	1	1048	1	21,24,25	1.02	2 (9%)	29,34,37	1.44	4 (13%)
2	5MC	2	875	2	18,22,23	0.94	2 (11%)	26,32,35	1.17	3 (11%)
1	4AC	1	22	1	21,24,25	1.04	2 (9%)	29,34,37	1.40	4 (13%)
1	4AC	1	1460	1	21,24,25	1.02	2 (9%)	29,34,37	1.40	4 (13%)
1	OMG	1	789	1	23,26,27	1.25	3 (13%)	33,38,41	2.00	7 (21%)
2	4AC	2	319	2	21,24,25	1.01	2 (9%)	29,34,37	1.39	4 (13%)
1	4AC	1	829	1	21,24,25	1.03	2 (9%)	29,34,37	1.37	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	1	615	1	19,22,23	0.80	0	26,31,34	0.80	0
1	4AC	1	2570	1	21,24,25	1.02	1 (4%)	29,34,37	1.37	4 (13%)
1	4AC	1	1243	1	21,24,25	1.05	2 (9%)	29,34,37	1.44	4 (13%)
2	4AC	2	286	2	21,24,25	1.03	2 (9%)	29,34,37	1.34	4 (13%)
2	5MC	2	1374	2	18,22,23	0.93	2 (11%)	26,32,35	1.10	2 (7%)
1	4AC	1	533	1	21,24,25	1.03	1 (4%)	29,34,37	1.40	4 (13%)
2	5MC	2	1498	2	18,22,23	0.94	2 (11%)	26,32,35	1.25	4 (15%)
2	4AC	2	626	2	21,24,25	1.02	2 (9%)	29,34,37	1.40	4 (13%)
1	4AC	1	2925	1	21,24,25	1.02	1 (4%)	29,34,37	1.42	4 (13%)
1	4AC	1	1662	1	21,24,25	1.03	2 (9%)	29,34,37	1.40	4 (13%)
1	4AC	1	1885	1	21,24,25	1.01	2 (9%)	29,34,37	1.39	4 (13%)
1	4AC	1	1934	1	21,24,25	1.01	2 (9%)	29,34,37	1.39	4 (13%)
2	4AC	2	1147	2	21,24,25	1.04	1 (4%)	29,34,37	1.54	5 (17%)
1	4AC	1	835	1	21,24,25	1.03	1 (4%)	29,34,37	1.40	4 (13%)
2	OMG	2	934	2	23,26,27	1.22	3 (13%)	33,38,41	1.94	6 (18%)
1	5MC	1	2163	1	18,22,23	0.94	2 (11%)	26,32,35	1.26	2 (7%)
2	5MC	2	1496	2	18,22,23	0.94	2 (11%)	26,32,35	1.18	2 (7%)
1	4AC	1	161	1	21,24,25	1.03	2 (9%)	29,34,37	1.40	4 (13%)
2	OMU	2	830	2	19,22,23	1.27	4 (21%)	26,31,34	1.69	5 (19%)
2	4AC	2	590	2	21,24,25	1.02	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	2908	1	21,24,25	1.04	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	2287	1	21,24,25	1.01	1 (4%)	29,34,37	1.43	4 (13%)
1	5MC	1	2183	1	18,22,23	0.93	2 (11%)	26,32,35	1.17	2 (7%)
2	OMG	2	873	2	23,26,27	1.21	3 (13%)	33,38,41	1.96	6 (18%)
2	4AC	2	1028	2	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
2	MA6	2	1488	2	23,26,27	1.45	4 (17%)	34,38,41	2.11	10 (29%)
1	OMG	1	2138	1	23,26,27	1.20	3 (13%)	33,38,41	1.91	6 (18%)
2	OMU	2	20	2	19,22,23	1.23	2 (10%)	26,31,34	1.81	5 (19%)
1	OMG	1	2678	1	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
1	4AC	1	1222	67,1	21,24,25	1.02	1 (4%)	29,34,37	1.44	4 (13%)
2	OMU	2	774	2	19,22,23	1.22	3 (15%)	26,31,34	1.73	4 (15%)
1	LHH	1	616	1	22,25,26	0.30	0	29,35,38	0.46	0
1	4AC	1	1617	1	21,24,25	1.02	1 (4%)	29,34,37	1.40	4 (13%)
1	4AC	1	211	1	21,24,25	1.03	2 (9%)	29,34,37	1.41	4 (13%)
2	LHH	2	250	2	22,25,26	0.30	0	29,35,38	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMG	2	1069	2	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
1	OMG	1	328	1	23,26,27	1.21	3 (13%)	33,38,41	1.91	6 (18%)
2	OMC	2	773	2	19,22,23	0.82	0	26,31,34	0.83	0
1	4AC	1	1594	67,1	21,24,25	1.01	1 (4%)	29,34,37	1.43	4 (13%)
1	5MC	1	2203	1	18,22,23	0.95	2 (11%)	26,32,35	1.20	2 (7%)
2	4AC	2	546	2	21,24,25	0.99	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	243	1	21,24,25	1.02	1 (4%)	29,34,37	1.39	4 (13%)
2	LHH	2	1041	2	22,25,26	0.31	0	29,35,38	0.49	0
3	4AC	3	32	3	21,24,25	1.04	1 (4%)	29,34,37	1.40	4 (13%)
2	4AC	2	868	2	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
2	OMU	2	1380	2	19,22,23	1.28	4 (21%)	26,31,34	1.71	4 (15%)
1	OMC	1	1948	1	19,22,23	0.81	0	26,31,34	0.74	0
1	4AC	1	2865	1	21,24,25	1.03	1 (4%)	29,34,37	1.39	4 (13%)
2	4AC	2	851	2	21,24,25	1.03	2 (9%)	29,34,37	1.36	4 (13%)
1	OMG	1	2144	1	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
2	OMC	2	1376	2	19,22,23	0.81	0	26,31,34	0.76	0
2	OMG	2	913	2	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
1	4AC	1	1873	1	21,24,25	1.02	1 (4%)	29,34,37	1.39	4 (13%)
2	4AC	2	1184	2	21,24,25	1.05	2 (9%)	29,34,37	1.56	4 (13%)
1	OMG	1	2147	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	4AC	1	2992	1	21,24,25	1.06	1 (4%)	29,34,37	0.86	2 (6%)
1	A2M	1	2173	1	22,25,26	1.46	4 (18%)	31,36,39	2.02	8 (25%)
1	4AC	1	91	1	21,24,25	1.04	2 (9%)	29,34,37	1.58	4 (13%)
1	4AC	1	2001	1	21,24,25	1.07	2 (9%)	29,34,37	1.50	4 (13%)
2	OMU	2	787	2	19,22,23	1.23	2 (10%)	26,31,34	1.80	5 (19%)
1	4AC	1	1867	1	21,24,25	1.04	2 (9%)	29,34,37	1.37	4 (13%)
1	A2M	1	1055	1	22,25,26	1.47	4 (18%)	31,36,39	2.11	10 (32%)
2	OMC	2	846	2	19,22,23	0.82	0	26,31,34	0.79	0
1	4AC	1	2642	1	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	2329	1	21,24,25	1.03	2 (9%)	29,34,37	1.39	4 (13%)
2	4AC	2	511	2	21,24,25	1.04	2 (9%)	29,34,37	1.34	4 (13%)
2	4AC	2	17	2	21,24,25	1.03	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	1	2249	1	21,24,25	1.04	2 (9%)	29,34,37	1.41	4 (13%)
1	4AC	1	2608	1	21,24,25	1.07	2 (9%)	29,34,37	1.76	6 (20%)
2	OMC	2	1040	2	19,22,23	0.84	0	26,31,34	0.96	1 (3%)
1	4AC	1	2083	1	21,24,25	1.04	2 (9%)	29,34,37	1.39	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMU	2	64	2	19,22,23	1.22	3 (15%)	26,31,34	1.70	5 (19%)
1	4AC	1	2718	1	21,24,25	1.01	1 (4%)	29,34,37	1.43	4 (13%)
1	4AC	1	1962	1	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	641	1	21,24,25	1.04	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	1554	1	21,24,25	1.02	1 (4%)	29,34,37	1.41	4 (13%)
1	4AC	1	458	1	21,24,25	1.00	1 (4%)	29,34,37	1.40	4 (13%)
1	4AC	1	1938	1	21,24,25	1.04	2 (9%)	29,34,37	1.38	4 (13%)
2	4AC	2	394	2	21,24,25	1.00	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	1878	1	21,24,25	1.01	1 (4%)	29,34,37	1.53	4 (13%)
2	4AC	2	53	2	21,24,25	1.02	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	1695	1	21,24,25	1.03	2 (9%)	29,34,37	1.37	4 (13%)
2	A2M	2	373	2	22,25,26	1.46	4 (18%)	31,36,39	2.11	9 (29%)
2	4AC	2	1233	2	21,24,25	1.02	1 (4%)	29,34,37	1.42	4 (13%)
2	4AC	2	636	2	21,24,25	1.01	2 (9%)	29,34,37	1.48	4 (13%)
2	4AC	2	828	2	21,24,25	1.00	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	802	1	21,24,25	1.02	1 (4%)	29,34,37	1.45	4 (13%)
1	4AC	1	2548	1	21,24,25	1.02	2 (9%)	29,34,37	1.50	4 (13%)
1	5MC	1	2198	1	18,22,23	0.95	2 (11%)	26,32,35	1.11	2 (7%)
1	4AC	1	341	1	21,24,25	1.04	2 (9%)	29,34,37	1.37	4 (13%)
2	4AC	2	957	2	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
2	4AC	2	303	2	21,24,25	1.02	2 (9%)	29,34,37	1.37	4 (13%)
1	5MC	1	2093	1	18,22,23	0.94	2 (11%)	26,32,35	1.12	2 (7%)
1	5MC	1	2162	1	18,22,23	0.96	2 (11%)	26,32,35	1.23	2 (7%)
1	4AC	1	3004	1	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	1068	1	21,24,25	1.05	2 (9%)	29,34,37	1.54	4 (13%)
1	4AC	1	451	1	21,24,25	1.05	2 (9%)	29,34,37	1.47	4 (13%)
1	4AC	1	1780	1	21,24,25	1.02	1 (4%)	29,34,37	1.62	4 (13%)
2	4AC	2	703	2	21,24,25	1.01	2 (9%)	29,34,37	1.43	4 (13%)
1	4AC	1	60	1	21,24,25	1.01	2 (9%)	29,34,37	1.43	5 (17%)
1	4AC	1	1065	1	21,24,25	1.01	1 (4%)	29,34,37	1.41	4 (13%)
1	4AC	1	2960	1	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	1	2937	67,1	21,24,25	1.02	2 (9%)	29,34,37	1.61	4 (13%)
2	OMU	2	1177	2	19,22,23	1.22	3 (15%)	26,31,34	1.69	5 (19%)
1	4AC	1	2062	1	21,24,25	1.03	2 (9%)	29,34,37	1.38	4 (13%)
2	4AC	2	1239	2	21,24,25	1.02	1 (4%)	29,34,37	1.35	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	1	923	67,1	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
1	4AC	1	1667	1	21,24,25	1.02	1 (4%)	29,34,37	1.37	4 (13%)
2	4AC	2	479	2	21,24,25	1.01	2 (9%)	29,34,37	1.39	4 (13%)
2	B8H	2	938	2	19,22,23	0.63	1 (5%)	22,32,35	0.71	1 (4%)
1	4AC	1	1550	1	21,24,25	1.02	1 (4%)	29,34,37	1.39	4 (13%)
2	OMG	2	467	2	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
1	4AC	1	2136	1	21,24,25	1.04	1 (4%)	29,34,37	1.46	5 (17%)
2	OMC	2	129	2	19,22,23	0.82	0	26,31,34	0.80	0
1	4AC	1	2545	1	21,24,25	1.05	2 (9%)	29,34,37	1.46	4 (13%)
2	5MC	2	693	2	18,22,23	0.93	2 (11%)	26,32,35	1.10	2 (7%)
2	MA6	2	1487	2	23,26,27	1.50	4 (17%)	34,38,41	2.18	11 (32%)
1	4AC	1	2966	1	21,24,25	1.04	2 (9%)	29,34,37	1.49	4 (13%)
1	4AC	1	314	1	21,24,25	1.03	1 (4%)	29,34,37	1.39	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6MZ	2	1469	67,2	-	0/9/27/28	0/3/3/3
1	4AC	1	1557	1	-	0/11/29/30	0/2/2/2
2	4AC	2	379	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2027	1	-	0/11/29/30	0/2/2/2
2	OMG	2	657	2	-	0/9/27/28	0/3/3/3
1	4AC	1	229	1	-	0/11/29/30	0/2/2/2
2	4AC	2	751	2	-	0/11/29/30	0/2/2/2
1	4AC	1	694	1	-	0/11/29/30	0/2/2/2
1	4AC	1	357	1	-	0/11/29/30	0/2/2/2
2	4AC	2	731	2	-	0/11/29/30	0/2/2/2
2	UR3	2	1467	2	-	0/7/25/26	0/2/2/2
1	4AC	1	2585	1	-	3/11/29/30	0/2/2/2
2	OMG	2	680	2	-	0/9/27/28	0/3/3/3
2	4AC	2	1479	2	-	0/11/29/30	0/2/2/2
1	4AC	1	981	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1765	1	-	0/11/29/30	0/2/2/2
2	4AC	2	839	2	-	0/11/29/30	0/2/2/2
2	OMG	2	519	2	-	0/9/27/28	0/3/3/3
2	5MC	2	1202	2	-	0/7/25/26	0/2/2/2
2	4AC	2	848	2	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	1	922	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2495	1	-	0/11/29/30	0/2/2/2
1	OMU	1	2784	1	-	0/9/27/28	0/2/2/2
1	4AC	1	1755	1	-	1/11/29/30	0/2/2/2
2	OMG	2	471	2	-	0/9/27/28	0/3/3/3
2	5MC	2	1505	66,2	-	0/7/25/26	0/2/2/2
2	5MC	2	535	2	-	0/7/25/26	0/2/2/2
1	4AC	1	1621	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1293	1	-	0/11/29/30	0/2/2/2
2	5MC	2	1025	2	-	0/7/25/26	0/2/2/2
2	4AC	2	718	2	-	0/11/29/30	0/2/2/2
1	5MC	1	2733	1	-	6/7/25/26	0/2/2/2
1	4AC	1	136	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1048	1	-	0/11/29/30	0/2/2/2
2	5MC	2	875	2	-	0/7/25/26	0/2/2/2
1	4AC	1	22	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1460	1	-	0/11/29/30	0/2/2/2
1	OMG	1	789	1	-	2/9/27/28	0/3/3/3
2	4AC	2	319	2	-	0/11/29/30	0/2/2/2
1	4AC	1	829	1	-	0/11/29/30	0/2/2/2
1	OMC	1	615	1	-	0/9/27/28	0/2/2/2
1	4AC	1	2570	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1243	1	-	0/11/29/30	0/2/2/2
2	4AC	2	286	2	-	0/11/29/30	0/2/2/2
2	5MC	2	1374	2	-	1/7/25/26	0/2/2/2
1	4AC	1	533	1	-	0/11/29/30	0/2/2/2
2	5MC	2	1498	2	-	3/7/25/26	0/2/2/2
2	4AC	2	626	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2925	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1662	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1885	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1934	1	-	0/11/29/30	0/2/2/2
2	4AC	2	1147	2	-	0/11/29/30	0/2/2/2
1	4AC	1	835	1	-	0/11/29/30	0/2/2/2
2	OMG	2	934	2	-	1/9/27/28	0/3/3/3
1	5MC	1	2163	1	-	0/7/25/26	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	OMU	2	830	2	-	1/9/27/28	0/2/2/2
2	4AC	2	590	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2908	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2287	1	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1	2183	1	-	0/7/25/26	0/2/2/2
2	OMG	2	873	2	-	1/9/27/28	0/3/3/3
2	4AC	2	1028	2	-	0/11/29/30	0/2/2/2
2	MA6	2	1488	2	-	2/11/29/30	0/3/3/3
1	OMG	1	2138	1	-	0/9/27/28	0/3/3/3
2	OMU	2	20	2	-	6/9/27/28	0/2/2/2
1	OMG	1	2678	1	-	1/9/27/28	0/3/3/3
1	4AC	1	1222	67,1	-	0/11/29/30	0/2/2/2
2	OMU	2	774	2	-	0/9/27/28	0/2/2/2
1	LHH	1	616	1	-	0/13/31/32	0/2/2/2
1	4AC	1	1617	1	-	0/11/29/30	0/2/2/2
1	4AC	1	211	1	-	0/11/29/30	0/2/2/2
2	LHH	2	250	2	-	0/13/31/32	0/2/2/2
2	OMG	2	1069	2	-	2/9/27/28	0/3/3/3
1	OMG	1	328	1	-	0/9/27/28	0/3/3/3
2	OMC	2	773	2	-	0/9/27/28	0/2/2/2
1	4AC	1	1594	67,1	-	0/11/29/30	0/2/2/2
1	5MC	1	2203	1	-	0/7/25/26	0/2/2/2
2	4AC	2	546	2	-	0/11/29/30	0/2/2/2
1	4AC	1	243	1	-	0/11/29/30	0/2/2/2
2	LHH	2	1041	2	-	0/13/31/32	0/2/2/2
3	4AC	3	32	3	-	1/11/29/30	0/2/2/2
2	4AC	2	868	2	-	0/11/29/30	0/2/2/2
2	OMU	2	1380	2	-	0/9/27/28	0/2/2/2
1	OMC	1	1948	1	-	0/9/27/28	0/2/2/2
1	4AC	1	2865	1	-	0/11/29/30	0/2/2/2
2	4AC	2	851	2	-	0/11/29/30	0/2/2/2
1	OMG	1	2144	1	-	2/9/27/28	0/3/3/3
2	OMC	2	1376	2	-	0/9/27/28	0/2/2/2
2	OMG	2	913	2	-	0/9/27/28	0/3/3/3
1	4AC	1	1873	1	-	0/11/29/30	0/2/2/2
2	4AC	2	1184	2	-	0/11/29/30	0/2/2/2
1	OMG	1	2147	1	-	2/9/27/28	0/3/3/3
1	4AC	1	2992	1	-	2/11/29/30	0/2/2/2
1	A2M	1	2173	1	-	0/9/27/28	0/3/3/3
1	4AC	1	91	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2001	1	-	0/11/29/30	0/2/2/2
2	OMU	2	787	2	-	4/9/27/28	0/2/2/2
1	4AC	1	1867	1	-	0/11/29/30	0/2/2/2
1	A2M	1	1055	1	-	0/9/27/28	0/3/3/3
2	OMC	2	846	2	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	1	2642	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2329	1	-	0/11/29/30	0/2/2/2
2	4AC	2	511	2	-	0/11/29/30	0/2/2/2
2	4AC	2	17	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2249	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2608	1	-	3/11/29/30	0/2/2/2
2	OMC	2	1040	2	-	1/9/27/28	0/2/2/2
1	4AC	1	2083	1	-	0/11/29/30	0/2/2/2
2	OMU	2	64	2	-	0/9/27/28	0/2/2/2
1	4AC	1	2718	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1962	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	1554	1	-	0/11/29/30	0/2/2/2
1	4AC	1	458	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1938	1	-	0/11/29/30	0/2/2/2
2	4AC	2	394	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1878	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	1695	1	-	0/11/29/30	0/2/2/2
2	A2M	2	373	2	-	0/9/27/28	0/3/3/3
2	4AC	2	1233	2	-	0/11/29/30	0/2/2/2
2	4AC	2	636	2	-	0/11/29/30	0/2/2/2
2	4AC	2	828	2	-	0/11/29/30	0/2/2/2
1	4AC	1	802	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2548	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	341	1	-	0/11/29/30	0/2/2/2
2	4AC	2	957	2	-	0/11/29/30	0/2/2/2
2	4AC	2	303	2	-	0/11/29/30	0/2/2/2
1	5MC	1	2093	1	-	0/7/25/26	0/2/2/2
1	5MC	1	2162	1	-	0/7/25/26	0/2/2/2
1	4AC	1	3004	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1068	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	1780	1	-	0/11/29/30	0/2/2/2
2	4AC	2	703	2	-	0/11/29/30	0/2/2/2
1	4AC	1	60	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	2960	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2937	67,1	-	1/11/29/30	0/2/2/2
2	OMU	2	1177	2	-	0/9/27/28	0/2/2/2
1	4AC	1	2062	1	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4AC	2	1239	2	-	0/11/29/30	0/2/2/2
1	OMG	1	923	67,1	-	2/9/27/28	0/3/3/3
1	4AC	1	1667	1	-	0/11/29/30	0/2/2/2
2	4AC	2	479	2	-	0/11/29/30	0/2/2/2
2	B8H	2	938	2	-	1/7/25/26	0/2/2/2
1	4AC	1	1550	1	-	0/11/29/30	0/2/2/2
2	OMG	2	467	2	-	0/9/27/28	0/3/3/3
1	4AC	1	2136	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	2545	1	-	0/11/29/30	0/2/2/2
2	5MC	2	693	2	-	0/7/25/26	0/2/2/2
2	MA6	2	1487	2	-	0/11/29/30	0/3/3/3
1	4AC	1	2966	1	-	0/11/29/30	0/2/2/2
1	4AC	1	314	1	-	0/11/29/30	0/2/2/2

All (298) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1469	6MZ	C5-C4	4.58	1.47	1.39
2	2	1487	MA6	C5-C4	4.52	1.47	1.39
1	1	1055	A2M	C5-C4	4.52	1.47	1.39
1	1	2173	A2M	C5-C4	4.50	1.47	1.39
2	2	1488	MA6	C5-C4	4.41	1.47	1.39
2	2	373	A2M	C5-C4	4.41	1.47	1.39
1	1	2992	4AC	C5-C4	3.25	1.47	1.40
2	2	657	OMG	C5-C4	3.18	1.47	1.38
1	1	789	OMG	C5-C4	3.17	1.47	1.38
1	1	2138	OMG	C5-C4	3.15	1.47	1.38
1	1	2144	OMG	C5-C4	3.14	1.47	1.38
2	2	471	OMG	C5-C4	3.13	1.47	1.38
1	1	328	OMG	C5-C4	3.12	1.47	1.38
1	1	923	OMG	C5-C4	3.10	1.47	1.38
1	1	1867	4AC	C5-C4	3.09	1.47	1.40
1	1	829	4AC	C5-C4	3.07	1.47	1.40
1	1	2495	4AC	C5-C4	3.07	1.47	1.40
1	1	2642	4AC	C5-C4	3.07	1.47	1.40
1	1	641	4AC	C5-C4	3.06	1.47	1.40
1	1	2733	5MC	C6-C5	3.06	1.39	1.34
1	1	2678	OMG	C5-C4	3.06	1.47	1.38
1	1	229	4AC	C5-C4	3.06	1.47	1.40
1	1	22	4AC	C5-C4	3.06	1.47	1.40
2	2	680	OMG	C5-C4	3.06	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2908	4AC	C5-C4	3.05	1.47	1.40
2	2	873	OMG	C5-C4	3.05	1.47	1.38
1	1	1695	4AC	C5-C4	3.04	1.47	1.40
1	1	341	4AC	C5-C4	3.04	1.47	1.40
1	1	1293	4AC	C5-C4	3.03	1.47	1.40
1	1	533	4AC	C5-C4	3.03	1.47	1.40
1	1	2865	4AC	C5-C4	3.03	1.47	1.40
1	1	3004	4AC	C5-C4	3.03	1.47	1.40
1	1	2147	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
1	1	314	4AC	C5-C4	3.02	1.47	1.40
1	1	211	4AC	C5-C4	3.02	1.47	1.40
2	2	511	4AC	C5-C4	3.02	1.47	1.40
1	1	1667	4AC	C5-C4	3.02	1.47	1.40
1	1	1557	4AC	C5-C4	3.02	1.47	1.40
1	1	1938	4AC	C5-C4	3.02	1.47	1.40
2	2	751	4AC	C5-C4	3.01	1.47	1.40
1	1	1621	4AC	C5-C4	3.01	1.47	1.40
1	1	136	4AC	C5-C4	3.01	1.47	1.40
1	1	357	4AC	C5-C4	3.01	1.47	1.40
1	1	694	4AC	C5-C4	3.00	1.47	1.40
1	1	1873	4AC	C5-C4	3.00	1.47	1.40
1	1	1460	4AC	C5-C4	3.00	1.47	1.40
2	2	1239	4AC	C5-C4	3.00	1.47	1.40
1	1	1617	4AC	C5-C4	2.99	1.47	1.40
1	1	2083	4AC	C5-C4	2.99	1.47	1.40
1	1	2329	4AC	C5-C4	2.99	1.47	1.40
1	1	2570	4AC	C5-C4	2.99	1.47	1.40
2	2	467	OMG	C5-C4	2.99	1.47	1.38
1	1	1222	4AC	C5-C4	2.99	1.47	1.40
2	2	934	OMG	C5-C4	2.99	1.47	1.38
1	1	243	4AC	C5-C4	2.98	1.47	1.40
1	1	1662	4AC	C5-C4	2.98	1.47	1.40
2	2	851	4AC	C5-C4	2.98	1.47	1.40
2	2	913	OMG	C5-C4	2.98	1.47	1.38
2	2	286	4AC	C5-C4	2.98	1.47	1.40
3	3	32	4AC	C5-C4	2.98	1.47	1.40
1	1	2960	4AC	C5-C4	2.98	1.47	1.40
2	2	519	OMG	C5-C4	2.98	1.47	1.38
1	1	1962	4AC	C5-C4	2.98	1.47	1.40
1	1	2249	4AC	C5-C4	2.97	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1048	4AC	C5-C4	2.97	1.47	1.40
1	1	458	4AC	C5-C4	2.97	1.47	1.40
1	1	1065	4AC	C5-C4	2.97	1.47	1.40
2	2	1028	4AC	C5-C4	2.97	1.47	1.40
1	1	2027	4AC	C5-C4	2.97	1.47	1.40
1	1	2966	4AC	C5-C4	2.97	1.47	1.40
1	1	1550	4AC	C5-C4	2.97	1.47	1.40
1	1	2136	4AC	C5-C4	2.97	1.47	1.40
2	2	17	4AC	C5-C4	2.96	1.47	1.40
1	1	451	4AC	C5-C4	2.96	1.47	1.40
2	2	957	4AC	C5-C4	2.96	1.47	1.40
1	1	1554	4AC	C5-C4	2.96	1.47	1.40
2	2	868	4AC	C5-C4	2.96	1.47	1.40
1	1	2925	4AC	C5-C4	2.96	1.47	1.40
1	1	922	4AC	C5-C4	2.95	1.47	1.40
1	1	1878	4AC	C5-C4	2.95	1.47	1.40
2	2	1233	4AC	C5-C4	2.95	1.47	1.40
1	1	1594	4AC	C5-C4	2.95	1.47	1.40
1	1	1243	4AC	C5-C4	2.94	1.47	1.40
1	1	835	4AC	C5-C4	2.94	1.47	1.40
1	1	60	4AC	C5-C4	2.94	1.47	1.40
1	1	2718	4AC	C5-C4	2.94	1.47	1.40
1	1	802	4AC	C5-C4	2.94	1.47	1.40
2	2	590	4AC	C5-C4	2.94	1.47	1.40
1	1	2062	4AC	C5-C4	2.94	1.47	1.40
1	1	161	4AC	C5-C4	2.93	1.47	1.40
2	2	479	4AC	C5-C4	2.93	1.47	1.40
2	2	731	4AC	C5-C4	2.93	1.47	1.40
1	1	2287	4AC	C5-C4	2.93	1.47	1.40
1	1	1934	4AC	C5-C4	2.92	1.47	1.40
1	1	2548	4AC	C5-C4	2.92	1.47	1.40
1	1	1885	4AC	C5-C4	2.91	1.47	1.40
2	2	303	4AC	C5-C4	2.91	1.47	1.40
2	2	848	4AC	C5-C4	2.91	1.47	1.40
1	1	981	4AC	C5-C4	2.90	1.47	1.40
1	1	2545	4AC	C5-C4	2.90	1.47	1.40
2	2	53	4AC	C5-C4	2.90	1.47	1.40
2	2	828	4AC	C5-C4	2.90	1.47	1.40
2	2	626	4AC	C5-C4	2.89	1.47	1.40
1	1	1068	4AC	C5-C4	2.89	1.47	1.40
2	2	319	4AC	C5-C4	2.89	1.47	1.40
2	2	1487	MA6	C5-C6	2.87	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	394	4AC	C5-C4	2.87	1.47	1.40
1	1	2937	4AC	C5-C4	2.87	1.47	1.40
2	2	546	4AC	C5-C4	2.87	1.47	1.40
2	2	703	4AC	C5-C4	2.86	1.47	1.40
2	2	379	4AC	C5-C4	2.86	1.47	1.40
2	2	1184	4AC	C5-C4	2.85	1.46	1.40
1	1	91	4AC	C5-C4	2.83	1.46	1.40
2	2	636	4AC	C5-C4	2.83	1.46	1.40
2	2	718	4AC	C5-C4	2.82	1.46	1.40
1	1	2608	4AC	C5-C4	2.81	1.46	1.40
2	2	1202	5MC	C6-C5	2.80	1.39	1.34
2	2	1469	6MZ	C5-C6	2.79	1.49	1.41
2	2	1479	4AC	C5-C4	2.78	1.46	1.40
2	2	1147	4AC	C5-C4	2.78	1.46	1.40
1	1	2198	5MC	C6-C5	2.75	1.39	1.34
2	2	1505	5MC	C6-C5	2.75	1.39	1.34
2	2	1488	MA6	C5-C6	2.73	1.48	1.41
1	1	2585	4AC	C5-C4	2.72	1.46	1.40
1	1	2093	5MC	C6-C5	2.72	1.39	1.34
2	2	1380	OMU	C4-N3	-2.71	1.33	1.38
2	2	20	OMU	C4-N3	-2.71	1.33	1.38
1	1	1055	A2M	C5-C6	2.69	1.48	1.41
2	2	830	OMU	C4-N3	-2.67	1.33	1.38
1	1	1780	4AC	C5-C4	2.67	1.46	1.40
2	2	471	OMG	C6-N1	-2.66	1.33	1.38
2	2	787	OMU	C4-N3	-2.66	1.33	1.38
1	1	2162	5MC	C6-C5	2.66	1.39	1.34
1	1	1755	4AC	C5-C4	2.64	1.46	1.40
2	2	839	4AC	C5-C4	2.64	1.46	1.40
2	2	657	OMG	C6-N1	-2.63	1.34	1.38
2	2	1025	5MC	C6-C5	2.63	1.38	1.34
2	2	693	5MC	C6-C5	2.63	1.38	1.34
2	2	680	OMG	C6-N1	-2.63	1.34	1.38
2	2	873	OMG	C6-N1	-2.61	1.34	1.38
1	1	2163	5MC	C6-N1	-2.61	1.33	1.38
2	2	373	A2M	C5-C6	2.61	1.48	1.41
2	2	934	OMG	C6-N1	-2.60	1.34	1.38
2	2	64	OMU	C4-N3	-2.59	1.33	1.38
1	1	2173	A2M	C5-C6	2.58	1.48	1.41
1	1	2001	4AC	C4-N3	-2.58	1.28	1.32
2	2	774	OMU	C4-N3	-2.58	1.33	1.38
1	1	2183	5MC	C6-C5	2.58	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2144	OMG	C6-N1	-2.57	1.34	1.38
1	1	2203	5MC	C6-N1	-2.57	1.33	1.38
2	2	1374	5MC	C6-C5	2.57	1.38	1.34
2	2	1069	OMG	C6-N1	-2.57	1.34	1.38
1	1	2001	4AC	C5-C4	2.56	1.46	1.40
1	1	2678	OMG	C6-N1	-2.56	1.34	1.38
2	2	839	4AC	C4-N3	-2.56	1.28	1.32
1	1	328	OMG	C6-N1	-2.55	1.34	1.38
2	2	535	5MC	C6-C5	2.55	1.38	1.34
2	2	1496	5MC	C6-C5	2.54	1.38	1.34
2	2	1177	OMU	C4-N3	-2.53	1.34	1.38
2	2	875	5MC	C6-C5	2.53	1.38	1.34
2	2	1498	5MC	C6-C5	2.53	1.38	1.34
1	1	2147	OMG	C6-N1	-2.52	1.34	1.38
1	1	2138	OMG	C6-N1	-2.52	1.34	1.38
2	2	519	OMG	C6-N1	-2.52	1.34	1.38
1	1	2162	5MC	C6-N1	-2.51	1.33	1.38
1	1	923	OMG	C6-N1	-2.51	1.34	1.38
2	2	467	OMG	C6-N1	-2.50	1.34	1.38
1	1	2203	5MC	C6-C5	2.48	1.38	1.34
2	2	913	OMG	C6-N1	-2.45	1.34	1.38
1	1	2173	A2M	C8-N7	2.44	1.36	1.31
2	2	1496	5MC	C6-N1	-2.44	1.33	1.38
1	1	2784	OMU	C4-N3	-2.43	1.34	1.38
2	2	787	OMU	C2-N3	-2.42	1.33	1.38
2	2	1374	5MC	C6-N1	-2.41	1.33	1.38
1	1	789	OMG	C6-N1	-2.41	1.34	1.38
2	2	20	OMU	C2-N3	-2.41	1.33	1.38
2	2	1498	5MC	C6-N1	-2.41	1.33	1.38
1	1	1055	A2M	C8-N7	2.40	1.36	1.31
2	2	535	5MC	C6-N1	-2.39	1.34	1.38
1	1	2163	5MC	C6-C5	2.39	1.38	1.34
2	2	657	OMG	C5-N7	-2.39	1.34	1.39
2	2	875	5MC	C6-N1	-2.39	1.34	1.38
1	1	2183	5MC	C6-N1	-2.35	1.34	1.38
2	2	1025	5MC	C6-N1	-2.35	1.34	1.38
2	2	373	A2M	C5-N7	-2.35	1.34	1.39
2	2	1505	5MC	C6-N1	-2.32	1.34	1.38
1	1	789	OMG	C5-N7	-2.30	1.34	1.39
2	2	373	A2M	C8-N7	2.30	1.35	1.31
1	1	923	OMG	C5-N7	-2.30	1.34	1.39
2	2	693	5MC	C6-N1	-2.29	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	471	OMG	C5-N7	-2.29	1.34	1.39
1	1	2585	4AC	C4-N3	-2.28	1.28	1.32
1	1	2198	5MC	C6-N1	-2.27	1.34	1.38
2	2	1380	OMU	C2-N3	-2.27	1.33	1.38
2	2	851	4AC	C4-N3	-2.25	1.28	1.32
2	2	1469	6MZ	C8-N7	2.24	1.35	1.31
2	2	934	OMG	C5-N7	-2.24	1.34	1.39
2	2	1069	OMG	C5-N7	-2.24	1.34	1.39
1	1	2608	4AC	C4-N3	-2.24	1.28	1.32
1	1	60	4AC	C4-N3	-2.23	1.28	1.32
2	2	774	OMU	C2-N3	-2.23	1.34	1.38
2	2	1488	MA6	C8-N7	2.23	1.35	1.31
1	1	2147	OMG	C5-N7	-2.22	1.34	1.39
2	2	1487	MA6	C8-N7	2.22	1.35	1.31
2	2	873	OMG	C5-N7	-2.22	1.34	1.39
1	1	2144	OMG	C5-N7	-2.21	1.34	1.39
2	2	511	4AC	C4-N3	-2.21	1.29	1.32
1	1	2093	5MC	C6-N1	-2.20	1.34	1.38
2	2	830	OMU	C2-N3	-2.20	1.34	1.38
2	2	1202	5MC	C6-N1	-2.20	1.34	1.38
2	2	731	4AC	C4-N3	-2.19	1.29	1.32
1	1	2083	4AC	C4-N3	-2.19	1.29	1.32
2	2	17	4AC	C4-N3	-2.19	1.29	1.32
2	2	913	OMG	C5-N7	-2.18	1.34	1.39
1	1	328	OMG	C5-N7	-2.18	1.34	1.39
2	2	1177	OMU	C2-N3	-2.18	1.34	1.38
2	2	680	OMG	C5-N7	-2.18	1.34	1.39
1	1	2138	OMG	C5-N7	-2.18	1.34	1.39
2	2	286	4AC	C4-N3	-2.18	1.29	1.32
2	2	467	OMG	C5-N7	-2.17	1.34	1.39
2	2	53	4AC	C4-N3	-2.17	1.29	1.32
2	2	830	OMU	C2-N1	2.17	1.41	1.38
1	1	1243	4AC	C4-N3	-2.16	1.29	1.32
2	2	751	4AC	C4-N3	-2.16	1.29	1.32
2	2	848	4AC	C4-N3	-2.16	1.29	1.32
1	1	1055	A2M	C5-N7	-2.16	1.34	1.39
2	2	519	OMG	C5-N7	-2.15	1.34	1.39
1	1	1962	4AC	C4-N3	-2.15	1.29	1.32
1	1	2784	OMU	C2-N3	-2.14	1.34	1.38
2	2	1028	4AC	C4-N3	-2.14	1.29	1.32
1	1	2678	OMG	C5-N7	-2.14	1.34	1.39
2	2	1380	OMU	C2-N1	2.14	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	303	4AC	C4-N3	-2.13	1.29	1.32
2	2	590	4AC	C4-N3	-2.13	1.29	1.32
2	2	718	4AC	C4-N3	-2.13	1.29	1.32
2	2	830	OMU	C5-C4	-2.13	1.38	1.43
2	2	319	4AC	C4-N3	-2.12	1.29	1.32
2	2	64	OMU	C2-N3	-2.12	1.34	1.38
1	1	1938	4AC	C4-N3	-2.12	1.29	1.32
1	1	1765	4AC	C4-N3	-2.11	1.29	1.32
1	1	829	4AC	C4-N3	-2.11	1.29	1.32
2	2	938	B8H	O4'-C1'	-2.10	1.40	1.43
2	2	868	4AC	C4-N3	-2.10	1.29	1.32
2	2	1469	6MZ	C5-N7	-2.10	1.35	1.39
1	1	22	4AC	C4-N3	-2.10	1.29	1.32
2	2	626	4AC	C4-N3	-2.09	1.29	1.32
1	1	1885	4AC	C4-N3	-2.09	1.29	1.32
1	1	2173	A2M	C5-N7	-2.09	1.35	1.39
1	1	2966	4AC	C4-N3	-2.09	1.29	1.32
1	1	2027	4AC	C4-N3	-2.09	1.29	1.32
1	1	1557	4AC	C4-N3	-2.08	1.29	1.32
1	1	451	4AC	C4-N3	-2.08	1.29	1.32
1	1	981	4AC	C4-N3	-2.08	1.29	1.32
2	2	1487	MA6	C5-N7	-2.08	1.35	1.39
2	2	636	4AC	C4-N3	-2.08	1.29	1.32
2	2	546	4AC	C4-N3	-2.07	1.29	1.32
1	1	2249	4AC	C4-N3	-2.07	1.29	1.32
1	1	229	4AC	C4-N3	-2.07	1.29	1.32
1	1	2545	4AC	C4-N3	-2.07	1.29	1.32
2	2	828	4AC	C4-N3	-2.07	1.29	1.32
2	2	1488	MA6	C5-N7	-2.07	1.35	1.39
2	2	703	4AC	C4-N3	-2.07	1.29	1.32
2	2	1184	4AC	C4-N3	-2.07	1.29	1.32
1	1	2937	4AC	C4-N3	-2.07	1.29	1.32
1	1	1293	4AC	C4-N3	-2.06	1.29	1.32
1	1	2495	4AC	C4-N3	-2.06	1.29	1.32
2	2	1479	4AC	C4-N3	-2.06	1.29	1.32
1	1	341	4AC	C4-N3	-2.05	1.29	1.32
2	2	394	4AC	C4-N3	-2.05	1.29	1.32
1	1	2908	4AC	C4-N3	-2.05	1.29	1.32
2	2	379	4AC	C4-N3	-2.05	1.29	1.32
2	2	479	4AC	C4-N3	-2.05	1.29	1.32
2	2	1177	OMU	C5-C4	-2.05	1.39	1.43
2	2	1380	OMU	C5-C4	-2.04	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	64	OMU	C5-C4	-2.04	1.39	1.43
1	1	2062	4AC	C4-N3	-2.04	1.29	1.32
1	1	91	4AC	C4-N3	-2.04	1.29	1.32
1	1	641	4AC	C4-N3	-2.04	1.29	1.32
1	1	2548	4AC	C4-N3	-2.04	1.29	1.32
2	2	774	OMU	C5-C4	-2.04	1.39	1.43
1	1	2642	4AC	C4-N3	-2.04	1.29	1.32
1	1	2329	4AC	C4-N3	-2.03	1.29	1.32
1	1	161	4AC	C4-N3	-2.02	1.29	1.32
1	1	922	4AC	C4-N3	-2.02	1.29	1.32
1	1	2960	4AC	C4-N3	-2.02	1.29	1.32
1	1	1934	4AC	C4-N3	-2.02	1.29	1.32
2	2	957	4AC	C4-N3	-2.02	1.29	1.32
1	1	211	4AC	C4-N3	-2.02	1.29	1.32
1	1	3004	4AC	C4-N3	-2.02	1.29	1.32
1	1	1068	4AC	C4-N3	-2.02	1.29	1.32
1	1	1695	4AC	C4-N3	-2.01	1.29	1.32
1	1	1460	4AC	C4-N3	-2.01	1.29	1.32
1	1	357	4AC	C4-N3	-2.01	1.29	1.32
1	1	1662	4AC	C4-N3	-2.01	1.29	1.32
1	1	1867	4AC	C4-N3	-2.01	1.29	1.32
1	1	1048	4AC	C4-N3	-2.00	1.29	1.32

All (647) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	657	OMG	C5-C4-N3	-6.59	117.77	128.46
2	2	471	OMG	C5-C4-N3	-6.38	118.12	128.46
2	2	680	OMG	C5-C4-N3	-6.37	118.13	128.46
1	1	789	OMG	C5-C4-N3	-6.33	118.18	128.46
1	1	2144	OMG	C5-C4-N3	-6.26	118.30	128.46
2	2	873	OMG	C5-C4-N3	-6.23	118.35	128.46
2	2	373	A2M	C5-C4-N3	-6.23	118.62	126.75
1	1	2138	OMG	C5-C4-N3	-6.16	118.47	128.46
1	1	1055	A2M	C5-C4-N3	-6.15	118.73	126.75
2	2	1069	OMG	C5-C4-N3	-6.04	118.67	128.46
2	2	1469	6MZ	C5-C4-N3	-6.04	118.87	126.75
1	1	2678	OMG	C5-C4-N3	-6.03	118.69	128.46
1	1	2147	OMG	C5-C4-N3	-6.03	118.69	128.46
2	2	519	OMG	C5-C4-N3	-6.02	118.69	128.46
2	2	467	OMG	C5-C4-N3	-6.02	118.70	128.46
1	1	923	OMG	C5-C4-N3	-5.99	118.73	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2173	A2M	C5-C4-N3	-5.95	118.99	126.75
2	2	913	OMG	C5-C4-N3	-5.90	118.89	128.46
1	1	328	OMG	C5-C4-N3	-5.87	118.94	128.46
2	2	1467	UR3	C4-N3-C2	-5.77	119.13	124.56
2	2	934	OMG	C5-C4-N3	-5.74	119.14	128.46
2	2	1487	MA6	C5-C4-N3	-5.69	119.33	126.75
1	1	2001	4AC	O7-C7-N4	5.61	130.90	121.82
2	2	1488	MA6	C5-C4-N3	-5.59	119.45	126.75
1	1	1755	4AC	O7-C7-N4	5.51	130.74	121.82
1	1	1780	4AC	O7-C7-N4	5.31	130.42	121.82
1	1	91	4AC	O7-C7-N4	5.17	130.19	121.82
2	2	1184	4AC	O7-C7-N4	5.13	130.13	121.82
1	1	2548	4AC	O7-C7-N4	5.12	130.10	121.82
2	2	839	4AC	O7-C7-N4	5.11	130.08	121.82
1	1	1068	4AC	O7-C7-N4	5.09	130.06	121.82
1	1	789	OMG	N9-C4-N3	5.07	136.13	125.94
1	1	451	4AC	O7-C7-N4	5.07	130.02	121.82
1	1	2937	4AC	C5-C4-N4	-5.05	114.15	122.92
2	2	657	OMG	N9-C4-N3	5.04	136.05	125.94
1	1	2966	4AC	O7-C7-N4	5.03	129.97	121.82
1	1	1878	4AC	O7-C7-N4	4.97	129.85	121.82
2	2	680	OMG	C2-N3-C4	4.94	121.11	112.30
2	2	519	OMG	C2-N3-C4	4.92	121.07	112.30
1	1	1243	4AC	O7-C7-N4	4.92	129.78	121.82
1	1	2608	4AC	N4-C4-N3	4.92	122.10	113.85
1	1	2937	4AC	N4-C4-N3	4.91	122.10	113.85
2	2	657	OMG	C2-N3-C4	4.90	121.03	112.30
2	2	373	A2M	N3-C4-N9	4.89	135.14	127.08
2	2	636	4AC	O7-C7-N4	4.88	129.71	121.82
2	2	873	OMG	C2-N3-C4	4.87	120.97	112.30
2	2	467	OMG	C2-N3-C4	4.86	120.95	112.30
1	1	2144	OMG	C2-N3-C4	4.85	120.95	112.30
2	2	680	OMG	N9-C4-N3	4.85	135.69	125.94
1	1	922	4AC	O7-C7-N4	4.85	129.67	121.82
1	1	923	OMG	N9-C4-N3	4.85	135.68	125.94
1	1	1055	A2M	N3-C4-N9	4.85	135.06	127.08
2	2	1069	OMG	C2-N3-C4	4.84	120.93	112.30
2	2	471	OMG	C2-N3-C4	4.83	120.91	112.30
2	2	471	OMG	N9-C4-N3	4.83	135.64	125.94
1	1	2138	OMG	C2-N3-C4	4.83	120.91	112.30
1	1	2585	4AC	N4-C4-N3	4.83	121.95	113.85
2	2	787	OMU	C4-N3-C2	-4.79	120.26	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	60	4AC	O7-C7-N4	4.79	129.56	121.82
1	1	2147	OMG	N9-C4-N3	4.78	135.55	125.94
2	2	913	OMG	C2-N3-C4	4.78	120.83	112.30
2	2	20	OMU	C4-N3-C2	-4.78	120.28	126.58
2	2	718	4AC	O7-C7-N4	4.76	129.53	121.82
1	1	2678	OMG	C2-N3-C4	4.75	120.76	112.30
1	1	2173	A2M	N3-C4-N9	4.74	134.88	127.08
2	2	873	OMG	N9-C4-N3	4.73	135.44	125.94
1	1	2147	OMG	C2-N3-C4	4.73	120.72	112.30
1	1	2144	OMG	N9-C4-N3	4.70	135.37	125.94
1	1	2545	4AC	O7-C7-N4	4.68	129.40	121.82
1	1	789	OMG	C2-N3-C4	4.67	120.61	112.30
2	2	703	4AC	O7-C7-N4	4.66	129.36	121.82
1	1	328	OMG	C2-N3-C4	4.65	120.59	112.30
1	1	2608	4AC	C5-C4-N4	-4.65	114.84	122.92
1	1	923	OMG	C2-N3-C4	4.65	120.58	112.30
1	1	981	4AC	O7-C7-N4	4.60	129.27	121.82
1	1	2925	4AC	O7-C7-N4	4.60	129.26	121.82
1	1	458	4AC	O7-C7-N4	4.60	129.26	121.82
1	1	1594	4AC	O7-C7-N4	4.59	129.24	121.82
3	3	32	4AC	O7-C7-N4	4.58	129.23	121.82
1	1	1048	4AC	O7-C7-N4	4.57	129.22	121.82
1	1	1554	4AC	O7-C7-N4	4.57	129.22	121.82
2	2	1233	4AC	O7-C7-N4	4.57	129.21	121.82
1	1	2718	4AC	O7-C7-N4	4.56	129.20	121.82
1	1	2138	OMG	N9-C4-N3	4.56	135.10	125.94
1	1	1222	4AC	O7-C7-N4	4.56	129.19	121.82
1	1	2585	4AC	C5-C4-N4	-4.55	115.01	122.92
1	1	1934	4AC	O7-C7-N4	4.55	129.19	121.82
1	1	229	4AC	O7-C7-N4	4.55	129.19	121.82
2	2	848	4AC	O7-C7-N4	4.55	129.19	121.82
1	1	2678	OMG	N9-C4-N3	4.55	135.08	125.94
1	1	161	4AC	O7-C7-N4	4.55	129.18	121.82
2	2	1479	4AC	O7-C7-N4	4.55	129.18	121.82
2	2	1069	OMG	N9-C4-N3	4.53	135.03	125.94
2	2	546	4AC	O7-C7-N4	4.52	129.14	121.82
1	1	802	4AC	O7-C7-N4	4.52	129.13	121.82
1	1	1885	4AC	O7-C7-N4	4.51	129.11	121.82
2	2	774	OMU	C4-N3-C2	-4.51	120.64	126.58
1	1	1617	4AC	O7-C7-N4	4.51	129.11	121.82
1	1	2784	OMU	C4-N3-C2	-4.50	120.64	126.58
1	1	1065	4AC	O7-C7-N4	4.50	129.10	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1460	4AC	O7-C7-N4	4.50	129.09	121.82
2	2	394	4AC	O7-C7-N4	4.50	129.09	121.82
2	2	1147	4AC	O7-C7-N4	4.49	129.09	121.82
1	1	2287	4AC	O7-C7-N4	4.49	129.09	121.82
1	1	533	4AC	O7-C7-N4	4.49	129.09	121.82
1	1	1621	4AC	O7-C7-N4	4.49	129.08	121.82
1	1	1873	4AC	O7-C7-N4	4.49	129.08	121.82
1	1	211	4AC	O7-C7-N4	4.49	129.08	121.82
1	1	314	4AC	O7-C7-N4	4.49	129.08	121.82
1	1	1938	4AC	O7-C7-N4	4.49	129.08	121.82
2	2	828	4AC	O7-C7-N4	4.48	129.07	121.82
2	2	1487	MA6	C2-N1-C6	4.48	122.34	111.75
1	1	1550	4AC	O7-C7-N4	4.48	129.07	121.82
1	1	136	4AC	O7-C7-N4	4.48	129.07	121.82
1	1	243	4AC	O7-C7-N4	4.48	129.06	121.82
1	1	1662	4AC	O7-C7-N4	4.47	129.06	121.82
2	2	303	4AC	O7-C7-N4	4.47	129.06	121.82
2	2	519	OMG	N9-C4-N3	4.47	134.92	125.94
2	2	17	4AC	O7-C7-N4	4.47	129.05	121.82
2	2	626	4AC	O7-C7-N4	4.47	129.05	121.82
1	1	22	4AC	O7-C7-N4	4.46	129.04	121.82
2	2	590	4AC	O7-C7-N4	4.46	129.04	121.82
2	2	53	4AC	O7-C7-N4	4.46	129.03	121.82
1	1	1667	4AC	O7-C7-N4	4.46	129.03	121.82
2	2	467	OMG	N9-C4-N3	4.45	134.88	125.94
2	2	479	4AC	O7-C7-N4	4.45	129.02	121.82
2	2	319	4AC	O7-C7-N4	4.45	129.02	121.82
2	2	934	OMG	C2-N3-C4	4.45	120.22	112.30
1	1	641	4AC	O7-C7-N4	4.45	129.01	121.82
2	2	1469	6MZ	N3-C4-N9	4.45	134.41	127.08
1	1	2865	4AC	O7-C7-N4	4.45	129.01	121.82
1	1	694	4AC	O7-C7-N4	4.44	129.01	121.82
1	1	2062	4AC	O7-C7-N4	4.44	129.01	121.82
1	1	2329	4AC	O7-C7-N4	4.44	129.00	121.82
1	1	835	4AC	O7-C7-N4	4.43	128.99	121.82
2	2	731	4AC	O7-C7-N4	4.43	128.99	121.82
1	1	1695	4AC	O7-C7-N4	4.43	128.99	121.82
1	1	1765	4AC	O7-C7-N4	4.43	128.99	121.82
2	2	20	OMU	N3-C2-N1	4.43	120.77	114.89
1	1	2027	4AC	O7-C7-N4	4.42	128.97	121.82
1	1	829	4AC	O7-C7-N4	4.41	128.96	121.82
1	1	2249	4AC	O7-C7-N4	4.41	128.96	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	328	OMG	N9-C4-N3	4.41	134.80	125.94
2	2	751	4AC	O7-C7-N4	4.41	128.96	121.82
2	2	379	4AC	O7-C7-N4	4.41	128.95	121.82
2	2	1028	4AC	O7-C7-N4	4.41	128.95	121.82
1	1	357	4AC	O7-C7-N4	4.40	128.94	121.82
1	1	1293	4AC	O7-C7-N4	4.40	128.94	121.82
1	1	2136	4AC	O7-C7-N4	4.40	128.94	121.82
2	2	851	4AC	O7-C7-N4	4.40	128.93	121.82
1	1	1557	4AC	O7-C7-N4	4.39	128.93	121.82
2	2	913	OMG	N9-C4-N3	4.39	134.75	125.94
1	1	1867	4AC	O7-C7-N4	4.39	128.92	121.82
1	1	341	4AC	O7-C7-N4	4.38	128.91	121.82
1	1	2908	4AC	O7-C7-N4	4.38	128.91	121.82
2	2	1488	MA6	C2-N1-C6	4.38	122.10	111.75
2	2	1380	OMU	C4-N3-C2	-4.38	120.81	126.58
1	1	2960	4AC	O7-C7-N4	4.38	128.90	121.82
1	1	3004	4AC	O7-C7-N4	4.37	128.90	121.82
1	1	2642	4AC	O7-C7-N4	4.37	128.89	121.82
1	1	2570	4AC	O7-C7-N4	4.37	128.89	121.82
1	1	2083	4AC	O7-C7-N4	4.37	128.88	121.82
2	2	787	OMU	N3-C2-N1	4.36	120.67	114.89
2	2	1469	6MZ	C6-C5-N7	4.36	137.10	132.39
2	2	1488	MA6	N3-C4-N9	4.35	134.25	127.08
2	2	511	4AC	O7-C7-N4	4.35	128.85	121.82
1	1	1962	4AC	O7-C7-N4	4.35	128.85	121.82
2	2	934	OMG	N9-C4-N3	4.34	134.66	125.94
2	2	64	OMU	C4-N3-C2	-4.34	120.86	126.58
2	2	957	4AC	O7-C7-N4	4.34	128.84	121.82
2	2	1239	4AC	O7-C7-N4	4.33	128.83	121.82
2	2	1487	MA6	N3-C4-N9	4.33	134.22	127.08
2	2	286	4AC	O7-C7-N4	4.33	128.83	121.82
2	2	868	4AC	O7-C7-N4	4.33	128.82	121.82
1	1	2495	4AC	O7-C7-N4	4.32	128.81	121.82
2	2	1177	OMU	C4-N3-C2	-4.31	120.90	126.58
2	2	774	OMU	N3-C2-N1	4.19	120.45	114.89
2	2	830	OMU	C4-N3-C2	-4.19	121.06	126.58
1	1	2162	5MC	C5-C6-N1	-4.16	119.06	123.34
1	1	2784	OMU	N3-C2-N1	4.15	120.39	114.89
1	1	2203	5MC	C5-C6-N1	-4.15	119.07	123.34
2	2	1380	OMU	N3-C2-N1	4.14	120.39	114.89
1	1	2163	5MC	C5-C6-N1	-4.06	119.16	123.34
2	2	830	OMU	N3-C2-N1	4.05	120.27	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	64	OMU	N3-C2-N1	4.04	120.25	114.89
1	1	1755	4AC	C5-C4-N4	-3.99	115.98	122.92
2	2	1487	MA6	C4-C5-N7	-3.99	105.75	110.62
2	2	1177	OMU	N3-C2-N1	3.98	120.17	114.89
2	2	1469	6MZ	C4-C5-N7	-3.96	105.80	110.62
1	1	1780	4AC	C5-C4-N4	-3.91	116.12	122.92
2	2	1469	6MZ	C2-N3-C4	3.90	120.97	111.75
2	2	373	A2M	C2-N3-C4	3.87	120.89	111.75
1	1	1780	4AC	N4-C4-N3	3.86	120.34	113.85
1	1	1055	A2M	C2-N3-C4	3.86	120.87	111.75
2	2	1487	MA6	C2-N3-C4	3.83	120.80	111.75
2	2	1488	MA6	C2-N3-C4	3.83	120.79	111.75
1	1	1755	4AC	N4-C4-N3	3.79	120.22	113.85
1	1	2173	A2M	C2-N3-C4	3.75	120.60	111.75
2	2	535	5MC	C5-C6-N1	-3.73	119.50	123.34
2	2	20	OMU	C5-C4-N3	3.65	120.29	114.84
1	1	2183	5MC	C5-C6-N1	-3.63	119.60	123.34
1	1	2093	5MC	C5-C6-N1	-3.62	119.61	123.34
2	2	787	OMU	C5-C4-N3	3.61	120.24	114.84
1	1	91	4AC	C5-C4-N4	-3.61	116.66	122.92
1	1	91	4AC	N4-C4-N3	3.60	119.90	113.85
2	2	1488	MA6	C4-C5-N7	-3.60	106.24	110.62
2	2	774	OMU	C5-C4-N3	3.56	120.16	114.84
1	1	2784	OMU	C5-C4-N3	3.56	120.16	114.84
1	1	2733	5MC	C5-C6-N1	-3.55	119.68	123.34
2	2	64	OMU	C5-C4-N3	3.54	120.14	114.84
2	2	1177	OMU	C5-C4-N3	3.53	120.12	114.84
1	1	1068	4AC	C5-C4-N4	-3.52	116.81	122.92
2	2	1025	5MC	C5-C6-N1	-3.52	119.72	123.34
2	2	1147	4AC	N4-C4-N3	3.49	119.71	113.85
2	2	875	5MC	C5-C6-N1	-3.48	119.76	123.34
1	1	802	4AC	N4-C4-N3	3.48	119.69	113.85
1	1	1068	4AC	N4-C4-N3	3.48	119.69	113.85
2	2	1380	OMU	C5-C4-N3	3.48	120.04	114.84
1	1	1222	4AC	N4-C4-N3	3.47	119.68	113.85
1	1	2287	4AC	N4-C4-N3	3.46	119.67	113.85
2	2	1184	4AC	C5-C4-N4	-3.45	116.93	122.92
2	2	693	5MC	C5-C6-N1	-3.44	119.80	123.34
1	1	2198	5MC	C5-C6-N1	-3.41	119.83	123.34
1	1	2718	4AC	N4-C4-N3	3.41	119.58	113.85
1	1	1878	4AC	C5-C4-N4	-3.41	116.99	122.92
2	2	830	OMU	C5-C4-N3	3.41	119.94	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2136	4AC	N4-C4-N3	3.40	119.56	113.85
2	2	1479	4AC	N4-C4-N3	3.40	119.55	113.85
1	1	2585	4AC	O7-C7-N4	3.39	127.31	121.82
1	1	2545	4AC	C5-C4-N4	-3.37	117.06	122.92
1	1	2937	4AC	O7-C7-N4	3.36	127.26	121.82
2	2	1233	4AC	N4-C4-N3	3.36	119.50	113.85
1	1	1065	4AC	N4-C4-N3	3.36	119.49	113.85
1	1	2608	4AC	O7-C7-N4	3.36	127.25	121.82
1	1	458	4AC	N4-C4-N3	3.34	119.47	113.85
2	2	1505	5MC	C5-C6-N1	-3.34	119.90	123.34
1	1	1885	4AC	CM7-C7-N4	-3.33	109.53	115.29
1	1	1594	4AC	N4-C4-N3	3.32	119.43	113.85
3	3	32	4AC	N4-C4-N3	3.32	119.43	113.85
1	1	1878	4AC	N4-C4-N3	3.32	119.43	113.85
1	1	1222	4AC	C5-C4-N4	-3.32	117.15	122.92
2	2	636	4AC	C5-C4-N4	-3.32	117.15	122.92
1	1	1878	4AC	CM7-C7-N4	-3.32	109.55	115.29
2	2	1469	6MZ	N1-C2-N3	-3.31	123.43	128.60
2	2	703	4AC	N4-C4-N3	3.31	119.40	113.85
2	2	1374	5MC	C5-C6-N1	-3.30	119.94	123.34
1	1	533	4AC	N4-C4-N3	3.30	119.39	113.85
2	2	1488	MA6	N1-C2-N3	-3.30	123.44	128.60
2	2	1147	4AC	C5-C4-N4	-3.30	117.19	122.92
2	2	703	4AC	C5-C4-N4	-3.30	117.19	122.92
1	1	136	4AC	N4-C4-N3	3.28	119.35	113.85
2	2	1184	4AC	CM7-C7-N4	-3.28	109.63	115.29
2	2	519	OMG	C6-C5-N7	3.27	136.34	130.25
1	1	2545	4AC	N4-C4-N3	3.27	119.34	113.85
2	2	636	4AC	N4-C4-N3	3.27	119.34	113.85
2	2	1487	MA6	N1-C2-N3	-3.27	123.49	128.60
1	1	2548	4AC	CM7-C7-N4	-3.27	109.65	115.29
2	2	626	4AC	N4-C4-N3	3.26	119.32	113.85
2	2	913	OMG	C6-C5-N7	3.25	136.30	130.25
2	2	1487	MA6	C5-N7-C8	3.24	108.12	103.51
1	1	1550	4AC	N4-C4-N3	3.24	119.30	113.85
1	1	802	4AC	C5-C4-N4	-3.24	117.29	122.92
1	1	2718	4AC	C5-C4-N4	-3.24	117.29	122.92
1	1	2966	4AC	C5-C4-N4	-3.23	117.30	122.92
1	1	1594	4AC	C5-C4-N4	-3.23	117.30	122.92
2	2	934	OMG	C6-C5-N7	3.23	136.26	130.25
2	2	1496	5MC	C5-C6-N1	-3.22	120.02	123.34
1	1	357	4AC	N4-C4-N3	3.22	119.26	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1662	4AC	N4-C4-N3	3.22	119.26	113.85
1	1	2287	4AC	C5-C4-N4	-3.22	117.32	122.92
2	2	467	OMG	C6-C5-N7	3.22	136.23	130.25
1	1	243	4AC	N4-C4-N3	3.22	119.25	113.85
2	2	1069	OMG	C6-C5-N7	3.21	136.22	130.25
1	1	1617	4AC	N4-C4-N3	3.21	119.23	113.85
2	2	1479	4AC	C5-C4-N4	-3.20	117.35	122.92
2	2	1233	4AC	C5-C4-N4	-3.20	117.35	122.92
1	1	1554	4AC	N4-C4-N3	3.20	119.22	113.85
2	2	1469	6MZ	C5-N7-C8	3.19	108.04	103.51
2	2	373	A2M	C4-C5-N7	-3.19	106.73	110.62
1	1	1065	4AC	C5-C4-N4	-3.19	117.38	122.92
1	1	2960	4AC	N4-C4-N3	3.19	119.20	113.85
1	1	533	4AC	C5-C4-N4	-3.18	117.39	122.92
2	2	379	4AC	N4-C4-N3	3.18	119.19	113.85
1	1	1934	4AC	N4-C4-N3	3.18	119.19	113.85
1	1	2865	4AC	N4-C4-N3	3.18	119.18	113.85
1	1	1055	A2M	C4-C5-N7	-3.17	106.75	110.62
1	1	1873	4AC	N4-C4-N3	3.17	119.17	113.85
1	1	1667	4AC	N4-C4-N3	3.17	119.17	113.85
1	1	2548	4AC	C5-C4-N4	-3.17	117.42	122.92
2	2	546	4AC	N4-C4-N3	3.17	119.17	113.85
1	1	2925	4AC	N4-C4-N3	3.16	119.16	113.85
1	1	2908	4AC	N4-C4-N3	3.16	119.16	113.85
1	1	1055	A2M	N3-C2-N1	-3.16	123.66	128.60
1	1	1460	4AC	N4-C4-N3	3.16	119.15	113.85
1	1	211	4AC	N4-C4-N3	3.15	119.15	113.85
1	1	314	4AC	N4-C4-N3	3.15	119.14	113.85
2	2	479	4AC	N4-C4-N3	3.15	119.14	113.85
2	2	1498	5MC	C5-C6-N1	-3.15	120.10	123.34
2	2	319	4AC	N4-C4-N3	3.15	119.13	113.85
1	1	835	4AC	N4-C4-N3	3.15	119.13	113.85
1	1	1048	4AC	N4-C4-N3	3.14	119.13	113.85
1	1	694	4AC	N4-C4-N3	3.14	119.13	113.85
1	1	2062	4AC	N4-C4-N3	3.14	119.13	113.85
1	1	451	4AC	C5-C4-N4	-3.14	117.47	122.92
1	1	2966	4AC	CM7-C7-N4	-3.14	109.86	115.29
1	1	2925	4AC	C5-C4-N4	-3.14	117.47	122.92
1	1	1780	4AC	CM7-C7-N4	-3.14	109.87	115.29
1	1	2585	4AC	O2-C2-N3	-3.13	117.24	122.33
1	1	161	4AC	CM7-C7-N4	-3.13	109.88	115.29
1	1	2027	4AC	N4-C4-N3	3.13	119.11	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2249	4AC	N4-C4-N3	3.13	119.11	113.85
1	1	1621	4AC	N4-C4-N3	3.12	119.10	113.85
1	1	1048	4AC	C5-C4-N4	-3.12	117.50	122.92
2	2	636	4AC	CM7-C7-N4	-3.12	109.89	115.29
1	1	328	OMG	C6-C5-N7	3.12	136.05	130.25
1	1	1617	4AC	C5-C4-N4	-3.12	117.50	122.92
1	1	2966	4AC	N4-C4-N3	3.11	119.08	113.85
1	1	981	4AC	N4-C4-N3	3.11	119.07	113.85
2	2	394	4AC	N4-C4-N3	3.11	119.07	113.85
2	2	1239	4AC	N4-C4-N3	3.11	119.07	113.85
1	1	1554	4AC	C5-C4-N4	-3.10	117.53	122.92
1	1	2329	4AC	N4-C4-N3	3.10	119.06	113.85
1	1	2570	4AC	N4-C4-N3	3.10	119.06	113.85
1	1	2548	4AC	N4-C4-N3	3.10	119.05	113.85
1	1	60	4AC	N4-C4-N3	3.10	119.05	113.85
1	1	2678	OMG	C6-C5-N7	3.10	136.01	130.25
1	1	211	4AC	C5-C4-N4	-3.09	117.55	122.92
1	1	60	4AC	CM7-C7-N4	-3.09	109.95	115.29
1	1	2001	4AC	CM7-C7-N4	-3.09	109.96	115.29
2	2	373	A2M	N3-C2-N1	-3.08	123.78	128.60
2	2	1184	4AC	N4-C4-N3	3.08	119.03	113.85
1	1	2173	A2M	C4-C5-N7	-3.08	106.87	110.62
1	1	922	4AC	C5-C4-N4	-3.08	117.57	122.92
1	1	1460	4AC	C5-C4-N4	-3.08	117.57	122.92
1	1	341	4AC	N4-C4-N3	3.08	119.01	113.85
1	1	2249	4AC	C5-C4-N4	-3.07	117.58	122.92
2	2	731	4AC	N4-C4-N3	3.07	119.01	113.85
1	1	1934	4AC	C5-C4-N4	-3.07	117.58	122.92
1	1	243	4AC	C5-C4-N4	-3.07	117.58	122.92
2	2	379	4AC	C5-C4-N4	-3.07	117.59	122.92
2	2	479	4AC	C5-C4-N4	-3.07	117.59	122.92
1	1	1662	4AC	C5-C4-N4	-3.07	117.59	122.92
1	1	981	4AC	C5-C4-N4	-3.06	117.60	122.92
1	1	1755	4AC	CM7-C7-N4	-3.06	110.00	115.29
1	1	1048	4AC	CM7-C7-N4	-3.06	110.00	115.29
2	2	303	4AC	N4-C4-N3	3.06	118.98	113.85
1	1	2173	A2M	N3-C2-N1	-3.06	123.82	128.60
1	1	2138	OMG	C6-C5-N7	3.06	135.93	130.25
2	2	53	4AC	N4-C4-N3	3.05	118.98	113.85
2	2	839	4AC	N4-C4-N3	3.05	118.97	113.85
1	1	22	4AC	CM7-C7-N4	-3.05	110.02	115.29
1	1	451	4AC	CM7-C7-N4	-3.05	110.02	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1293	4AC	N4-C4-N3	3.04	118.96	113.85
1	1	2144	OMG	C6-C5-N7	3.04	135.90	130.25
2	2	839	4AC	CM7-C7-N4	-3.04	110.03	115.29
2	2	626	4AC	C5-C4-N4	-3.04	117.64	122.92
1	1	136	4AC	C5-C4-N4	-3.04	117.64	122.92
1	1	229	4AC	CM7-C7-N4	-3.04	110.04	115.29
1	1	1243	4AC	C5-C4-N4	-3.04	117.64	122.92
1	1	922	4AC	CM7-C7-N4	-3.03	110.05	115.29
2	2	17	4AC	CM7-C7-N4	-3.03	110.05	115.29
2	2	957	4AC	N4-C4-N3	3.03	118.94	113.85
2	2	848	4AC	CM7-C7-N4	-3.03	110.05	115.29
1	1	2925	4AC	CM7-C7-N4	-3.03	110.05	115.29
1	1	1867	4AC	N4-C4-N3	3.03	118.94	113.85
1	1	1554	4AC	CM7-C7-N4	-3.03	110.05	115.29
2	2	873	OMG	C6-C5-N7	3.03	135.88	130.25
1	1	1243	4AC	CM7-C7-N4	-3.02	110.06	115.29
1	1	1594	4AC	CM7-C7-N4	-3.02	110.07	115.29
2	2	868	4AC	N4-C4-N3	3.02	118.92	113.85
1	1	161	4AC	C5-C4-N4	-3.02	117.67	122.92
1	1	2784	OMU	O4-C4-C5	-3.02	119.85	125.16
2	2	718	4AC	C5-C4-N4	-3.01	117.68	122.92
1	1	922	4AC	N4-C4-N3	3.01	118.91	113.85
1	1	2865	4AC	C5-C4-N4	-3.01	117.68	122.92
2	2	319	4AC	C5-C4-N4	-3.01	117.68	122.92
1	1	2001	4AC	N4-C4-N3	3.01	118.91	113.85
2	2	839	4AC	C5-C4-N4	-3.01	117.69	122.92
1	1	1695	4AC	N4-C4-N3	3.01	118.91	113.85
1	1	1667	4AC	C5-C4-N4	-3.01	117.69	122.92
1	1	161	4AC	N4-C4-N3	3.01	118.90	113.85
2	2	774	OMU	O4-C4-C5	-3.01	119.87	125.16
2	2	828	4AC	N4-C4-N3	3.01	118.90	113.85
2	2	64	OMU	O4-C4-C5	-3.01	119.88	125.16
1	1	2908	4AC	C5-C4-N4	-3.00	117.70	122.92
2	2	590	4AC	N4-C4-N3	3.00	118.89	113.85
1	1	1765	4AC	N4-C4-N3	3.00	118.89	113.85
1	1	1938	4AC	CM7-C7-N4	-3.00	110.11	115.29
1	1	2329	4AC	C5-C4-N4	-3.00	117.71	122.92
1	1	2495	4AC	N4-C4-N3	3.00	118.88	113.85
1	1	1550	4AC	C5-C4-N4	-3.00	117.71	122.92
2	2	1177	OMU	O4-C4-C5	-3.00	119.89	125.16
1	1	641	4AC	N4-C4-N3	2.99	118.88	113.85
1	1	981	4AC	CM7-C7-N4	-2.99	110.12	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	451	4AC	N4-C4-N3	2.99	118.87	113.85
1	1	3004	4AC	N4-C4-N3	2.99	118.87	113.85
1	1	357	4AC	C5-C4-N4	-2.99	117.73	122.92
1	1	2608	4AC	O2-C2-N3	-2.98	117.48	122.33
1	1	229	4AC	N4-C4-N3	2.98	118.85	113.85
1	1	2062	4AC	C5-C4-N4	-2.98	117.75	122.92
1	1	1621	4AC	C5-C4-N4	-2.97	117.75	122.92
1	1	314	4AC	C5-C4-N4	-2.97	117.75	122.92
1	1	1873	4AC	C5-C4-N4	-2.97	117.75	122.92
1	1	694	4AC	C5-C4-N4	-2.97	117.76	122.92
2	2	546	4AC	C5-C4-N4	-2.97	117.77	122.92
1	1	1460	4AC	CM7-C7-N4	-2.97	110.17	115.29
1	1	1621	4AC	CM7-C7-N4	-2.96	110.17	115.29
1	1	1938	4AC	N4-C4-N3	2.96	118.83	113.85
1	1	829	4AC	CM7-C7-N4	-2.95	110.19	115.29
2	2	53	4AC	CM7-C7-N4	-2.95	110.19	115.29
2	2	394	4AC	C5-C4-N4	-2.95	117.80	122.92
1	1	211	4AC	CM7-C7-N4	-2.95	110.19	115.29
2	2	828	4AC	CM7-C7-N4	-2.95	110.20	115.29
2	2	731	4AC	CM7-C7-N4	-2.94	110.20	115.29
2	2	851	4AC	CM7-C7-N4	-2.94	110.20	115.29
1	1	2027	4AC	C5-C4-N4	-2.94	117.81	122.92
2	2	1487	MA6	N1-C6-N6	2.94	120.30	117.08
1	1	2545	4AC	CM7-C7-N4	-2.94	110.22	115.29
1	1	229	4AC	C5-C4-N4	-2.93	117.82	122.92
2	2	1488	MA6	C4-N9-C8	2.93	108.91	105.73
1	1	2083	4AC	CM7-C7-N4	-2.93	110.22	115.29
2	2	394	4AC	CM7-C7-N4	-2.93	110.22	115.29
2	2	828	4AC	C5-C4-N4	-2.93	117.83	122.92
2	2	511	4AC	CM7-C7-N4	-2.93	110.23	115.29
2	2	718	4AC	N4-C4-N3	2.93	118.77	113.85
2	2	1488	MA6	C5-N7-C8	2.93	107.67	103.51
1	1	2249	4AC	CM7-C7-N4	-2.93	110.23	115.29
2	2	1239	4AC	C5-C4-N4	-2.92	117.84	122.92
2	2	680	OMG	C6-C5-N7	2.92	135.68	130.25
2	2	1028	4AC	N4-C4-N3	2.92	118.76	113.85
1	1	1962	4AC	CM7-C7-N4	-2.92	110.24	115.29
2	2	546	4AC	CM7-C7-N4	-2.92	110.24	115.29
1	1	2960	4AC	C5-C4-N4	-2.92	117.84	122.92
2	2	53	4AC	C5-C4-N4	-2.92	117.85	122.92
1	1	1934	4AC	CM7-C7-N4	-2.92	110.25	115.29
1	1	2136	4AC	C5-C4-N4	-2.92	117.85	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1028	4AC	CM7-C7-N4	-2.92	110.25	115.29
2	2	957	4AC	C5-C4-N4	-2.91	117.86	122.92
1	1	1873	4AC	CM7-C7-N4	-2.91	110.25	115.29
2	2	303	4AC	CM7-C7-N4	-2.91	110.25	115.29
2	2	1380	OMU	O4-C4-C5	-2.91	120.04	125.16
2	2	731	4AC	C5-C4-N4	-2.91	117.86	122.92
2	2	787	OMU	O4-C4-C5	-2.91	120.04	125.16
1	1	2642	4AC	CM7-C7-N4	-2.91	110.26	115.29
1	1	458	4AC	C5-C4-N4	-2.91	117.87	122.92
1	1	1765	4AC	C5-C4-N4	-2.91	117.87	122.92
1	1	1557	4AC	N4-C4-N3	2.91	118.73	113.85
2	2	303	4AC	C5-C4-N4	-2.91	117.87	122.92
2	2	751	4AC	CM7-C7-N4	-2.91	110.27	115.29
2	2	286	4AC	CM7-C7-N4	-2.90	110.27	115.29
1	1	3004	4AC	C5-C4-N4	-2.90	117.88	122.92
1	1	341	4AC	C5-C4-N4	-2.90	117.88	122.92
1	1	2570	4AC	C5-C4-N4	-2.90	117.88	122.92
1	1	3004	4AC	CM7-C7-N4	-2.90	110.28	115.29
2	2	1487	MA6	C4-N9-C8	2.90	108.87	105.73
2	2	20	OMU	O4-C4-C5	-2.90	120.06	125.16
1	1	2570	4AC	CM7-C7-N4	-2.90	110.28	115.29
1	1	1867	4AC	C5-C4-N4	-2.90	117.88	122.92
2	2	1202	5MC	C5-C4-N3	-2.90	118.55	121.67
1	1	2027	4AC	CM7-C7-N4	-2.90	110.28	115.29
2	2	830	OMU	O4-C4-C5	-2.90	120.07	125.16
1	1	829	4AC	N4-C4-N3	2.89	118.71	113.85
1	1	1055	A2M	C2'-C1'-N9	-2.89	108.66	113.53
2	2	703	4AC	CM7-C7-N4	-2.89	110.29	115.29
1	1	2083	4AC	N4-C4-N3	2.89	118.71	113.85
1	1	641	4AC	CM7-C7-N4	-2.89	110.29	115.29
1	1	314	4AC	CM7-C7-N4	-2.89	110.30	115.29
1	1	2718	4AC	CM7-C7-N4	-2.89	110.30	115.29
1	1	1293	4AC	CM7-C7-N4	-2.89	110.30	115.29
1	1	243	4AC	CM7-C7-N4	-2.89	110.30	115.29
2	2	590	4AC	CM7-C7-N4	-2.88	110.31	115.29
1	1	1222	4AC	CM7-C7-N4	-2.88	110.31	115.29
3	3	32	4AC	C5-C4-N4	-2.88	117.91	122.92
1	1	1695	4AC	C5-C4-N4	-2.88	117.91	122.92
2	2	868	4AC	C5-C4-N4	-2.88	117.92	122.92
2	2	848	4AC	N4-C4-N3	2.87	118.68	113.85
1	1	2865	4AC	CM7-C7-N4	-2.87	110.32	115.29
1	1	2585	4AC	C1'-N1-C2	2.87	124.83	118.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2642	4AC	N4-C4-N3	2.87	118.67	113.85
1	1	1667	4AC	CM7-C7-N4	-2.87	110.33	115.29
1	1	641	4AC	C5-C4-N4	-2.87	117.93	122.92
1	1	835	4AC	CM7-C7-N4	-2.87	110.33	115.29
1	1	1068	4AC	CM7-C7-N4	-2.87	110.33	115.29
2	2	1202	5MC	C5-C6-N1	-2.87	120.39	123.34
1	1	802	4AC	CM7-C7-N4	-2.87	110.34	115.29
1	1	22	4AC	N4-C4-N3	2.86	118.66	113.85
1	1	1765	4AC	CM7-C7-N4	-2.86	110.34	115.29
2	2	751	4AC	N4-C4-N3	2.86	118.65	113.85
2	2	479	4AC	CM7-C7-N4	-2.86	110.35	115.29
1	1	1867	4AC	CM7-C7-N4	-2.85	110.36	115.29
1	1	2062	4AC	CM7-C7-N4	-2.85	110.36	115.29
1	1	2495	4AC	CM7-C7-N4	-2.85	110.36	115.29
1	1	458	4AC	CM7-C7-N4	-2.85	110.37	115.29
1	1	1617	4AC	CM7-C7-N4	-2.85	110.37	115.29
1	1	533	4AC	CM7-C7-N4	-2.85	110.37	115.29
2	2	379	4AC	CM7-C7-N4	-2.85	110.37	115.29
1	1	22	4AC	C5-C4-N4	-2.84	117.98	122.92
1	1	1550	4AC	CM7-C7-N4	-2.84	110.38	115.29
1	1	1662	4AC	CM7-C7-N4	-2.84	110.38	115.29
2	2	626	4AC	CM7-C7-N4	-2.84	110.38	115.29
2	2	718	4AC	CM7-C7-N4	-2.84	110.38	115.29
2	2	590	4AC	C5-C4-N4	-2.84	117.99	122.92
2	2	471	OMG	C6-C5-N7	2.84	135.53	130.25
2	2	1233	4AC	CM7-C7-N4	-2.84	110.39	115.29
1	1	136	4AC	CM7-C7-N4	-2.84	110.39	115.29
1	1	1885	4AC	C5-C4-N4	-2.83	118.00	122.92
2	2	319	4AC	CM7-C7-N4	-2.83	110.39	115.29
1	1	923	OMG	C6-C5-N7	2.83	135.51	130.25
1	1	1293	4AC	C5-C4-N4	-2.83	118.00	122.92
1	1	1695	4AC	CM7-C7-N4	-2.83	110.40	115.29
2	2	848	4AC	C5-C4-N4	-2.83	118.01	122.92
1	1	694	4AC	CM7-C7-N4	-2.83	110.40	115.29
1	1	2083	4AC	C5-C4-N4	-2.83	118.01	122.92
1	1	829	4AC	C5-C4-N4	-2.82	118.02	122.92
1	1	2495	4AC	C5-C4-N4	-2.82	118.02	122.92
1	1	2329	4AC	CM7-C7-N4	-2.82	110.42	115.29
2	2	17	4AC	N4-C4-N3	2.82	118.58	113.85
2	2	957	4AC	CM7-C7-N4	-2.81	110.43	115.29
1	1	2147	OMG	C6-C5-N7	2.81	135.47	130.25
2	2	1479	4AC	CM7-C7-N4	-2.81	110.44	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	868	4AC	CM7-C7-N4	-2.80	110.45	115.29
1	1	1962	4AC	N4-C4-N3	2.80	118.55	113.85
1	1	1938	4AC	C5-C4-N4	-2.80	118.06	122.92
1	1	835	4AC	C5-C4-N4	-2.80	118.06	122.92
1	1	341	4AC	CM7-C7-N4	-2.80	110.46	115.29
1	1	1065	4AC	CM7-C7-N4	-2.79	110.47	115.29
2	2	286	4AC	N4-C4-N3	2.79	118.53	113.85
1	1	1243	4AC	N4-C4-N3	2.78	118.53	113.85
1	1	2733	5MC	C5-C4-N3	-2.77	118.68	121.67
2	2	17	4AC	C5-C4-N4	-2.77	118.11	122.92
1	1	1557	4AC	CM7-C7-N4	-2.77	110.51	115.29
1	1	2287	4AC	CM7-C7-N4	-2.77	110.51	115.29
2	2	1202	5MC	O2-C2-N3	-2.75	117.86	122.33
2	2	511	4AC	N4-C4-N3	2.75	118.46	113.85
1	1	357	4AC	CM7-C7-N4	-2.74	110.55	115.29
2	2	751	4AC	C5-C4-N4	-2.72	118.19	122.92
1	1	1885	4AC	N4-C4-N3	2.72	118.42	113.85
2	2	1028	4AC	C5-C4-N4	-2.72	118.19	122.92
1	1	2642	4AC	C5-C4-N4	-2.71	118.20	122.92
1	1	2960	4AC	CM7-C7-N4	-2.71	110.60	115.29
1	1	2908	4AC	CM7-C7-N4	-2.71	110.61	115.29
1	1	2173	A2M	C4-N9-C8	2.71	108.66	105.73
1	1	1962	4AC	C5-C4-N4	-2.71	118.22	122.92
2	2	286	4AC	C5-C4-N4	-2.70	118.22	122.92
2	2	851	4AC	N4-C4-N3	2.70	118.39	113.85
1	1	91	4AC	CM7-C7-N4	-2.70	110.62	115.29
2	2	1496	5MC	C5-C4-N3	-2.70	118.76	121.67
1	1	1055	A2M	C5-N7-C8	2.69	107.33	103.51
1	1	1557	4AC	C5-C4-N4	-2.68	118.26	122.92
2	2	373	A2M	C5-N7-C8	2.68	107.32	103.51
2	2	934	OMG	C4-C5-N7	-2.68	106.48	110.72
2	2	1505	5MC	C5-C4-N3	-2.66	118.80	121.67
2	2	851	4AC	C5-C4-N4	-2.65	118.32	122.92
2	2	1239	4AC	CM7-C7-N4	-2.64	110.72	115.29
1	1	60	4AC	C5-C4-N4	-2.63	118.36	122.92
2	2	519	OMG	C4-C5-N7	-2.63	106.57	110.72
1	1	2608	4AC	C1'-N1-C2	2.61	124.25	118.42
2	2	467	OMG	C4-C5-N7	-2.61	106.59	110.72
1	1	2138	OMG	C4-C5-N7	-2.60	106.60	110.72
2	2	787	OMU	O2-C2-N1	-2.60	119.33	122.79
2	2	1069	OMG	C4-C5-N7	-2.59	106.61	110.72
1	1	1055	A2M	C4-N9-C8	2.59	108.53	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2001	4AC	C5-C4-N4	-2.59	118.42	122.92
2	2	511	4AC	C5-C4-N4	-2.58	118.43	122.92
2	2	913	OMG	C4-C5-N7	-2.58	106.63	110.72
2	2	20	OMU	O2-C2-N1	-2.57	119.37	122.79
2	2	830	OMU	C1'-N1-C2	2.57	122.23	117.57
2	2	875	5MC	C5-C4-N3	-2.57	118.91	121.67
1	1	2144	OMG	C4-C5-N7	-2.56	106.66	110.72
1	1	2136	4AC	CM7-C7-N4	-2.56	110.86	115.29
2	2	657	OMG	C6-C5-N7	2.56	135.01	130.25
1	1	789	OMG	O6-C6-C5	-2.56	119.81	126.60
1	1	2678	OMG	C4-C5-N7	-2.56	106.67	110.72
1	1	2173	A2M	C5-N7-C8	2.55	107.13	103.51
2	2	873	OMG	C4-C5-N7	-2.55	106.69	110.72
2	2	1147	4AC	CM7-C7-N4	-2.54	110.91	115.29
2	2	1498	5MC	C5-C4-N3	-2.53	118.94	121.67
1	1	789	OMG	C6-C5-N7	2.53	134.96	130.25
2	2	373	A2M	C2'-C1'-N9	-2.53	109.28	113.53
2	2	471	OMG	C4-C5-N7	-2.52	106.73	110.72
2	2	373	A2M	C4-N9-C8	2.51	108.45	105.73
2	2	1374	5MC	C5-C4-N3	-2.51	118.97	121.67
2	2	680	OMG	C4-C5-N7	-2.51	106.75	110.72
1	1	2198	5MC	C5-C4-N3	-2.51	118.97	121.67
1	1	2733	5MC	O2-C2-N3	-2.50	118.27	122.33
2	2	1498	5MC	O2-C2-N3	-2.50	118.27	122.33
2	2	535	5MC	C5-C4-N3	-2.48	118.99	121.67
2	2	1488	MA6	C6-C5-N7	2.46	137.41	133.28
2	2	1487	MA6	C6-C5-N7	2.45	137.40	133.28
1	1	328	OMG	C4-C5-N7	-2.45	106.85	110.72
2	2	1040	OMC	O2-C2-N3	-2.44	118.36	122.33
2	2	1469	6MZ	C4-N9-C8	2.44	108.37	105.73
1	1	2093	5MC	C5-C4-N3	-2.42	119.07	121.67
2	2	1025	5MC	C5-C4-N3	-2.41	119.08	121.67
3	3	32	4AC	CM7-C7-N4	-2.40	111.14	115.29
2	2	657	OMG	C4-C5-N7	-2.39	106.94	110.72
1	1	2147	OMG	O6-C6-C5	-2.38	120.28	126.60
1	1	2992	4AC	CM7-C7-N4	2.38	119.41	115.29
2	2	693	5MC	C5-C4-N3	-2.37	119.12	121.67
1	1	2183	5MC	C5-C4-N3	-2.34	119.14	121.67
1	1	2784	OMU	O2-C2-N1	-2.32	119.70	122.79
2	2	1498	5MC	C1'-N1-C6	-2.29	117.32	121.12
1	1	2937	4AC	CM7-C7-N4	-2.28	111.34	115.29
2	2	1505	5MC	O2-C2-N3	-2.28	118.62	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	923	OMG	C4-C5-N7	-2.27	107.12	110.72
2	2	1487	MA6	N9-C8-N7	-2.27	110.80	113.91
1	1	923	OMG	O6-C6-C5	-2.26	120.61	126.60
1	1	2163	5MC	C5-C4-N3	-2.24	119.26	121.67
1	1	789	OMG	C4-C5-N7	-2.23	107.19	110.72
2	2	1147	4AC	O3'-C3'-C2'	2.22	119.01	111.82
2	2	1488	MA6	N9-C8-N7	-2.22	110.88	113.91
2	2	1467	UR3	C1'-N1-C2	2.22	120.73	116.99
1	1	2136	4AC	O2-C2-N3	-2.22	118.73	122.33
1	1	2147	OMG	C4-C5-N7	-2.22	107.22	110.72
1	1	2585	4AC	CM7-C7-N4	-2.21	111.47	115.29
1	1	2162	5MC	C5-C4-N3	-2.19	119.31	121.67
1	1	2608	4AC	CM7-C7-N4	-2.18	111.52	115.29
2	2	875	5MC	O2-C2-N3	-2.18	118.78	122.33
1	1	2203	5MC	C5-C4-N3	-2.18	119.33	121.67
2	2	938	B8H	O4'-C1'-C2'	2.17	108.21	105.14
2	2	1177	OMU	C1'-N1-C2	2.17	121.50	117.57
2	2	680	OMG	O6-C6-C5	-2.16	120.86	126.60
2	2	1469	6MZ	C2-N1-C6	2.16	122.49	115.25
2	2	467	OMG	O6-C6-C5	-2.16	120.88	126.60
1	1	2144	OMG	O6-C6-C5	-2.16	120.88	126.60
1	1	1055	A2M	C6-C5-N7	2.15	136.03	132.02
2	2	657	OMG	O6-C6-C5	-2.14	120.91	126.60
2	2	873	OMG	O6-C6-C5	-2.14	120.91	126.60
2	2	913	OMG	O6-C6-C5	-2.14	120.92	126.60
2	2	64	OMU	C1'-N1-C2	2.14	121.45	117.57
1	1	2173	A2M	C6-C5-N7	2.14	136.00	132.02
2	2	471	OMG	O6-C6-C5	-2.13	120.95	126.60
2	2	1069	OMG	O6-C6-C5	-2.10	121.02	126.60
2	2	373	A2M	C6-C5-N7	2.10	135.94	132.02
2	2	519	OMG	O6-C6-C5	-2.10	121.03	126.60
1	1	2733	5MC	N1-C2-N3	2.10	122.63	118.81
1	1	2678	OMG	O6-C6-C5	-2.09	121.05	126.60
1	1	328	OMG	O6-C6-C5	-2.08	121.08	126.60
2	2	1469	6MZ	N9-C8-N7	-2.07	111.08	113.91
2	2	934	OMG	O6-C6-C5	-2.07	121.12	126.60
1	1	789	OMG	CM2-O2'-C2'	-2.05	109.14	114.52
1	1	2992	4AC	O7-C7-CM7	-2.04	118.27	122.06
1	1	2138	OMG	O6-C6-C5	-2.04	121.20	126.60
1	1	60	4AC	O2-C2-N3	-2.04	119.02	122.33
2	2	839	4AC	O2-C2-N3	-2.01	119.07	122.33
1	1	1055	A2M	N9-C8-N7	-2.00	111.17	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2083	4AC	O2-C2-N3	-2.00	119.08	122.33

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	789	OMG	C3'-C4'-C5'-O5'
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
1	1	789	OMG	O4'-C4'-C5'-O5'
2	2	1488	MA6	O4'-C4'-C5'-O5'
1	1	2147	OMG	O4'-C4'-C5'-O5'
2	2	1488	MA6	C3'-C4'-C5'-O5'
1	1	2733	5MC	C2'-C1'-N1-C6
2	2	20	OMU	C2'-C1'-N1-C6
2	2	20	OMU	O4'-C4'-C5'-O5'
1	1	2992	4AC	O7-C7-N4-C4
1	1	2992	4AC	CM7-C7-N4-C4
2	2	1498	5MC	O4'-C1'-N1-C6
1	1	2678	OMG	C3'-C2'-O2'-CM2
1	1	2733	5MC	O4'-C1'-N1-C6
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	20	OMU	C3'-C4'-C5'-O5'
2	2	1498	5MC	O4'-C1'-N1-C2
1	1	2733	5MC	C2'-C1'-N1-C2
2	2	20	OMU	C2'-C1'-N1-C2
1	1	2733	5MC	O4'-C1'-N1-C2
2	2	20	OMU	O4'-C1'-N1-C2
2	2	934	OMG	O4'-C4'-C5'-O5'
2	2	787	OMU	C2'-C1'-N1-C6
2	2	938	B8H	O4'-C1'-C5-C4
2	2	873	OMG	C4'-C5'-O5'-P
2	2	787	OMU	O4'-C1'-N1-C6
1	1	2733	5MC	O4'-C4'-C5'-O5'
2	2	1040	OMC	C2'-C1'-N1-C2
2	2	1374	5MC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	1	923	OMG	C1'-C2'-O2'-CM2
1	1	2144	OMG	C1'-C2'-O2'-CM2
2	2	1069	OMG	C1'-C2'-O2'-CM2
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-C2
1	1	1755	4AC	C3'-C4'-C5'-O5'
2	2	1498	5MC	O4'-C4'-C5'-O5'
3	3	32	4AC	C3'-C4'-C5'-O5'
2	2	830	OMU	C2'-C1'-N1-C2
1	1	2733	5MC	C3'-C4'-C5'-O5'
2	2	787	OMU	C2'-C1'-N1-C2

There are no ring outliers.

107 monomers are involved in 177 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	1557	4AC	1	0
2	2	379	4AC	1	0
1	1	2027	4AC	1	0
1	1	229	4AC	2	0
1	1	694	4AC	1	0
1	1	357	4AC	1	0
2	2	731	4AC	2	0
1	1	2585	4AC	2	0
2	2	680	OMG	1	0
2	2	1479	4AC	2	0
1	1	981	4AC	1	0
1	1	1765	4AC	2	0
2	2	839	4AC	2	0
2	2	848	4AC	1	0
1	1	922	4AC	2	0
1	1	2495	4AC	1	0
1	1	1755	4AC	3	0
2	2	471	OMG	1	0
1	1	1621	4AC	1	0
1	1	1293	4AC	1	0
2	2	1025	5MC	1	0
2	2	718	4AC	1	0
1	1	2733	5MC	2	0
1	1	136	4AC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	1048	4AC	2	0
1	1	1460	4AC	3	0
1	1	789	OMG	2	0
2	2	319	4AC	1	0
1	1	829	4AC	1	0
1	1	615	OMC	1	0
1	1	1243	4AC	1	0
1	1	533	4AC	2	0
2	2	626	4AC	2	0
1	1	2925	4AC	2	0
1	1	1662	4AC	2	0
1	1	1934	4AC	2	0
2	2	1147	4AC	1	0
1	1	835	4AC	2	0
1	1	2163	5MC	3	0
2	2	1496	5MC	1	0
1	1	161	4AC	1	0
2	2	590	4AC	1	0
1	1	2908	4AC	2	0
1	1	2287	4AC	5	0
2	2	873	OMG	1	0
2	2	1488	MA6	1	0
1	1	2678	OMG	2	0
1	1	1222	4AC	2	0
1	1	1617	4AC	4	0
1	1	211	4AC	2	0
2	2	1069	OMG	1	0
1	1	1594	4AC	1	0
2	2	546	4AC	1	0
1	1	243	4AC	1	0
3	3	32	4AC	1	0
2	2	868	4AC	1	0
2	2	1380	OMU	2	0
1	1	2865	4AC	1	0
2	2	1376	OMC	2	0
2	2	913	OMG	1	0
2	2	1184	4AC	2	0
1	1	2992	4AC	1	0
1	1	91	4AC	2	0
1	1	2001	4AC	4	0
1	1	1867	4AC	1	0
1	1	1055	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	2642	4AC	1	0
1	1	2329	4AC	1	0
2	2	511	4AC	1	0
1	1	2249	4AC	2	0
1	1	2608	4AC	3	0
1	1	2083	4AC	2	0
2	2	64	OMU	1	0
1	1	2718	4AC	2	0
1	1	1554	4AC	1	0
1	1	458	4AC	3	0
1	1	1938	4AC	1	0
2	2	394	4AC	1	0
1	1	1878	4AC	2	0
2	2	53	4AC	2	0
1	1	1695	4AC	1	0
2	2	373	A2M	2	0
2	2	1233	4AC	1	0
2	2	636	4AC	2	0
2	2	828	4AC	1	0
1	1	802	4AC	2	0
1	1	2548	4AC	2	0
1	1	2198	5MC	1	0
1	1	341	4AC	1	0
2	2	957	4AC	1	0
1	1	2162	5MC	2	0
1	1	3004	4AC	2	0
1	1	1068	4AC	2	0
1	1	451	4AC	3	0
1	1	1780	4AC	3	0
2	2	703	4AC	4	0
1	1	1065	4AC	3	0
1	1	2960	4AC	2	0
2	2	1177	OMU	2	0
1	1	2062	4AC	1	0
2	2	1239	4AC	1	0
1	1	1667	4AC	4	0
2	2	479	4AC	2	0
1	1	1550	4AC	2	0
1	1	2136	4AC	2	0
1	1	2545	4AC	3	0
1	1	314	4AC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 257 ligands modelled in this entry, 257 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	11.57

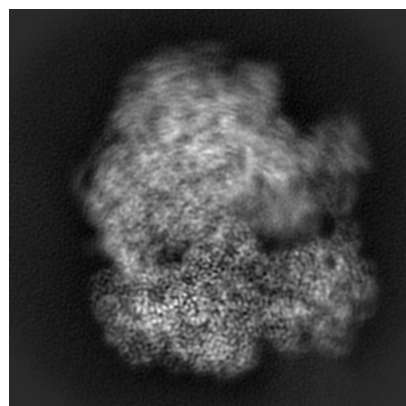
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55135. These allow visual inspection of the internal detail of the map and identification of artifacts.

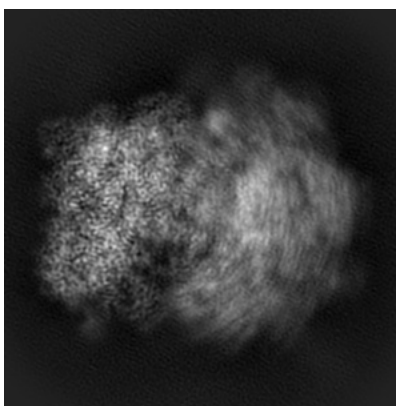
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

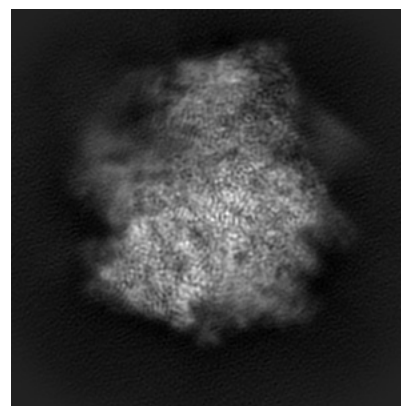
6.1.1 Primary map



X

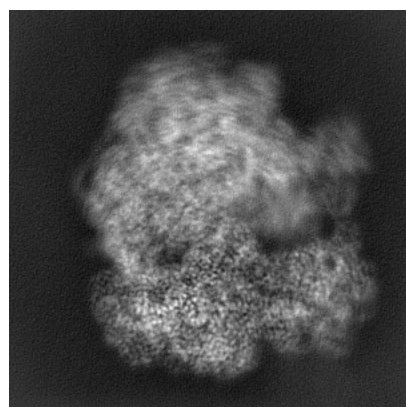


Y

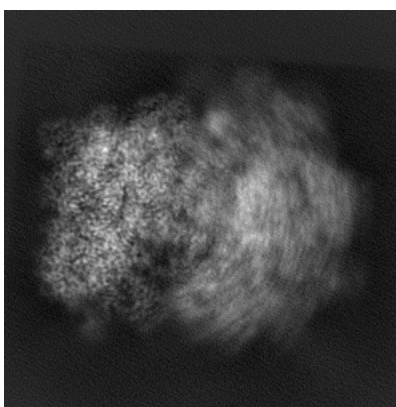


Z

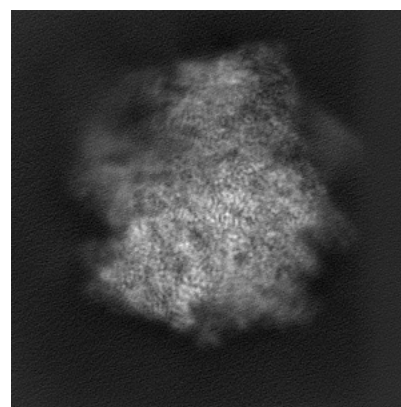
6.1.2 Raw map



X



Y

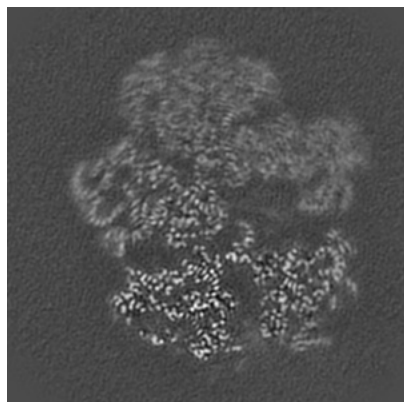


Z

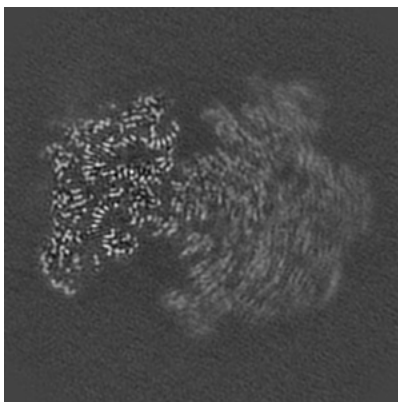
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

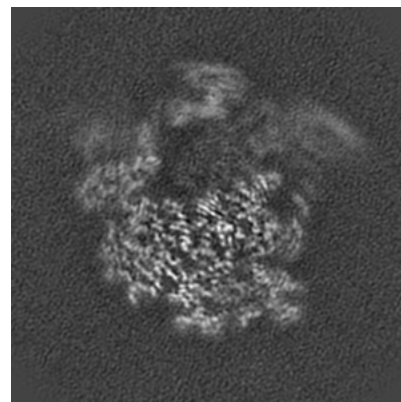
6.2.1 Primary map



X Index: 180

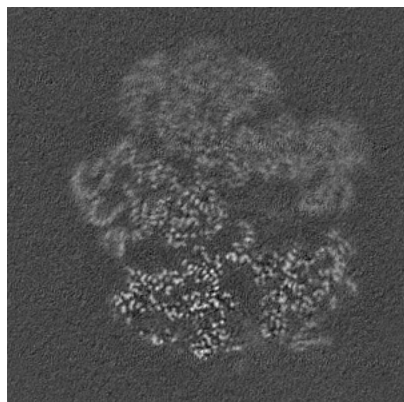


Y Index: 180

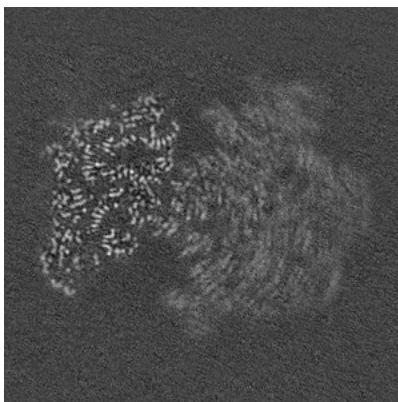


Z Index: 180

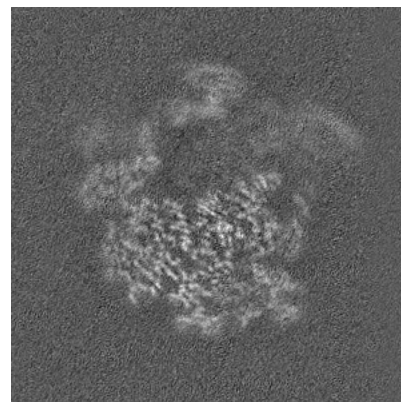
6.2.2 Raw map



X Index: 180



Y Index: 180

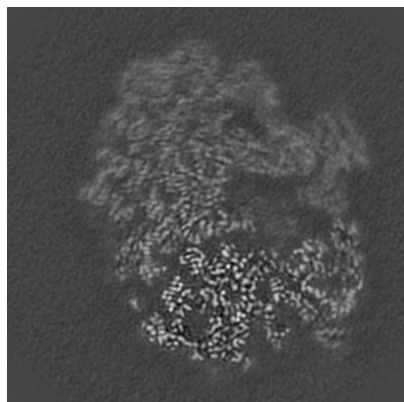


Z Index: 180

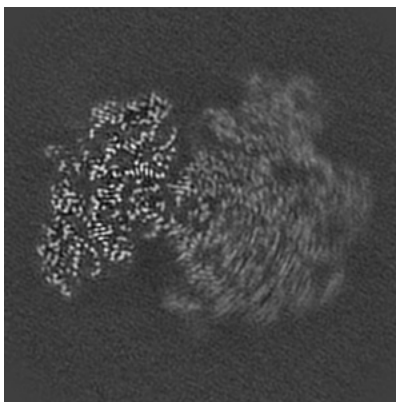
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

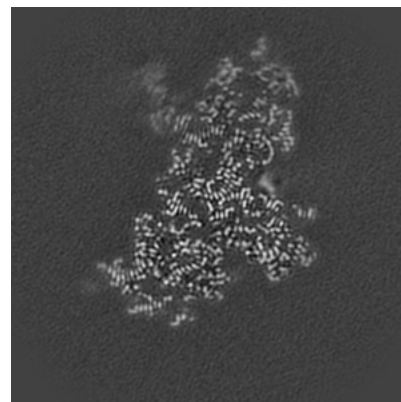
6.3.1 Primary map



X Index: 196

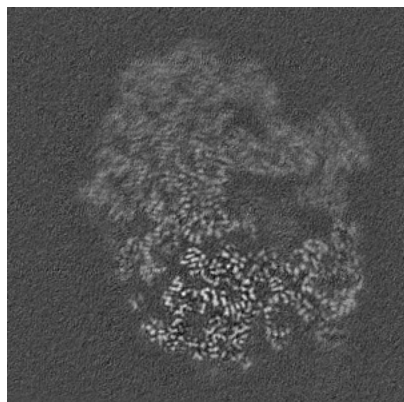


Y Index: 175

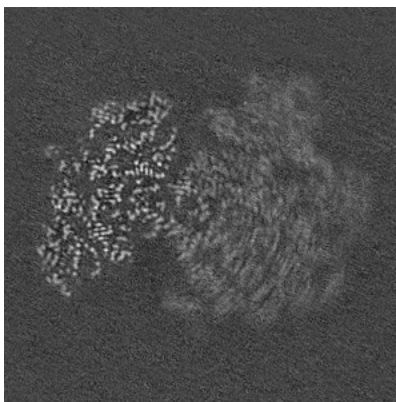


Z Index: 91

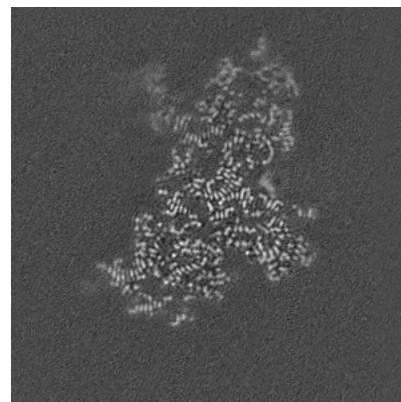
6.3.2 Raw map



X Index: 195



Y Index: 175

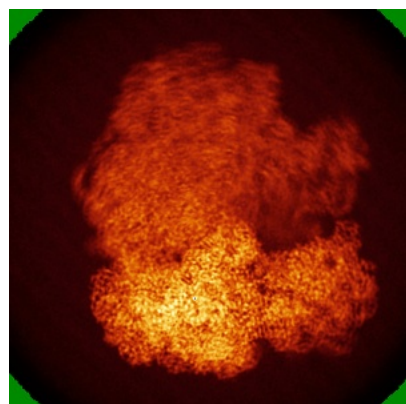


Z Index: 91

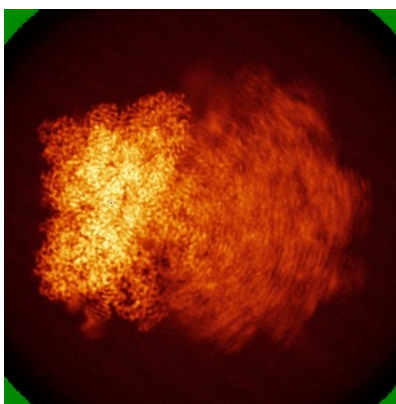
The images above show the largest variance slices of the map in three orthogonal directions.

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

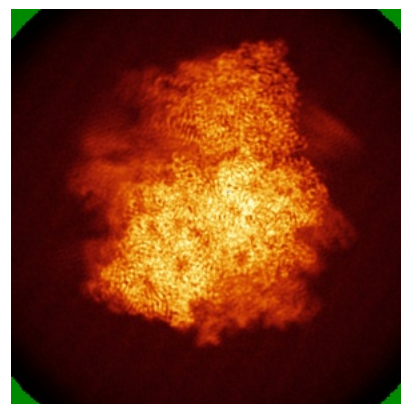
6.4.1 Primary map



X

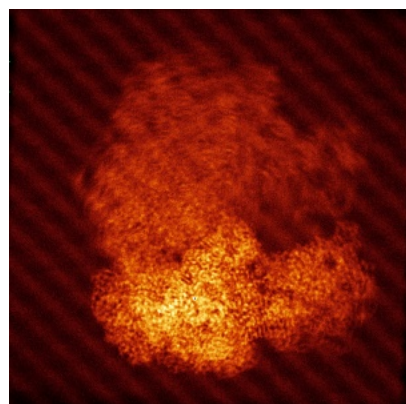


Y

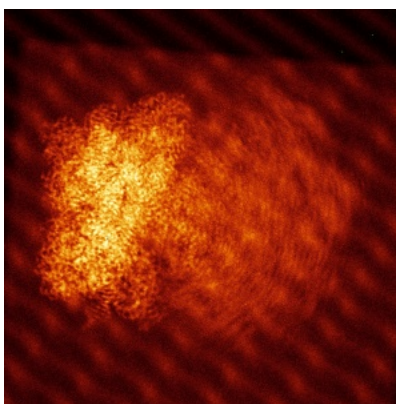


Z

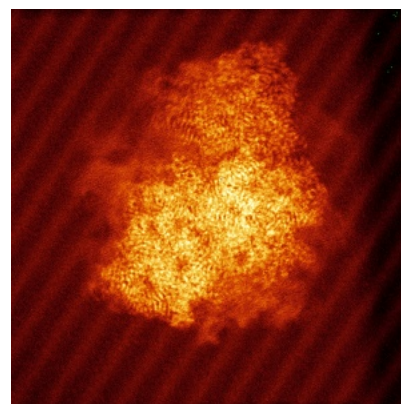
6.4.2 Raw map



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



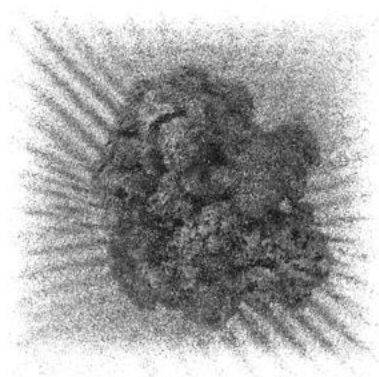
Y



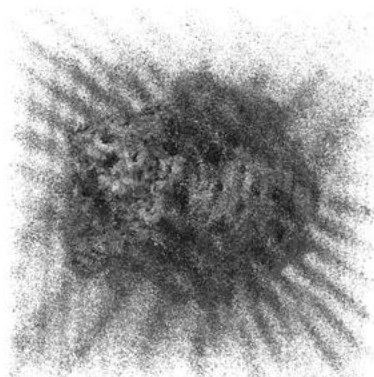
Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

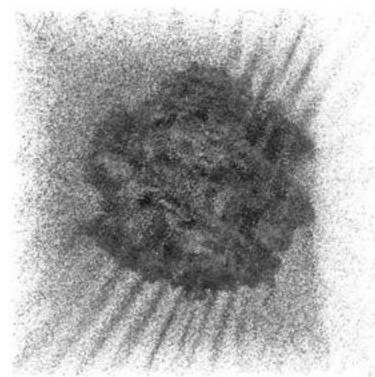
6.5.2 Raw map



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.

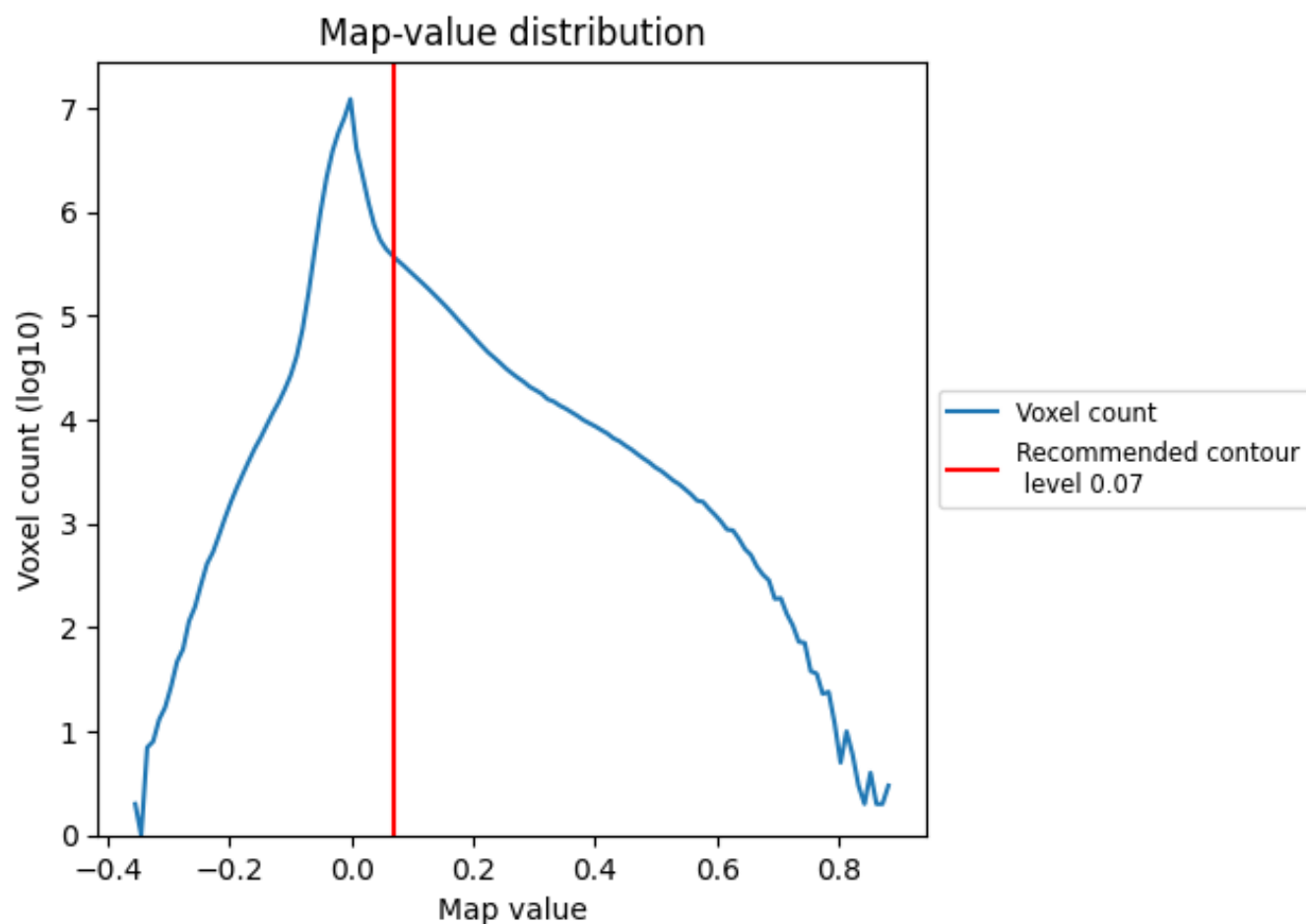
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

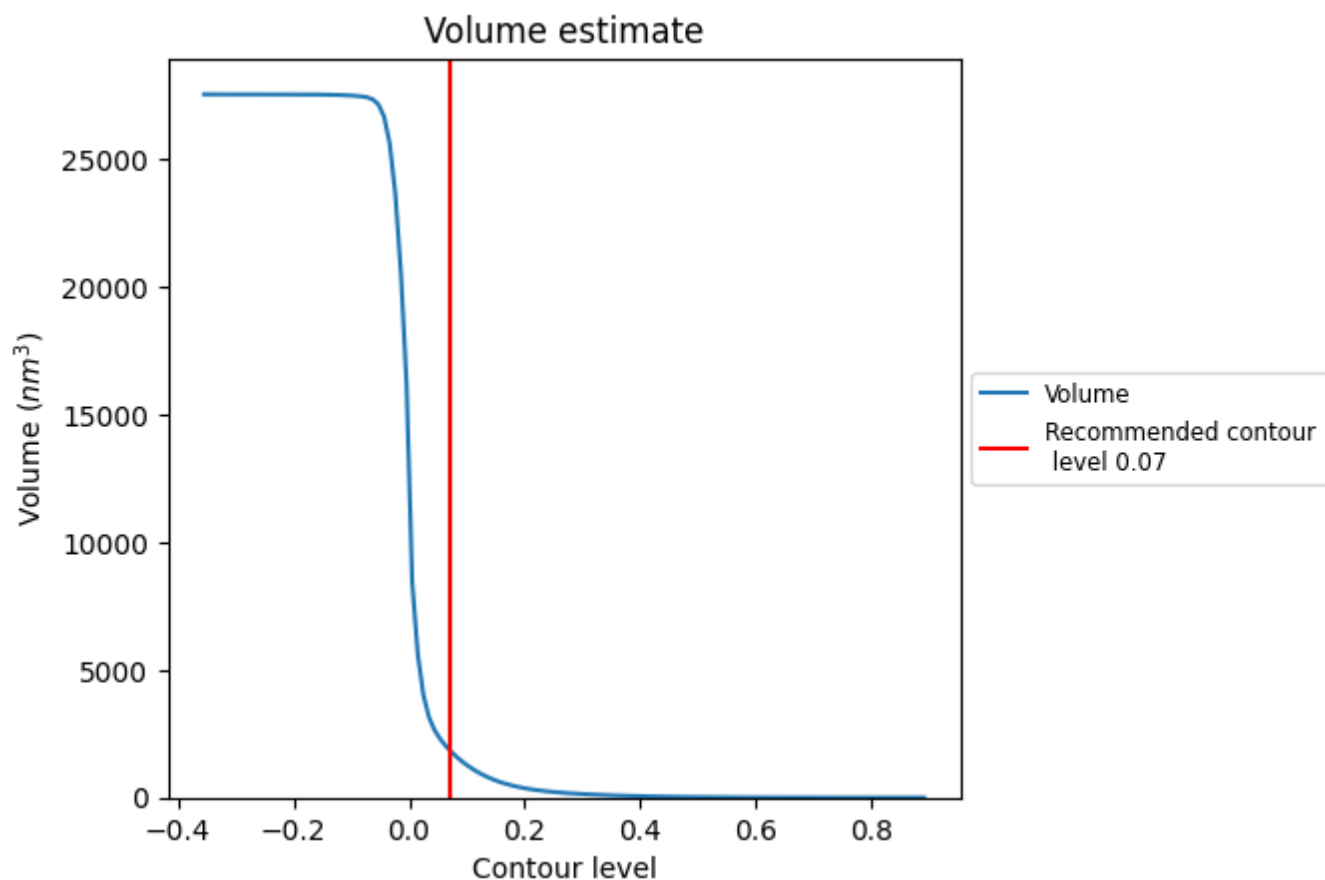
This section contains the results of statistical analysis of the map.

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.

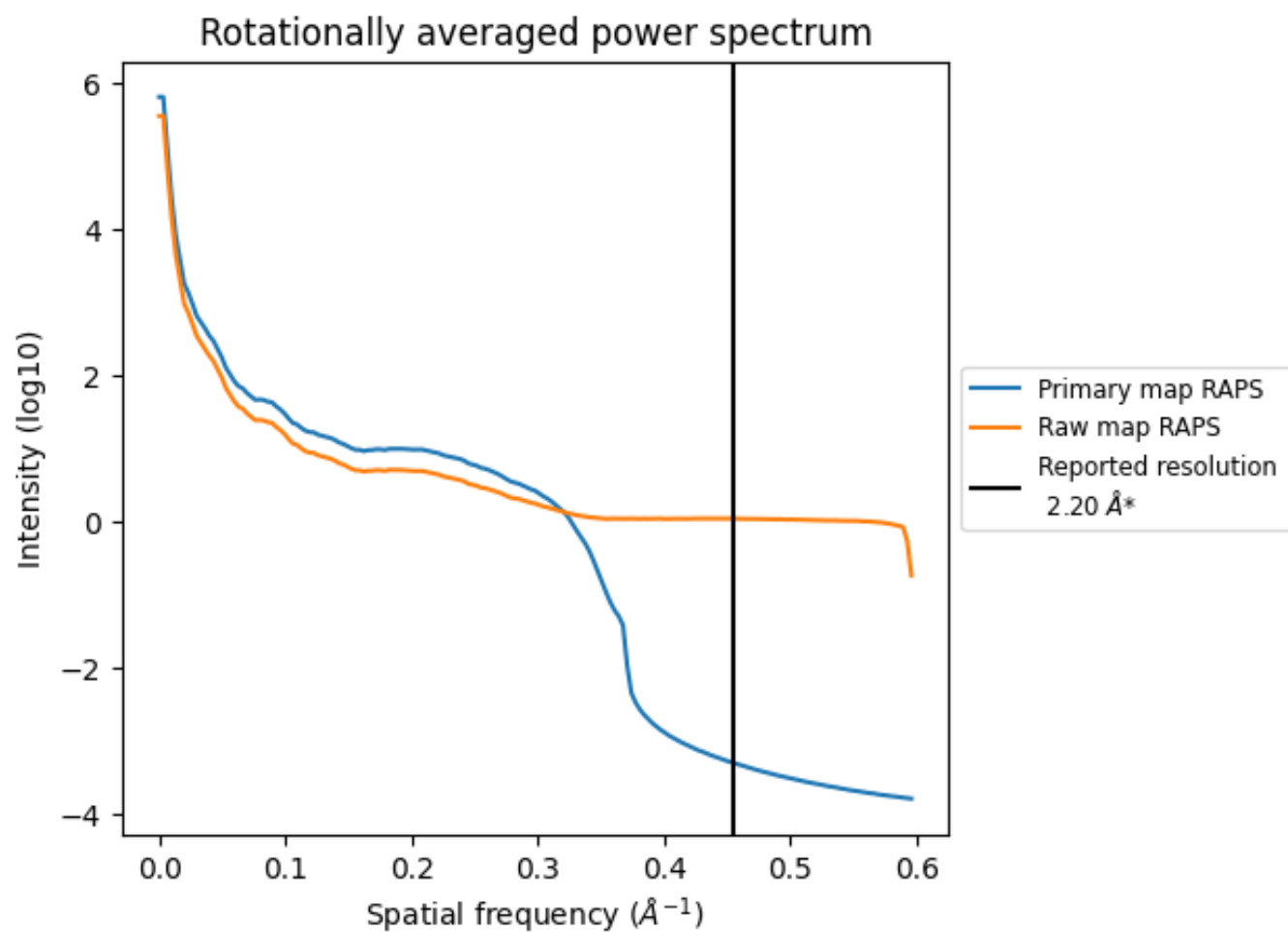
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1867 nm^3 ; this corresponds to an approximate mass of 1686 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

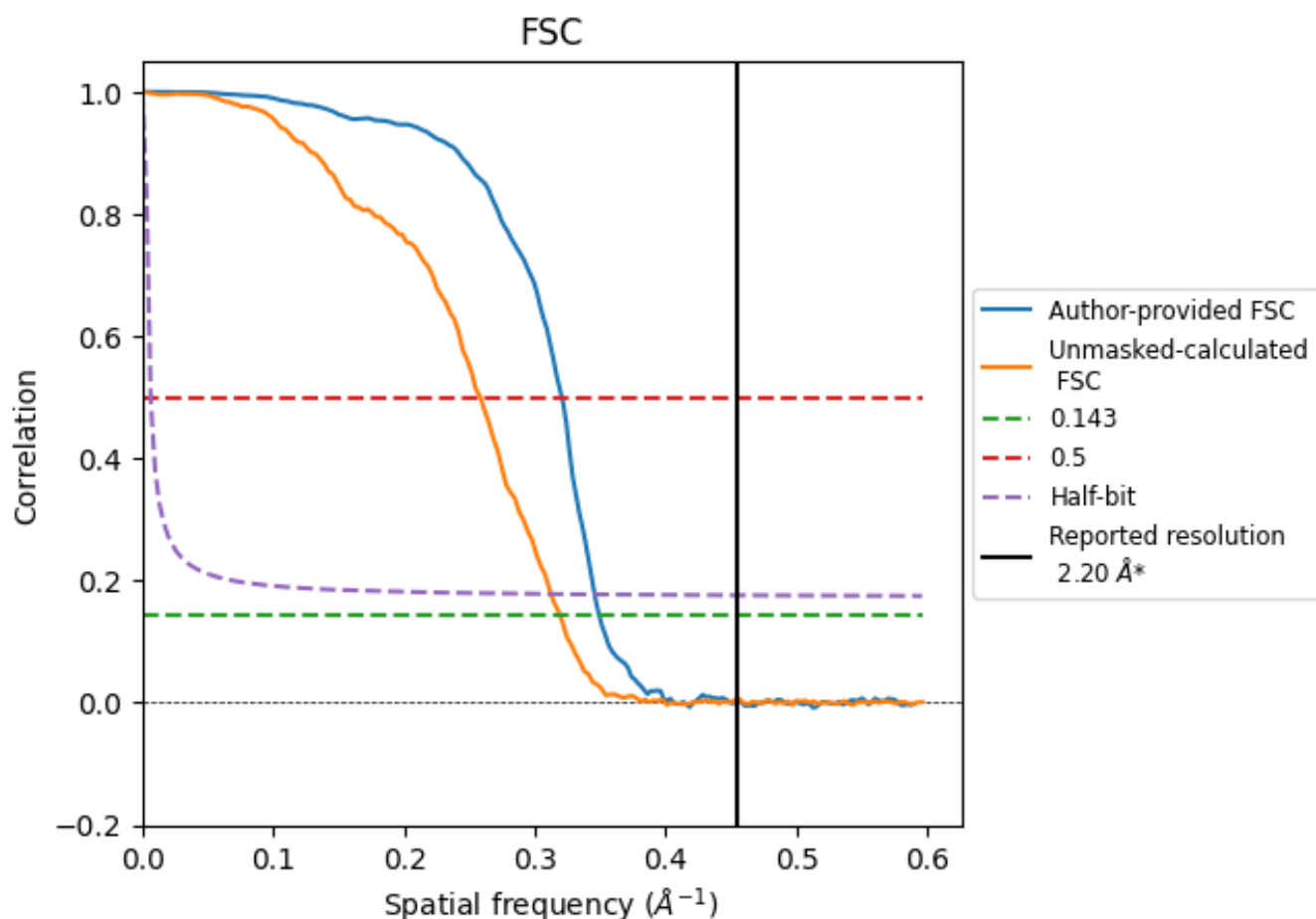


*Reported resolution corresponds to spatial frequency of 0.455 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.86	3.12	2.89
Unmasked-calculated*	3.13	3.87	3.20

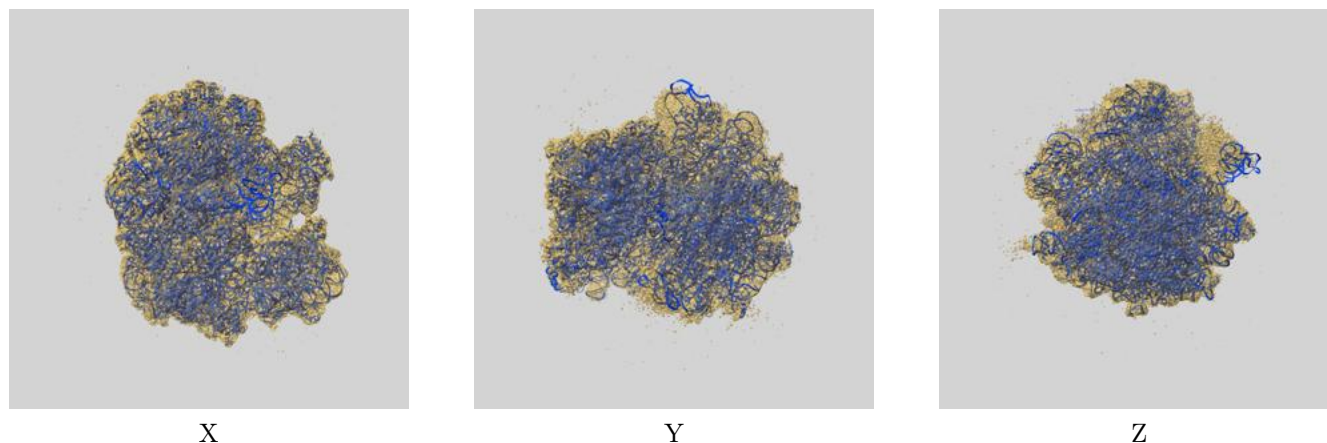
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.86 differs from the reported value 2.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.13 differs from the reported value 2.2 by more than 10 %

9 Map-model fit [i](#)

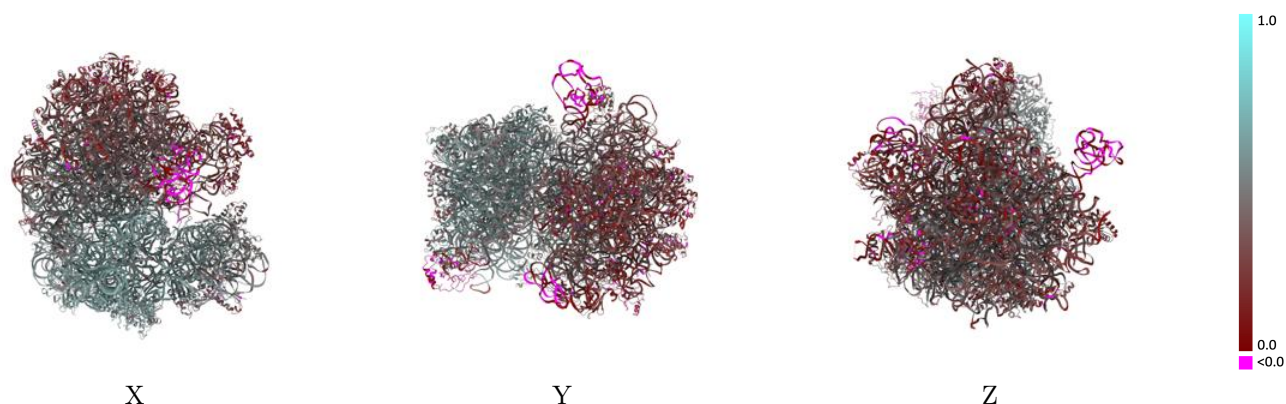
This section contains information regarding the fit between EMDB map EMD-55135 and PDB model 9SRA. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



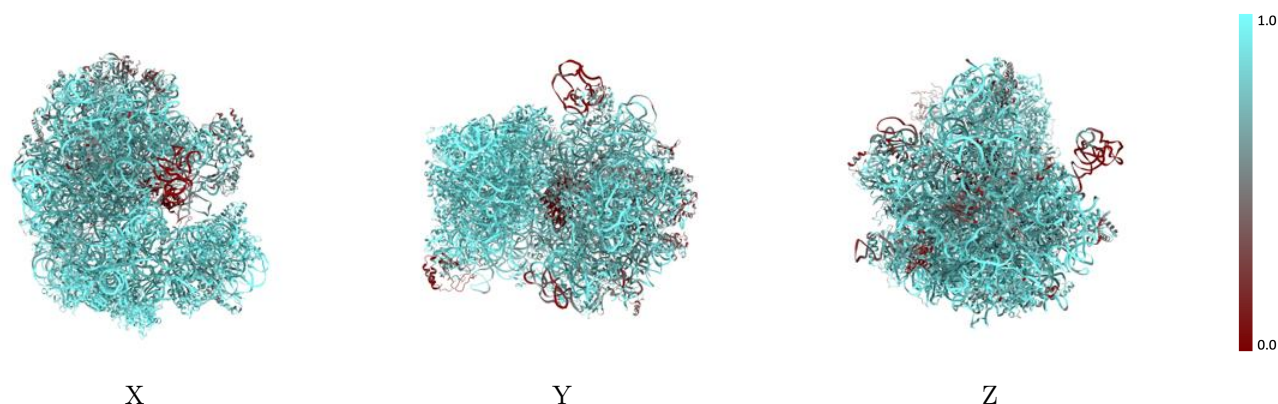
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



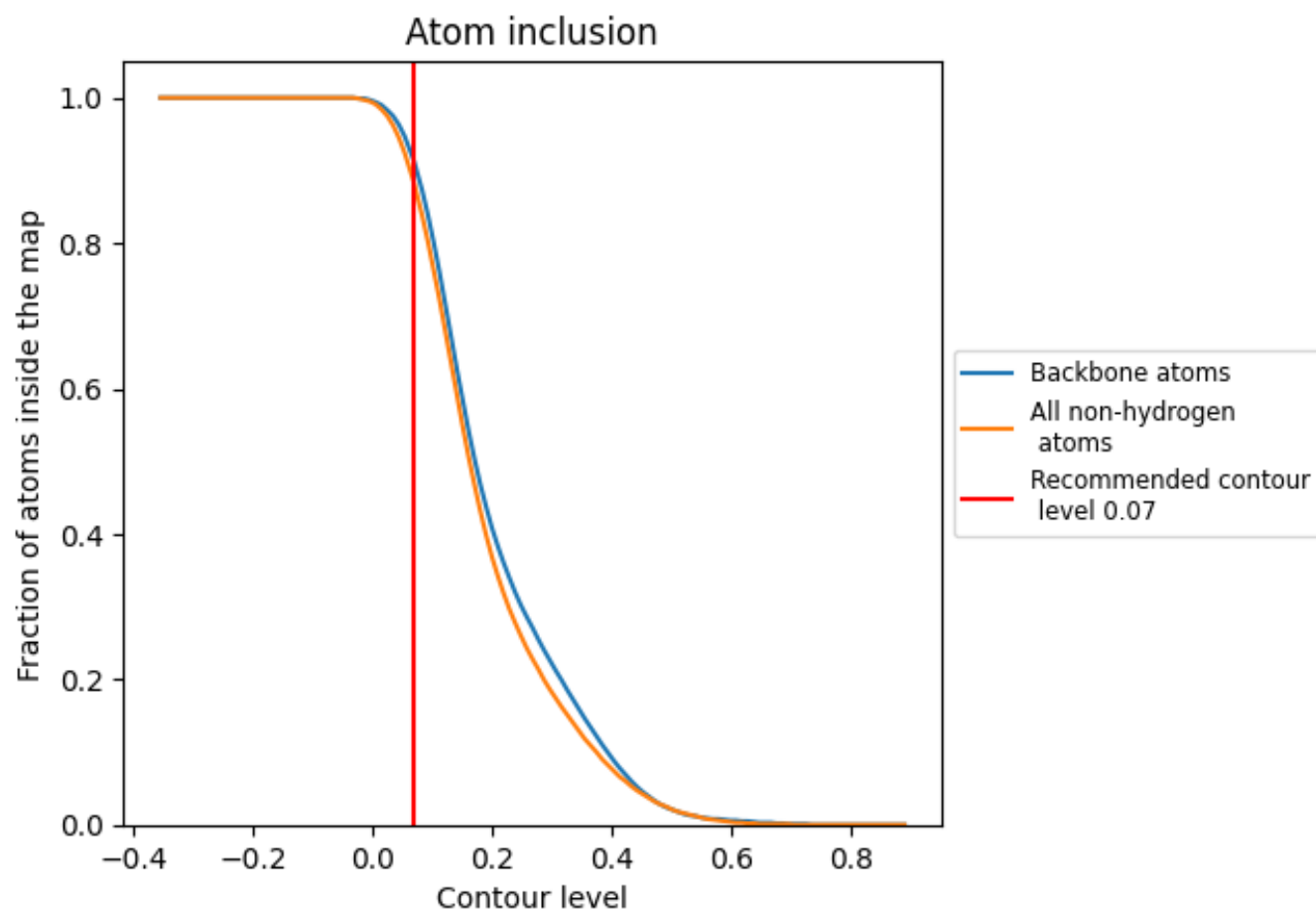
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8820	 0.4130
1	 0.9040	 0.3630
2	 0.9930	 0.5590
3	 0.9120	 0.2480
A0	 0.9500	 0.5960
A3	 0.3670	 0.0910
AA	 0.9400	 0.5430
AB	 0.9630	 0.5590
AC	 0.9660	 0.5740
AD	 0.9680	 0.5590
AE	 0.9680	 0.5650
AF	 0.9620	 0.5750
AG	 0.9380	 0.5040
AH	 0.9670	 0.5550
AI	 0.9790	 0.5980
AJ	 0.9540	 0.5500
AK	 0.9420	 0.5120
AL	 0.8550	 0.4280
AM	 0.9440	 0.5610
AN	 0.9540	 0.5760
AO	 0.9010	 0.4330
AP	 0.9290	 0.5180
AQ	 0.9590	 0.5670
AR	 0.9700	 0.5860
AS	 0.9330	 0.4910
AT	 0.8780	 0.4330
AU	 0.9380	 0.4730
AV	 0.9390	 0.5140
AW	 0.9740	 0.5280
AX	 0.8970	 0.4850
AY	 0.2330	 0.0680
AZ	 0.8930	 0.4620
B4	 0.3280	 0.1520
B5	 0.8530	 0.4050
B6	 0.3360	 0.1680



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Chain	Atom inclusion	Q-score
BB	 0.8710	 0.4790
BC	 0.8510	 0.3840
BD	 0.7510	 0.2670
BE	 0.7160	 0.1880
BF	 0.8040	 0.2580
BG	 0.6820	 0.2780
BI	 0.7730	 0.3000
BJ	 0.8560	 0.4420
BK	 0.7020	 0.1860
BL	 0.6410	 0.2590
BM	 0.8230	 0.3600
BN	 0.7610	 0.2940
BO	 0.6370	 0.2020
BP	 0.7400	 0.2220
BQ	 0.8810	 0.4570
BR	 0.7500	 0.2660
BS	 0.8760	 0.4130
BT	 0.7910	 0.3520
BU	 0.7700	 0.2700
BV	 0.9100	 0.4140
BW	 0.6870	 0.2640
BY	 0.7130	 0.2530
BZ	 0.8630	 0.4450
Ba	 0.8820	 0.4430
Bb	 0.7500	 0.2990
Bc	 0.7190	 0.2510
Bd	 0.9000	 0.4510
Be	 0.8310	 0.4000
Bf	 0.8380	 0.3500
Bg	 0.8730	 0.2910
Bi	 0.8790	 0.5000
Bj	 0.6700	 0.3110
Bk	 0.7950	 0.2740
Bl	 0.5770	 0.1920
H	 0.3280	 0.3540
sd	 0.9400	 0.4010