



Full wwPDB EM Validation Report ⓘ

Aug 3, 2026 – 02:01 pm BST

PDB ID : 9T7H / pdb_00009t7h
EMDB ID : EMD-55636
Title : Cryo-EM structure of P. abyssi 70S ribosome in complex with hibernation factor HibA (L1 stalk conformation)
Authors : Madru, C.M.; Bourgeois, G.B.; Mechulam, Y.M.; Schmitt, E.S.
Deposited on : 2025-11-10
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

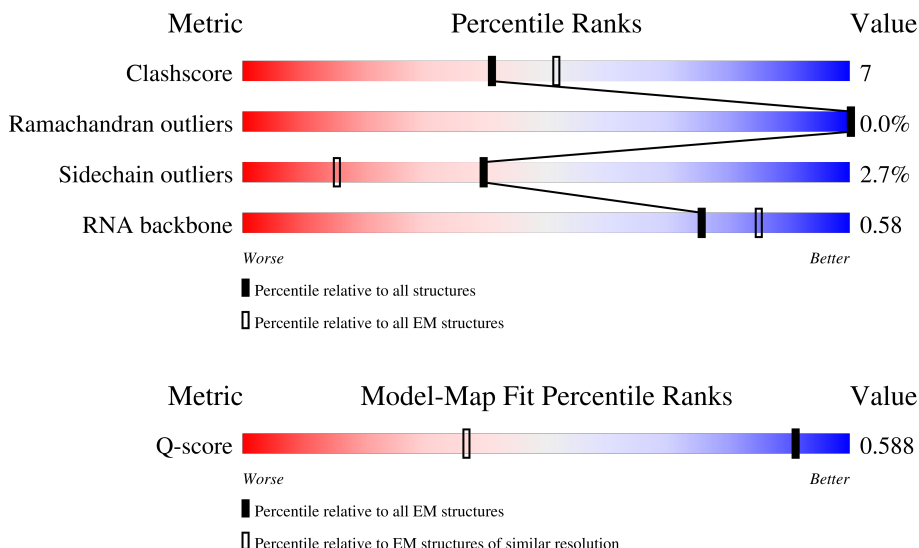
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.10 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	2317 (1.60 - 2.60)

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.

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1	1	3018	
2	2	1512	
3	3	128	

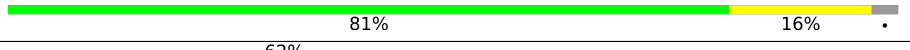
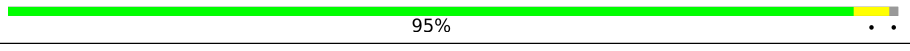
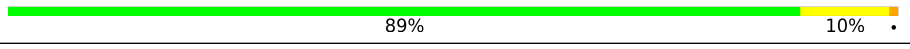
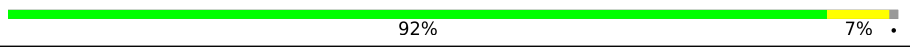
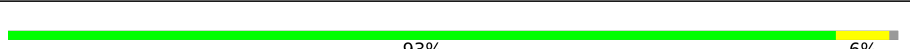
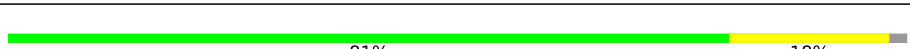
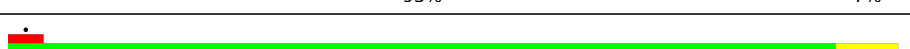
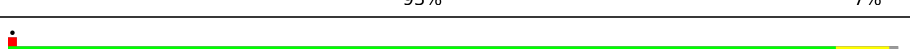
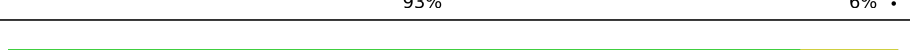
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Mol	Chain	Length	Quality of chain
4	H	392	
5	AA	199	
6	AB	202	
7	AC	63	
8	AD	180	
9	AE	243	
10	AF	236	
11	AG	125	
12	AH	215	
13	AI	130	
14	AJ	127	
15	AK	135	
16	AL	102	
17	AM	137	
18	AN	147	
19	AP	56	
20	AQ	158	
21	AR	113	
22	AS	67	
23	AU	150	
24	AV	99	
24	B6	99	
25	AW	65	
26	AX	71	
27	AY	51	

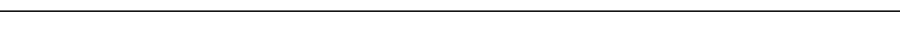
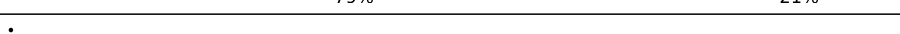
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Mol	Chain	Length	Quality of chain
28	AZ	210	
29	A0	37	
30	A3	123	
30	B4	123	
30	BG	123	
31	AT	132	
32	AO	148	
33	BB	239	
34	BY	155	
35	BO	203	
36	BC	361	
37	B5	82	
37	BK	82	
38	BL	147	
39	Bf	51	
40	BU	121	
41	Bb	130	
42	Be	62	
43	BE	188	
44	Ba	94	
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	 86% 13% .
51	BV	67	 82% 12% 6%
52	Bj	94	 90% 10%
53	BD	255	 85% 13% .
54	BF	184	 82% 16% ..
55	BZ	99	 82% 17% .
56	BP	120	 88% 12%
57	BM	194	 91% 8% .
58	BS	155	 86% 12% ..
59	Bd	91	 91% 8% .
60	BN	181	 80% 17% ..
61	Bg	51	 78% 16% 6%
62	Bc	87	 89% 10% .
63	BJ	141	 91% 8% .
64	Bl	77	 79% 21%
65	Bk	65	 88% 9% .
66	BA	219	 36% 52% 44% ..

2 Entry composition

There are 68 unique types of molecules in this entry. The entry contains 171964 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called rRNA 23S.

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

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

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

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

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

- Molecule 4 is a protein called 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	29	Total	C	N	O	S	0	0
			227	141	44	37	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 Small ribosomal subunit protein 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 protein called Large ribosomal subunit protein uL1.

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

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

Mol	Chain	Residues	Atoms		AltConf
67	1	165	Total	Mg	0
			165	165	
67	2	61	Total	Mg	0
			61	61	
67	3	1	Total	Mg	0
			1	1	
67	AD	1	Total	Mg	0
			1	1	
67	AE	1	Total	Mg	0
			1	1	
67	AF	1	Total	Mg	0
			1	1	
67	AK	1	Total	Mg	0
			1	1	
67	AN	1	Total	Mg	0
			1	1	
67	AR	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
67	AU	1	Total 1	Mg 1	0
67	AT	1	Total 1	Mg 1	0
67	BB	2	Total 2	Mg 2	0
67	Bb	1	Total 1	Mg 1	0
67	BD	1	Total 1	Mg 1	0
67	BM	1	Total 1	Mg 1	0
67	BS	1	Total 1	Mg 1	0

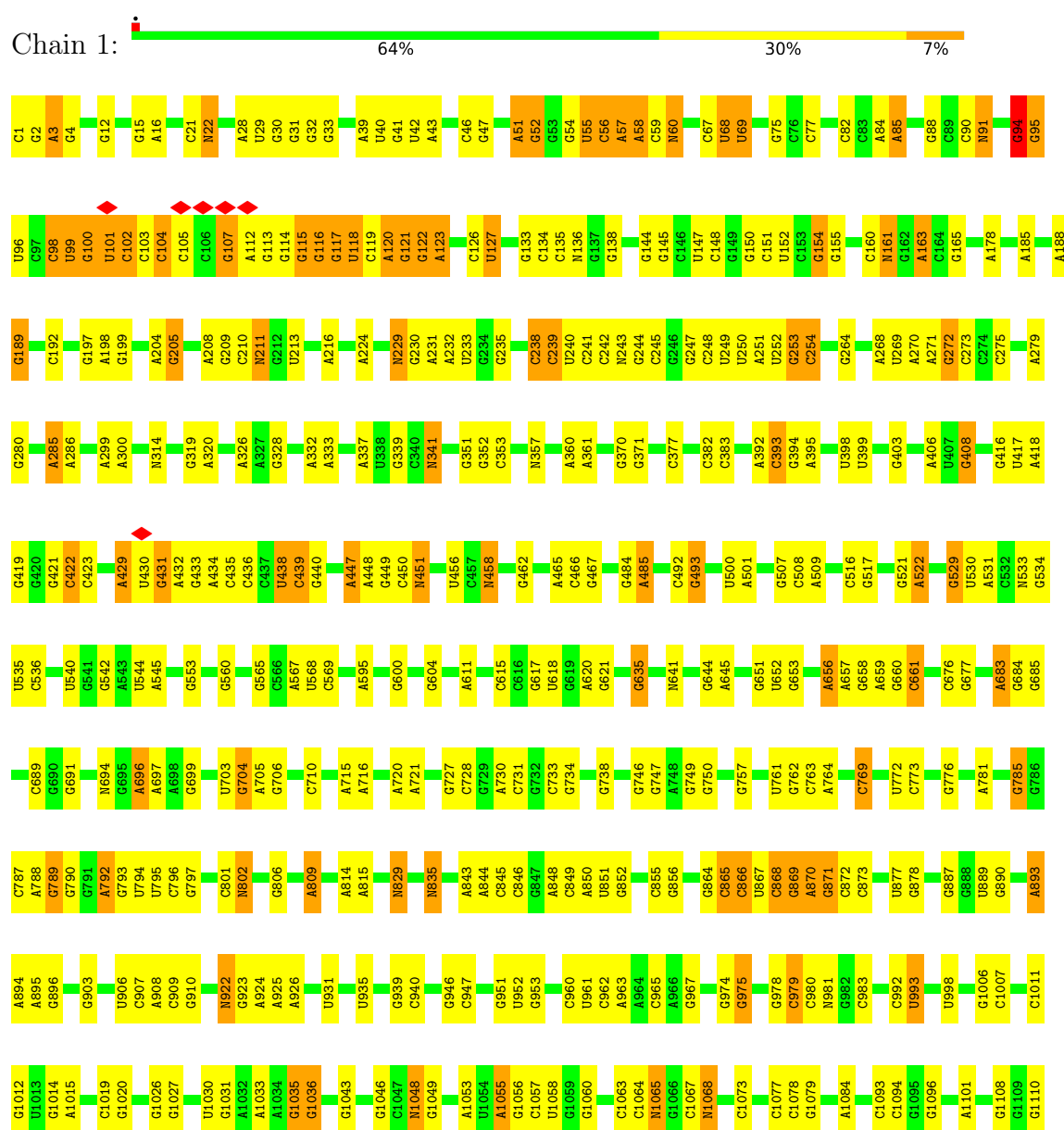
- Molecule 68 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

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

• Molecule 1: rRNA 23S

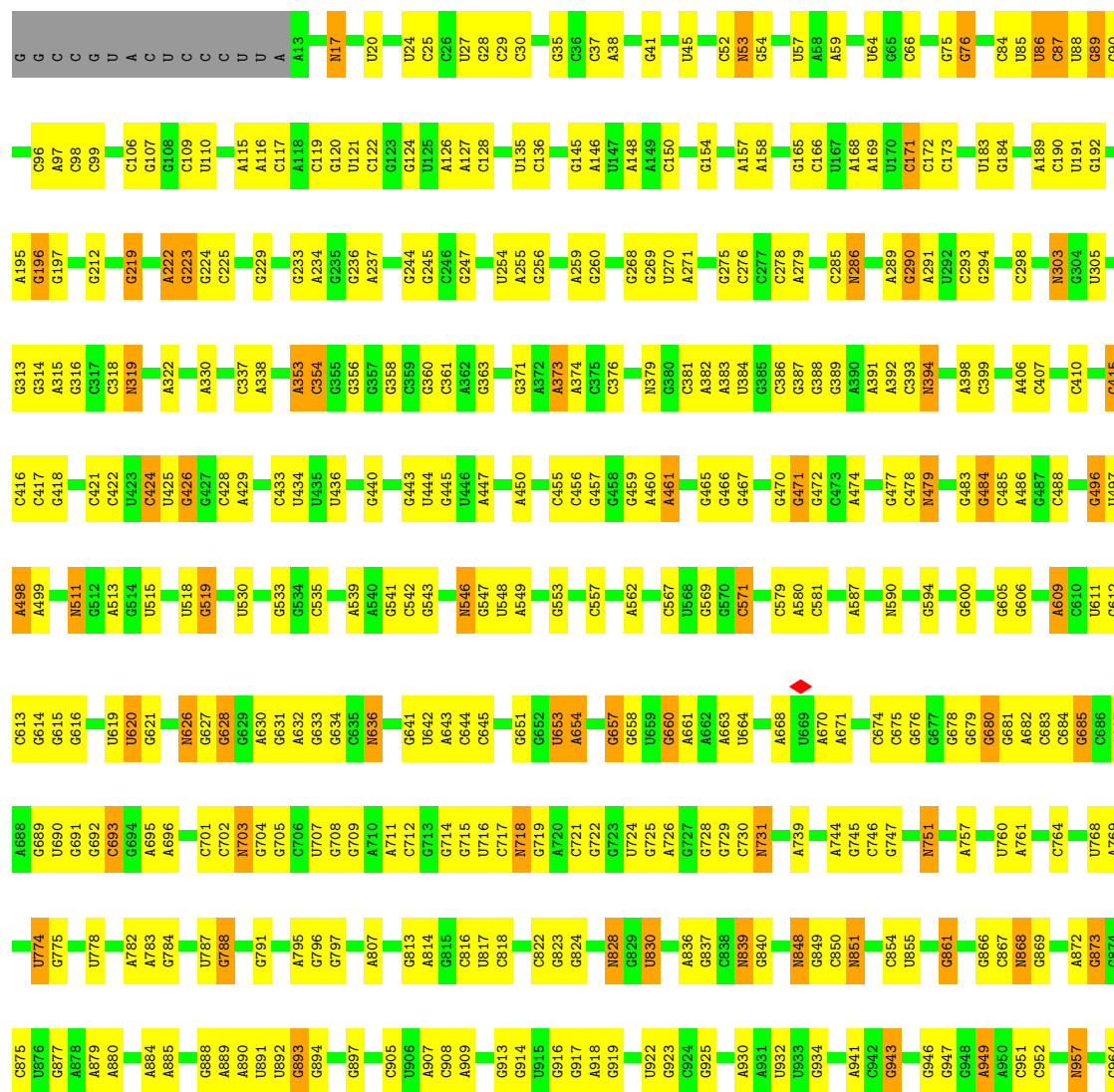


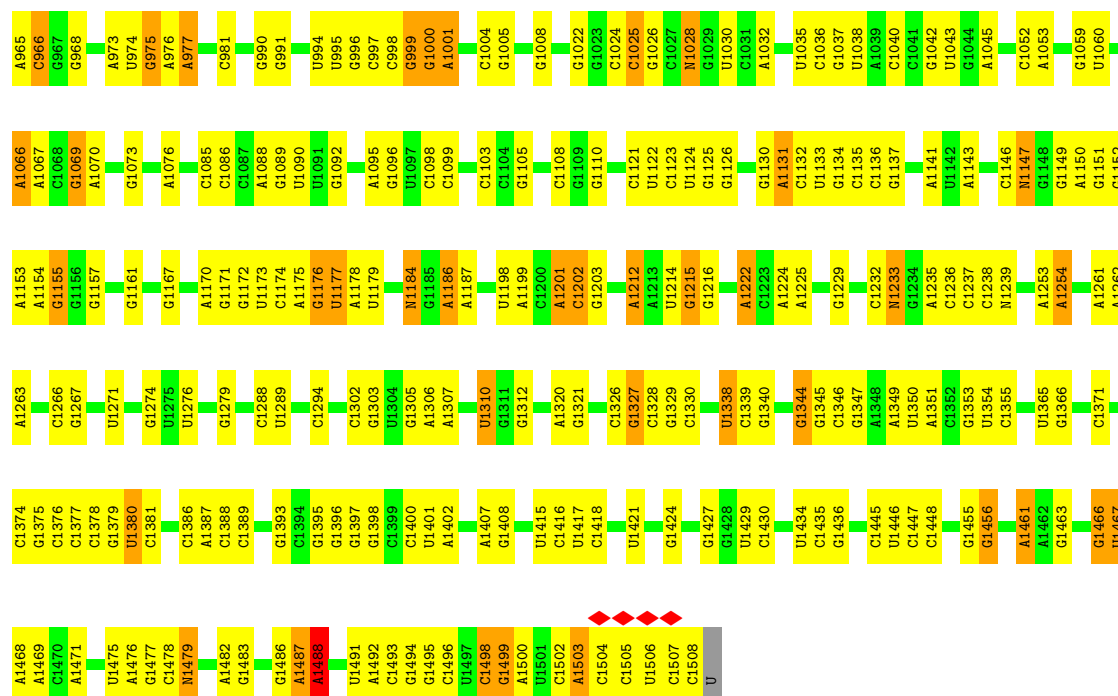




• Molecule 2: rRNA 16S

Chain 2: 57% 35% 7% .

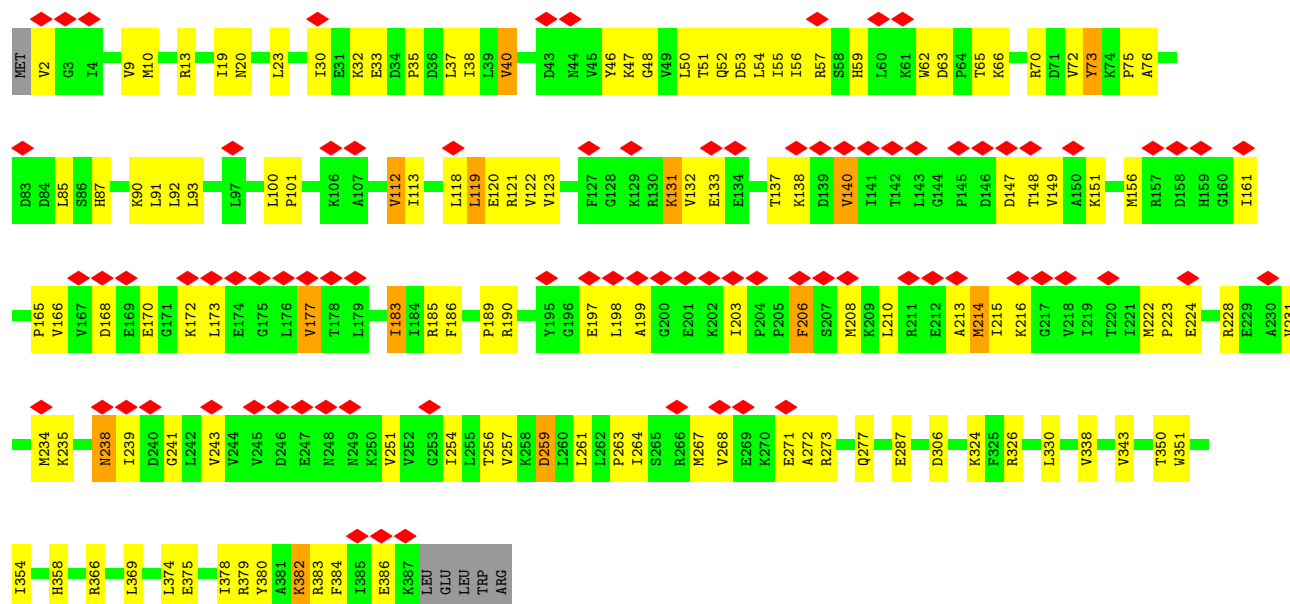




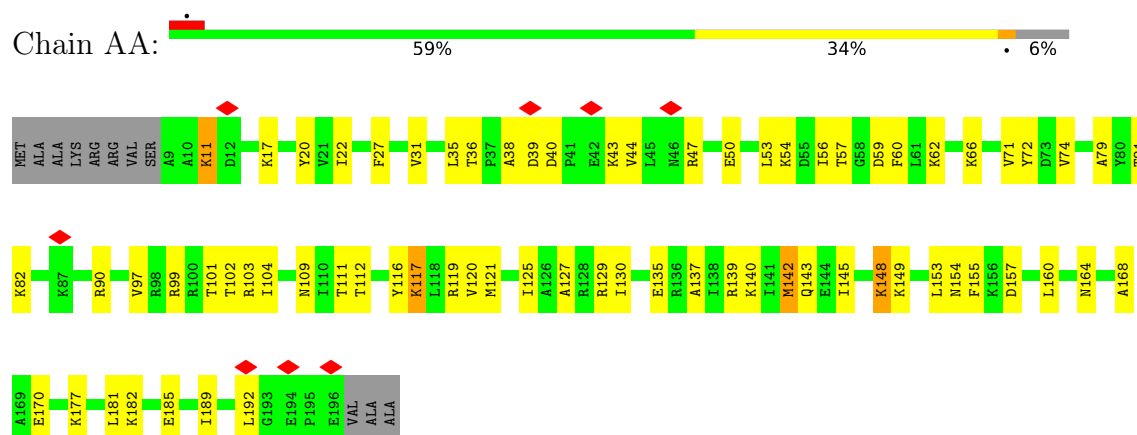
• Molecule 3: rRNA 5S



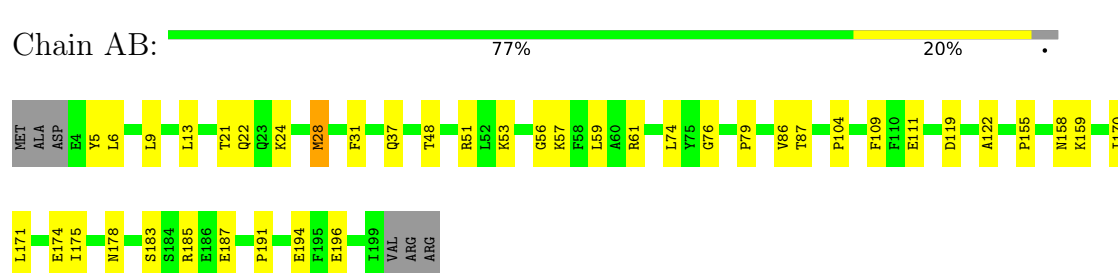
• Molecule 4: Dehydrogenase



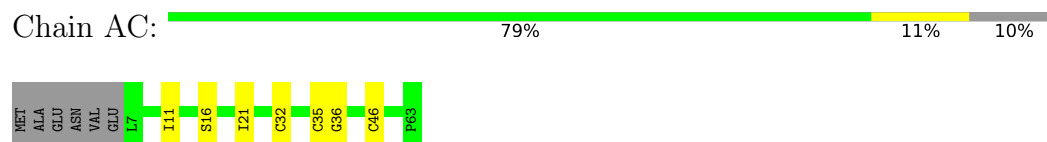
- Molecule 5: 30S ribosomal protein S3Ae



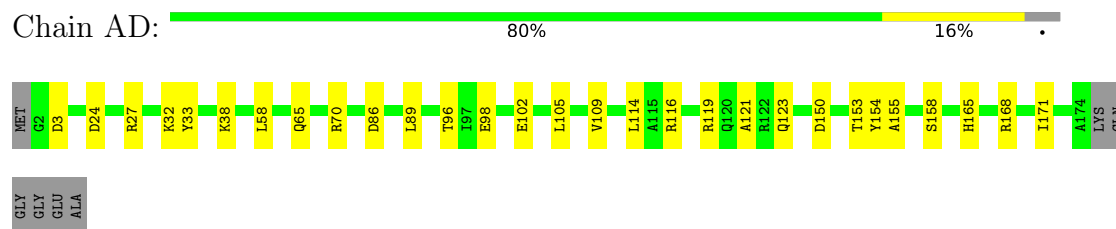
- Molecule 6: 30S ribosomal protein S2



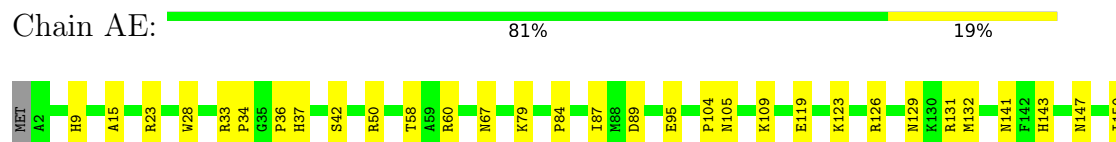
- Molecule 7: Zn-ribbon RNA-binding protein involved in translation



- Molecule 8: 30S ribosomal protein S4



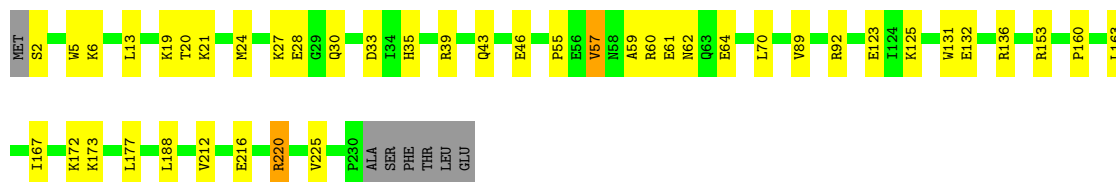
- Molecule 9: 30S ribosomal protein S4e





- Molecule 10: 30S ribosomal protein S5

Chain AF: 79% 17% ..



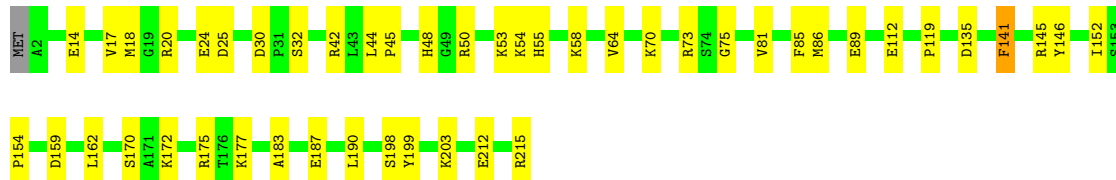
- Molecule 11: 30S ribosomal protein S6e

Chain AG: 74% 23% ..



- Molecule 12: 30S ribosomal protein S7

Chain AH: 78% 21%



- Molecule 13: 30S ribosomal protein S8

Chain AI: 84% 15% ..



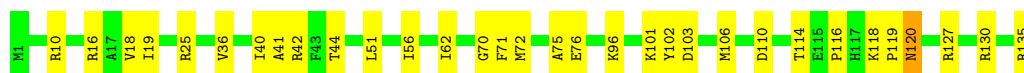
- Molecule 14: 30S ribosomal protein S8e

Chain AJ: 75% 20% ..

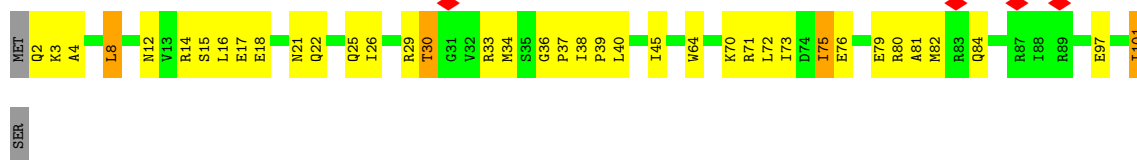


- Molecule 15: 30S ribosomal protein S9

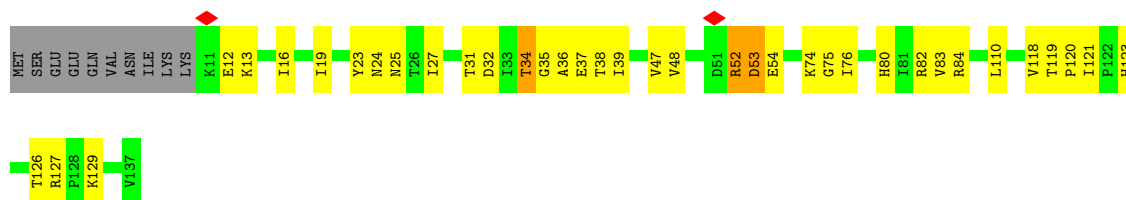
Chain AK: 76% 23%



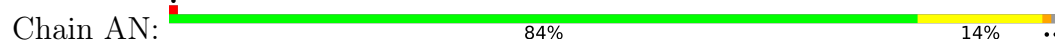
- Molecule 16: 30S ribosomal protein S10



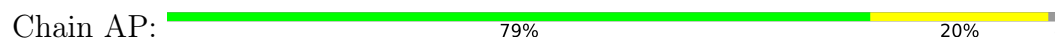
- Molecule 17: 30S ribosomal protein S11



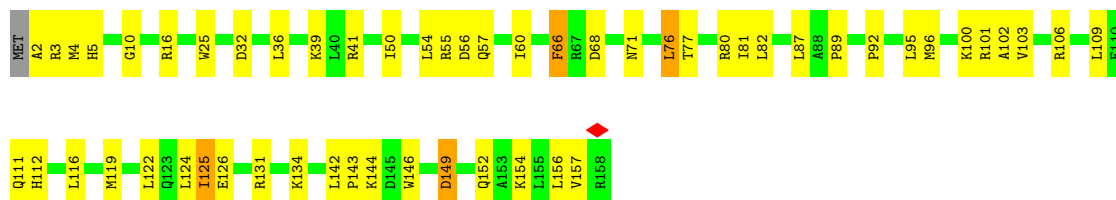
- Molecule 18: 30S ribosomal protein S12



- Molecule 19: 30S ribosomal protein S14 type Z



- Molecule 20: 30S ribosomal protein S15



- Molecule 21: 30S ribosomal protein S17

Chain AR:  80% 14% 5%



- Molecule 22: 30S ribosomal protein S17e

Chain AS:  73% 22% 5%



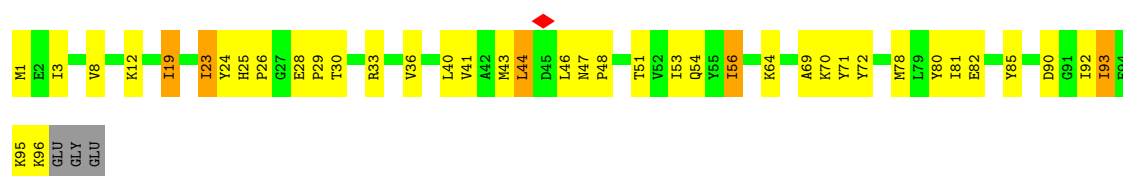
- Molecule 23: 30S ribosomal protein S19e

Chain AU:  83% 16% 1%



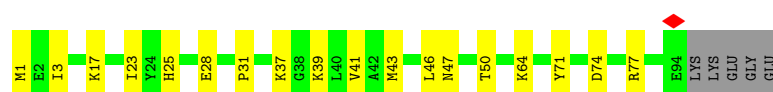
- Molecule 24: 30S ribosomal protein S24e

Chain AV:  57% 35% 5%



- Molecule 24: 30S ribosomal protein S24e

Chain B6:  77% 18% 5%



- Molecule 25: 30S ribosomal protein S27e

Chain AW:  68% 25% 6%

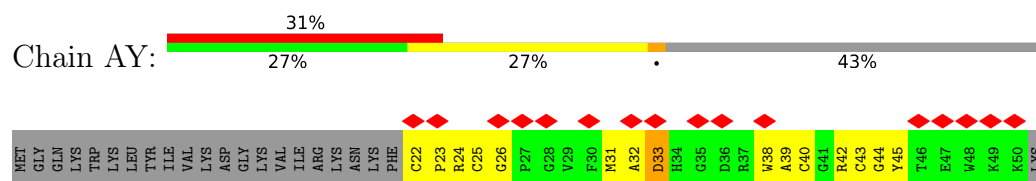


- Molecule 26: 30S ribosomal protein S28e

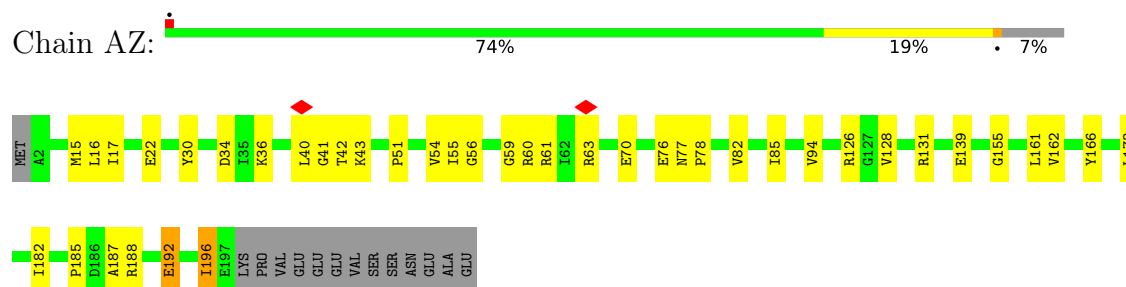
Chain AX:  59% 30% 8%



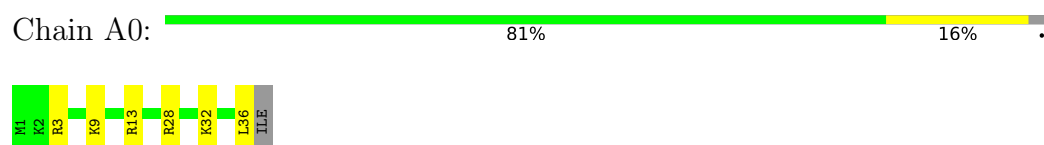
- Molecule 27: 30S ribosomal protein S27ae



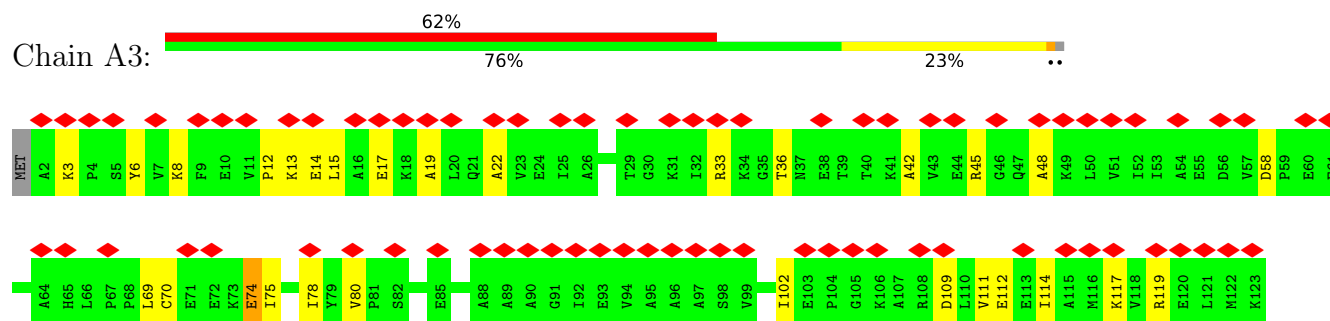
- Molecule 28: 30S ribosomal protein S3



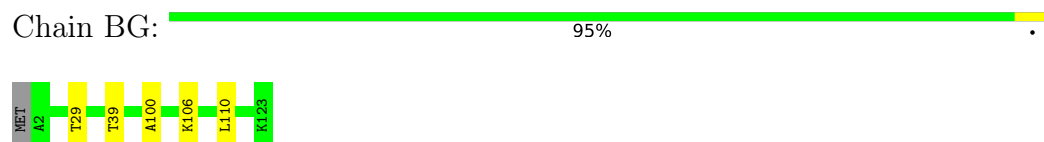
- Molecule 29: Small ribosomal subunit protein eS32



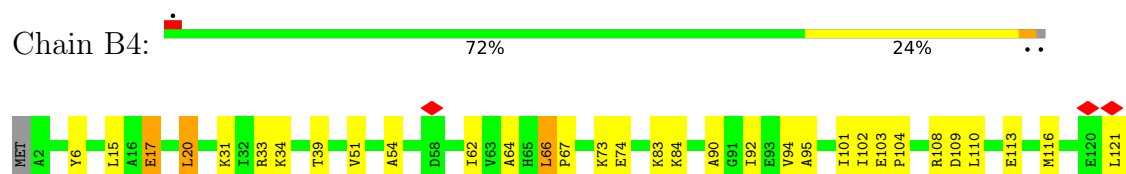
- Molecule 30: 50S ribosomal protein L7Ae



- Molecule 30: 50S ribosomal protein L7Ae



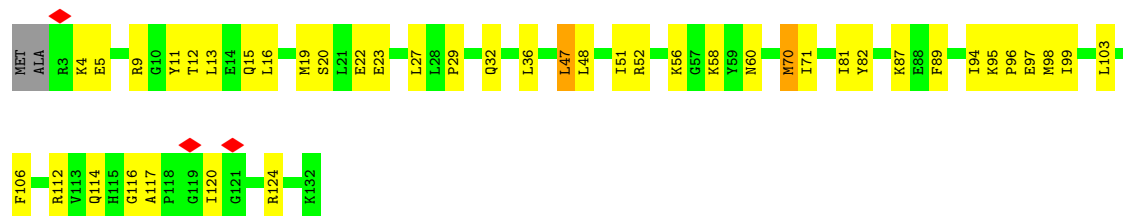
- Molecule 30: 50S ribosomal protein L7Ae



K123

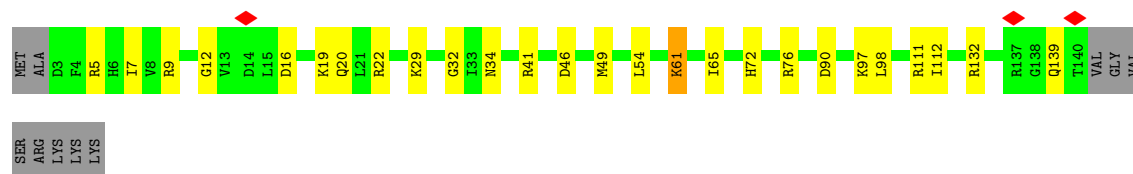
- Molecule 31: 30S ribosomal protein S19

Chain AT:  66% 31% . .



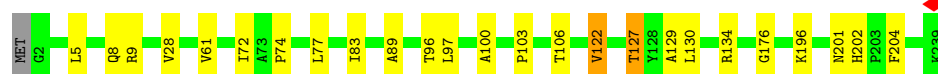
- Molecule 32: 30S ribosomal protein S13

Chain AO:  76% 17% . 7%

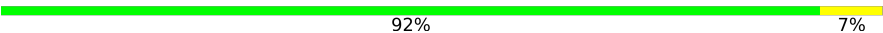


- Molecule 33: Large ribosomal subunit protein uL2

Chain BB:  89% 10% .



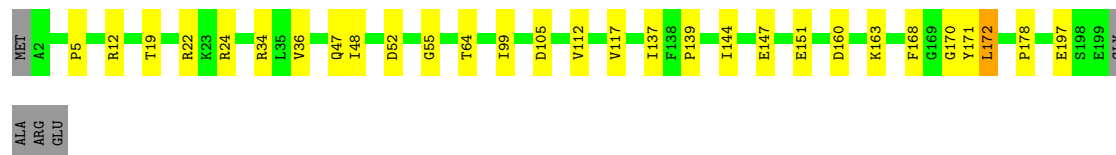
- Molecule 34: Large ribosomal subunit protein uL30

Chain BY:  92% 7% .



- Molecule 35: Large ribosomal subunit protein uL18

Chain BO:  83% 14% .



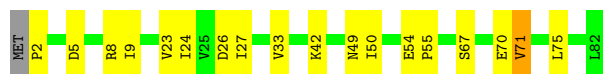
- Molecule 36: Large ribosomal subunit protein uL3

Chain BC:  91% 9%



- Molecule 37: Large ribosomal subunit protein eL14

Chain B5:  77% 21% ..



- Molecule 37: Large ribosomal subunit protein eL14

Chain BK:  87% 11% .



- Molecule 38: Large ribosomal subunit protein uL15

Chain BL:  85% 15%



- Molecule 39: Large ribosomal subunit protein eL39

Chain Bf:  86% 10% ..



- Molecule 40: Large ribosomal subunit protein uL24

Chain BU:  83% 17%



- Molecule 41: Large ribosomal subunit protein eL32

Chain Bb:  93% 6% .



- Molecule 42: Large ribosomal subunit protein eL37

Chain Be:  81% 18%



- Molecule 43: Large ribosomal subunit protein uL5

Chain BE:  70% 26%



- Molecule 44: Large ribosomal subunit protein eL31

Chain Ba:  86% 14%

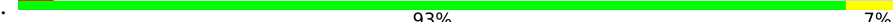


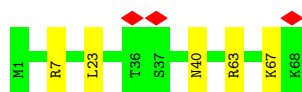
- Molecule 45: Large ribosomal subunit protein uL23

Chain BT:  93% 7%



- Molecule 46: Large ribosomal subunit protein uL29

Chain BW:  93% 7%



- Molecule 47: Large ribosomal subunit protein eL43

Chain Bi:  93% 6%



- Molecule 48: Large ribosomal subunit protein uL13

Chain BI:  89% 11%



- Molecule 49: Large ribosomal subunit protein eL21

Chain BR: 88% 11%



- Molecule 50: Large ribosomal subunit protein eL19

Chain BQ: 86% 13%



- Molecule 51: Large ribosomal subunit protein eL24

Chain BV: 82% 12% 6%



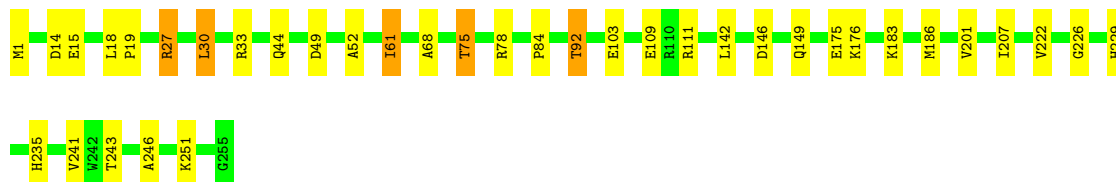
- Molecule 52: Large ribosomal subunit protein eL42

Chain Bj: 90% 10%



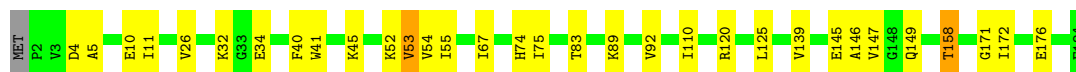
- Molecule 53: Large ribosomal subunit protein uL4

Chain BD: 85% 13%



- Molecule 54: Large ribosomal subunit protein uL6

Chain BF: 82% 16%



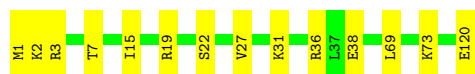
- Molecule 55: Large ribosomal subunit protein eL30

Chain BZ:  82% 17% .



- Molecule 56: Large ribosomal subunit protein eL18

Chain BP:  88% 12%



- Molecule 57: Large ribosomal subunit protein eL15

Chain BM:  91% 8% .



- Molecule 58: Large ribosomal subunit protein uL22

Chain BS:  86% 12% ..



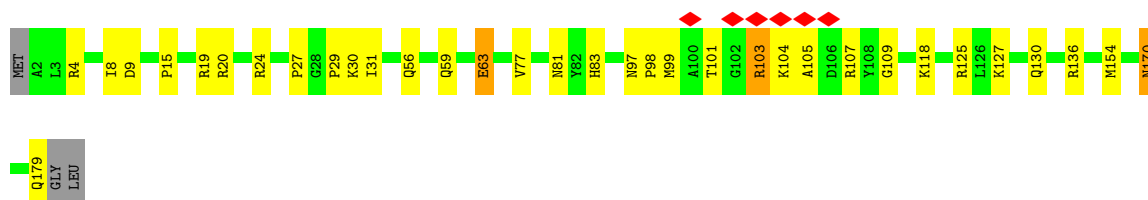
- Molecule 59: Large ribosomal subunit protein eL34

Chain Bd:  91% 8% .



- Molecule 60: Large ribosomal subunit protein uL16

Chain BN:  80% 17% ..



- Molecule 61: Large ribosomal subunit protein eL40

Chain Bg:  78% 16% 6%





- Molecule 62: Large ribosomal subunit protein eL33

Chain Bc: 89% 10%



- Molecule 63: Large ribosomal subunit protein uL14

Chain BJ: 91% 8%



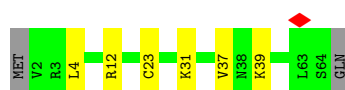
- Molecule 64: Large ribosomal subunit protein eL20

Chain Bl: 79% 21%



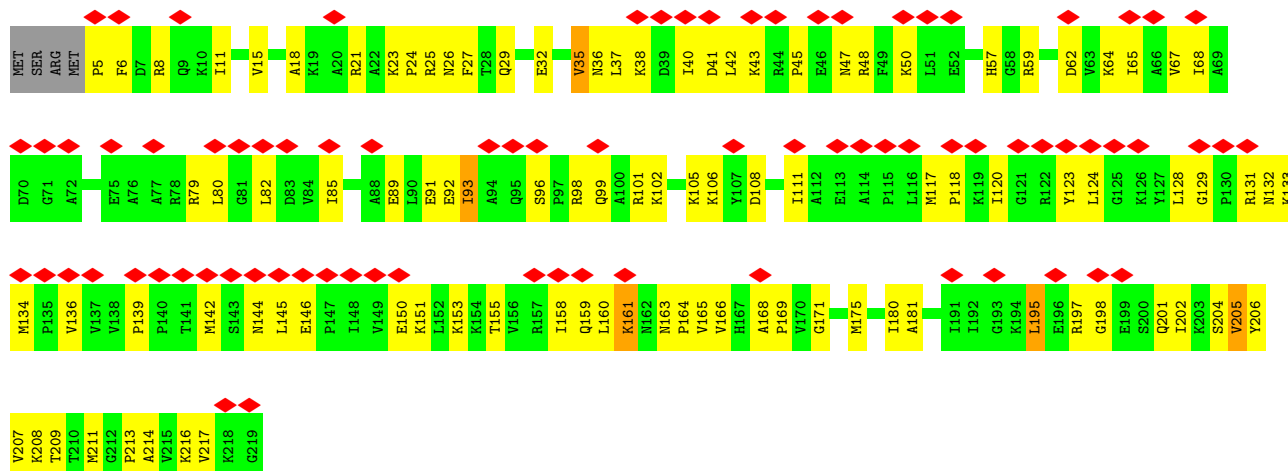
- Molecule 65: C2H2-type domain-containing protein

Chain Bk: 88% 9%



- Molecule 66: Large ribosomal subunit protein uL1

Chain BA: 36% 52% 44%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170000	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	0.015	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0008	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: MA6, OMU, LHH, UR3, 4AC, B8H, OMC, A2M, ZN, MG, 5MC, 6MZ, OMG

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	0.23	2/70601 (0.0%)	0.31	0/110066
2	2	0.18	0/34435	0.26	0/53681
3	3	0.18	0/2995	0.25	0/4669
4	H	0.13	0/3120	0.31	0/4209
5	AA	0.11	0/1557	0.27	0/2087
6	AB	0.12	0/1602	0.24	0/2165
7	AC	0.12	0/463	0.27	0/628
8	AD	0.12	0/1476	0.21	0/1980
9	AE	0.14	0/2032	0.27	0/2742
10	AF	0.15	0/1838	0.26	0/2478
11	AG	0.12	0/993	0.30	0/1329
12	AH	0.11	0/1762	0.23	0/2366
13	AI	0.15	0/1055	0.26	0/1415
14	AJ	0.14	0/995	0.24	0/1327
15	AK	0.13	0/1089	0.31	0/1459
16	AL	0.13	0/817	0.30	0/1097
17	AM	0.12	0/973	0.30	0/1311
18	AN	0.15	0/1165	0.29	0/1547
19	AP	0.15	0/465	0.29	0/613
20	AQ	0.11	0/1333	0.28	0/1791
21	AR	0.14	0/907	0.29	0/1225
22	AS	0.12	0/548	0.25	0/725
23	AU	0.11	0/1253	0.22	0/1689
24	AV	0.14	0/826	0.29	0/1108
24	B6	0.10	0/808	0.23	0/1086
25	AW	0.11	0/476	0.24	0/641
26	AX	0.14	0/518	0.28	0/694
27	AY	0.09	0/235	0.27	0/315
28	AZ	0.13	0/1563	0.26	0/2099
29	A0	0.16	0/349	0.25	0/451
30	A3	0.11	0/945	0.31	0/1274
30	B4	0.12	0/945	0.32	0/1274

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	BG	0.13	0/944	0.25	0/1274
31	AT	0.12	0/1077	0.26	0/1439
32	AO	0.12	0/1135	0.29	0/1526
33	BB	0.19	0/1882	0.29	0/2538
34	BY	0.16	0/1254	0.26	0/1677
35	BO	0.15	0/1645	0.26	0/2209
36	BC	0.17	0/2933	0.28	0/3943
37	B5	0.14	0/619	0.28	0/830
37	BK	0.14	0/611	0.29	0/819
38	BL	0.17	0/1167	0.31	0/1552
39	Bf	0.18	0/443	0.25	0/589
40	BU	0.15	0/1027	0.25	0/1368
41	Bb	0.17	0/1120	0.26	0/1494
42	Be	0.20	0/514	0.28	0/676
43	BE	0.14	0/1509	0.28	0/2022
44	Ba	0.16	0/793	0.26	0/1064
45	BT	0.17	0/705	0.28	0/945
46	BW	0.13	0/566	0.22	0/747
47	Bi	0.15	0/630	0.28	0/839
48	BI	0.18	0/1166	0.25	0/1559
49	BR	0.17	0/819	0.24	0/1098
50	BQ	0.17	0/1281	0.24	0/1689
51	BV	0.18	0/547	0.28	0/729
52	Bj	0.16	0/807	0.24	0/1070
53	BD	0.17	0/2069	0.28	0/2787
54	BF	0.15	0/1485	0.27	0/2003
55	BZ	0.15	0/759	0.27	0/1023
56	BP	0.16	0/984	0.25	0/1314
57	BM	0.19	0/1627	0.29	0/2170
58	BS	0.19	0/1275	0.30	0/1715
59	Bd	0.21	0/778	0.37	0/1036
60	BN	0.16	0/1483	0.26	0/1992
61	Bg	0.13	0/396	0.23	0/526
62	Bc	0.17	0/693	0.29	0/926
63	BJ	0.17	0/1080	0.27	0/1456
64	Bl	0.15	0/669	0.25	0/886
65	Bk	0.19	0/538	0.27	0/709
66	BA	0.11	0/1700	0.28	0/2288
All	All	0.19	2/180869 (0.0%)	0.28	0/266068

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	94	G	O3'-P	-6.15	1.51	1.61
1	1	96	U	C1'-N1	5.73	1.57	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	65181	0	32949	665	0
2	2	32291	0	16340	427	0
3	3	2703	0	1375	23	0
4	H	3074	0	3190	100	0
5	AA	1531	0	1623	50	0
6	AB	1571	0	1630	25	0
7	AC	449	0	435	5	0
8	AD	1452	0	1521	20	0
9	AE	1983	0	2060	30	0
10	AF	1808	0	1879	34	0
11	AG	977	0	1037	19	0
12	AH	1725	0	1780	33	0
13	AI	1034	0	1069	15	0
14	AJ	986	0	1070	22	0
15	AK	1073	0	1133	23	0
16	AL	809	0	859	31	0
17	AM	955	0	981	33	0
18	AN	1148	0	1248	13	0
19	AP	455	0	475	11	0
20	AQ	1305	0	1388	41	0
21	AR	884	0	906	11	0
22	AS	541	0	573	10	0
23	AU	1223	0	1263	19	0
24	AV	808	0	832	26	0
24	B6	790	0	806	12	0
25	AW	470	0	495	13	0
26	AX	516	0	544	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	AY	227	0	207	11	0
28	AZ	1541	0	1624	26	0
29	A0	343	0	407	4	0
30	A3	933	0	982	19	0
30	B4	933	0	982	21	0
30	BG	932	0	982	3	0
31	AT	1057	0	1131	27	0
32	AO	1116	0	1152	19	0
33	BB	1838	0	1903	17	0
34	BY	1235	0	1314	10	0
35	BO	1607	0	1638	16	0
36	BC	2870	0	3020	18	0
37	B5	614	0	671	12	0
37	BK	607	0	663	7	0
38	BL	1149	0	1218	16	0
39	Bf	435	0	494	4	0
40	BU	1011	0	1078	14	0
41	Bb	1095	0	1190	6	0
42	Be	503	0	533	11	0
43	BE	1485	0	1539	32	0
44	Ba	778	0	851	9	0
45	BT	696	0	758	3	0
46	BW	565	0	628	3	0
47	Bi	620	0	668	2	0
48	BI	1148	0	1237	11	0
49	BR	797	0	835	7	0
50	BQ	1265	0	1391	13	0
51	BV	532	0	523	7	0
52	Bj	789	0	842	7	0
53	BD	2026	0	2131	27	0
54	BF	1456	0	1514	18	0
55	BZ	749	0	796	11	0
56	BP	971	0	1039	10	0
57	BM	1588	0	1683	10	0
58	BS	1247	0	1280	11	0
59	Bd	759	0	825	10	0
60	BN	1452	0	1491	26	0
61	Bg	387	0	397	5	0
62	Bc	684	0	748	7	0
63	BJ	1066	0	1133	7	0
64	Bl	659	0	702	11	0
65	Bk	528	0	575	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
66	BA	1675	0	1787	86	0
67	1	165	0	0	0	0
67	2	61	0	0	0	0
67	3	1	0	0	0	0
67	AD	1	0	0	0	0
67	AE	1	0	0	0	0
67	AF	1	0	0	0	0
67	AK	1	0	0	0	0
67	AN	1	0	0	0	0
67	AR	1	0	0	0	0
67	AT	1	0	0	0	0
67	AU	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	171964	0	126023	2034	0

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

All (2034) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2585:4AC:H5	1:1:2597:G:H1	1.13	1.09
1:1:2608:4AC:H5	1:1:2613:G:H1	1.19	1.01
1:1:2887:A:HO2'	63:BJ:2:ALA:N	1.59	0.99
1:1:102:C:N4	1:1:117:G:O6	1.97	0.97
1:1:2359:A:H61	1:1:2408:G:H8	1.18	0.91
1:1:235:G:H1	1:1:242:C:H5	1.23	0.86
1:1:3020:U:OP2	1:1:3022:C:H5'	1.76	0.86
2:2:440:G:N2	2:2:456:C:O2	2.09	0.85
1:1:931:U:H3	1:1:1046:G:H1	1.25	0.84
1:1:438:U:O2'	1:1:440:G:N7	2.11	0.83
1:1:2348:G:N2	1:1:2421:C:O2	2.10	0.83
66:BA:37:LEU:HB3	66:BA:201:GLN:HE21	1.43	0.83
1:1:1713:G:H21	1:1:1787:A:H8	1.27	0.83
2:2:631:G:H22	2:2:708:G:H1	1.25	0.83
1:1:2536:U:H5''	43:BE:116:GLY:HA3	1.62	0.82
2:2:651:G:H21	17:AM:38:THR:HG21	1.44	0.81
5:AA:127:ALA:HB2	5:AA:182:LYS:HB2	1.63	0.80
1:1:3021:U:H3'	1:1:3021:U:OP2	1.81	0.80
66:BA:62:ASP:HA	66:BA:153:LYS:HE2	1.64	0.79
1:1:720:A:H2'	1:1:721:A:H8	1.48	0.79
2:2:150:C:O2	2:2:165:G:N2	2.15	0.78
25:AW:27:GLN:HE22	25:AW:40:ASN:H	1.29	0.77
1:1:2408:G:H21	66:BA:101:ARG:HE	1.29	0.77
27:AY:25:CYS:HB3	30:A3:45:ARG:HH22	1.49	0.77
2:2:703:4AC:H2'	2:2:704:G:H8	1.49	0.77
66:BA:18:ALA:O	66:BA:21:ARG:NH1	2.18	0.76
3:3:74:C:O2	3:3:109:G:N2	2.17	0.76
4:H:35:PRO:O	4:H:52:GLN:NE2	2.19	0.76
4:H:133:GLU:O	4:H:138:LYS:NZ	2.19	0.75
2:2:634:G:N1	2:2:707:U:C2	2.54	0.75
37:B5:23:VAL:HG21	37:B5:71:VAL:HG21	1.67	0.75
4:H:131:LYS:NZ	4:H:223:PRO:O	2.18	0.75
1:1:793:G:OP2	38:BL:12:ARG:NH2	2.19	0.75
10:AF:212:VAL:H	13:AI:70:ASN:HD21	1.32	0.75
38:BL:1:MET:HE1	53:BD:30:LEU:HD12	1.68	0.74
1:1:785:G:H5''	1:1:2259:U:H5''	1.68	0.74
4:H:214:MET:SD	4:H:216:LYS:NZ	2.59	0.74
17:AM:39:ILE:HG23	17:AM:74:LYS:HD2	1.70	0.74
30:A3:14:GLU:OE1	30:A3:117:LYS:NZ	2.20	0.74
1:1:2535:G:H22	1:1:2543:U:H3	1.35	0.74
2:2:415:G:H21	8:AD:123:GLN:HE22	1.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AE:89:ASP:OD1	9:AE:123:LYS:NZ	2.20	0.73
20:AQ:54:LEU:HB3	20:AQ:60:ILE:HD11	1.69	0.73
1:1:103:C:H2'	1:1:104:C:C6	2.23	0.73
2:2:444:U:H4'	24:AV:56:ILE:HD11	1.71	0.73
1:1:1140:G:O2'	1:1:1143:A:N6	2.21	0.73
2:2:424:C:O2'	2:2:426:G:O6	2.07	0.73
2:2:633:G:H5'	2:2:693:5MC:H1'	1.70	0.73
49:BR:19:HIS:HD2	49:BR:21:ARG:H	1.35	0.73
1:1:117:G:O2'	1:1:118:U:P	2.47	0.72
1:1:2103:U:O2'	1:1:2104:A:N7	2.21	0.72
66:BA:38:LYS:O	66:BA:201:GLN:NE2	2.21	0.72
30:B4:51:VAL:HG11	30:B4:66:LEU:HD11	1.70	0.72
1:1:710:C:O2	1:1:747:G:N2	2.17	0.72
2:2:778:U:O2'	2:2:872:A:N1	2.22	0.72
31:AT:82:TYR:HB3	31:AT:89:PHE:HB3	1.70	0.72
1:1:102:C:C4	1:1:103:C:C4	2.78	0.72
2:2:1396:G:N2	2:2:1447:C:O2	2.17	0.72
1:1:103:C:H2'	1:1:104:C:H6	1.55	0.71
66:BA:124:LEU:HB3	66:BA:128:LEU:HD12	1.72	0.71
6:AB:59:LEU:HB2	6:AB:175:ILE:HD11	1.72	0.71
3:3:2:G:N2	3:3:123:C:O2	2.16	0.71
20:AQ:143:PRO:HG2	20:AQ:146:TRP:HB2	1.72	0.71
30:B4:83:LYS:HG2	30:B4:95:ALA:HB1	1.72	0.71
2:2:660:G:OP2	4:H:383:ARG:NH2	2.24	0.71
2:2:1177:OMU:HM22	2:2:1178:A:H5'	1.71	0.71
14:AJ:73:ARG:HH21	14:AJ:105:ILE:HD13	1.54	0.71
1:1:102:C:N4	1:1:103:C:N4	2.38	0.71
1:1:2585:4AC:H5	1:1:2597:G:N1	1.98	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
1:1:1285:G:H4'	60:BN:154:MET:HE1	1.71	0.71
2:2:496:G:N2	4:H:324:LYS:O	2.22	0.70
3:3:2:G:N1	3:3:123:C:N3	2.32	0.70
27:AY:40:CYS:HB3	27:AY:44:GLY:H	1.57	0.70
2:2:681:G:H2'	2:2:682:A:H8	1.56	0.70
2:2:872:A:OP1	29:A0:28:ARG:NH2	2.25	0.69
1:1:792:A:H62	1:1:1509:C:H5	1.37	0.69
30:B4:84:LYS:HD2	30:B4:95:ALA:HB2	1.75	0.69
6:AB:174:GLU:OE1	6:AB:185:ARG:NH1	2.26	0.69
1:1:253:G:H2'	1:1:254:C:H6	1.58	0.69
6:AB:61:ARG:NH1	7:AC:32:CYS:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:BE:64:THR:HG23	43:BE:71:ARG:HA	1.75	0.68
59:Bd:89:MET:HE3	59:Bd:89:MET:C	2.17	0.68
2:2:1271:U:O2'	12:AH:177:LYS:NZ	2.26	0.68
2:2:634:G:C2	2:2:707:U:O2	2.47	0.68
2:2:717:C:OP2	20:AQ:16:ARG:NH2	2.26	0.68
5:AA:53:LEU:HD22	5:AA:62:LYS:HB2	1.76	0.68
2:2:714:G:O2'	20:AQ:55:ARG:NH1	2.27	0.68
1:1:1310:G:O2'	1:1:1339:A:N6	2.27	0.68
2:2:609:A:N7	13:AI:107:SER:HA	2.08	0.68
5:AA:160:LEU:O	5:AA:164:ASN:ND2	2.26	0.68
2:2:965:A:H5''	2:2:966:C:H5	1.59	0.68
54:BF:10:GLU:HB3	54:BF:52:LYS:HD3	1.74	0.68
2:2:634:G:C2	2:2:707:U:C2	2.82	0.68
28:AZ:60:ARG:HH21	28:AZ:63:ARG:HD2	1.59	0.67
33:BB:28:VAL:HG11	33:BB:72:ILE:HG13	1.76	0.67
1:1:102:C:C4	1:1:103:C:C5	2.81	0.67
1:1:1568:G:N7	39:Bf:3:ARG:NH2	2.41	0.67
5:AA:27:PHE:HZ	5:AA:160:LEU:HB3	1.59	0.67
60:BN:56:GLN:HE21	60:BN:125:ARG:HE	1.43	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
5:AA:47:ARG:HD3	17:AM:34:THR:HG21	1.77	0.67
27:AY:31:MET:HE3	27:AY:32:ALA:H	1.59	0.67
2:2:951:C:O2	19:AP:12:ARG:NH2	2.28	0.67
2:2:976:A:N6	2:2:1001:A:O4'	2.28	0.67
24:B6:1:MET:O	24:B6:39:LYS:NZ	2.28	0.67
4:H:13:ARG:NH2	4:H:33:GLU:O	2.27	0.67
2:2:428:C:H2'	2:2:429:A:H8	1.59	0.67
1:1:418:A:H2'	1:1:419:G:C8	2.30	0.67
1:1:653:G:N1	1:1:656:A:OP2	2.28	0.67
2:2:918:A:H2'	2:2:919:G:H8	1.60	0.67
30:B4:101:ILE:HD11	30:B4:104:PRO:HA	1.77	0.67
43:BE:64:THR:HG22	43:BE:66:ARG:HH12	1.58	0.66
37:BK:45:ARG:NH2	37:BK:66:ALA:O	2.27	0.66
2:2:1380:OMU:HM22	2:2:1381:C:H5'	1.78	0.66
1:1:2242:C:O2'	44:Ba:24:ARG:NH2	2.29	0.66
66:BA:195:LEU:HD13	66:BA:197:ARG:H	1.60	0.66
1:1:2409:A:OP2	66:BA:101:ARG:NH2	2.29	0.66
1:1:2701:A:N6	1:1:2713:G:O2'	2.28	0.66
4:H:46:TYR:OH	4:H:76:ALA:O	2.13	0.66
2:2:918:A:H2'	2:2:919:G:C8	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:634:G:N1	2:2:707:U:N3	2.44	0.66
31:AT:48:LEU:HD11	31:AT:52:ARG:HH21	1.61	0.66
1:1:2608:4AC:H5	1:1:2613:G:N1	2.02	0.66
2:2:651:G:O2'	17:AM:37:GLU:OE1	2.14	0.66
24:AV:33:ARG:NH2	24:AV:53:ILE:O	2.28	0.66
1:1:2498:A:H2	1:1:2503:U:H3	1.44	0.66
1:1:908:A:N3	53:BD:33:ARG:NH2	2.44	0.66
1:1:2109:A:H2'	1:1:2110:A:C8	2.31	0.66
2:2:1095:A:H2'	2:2:1096:G:C8	2.31	0.65
17:AM:31:THR:HB	17:AM:35:GLY:HA2	1.77	0.65
4:H:382:LYS:HZ2	17:AM:52:ARG:HD3	1.61	0.65
9:AE:129:ASN:HB3	9:AE:141:ASN:HD22	1.61	0.65
1:1:230:G:OP1	42:Be:21:ARG:NH1	2.30	0.65
1:1:869:G:O2'	1:1:870:A:O5'	2.13	0.65
1:1:2311:A:H2'	1:1:2312:G:C8	2.31	0.65
2:2:150:C:N3	2:2:165:G:N1	2.33	0.65
2:2:484:G:N2	18:AN:65:PRO:O	2.30	0.65
33:BB:202:HIS:HD2	33:BB:204:PHE:H	1.42	0.65
2:2:330:A:OP1	14:AJ:2:ALA:N	2.29	0.65
34:BY:60:ASN:H	34:BY:148:ASN:HD21	1.44	0.65
1:1:1739:G:HO2'	1:1:1816:U:HO2'	1.39	0.65
1:1:894:A:H2'	1:1:895:A:C8	2.32	0.65
2:2:219:G:H21	2:2:222:A:H8	1.45	0.65
2:2:626:4AC:H2'	2:2:627:G:H8	1.62	0.65
5:AA:97:VAL:HG11	5:AA:103:ARG:HD2	1.79	0.65
9:AE:95:GLU:OE1	24:AV:12:LYS:NZ	2.29	0.65
2:2:1398:G:N2	2:2:1445:C:O2	2.19	0.65
13:AI:90:GLU:OE2	13:AI:113:HIS:NE2	2.27	0.65
31:AT:116:GLY:HA2	31:AT:124:ARG:HH11	1.62	0.65
30:B4:92:ILE:HG22	30:B4:94:VAL:H	1.61	0.65
61:Bg:32:ARG:HG3	61:Bg:33:LYS:HD2	1.79	0.65
20:AQ:57:GLN:OE1	25:AW:38:ARG:NH1	2.31	0.64
2:2:675:C:H2'	2:2:676:G:H8	1.62	0.64
4:H:259:ASP:N	4:H:259:ASP:OD1	2.29	0.64
30:A3:70:CYS:HA	30:A3:75:ILE:HD12	1.80	0.64
2:2:679:G:H2'	2:2:680:OMG:H8	1.62	0.64
37:BK:21:LYS:O	37:BK:41:ASN:ND2	2.30	0.64
2:2:627:G:H2'	2:2:628:G:C8	2.32	0.64
9:AE:15:ALA:O	9:AE:23:ARG:NH2	2.29	0.64
12:AH:112:GLU:HB3	12:AH:119:PRO:HG3	1.80	0.64
66:BA:41:ASP:O	66:BA:47:ASN:ND2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:116:G:H2'	1:1:117:G:H8	1.62	0.64
1:1:418:A:H2'	1:1:419:G:H8	1.62	0.64
9:AE:126:ARG:H	9:AE:143:HIS:HD2	1.46	0.64
13:AI:96:ALA:HB3	13:AI:99:PHE:HB2	1.78	0.64
66:BA:129:GLY:HA2	66:BA:134:MET:HE1	1.80	0.64
2:2:1379:G:H2'	2:2:1380:OMU:H6	1.79	0.64
33:BB:5:LEU:H	33:BB:8:GLN:HE21	1.45	0.64
1:1:2343:G:OP1	1:1:2343:G:H4'	1.97	0.64
58:BS:46:ASP:OD1	58:BS:49:ARG:NH2	2.31	0.64
64:BI:10:GLY:HA2	64:BI:55:LYS:HG2	1.78	0.64
1:1:102:C:C2	1:1:103:C:C6	2.86	0.64
1:1:1905:G:N1	1:1:1908:A:OP2	2.29	0.64
5:AA:50:GLU:OE1	17:AM:82:ARG:NH2	2.30	0.64
10:AF:59:ALA:HB3	10:AF:62:ASN:HD22	1.62	0.64
56:BP:36:ARG:NH1	56:BP:120:GLU:OE2	2.26	0.64
1:1:2361:G:O2'	66:BA:161:LYS:NZ	2.31	0.64
1:1:2990:G:H21	54:BF:149:GLN:HE22	1.46	0.63
10:AF:167:ILE:O	10:AF:172:LYS:NZ	2.25	0.63
37:B5:67:SER:OG	37:B5:70:GLU:OE1	2.13	0.63
2:2:1089:G:N2	2:2:1090:U:O4	2.29	0.63
1:1:67:C:OP2	1:1:68:U:O2'	2.16	0.63
18:AN:143:GLU:HG2	18:AN:147:ARG:HH21	1.63	0.63
1:1:764:A:O2'	62:Bc:17:GLN:NE2	2.30	0.63
33:BB:122:VAL:HG21	33:BB:129:ALA:HB2	1.79	0.63
12:AH:215:ARG:OXT	26:AX:62:ARG:NH1	2.32	0.63
20:AQ:122:LEU:HD12	20:AQ:125:ILE:HD11	1.80	0.63
1:1:1653:U:OP2	50:BQ:42:ARG:NH2	2.32	0.63
1:1:2426:C:H2'	1:1:2427:G:H8	1.63	0.63
31:AT:47:LEU:HD12	31:AT:70:MET:HG3	1.81	0.63
1:1:31:G:H4'	44:Ba:14:PRO:HG3	1.81	0.63
1:1:112:A:H3'	1:1:113:G:H8	1.63	0.63
2:2:511:4AC:OP1	8:AD:38:LYS:NZ	2.29	0.63
3:3:52:A:H5''	35:BO:170:GLY:H	1.64	0.63
30:A3:114:ILE:HA	30:A3:117:LYS:HE3	1.80	0.63
49:BR:45:ILE:H	49:BR:59:HIS:HD2	1.44	0.62
66:BA:79:ARG:HH22	66:BA:145:LEU:H	1.44	0.62
1:1:1283:A:H2'	1:1:1284:A:C8	2.34	0.62
32:AO:61:LYS:O	32:AO:61:LYS:NZ	2.30	0.62
43:BE:30:ILE:HG22	43:BE:139:VAL:HG22	1.80	0.62
17:AM:25:ASN:ND2	17:AM:54:GLU:OE1	2.32	0.62
1:1:761:U:H2'	1:1:762:G:H8	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:687:C:O2'	5:AA:101:THR:O	2.16	0.62
6:AB:6:LEU:HD21	6:AB:53:LYS:HG3	1.80	0.62
15:AK:36:VAL:O	15:AK:42:ARG:NH1	2.32	0.62
2:2:548:U:OP1	20:AQ:134:LYS:NZ	2.31	0.62
4:H:186:PHE:HB3	4:H:206:PHE:HE1	1.63	0.62
26:AX:15:ILE:HD11	26:AX:28:LYS:HG3	1.82	0.62
30:B4:6:TYR:OH	30:B4:54:ALA:O	2.17	0.62
2:2:925:G:N7	32:AO:132:ARG:NH2	2.48	0.62
2:2:1103:C:O2'	23:AU:130:ASP:OD2	2.18	0.62
11:AG:113:SER:OG	11:AG:115:GLU:OE1	2.18	0.62
2:2:774:OMU:HM22	2:2:775:G:H5'	1.82	0.62
2:2:1378:C:H2'	2:2:1379:G:C8	2.35	0.62
9:AE:58:THR:HG22	9:AE:60:ARG:H	1.65	0.62
24:B6:47:ASN:HB3	24:B6:50:THR:HG22	1.81	0.62
66:BA:151:LYS:O	66:BA:155:THR:OG1	2.18	0.62
1:1:2368:G:OP2	66:BA:26:ASN:ND2	2.33	0.62
17:AM:47:VAL:HG23	17:AM:48:VAL:HG23	1.82	0.62
1:1:189:G:H22	1:1:224:A:H2	1.47	0.61
2:2:1482:A:H2'	2:2:1483:G:H8	1.65	0.61
32:AO:76:ARG:NE	32:AO:90:ASP:OD2	2.33	0.61
40:BU:28:ALA:HA	40:BU:45:PRO:HA	1.82	0.61
1:1:1317:G:H2'	1:1:1318:G:H8	1.63	0.61
1:1:763:C:H2'	1:1:764:A:C8	2.35	0.61
37:B5:55:PRO:O	55:BZ:51:TYR:OH	2.16	0.61
60:BN:105:ALA:O	60:BN:109:GLY:N	2.34	0.61
1:1:2823:C:H2'	1:1:2824:G:C8	2.36	0.61
1:1:1676:A:N1	1:1:1692:G:O2'	2.32	0.61
1:1:1806:G:OP2	1:1:1806:G:N2	2.27	0.61
47:Bi:82:VAL:HG12	47:Bi:83:GLU:HG3	1.83	0.61
1:1:595:A:O2'	53:BD:44:GLN:NE2	2.33	0.61
17:AM:84:ARG:HB3	17:AM:118:VAL:HG23	1.82	0.61
1:1:806:G:OP1	53:BD:27:ARG:NH2	2.34	0.61
14:AJ:83:ASN:HD21	14:AJ:96:THR:HG22	1.65	0.61
2:2:557:C:OP1	13:AI:32:LYS:NZ	2.29	0.61
6:AB:111:GLU:OE2	10:AF:43:GLN:NE2	2.31	0.61
1:1:253:G:H2'	1:1:254:C:C6	2.35	0.61
1:1:2559:A:H2'	1:1:2560:G:C8	2.36	0.61
4:H:123:VAL:O	4:H:228:ARG:NH2	2.34	0.61
16:AL:8:LEU:HB2	16:AL:71:ARG:HB2	1.82	0.61
31:AT:9:ARG:HG3	31:AT:27:LEU:HB3	1.82	0.61
60:BN:97:ASN:HD22	60:BN:98:PRO:HD2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2362:C:H2'	1:1:2363:G:C8	2.37	0.60
4:H:50:LEU:HD21	4:H:72:VAL:HG13	1.83	0.60
13:AI:51:GLU:OE2	13:AI:62:ARG:NH2	2.34	0.60
36:BC:278:GLU:HG3	36:BC:325:PRO:HD3	1.83	0.60
1:1:2036:A:HO2'	42:Be:2:SER:N	1.99	0.60
66:BA:67:VAL:HG22	66:BA:111:ILE:HB	1.83	0.60
2:2:1025:5MC:H2'	2:2:1026:G:H8	1.66	0.60
5:AA:71:VAL:HG21	5:AA:79:ALA:HB1	1.83	0.60
57:BM:33:GLU:O	57:BM:65:ARG:NH2	2.34	0.60
1:1:1775:A:N1	55:BZ:67:SER:OG	2.28	0.60
11:AG:68:ASP:HA	11:AG:116:ILE:HA	1.82	0.60
21:AR:16:CYS:HB3	21:AR:77:CYS:HB3	1.83	0.60
1:1:2878:G:OP2	1:1:2962:C:O2'	2.20	0.60
1:1:3007:A:H2	1:1:3009:A:H62	1.49	0.60
2:2:730:C:H2'	2:2:731:4AC:H6	1.84	0.60
20:AQ:96:MET:O	20:AQ:100:LYS:HG2	2.00	0.60
34:BY:123:ARG:NH1	34:BY:155:LEU:O	2.34	0.60
1:1:113:G:H2'	1:1:114:G:C8	2.36	0.60
1:1:2408:G:H21	66:BA:101:ARG:NE	1.97	0.60
12:AH:50:ARG:NH1	15:AK:110:ASP:OD2	2.34	0.60
1:1:1998:A:H2'	1:1:1999:C:C6	2.37	0.60
6:AB:191:PRO:HG2	6:AB:194:GLU:HB2	1.83	0.60
23:AU:137:LYS:NZ	23:AU:141:GLU:OE2	2.33	0.60
66:BA:163:ASN:HD22	66:BA:165:VAL:HG12	1.67	0.60
1:1:710:C:N3	1:1:747:G:N1	2.37	0.60
24:AV:54:GLN:HB2	24:AV:70:LYS:HZ1	1.65	0.60
66:BA:96:SER:O	66:BA:99:GLN:NE2	2.30	0.60
2:2:975:G:N2	2:2:1000:G:O2'	2.33	0.60
25:AW:50:THR:OG1	25:AW:53:LYS:O	2.19	0.60
48:BI:17:ARG:NH1	48:BI:117:GLU:OE2	2.33	0.60
2:2:660:G:H1'	4:H:379:ARG:HG2	1.84	0.60
2:2:1395:G:N2	2:2:1448:C:O2	2.18	0.60
3:3:97:G:H2'	3:3:98:G:H8	1.66	0.60
16:AL:38:ILE:HB	16:AL:72:LEU:HB3	1.83	0.60
2:2:643:A:H5''	17:AM:120:PRO:HB2	1.84	0.59
2:2:681:G:H2'	2:2:682:A:C8	2.37	0.59
2:2:1146:C:H2'	2:2:1147:4AC:H6	1.84	0.59
12:AH:48:HIS:NE2	15:AK:76:GLU:OE2	2.35	0.59
40:BU:5:SER:O	40:BU:11:GLN:NE2	2.33	0.59
43:BE:103:LYS:HA	43:BE:184:VAL:HG22	1.84	0.59
1:1:209:G:O2'	46:BW:40:ASN:ND2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1266:C:H2'	2:2:1267:G:H8	1.67	0.59
1:1:2342:C:H3'	1:1:2343:G:H5''	1.83	0.59
2:2:1310:U:O2'	12:AH:85:PHE:O	2.19	0.59
11:AG:40:VAL:HG11	11:AG:47:LEU:HD22	1.84	0.59
49:BR:89:HIS:HD2	49:BR:91:VAL:H	1.49	0.59
1:1:1415:C:OP2	34:BY:118:ARG:NH2	2.34	0.59
1:1:1734:G:H2'	1:1:1735:G:H8	1.68	0.59
2:2:1365:U:H2'	2:2:1366:G:C8	2.38	0.59
3:3:9:G:OP1	35:BO:24:ARG:NH1	2.36	0.59
4:H:20:ASN:OD1	4:H:70:ARG:NH1	2.36	0.59
9:AE:154:GLU:OE1	9:AE:154:GLU:N	2.35	0.59
35:BO:34:ARG:NH1	35:BO:105:ASP:OD2	2.36	0.59
54:BF:4:ASP:OD1	54:BF:5:ALA:N	2.35	0.59
1:1:2405:C:H2'	1:1:2406:A:C8	2.37	0.59
2:2:259:A:OP1	14:AJ:10:ARG:NH2	2.34	0.59
2:2:386:C:H2'	2:2:387:G:H8	1.67	0.59
2:2:977:A:H62	2:2:999:G:H21	1.49	0.59
4:H:63:ASP:OD2	4:H:65:THR:OG1	2.21	0.59
1:1:205:G:N7	39:Bf:34:ARG:NH2	2.49	0.59
19:AP:22:ILE:HD13	28:AZ:16:LEU:HD11	1.85	0.59
20:AQ:66:PHE:HB2	20:AQ:76:LEU:HD23	1.84	0.59
52:Bj:1:MET:N	52:Bj:88:LYS:O	2.35	0.59
1:1:1164:C:OP1	60:BN:19:ARG:NH1	2.35	0.59
9:AE:105:ASN:N	9:AE:109:LYS:O	2.35	0.59
16:AL:79:GLU:HA	16:AL:82:MET:HE1	1.84	0.59
33:BB:74:PRO:HD2	33:BB:77:LEU:HD22	1.85	0.59
43:BE:5:ILE:HB	43:BE:8:ARG:HB2	1.85	0.59
2:2:1321:G:O6	15:AK:10:ARG:NH2	2.33	0.59
4:H:19:ILE:HG13	4:H:70:ARG:HH11	1.67	0.59
4:H:51:THR:HG22	4:H:54:LEU:HG	1.83	0.59
11:AG:77:ASP:OD1	11:AG:77:ASP:N	2.34	0.59
53:BD:226:GLY:H	53:BD:229:HIS:HD2	1.51	0.58
2:2:869:G:N2	2:2:872:A:OP2	2.31	0.58
5:AA:27:PHE:CZ	5:AA:160:LEU:HB3	2.38	0.58
53:BD:49:ASP:HB3	53:BD:52:ALA:HB2	1.84	0.58
1:1:1756:G:OP1	59:Bd:77:ARG:NH1	2.26	0.58
1:1:2035:U:OP2	1:1:2040:A:N6	2.29	0.58
1:1:2408:G:H1'	1:1:2410:G:N7	2.18	0.58
2:2:410:C:O2'	2:2:587:A:N3	2.35	0.58
4:H:186:PHE:O	4:H:190:ARG:NH1	2.35	0.58
14:AJ:87:ARG:HG3	14:AJ:88:GLN:HG2	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1710:C:H2'	1:1:1711:G:H8	1.69	0.58
66:BA:37:LEU:HD22	66:BA:201:GLN:HG3	1.86	0.58
1:1:1421:C:H2'	1:1:1422:A:C8	2.38	0.58
1:1:2164:U:H2'	1:1:2165:C:C6	2.39	0.58
2:2:1466:G:H1'	2:2:1487:MA6:H2	1.85	0.58
2:2:1491:U:H2'	2:2:1492:A:H8	1.68	0.58
10:AF:61:GLU:O	10:AF:92:ARG:NH1	2.37	0.58
53:BD:75:THR:O	53:BD:78:ARG:HG2	2.03	0.58
1:1:2887:A:O2'	63:BJ:2:ALA:N	2.34	0.58
2:2:145:G:H2'	2:2:146:A:C8	2.39	0.58
2:2:184:G:H4'	14:AJ:123:ILE:HD11	1.84	0.58
2:2:183:U:H2'	2:2:184:G:H8	1.69	0.58
2:2:244:G:H2'	2:2:245:G:H8	1.69	0.58
11:AG:47:LEU:HA	11:AG:50:LEU:HD13	1.85	0.58
21:AR:15:LYS:HD3	21:AR:24:HIS:CD2	2.38	0.58
24:AV:92:ILE:HG22	24:AV:93:ILE:HG23	1.86	0.58
29:A0:9:LYS:O	29:A0:13:ARG:NH1	2.26	0.58
2:2:791:G:OP1	20:AQ:2:ALA:N	2.36	0.58
4:H:85:LEU:HD12	4:H:118:LEU:HD12	1.85	0.58
28:AZ:55:ILE:HG22	28:AZ:59:GLY:H	1.69	0.58
37:B5:9:ILE:HG12	37:B5:23:VAL:HG12	1.85	0.58
66:BA:208:LYS:HB3	66:BA:214:ALA:HA	1.85	0.58
1:1:772:U:H2'	1:1:773:C:C6	2.38	0.57
2:2:75:G:H2'	2:2:76:G:C8	2.38	0.57
4:H:156:MET:HE1	4:H:161:ILE:HG13	1.86	0.57
1:1:720:A:H2'	1:1:721:A:C8	2.34	0.57
1:1:1601:U:O4	45:BT:15:LYS:NZ	2.36	0.57
2:2:619:U:O4	2:2:719:G:O2'	2.20	0.57
16:AL:97:GLU:OE1	16:AL:97:GLU:N	2.37	0.57
1:1:116:G:H2'	1:1:117:G:C8	2.40	0.57
1:1:567:A:H1'	1:1:2121:A:C2	2.39	0.57
1:1:1489:C:H2'	1:1:1490:G:H8	1.68	0.57
2:2:247:G:OP1	21:AR:66:ARG:NH1	2.37	0.57
2:2:712:C:OP1	2:2:822:C:O2'	2.20	0.57
5:AA:120:VAL:HG12	5:AA:189:ILE:HG12	1.86	0.57
66:BA:8:ARG:HH21	66:BA:181:ALA:HB1	1.69	0.57
1:1:763:C:H2'	1:1:764:A:H8	1.69	0.57
1:1:1327:C:N4	1:1:1352:C:O3'	2.31	0.57
2:2:470:G:H2'	2:2:471:OMG:H8	1.69	0.57
2:2:1328:C:H2'	2:2:1329:G:H8	1.70	0.57
45:BT:21:GLU:OE1	45:BT:21:GLU:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:BA:205:VAL:HG13	66:BA:217:VAL:HB	1.85	0.57
1:1:1283:A:H2'	1:1:1284:A:H8	1.70	0.57
2:2:634:G:C6	2:2:707:U:N3	2.73	0.57
2:2:813:G:OP1	5:AA:177:LYS:NZ	2.37	0.57
5:AA:57:THR:HG22	5:AA:59:ASP:H	1.70	0.57
36:BC:68:MET:HE3	36:BC:69:PRO:HD2	1.85	0.57
38:BL:47:TRP:CZ2	38:BL:51:ILE:HD11	2.40	0.57
2:2:679:G:H2'	2:2:680:OMG:C8	2.39	0.57
66:BA:206:TYR:HE1	66:BA:216:LYS:HD3	1.68	0.57
1:1:2314:U:H2'	1:1:2315:U:C6	2.40	0.57
23:AU:33:PRO:HB3	32:AO:41:ARG:HD3	1.87	0.57
55:BZ:28:LYS:HE3	55:BZ:52:TYR:CZ	2.39	0.57
66:BA:117:MET:HG3	66:BA:118:PRO:HD3	1.86	0.57
1:1:2823:C:H2'	1:1:2824:G:H8	1.69	0.57
4:H:156:MET:HE2	4:H:156:MET:HA	1.87	0.57
6:AB:183:SER:N	6:AB:187:GLU:OE2	2.37	0.57
37:BK:45:ARG:NH1	64:BL:1:MET:O	2.38	0.57
2:2:382:A:H1'	2:2:447:A:H5'	1.86	0.56
16:AL:81:ALA:HA	16:AL:84:GLN:HE22	1.69	0.56
61:Bg:6:GLU:OE1	61:Bg:6:GLU:N	2.30	0.56
1:1:1715:U:H5	1:1:1824:A:N7	2.03	0.56
2:2:1302:C:OP1	32:AO:34:ASN:ND2	2.34	0.56
9:AE:172:GLU:N	9:AE:172:GLU:OE1	2.38	0.56
15:AK:41:ALA:O	15:AK:44:THR:OG1	2.23	0.56
17:AM:84:ARG:HE	17:AM:120:PRO:HD3	1.70	0.56
60:BN:98:PRO:HG3	60:BN:118:LYS:HG2	1.86	0.56
1:1:100:G:O2'	1:1:101:U:H5'	2.05	0.56
1:1:1146:C:H2'	1:1:1147:C:C6	2.41	0.56
4:H:119:LEU:HD21	4:H:257:VAL:HG13	1.87	0.56
12:AH:135:ASP:HB2	12:AH:152:ILE:HD11	1.88	0.56
5:AA:20:TYR:O	5:AA:35:LEU:HB2	2.06	0.56
18:AN:73:VAL:HG11	18:AN:97:ILE:HG21	1.88	0.56
24:B6:3:ILE:HG12	24:B6:23:ILE:HD13	1.86	0.56
1:1:1278:C:OP1	1:1:1281:C:N4	2.38	0.56
1:1:1498:C:H2'	1:1:1499:G:H8	1.69	0.56
1:1:1685:A:N3	1:1:1755:4AC:O2'	2.36	0.56
2:2:1032:A:N1	2:2:1073:G:O2'	2.35	0.56
2:2:1350:U:H2'	2:2:1351:A:H8	1.71	0.56
1:1:1303:A:H61	1:1:1367:G:H1'	1.71	0.56
2:2:849:G:OP2	18:AN:4:LYS:NZ	2.39	0.56
6:AB:56:GLY:HA3	6:AB:174:GLU:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AH:17:VAL:HG21	12:AH:64:VAL:HG21	1.85	0.56
24:AV:72:TYR:OH	24:AV:82:GLU:OE1	2.20	0.56
12:AH:190:LEU:HB2	12:AH:198:SER:HB3	1.86	0.56
17:AM:53:ASP:OD1	17:AM:53:ASP:N	2.32	0.56
35:BO:160:ASP:HB3	35:BO:163:LYS:HB3	1.87	0.56
1:1:382:C:H2'	1:1:383:C:H6	1.69	0.56
1:1:2130:A:H2'	1:1:2131:A:C8	2.41	0.56
1:1:2543:U:O2'	43:BE:31:ASN:ND2	2.38	0.56
12:AH:70:LYS:HG3	12:AH:162:LEU:HB3	1.88	0.56
1:1:1173:C:H2'	1:1:1174:A:H8	1.71	0.56
10:AF:220:ARG:NH1	13:AI:98:GLU:OE1	2.38	0.56
1:1:210:C:H2'	1:1:211:4AC:H6	1.86	0.55
1:1:1049:G:OP1	42:Be:53:LYS:NZ	2.38	0.55
19:AP:9:ARG:NH1	19:AP:27:TYR:OH	2.39	0.55
32:AO:97:LYS:O	32:AO:97:LYS:NZ	2.35	0.55
36:BC:293:VAL:HG22	36:BC:298:GLU:HG2	1.87	0.55
2:2:861:G:O2'	2:2:877:G:O6	2.24	0.55
2:2:1237:C:OP1	23:AU:119:ARG:NH1	2.39	0.55
66:BA:42:LEU:HD12	66:BA:160:LEU:HD21	1.87	0.55
1:1:1303:A:H1'	1:1:1304:C:H5'	1.88	0.55
1:1:2009:G:N2	1:1:2012:G:OP2	2.35	0.55
1:1:2304:C:H2'	1:1:2305:C:C6	2.41	0.55
1:1:2363:G:N2	66:BA:208:LYS:HZ3	2.04	0.55
2:2:907:A:H2'	2:2:908:C:H6	1.69	0.55
52:Bj:2:LYS:HD2	52:Bj:92:VAL:HG11	1.89	0.55
30:B4:31:LYS:H	30:B4:103:GLU:HB3	1.72	0.55
1:1:107:G:N2	1:1:112:A:H8	1.93	0.55
31:AT:32:GLN:HG3	31:AT:71:ILE:HD12	1.87	0.55
33:BB:202:HIS:CD2	33:BB:204:PHE:H	2.23	0.55
55:BZ:98:LYS:HG3	55:BZ:99:ARG:HH11	1.71	0.55
60:BN:83:HIS:HD2	60:BN:136:ARG:HE	1.54	0.55
1:1:705:A:H2'	1:1:706:G:C8	2.42	0.55
1:1:978:G:O2'	1:1:1014:G:H4'	2.06	0.55
1:1:2944:C:O2'	1:1:2946:C:OP2	2.17	0.55
1:1:3014:C:H2'	1:1:3015:G:H8	1.72	0.55
54:BF:11:ILE:HB	54:BF:53:VAL:HG13	1.89	0.55
2:2:579:C:H2'	2:2:580:A:H8	1.72	0.55
2:2:678:G:H2'	2:2:679:G:H8	1.71	0.55
4:H:38:ILE:N	4:H:50:LEU:O	2.26	0.55
2:2:1069:OMG:HM22	2:2:1070:A:H5'	1.88	0.55
12:AH:58:LYS:NZ	12:AH:159:ASP:OD2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AL:4:ALA:HB3	16:AL:75:ILE:HD12	1.89	0.55
53:BD:175:GLU:OE1	53:BD:176:LYS:NZ	2.32	0.55
60:BN:127:LYS:H	60:BN:130:GLN:NE2	2.04	0.55
1:1:1401:C:O2'	64:BL:42:GLY:O	2.24	0.55
1:1:1740:C:O3'	59:Bd:16:ARG:NH2	2.34	0.55
1:1:2118:U:N3	1:1:2121:A:OP2	2.33	0.55
4:H:208:MET:HE1	4:H:213:ALA:HB3	1.88	0.55
14:AJ:33:SER:HB3	14:AJ:56:ARG:HD3	1.89	0.55
49:BR:45:ILE:H	49:BR:59:HIS:CD2	2.24	0.55
1:1:1116:G:H2'	1:1:1117:C:C6	2.41	0.55
1:1:1321:U:N3	1:1:1324:A:OP2	2.36	0.55
1:1:2535:G:N2	1:1:2543:U:H3	2.03	0.55
2:2:121:U:H2'	2:2:122:C:C6	2.42	0.55
2:2:1482:A:H2'	2:2:1483:G:C8	2.41	0.55
4:H:37:LEU:HD22	4:H:112:VAL:HG21	1.89	0.55
4:H:120:GLU:HG3	4:H:235:LYS:HD2	1.89	0.55
10:AF:13:LEU:O	10:AF:27:LYS:NZ	2.34	0.55
1:1:102:C:N3	1:1:103:C:C5	2.74	0.55
1:1:1612:A:H2'	1:1:1613:A:C8	2.42	0.55
1:1:1842:A:H2'	1:1:1843:A:C8	2.42	0.55
1:1:2408:G:H1'	1:1:2410:G:C8	2.41	0.55
2:2:24:U:H2'	2:2:25:C:C6	2.42	0.55
8:AD:24:ASP:OD1	8:AD:27:ARG:NH2	2.40	0.55
8:AD:109:VAL:HG23	8:AD:114:LEU:HB2	1.88	0.55
15:AK:19:ILE:HG13	15:AK:62:ILE:HG12	1.88	0.55
24:AV:51:THR:HG22	24:AV:71:TYR:HD1	1.71	0.55
1:1:850:A:N6	38:BL:117:LYS:O	2.35	0.54
2:2:1130:G:N7	22:AS:44:LYS:NZ	2.43	0.54
9:AE:202:ILE:HG13	9:AE:213:VAL:HG12	1.89	0.54
16:AL:8:LEU:HB3	16:AL:16:LEU:HD22	1.88	0.54
1:1:1324:A:H4'	1:1:1325:A:H5''	1.89	0.54
1:1:2370:G:O2'	1:1:2374:A:N7	2.37	0.54
4:H:30:ILE:HD13	4:H:35:PRO:HD2	1.89	0.54
8:AD:165:HIS:HB3	8:AD:168:ARG:HB3	1.89	0.54
66:BA:43:LYS:HA	66:BA:48:ARG:HH21	1.72	0.54
1:1:2426:C:H2'	1:1:2427:G:C8	2.42	0.54
2:2:683:C:H2'	2:2:684:C:C6	2.41	0.54
60:BN:170:ASN:OD1	60:BN:170:ASN:N	2.40	0.54
1:1:1064:C:H2'	1:1:1065:4AC:H6	1.89	0.54
38:BL:36:MET:HE3	38:BL:39:THR:HG21	1.88	0.54
2:2:626:4AC:H2'	2:2:627:G:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AC:35:CYS:SG	7:AC:36:GLY:N	2.81	0.54
24:AV:46:LEU:HD13	24:AV:51:THR:HG21	1.88	0.54
54:BF:139:VAL:HG12	54:BF:147:VAL:HG13	1.89	0.54
66:BA:131:ARG:HB3	66:BA:133:LYS:HG2	1.88	0.54
1:1:353:C:OP2	1:1:2628:C:O2'	2.18	0.54
2:2:724:U:H2'	2:2:725:G:O4'	2.07	0.54
2:2:1214:U:O4	12:AH:170:SER:OG	2.22	0.54
10:AF:33:ASP:OD2	10:AF:35:HIS:ND1	2.26	0.54
16:AL:45:ILE:HG12	19:AP:34:HIS:HD2	1.73	0.54
18:AN:139:LYS:HB3	18:AN:141:ARG:HE	1.72	0.54
26:AX:11:VAL:HG22	26:AX:53:ASP:H	1.71	0.54
1:1:1742:A:H2'	1:1:1743:A:C8	2.43	0.54
1:1:3014:C:H2'	1:1:3015:G:C8	2.43	0.54
5:AA:104:ILE:HG12	5:AA:135:GLU:HG3	1.89	0.54
20:AQ:103:VAL:HG21	20:AQ:157:VAL:HG11	1.88	0.54
26:AX:10:GLU:HB2	26:AX:32:LEU:HD21	1.89	0.54
48:BI:56:ARG:HA	48:BI:65:PRO:HD2	1.89	0.54
24:B6:23:ILE:HG21	24:B6:31:PRO:HG3	1.90	0.54
1:1:635:G:O2'	1:1:659:A:N1	2.37	0.54
2:2:285:C:OP1	21:AR:40:SER:OG	2.24	0.54
2:2:977:A:H62	2:2:999:G:N2	2.06	0.54
30:B4:109:ASP:O	30:B4:113:GLU:N	2.38	0.54
1:1:94:G:H3'	1:1:95:G:H5'	1.89	0.54
2:2:384:U:OP1	9:AE:50:ARG:NH1	2.40	0.54
2:2:908:C:C2	2:2:909:A:C8	2.96	0.54
1:1:360:A:H2'	1:1:361:A:C8	2.42	0.54
1:1:382:C:H2'	1:1:383:C:C6	2.42	0.54
2:2:483:G:H4'	2:2:485:C:C2	2.43	0.54
2:2:641:G:N2	17:AM:123:HIS:O	2.41	0.54
7:AC:16:SER:OG	7:AC:46:CYS:SG	2.62	0.54
28:AZ:36:LYS:HB2	28:AZ:43:LYS:HG3	1.88	0.54
1:1:2305:C:H2'	1:1:2306:C:H6	1.73	0.53
17:AM:19:ILE:HB	17:AM:83:VAL:HA	1.89	0.53
34:BY:148:ASN:O	34:BY:152:GLU:HG2	2.07	0.53
22:AS:25:THR:HG23	22:AS:27:ASP:H	1.72	0.53
28:AZ:128:VAL:HG23	28:AZ:182:ILE:HG12	1.90	0.53
31:AT:81:ILE:HG12	31:AT:94:ILE:HD11	1.91	0.53
56:BP:22:SER:OG	56:BP:27:VAL:O	2.22	0.53
58:BS:37:ARG:NH1	58:BS:38:GLU:OE2	2.41	0.53
1:1:600:G:H2'	53:BD:183:LYS:HE3	1.90	0.53
1:1:1575:A:H2'	1:1:1576:C:C6	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1754:C:OP1	59:Bd:41:ARG:NH1	2.40	0.53
2:2:1261:A:H2'	2:2:1262:A:C8	2.43	0.53
18:AN:98:ASP:OD1	18:AN:99:GLU:N	2.37	0.53
2:2:746:C:H2'	2:2:747:G:O4'	2.08	0.53
9:AE:87:ILE:HD12	9:AE:104:PRO:HD3	1.90	0.53
23:AU:25:GLU:OE1	23:AU:25:GLU:N	2.42	0.53
53:BD:1:MET:HG2	53:BD:18:LEU:HD12	1.89	0.53
53:BD:149:GLN:HA	53:BD:207:ILE:HB	1.89	0.53
1:1:133:G:H2'	1:1:134:C:C6	2.44	0.53
2:2:1229:G:O2'	2:2:1232:C:O2	2.21	0.53
23:AU:63:TYR:HE2	23:AU:126:ARG:HG3	1.73	0.53
26:AX:9:ALA:N	26:AX:55:LEU:O	2.42	0.53
41:Bb:80:GLU:OE1	24:B6:64:LYS:NZ	2.31	0.53
48:BI:57:THR:H	48:BI:64:GLY:HA3	1.73	0.53
57:BM:76:TRP:CD1	57:BM:76:TRP:H	2.25	0.53
1:1:773:C:H5'	38:BL:22:LYS:HE2	1.90	0.53
2:2:96:C:H2'	2:2:97:A:C8	2.44	0.53
4:H:2:VAL:HG21	4:H:121:ARG:HH22	1.74	0.53
5:AA:11:LYS:HD3	5:AA:11:LYS:H	1.74	0.53
16:AL:33:ARG:O	16:AL:33:ARG:NH1	2.36	0.53
1:1:102:C:C2	1:1:103:C:C5	2.97	0.53
2:2:916:G:N1	2:2:1312:G:OP2	2.39	0.53
30:A3:33:ARG:HH22	30:A3:42:ALA:HB2	1.74	0.53
32:AO:16:ASP:HB3	32:AO:19:LYS:HD2	1.89	0.53
66:BA:15:VAL:HG22	66:BA:207:VAL:HG11	1.91	0.53
66:BA:102:LYS:O	66:BA:106:LYS:HG2	2.08	0.53
1:1:462:G:H21	1:1:485:A:H62	1.56	0.53
1:1:795:U:H2'	1:1:796:C:C6	2.44	0.53
1:1:1108:G:OP1	49:BR:97:LYS:NZ	2.42	0.53
1:1:2405:C:OP1	66:BA:102:LYS:NZ	2.34	0.53
4:H:50:LEU:HA	4:H:54:LEU:HD12	1.91	0.53
9:AE:36:PRO:HD2	9:AE:84:PRO:HG2	1.89	0.53
14:AJ:42:LYS:HB3	14:AJ:59:ALA:HB3	1.91	0.53
33:BB:122:VAL:HG13	33:BB:127:THR:HG22	1.90	0.53
38:BL:79:LYS:HB3	38:BL:116:GLY:HA3	1.91	0.53
45:BT:78:GLU:OE1	45:BT:78:GLU:N	2.42	0.53
66:BA:35:VAL:HG23	66:BA:202:ILE:HD13	1.90	0.53
1:1:508:C:H2'	1:1:509:A:C8	2.44	0.53
1:1:889:U:H2'	1:1:890:G:C8	2.44	0.53
1:1:1301:A:H4'	1:1:1302:G:H5'	1.91	0.53
1:1:1755:4AC:O7	1:1:1755:4AC:H5	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:135:U:O2	9:AE:147:ASN:ND2	2.36	0.53
2:2:594:G:O2'	8:AD:65:GLN:NE2	2.40	0.53
10:AF:132:GLU:HG3	10:AF:160:PRO:HG3	1.91	0.53
25:AW:29:VAL:HG11	25:AW:47:VAL:HG21	1.90	0.53
1:1:1266:G:N2	64:Bl:43:SER:HB2	2.24	0.53
2:2:122:C:OP1	2:2:571:C:O2'	2.26	0.53
2:2:386:C:H2'	2:2:387:G:C8	2.44	0.53
4:H:137:THR:OG1	4:H:254:ILE:O	2.26	0.53
31:AT:11:TYR:HD2	31:AT:19:MET:HE1	1.73	0.53
37:BK:58:GLU:OE1	37:BK:58:GLU:N	2.42	0.53
1:1:431:G:OP2	1:1:431:G:H8	1.92	0.52
1:1:974:G:OP1	50:BQ:92:LYS:NZ	2.33	0.52
1:1:1055:A2M:HM'2	1:1:1057:C:C6	2.44	0.52
1:1:1421:C:H2'	1:1:1422:A:H8	1.74	0.52
1:1:2050:U:H2'	1:1:2051:C:H6	1.75	0.52
1:1:2359:A:N6	1:1:2408:G:H8	1.96	0.52
1:1:2723:C:H5'	1:1:2802:G:H5''	1.90	0.52
10:AF:125:LYS:HG2	10:AF:225:VAL:HG22	1.89	0.52
31:AT:97:GLU:OE2	32:AO:111:ARG:NH1	2.42	0.52
1:1:2272:C:OP1	1:1:2686:G:O2'	2.26	0.52
2:2:768:U:H2'	2:2:769:A:H8	1.74	0.52
1:1:1524:G:N7	58:BS:28:SER:OG	2.37	0.52
2:2:1024:C:O3'	19:AP:44:ARG:NH2	2.42	0.52
2:2:1136:C:H2'	2:2:1137:G:H8	1.75	0.52
33:BB:100:ALA:O	33:BB:134:ARG:NH2	2.38	0.52
24:B6:41:VAL:HG23	24:B6:46:LEU:HB2	1.90	0.52
1:1:1035:G:H5'	1:1:1036:G:OP1	2.09	0.52
2:2:195:A:O2'	2:2:197:G:N7	2.34	0.52
5:AA:137:ALA:O	5:AA:140:LYS:HG2	2.09	0.52
64:Bl:9:SER:OG	64:Bl:56:GLU:OE1	2.27	0.52
1:1:1317:G:H2'	1:1:1318:G:C8	2.43	0.52
2:2:907:A:H2'	2:2:908:C:C6	2.43	0.52
7:AC:21:ILE:O	10:AF:39:ARG:NH1	2.41	0.52
13:AI:55:ASP:N	13:AI:55:ASP:OD1	2.41	0.52
21:AR:84:ASP:HB2	21:AR:107:GLU:O	2.10	0.52
1:1:2363:G:H2'	1:1:2364:G:C8	2.44	0.52
2:2:28:G:H2'	2:2:29:C:C6	2.44	0.52
2:2:974:U:H5''	30:A3:36:THR:HG21	1.91	0.52
2:2:1212:A:H2	2:2:1215:G:N3	2.08	0.52
4:H:380:TYR:HA	12:AH:145:ARG:HB2	1.91	0.52
28:AZ:126:ARG:HG3	28:AZ:185:PRO:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BQ:140:MET:O	50:BQ:144:GLU:HG2	2.10	0.52
66:BA:65:ILE:HB	66:BA:82:LEU:HD11	1.92	0.52
1:1:435:C:H2'	1:1:436:C:H6	1.74	0.52
2:2:1435:C:H2'	2:2:1436:G:O4'	2.10	0.52
2:2:1491:U:H2'	2:2:1492:A:C8	2.44	0.52
4:H:338:VAL:HG11	15:AK:135:ARG:HG3	1.91	0.52
66:BA:32:GLU:HA	66:BA:169:PRO:HA	1.92	0.52
2:2:485:C:H2'	2:2:486:A:O4'	2.10	0.52
4:H:386:GLU:HG3	17:AM:23:TYR:CZ	2.45	0.52
5:AA:112:THR:HG21	5:AA:155:PHE:HB2	1.91	0.52
16:AL:33:ARG:HH12	16:AL:75:ILE:HA	1.73	0.52
20:AQ:92:PRO:HD2	20:AQ:95:LEU:HD12	1.90	0.52
1:1:451:4AC:H5''	40:BU:119:ARG:HG2	1.90	0.52
1:1:2373:G:H8	1:1:2373:G:OP2	1.93	0.52
2:2:684:C:O2'	2:2:701:C:O4'	2.17	0.52
5:AA:54:LYS:HE3	5:AA:60:PHE:HB3	1.90	0.52
31:AT:112:ARG:HH12	31:AT:114:GLN:HE21	1.58	0.52
43:BE:43:LYS:HD3	43:BE:132:ILE:HA	1.91	0.52
65:Bk:4:LEU:HD13	65:Bk:37:VAL:HG13	1.92	0.52
1:1:691:G:OP1	62:Bc:49:SER:OG	2.21	0.52
1:1:1331:C:H2'	1:1:1332:A:C8	2.44	0.52
2:2:421:C:H2'	2:2:422:C:C6	2.45	0.52
2:2:484:G:O2'	4:H:324:LYS:O	2.26	0.52
30:A3:3:LYS:HE2	30:A3:58:ASP:HB3	1.92	0.52
40:BU:31:LEU:HD23	40:BU:102:ILE:HB	1.90	0.52
2:2:1321:G:OP2	12:AH:53:LYS:NZ	2.38	0.51
31:AT:98:MET:HG2	31:AT:106:PHE:CZ	2.45	0.51
1:1:2416:G:H2'	1:1:2417:C:H6	1.76	0.51
2:2:484:G:H8	2:2:496:G:H5'	1.75	0.51
2:2:498:A:O2'	28:AZ:139:GLU:OE2	2.20	0.51
2:2:579:C:H2'	2:2:580:A:C8	2.45	0.51
2:2:663:A:H2'	2:2:664:U:H6	1.74	0.51
2:2:1416:C:H2'	2:2:1417:U:C6	2.45	0.51
25:AW:38:ARG:HD3	25:AW:38:ARG:H	1.76	0.51
53:BD:201:VAL:HG11	53:BD:207:ILE:HG21	1.92	0.51
1:1:42:U:H4'	1:1:43:A:H5'	1.92	0.51
1:1:299:A:H5''	38:BL:37:ALA:HB2	1.92	0.51
1:1:1210:U:H4'	60:BN:8:ILE:HG23	1.92	0.51
2:2:416:C:H5''	8:AD:119:ARG:HE	1.73	0.51
11:AG:24:PRO:O	11:AG:28:LYS:NZ	2.43	0.51
30:A3:48:ALA:HA	30:A3:102:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2363:G:H2'	1:1:2364:G:H8	1.75	0.51
2:2:511:4AC:O2'	2:2:515:U:OP1	2.27	0.51
2:2:658:G:O2'	2:2:764:C:H4'	2.10	0.51
5:AA:153:LEU:HG	5:AA:157:ASP:HB3	1.92	0.51
8:AD:116:ARG:HG3	8:AD:171:ILE:HA	1.91	0.51
11:AG:75:ARG:HG2	11:AG:92:PRO:HG2	1.93	0.51
62:Bc:8:LEU:HD11	62:Bc:25:LYS:HB2	1.92	0.51
1:1:1687:C:H5'	59:Bd:64:PRO:HB3	1.91	0.51
2:2:1092:G:H5'	2:2:1254:A:O2'	2.10	0.51
2:2:1386:C:H2'	2:2:1387:A:C8	2.45	0.51
3:3:10:G:O6	35:BO:12:ARG:NH1	2.43	0.51
8:AD:109:VAL:HG13	8:AD:121:ALA:HB1	1.92	0.51
14:AJ:75:VAL:HG11	14:AJ:105:ILE:HD11	1.91	0.51
43:BE:71:ARG:N	43:BE:74:GLU:OE2	2.38	0.51
55:BZ:17:ILE:HD12	55:BZ:26:LEU:HD11	1.92	0.51
23:AU:42:GLU:HG3	23:AU:43:ARG:HG3	1.93	0.51
1:1:122:G:H2'	1:1:123:A:C8	2.45	0.51
1:1:908:A:H2'	1:1:909:C:C6	2.46	0.51
1:1:1943:G:O2'	1:1:2232:U:O4	2.22	0.51
6:AB:48:THR:OG1	6:AB:155:PRO:O	2.27	0.51
10:AF:160:PRO:HD2	10:AF:163:LEU:HD22	1.93	0.51
33:BB:61:VAL:HG11	33:BB:83:ILE:HD11	1.93	0.51
39:Bf:21:ARG:O	39:Bf:38:HIS:HE1	1.94	0.51
1:1:115:G:N3	1:1:115:G:H2'	2.26	0.51
1:1:1048:4AC:O2'	42:Be:51:TRP:O	2.28	0.51
1:1:2416:G:H2'	1:1:2417:C:C6	2.46	0.51
2:2:1224:A:H2'	2:2:1225:A:C8	2.45	0.51
9:AE:119:GLU:OE2	9:AE:241:SER:N	2.31	0.51
17:AM:34:THR:HG23	17:AM:36:ALA:H	1.76	0.51
30:A3:15:LEU:HG	30:A3:114:ILE:HD11	1.93	0.51
2:2:29:C:H2'	2:2:30:C:C6	2.46	0.51
2:2:611:U:C2	2:2:612:G:C8	2.99	0.51
2:2:1416:C:H2'	2:2:1417:U:H6	1.76	0.51
3:3:30:C:H5'	43:BE:149:ARG:HD3	1.92	0.51
3:3:98:G:H2'	3:3:99:G:C8	2.46	0.51
4:H:87:HIS:O	4:H:90:LYS:HG2	2.11	0.51
31:AT:95:LYS:HB2	32:AO:112:ILE:HD11	1.93	0.51
1:1:952:U:H2'	1:1:953:G:O4'	2.11	0.51
1:1:1787:A:OP1	59:Bd:30:LYS:NZ	2.33	0.51
1:1:2311:A:H2'	1:1:2312:G:H8	1.75	0.51
8:AD:96:THR:HG22	8:AD:98:GLU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AL:30:THR:HG21	16:AL:80:ARG:CZ	2.41	0.51
36:BC:188:SER:HB3	36:BC:191:GLU:HB2	1.93	0.51
38:BL:5:ARG:NH2	38:BL:10:LYS:HD2	2.26	0.51
41:Bb:103:ALA:HB3	41:Bb:106:VAL:HG23	1.93	0.51
63:BJ:85:GLN:HA	63:BJ:102:ASN:HD22	1.76	0.51
1:1:32:G:H2'	1:1:33:G:H8	1.75	0.50
1:1:1841:A:H2'	1:1:1842:A:C8	2.45	0.50
1:1:2337:C:H2'	1:1:2338:G:H8	1.77	0.50
58:BS:60:PRO:HG2	58:BS:78:PHE:CZ	2.46	0.50
64:Bl:64:GLU:OE1	64:Bl:64:GLU:N	2.43	0.50
66:BA:93:ILE:HA	66:BA:99:GLN:HE22	1.76	0.50
1:1:1740:C:H4'	59:Bd:16:ARG:HH12	1.76	0.50
2:2:190:C:H2'	2:2:191:U:C6	2.46	0.50
2:2:1499:G:H2'	2:2:1500:A:C8	2.47	0.50
43:BE:123:ILE:HD11	43:BE:126:VAL:HG13	1.93	0.50
1:1:2522:U:H2'	1:1:2523:C:C6	2.47	0.50
2:2:37:C:H2'	2:2:38:A:H8	1.76	0.50
2:2:353:A:H3'	2:2:354:C:H6	1.76	0.50
2:2:1089:G:O4'	16:AL:38:ILE:HD11	2.11	0.50
9:AE:33:ARG:HG3	9:AE:34:PRO:HD2	1.93	0.50
44:Ba:25:TRP:HA	44:Ba:64:GLU:HG2	1.93	0.50
57:BM:157:ARG:HB2	57:BM:162:LEU:HB2	1.93	0.50
1:1:658:G:H5''	1:1:661:C:H1'	1.94	0.50
1:1:1549:C:H2'	1:1:1550:4AC:H6	1.92	0.50
1:1:2066:A:H2'	1:1:2067:G:O4'	2.11	0.50
1:1:2455:A:H4'	1:1:2456:C:O5'	2.11	0.50
2:2:653:U:H1'	2:2:654:A:C8	2.45	0.50
2:2:1121:C:O2	15:AK:16:ARG:NH1	2.45	0.50
20:AQ:25:TRP:CG	25:AW:64:LEU:HD21	2.47	0.50
20:AQ:149:ASP:H	20:AQ:152:GLN:HE21	1.60	0.50
37:B5:26:ASP:OD1	37:B5:27:ILE:N	2.45	0.50
38:BL:38:GLY:HA2	38:BL:43:ASN:HB3	1.93	0.50
1:1:2370:G:N2	1:1:2374:A:N1	2.55	0.50
1:1:2858:U:H3	1:1:3007:A:H62	1.58	0.50
66:BA:27:PHE:O	66:BA:29:GLN:NE2	2.43	0.50
1:1:1006:G:H2'	1:1:1007:C:C6	2.47	0.50
1:1:2341:G:H5'	1:1:2342:C:OP2	2.12	0.50
2:2:392:A:H4'	24:AV:80:TYR:HE1	1.75	0.50
66:BA:8:ARG:HH22	66:BA:11:ILE:HD12	1.77	0.50
66:BA:68:ILE:HG12	66:BA:85:ILE:HD12	1.93	0.50
1:1:434:A:H2'	1:1:435:C:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1211:A:H2'	1:1:1212:A:C8	2.47	0.50
1:1:2477:G:H2'	1:1:2478:C:H6	1.76	0.50
1:1:2480:G:O2'	1:1:2728:U:OP1	2.23	0.50
2:2:433:C:H2'	2:2:434:U:C6	2.46	0.50
2:2:678:G:H2'	2:2:679:G:C8	2.47	0.50
2:2:922:U:H2'	2:2:923:G:H8	1.76	0.50
2:2:973:A:OP1	2:2:974:U:O2'	2.25	0.50
2:2:1502:C:H2'	2:2:1503:A:H4'	1.93	0.50
4:H:185:ARG:C	4:H:185:ARG:HD3	2.37	0.50
5:AA:111:THR:HA	5:AA:117:LYS:HA	1.93	0.50
43:BE:60:LYS:HA	43:BE:75:PRO:HA	1.93	0.50
66:BA:64:LYS:O	66:BA:108:ASP:N	2.45	0.50
1:1:154:G:C5	1:1:155:G:C8	3.00	0.50
1:1:3020:U:H2'	1:1:3021:U:C5	2.47	0.50
2:2:977:A:N6	2:2:999:G:H21	2.10	0.50
2:2:1076:A:H4'	22:AS:6:GLN:HE22	1.75	0.50
2:2:1326:C:H2'	2:2:1327:G:C8	2.46	0.50
4:H:48:GLY:HA2	4:H:75:PRO:HA	1.92	0.50
12:AH:14:GLU:OE1	12:AH:14:GLU:N	2.45	0.50
21:AR:16:CYS:H	21:AR:24:HIS:CD2	2.30	0.50
26:AX:36:ASP:HB3	26:AX:39:ARG:HD3	1.92	0.50
30:A3:74:GLU:OE1	30:A3:119:ARG:NH2	2.45	0.50
1:1:229:4AC:O2'	42:Be:21:ARG:HG2	2.12	0.50
1:1:535:U:H2'	1:1:536:C:C6	2.47	0.50
1:1:776:G:H2'	1:1:2270:C:C5	2.47	0.50
1:1:1842:A:H2'	1:1:1843:A:H8	1.76	0.50
1:1:2305:C:H2'	1:1:2306:C:C6	2.47	0.50
1:1:2558:A:H2'	1:1:2559:A:C8	2.47	0.50
2:2:353:A:H5''	2:2:354:C:H5	1.77	0.50
2:2:445:G:N2	2:2:450:A:N7	2.60	0.50
2:2:658:G:N7	17:AM:24:ASN:ND2	2.60	0.50
4:H:40:VAL:HG11	4:H:73:TYR:HB2	1.93	0.50
4:H:235:LYS:O	4:H:238:ASN:ND2	2.45	0.50
24:AV:43:MET:HG2	24:AV:44:LEU:HD22	1.93	0.50
31:AT:20:SER:OG	31:AT:22:GLU:OE1	2.28	0.50
31:AT:94:ILE:HA	31:AT:98:MET:SD	2.52	0.50
1:1:32:G:H2'	1:1:33:G:C8	2.47	0.49
1:1:118:U:H2'	1:1:118:U:O2	2.11	0.49
1:1:1110:G:N3	1:1:2499:A:H2'	2.27	0.49
1:1:1176:C:H2'	1:1:1177:G:H8	1.77	0.49
1:1:1393:G:H5'	48:BI:78:THR:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1763:G:H2'	1:1:1764:C:C6	2.46	0.49
1:1:2650:G:H2'	1:1:2651:C:H6	1.76	0.49
2:2:1415:U:H2'	2:2:1416:C:C6	2.47	0.49
9:AE:131:ARG:HE	9:AE:141:ASN:HD21	1.58	0.49
17:AM:84:ARG:HA	17:AM:119:THR:HG22	1.94	0.49
23:AU:45:PRO:O	32:AO:41:ARG:NH2	2.45	0.49
38:BL:1:MET:HE2	53:BD:33:ARG:HD2	1.93	0.49
56:BP:15:ILE:HD13	56:BP:38:GLU:HG3	1.93	0.49
1:1:2537:C:N4	43:BE:33:GLY:O	2.44	0.49
5:AA:117:LYS:HG2	5:AA:192:LEU:HB2	1.93	0.49
10:AF:19:LYS:N	10:AF:46:GLU:OE2	2.38	0.49
22:AS:29:GLU:O	22:AS:33:LYS:HD3	2.12	0.49
1:1:360:A:H2'	1:1:361:A:H8	1.77	0.49
1:1:1077:C:H5'	1:1:2662:A:O2'	2.12	0.49
2:2:965:A:H5''	2:2:966:C:C5	2.44	0.49
32:AO:9:ARG:NH1	32:AO:12:GLY:HA2	2.27	0.49
54:BF:92:VAL:HG22	54:BF:172:ILE:HG12	1.95	0.49
1:1:107:G:C2	1:1:112:A:N7	2.75	0.49
1:1:848:A:O2'	1:1:887:G:O2'	2.23	0.49
1:1:2504:A:H2'	1:1:2505:U:C6	2.47	0.49
2:2:456:C:H2'	2:2:457:G:H8	1.76	0.49
2:2:952:C:O2	19:AP:17:GLY:N	2.39	0.49
2:2:1492:A:H2'	2:2:1493:C:C6	2.46	0.49
5:AA:154:ASN:OD1	5:AA:155:PHE:N	2.45	0.49
30:A3:114:ILE:HD12	30:A3:117:LYS:HE3	1.94	0.49
61:Bg:8:GLU:OE1	61:Bg:44:ARG:NH2	2.37	0.49
1:1:757:G:O2'	1:1:1478:G:OP1	2.26	0.49
1:1:1355:C:H2'	1:1:1356:U:O4'	2.12	0.49
1:1:1574:C:H2'	1:1:1575:A:C8	2.48	0.49
1:1:2473:U:H2'	1:1:2474:U:C6	2.47	0.49
2:2:373:A2M:HM'2	2:2:374:A:C5	2.48	0.49
2:2:702:C:H2'	2:2:703:4AC:H6	1.94	0.49
2:2:922:U:H2'	2:2:923:G:C8	2.47	0.49
43:BE:129:ASP:HB3	43:BE:132:ILE:HG12	1.95	0.49
1:1:1993:G:N2	1:1:1995:G:H3'	2.27	0.49
1:1:2986:U:H1'	1:1:2987:A:H5''	1.93	0.49
2:2:994:U:H2'	2:2:995:U:C6	2.47	0.49
1:1:1363:U:O2'	1:1:1364:C:OP1	2.30	0.49
1:1:1393:G:OP2	48:BI:52:ARG:NH2	2.32	0.49
1:1:2347:G:H1	1:1:2422:U:H3	1.61	0.49
5:AA:109:ASN:HD21	5:AA:119:ARG:HE	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:BE:29:THR:HG23	43:BE:81:THR:HG22	1.95	0.49
66:BA:206:TYR:HB3	66:BA:214:ALA:HB1	1.95	0.49
1:1:727:G:N2	1:1:730:A:OP2	2.43	0.49
1:1:2399:G:H2'	1:1:2400:C:H6	1.78	0.49
4:H:140:VAL:HG21	4:H:254:ILE:HG12	1.95	0.49
8:AD:58:LEU:HD13	8:AD:70:ARG:HA	1.95	0.49
16:AL:37:PRO:HA	16:AL:73:ILE:HG13	1.95	0.49
20:AQ:111:GLN:HG2	20:AQ:112:HIS:HD2	1.77	0.49
24:AV:24:TYR:CZ	24:AV:26:PRO:HG3	2.48	0.49
60:BN:179:GLN:OE1	60:BN:179:GLN:N	2.45	0.49
1:1:2988:A:N1	54:BF:74:HIS:HE1	2.10	0.49
2:2:548:U:C2	2:2:549:A:C8	3.01	0.49
2:2:1088:A:H4'	16:AL:36:GLY:HA3	1.94	0.49
3:3:97:G:H2'	3:3:98:G:C8	2.48	0.49
21:AR:15:LYS:HD3	21:AR:24:HIS:HD2	1.78	0.49
26:AX:8:PRO:HB2	26:AX:32:LEU:HD12	1.94	0.49
28:AZ:41:GLY:HA3	28:AZ:77:ASN:HB3	1.94	0.49
30:A3:22:ALA:HB1	30:A3:111:VAL:HG22	1.95	0.49
32:AO:65:ILE:HG12	32:AO:72:HIS:HD2	1.78	0.49
51:BV:24:ARG:HH11	51:BV:28:ARG:NH2	2.11	0.49
60:BN:20:ARG:NH2	60:BN:27:PRO:O	2.34	0.49
66:BA:195:LEU:HG	66:BA:201:GLN:HG2	1.93	0.49
1:1:1324:A:O2'	1:1:1329:G:O6	2.30	0.49
2:2:680:OMG:H2'	2:2:681:G:C8	2.48	0.49
4:H:9:VAL:HG13	4:H:113:ILE:HD13	1.94	0.49
12:AH:75:GLY:HA3	12:AH:86:MET:HE3	1.94	0.49
24:AV:19:ILE:HD11	24:AV:69:ALA:HB3	1.94	0.49
30:BG:29:THR:HG21	30:BG:106:LYS:HG3	1.95	0.49
1:1:2255:A:H2'	1:1:2256:A:C8	2.48	0.48
1:1:2719:G:H2'	1:1:2720:A:H8	1.77	0.48
1:1:2792:C:H2'	1:1:2793:A:C8	2.48	0.48
2:2:459:G:O2'	2:2:461:A:H1'	2.13	0.48
2:2:879:A:H2'	2:2:880:A:C8	2.48	0.48
2:2:1346:C:H2'	2:2:1347:G:O4'	2.13	0.48
2:2:1478:C:H2'	2:2:1479:4AC:H6	1.94	0.48
8:AD:155:ALA:HB3	8:AD:158:SER:HB2	1.95	0.48
30:A3:19:ALA:HA	30:A3:78:ILE:HD12	1.94	0.48
1:1:895:A:H2'	1:1:896:G:O4'	2.14	0.48
1:1:910:G:H21	56:BP:1:MET:HE1	1.78	0.48
1:1:1489:C:H2'	1:1:1490:G:C8	2.47	0.48
1:1:1666:C:H2'	1:1:1667:4AC:H6	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:35:G:O2'	2:2:305:U:OP1	2.31	0.48
2:2:89:G:H2'	2:2:90:G:C8	2.48	0.48
2:2:124:G:O2'	21:AR:30:HIS:ND1	2.46	0.48
3:3:115:G:H2'	3:3:116:C:C6	2.48	0.48
60:BN:56:GLN:NE2	60:BN:125:ARG:HH21	2.12	0.48
1:1:727:G:N7	37:BK:17:ARG:NH2	2.61	0.48
1:1:1145:C:H2'	1:1:1146:C:C6	2.48	0.48
1:1:1232:A:N1	1:1:2267:G:O2'	2.43	0.48
1:1:1342:G:N2	1:1:1345:U:O4	2.47	0.48
1:1:1667:4AC:H2'	1:1:1668:G:H8	1.78	0.48
2:2:1212:A:H5'	12:AH:175:ARG:HG2	1.95	0.48
5:AA:40:ASP:HB3	5:AA:43:LYS:HG3	1.94	0.48
27:AY:33:ASP:OD1	27:AY:33:ASP:N	2.47	0.48
66:BA:36:ASN:ND2	66:BA:204:SER:O	2.40	0.48
1:1:264:G:OP1	1:1:403:G:O2'	2.26	0.48
1:1:1780:4AC:O7	1:1:1780:4AC:H5	2.13	0.48
1:1:2931:U:H2'	1:1:2932:C:C6	2.48	0.48
2:2:443:G:O2'	24:AV:30:THR:O	2.31	0.48
2:2:1141:A:O2'	2:2:1143:A:N7	2.38	0.48
4:H:185:ARG:HD2	4:H:186:PHE:CE2	2.49	0.48
4:H:256:THR:OG1	4:H:259:ASP:OD1	2.31	0.48
32:AO:5:ARG:NH2	32:AO:54:LEU:O	2.40	0.48
30:B4:17:GLU:HA	30:B4:20:LEU:HD23	1.95	0.48
66:BA:36:ASN:ND2	66:BA:204:SER:OG	2.46	0.48
2:2:746:C:H5''	17:AM:129:LYS:HB2	1.95	0.48
5:AA:90:ARG:NH2	17:AM:119:THR:O	2.45	0.48
11:AG:113:SER:H	11:AG:116:ILE:HD12	1.78	0.48
20:AQ:56:ASP:OD2	25:AW:34:ALA:N	2.40	0.48
23:AU:143:ILE:HG13	23:AU:144:ILE:HG13	1.94	0.48
30:A3:19:ALA:HB1	30:A3:80:VAL:HG22	1.96	0.48
62:Bc:41:ARG:HE	62:Bc:87:ILE:C	2.22	0.48
30:B4:108:ARG:HH11	30:B4:108:ARG:HA	1.78	0.48
1:1:21:C:H2'	1:1:22:4AC:H6	1.95	0.48
1:1:238:C:H4'	1:1:239:C:O5'	2.12	0.48
2:2:98:C:H2'	2:2:99:C:H6	1.79	0.48
2:2:191:U:H2'	2:2:192:G:O4'	2.14	0.48
2:2:866:G:H2'	2:2:867:C:H6	1.78	0.48
48:BI:126:PRO:HG3	54:BF:40:PHE:HE2	1.78	0.48
55:BZ:40:ASN:HB2	55:BZ:66:THR:HA	1.96	0.48
1:1:117:G:N3	1:1:118:U:C6	2.82	0.48
1:1:993:U:OP2	1:1:1951:C:O2'	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1124:U:H2'	1:1:1125:G:C8	2.48	0.48
1:1:2065:A:H2'	1:1:2066:A:C8	2.49	0.48
2:2:1329:G:H2'	2:2:1330:C:C6	2.49	0.48
4:H:2:VAL:HG21	4:H:121:ARG:NH2	2.28	0.48
4:H:100:LEU:HG	4:H:101:PRO:HD2	1.95	0.48
30:BG:39:THR:HG23	30:BG:100:ALA:HB2	1.95	0.48
64:BL:31:GLU:H	64:BL:31:GLU:CD	2.21	0.48
66:BA:6:PHE:HB3	66:BA:11:ILE:HD11	1.96	0.48
1:1:102:C:N3	1:1:103:C:C4	2.81	0.48
1:1:3022:C:O2	1:1:3022:C:H2'	2.13	0.48
2:2:391:A:H2'	2:2:392:A:C8	2.49	0.48
5:AA:72:TYR:HE2	5:AA:82:LYS:HB2	1.79	0.48
21:AR:38:VAL:HG12	21:AR:49:VAL:HG22	1.96	0.48
31:AT:12:THR:HB	31:AT:15:GLN:HG3	1.96	0.48
43:BE:123:ILE:HG12	43:BE:126:VAL:HG22	1.94	0.48
1:1:98:C:H6	1:1:98:C:H5''	1.79	0.48
1:1:703:U:H3'	1:1:704:G:H5'	1.94	0.48
1:1:704:G:H8	1:1:704:G:OP2	1.97	0.48
1:1:1698:A:H2'	1:1:1699:G:H8	1.79	0.48
1:1:1706:G:H2'	1:1:1707:C:H6	1.78	0.48
4:H:271:GLU:HG3	4:H:272:ALA:H	1.78	0.48
10:AF:70:LEU:HD23	10:AF:70:LEU:H	1.79	0.48
37:B5:49:ASN:OD1	37:B5:50:ILE:N	2.46	0.48
66:BA:21:ARG:NH2	66:BA:213:PRO:O	2.30	0.48
1:1:90:C:H2'	1:1:91:4AC:H6	1.96	0.48
1:1:1011:C:H2'	1:1:1012:G:O4'	2.13	0.48
1:1:2130:A:H2'	1:1:2131:A:H8	1.77	0.48
2:2:1401:U:H2'	2:2:1402:A:C8	2.49	0.48
20:AQ:111:GLN:HG2	20:AQ:112:HIS:CD2	2.49	0.48
1:1:1145:C:H2'	1:1:1146:C:H6	1.78	0.47
1:1:1616:C:H2'	1:1:1617:4AC:H6	1.95	0.47
1:1:2535:G:H1	1:1:2543:U:H3	1.60	0.47
4:H:197:GLU:OE1	4:H:199:ALA:N	2.47	0.47
15:AK:119:PRO:O	15:AK:120:ASN:HB2	2.13	0.47
20:AQ:25:TRP:NE1	25:AW:65:GLU:OE2	2.38	0.47
23:AU:15:ARG:HH21	23:AU:135:GLU:CD	2.22	0.47
1:1:54:G:C2	1:1:55:U:H1'	2.48	0.47
1:1:855:C:H2'	1:1:856:G:O4'	2.13	0.47
1:1:889:U:H2'	1:1:890:G:H8	1.77	0.47
1:1:1933:C:H2'	1:1:1934:4AC:H6	1.96	0.47
1:1:2304:C:H2'	1:1:2305:C:H6	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2390:U:H2'	1:1:2391:C:C6	2.49	0.47
2:2:393:C:H2'	2:2:394:4AC:H6	1.96	0.47
2:2:547:G:N1	2:2:726:A:OP2	2.38	0.47
2:2:1222:A:OP2	23:AU:61:ARG:NH1	2.41	0.47
36:BC:91:LEU:O	48:BI:141:LYS:NZ	2.47	0.47
42:Be:28:PHE:HA	42:Be:35:CYS:HA	1.95	0.47
51:BV:21:MET:HE3	63:BJ:97:ILE:HD12	1.96	0.47
1:1:1806:G:H2'	1:1:1807:U:H5''	1.95	0.47
2:2:278:C:H2'	2:2:279:A:C8	2.50	0.47
2:2:567:C:OP1	13:AI:84:ARG:NH2	2.46	0.47
4:H:57:ARG:HH12	4:H:183:ILE:HD12	1.79	0.47
4:H:375:GLU:O	4:H:378:ILE:HG12	2.13	0.47
5:AA:168:ALA:HB1	5:AA:185:GLU:HA	1.96	0.47
10:AF:131:TRP:CE2	13:AI:97:PHE:HA	2.48	0.47
10:AF:136:ARG:HE	10:AF:220:ARG:HA	1.79	0.47
15:AK:101:LYS:HE3	15:AK:101:LYS:HB3	1.64	0.47
15:AK:103:ASP:HB3	15:AK:106:MET:HG3	1.96	0.47
23:AU:3:THR:OG1	23:AU:4:VAL:N	2.39	0.47
40:BU:84:ARG:HD2	40:BU:90:GLU:HG3	1.96	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
1:1:1067:C:H2'	1:1:1068:4AC:H6	1.97	0.47
1:1:1133:A:O2'	1:1:1134:G:H5'	2.14	0.47
1:1:2050:U:H2'	1:1:2051:C:C6	2.49	0.47
1:1:2109:A:H2'	1:1:2110:A:H8	1.78	0.47
1:1:2372:C:H4'	1:1:2373:G:OP2	2.15	0.47
2:2:37:C:H2'	2:2:38:A:C8	2.49	0.47
2:2:695:A:H2'	2:2:696:A:C8	2.49	0.47
8:AD:105:LEU:O	8:AD:109:VAL:HG12	2.15	0.47
13:AI:20:VAL:HG23	13:AI:22:LYS:HD3	1.96	0.47
35:BO:139:PRO:HG2	35:BO:144:ILE:HD11	1.96	0.47
1:1:102:C:OP2	1:1:102:C:H6	1.96	0.47
1:1:869:G:H2'	1:1:871:G:C8	2.49	0.47
1:1:2162:5MC:H2'	1:1:2163:5MC:H6	1.78	0.47
1:1:2416:G:H1'	66:BA:208:LYS:NZ	2.30	0.47
8:AD:150:ASP:N	8:AD:150:ASP:OD1	2.47	0.47
20:AQ:57:GLN:HG2	25:AW:37:VAL:HG22	1.97	0.47
2:2:745:G:H2'	2:2:746:C:O4'	2.15	0.47
2:2:908:C:H2'	2:2:909:A:H8	1.79	0.47
2:2:998:C:N4	2:2:999:G:O6	2.47	0.47
9:AE:132:MET:HE1	9:AE:152:LEU:HD23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AF:30:GLN:OE1	10:AF:30:GLN:N	2.47	0.47
17:AM:13:LYS:HG3	17:AM:75:GLY:O	2.15	0.47
20:AQ:106:ARG:NH2	20:AQ:126:GLU:OE2	2.47	0.47
27:AY:24:ARG:NH2	27:AY:25:CYS:SG	2.84	0.47
1:1:144:G:H2'	1:1:145:G:C8	2.50	0.47
1:1:197:G:OP1	40:BU:25:LYS:NZ	2.47	0.47
1:1:792:A:N1	1:1:1060:G:O2'	2.39	0.47
1:1:801:C:H2'	1:1:802:4AC:H6	1.97	0.47
1:1:814:A:H2'	1:1:815:A:C8	2.50	0.47
1:1:1084:A:H62	1:1:1198:A:H2	1.63	0.47
1:1:1481:G:N2	1:1:1484:A:OP2	2.40	0.47
1:1:1939:G:O2'	1:1:2919:G:H4'	2.14	0.47
1:1:2108:G:N1	1:1:2130:A:OP2	2.41	0.47
1:1:2593:A:H2	1:1:2662:A:H61	1.63	0.47
1:1:2635:G:O2'	1:1:2636:C:O5'	2.28	0.47
1:1:2693:C:H2'	1:1:2694:U:C6	2.50	0.47
1:1:2808:G:O2'	1:1:2811:C:OP2	2.32	0.47
2:2:270:U:OP2	14:AJ:56:ARG:NH2	2.42	0.47
2:2:541:G:O2'	2:2:788:G:H5'	2.14	0.47
2:2:630:A:H2'	2:2:631:G:C8	2.49	0.47
2:2:891:U:H2'	2:2:892:U:C6	2.49	0.47
2:2:1176:G:N2	19:AP:45:GLU:OE2	2.43	0.47
4:H:93:LEU:HD11	4:H:261:LEU:O	2.14	0.47
11:AG:6:LEU:HD12	11:AG:119:VAL:HB	1.97	0.47
12:AH:30:ASP:OD1	12:AH:32:SER:OG	2.28	0.47
12:AH:32:SER:HB2	12:AH:154:PRO:HB3	1.97	0.47
14:AJ:67:ASP:HB3	14:AJ:124:LEU:HD23	1.95	0.47
21:AR:39:VAL:HG13	21:AR:50:GLU:OE1	2.15	0.47
22:AS:5:ARG:HB2	22:AS:10:LYS:HD2	1.97	0.47
26:AX:18:THR:OG1	26:AX:19:GLY:N	2.46	0.47
31:AT:117:ALA:HB3	31:AT:120:ILE:HB	1.95	0.47
54:BF:32:LYS:NZ	54:BF:83:THR:O	2.45	0.47
56:BP:19:ARG:NH2	56:BP:38:GLU:OE1	2.40	0.47
1:1:705:A:H2'	1:1:706:G:H8	1.78	0.47
1:1:789:OMG:HM22	1:1:790:G:H5'	1.97	0.47
2:2:930:A:C5	31:AT:87:LYS:HD2	2.50	0.47
10:AF:20:THR:OG1	10:AF:46:GLU:OE1	2.24	0.47
14:AJ:41:ASP:OD1	14:AJ:61:ALA:N	2.40	0.47
16:AL:22:GLN:HA	16:AL:25:GLN:HG2	1.97	0.47
18:AN:75:VAL:HG21	18:AN:105:ILE:HG21	1.96	0.47
54:BF:125:LEU:HD12	54:BF:146:ALA:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:117:G:C5	1:1:118:U:C5	3.02	0.47
1:1:703:U:O4	30:B4:83:LYS:NZ	2.42	0.47
2:2:605:G:C2	2:2:606:G:C8	3.03	0.47
2:2:1378:C:H2'	2:2:1379:G:H8	1.78	0.47
4:H:271:GLU:O	4:H:273:ARG:NE	2.43	0.47
4:H:354:ILE:HG22	4:H:358:HIS:CE1	2.50	0.47
13:AI:28:LYS:HB3	13:AI:29:PRO:HD3	1.97	0.47
24:AV:95:LYS:NZ	24:AV:96:LYS:O	2.48	0.47
53:BD:146:ASP:O	53:BD:149:GLN:HG2	2.14	0.47
1:1:1706:G:H2'	1:1:1707:C:C6	2.50	0.47
1:1:2611:A:H2'	1:1:2612:A:C8	2.50	0.47
2:2:1344:G:OP2	15:AK:114:THR:HG21	2.14	0.47
5:AA:17:LYS:HA	5:AA:39:ASP:HA	1.96	0.47
5:AA:102:THR:HG21	5:AA:130:ILE:H	1.80	0.47
18:AN:139:LYS:HG2	18:AN:141:ARG:HH21	1.80	0.47
22:AS:30:HIS:O	22:AS:34:LYS:HG2	2.14	0.47
50:BQ:24:ILE:HG23	50:BQ:32:VAL:HG21	1.97	0.47
60:BN:99:MET:HG3	60:BN:101:THR:HG23	1.97	0.47
1:1:1146:C:H2'	1:1:1147:C:H6	1.78	0.46
1:1:2362:C:H5'	66:BA:161:LYS:NZ	2.30	0.46
1:1:2534:G:O3'	43:BE:106:SER:HA	2.15	0.46
2:2:135:U:H2'	2:2:136:C:C6	2.50	0.46
2:2:316:G:N1	8:AD:3:ASP:OD1	2.42	0.46
2:2:728:G:H2'	2:2:729:G:H8	1.80	0.46
2:2:893:G:H2'	2:2:894:G:C8	2.50	0.46
2:2:925:G:O2'	4:H:277:GLN:NE2	2.48	0.46
2:2:964:G:H22	2:2:1186:A:P	2.38	0.46
2:2:1022:G:H22	2:2:1177:OMU:HN3	1.62	0.46
24:AV:72:TYR:CD1	24:AV:78:MET:HG3	2.50	0.46
51:BV:3:ARG:CZ	51:BV:4:TRP:H	2.28	0.46
66:BA:6:PHE:HE2	66:BA:202:ILE:HG21	1.79	0.46
1:1:794:U:H2'	1:1:795:U:C6	2.50	0.46
1:1:1998:A:H2'	1:1:1999:C:H6	1.80	0.46
1:1:2332:U:N3	1:1:2456:C:OP2	2.48	0.46
2:2:711:A:OP1	20:AQ:3:ARG:NH1	2.40	0.46
2:2:1401:U:H2'	2:2:1402:A:H8	1.79	0.46
4:H:131:LYS:HD3	4:H:224:GLU:HA	1.97	0.46
53:BD:84:PRO:HB3	53:BD:92:THR:HG22	1.97	0.46
1:1:120:A:H5''	1:1:120:A:C8	2.49	0.46
1:1:429:A:H1'	1:1:431:G:N7	2.30	0.46
1:1:431:G:H2'	1:1:432:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1591:A:H2'	1:1:1593:C:C5	2.50	0.46
1:1:1698:A:H2'	1:1:1699:G:C8	2.50	0.46
1:1:2524:G:H2'	1:1:2525:G:H8	1.81	0.46
2:2:836:A:H5'	2:2:1043:U:C5	2.50	0.46
2:2:1434:U:H2'	2:2:1435:C:C6	2.51	0.46
4:H:165:PRO:HG3	4:H:254:ILE:HD11	1.97	0.46
12:AH:54:LYS:HD2	12:AH:55:HIS:O	2.15	0.46
37:B5:70:GLU:OE1	37:B5:70:GLU:N	2.46	0.46
60:BN:77:VAL:HG12	60:BN:81:ASN:HB2	1.96	0.46
66:BA:91:GLU:OE1	66:BA:123:TYR:OH	2.29	0.46
1:1:1111:G:O2'	1:1:1168:G:O6	2.31	0.46
1:1:1161:A:H2'	1:1:1164:C:C5	2.50	0.46
2:2:168:A:H2'	2:2:169:A:C8	2.51	0.46
2:2:1131:A:H5'	2:2:1132:C:C6	2.51	0.46
2:2:1375:G:O6	4:H:366:ARG:NH2	2.46	0.46
4:H:287:GLU:CD	4:H:287:GLU:H	2.23	0.46
1:1:992:C:H3'	1:1:993:U:H4'	1.98	0.46
2:2:384:U:O2'	9:AE:28:TRP:O	2.33	0.46
2:2:709:G:OP1	20:AQ:101:ARG:NH2	2.49	0.46
2:2:797:G:H5''	6:AB:24:LYS:O	2.16	0.46
2:2:1152:G:N2	2:2:1155:G:OP2	2.47	0.46
8:AD:98:GLU:O	8:AD:102:GLU:HG2	2.15	0.46
10:AF:28:GLU:HG3	10:AF:30:GLN:OE1	2.16	0.46
16:AL:14:ARG:O	16:AL:18:GLU:HG2	2.15	0.46
43:BE:118:ASP:N	43:BE:118:ASP:OD1	2.46	0.46
53:BD:61:ILE:H	53:BD:61:ILE:HG13	1.54	0.46
1:1:1734:G:H2'	1:1:1735:G:C8	2.49	0.46
2:2:1215:G:H2'	2:2:1216:G:H8	1.81	0.46
2:2:1236:C:H2'	2:2:1237:C:H6	1.80	0.46
2:2:1354:U:H2'	2:2:1355:C:C6	2.51	0.46
9:AE:126:ARG:H	9:AE:143:HIS:CD2	2.29	0.46
38:BL:134:GLU:O	38:BL:138:LYS:HG2	2.15	0.46
53:BD:33:ARG:NH1	53:BD:109:GLU:OE2	2.49	0.46
1:1:84:A:OP1	44:Ba:2:PRO:HD2	2.15	0.46
1:1:120:A:C8	1:1:120:A:C5'	2.98	0.46
1:1:394:G:H2'	1:1:395:A:C8	2.50	0.46
1:1:845:C:H2'	1:1:846:C:C6	2.51	0.46
1:1:2277:C:H2'	1:1:2278:A:C8	2.51	0.46
1:1:2337:C:H2'	1:1:2338:G:C8	2.51	0.46
2:2:615:G:H2'	2:2:616:G:H8	1.81	0.46
2:2:1375:G:H2'	2:2:1376:OMC:O4'	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1415:U:H2'	2:2:1416:C:H6	1.80	0.46
12:AH:187:GLU:OE2	12:AH:199:TYR:N	2.48	0.46
20:AQ:5:HIS:CG	20:AQ:124:LEU:HD22	2.51	0.46
24:AV:25:HIS:ND1	24:AV:25:HIS:O	2.49	0.46
40:BU:34:GLU:OE1	40:BU:34:GLU:N	2.40	0.46
1:1:492:C:H2'	1:1:493:G:O4'	2.15	0.46
1:1:617:G:N2	1:1:620:A:OP2	2.33	0.46
1:1:877:U:H2'	1:1:878:G:O4'	2.15	0.46
2:2:416:C:H5'	8:AD:119:ARG:HH21	1.81	0.46
2:2:917:G:C2	2:2:918:A:C8	3.03	0.46
2:2:1066:A:H4'	2:2:1067:A:O5'	2.16	0.46
2:2:1288:C:H2'	2:2:1289:U:C6	2.50	0.46
4:H:382:LYS:NZ	17:AM:52:ARG:HH11	2.14	0.46
20:AQ:68:ASP:HB3	20:AQ:71:ASN:O	2.16	0.46
32:AO:20:GLN:HE22	32:AO:22:ARG:HH21	1.62	0.46
35:BO:52:ASP:HB3	35:BO:55:GLY:O	2.16	0.46
40:BU:96:HIS:HD2	40:BU:98:SER:H	1.62	0.46
30:B4:108:ARG:HA	30:B4:108:ARG:NH1	2.31	0.46
66:BA:171:GLY:HA3	66:BA:175:MET:HE1	1.98	0.46
1:1:107:G:C2	1:1:113:G:C6	3.04	0.46
2:2:687:C:OP1	5:AA:99:ARG:HD3	2.16	0.46
2:2:1174:C:O2'	2:2:1179:U:O4	2.27	0.46
4:H:131:LYS:HD2	4:H:132:VAL:H	1.80	0.46
4:H:263:PRO:O	4:H:267:MET:HG3	2.16	0.46
36:BC:79:ARG:HH21	36:BC:167:GLN:HE22	1.62	0.46
1:1:1305:A:C6	1:1:1306:G:C6	3.03	0.46
1:1:1574:C:H2'	1:1:1575:A:H8	1.81	0.46
1:1:1806:G:O2'	1:1:1808:U:OP1	2.18	0.46
1:1:2407:U:H5	66:BA:98:ARG:HH22	1.64	0.46
2:2:41:G:H4'	18:AN:133:SER:HB2	1.98	0.46
2:2:569:G:OP2	9:AE:191:LYS:NZ	2.39	0.46
2:2:1150:A:H3'	2:2:1151:G:H8	1.80	0.46
8:AD:70:ARG:HD3	8:AD:89:LEU:HD22	1.98	0.46
10:AF:64:GLU:HG2	10:AF:173:LYS:HB3	1.98	0.46
15:AK:51:LEU:HD11	15:AK:102:TYR:CG	2.50	0.46
16:AL:64:TRP:HB3	19:AP:52:PHE:HB3	1.98	0.46
18:AN:129:VAL:O	18:AN:132:VAL:HG12	2.16	0.46
44:Ba:46:GLN:NE2	44:Ba:87:ARG:H	2.14	0.46
51:BV:24:ARG:HH11	51:BV:28:ARG:HH21	1.63	0.46
1:1:117:G:C6	1:1:118:U:C5	3.04	0.45
1:1:271:A:H2'	1:1:272:G:H4'	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2951:C:O2'	36:BC:361:GLN:O	2.24	0.45
2:2:424:C:H5'	2:2:425:U:H5	1.80	0.45
2:2:892:U:H2'	2:2:893:G:O4'	2.16	0.45
4:H:243:VAL:HA	4:H:254:ILE:HD13	1.98	0.45
24:AV:3:ILE:HD13	24:AV:23:ILE:HB	1.98	0.45
52:Bj:5:LYS:HG2	52:Bj:91:LEU:HB3	1.97	0.45
54:BF:110:ILE:HB	54:BF:120:ARG:HB2	1.98	0.45
1:1:1368:G:C5	1:1:1369:U:C5	3.03	0.45
1:1:2102:G:H2'	1:1:2103:U:O4'	2.16	0.45
1:1:2565:A:N6	35:BO:19:THR:O	2.47	0.45
2:2:1037:G:H2'	2:2:1038:U:C6	2.51	0.45
2:2:1262:A:H2'	2:2:1263:A:C8	2.52	0.45
2:2:1476:A:H2'	2:2:1477:G:C8	2.51	0.45
5:AA:121:MET:N	5:AA:121:MET:SD	2.89	0.45
8:AD:153:THR:OG1	8:AD:154:TYR:N	2.48	0.45
28:AZ:188:ARG:HG3	28:AZ:192:GLU:HG3	1.97	0.45
43:BE:10:GLU:OE1	43:BE:10:GLU:N	2.42	0.45
43:BE:27:LYS:HD3	43:BE:83:ARG:NH2	2.30	0.45
54:BF:10:GLU:HG2	54:BF:54:VAL:HG22	1.98	0.45
66:BA:105:LYS:HE2	66:BA:131:ARG:HH21	1.81	0.45
2:2:447:A:H5''	24:AV:85:TYR:CE2	2.51	0.45
4:H:386:GLU:CD	4:H:386:GLU:H	2.25	0.45
17:AM:13:LYS:HB3	17:AM:76:ILE:HD12	1.99	0.45
1:1:2128:U:H2'	1:1:2129:G:O4'	2.17	0.45
1:1:2268:C:H2'	1:1:2269:G:O4'	2.17	0.45
1:1:2645:U:H2'	1:1:2646:G:C8	2.51	0.45
2:2:157:A:H2'	2:2:158:A:O4'	2.15	0.45
7:AC:11:ILE:HG23	10:AF:39:ARG:HD3	1.99	0.45
14:AJ:81:ILE:HD11	14:AJ:102:GLU:HB2	1.99	0.45
24:AV:41:VAL:HG11	24:AV:48:PRO:HB3	1.98	0.45
26:AX:28:LYS:HA	26:AX:42:ARG:HA	1.99	0.45
43:BE:45:GLU:OE1	43:BE:58:ARG:NH1	2.49	0.45
66:BA:139:PRO:HG2	66:BA:142:MET:HB2	1.99	0.45
1:1:208:A:H2'	1:1:209:G:O4'	2.17	0.45
1:1:1170:A:H5''	3:3:102:G:O2'	2.16	0.45
1:1:1625:A:H2'	1:1:1626:C:C6	2.52	0.45
1:1:2081:G:OP1	33:BB:202:HIS:HE1	2.00	0.45
1:1:2645:U:H2'	1:1:2646:G:H8	1.81	0.45
4:H:30:ILE:HD12	4:H:52:GLN:HG3	1.98	0.45
22:AS:23:GLU:OE2	22:AS:34:LYS:HE2	2.16	0.45
27:AY:42:ARG:NH1	27:AY:43:CYS:SG	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BK:76:GLU:OE1	37:BK:76:GLU:N	2.49	0.45
66:BA:21:ARG:HH22	66:BA:209:THR:H	1.63	0.45
1:1:16:A:N1	1:1:2287:4AC:O2'	2.46	0.45
1:1:1019:C:H2'	1:1:1020:G:H8	1.81	0.45
1:1:1176:C:H2'	1:1:1177:G:C8	2.52	0.45
1:1:2423:C:H2'	1:1:2424:C:C6	2.51	0.45
2:2:196:G:H2'	2:2:196:G:N3	2.31	0.45
2:2:914:G:OP1	12:AH:89:GLU:HG2	2.16	0.45
10:AF:153:ARG:HB2	10:AF:188:LEU:HB2	1.98	0.45
31:AT:4:LYS:HD3	31:AT:5:GLU:H	1.82	0.45
37:B5:2:PRO:HD2	37:B5:5:ASP:HB3	1.98	0.45
60:BN:30:LYS:H	60:BN:59:GLN:NE2	2.15	0.45
30:B4:116:MET:N	30:B4:116:MET:SD	2.90	0.45
1:1:2419:C:H2'	1:1:2420:A:H8	1.82	0.45
2:2:1122:U:H2'	2:2:1123:C:O4'	2.17	0.45
20:AQ:68:ASP:OD2	20:AQ:71:ASN:N	2.33	0.45
28:AZ:196:ILE:H	28:AZ:196:ILE:HG13	1.60	0.45
34:BY:3:LYS:HD3	34:BY:3:LYS:HA	1.83	0.45
53:BD:61:ILE:HD11	53:BD:68:ALA:O	2.17	0.45
1:1:1253:G:H2'	1:1:1254:C:C6	2.52	0.45
1:1:2725:U:H2'	1:1:2726:G:O4'	2.17	0.45
2:2:236:G:H2'	2:2:237:A:H8	1.81	0.45
2:2:268:G:H2'	2:2:269:G:C8	2.51	0.45
5:AA:72:TYR:CE2	5:AA:82:LYS:HB2	2.52	0.45
22:AS:25:THR:HG22	22:AS:30:HIS:CD2	2.51	0.45
28:AZ:51:PRO:O	28:AZ:55:ILE:HG12	2.17	0.45
31:AT:48:LEU:HD13	31:AT:52:ARG:HE	1.82	0.45
35:BO:48:ILE:HG21	35:BO:99:ILE:HD13	1.98	0.45
36:BC:74:GLU:OE1	36:BC:310:TYR:OH	2.24	0.45
36:BC:194:ASN:O	36:BC:198:GLU:HG2	2.17	0.45
24:B6:17:LYS:HD3	24:B6:71:TYR:CD2	2.51	0.45
58:BS:20:ALA:HB1	58:BS:97:ASN:HD22	1.82	0.45
60:BN:127:LYS:H	60:BN:130:GLN:HE21	1.63	0.45
1:1:29:U:H2'	1:1:30:G:H8	1.82	0.45
1:1:961:U:H2'	1:1:962:C:C6	2.52	0.45
1:1:1019:C:H2'	1:1:1020:G:C8	2.52	0.45
1:1:1703:G:OP2	59:Bd:32:LYS:NZ	2.49	0.45
1:1:2044:C:H5'	33:BB:196:LYS:HE2	1.98	0.45
1:1:2523:C:H2'	1:1:2524:G:H8	1.82	0.45
2:2:172:C:H2'	2:2:173:C:H6	1.82	0.45
2:2:255:A:C2	2:2:291:A:C5	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:729:G:H2'	2:2:730:C:C6	2.52	0.45
16:AL:81:ALA:O	16:AL:84:GLN:NE2	2.50	0.45
1:1:447:A:N7	1:1:500:U:O2'	2.45	0.45
1:1:787:C:H2'	1:1:788:A:C8	2.52	0.45
2:2:289:A:H3'	2:2:290:G:H5'	1.99	0.45
4:H:214:MET:HE1	4:H:216:LYS:HG3	1.98	0.45
28:AZ:34:ASP:N	28:AZ:34:ASP:OD1	2.47	0.45
35:BO:36:VAL:HG22	35:BO:47:GLN:HB2	1.97	0.45
66:BA:175:MET:HE3	66:BA:180:ILE:HG12	1.99	0.45
1:1:1015:A:H5'	33:BB:176:GLY:HA2	1.99	0.44
1:1:1140:G:HO2'	1:1:1143:A:H62	1.61	0.44
1:1:1653:U:P	50:BQ:42:ARG:HH22	2.39	0.44
1:1:1806:G:H1'	1:1:1809:A:C8	2.52	0.44
1:1:2326:U:H2'	1:1:2327:G:H8	1.81	0.44
1:1:2551:A:H2'	1:1:2551:A:N3	2.32	0.44
1:1:2584:C:H2'	1:1:2585:4AC:O2	2.17	0.44
2:2:171:C:H2'	2:2:172:C:H6	1.82	0.44
2:2:322:A:H5''	14:AJ:21:ARG:HB3	1.99	0.44
2:2:703:4AC:O7	2:2:703:4AC:H5	2.17	0.44
2:2:1167:G:OP2	28:AZ:131:ARG:NH2	2.50	0.44
9:AE:191:LYS:HB3	9:AE:191:LYS:HE2	1.80	0.44
10:AF:57:VAL:HG22	10:AF:89:VAL:HB	1.98	0.44
20:AQ:36:LEU:HA	20:AQ:39:LYS:HZ2	1.81	0.44
50:BQ:105:GLU:OE2	50:BQ:139:TYR:OH	2.35	0.44
66:BA:50:LYS:HG2	66:BA:159:GLN:OE1	2.17	0.44
1:1:618:U:O2'	42:Be:17:HIS:HD2	1.99	0.44
1:1:762:G:H2'	1:1:763:C:C6	2.51	0.44
1:1:951:G:OP1	50:BQ:86:THR:HG23	2.17	0.44
1:1:2166:U:H2'	1:1:2167:U:C6	2.52	0.44
1:1:2498:A:N3	1:1:2498:A:H2'	2.32	0.44
1:1:2564:A:H5''	35:BO:22:ARG:NH2	2.31	0.44
2:2:223:G:H2'	2:2:224:G:H8	1.82	0.44
2:2:553:G:N1	2:2:721:C:OP2	2.48	0.44
2:2:1320:A:OP1	15:AK:127:ARG:NH1	2.47	0.44
3:3:98:G:H2'	3:3:99:G:H8	1.82	0.44
11:AG:64:ARG:HD2	11:AG:122:LYS:HD2	1.99	0.44
12:AH:18:MET:O	12:AH:20:ARG:NH1	2.50	0.44
23:AU:130:ASP:O	23:AU:134:THR:HG23	2.17	0.44
31:AT:47:LEU:HD13	31:AT:51:ILE:HD11	1.99	0.44
44:Ba:21:ILE:HG13	44:Ba:22:VAL:HG13	1.99	0.44
1:1:893:A:N1	1:1:2603:A:O2'	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:488:C:N4	18:AN:118:ASP:OD2	2.50	0.44
2:2:1388:C:H2'	2:2:1389:C:H6	1.82	0.44
3:3:28:C:H2'	3:3:29:A:O4'	2.16	0.44
3:3:93:G:H2'	3:3:94:A:C8	2.53	0.44
6:AB:104:PRO:HA	6:AB:109:PHE:CG	2.53	0.44
16:AL:21:ASN:O	16:AL:25:GLN:HG2	2.18	0.44
20:AQ:4:MET:HG2	20:AQ:5:HIS:CD2	2.53	0.44
28:AZ:173:LEU:HD23	28:AZ:173:LEU:HA	1.86	0.44
49:BR:46:GLU:OE1	49:BR:48:SER:OG	2.29	0.44
60:BN:4:ARG:NH2	60:BN:9:ASP:OD1	2.51	0.44
65:Bk:39:LYS:HE2	65:Bk:39:LYS:HB3	1.88	0.44
66:BA:6:PHE:CE2	66:BA:202:ILE:HG21	2.52	0.44
1:1:3:A:H5'	1:1:4:G:OP2	2.17	0.44
1:1:894:A:H2'	1:1:895:A:H8	1.81	0.44
1:1:1680:G:OP1	37:B5:42:LYS:NZ	2.33	0.44
1:1:1710:C:H2'	1:1:1711:G:C8	2.51	0.44
1:1:2810:G:H2'	1:1:2811:C:H6	1.82	0.44
2:2:145:G:H2'	2:2:146:A:H8	1.81	0.44
2:2:236:G:H2'	2:2:237:A:C8	2.52	0.44
2:2:1172:G:H2'	2:2:1173:U:C6	2.52	0.44
4:H:122:VAL:HG11	4:H:264:ILE:HD13	1.98	0.44
4:H:383:ARG:O	4:H:384:PHE:HB3	2.18	0.44
6:AB:158:ASN:OD1	6:AB:159:LYS:NZ	2.50	0.44
20:AQ:102:ALA:O	20:AQ:106:ARG:HG3	2.16	0.44
30:A3:12:PRO:HG2	30:A3:15:LEU:HD22	1.98	0.44
53:BD:14:ASP:OD1	53:BD:15:GLU:N	2.44	0.44
24:B6:47:ASN:H	24:B6:71:TYR:HE1	1.64	0.44
1:1:120:A:C5'	1:1:120:A:H8	2.31	0.44
1:1:192:C:OP1	46:BW:7:ARG:NH2	2.50	0.44
1:1:422:C:H2'	1:1:423:C:H6	1.81	0.44
1:1:1216:G:H21	1:1:2498:A:H62	1.63	0.44
2:2:668:A:O2'	4:H:170:GLU:OE2	2.30	0.44
2:2:866:G:H2'	2:2:867:C:C6	2.53	0.44
2:2:1184:4AC:O7	2:2:1184:4AC:H5	2.17	0.44
10:AF:24:MET:O	10:AF:28:GLU:HG2	2.17	0.44
11:AG:7:VAL:HG11	11:AG:120:ASN:HD22	1.82	0.44
12:AH:212:GLU:OE1	12:AH:215:ARG:NH2	2.50	0.44
13:AI:104:VAL:HG22	13:AI:125:LEU:HD23	2.00	0.44
28:AZ:40:LEU:HD23	28:AZ:40:LEU:H	1.82	0.44
1:1:197:G:P	40:BU:118:ARG:HH22	2.39	0.44
1:1:394:G:H2'	1:1:395:A:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:398:A:H3'	2:2:399:C:H6	1.82	0.44
2:2:1306:A:H2'	2:2:1307:A:C8	2.53	0.44
4:H:32:LYS:HB2	4:H:33:GLU:OE1	2.17	0.44
4:H:338:VAL:HG22	4:H:343:VAL:HG13	1.99	0.44
12:AH:25:ASP:OD1	12:AH:25:ASP:N	2.45	0.44
20:AQ:32:ASP:N	20:AQ:32:ASP:OD1	2.50	0.44
20:AQ:154:LYS:HB3	20:AQ:154:LYS:HE3	1.82	0.44
1:1:521:G:H4'	1:1:522:A:N7	2.32	0.44
1:1:1847:C:H2'	1:1:1848:U:C6	2.51	0.44
1:1:2577:A:N1	52:Bj:1:MET:HE1	2.33	0.44
2:2:1134:G:C2	2:2:1135:C:C6	3.06	0.44
5:AA:17:LYS:NZ	17:AM:37:GLU:HG2	2.33	0.44
15:AK:71:PHE:CE2	15:AK:72:MET:HG2	2.53	0.44
16:AL:45:ILE:HG12	19:AP:34:HIS:CD2	2.53	0.44
20:AQ:57:GLN:HE22	25:AW:38:ARG:HD3	1.81	0.44
22:AS:27:ASP:OD1	22:AS:30:HIS:N	2.35	0.44
37:B5:8:ARG:HB3	37:B5:24:ILE:HD12	1.99	0.44
37:B5:54:GLU:OE2	59:Bd:85:ARG:NE	2.47	0.44
43:BE:11:ILE:HG21	43:BE:173:VAL:HG11	1.98	0.44
50:BQ:15:LEU:HD13	50:BQ:52:LYS:HB2	1.99	0.44
53:BD:251:LYS:HE3	53:BD:251:LYS:HB2	1.81	0.44
1:1:51:A:H5''	1:1:52:G:OP2	2.18	0.44
1:1:68:U:H4'	1:1:69:U:O5'	2.18	0.44
1:1:94:G:H3'	1:1:95:G:C5'	2.47	0.44
1:1:371:G:O2'	65:Bk:23:CYS:SG	2.68	0.44
1:1:465:A:C4	1:1:467:G:C8	3.06	0.44
1:1:696:A:H2'	1:1:697:A:C8	2.53	0.44
1:1:2712:C:H2'	1:1:2713:G:O4'	2.17	0.44
2:2:683:C:H2'	2:2:684:C:H6	1.83	0.44
2:2:817:U:H2'	2:2:818:C:C6	2.53	0.44
2:2:1339:C:H2'	2:2:1340:G:C8	2.53	0.44
2:2:1388:C:H2'	2:2:1389:C:C6	2.53	0.44
4:H:168:ASP:OD1	4:H:172:LYS:N	2.50	0.44
5:AA:97:VAL:HG12	5:AA:125:ILE:HD11	2.00	0.44
5:AA:117:LYS:H	5:AA:117:LYS:HD2	1.82	0.44
5:AA:148:LYS:HE2	5:AA:148:LYS:HB3	1.68	0.44
10:AF:64:GLU:HB2	10:AF:177:LEU:HD11	2.00	0.44
11:AG:29:LEU:HD21	11:AG:43:LEU:HD11	2.00	0.44
11:AG:63:ILE:HA	11:AG:121:VAL:HG23	2.00	0.44
16:AL:12:ASN:OD1	16:AL:15:SER:N	2.48	0.44
35:BO:168:PHE:CG	35:BO:178:PRO:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B6:17:LYS:HD3	24:B6:71:TYR:HD2	1.83	0.44
58:BS:116:HIS:HB3	58:BS:149:VAL:HB	2.00	0.44
1:1:102:C:OP2	1:1:102:C:C6	2.71	0.44
1:1:144:G:H2'	1:1:145:G:H8	1.83	0.44
1:1:351:G:OP2	1:1:353:C:N4	2.43	0.44
1:1:787:C:H2'	1:1:788:A:H8	1.81	0.44
1:1:1259:A:N6	62:Bc:14:LYS:HB2	2.33	0.44
1:1:1809:A:C5	1:1:1810:G:H1'	2.53	0.44
2:2:879:A:H2'	2:2:880:A:H8	1.82	0.44
2:2:1052:C:H2'	2:2:1053:A:H8	1.83	0.44
2:2:1123:C:H2'	2:2:1124:U:C6	2.52	0.44
6:AB:57:LYS:HG2	6:AB:178:ASN:HD21	1.83	0.44
9:AE:9:HIS:HB3	9:AE:28:TRP:CZ3	2.53	0.44
28:AZ:54:VAL:HG21	28:AZ:82:VAL:HG11	2.00	0.44
55:BZ:90:GLU:H	55:BZ:90:GLU:HG3	1.71	0.44
1:1:163:A:H5''	1:1:165:G:O4'	2.17	0.43
1:1:1174:A:H2'	1:1:1175:C:H6	1.83	0.43
1:1:1487:U:H2'	1:1:1488:C:C6	2.53	0.43
1:1:2366:A:N1	1:1:2402:G:O2'	2.43	0.43
1:1:2537:C:OP2	1:1:2538:A:O2'	2.31	0.43
1:1:2577:A:H61	52:Bj:1:MET:HE1	1.83	0.43
2:2:609:A:C5	13:AI:107:SER:HA	2.53	0.43
2:2:626:4AC:O7	2:2:626:4AC:H5	2.17	0.43
2:2:661:A:OP1	4:H:383:ARG:HB2	2.18	0.43
2:2:1035:U:H2'	2:2:1036:C:H6	1.83	0.43
5:AA:35:LEU:HD11	17:AM:13:LYS:NZ	2.32	0.43
6:AB:86:VAL:HG23	6:AB:87:THR:HG23	1.99	0.43
43:BE:65:ASN:HB3	43:BE:68:PHE:HB2	1.99	0.43
30:BG:110:LEU:HD23	30:BG:110:LEU:HA	1.86	0.43
66:BA:23:LYS:HG2	66:BA:24:PRO:HD2	1.99	0.43
1:1:99:U:O4	1:1:120:A:N1	2.51	0.43
1:1:150:G:N3	1:1:604:G:O2'	2.51	0.43
1:1:189:G:H2'	1:1:189:G:N3	2.33	0.43
1:1:392:A:O2'	1:1:393:C:H5''	2.18	0.43
1:1:651:G:O6	58:BS:2:GLY:N	2.50	0.43
1:1:749:G:C2	1:1:750:G:C8	3.06	0.43
1:1:960:C:H2'	1:1:961:U:H6	1.83	0.43
1:1:1580:C:C5	1:1:1589:U:H5''	2.53	0.43
1:1:1697:G:H2'	1:1:1698:A:H8	1.83	0.43
1:1:2799:G:H2'	1:1:2800:G:C8	2.52	0.43
2:2:1215:G:H2'	2:2:1216:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1446:U:H2'	2:2:1447:C:C6	2.53	0.43
24:AV:78:MET:HE1	24:AV:92:ILE:HG21	2.00	0.43
27:AY:26:GLY:H	30:A3:45:ARG:NH1	2.16	0.43
31:AT:13:LEU:HA	31:AT:16:LEU:HD12	2.00	0.43
41:Bb:29:TRP:CD1	41:Bb:29:TRP:H	2.36	0.43
50:BQ:115:ILE:HB	50:BQ:119:THR:HG23	2.00	0.43
53:BD:142:LEU:HD23	53:BD:241:VAL:HG22	2.00	0.43
60:BN:24:ARG:HA	60:BN:24:ARG:HD3	1.76	0.43
66:BA:158:ILE:HG21	66:BA:168:ALA:HB2	2.00	0.43
1:1:40:U:H2'	1:1:41:G:O4'	2.19	0.43
1:1:946:G:H2'	1:1:947:C:C6	2.53	0.43
1:1:1250:A:H2'	1:1:1251:A:C8	2.53	0.43
1:1:1422:A:H2'	1:1:1423:C:C6	2.54	0.43
1:1:1617:4AC:H2'	1:1:1618:G:H8	1.83	0.43
1:1:2517:U:H4'	1:1:2518:A:O4'	2.18	0.43
2:2:658:G:C8	17:AM:24:ASN:ND2	2.86	0.43
2:2:711:A:H4'	2:2:823:G:O2'	2.19	0.43
2:2:868:4AC:N3	2:2:873:OMG:N1	2.53	0.43
2:2:1407:A:H2'	2:2:1408:G:O4'	2.18	0.43
4:H:231:VAL:HA	4:H:234:MET:HG2	2.00	0.43
49:BR:89:HIS:CD2	49:BR:91:VAL:H	2.33	0.43
57:BM:75:ARG:HE	57:BM:87:GLN:HE22	1.66	0.43
1:1:285:A:H2'	1:1:286:A:C8	2.53	0.43
1:1:1310:G:H5'	1:1:1311:G:N2	2.33	0.43
1:1:1362:G:O2'	1:1:1363:U:H5'	2.18	0.43
1:1:2477:G:H2'	1:1:2478:C:C6	2.53	0.43
2:2:456:C:H2'	2:2:457:G:C8	2.53	0.43
2:2:836:A:H2'	2:2:837:G:C8	2.54	0.43
2:2:854:C:O2'	2:2:855:U:H5'	2.18	0.43
9:AE:184:TYR:CE1	9:AE:238:PRO:HG3	2.53	0.43
43:BE:185:GLU:CD	43:BE:186:GLU:HG2	2.43	0.43
66:BA:41:ASP:OD1	66:BA:43:LYS:HG2	2.19	0.43
1:1:728:C:H5''	37:BK:46:ARG:NH2	2.34	0.43
1:1:1031:G:H1	33:BB:201:ASN:HD21	1.66	0.43
1:1:1368:G:C6	1:1:1369:U:C4	3.06	0.43
1:1:2281:G:OP1	48:BI:77:ARG:NH2	2.46	0.43
2:2:244:G:H2'	2:2:245:G:C8	2.50	0.43
2:2:293:C:H2'	2:2:294:G:H8	1.83	0.43
2:2:417:C:H2'	2:2:418:G:H8	1.82	0.43
2:2:613:C:H2'	2:2:614:G:H8	1.84	0.43
2:2:889:A:H2'	2:2:890:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:139:ARG:HA	5:AA:142:MET:SD	2.58	0.43
55:BZ:30:GLY:HA2	55:BZ:58:ILE:HD11	2.00	0.43
66:BA:161:LYS:HE3	66:BA:161:LYS:HB2	1.67	0.43
1:1:99:U:H3	1:1:120:A:H2	1.66	0.43
1:1:377:C:O2'	1:1:422:C:H5''	2.18	0.43
1:1:835:4AC:O2'	1:1:906:U:OP1	2.29	0.43
1:1:870:A:H62	56:BP:31:LYS:NZ	2.17	0.43
1:1:1413:C:H2'	1:1:1414:C:H6	1.83	0.43
1:1:1755:4AC:H2'	1:1:1756:G:H8	1.82	0.43
1:1:2247:C:H2'	1:1:2248:C:C6	2.54	0.43
2:2:119:C:H2'	2:2:120:G:H8	1.84	0.43
2:2:1110:G:H5''	15:AK:25:ARG:HH12	1.83	0.43
4:H:52:GLN:H	4:H:52:GLN:CD	2.26	0.43
4:H:53:ASP:O	4:H:57:ARG:HG2	2.19	0.43
4:H:338:VAL:HG13	4:H:343:VAL:HG22	2.00	0.43
23:AU:146:GLU:OE1	23:AU:146:GLU:N	2.49	0.43
1:1:114:G:N3	1:1:115:G:C8	2.86	0.43
1:1:204:A:H1'	39:Bf:30:LYS:HE2	2.00	0.43
1:1:872:C:H2'	1:1:873:C:C6	2.53	0.43
1:1:1084:A:N6	1:1:1198:A:H2	2.16	0.43
1:1:1166:C:H4'	35:BO:5:PRO:HB2	2.01	0.43
1:1:1434:G:H2'	1:1:1435:U:C6	2.54	0.43
1:1:1733:A:C2	1:1:1734:G:H1'	2.54	0.43
1:1:1953:A:H2'	1:1:1954:A:H8	1.84	0.43
1:1:2524:G:H2'	1:1:2525:G:C8	2.54	0.43
2:2:1042:G:N2	2:2:1045:A:OP2	2.41	0.43
2:2:1076:A:H61	28:AZ:155:GLY:HA3	1.83	0.43
24:AV:64:LYS:HE3	24:AV:64:LYS:HB3	1.89	0.43
40:BU:33:LYS:O	40:BU:37:GLU:HG2	2.18	0.43
30:B4:64:ALA:O	30:B4:67:PRO:HD2	2.19	0.43
66:BA:195:LEU:HD12	66:BA:198:GLY:H	1.83	0.43
1:1:117:G:N2	1:1:118:U:H1'	2.34	0.43
1:1:788:A:H2'	1:1:789:OMG:H8	1.83	0.43
1:1:796:C:H2'	1:1:797:G:H8	1.84	0.43
1:1:960:C:H2'	1:1:961:U:C6	2.54	0.43
1:1:1270:A:N1	1:1:1395:U:O2'	2.52	0.43
1:1:1847:C:OP1	1:1:1862:U:H5	2.00	0.43
1:1:1933:C:H5''	36:BC:246:GLY:HA3	1.99	0.43
1:1:2249:4AC:OP1	58:BS:70:GLN:NE2	2.52	0.43
2:2:148:A:OP2	2:2:166:C:N4	2.46	0.43
2:2:478:C:H2'	2:2:479:4AC:H6	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:739:A:N6	2:2:775:G:O6	2.52	0.43
2:2:949:A:N6	2:2:1198:U:O5'	2.51	0.43
4:H:197:GLU:HB3	4:H:198:LEU:H	1.62	0.43
11:AG:5:LYS:HG3	11:AG:20:GLU:HG3	2.00	0.43
12:AH:42:ARG:NH2	15:AK:102:TYR:O	2.51	0.43
31:AT:56:LYS:HG2	31:AT:58:LYS:HE3	2.01	0.43
58:BS:84:PRO:HB2	58:BS:87:VAL:HB	2.00	0.43
66:BA:80:LEU:HD21	66:BA:146:GLU:HG2	2.01	0.43
1:1:42:U:C4	51:BV:51:LYS:HB2	2.54	0.43
1:1:54:G:H1'	1:1:58:A:H61	1.84	0.43
1:1:1662:4AC:O7	1:1:1662:4AC:H5	2.18	0.43
1:1:1787:A:H1'	1:1:1828:C:H1'	2.01	0.43
1:1:1877:C:H2'	1:1:1878:4AC:H6	2.01	0.43
1:1:2725:U:H4'	60:BN:103:ARG:HG2	2.00	0.43
2:2:106:C:H2'	2:2:107:G:O4'	2.18	0.43
2:2:702:C:H2'	2:2:703:4AC:C6	2.48	0.43
2:2:703:4AC:H2'	2:2:704:G:C8	2.40	0.43
2:2:849:G:H2'	2:2:850:C:C6	2.54	0.43
2:2:1429:U:H2'	2:2:1430:C:C6	2.54	0.43
3:3:51:G:H5'	35:BO:171:TYR:HE1	1.84	0.43
4:H:228:ARG:HA	4:H:231:VAL:HG12	2.00	0.43
29:A0:3:ARG:HA	29:A0:3:ARG:HD2	1.94	0.43
31:AT:29:PRO:HG2	31:AT:32:GLN:OE1	2.18	0.43
36:BC:190:GLU:OE1	36:BC:190:GLU:N	2.40	0.43
30:B4:121:LEU:HD23	30:B4:122:MET:H	1.83	0.43
66:BA:32:GLU:HG2	66:BA:208:LYS:HG3	2.01	0.43
66:BA:59:ARG:HA	66:BA:171:GLY:HA2	2.01	0.43
1:1:197:G:OP2	40:BU:118:ARG:NH2	2.52	0.43
1:1:540:U:O2'	1:1:542:G:N7	2.43	0.43
1:1:843:A:H2'	1:1:844:A:C8	2.54	0.43
1:1:906:U:H2'	1:1:907:C:C6	2.54	0.43
1:1:1058:U:O2'	1:1:2300:A:N1	2.49	0.43
1:1:1364:C:H4'	1:1:1365:G:OP1	2.19	0.43
1:1:1618:G:H2'	1:1:1619:C:H6	1.84	0.43
1:1:2406:A:H3'	66:BA:98:ARG:NH2	2.34	0.43
1:1:2804:A:OP2	1:1:2804:A:H8	2.02	0.43
2:2:546:4AC:O7	2:2:546:4AC:H5	2.18	0.43
2:2:830:OMU:OP2	2:2:840:G:N1	2.40	0.43
2:2:1161:G:O5'	15:AK:118:LYS:HE3	2.19	0.43
2:2:1202:5MC:H2'	2:2:1203:G:C8	2.53	0.43
2:2:1493:C:H2'	2:2:1494:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:43:C:O2	43:BE:83:ARG:NH1	2.46	0.43
4:H:189:PRO:HB2	4:H:203:ILE:HG12	2.00	0.43
10:AF:39:ARG:NE	10:AF:123:GLU:OE2	2.48	0.43
20:AQ:41:ARG:CZ	20:AQ:82:LEU:HD13	2.49	0.43
24:AV:95:LYS:HE2	24:AV:95:LYS:HB2	1.89	0.43
50:BQ:60:ARG:HG2	50:BQ:63:ALA:HB3	1.99	0.43
54:BF:89:LYS:HG2	54:BF:176:GLU:HB3	2.00	0.43
66:BA:124:LEU:O	66:BA:128:LEU:HB2	2.18	0.43
1:1:102:C:N3	1:1:117:G:N1	2.37	0.42
1:1:431:G:H2'	1:1:432:A:H8	1.84	0.42
1:1:733:C:H2'	1:1:734:G:H8	1.84	0.42
1:1:1142:A:H4'	1:1:1143:A:C8	2.54	0.42
1:1:1667:4AC:H2'	1:1:1668:G:C8	2.54	0.42
1:1:1729:G:N1	1:1:1732:G:OP2	2.52	0.42
1:1:2871:A:H2'	1:1:2872:G:O4'	2.19	0.42
2:2:479:4AC:O7	2:2:479:4AC:H5	2.19	0.42
2:2:704:G:C2	2:2:705:G:C8	3.07	0.42
2:2:839:4AC:H2'	2:2:840:G:O4'	2.19	0.42
2:2:1455:G:H2'	2:2:1456:G:C8	2.54	0.42
4:H:131:LYS:NZ	4:H:133:GLU:HB2	2.34	0.42
5:AA:50:GLU:OE2	5:AA:66:LYS:HD2	2.19	0.42
5:AA:145:ILE:HD13	5:AA:170:GLU:HG3	2.01	0.42
6:AB:21:THR:OG1	6:AB:22:GLN:N	2.51	0.42
15:AK:44:THR:OG1	15:AK:75:ALA:HB1	2.19	0.42
24:AV:53:ILE:N	24:AV:90:ASP:OD2	2.44	0.42
60:BN:29:PRO:HA	60:BN:59:GLN:HE22	1.84	0.42
64:Bl:61:ARG:HB2	64:Bl:64:GLU:OE1	2.19	0.42
1:1:56:C:H5'	1:1:57:A:C4	2.54	0.42
1:1:2197:G:C8	1:1:2198:5MC:HM52	2.54	0.42
1:1:2427:G:H2'	1:1:2428:C:C6	2.54	0.42
1:1:2607:C:H2'	1:1:2608:4AC:O2	2.19	0.42
2:2:455:C:O2'	24:AV:29:PRO:HD3	2.19	0.42
2:2:470:G:H2'	2:2:471:OMG:C8	2.54	0.42
2:2:692:G:OP1	2:2:824:G:N2	2.46	0.42
2:2:1125:G:O4'	16:AL:39:PRO:HB2	2.19	0.42
2:2:1446:U:H2'	2:2:1447:C:H6	1.84	0.42
36:BC:153:LYS:HE2	36:BC:153:LYS:HB2	1.92	0.42
54:BF:55:ILE:HD11	54:BF:75:ILE:HD12	2.02	0.42
57:BM:152:LYS:HG3	65:Bk:12:ARG:HA	2.00	0.42
63:BJ:91:ARG:NE	63:BJ:125:GLU:OE2	2.52	0.42
1:1:676:C:H2'	1:1:677:G:O4'	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:788:A:H2'	1:1:789:OMG:C8	2.54	0.42
1:1:1303:A:N6	1:1:1367:G:H1'	2.34	0.42
1:1:1615:C:H2'	1:1:1616:C:H6	1.84	0.42
1:1:1769:A:N1	1:1:1831:G:O2'	2.43	0.42
5:AA:102:THR:HG23	5:AA:129:ARG:HA	2.01	0.42
10:AF:5:TRP:HB3	10:AF:55:PRO:HB2	2.01	0.42
10:AF:212:VAL:N	13:AI:70:ASN:HD21	2.07	0.42
11:AG:78:ILE:O	11:AG:110:ASN:N	2.52	0.42
20:AQ:142:LEU:HD13	20:AQ:143:PRO:HD2	2.01	0.42
52:Bj:45:LYS:HB3	52:Bj:45:LYS:HE2	1.85	0.42
53:BD:243:THR:HG23	53:BD:246:ALA:H	1.83	0.42
1:1:29:U:H2'	1:1:30:G:C8	2.54	0.42
1:1:133:G:H2'	1:1:134:C:H6	1.82	0.42
1:1:151:C:H2'	1:1:152:U:C6	2.54	0.42
1:1:2162:5MC:H2'	1:1:2163:5MC:C6	2.55	0.42
1:1:2336:A:H2'	1:1:2337:C:C6	2.55	0.42
1:1:2559:A:H2'	1:1:2560:G:H8	1.80	0.42
2:2:484:G:C8	2:2:496:G:H5'	2.53	0.42
2:2:644:C:H2'	2:2:645:C:H6	1.83	0.42
2:2:731:4AC:O7	2:2:731:4AC:H5	2.18	0.42
2:2:1149:G:H2'	2:2:1150:A:H8	1.84	0.42
15:AK:116:PRO:O	15:AK:118:LYS:NZ	2.44	0.42
16:AL:26:ILE:HD13	16:AL:84:GLN:HG2	2.01	0.42
27:AY:22:CYS:HB2	27:AY:25:CYS:HB2	2.01	0.42
36:BC:17:ARG:HB2	36:BC:233:ARG:NH2	2.34	0.42
66:BA:45:PRO:HA	66:BA:48:ARG:HD2	2.02	0.42
1:1:77:C:H4'	36:BC:311:GLY:HA2	2.01	0.42
1:1:103:C:C2	1:1:117:G:C2	3.08	0.42
1:1:279:A:H2'	1:1:280:G:C8	2.54	0.42
1:1:398:U:H2'	1:1:399:U:C6	2.55	0.42
1:1:529:G:OP2	57:BM:44:ARG:NH1	2.52	0.42
1:1:809:A:N7	1:1:903:G:O2'	2.40	0.42
1:1:1206:G:H2'	1:1:1207:G:H8	1.85	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:H8	1.82	0.42
2:2:1085:C:H2'	2:2:1086:C:H6	1.83	0.42
2:2:1266:C:H2'	2:2:1267:G:C8	2.50	0.42
2:2:1303:G:H5''	32:AO:32:GLY:N	2.33	0.42
3:3:5:C:O2'	3:3:27:A:N3	2.50	0.42
4:H:149:VAL:HG21	4:H:186:PHE:CZ	2.54	0.42
12:AH:32:SER:HA	26:AX:54:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AJ:65:VAL:HG22	14:AJ:124:LEU:HD22	2.01	0.42
16:AL:3:LYS:HG2	16:AL:101:ILE:HD11	2.00	0.42
17:AM:32:ASP:OD1	17:AM:34:THR:HG22	2.20	0.42
20:AQ:144:LYS:H	20:AQ:144:LYS:HD2	1.84	0.42
27:AY:23:PRO:HD2	27:AY:45:TYR:CZ	2.55	0.42
32:AO:20:GLN:NE2	32:AO:22:ARG:HE	2.17	0.42
36:BC:218:VAL:HG11	36:BC:324:VAL:HG13	2.01	0.42
43:BE:104:ALA:O	43:BE:168:LYS:NZ	2.52	0.42
44:Ba:82:ASP:OD1	44:Ba:82:ASP:N	2.52	0.42
46:BW:67:LYS:HB3	46:BW:67:LYS:HE3	1.82	0.42
66:BA:67:VAL:HG23	66:BA:82:LEU:HD22	2.01	0.42
66:BA:79:ARG:HH12	66:BA:144:ASN:HA	1.84	0.42
1:1:46:C:H2'	1:1:47:G:H8	1.85	0.42
1:1:1305:A:N6	1:1:2981:G:C6	2.87	0.42
1:1:2259:U:O2	41:Bb:30:ARG:NH2	2.51	0.42
2:2:1201:A:H4'	32:AO:139:GLN:HG2	2.00	0.42
4:H:19:ILE:HD13	4:H:47:LYS:NZ	2.35	0.42
9:AE:150:ILE:HD13	9:AE:158:TYR:CD1	2.54	0.42
14:AJ:3:ILE:H	14:AJ:3:ILE:HD12	1.84	0.42
16:AL:26:ILE:HG12	16:AL:29:ARG:NH2	2.35	0.42
20:AQ:109:LEU:HD13	20:AQ:119:MET:SD	2.59	0.42
21:AR:74:ASN:HD21	21:AR:80:ALA:H	1.67	0.42
25:AW:19:LYS:HE2	25:AW:19:LYS:HB2	1.91	0.42
28:AZ:161:LEU:HD13	28:AZ:187:ALA:HB1	2.01	0.42
31:AT:19:MET:HG3	31:AT:23:GLU:HG3	2.01	0.42
38:BL:47:TRP:CH2	38:BL:51:ILE:HD11	2.54	0.42
47:Bi:6:LYS:HD2	47:Bi:23:ARG:NH2	2.33	0.42
55:BZ:98:LYS:HG3	55:BZ:99:ARG:HD2	2.02	0.42
63:BJ:107:VAL:HG12	63:BJ:108:THR:O	2.20	0.42
66:BA:89:GLU:O	66:BA:93:ILE:HB	2.20	0.42
1:1:458:4AC:O7	1:1:458:4AC:H5	2.20	0.42
1:1:493:G:H5'	40:BU:1:MET:HG2	2.01	0.42
1:1:568:U:H2'	1:1:569:C:C6	2.55	0.42
1:1:1760:A:N1	1:1:1773:C:O2'	2.51	0.42
1:1:1809:A:H5'	50:BQ:43:ARG:HD3	2.01	0.42
1:1:2907:C:O2'	63:BJ:47:HIS:O	2.38	0.42
2:2:383:A:C6	2:2:384:U:C4	3.08	0.42
2:2:1098:C:H2'	2:2:1099:C:H6	1.84	0.42
3:3:45:A:C4	3:3:46:A:C8	3.08	0.42
5:AA:140:LYS:HA	5:AA:143:GLN:HE21	1.85	0.42
6:AB:196:GLU:H	6:AB:196:GLU:HG2	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AM:16:ILE:HD13	17:AM:80:HIS:HB2	2.01	0.42
42:Be:55:TRP:CD1	42:Be:55:TRP:H	2.38	0.42
64:Bl:75:LEU:HD12	64:Bl:76:GLU:HG2	2.01	0.42
30:B4:73:LYS:C	30:B4:74:GLU:HG3	2.44	0.42
1:1:1174:A:H2'	1:1:1175:C:C6	2.55	0.42
1:1:1953:A:H2'	1:1:1954:A:C8	2.55	0.42
1:1:2374:A:H2'	1:1:2398:A:C8	2.55	0.42
2:2:636:4AC:O7	2:2:636:4AC:H5	2.19	0.42
2:2:657:OMG:HM22	2:2:658:G:O4'	2.19	0.42
2:2:1235:A:H4'	23:AU:72:ARG:HH12	1.84	0.42
2:2:1329:G:H2'	2:2:1330:C:H6	1.85	0.42
2:2:1417:U:H2'	2:2:1418:C:C6	2.55	0.42
4:H:53:ASP:O	4:H:56:ILE:HG22	2.20	0.42
4:H:87:HIS:O	4:H:91:LEU:HG	2.19	0.42
4:H:374:LEU:HD23	4:H:374:LEU:HA	1.94	0.42
6:AB:28:MET:HE3	6:AB:31:PHE:HD2	1.85	0.42
8:AD:32:LYS:HD2	8:AD:33:TYR:CE2	2.55	0.42
12:AH:141:PHE:CE2	26:AX:65:ARG:HD3	2.55	0.42
14:AJ:39:GLU:OE1	14:AJ:39:GLU:N	2.46	0.42
16:AL:34:MET:HE3	16:AL:34:MET:HB3	1.94	0.42
18:AN:98:ASP:HB3	18:AN:101:ASP:OD1	2.19	0.42
25:AW:36:ARG:HA	25:AW:49:PRO:HD3	2.02	0.42
25:AW:46:LEU:C	25:AW:57:ARG:HH21	2.27	0.42
33:BB:130:LEU:HD12	33:BB:130:LEU:HA	1.90	0.42
30:B4:66:LEU:HB3	30:B4:67:PRO:HD3	2.01	0.42
1:1:60:4AC:O7	1:1:60:4AC:H5	2.19	0.42
1:1:683:A:O2'	1:1:769:C:H5''	2.20	0.42
1:1:2719:G:H2'	1:1:2720:A:C8	2.54	0.42
1:1:2834:A:O2'	60:BN:107:ARG:NH2	2.53	0.42
2:2:465:G:H2'	2:2:466:G:C8	2.55	0.42
2:2:670:A:H4'	2:2:671:A:H5'	2.02	0.42
2:2:783:A:OP1	2:2:1495:G:O2'	2.31	0.42
2:2:795:A:H2'	2:2:796:G:O4'	2.20	0.42
2:2:1345:G:O3'	15:AK:70:GLY:HA3	2.19	0.42
2:2:1349:A:H2'	2:2:1350:U:O4'	2.20	0.42
5:AA:38:ALA:HB3	5:AA:44:VAL:HG22	2.02	0.42
5:AA:148:LYS:HE3	5:AA:149:LYS:HE2	2.01	0.42
5:AA:157:ASP:O	5:AA:160:LEU:HG	2.20	0.42
10:AF:136:ARG:HG2	10:AF:220:ARG:O	2.19	0.42
12:AH:44:LEU:HD11	15:AK:40:ILE:HG13	2.01	0.42
19:AP:13:LYS:HD2	19:AP:13:LYS:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AV:8:VAL:HG22	24:AV:19:ILE:HG22	2.02	0.42
30:A3:6:TYR:O	30:A3:8:LYS:NZ	2.51	0.42
48:BI:106:GLU:OE1	48:BI:106:GLU:N	2.45	0.42
60:BN:31:ILE:HB	60:BN:63:GLU:HG2	2.01	0.42
66:BA:128:LEU:HD22	66:BA:133:LYS:HB2	2.02	0.42
1:1:864:G:H2'	1:1:865:C:O4'	2.19	0.42
1:1:1709:U:H2'	1:1:1710:C:C6	2.55	0.42
1:1:2886:U:OP2	1:1:2887:A:O2'	2.38	0.42
2:2:259:A:P	14:AJ:10:ARG:HH22	2.40	0.42
2:2:547:G:P	20:AQ:131:ARG:HH21	2.43	0.42
2:2:674:C:H2'	2:2:675:C:H6	1.84	0.42
2:2:807:A:N3	6:AB:37:GLN:NE2	2.67	0.42
2:2:1350:U:H2'	2:2:1351:A:C8	2.53	0.42
4:H:148:THR:OG1	4:H:151:LYS:HD2	2.19	0.42
6:AB:51:ARG:HA	6:AB:51:ARG:HD3	1.83	0.42
28:AZ:70:GLU:CD	28:AZ:78:PRO:HD3	2.45	0.42
32:AO:46:ASP:O	32:AO:49:MET:HG3	2.20	0.42
58:BS:29:PRO:HG3	58:BS:144:THR:HG22	2.01	0.42
60:BN:97:ASN:HD22	60:BN:98:PRO:CD	2.31	0.42
1:1:54:G:N2	1:1:55:U:O2'	2.52	0.41
1:1:1115:A:H2'	1:1:1116:G:C8	2.55	0.41
1:1:1171:C:H2'	1:1:1172:C:C6	2.55	0.41
1:1:1932:C:H2'	1:1:1933:C:H6	1.85	0.41
1:1:2593:A:H4'	38:BL:51:ILE:HG22	2.02	0.41
2:2:389:G:N2	2:2:392:A:OP2	2.47	0.41
4:H:177:VAL:HG11	4:H:210:LEU:HD22	2.01	0.41
9:AE:219:GLU:HB2	9:AE:221:GLU:OE1	2.20	0.41
20:AQ:76:LEU:HD12	20:AQ:81:ILE:HD11	2.02	0.41
27:AY:31:MET:HE2	27:AY:39:ALA:HB3	2.01	0.41
35:BO:147:GLU:O	35:BO:151:GLU:HG2	2.20	0.41
54:BF:158:THR:HG21	54:BF:171:GLY:CA	2.50	0.41
24:B6:25:HIS:HB2	24:B6:28:GLU:HB2	2.01	0.41
56:BP:73:LYS:HE3	56:BP:73:LYS:HB2	1.92	0.41
1:1:659:A:H5''	1:1:660:G:H3'	2.02	0.41
1:1:868:C:H5''	1:1:869:G:C2	2.55	0.41
1:1:1529:A:N3	1:1:2244:G:O2'	2.47	0.41
1:1:1697:G:H2'	1:1:1698:A:C8	2.55	0.41
1:1:1878:4AC:O7	1:1:1878:4AC:H5	2.19	0.41
1:1:2042:A:H1'	1:1:2179:A:N6	2.34	0.41
1:1:2686:G:C4	1:1:2687:A:C8	3.07	0.41
2:2:109:C:H2'	2:2:110:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:286:4AC:O7	2:2:286:4AC:H5	2.20	0.41
2:2:417:C:H2'	2:2:418:G:C8	2.55	0.41
2:2:888:G:H2'	2:2:889:A:C8	2.55	0.41
4:H:206:PHE:HD1	4:H:206:PHE:HA	1.78	0.41
5:AA:145:ILE:O	5:AA:149:LYS:HG2	2.20	0.41
12:AH:44:LEU:HD12	12:AH:45:PRO:HD2	2.02	0.41
31:AT:103:LEU:HD12	31:AT:103:LEU:HA	1.88	0.41
52:Bj:48:GLY:HA2	57:BM:83:SER:HA	2.02	0.41
60:BN:104:LYS:HG3	60:BN:107:ARG:HG3	2.01	0.41
61:Bg:3:ARG:NH1	61:Bg:45:GLU:OE2	2.50	0.41
65:Bk:31:LYS:HE3	65:Bk:31:LYS:HB3	1.93	0.41
66:BA:35:VAL:HG13	66:BA:166:VAL:HB	2.02	0.41
1:1:68:U:O2'	51:BV:51:LYS:NZ	2.53	0.41
1:1:802:4AC:O7	1:1:802:4AC:H5	2.21	0.41
1:1:953:G:N2	1:1:975:G:O2'	2.48	0.41
1:1:1093:C:H2'	1:1:1094:C:H6	1.85	0.41
1:1:2382:C:H2'	1:1:2383:C:C1'	2.50	0.41
2:2:290:G:H8	2:2:290:G:OP2	2.02	0.41
2:2:373:A2M:O5'	2:2:373:A2M:H8	2.19	0.41
2:2:1131:A:C2	2:2:1155:G:C4	3.09	0.41
9:AE:37:HIS:HB2	9:AE:42:SER:HB3	2.03	0.41
10:AF:60:ARG:HD3	10:AF:60:ARG:HA	1.88	0.41
12:AH:24:GLU:OE1	12:AH:24:GLU:N	2.49	0.41
24:B6:74:ASP:OD1	24:B6:77:ARG:HB2	2.21	0.41
66:BA:5:PRO:HB2	66:BA:6:PHE:H	1.56	0.41
66:BA:132:ASN:O	66:BA:133:LYS:HD2	2.20	0.41
1:1:869:G:H4'	1:1:870:A:OP1	2.20	0.41
1:1:1453:G:OP1	56:BP:2:LYS:NZ	2.44	0.41
1:1:1460:4AC:H5	1:1:1460:4AC:O7	2.20	0.41
1:1:2265:U:H2'	1:1:2266:G:C8	2.55	0.41
2:2:268:G:OP2	14:Aj:113:ARG:NH1	2.39	0.41
2:2:269:G:H5'	14:Aj:32:PRO:HA	2.02	0.41
2:2:270:U:P	14:Aj:56:ARG:HH22	2.44	0.41
2:2:718:4AC:H2'	2:2:719:G:O4'	2.21	0.41
2:2:828:4AC:O7	2:2:828:4AC:H5	2.21	0.41
2:2:1222:A:P	23:AU:60:ARG:HH12	2.40	0.41
2:2:1376:OMC:H2'	2:2:1377:C:O4'	2.20	0.41
2:2:1487:MA6:H93	2:2:1488:MA6:H92	2.03	0.41
4:H:63:ASP:HB3	4:H:66:LYS:HE2	2.02	0.41
4:H:147:ASP:O	4:H:210:LEU:N	2.43	0.41
6:AB:5:TYR:CZ	6:AB:9:LEU:HD21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AL:2:GLN:OE1	16:AL:3:LYS:NZ	2.45	0.41
16:AL:76:GLU:OE1	16:AL:76:GLU:N	2.52	0.41
17:AM:12:GLU:H	17:AM:12:GLU:CD	2.27	0.41
18:AN:103:VAL:HG23	18:AN:126:VAL:HG13	2.01	0.41
24:AV:47:ASN:HB3	24:AV:71:TYR:HE1	1.86	0.41
28:AZ:56:GLY:HA3	28:AZ:61:ARG:HB3	2.03	0.41
30:A3:13:LYS:O	30:A3:17:GLU:HG2	2.21	0.41
30:A3:109:ASP:O	30:A3:112:GLU:HG3	2.20	0.41
33:BB:89:ALA:HB3	33:BB:97:LEU:HG	2.02	0.41
33:BB:103:PRO:HA	33:BB:134:ARG:NH1	2.35	0.41
36:BC:150:ASP:O	36:BC:154:GLU:HG2	2.21	0.41
38:BL:3:ARG:NH2	53:BD:103:GLU:OE2	2.50	0.41
43:BE:12:LEU:O	43:BE:16:GLU:HG2	2.21	0.41
43:BE:48:LEU:HD23	43:BE:78:VAL:HG12	2.02	0.41
24:B6:3:ILE:HB	24:B6:43:MET:HE1	2.02	0.41
57:BM:41:ARG:HD3	57:BM:42:PRO:HD2	2.02	0.41
1:1:161:4AC:O7	1:1:161:4AC:H5	2.21	0.41
1:1:796:C:H2'	1:1:797:G:C8	2.54	0.41
1:1:1348:G:N1	1:1:1349:U:O4	2.53	0.41
1:1:1406:G:OP2	34:BY:127:ARG:NH1	2.50	0.41
1:1:1867:4AC:O7	1:1:1867:4AC:H5	2.21	0.41
1:1:2287:4AC:O7	1:1:2287:4AC:H5	2.20	0.41
1:1:2706:C:N4	61:Bg:47:ARG:O	2.53	0.41
1:1:2724:U:H2'	1:1:2725:U:O4'	2.21	0.41
2:2:313:G:H2'	2:2:314:G:O4'	2.20	0.41
2:2:518:U:H2'	2:2:519:OMG:H8	1.86	0.41
2:2:580:A:H2'	2:2:581:C:C6	2.56	0.41
2:2:1022:G:O2'	28:AZ:166:TYR:OH	2.28	0.41
10:AF:216:GLU:OE1	10:AF:216:GLU:N	2.49	0.41
17:AM:52:ARG:HG2	17:AM:53:ASP:N	2.35	0.41
20:AQ:32:ASP:O	20:AQ:36:LEU:HG	2.20	0.41
27:AY:40:CYS:HB3	27:AY:44:GLY:N	2.29	0.41
36:BC:57:GLU:HG3	36:BC:58:PRO:HD2	2.02	0.41
43:BE:30:ILE:HD11	43:BE:52:THR:HG21	2.02	0.41
48:BI:49:TYR:HB3	48:BI:138:LEU:HD11	2.02	0.41
66:BA:25:ARG:CZ	66:BA:211:MET:HB3	2.51	0.41
1:1:113:G:H8	1:1:113:G:O5'	2.03	0.41
1:1:213:U:O4	40:BU:47:ARG:NH2	2.53	0.41
1:1:569:C:O2'	1:1:2119:A:N6	2.53	0.41
1:1:866:C:N3	1:1:869:G:N1	2.69	0.41
1:1:1173:C:H2'	1:1:1174:A:C8	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1303:A:O2'	1:1:1304:C:O5'	2.35	0.41
1:1:2425:U:H2'	1:1:2426:C:C2	2.56	0.41
1:1:2881:G:H2'	1:1:2882:C:C6	2.56	0.41
2:2:422:C:N4	2:2:424:C:H1'	2.35	0.41
2:2:816:C:H2'	2:2:817:U:C6	2.55	0.41
2:2:1085:C:H2'	2:2:1086:C:C6	2.56	0.41
3:3:71:U:H2'	3:3:72:C:C6	2.55	0.41
4:H:306:ASP:N	4:H:306:ASP:OD1	2.53	0.41
16:AL:38:ILE:HA	16:AL:38:ILE:HD13	1.69	0.41
20:AQ:41:ARG:NH2	20:AQ:89:PRO:HD3	2.35	0.41
31:AT:112:ARG:HH12	31:AT:114:GLN:NE2	2.17	0.41
66:BA:120:ILE:HG23	66:BA:124:LEU:HD12	2.02	0.41
1:1:15:G:H2'	1:1:16:A:H5''	2.02	0.41
1:1:939:G:H2'	1:1:940:C:C6	2.55	0.41
1:1:1065:4AC:O7	1:1:1065:4AC:H5	2.21	0.41
1:1:1379:C:H2'	1:1:1380:G:O4'	2.21	0.41
1:1:1431:U:O2	56:BP:7:THR:HG23	2.19	0.41
1:1:1462:G:O2'	53:BD:235:HIS:HD2	2.02	0.41
1:1:1551:G:H5'	50:BQ:24:ILE:O	2.21	0.41
1:1:1594:4AC:O7	1:1:1594:4AC:H5	2.21	0.41
1:1:2047:A:N6	1:1:2084:G:O2'	2.47	0.41
1:1:2058:A:H2'	1:1:2059:G:C8	2.55	0.41
1:1:2362:C:H5'	66:BA:161:LYS:HZ3	1.86	0.41
1:1:2531:G:H2'	1:1:2532:C:C6	2.56	0.41
2:2:318:C:H2'	2:2:319:4AC:H6	2.01	0.41
2:2:319:4AC:O7	2:2:319:4AC:H5	2.20	0.41
2:2:1052:C:H2'	2:2:1053:A:C8	2.56	0.41
2:2:1233:4AC:O7	2:2:1233:4AC:H5	2.19	0.41
4:H:173:LEU:HD13	4:H:251:VAL:HG11	2.02	0.41
6:AB:119:ASP:HB3	6:AB:122:ALA:HB3	2.02	0.41
12:AH:199:TYR:OH	12:AH:203:LYS:HD2	2.21	0.41
17:AM:126:THR:OG1	17:AM:127:ARG:N	2.54	0.41
36:BC:25:PRO:HB2	36:BC:219:ILE:HG22	2.03	0.41
42:Be:56:LYS:HB3	42:Be:62:HIS:HB3	2.02	0.41
43:BE:108:ASP:OD2	43:BE:112:ASN:HB2	2.21	0.41
48:BI:51:GLN:HE21	48:BI:51:GLN:HB3	1.69	0.41
66:BA:40:ILE:HB	66:BA:201:GLN:HE22	1.85	0.41
1:1:1:C:H2'	1:1:2:G:O4'	2.21	0.41
1:1:279:A:H1'	57:BM:110:ASN:ND2	2.35	0.41
1:1:715:A:H2'	1:1:716:A:C8	2.55	0.41
1:1:1731:U:H4'	1:1:1732:G:O5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1934:4AC:H5	1:1:1934:4AC:O7	2.21	0.41
1:1:2664:A:O2'	1:1:2665:A:H2'	2.20	0.41
2:2:27:U:H2'	2:2:28:G:O4'	2.21	0.41
2:2:957:4AC:O7	2:2:957:4AC:H5	2.21	0.41
2:2:1153:A:H2'	2:2:1154:A:O4'	2.21	0.41
2:2:1237:C:H2'	2:2:1238:C:H6	1.85	0.41
4:H:56:ILE:HA	4:H:59:HIS:HE1	1.85	0.41
4:H:131:LYS:HE3	4:H:131:LYS:HB3	1.78	0.41
4:H:222:MET:SD	4:H:223:PRO:HD2	2.61	0.41
5:AA:22:ILE:HD11	5:AA:36:THR:HG22	2.02	0.41
16:AL:17:GLU:O	16:AL:21:ASN:HB2	2.20	0.41
22:AS:60:MET:HB3	22:AS:65:LYS:HG3	2.03	0.41
23:AU:3:THR:HG1	23:AU:63:TYR:HH	1.66	0.41
26:AX:13:GLU:OE1	26:AX:28:LYS:HB2	2.20	0.41
28:AZ:15:MET:HE3	28:AZ:15:MET:HB3	1.96	0.41
29:A0:32:LYS:HB2	29:A0:32:LYS:HE2	1.77	0.41
37:B5:50:ILE:HD13	37:B5:50:ILE:HA	1.81	0.41
57:BM:73:ARG:HD2	57:BM:90:TYR:CD1	2.55	0.41
66:BA:40:ILE:HD11	66:BA:47:ASN:HB3	2.01	0.41
66:BA:79:ARG:HE	66:BA:80:LEU:HG	1.85	0.41
1:1:85:A:OP1	44:Ba:44:LYS:NZ	2.45	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
1:1:127:U:H6	1:1:127:U:H5''	1.86	0.41
1:1:147:U:OP2	53:BD:186:MET:HG2	2.20	0.41
1:1:422:C:H2'	1:1:423:C:C6	2.56	0.41
1:1:439:C:H2'	1:1:440:G:H5'	2.02	0.41
1:1:450:C:H2'	1:1:451:4AC:H6	2.02	0.41
1:1:530:U:H2'	1:1:531:A:H8	1.86	0.41
1:1:652:U:H2'	1:1:653:G:O4'	2.21	0.41
1:1:1030:U:OP2	33:BB:9:ARG:HD2	2.20	0.41
1:1:1369:U:N3	1:1:1370:C:C5	2.89	0.41
1:1:1648:C:H2'	1:1:1649:G:H8	1.86	0.41
1:1:2058:A:H2'	1:1:2059:G:H8	1.86	0.41
1:1:2144:OMG:HM22	1:1:2145:G:H5'	2.02	0.41
1:1:2302:A:H2'	1:1:2303:C:H5'	2.03	0.41
1:1:2433:U:H2'	1:1:2434:G:H8	1.85	0.41
1:1:2536:U:C2	43:BE:136:GLY:HA3	2.56	0.41
1:1:2705:C:O2	1:1:2705:C:H2'	2.20	0.41
1:1:2782:G:H2'	1:1:2783:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2992:4AC:CM7	1:1:2992:4AC:H5	2.50	0.41
2:2:17:4AC:O7	2:2:17:4AC:H5	2.21	0.41
2:2:89:G:H2'	2:2:90:G:H8	1.86	0.41
2:2:303:4AC:O7	2:2:303:4AC:H5	2.21	0.41
2:2:387:G:H2'	2:2:388:G:C8	2.56	0.41
2:2:518:U:H2'	2:2:519:OMG:C8	2.56	0.41
2:2:644:C:H2'	2:2:645:C:C6	2.56	0.41
2:2:751:4AC:O7	2:2:751:4AC:H5	2.21	0.41
2:2:1028:4AC:O7	2:2:1028:4AC:H5	2.20	0.41
2:2:1365:U:H2'	2:2:1366:G:H8	1.82	0.41
2:2:1445:C:H2'	2:2:1446:U:O4'	2.21	0.41
3:3:98:G:H5''	64:BI:51:LYS:HE3	2.03	0.41
5:AA:39:ASP:OD1	5:AA:39:ASP:N	2.54	0.41
12:AH:172:LYS:HB3	12:AH:183:ALA:HB1	2.03	0.41
28:AZ:42:THR:HG22	28:AZ:76:GLU:O	2.21	0.41
34:BY:33:HIS:CE1	34:BY:118:ARG:HG2	2.56	0.41
55:BZ:55:LEU:HD23	55:BZ:55:LEU:HA	1.89	0.41
56:BP:3:ARG:NH2	56:BP:38:GLU:O	2.54	0.41
30:B4:33:ARG:HG2	30:B4:102:ILE:HD13	2.02	0.41
30:B4:34:LYS:HE3	30:B4:34:LYS:HB2	1.87	0.41
1:1:198:A:C2	1:1:216:A:C5	3.08	0.41
1:1:829:4AC:OP2	53:BD:111:ARG:NH2	2.53	0.41
1:1:979:C:H2'	1:1:980:C:H6	1.85	0.41
1:1:2136:4AC:H5	1:1:2136:4AC:O7	2.21	0.41
1:1:2380:G:C6	1:1:2392:G:C6	3.09	0.41
1:1:2535:G:H5'	1:1:2536:U:OP2	2.21	0.41
1:1:2960:4AC:O7	1:1:2960:4AC:H5	2.21	0.41
2:2:416:C:H2'	2:2:417:C:C6	2.55	0.41
2:2:1147:4AC:O7	2:2:1147:4AC:H5	2.21	0.41
3:3:74:C:N3	3:3:109:G:N1	2.44	0.41
6:AB:76:GLY:C	6:AB:79:PRO:HD2	2.46	0.41
9:AE:67:ASN:HA	9:AE:79:LYS:HG3	2.03	0.41
16:AL:40:LEU:HB2	16:AL:70:LYS:HB2	2.03	0.41
26:AX:11:VAL:HG12	26:AX:29:VAL:HG23	2.01	0.41
26:AX:65:ARG:H	26:AX:65:ARG:HD2	1.86	0.41
28:AZ:85:ILE:HD13	28:AZ:94:VAL:HG11	2.02	0.41
31:AT:96:PRO:O	31:AT:99:ILE:HG12	2.20	0.41
43:BE:109:GLU:OE1	43:BE:109:GLU:N	2.54	0.41
54:BF:45:LYS:HE2	54:BF:45:LYS:HB3	1.98	0.41
66:BA:206:TYR:CE1	66:BA:216:LYS:HD3	2.54	0.41
1:1:91:4AC:O7	1:1:91:4AC:H5	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:285:A:H5''	42:Be:55:TRP:HZ3	1.86	0.40
1:1:1207:G:OP1	60:BN:15:PRO:HG3	2.21	0.40
1:1:1618:G:H2'	1:1:1619:C:C6	2.56	0.40
1:1:1765:4AC:O7	1:1:1765:4AC:H5	2.21	0.40
1:1:2165:C:H2'	1:1:2166:U:C6	2.56	0.40
1:1:2406:A:H2'	1:1:2407:U:C6	2.56	0.40
1:1:2908:4AC:O7	1:1:2908:4AC:H5	2.21	0.40
1:1:2981:G:H5''	1:1:2982:C:H5	1.85	0.40
2:2:24:U:H2'	2:2:25:C:H6	1.85	0.40
2:2:233:G:H2'	2:2:234:A:C8	2.56	0.40
2:2:356:G:O5'	11:AG:83:ARG:NH2	2.53	0.40
2:2:1461:A:C8	4:H:326:ARG:HG3	2.56	0.40
3:3:32:4AC:H5	3:3:32:4AC:O7	2.20	0.40
4:H:51:THR:O	4:H:55:ILE:HD12	2.20	0.40
4:H:239:ILE:HG13	4:H:241:GLY:H	1.86	0.40
4:H:330:LEU:HB2	4:H:351:TRP:CZ3	2.56	0.40
5:AA:71:VAL:HA	5:AA:81:THR:HA	2.03	0.40
9:AE:126:ARG:HB3	9:AE:143:HIS:HB3	2.03	0.40
11:AG:17:LYS:HD3	11:AG:50:LEU:HB3	2.02	0.40
11:AG:63:ILE:HD13	11:AG:121:VAL:HG23	2.02	0.40
14:AJ:39:GLU:HG2	14:AJ:40:GLN:OE1	2.20	0.40
32:AO:29:LYS:HD3	32:AO:98:LEU:HD23	2.02	0.40
40:BU:16:TYR:O	40:BU:23:ARG:NH2	2.54	0.40
51:BV:60:ARG:HG3	51:BV:61:LEU:N	2.36	0.40
62:Bc:26:PRO:HB2	62:Bc:29:VAL:CG1	2.51	0.40
64:Bl:34:LYS:HE3	64:Bl:34:LYS:HB2	1.89	0.40
30:B4:90:ALA:O	30:B4:92:ILE:HG12	2.21	0.40
1:1:279:A:H2'	1:1:280:G:H8	1.86	0.40
1:1:341:4AC:O7	1:1:341:4AC:H5	2.22	0.40
1:1:451:4AC:O7	1:1:451:4AC:H5	2.21	0.40
1:1:922:4AC:O7	1:1:922:4AC:H5	2.21	0.40
1:1:1909:A:H2'	1:1:1910:G:C8	2.56	0.40
1:1:1985:C:OP1	50:BQ:69:GLN:NE2	2.54	0.40
1:1:2163:5MC:C4	1:1:2164:U:C4	3.10	0.40
1:1:2630:C:H2'	1:1:2631:C:H6	1.86	0.40
1:1:2705:C:C2	1:1:2706:C:O2	2.74	0.40
2:2:233:G:H2'	2:2:234:A:H8	1.86	0.40
2:2:1125:G:C2	2:2:1126:G:C5	3.09	0.40
34:BY:82:ASP:OD1	34:BY:82:ASP:N	2.54	0.40
44:Ba:33:LYS:HE3	44:Ba:33:LYS:HB2	1.92	0.40
54:BF:41:TRP:CG	54:BF:67:ILE:HG21	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:Bc:72:GLU:H	62:Bc:72:GLU:CD	2.29	0.40
1:1:406:A:H5''	1:1:408:G:O4'	2.22	0.40
1:1:1667:4AC:H5	1:1:1667:4AC:O7	2.21	0.40
1:1:1986:U:H2'	1:1:1987:G:O4'	2.21	0.40
1:1:2310:G:H2'	1:1:2311:A:C8	2.56	0.40
1:1:2342:C:H3'	1:1:2343:G:C5'	2.48	0.40
1:1:2976:U:O2'	54:BF:145:GLU:OE2	2.34	0.40
2:2:29:C:O2'	2:2:884:A:N1	2.50	0.40
2:2:53:4AC:O7	2:2:53:4AC:H5	2.20	0.40
2:2:546:4AC:H2'	2:2:547:G:O4'	2.21	0.40
2:2:620:U:O2'	2:2:621:G:H8	2.04	0.40
2:2:848:4AC:O7	2:2:848:4AC:H5	2.20	0.40
2:2:1467:UR3:H6	2:2:1467:UR3:O5'	2.20	0.40
11:AG:38:ILE:HB	11:AG:61:MET:HG2	2.03	0.40
23:AU:27:LYS:HE2	23:AU:27:LYS:HB2	1.93	0.40
28:AZ:22:GLU:HG3	28:AZ:30:TYR:CE2	2.55	0.40
34:BY:59:ILE:HA	34:BY:148:ASN:HD21	1.86	0.40
35:BO:168:PHE:O	35:BO:172:LEU:HD22	2.20	0.40
41:Bb:37:ASP:N	41:Bb:37:ASP:OD1	2.55	0.40
58:BS:72:HIS:HA	58:BS:79:GLY:O	2.21	0.40
59:Bd:89:MET:O	59:Bd:89:MET:SD	2.78	0.40
30:B4:83:LYS:HB3	30:B4:83:LYS:HE2	1.84	0.40
1:1:534:G:H2'	1:1:535:U:C6	2.57	0.40
1:1:871:G:H2'	1:1:872:C:H6	1.86	0.40
1:1:2447:A:H2'	1:1:2448:A:C8	2.56	0.40
1:1:2718:4AC:O7	1:1:2718:4AC:H5	2.21	0.40
2:2:84:C:H2'	2:2:85:U:O4'	2.21	0.40
2:2:394:4AC:O7	2:2:394:4AC:H5	2.20	0.40
2:2:685:G:H2'	2:2:685:G:N3	2.37	0.40
2:2:823:G:H4'	20:AQ:10:GLY:HA2	2.02	0.40
2:2:850:C:H2'	2:2:851:4AC:H6	2.04	0.40
2:2:1338:U:P	23:AU:83:ARG:HH22	2.44	0.40
6:AB:57:LYS:HG2	6:AB:178:ASN:ND2	2.36	0.40
6:AB:111:GLU:O	10:AF:21:LYS:HE2	2.22	0.40
19:AP:22:ILE:HG13	19:AP:37:MET:O	2.22	0.40
20:AQ:77:THR:HG23	20:AQ:80:ARG:HD2	2.03	0.40
28:AZ:54:VAL:HG21	28:AZ:82:VAL:HG21	2.03	0.40
34:BY:33:HIS:NE2	34:BY:118:ARG:HG2	2.36	0.40
38:BL:86:ASP:OD1	38:BL:87:GLU:N	2.54	0.40
41:Bb:127:ASN:OD1	41:Bb:127:ASN:N	2.54	0.40
53:BD:19:PRO:HG3	53:BD:251:LYS:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:BZ:42:PRO:HG2	55:BZ:45:ILE:HD12	2.04	0.40
66:BA:40:ILE:HB	66:BA:201:GLN:NE2	2.37	0.40
66:BA:163:ASN:HA	66:BA:164:PRO:HD3	1.96	0.40
1:1:134:C:H2'	1:1:135:C:C6	2.57	0.40
1:1:644:G:H2'	1:1:645:A:C8	2.56	0.40
1:1:1202:U:C2	1:1:1203:G:C8	3.09	0.40
1:1:1885:4AC:O2	42:Be:9:GLY:HA2	2.21	0.40
1:1:2336:A:H2'	1:1:2337:C:H6	1.87	0.40
2:2:86:U:H5'	2:2:87:C:OP2	2.21	0.40
2:2:471:OMG:HM22	2:2:472:G:H5'	2.03	0.40
2:2:511:4AC:H5	2:2:511:4AC:O7	2.22	0.40
2:2:718:4AC:O7	2:2:718:4AC:H5	2.21	0.40
2:2:943:G:P	15:AK:130:ARG:HH22	2.44	0.40
4:H:56:ILE:HA	4:H:59:HIS:CE1	2.56	0.40
6:AB:175:ILE:HD13	6:AB:175:ILE:HA	1.79	0.40
9:AE:151:PRO:HG2	9:AE:154:GLU:OE1	2.20	0.40
10:AF:2:SER:O	10:AF:6:LYS:HG2	2.22	0.40
10:AF:216:GLU:H	10:AF:216:GLU:CD	2.29	0.40
17:AM:19:ILE:N	17:AM:82:ARG:O	2.42	0.40
66:BA:64:LYS:HD2	66:BA:108:ASP:OD1	2.21	0.40
66:BA:159:GLN:HG3	66:BA:161:LYS:HG3	2.03	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%)	368 (96%)	15 (4%)	1 (0%)	36	36
5	AA	186/199 (94%)	181 (97%)	5 (3%)	0	100	100
6	AB	194/202 (96%)	191 (98%)	3 (2%)	0	100	100
7	AC	55/63 (87%)	53 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	AD	171/180 (95%)	169 (99%)	2 (1%)	0	100	100
9	AE	240/243 (99%)	234 (98%)	6 (2%)	0	100	100
10	AF	227/236 (96%)	221 (97%)	6 (3%)	0	100	100
11	AG	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
12	AH	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
13	AI	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
14	AJ	123/127 (97%)	121 (98%)	2 (2%)	0	100	100
15	AK	133/135 (98%)	129 (97%)	3 (2%)	1 (1%)	16	12
16	AL	98/102 (96%)	95 (97%)	3 (3%)	0	100	100
17	AM	125/137 (91%)	119 (95%)	6 (5%)	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%)	102 (97%)	3 (3%)	0	100	100
22	AS	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
23	AU	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
24	AV	94/99 (95%)	90 (96%)	4 (4%)	0	100	100
24	B6	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
25	AW	59/65 (91%)	55 (93%)	4 (7%)	0	100	100
26	AX	63/71 (89%)	63 (100%)	0	0	100	100
27	AY	27/51 (53%)	23 (85%)	4 (15%)	0	100	100
28	AZ	194/210 (92%)	186 (96%)	8 (4%)	0	100	100
29	A0	34/37 (92%)	34 (100%)	0	0	100	100
30	A3	120/123 (98%)	111 (92%)	9 (8%)	0	100	100
30	B4	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
30	BG	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
31	AT	128/132 (97%)	128 (100%)	0	0	100	100
32	AO	136/148 (92%)	130 (96%)	6 (4%)	0	100	100
33	BB	236/239 (99%)	229 (97%)	6 (2%)	1 (0%)	30	28
34	BY	152/155 (98%)	150 (99%)	2 (1%)	0	100	100
35	BO	196/203 (97%)	195 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BC	358/361 (99%)	349 (98%)	8 (2%)	1 (0%)	36	36
37	B5	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
37	BK	78/82 (95%)	75 (96%)	3 (4%)	0	100	100
38	BL	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
39	Bf	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
40	BU	119/121 (98%)	119 (100%)	0	0	100	100
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%)	181 (99%)	2 (1%)	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%)	146 (99%)	2 (1%)	0	100	100
51	BV	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
52	Bj	92/94 (98%)	92 (100%)	0	0	100	100
53	BD	253/255 (99%)	249 (98%)	4 (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%)	189 (99%)	2 (1%)	0	100	100
58	BS	152/155 (98%)	149 (98%)	3 (2%)	0	100	100
59	Bd	89/91 (98%)	89 (100%)	0	0	100	100
60	BN	176/181 (97%)	171 (97%)	5 (3%)	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%)	73 (97%)	2 (3%)	0	100	100
65	Bk	61/65 (94%)	61 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	BA	213/219 (97%)	207 (97%)	6 (3%)	0	100	100
All	All	8761/9080 (96%)	8568 (98%)	189 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	AK	120	ASN
4	H	268	VAL
36	BC	347	VAL
33	BB	122	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	332/338 (98%)	311 (94%)	21 (6%)	16	14
5	AA	160/167 (96%)	151 (94%)	9 (6%)	19	18
6	AB	168/173 (97%)	163 (97%)	5 (3%)	36	41
7	AC	50/55 (91%)	50 (100%)	0	100	100
8	AD	156/160 (98%)	155 (99%)	1 (1%)	78	86
9	AE	213/214 (100%)	212 (100%)	1 (0%)	81	88
10	AF	192/198 (97%)	190 (99%)	2 (1%)	68	76
11	AG	107/108 (99%)	104 (97%)	3 (3%)	38	43
12	AH	183/184 (100%)	179 (98%)	4 (2%)	45	53
13	AI	106/107 (99%)	104 (98%)	2 (2%)	50	58
14	AJ	101/103 (98%)	94 (93%)	7 (7%)	14	12
15	AK	111/111 (100%)	108 (97%)	3 (3%)	39	45
16	AL	89/91 (98%)	85 (96%)	4 (4%)	24	25
17	AM	94/104 (90%)	88 (94%)	6 (6%)	16	14
18	AN	120/121 (99%)	116 (97%)	4 (3%)	33	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AP	45/46 (98%)	45 (100%)	0	100	100
20	AQ	142/143 (99%)	134 (94%)	8 (6%)	19	18
21	AR	96/102 (94%)	93 (97%)	3 (3%)	35	39
22	AS	58/61 (95%)	56 (97%)	2 (3%)	32	35
23	AU	126/127 (99%)	126 (100%)	0	100	100
24	AV	88/90 (98%)	78 (89%)	10 (11%)	5	3
24	B6	86/90 (96%)	85 (99%)	1 (1%)	63	72
25	AW	53/56 (95%)	51 (96%)	2 (4%)	29	32
26	AX	55/60 (92%)	49 (89%)	6 (11%)	6	4
27	AY	22/42 (52%)	20 (91%)	2 (9%)	9	6
28	AZ	155/168 (92%)	151 (97%)	4 (3%)	40	46
29	A0	34/35 (97%)	33 (97%)	1 (3%)	37	42
30	A3	98/99 (99%)	96 (98%)	2 (2%)	48	56
30	B4	98/99 (99%)	91 (93%)	7 (7%)	13	11
30	BG	98/99 (99%)	98 (100%)	0	100	100
31	AT	113/114 (99%)	109 (96%)	4 (4%)	32	35
32	AO	115/123 (94%)	113 (98%)	2 (2%)	53	62
33	BB	188/189 (100%)	185 (98%)	3 (2%)	55	64
34	BY	132/133 (99%)	132 (100%)	0	100	100
35	BO	167/170 (98%)	161 (96%)	6 (4%)	31	34
36	BC	306/307 (100%)	304 (99%)	2 (1%)	76	83
37	B5	65/66 (98%)	62 (95%)	3 (5%)	24	25
37	BK	64/66 (97%)	63 (98%)	1 (2%)	55	64
38	BL	118/118 (100%)	116 (98%)	2 (2%)	53	62
39	Bf	46/47 (98%)	44 (96%)	2 (4%)	26	27
40	BU	109/109 (100%)	108 (99%)	1 (1%)	70	78
41	Bb	117/118 (99%)	116 (99%)	1 (1%)	70	78
42	Be	52/53 (98%)	52 (100%)	0	100	100
43	BE	158/160 (99%)	148 (94%)	10 (6%)	16	14
44	Ba	84/84 (100%)	83 (99%)	1 (1%)	63	72
45	BT	77/77 (100%)	74 (96%)	3 (4%)	28	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	BW	63/63 (100%)	61 (97%)	2 (3%)	34	38
47	Bi	61/62 (98%)	60 (98%)	1 (2%)	55	64
48	BI	122/122 (100%)	121 (99%)	1 (1%)	73	81
49	BR	86/87 (99%)	84 (98%)	2 (2%)	44	51
50	BQ	132/133 (99%)	129 (98%)	3 (2%)	44	51
51	BV	54/58 (93%)	54 (100%)	0	100	100
52	Bj	83/84 (99%)	82 (99%)	1 (1%)	63	72
53	BD	212/212 (100%)	206 (97%)	6 (3%)	38	43
54	BF	156/157 (99%)	152 (97%)	4 (3%)	40	46
55	BZ	79/80 (99%)	78 (99%)	1 (1%)	61	69
56	BP	102/102 (100%)	101 (99%)	1 (1%)	68	76
57	BM	160/161 (99%)	159 (99%)	1 (1%)	78	86
58	BS	130/131 (99%)	128 (98%)	2 (2%)	57	65
59	Bd	82/82 (100%)	81 (99%)	1 (1%)	63	72
60	BN	149/151 (99%)	146 (98%)	3 (2%)	48	56
61	Bg	37/39 (95%)	37 (100%)	0	100	100
62	Bc	74/74 (100%)	73 (99%)	1 (1%)	59	67
63	BJ	108/109 (99%)	106 (98%)	2 (2%)	50	58
64	Bl	72/72 (100%)	70 (97%)	2 (3%)	38	43
65	Bk	55/57 (96%)	55 (100%)	0	100	100
66	BA	182/186 (98%)	173 (95%)	9 (5%)	22	22
All	All	7546/7707 (98%)	7342 (97%)	204 (3%)	40	45

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	10	MET
4	H	23	LEU
4	H	40	VAL
4	H	62	TRP
4	H	73	TYR
4	H	92	LEU
4	H	112	VAL
4	H	119	LEU
4	H	131	LYS

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Mol	Chain	Res	Type
4	H	140	VAL
4	H	166	VAL
4	H	177	VAL
4	H	183	ILE
4	H	206	PHE
4	H	214	MET
4	H	215	ILE
4	H	238	ASN
4	H	259	ASP
4	H	350	THR
4	H	369	LEU
4	H	382	LYS
5	AA	11	LYS
5	AA	31	VAL
5	AA	56	ILE
5	AA	74	VAL
5	AA	116	TYR
5	AA	117	LYS
5	AA	142	MET
5	AA	148	LYS
5	AA	181	LEU
6	AB	13	LEU
6	AB	28	MET
6	AB	74	LEU
6	AB	170	ILE
6	AB	171	LEU
8	AD	86	ASP
9	AE	164	VAL
10	AF	57	VAL
10	AF	220	ARG
11	AG	19	ILE
11	AG	77	ASP
11	AG	121	VAL
12	AH	73	ARG
12	AH	81	VAL
12	AH	141	PHE
12	AH	146	TYR
13	AI	33	LEU
13	AI	98	GLU
14	AJ	18	VAL
14	AJ	40	GLN
14	AJ	88	GLN

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Mol	Chain	Res	Type
14	AJ	95	ILE
14	AJ	96	THR
14	AJ	124	LEU
14	AJ	125	LEU
15	AK	18	VAL
15	AK	56	ILE
15	AK	96	LYS
16	AL	8	LEU
16	AL	30	THR
16	AL	75	ILE
16	AL	101	ILE
17	AM	27	ILE
17	AM	34	THR
17	AM	52	ARG
17	AM	53	ASP
17	AM	110	LEU
17	AM	121	ILE
18	AN	53	ILE
18	AN	58	ILE
18	AN	75	VAL
18	AN	106	GLU
20	AQ	50	ILE
20	AQ	66	PHE
20	AQ	76	LEU
20	AQ	87	LEU
20	AQ	116	LEU
20	AQ	125	ILE
20	AQ	149	ASP
20	AQ	156	LEU
21	AR	37	ILE
21	AR	38	VAL
21	AR	102	VAL
22	AS	16	LEU
22	AS	43	SER
24	AV	1	MET
24	AV	19	ILE
24	AV	23	ILE
24	AV	28	GLU
24	AV	36	VAL
24	AV	40	LEU
24	AV	44	LEU
24	AV	56	ILE

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Mol	Chain	Res	Type
24	AV	81	ILE
24	AV	93	ILE
25	AW	27	GLN
25	AW	60	ILE
26	AX	12	ILE
26	AX	29	VAL
26	AX	49	VAL
26	AX	53	ASP
26	AX	58	ARG
26	AX	59	GLU
27	AY	33	ASP
27	AY	38	TRP
28	AZ	17	ILE
28	AZ	162	VAL
28	AZ	192	GLU
28	AZ	196	ILE
29	A0	36	LEU
30	A3	69	LEU
30	A3	74	GLU
31	AT	36	LEU
31	AT	47	LEU
31	AT	60	ASN
31	AT	70	MET
32	AO	7	ILE
32	AO	61	LYS
33	BB	96	THR
33	BB	106	THR
33	BB	127	THR
35	BO	64	THR
35	BO	112	VAL
35	BO	117	VAL
35	BO	137	ILE
35	BO	172	LEU
35	BO	197	GLU
36	BC	56	ASP
36	BC	170	VAL
37	B5	33	VAL
37	B5	71	VAL
37	B5	75	LEU
38	BL	69	VAL
38	BL	123	VAL
39	Bf	3	ARG

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Mol	Chain	Res	Type
39	Bf	47	THR
40	BU	89	THR
41	Bb	91	GLU
43	BE	3	ILE
43	BE	22	LYS
43	BE	30	ILE
43	BE	65	ASN
43	BE	94	LEU
43	BE	120	HIS
43	BE	123	ILE
43	BE	138	ASP
43	BE	167	THR
43	BE	184	VAL
44	Ba	1	MET
45	BT	12	ILE
45	BT	27	THR
45	BT	85	LEU
46	BW	23	LEU
46	BW	63	ARG
47	Bi	51	THR
48	BI	1	MET
49	BR	2	VAL
49	BR	64	THR
37	BK	75	LEU
50	BQ	71	LYS
50	BQ	76	ARG
50	BQ	122	MET
52	Bj	86	VAL
53	BD	27	ARG
53	BD	30	LEU
53	BD	61	ILE
53	BD	75	THR
53	BD	92	THR
53	BD	222	VAL
54	BF	26	VAL
54	BF	34	GLU
54	BF	53	VAL
54	BF	158	THR
55	BZ	96	LEU
24	B6	37	LYS
56	BP	69	LEU
57	BM	3	MET

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Mol	Chain	Res	Type
58	BS	144	THR
58	BS	155	ARG
59	Bd	89	MET
60	BN	63	GLU
60	BN	103	ARG
60	BN	170	ASN
62	Bc	29	VAL
63	BJ	63	VAL
63	BJ	117	GLU
64	Bl	4	LYS
64	Bl	59	GLU
30	B4	15	LEU
30	B4	17	GLU
30	B4	20	LEU
30	B4	39	THR
30	B4	62	ILE
30	B4	66	LEU
30	B4	110	LEU
66	BA	35	VAL
66	BA	57	HIS
66	BA	92	GLU
66	BA	93	ILE
66	BA	136	VAL
66	BA	150	GLU
66	BA	161	LYS
66	BA	195	LEU
66	BA	205	VAL

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

Mol	Chain	Res	Type
4	H	59	HIS
4	H	87	HIS
4	H	159	HIS
4	H	249	ASN
4	H	277	GLN
4	H	295	ASN
4	H	322	ASN
4	H	329	HIS
4	H	370	GLN
5	AA	18	GLN
5	AA	109	ASN

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Mol	Chain	Res	Type
5	AA	143	GLN
6	AB	11	GLN
6	AB	18	HIS
6	AB	22	GLN
8	AD	47	GLN
8	AD	65	GLN
8	AD	72	GLN
8	AD	123	GLN
9	AE	37	HIS
9	AE	139	GLN
9	AE	141	ASN
9	AE	143	HIS
9	AE	148	HIS
9	AE	157	ASN
10	AF	17	GLN
10	AF	62	ASN
10	AF	63	GLN
10	AF	120	ASN
10	AF	196	ASN
10	AF	209	ASN
11	AG	79	HIS
11	AG	118	GLN
12	AH	55	HIS
12	AH	69	ASN
12	AH	90	HIS
12	AH	193	ASN
13	AI	9	ASN
13	AI	16	ASN
13	AI	64	GLN
13	AI	70	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
17	AM	99	GLN
18	AN	66	ASN
19	AP	7	ASN
19	AP	34	HIS
20	AQ	5	HIS
21	AR	26	HIS

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Mol	Chain	Res	Type
21	AR	52	GLN
21	AR	55	HIS
21	AR	74	ASN
22	AS	6	GLN
22	AS	30	HIS
24	AV	54	GLN
25	AW	27	GLN
29	A0	29	GLN
30	A3	21	GLN
30	A3	37	ASN
30	A3	65	HIS
31	AT	15	GLN
31	AT	60	ASN
31	AT	114	GLN
32	AO	20	GLN
32	AO	72	HIS
33	BB	8	GLN
33	BB	34	ASN
33	BB	50	HIS
33	BB	201	ASN
33	BB	202	HIS
33	BB	229	HIS
34	BY	48	GLN
34	BY	98	GLN
34	BY	148	ASN
35	BO	42	ASN
35	BO	43	HIS
35	BO	44	HIS
35	BO	76	HIS
35	BO	109	HIS
36	BC	167	GLN
36	BC	241	HIS
36	BC	257	HIS
36	BC	270	GLN
36	BC	274	HIS
36	BC	309	HIS
36	BC	348	GLN
38	BL	57	HIS
39	Bf	19	GLN
39	Bf	20	ASN
39	Bf	38	HIS
40	BU	7	GLN

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Mol	Chain	Res	Type
40	BU	96	HIS
41	Bb	26	GLN
42	Be	17	HIS
43	BE	31	ASN
43	BE	164	HIS
44	Ba	42	HIS
44	Ba	46	GLN
46	BW	40	ASN
48	BI	51	GLN
48	BI	119	HIS
49	BR	6	HIS
49	BR	19	HIS
49	BR	33	GLN
49	BR	39	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	67	HIS
50	BQ	75	HIS
50	BQ	136	HIS
50	BQ	137	GLN
51	BV	57	GLN
30	BG	47	GLN
53	BD	44	GLN
53	BD	213	ASN
53	BD	214	HIS
53	BD	229	HIS
53	BD	235	HIS
54	BF	24	ASN
54	BF	74	HIS
54	BF	104	GLN
54	BF	149	GLN
54	BF	156	GLN
55	BZ	21	ASN
56	BP	10	ASN
56	BP	23	ASN
56	BP	110	ASN
57	BM	87	GLN
57	BM	97	GLN

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Mol	Chain	Res	Type
57	BM	110	ASN
57	BM	154	HIS
57	BM	174	ASN
57	BM	189	ASN
58	BS	45	ASN
58	BS	97	ASN
59	Bd	35	HIS
59	Bd	70	HIS
60	BN	38	ASN
60	BN	56	GLN
60	BN	59	GLN
60	BN	70	ASN
60	BN	81	ASN
60	BN	83	HIS
60	BN	97	ASN
60	BN	110	ASN
60	BN	130	GLN
62	Bc	17	GLN
62	Bc	18	HIS
62	Bc	28	ASN
63	BJ	47	HIS
63	BJ	102	ASN
64	Bl	2	ASN
66	BA	36	ASN
66	BA	162	ASN
66	BA	163	ASN
66	BA	167	HIS
66	BA	201	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3016/3018 (99%)	427 (14%)	19 (0%)
2	2	1495/1512 (98%)	175 (11%)	2 (0%)
3	3	125/128 (97%)	13 (10%)	0
All	All	4636/4658 (99%)	615 (13%)	21 (0%)

All (615) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	3	A

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Mol	Chain	Res	Type
1	1	12	G
1	1	28	A
1	1	39	A
1	1	51	A
1	1	52	G
1	1	55	U
1	1	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	85	A
1	1	88	G
1	1	94	G
1	1	95	G
1	1	98	C
1	1	99	U
1	1	100	G
1	1	101	U
1	1	102	C
1	1	104	C
1	1	105	C
1	1	107	G
1	1	115	G
1	1	116	G
1	1	118	U
1	1	120	A
1	1	121	G
1	1	122	G
1	1	123	A
1	1	126	C
1	1	127	U
1	1	138	G
1	1	148	C
1	1	154	G
1	1	160	C
1	1	163	A
1	1	178	A
1	1	185	A
1	1	188	A

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Mol	Chain	Res	Type
1	1	189	G
1	1	199	G
1	1	205	G
1	1	231	A
1	1	232	A
1	1	233	U
1	1	238	C
1	1	239	C
1	1	240	U
1	1	241	C
1	1	244	G
1	1	245	C
1	1	247	G
1	1	248	C
1	1	249	U
1	1	250	U
1	1	251	A
1	1	252	U
1	1	253	G
1	1	254	C
1	1	268	A
1	1	269	U
1	1	270	A
1	1	272	G
1	1	273	C
1	1	275	C
1	1	285	A
1	1	300	A
1	1	319	G
1	1	320	A
1	1	326	A
1	1	332	A
1	1	333	A
1	1	337	A
1	1	339	G
1	1	352	G
1	1	370	G
1	1	393	C
1	1	408	G
1	1	416	G
1	1	417	U
1	1	421	G

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Mol	Chain	Res	Type
1	1	422	C
1	1	429	A
1	1	430	U
1	1	431	G
1	1	433	G
1	1	438	U
1	1	439	C
1	1	447	A
1	1	448	A
1	1	449	G
1	1	456	U
1	1	466	C
1	1	484	G
1	1	485	A
1	1	493	G
1	1	501	A
1	1	507	G
1	1	516	C
1	1	517	G
1	1	522	A
1	1	529	G
1	1	544	U
1	1	545	A
1	1	553	G
1	1	560	G
1	1	565	G
1	1	611	A
1	1	621	G
1	1	635	G
1	1	657	A
1	1	661	C
1	1	683	A
1	1	684	G
1	1	685	G
1	1	689	C
1	1	696	A
1	1	699	G
1	1	704	G
1	1	731	C
1	1	738	G
1	1	746	G
1	1	769	C

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Mol	Chain	Res	Type
1	1	781	A
1	1	785	G
1	1	792	A
1	1	809	A
1	1	849	C
1	1	851	U
1	1	852	G
1	1	865	C
1	1	866	C
1	1	867	U
1	1	868	C
1	1	869	G
1	1	870	A
1	1	871	G
1	1	893	A
1	1	924	A
1	1	925	A
1	1	926	A
1	1	935	U
1	1	963	A
1	1	965	C
1	1	967	G
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
1	1	1043	G
1	1	1053	A
1	1	1056	G
1	1	1063	C
1	1	1073	C
1	1	1078	C
1	1	1079	G
1	1	1096	G
1	1	1101	A
1	1	1111	G

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Mol	Chain	Res	Type
1	1	1118	A
1	1	1131	G
1	1	1132	C
1	1	1133	A
1	1	1134	G
1	1	1140	G
1	1	1141	A
1	1	1143	A
1	1	1144	G
1	1	1145	C
1	1	1148	C
1	1	1149	C
1	1	1159	U
1	1	1162	A
1	1	1164	C
1	1	1199	G
1	1	1200	G
1	1	1225	G
1	1	1231	A
1	1	1234	A
1	1	1236	C
1	1	1240	G
1	1	1241	A
1	1	1252	G
1	1	1261	G
1	1	1262	U
1	1	1263	G
1	1	1272	G
1	1	1280	C
1	1	1281	C
1	1	1282	A
1	1	1288	U
1	1	1289	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

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Mol	Chain	Res	Type
1	1	1316	A
1	1	1317	G
1	1	1322	A
1	1	1325	A
1	1	1326	G
1	1	1339	A
1	1	1343	A
1	1	1344	G
1	1	1345	U
1	1	1346	G
1	1	1353	A
1	1	1359	C
1	1	1362	G
1	1	1363	U
1	1	1364	C
1	1	1365	G
1	1	1366	A
1	1	1367	G
1	1	1371	C
1	1	1376	C
1	1	1387	G
1	1	1389	C
1	1	1393	G
1	1	1397	A
1	1	1411	G
1	1	1433	G
1	1	1443	C
1	1	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	1639	A
1	1	1641	A
1	1	1645	A
1	1	1648	C
1	1	1657	A

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Mol	Chain	Res	Type
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	1796	U
1	1	1799	C
1	1	1805	C
1	1	1808	U
1	1	1809	A
1	1	1810	G
1	1	1830	G
1	1	1840	A
1	1	1856	U
1	1	1857	U
1	1	1883	A
1	1	1890	C
1	1	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	1996	U
1	1	1997	A

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Mol	Chain	Res	Type
1	1	2020	G
1	1	2029	A
1	1	2042	A
1	1	2056	C
1	1	2085	A
1	1	2095	A
1	1	2119	A
1	1	2142	A
1	1	2147	OMG
1	1	2154	A
1	1	2155	C
1	1	2156	U
1	1	2157	A
1	1	2170	G
1	1	2171	G
1	1	2177	A
1	1	2178	A
1	1	2179	A
1	1	2181	U
1	1	2196	U
1	1	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	2300	A
1	1	2301	G
1	1	2303	C
1	1	2309	G
1	1	2310	G
1	1	2333	G
1	1	2342	C
1	1	2343	G

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Mol	Chain	Res	Type
1	1	2344	G
1	1	2348	G
1	1	2351	C
1	1	2352	G
1	1	2372	C
1	1	2373	G
1	1	2375	A
1	1	2383	C
1	1	2384	U
1	1	2388	G
1	1	2389	G
1	1	2397	G
1	1	2398	A
1	1	2399	G
1	1	2408	G
1	1	2412	C
1	1	2416	G
1	1	2425	U
1	1	2426	C
1	1	2427	G
1	1	2430	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

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Mol	Chain	Res	Type
1	1	2574	C
1	1	2588	A
1	1	2592	G
1	1	2617	G
1	1	2619	C
1	1	2636	C
1	1	2659	G
1	1	2664	A
1	1	2666	A
1	1	2673	C
1	1	2677	G
1	1	2680	A
1	1	2691	G
1	1	2706	C
1	1	2710	A
1	1	2723	C
1	1	2730	C
1	1	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	2831	G
1	1	2834	A
1	1	2845	U
1	1	2846	A
1	1	2861	U
1	1	2877	A
1	1	2878	G
1	1	2896	G
1	1	2906	G
1	1	2922	U
1	1	2945	G
1	1	2957	C
1	1	2964	G
1	1	2978	A
1	1	2981	G

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Mol	Chain	Res	Type
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	76	G
2	2	86	U
2	2	87	C
2	2	88	U
2	2	89	G
2	2	115	A
2	2	116	A
2	2	117	C
2	2	126	A
2	2	127	A
2	2	128	C
2	2	154	G
2	2	171	C
2	2	189	A
2	2	196	G
2	2	212	G
2	2	219	G
2	2	222	A
2	2	223	G
2	2	225	C
2	2	229	G
2	2	254	U
2	2	256	G
2	2	260	G
2	2	271	A
2	2	275	G
2	2	276	C
2	2	290	G
2	2	298	C
2	2	315	A

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Mol	Chain	Res	Type
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	407	C
2	2	415	G
2	2	424	C
2	2	426	G
2	2	436	U
2	2	460	A
2	2	461	A
2	2	474	A
2	2	477	G
2	2	484	G
2	2	496	G
2	2	497	U
2	2	498	A
2	2	499	A
2	2	513	A
2	2	530	U
2	2	533	G
2	2	539	A
2	2	542	C
2	2	543	G
2	2	562	A
2	2	571	C
2	2	600	G
2	2	609	A
2	2	620	U
2	2	628	G
2	2	632	A
2	2	642	U
2	2	654	A
2	2	660	G

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Mol	Chain	Res	Type
2	2	685	G
2	2	689	G
2	2	690	U
2	2	691	G
2	2	715	G
2	2	716	U
2	2	722	G
2	2	744	A
2	2	757	A
2	2	760	U
2	2	761	A
2	2	782	A
2	2	784	G
2	2	788	G
2	2	814	A
2	2	861	G
2	2	885	A
2	2	893	G
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	966	C
2	2	968	G
2	2	975	G
2	2	977	A
2	2	981	C
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
2	2	1004	C
2	2	1005	G
2	2	1008	G
2	2	1030	U

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Mol	Chain	Res	Type
2	2	1059	G
2	2	1060	U
2	2	1066	A
2	2	1105	G
2	2	1108	C
2	2	1131	A
2	2	1133	U
2	2	1155	G
2	2	1157	G
2	2	1170	A
2	2	1171	G
2	2	1175	A
2	2	1176	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	1253	A
2	2	1254	A
2	2	1274	G
2	2	1276	U
2	2	1279	G
2	2	1294	C
2	2	1305	G
2	2	1310	U
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	1397	G
2	2	1400	C
2	2	1421	U
2	2	1424	G
2	2	1427	G
2	2	1456	G
2	2	1461	A
2	2	1463	G

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Mol	Chain	Res	Type
2	2	1466	G
2	2	1468	A
2	2	1471	A
2	2	1475	U
2	2	1486	G
2	2	1488	MA6
2	2	1498	5MC
2	2	1499	G
2	2	1503	A
2	2	1504	C
2	2	1506	U
2	2	1507	C
2	2	1508	C
3	3	5	C
3	3	9	G
3	3	25	C
3	3	30	C
3	3	53	A
3	3	56	U
3	3	57	A
3	3	58	A
3	3	79	G
3	3	89	C
3	3	95	G
3	3	96	G
3	3	115	G

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	68	U
1	1	117	G
1	1	120	A
1	1	122	G
1	1	238	C
1	1	656	A
1	1	866	C
1	1	867	U
1	1	869	G
1	1	1035	G
1	1	1303	A
1	1	1363	U

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Mol	Chain	Res	Type
1	1	1364	C
1	1	1731	U
1	1	2397	G
1	1	2455	A
1	1	2733	5MC
1	1	2986	U
1	1	3021	U
2	2	406	A
2	2	653	U

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

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	OMU	2	1177	2	19,22,23	1.22	3 (15%)	26,31,34	1.70	5 (19%)
1	4AC	1	641	1	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
2	5MC	2	1374	2	18,22,23	0.92	2 (11%)	26,32,35	1.13	2 (7%)
2	5MC	2	535	2	18,22,23	0.93	2 (11%)	26,32,35	1.14	2 (7%)
2	4AC	2	636	2	21,24,25	1.02	1 (4%)	29,34,37	1.40	4 (13%)
2	OMC	2	1040	2	19,22,23	1.08	2 (10%)	26,31,34	0.85	0
1	4AC	1	2570	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
2	4AC	2	286	2	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
2	4AC	2	1147	2	21,24,25	1.01	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	922	1	21,24,25	1.05	2 (9%)	29,34,37	1.44	4 (13%)
2	4AC	2	319	2	21,24,25	1.02	2 (9%)	29,34,37	1.38	4 (13%)
2	4AC	2	848	2	21,24,25	1.01	2 (9%)	29,34,37	1.36	4 (13%)
1	OMG	1	789	1	23,26,27	1.25	3 (13%)	33,38,41	1.92	6 (18%)
2	4AC	2	1184	2	21,24,25	1.03	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	1	458	1	21,24,25	1.01	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	OMU	1	2784	1	19,22,23	1.22	3 (15%)	26,31,34	1.71	5 (19%)
2	4AC	2	546	67,2	21,24,25	1.01	2 (9%)	29,34,37	1.38	4 (13%)
2	OMC	2	846	2	19,22,23	0.81	0	26,31,34	0.81	0
1	5MC	1	2093	1	18,22,23	0.94	2 (11%)	26,32,35	1.14	2 (7%)
1	OMC	1	1948	1	19,22,23	0.82	0	26,31,34	0.79	0
1	5MC	1	2163	1	18,22,23	0.94	2 (11%)	26,32,35	1.14	3 (11%)
2	4AC	2	479	2	21,24,25	1.01	2 (9%)	29,34,37	1.39	4 (13%)
2	4AC	2	718	2	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	1695	1	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
2	6MZ	2	1469	67,2	22,25,26	1.48	4 (18%)	30,36,39	2.19	9 (30%)
1	4AC	1	2642	1	21,24,25	1.02	2 (9%)	29,34,37	1.32	4 (13%)
1	4AC	1	211	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	5MC	1	2733	1	18,22,23	0.96	2 (11%)	26,32,35	1.26	3 (11%)
1	A2M	1	1055	1	22,25,26	1.45	4 (18%)	31,36,39	2.07	9 (29%)
1	4AC	1	1293	1	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
2	4AC	2	53	2	21,24,25	1.00	2 (9%)	29,34,37	1.37	4 (13%)
2	4AC	2	751	2	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
2	4AC	2	626	2	21,24,25	1.02	1 (4%)	29,34,37	1.44	4 (13%)
2	OMU	2	774	2	19,22,23	1.21	2 (10%)	26,31,34	1.73	5 (19%)
2	OMC	2	129	2	19,22,23	0.81	0	26,31,34	0.83	0
1	4AC	1	341	1	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	1222	1,67	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	2865	1	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	2937	1,67	21,24,25	1.03	2 (9%)	29,34,37	1.57	4 (13%)
1	4AC	1	1873	1	21,24,25	1.03	2 (9%)	29,34,37	1.31	4 (13%)
1	4AC	1	835	1	21,24,25	1.03	2 (9%)	29,34,37	1.34	4 (13%)
2	OMU	2	20	2	19,22,23	1.25	3 (15%)	26,31,34	1.78	5 (19%)
1	5MC	1	2162	1	18,22,23	0.95	2 (11%)	26,32,35	1.21	3 (11%)
2	4AC	2	868	2	21,24,25	1.01	2 (9%)	29,34,37	1.31	4 (13%)
1	4AC	1	1885	1	21,24,25	1.02	2 (9%)	29,34,37	1.31	4 (13%)
1	4AC	1	829	1	21,24,25	1.03	2 (9%)	29,34,37	1.31	4 (13%)
1	4AC	1	2585	1	21,24,25	1.06	2 (9%)	29,34,37	1.75	5 (17%)
2	5MC	2	1025	2	18,22,23	0.94	2 (11%)	26,32,35	1.16	3 (11%)
1	4AC	1	243	1	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	1617	1	21,24,25	1.01	2 (9%)	29,34,37	1.38	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	1	2608	1	21,24,25	1.06	2 (9%)	29,34,37	1.73	5 (17%)
2	B8H	2	938	2	19,22,23	0.53	0	22,32,35	0.61	0
2	5MC	2	875	2	18,22,23	0.95	2 (11%)	26,32,35	1.18	3 (11%)
2	OMG	2	519	2	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
2	OMC	2	773	2	19,22,23	0.82	0	26,31,34	0.83	0
1	4AC	1	2548	1	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
1	OMG	1	2144	1	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)
1	4AC	1	533	1	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	2329	1	21,24,25	1.02	2 (9%)	29,34,37	1.37	4 (13%)
2	4AC	2	590	2	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
2	5MC	2	1202	2	18,22,23	0.96	2 (11%)	26,32,35	1.16	3 (11%)
2	OMG	2	934	2	23,26,27	1.21	3 (13%)	33,38,41	1.97	6 (18%)
1	4AC	1	229	1	21,24,25	1.04	2 (9%)	29,34,37	1.33	4 (13%)
1	5MC	1	2198	1	18,22,23	0.91	2 (11%)	26,32,35	1.15	2 (7%)
1	4AC	1	2966	1	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	451	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
2	LHH	2	250	2	22,25,26	0.32	0	29,35,38	0.43	0
2	UR3	2	1467	2	19,22,23	0.94	0	26,32,35	1.43	2 (7%)
1	4AC	1	1243	1	21,24,25	1.03	2 (9%)	29,34,37	1.36	4 (13%)
2	OMG	2	680	2	23,26,27	1.23	3 (13%)	33,38,41	1.99	6 (18%)
2	4AC	2	1233	2	21,24,25	1.02	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	2249	1	21,24,25	1.05	2 (9%)	29,34,37	1.39	4 (13%)
2	5MC	2	1496	2	18,22,23	0.93	2 (11%)	26,32,35	1.17	3 (11%)
1	4AC	1	1557	1	21,24,25	1.03	2 (9%)	29,34,37	1.30	4 (13%)
1	4AC	1	1594	1,67	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
2	OMG	2	467	2	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
1	4AC	1	802	1	21,24,25	1.01	2 (9%)	29,34,37	1.37	4 (13%)
2	5MC	2	693	2	18,22,23	0.94	2 (11%)	26,32,35	1.17	3 (11%)
2	4AC	2	703	2	21,24,25	1.03	1 (4%)	29,34,37	1.46	4 (13%)
1	4AC	1	1878	1	21,24,25	1.02	2 (9%)	29,34,37	1.46	4 (13%)
1	LHH	1	616	1	22,25,26	0.31	0	29,35,38	0.47	0
1	4AC	1	2001	1	21,24,25	1.06	2 (9%)	29,34,37	1.48	4 (13%)
1	4AC	1	1867	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	2960	1	21,24,25	1.00	2 (9%)	29,34,37	1.32	4 (13%)
1	4AC	1	314	1	21,24,25	1.04	2 (9%)	29,34,37	1.30	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	1	2203	1	18,22,23	0.93	2 (11%)	26,32,35	1.14	2 (7%)
2	5MC	2	1505	2	18,22,23	0.98	2 (11%)	26,32,35	1.13	3 (11%)
2	4AC	2	17	2	21,24,25	1.02	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	161	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
2	LHH	2	1041	2	22,25,26	0.32	0	29,35,38	0.48	0
2	OMU	2	1380	2	19,22,23	1.29	3 (15%)	26,31,34	1.74	4 (15%)
1	4AC	1	1667	1	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	2718	1	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
2	4AC	2	731	2	21,24,25	1.01	2 (9%)	29,34,37	1.46	4 (13%)
1	4AC	1	1550	1	21,24,25	1.01	2 (9%)	29,34,37	1.31	4 (13%)
1	4AC	1	981	1	21,24,25	1.01	2 (9%)	29,34,37	1.29	4 (13%)
1	OMG	1	328	1	23,26,27	1.22	3 (13%)	33,38,41	1.95	6 (18%)
1	4AC	1	1938	1	21,24,25	1.04	2 (9%)	29,34,37	1.35	4 (13%)
2	5MC	2	1498	2	18,22,23	0.94	2 (11%)	26,32,35	1.27	4 (15%)
2	OMG	2	873	2	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
2	OMC	2	1376	2	19,22,23	0.80	0	26,31,34	0.77	0
1	4AC	1	91	1	21,24,25	1.01	2 (9%)	29,34,37	1.39	4 (13%)
1	4AC	1	2136	1	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
1	5MC	1	2183	1	18,22,23	0.94	2 (11%)	26,32,35	1.15	2 (7%)
1	OMG	1	2147	1	23,26,27	1.22	3 (13%)	33,38,41	1.95	6 (18%)
2	OMU	2	64	2	19,22,23	1.23	3 (15%)	26,31,34	1.71	4 (15%)
1	4AC	1	1662	1	21,24,25	0.99	2 (9%)	29,34,37	1.39	4 (13%)
2	4AC	2	1028	2	21,24,25	1.01	2 (9%)	29,34,37	1.36	4 (13%)
1	OMC	1	615	1	19,22,23	0.80	0	26,31,34	0.83	1 (3%)
2	OMU	2	830	2	19,22,23	1.25	3 (15%)	26,31,34	1.69	4 (15%)
1	4AC	1	1755	1	21,24,25	1.09	2 (9%)	29,34,37	1.63	5 (17%)
1	4AC	1	2027	1	21,24,25	1.01	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	1	2287	1	21,24,25	1.00	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	1934	1	21,24,25	1.01	2 (9%)	29,34,37	1.38	4 (13%)
2	OMU	2	787	2	19,22,23	1.24	2 (10%)	26,31,34	1.82	5 (19%)
2	OMG	2	657	2	23,26,27	1.23	3 (13%)	33,38,41	1.93	5 (15%)
1	4AC	1	1065	1	21,24,25	1.01	2 (9%)	29,34,37	1.38	4 (13%)
2	4AC	2	828	2	21,24,25	1.00	2 (9%)	29,34,37	1.34	4 (13%)
2	4AC	2	394	2	21,24,25	1.00	2 (9%)	29,34,37	1.39	4 (13%)
2	MA6	2	1487	2	23,26,27	1.47	4 (17%)	34,38,41	2.10	10 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	1	2062	1	21,24,25	1.01	2 (9%)	29,34,37	1.31	4 (13%)
1	4AC	1	1765	1	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
1	A2M	1	2173	1	22,25,26	1.44	4 (18%)	31,36,39	2.05	8 (25%)
1	4AC	1	2925	1	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	1554	1	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	1048	1	21,24,25	1.04	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	694	1	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
2	MA6	2	1488	2	23,26,27	1.47	4 (17%)	34,38,41	2.10	9 (26%)
1	4AC	1	1780	1	21,24,25	1.04	2 (9%)	29,34,37	1.50	4 (13%)
1	4AC	1	60	1	21,24,25	1.02	2 (9%)	29,34,37	1.39	4 (13%)
2	4AC	2	839	2	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
2	4AC	2	1479	2	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	1460	1	21,24,25	1.00	2 (9%)	29,34,37	1.37	4 (13%)
2	A2M	2	373	2	22,25,26	1.46	4 (18%)	31,36,39	2.08	9 (29%)
2	4AC	2	1239	2	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	1068	1	21,24,25	1.04	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	2992	1	21,24,25	1.04	2 (9%)	29,34,37	0.86	2 (6%)
1	4AC	1	2083	1	21,24,25	1.04	2 (9%)	29,34,37	1.28	4 (13%)
1	OMG	1	2138	1	23,26,27	1.21	3 (13%)	33,38,41	1.91	6 (18%)
1	4AC	1	2495	1	21,24,25	1.04	2 (9%)	29,34,37	1.32	4 (13%)
2	OMG	2	471	2	23,26,27	1.22	3 (13%)	33,38,41	1.92	6 (18%)
1	4AC	1	136	1	21,24,25	1.01	2 (9%)	29,34,37	1.30	4 (13%)
1	4AC	1	1621	1	21,24,25	1.04	2 (9%)	29,34,37	1.32	4 (13%)
1	OMG	1	923	1,67	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)
2	4AC	2	957	2	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	22	1	21,24,25	1.04	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	357	1	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	2908	1	21,24,25	1.01	2 (9%)	29,34,37	1.32	4 (13%)
3	4AC	3	32	3	21,24,25	1.01	2 (9%)	29,34,37	1.37	4 (13%)
2	4AC	2	511	2	21,24,25	1.03	2 (9%)	29,34,37	1.36	4 (13%)
1	OMG	1	2678	1	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
2	OMG	2	913	2	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
1	4AC	1	3004	1	21,24,25	1.03	2 (9%)	29,34,37	1.28	4 (13%)
2	4AC	2	303	2	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
2	4AC	2	851	2	21,24,25	1.02	2 (9%)	29,34,37	1.29	4 (13%)

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	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	4AC	1	2545	1	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
2	4AC	2	379	2	21,24,25	1.01	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	1962	1	21,24,25	1.01	2 (9%)	29,34,37	1.37	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	OMU	2	1177	2	-	0/9/27/28	0/2/2/2
1	4AC	1	641	1	-	0/11/29/30	0/2/2/2
2	5MC	2	1374	2	-	0/7/25/26	0/2/2/2
2	5MC	2	535	2	-	0/7/25/26	0/2/2/2
2	4AC	2	636	2	-	0/11/29/30	0/2/2/2
2	OMC	2	1040	2	-	0/9/27/28	0/2/2/2
1	4AC	1	2570	1	-	0/11/29/30	0/2/2/2
2	4AC	2	286	2	-	0/11/29/30	0/2/2/2
2	4AC	2	1147	2	-	0/11/29/30	0/2/2/2
1	4AC	1	922	1	-	0/11/29/30	0/2/2/2
2	4AC	2	319	2	-	0/11/29/30	0/2/2/2
2	4AC	2	848	2	-	0/11/29/30	0/2/2/2
1	OMG	1	789	1	-	3/9/27/28	0/3/3/3
2	4AC	2	1184	2	-	0/11/29/30	0/2/2/2
1	4AC	1	458	1	-	0/11/29/30	0/2/2/2
1	OMU	1	2784	1	-	0/9/27/28	0/2/2/2
2	4AC	2	546	67,2	-	0/11/29/30	0/2/2/2
2	OMC	2	846	2	-	0/9/27/28	0/2/2/2
1	5MC	1	2093	1	-	0/7/25/26	0/2/2/2
1	OMC	1	1948	1	-	0/9/27/28	0/2/2/2
1	5MC	1	2163	1	-	0/7/25/26	0/2/2/2
2	4AC	2	479	2	-	0/11/29/30	0/2/2/2
2	4AC	2	718	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1695	1	-	0/11/29/30	0/2/2/2
2	6MZ	2	1469	67,2	-	0/9/27/28	0/3/3/3
1	4AC	1	2642	1	-	0/11/29/30	0/2/2/2
1	4AC	1	211	1	-	0/11/29/30	0/2/2/2
1	5MC	1	2733	1	-	4/7/25/26	0/2/2/2
1	A2M	1	1055	1	-	0/9/27/28	0/3/3/3
1	4AC	1	1293	1	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4AC	2	53	2	-	0/11/29/30	0/2/2/2
2	4AC	2	751	2	-	0/11/29/30	0/2/2/2
2	4AC	2	626	2	-	0/11/29/30	0/2/2/2
2	OMU	2	774	2	-	0/9/27/28	0/2/2/2
2	OMC	2	129	2	-	0/9/27/28	0/2/2/2
1	4AC	1	341	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1222	1,67	-	0/11/29/30	0/2/2/2
1	4AC	1	2865	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2937	1,67	-	1/11/29/30	0/2/2/2
1	4AC	1	1873	1	-	0/11/29/30	0/2/2/2
1	4AC	1	835	1	-	0/11/29/30	0/2/2/2
2	OMU	2	20	2	-	6/9/27/28	0/2/2/2
1	5MC	1	2162	1	-	0/7/25/26	0/2/2/2
2	4AC	2	868	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1885	1	-	0/11/29/30	0/2/2/2
1	4AC	1	829	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2585	1	-	3/11/29/30	0/2/2/2
2	5MC	2	1025	2	-	0/7/25/26	0/2/2/2
1	4AC	1	243	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1617	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2608	1	-	3/11/29/30	0/2/2/2
2	B8H	2	938	2	-	1/7/25/26	0/2/2/2
2	5MC	2	875	2	-	0/7/25/26	0/2/2/2
2	OMG	2	519	2	-	0/9/27/28	0/3/3/3
2	OMC	2	773	2	-	0/9/27/28	0/2/2/2
1	4AC	1	2548	1	-	0/11/29/30	0/2/2/2
1	OMG	1	2144	1	-	1/9/27/28	0/3/3/3
1	4AC	1	533	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	590	2	-	0/11/29/30	0/2/2/2
2	5MC	2	1202	2	-	0/7/25/26	0/2/2/2
2	OMG	2	934	2	-	2/9/27/28	0/3/3/3
1	4AC	1	229	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	2966	1	-	0/11/29/30	0/2/2/2
1	4AC	1	451	1	-	0/11/29/30	0/2/2/2
2	LHH	2	250	2	-	0/13/31/32	0/2/2/2
2	UR3	2	1467	2	-	0/7/25/26	0/2/2/2
1	4AC	1	1243	1	-	0/11/29/30	0/2/2/2
2	OMG	2	680	2	-	1/9/27/28	0/3/3/3
2	4AC	2	1233	2	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	1	2249	1	-	0/11/29/30	0/2/2/2
2	5MC	2	1496	2	-	0/7/25/26	0/2/2/2
1	4AC	1	1557	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1594	1,67	-	0/11/29/30	0/2/2/2
2	OMG	2	467	2	-	0/9/27/28	0/3/3/3
1	4AC	1	802	1	-	0/11/29/30	0/2/2/2
2	5MC	2	693	2	-	0/7/25/26	0/2/2/2
2	4AC	2	703	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1878	1	-	0/11/29/30	0/2/2/2
1	LHH	1	616	1	-	0/13/31/32	0/2/2/2
1	4AC	1	2001	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1867	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	314	1	-	0/11/29/30	0/2/2/2
1	5MC	1	2203	1	-	0/7/25/26	0/2/2/2
2	5MC	2	1505	2	-	4/7/25/26	0/2/2/2
2	4AC	2	17	2	-	0/11/29/30	0/2/2/2
1	4AC	1	161	1	-	0/11/29/30	0/2/2/2
2	LHH	2	1041	2	-	0/13/31/32	0/2/2/2
2	OMU	2	1380	2	-	0/9/27/28	0/2/2/2
1	4AC	1	1667	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2718	1	-	0/11/29/30	0/2/2/2
2	4AC	2	731	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1550	1	-	0/11/29/30	0/2/2/2
1	4AC	1	981	1	-	0/11/29/30	0/2/2/2
1	OMG	1	328	1	-	0/9/27/28	0/3/3/3
1	4AC	1	1938	1	-	0/11/29/30	0/2/2/2
2	5MC	2	1498	2	-	4/7/25/26	0/2/2/2
2	OMG	2	873	2	-	1/9/27/28	0/3/3/3
2	OMC	2	1376	2	-	0/9/27/28	0/2/2/2
1	4AC	1	91	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2136	1	-	0/11/29/30	0/2/2/2
1	5MC	1	2183	1	-	0/7/25/26	0/2/2/2
1	OMG	1	2147	1	-	2/9/27/28	0/3/3/3
2	OMU	2	64	2	-	2/9/27/28	0/2/2/2
1	4AC	1	1662	1	-	0/11/29/30	0/2/2/2
2	4AC	2	1028	2	-	0/11/29/30	0/2/2/2
1	OMC	1	615	1	-	0/9/27/28	0/2/2/2
2	OMU	2	830	2	-	0/9/27/28	0/2/2/2
1	4AC	1	1755	1	-	2/11/29/30	0/2/2/2
1	4AC	1	2027	1	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	1	2287	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1934	1	-	0/11/29/30	0/2/2/2
2	OMU	2	787	2	-	4/9/27/28	0/2/2/2
2	OMG	2	657	2	-	0/9/27/28	0/3/3/3
1	4AC	1	1065	1	-	0/11/29/30	0/2/2/2
2	4AC	2	828	2	-	0/11/29/30	0/2/2/2
2	4AC	2	394	2	-	0/11/29/30	0/2/2/2
2	MA6	2	1487	2	-	0/11/29/30	0/3/3/3
1	4AC	1	2062	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1765	1	-	0/11/29/30	0/2/2/2
1	A2M	1	2173	1	-	0/9/27/28	0/3/3/3
1	4AC	1	2925	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	1048	1	-	0/11/29/30	0/2/2/2
1	4AC	1	694	1	-	0/11/29/30	0/2/2/2
2	MA6	2	1488	2	-	1/11/29/30	0/3/3/3
1	4AC	1	1780	1	-	0/11/29/30	0/2/2/2
1	4AC	1	60	1	-	0/11/29/30	0/2/2/2
2	4AC	2	839	2	-	0/11/29/30	0/2/2/2
2	4AC	2	1479	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1460	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	1239	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1068	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2992	1	-	2/11/29/30	0/2/2/2
1	4AC	1	2083	1	-	0/11/29/30	0/2/2/2
1	OMG	1	2138	1	-	0/9/27/28	0/3/3/3
1	4AC	1	2495	1	-	0/11/29/30	0/2/2/2
2	OMG	2	471	2	-	0/9/27/28	0/3/3/3
1	4AC	1	136	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1621	1	-	0/11/29/30	0/2/2/2
1	OMG	1	923	1,67	-	1/9/27/28	0/3/3/3
2	4AC	2	957	2	-	0/11/29/30	0/2/2/2
1	4AC	1	22	1	-	0/11/29/30	0/2/2/2
1	4AC	1	357	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2908	1	-	0/11/29/30	0/2/2/2
3	4AC	3	32	3	-	0/11/29/30	0/2/2/2
2	4AC	2	511	2	-	0/11/29/30	0/2/2/2
1	OMG	1	2678	1	-	0/9/27/28	0/3/3/3
2	OMG	2	913	2	-	0/9/27/28	0/3/3/3
1	4AC	1	3004	1	-	0/11/29/30	0/2/2/2
2	4AC	2	303	2	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4AC	2	851	2	-	0/11/29/30	0/2/2/2
2	OMG	2	1069	2	-	1/9/27/28	0/3/3/3
1	4AC	1	2545	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	1962	1	-	0/11/29/30	0/2/2/2

All (327) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1488	MA6	C5-C4	4.60	1.47	1.39
2	2	1469	6MZ	C5-C4	4.55	1.47	1.39
2	2	373	A2M	C5-C4	4.42	1.47	1.39
2	2	1487	MA6	C5-C4	4.41	1.47	1.39
1	1	1055	A2M	C5-C4	4.28	1.47	1.39
1	1	2173	A2M	C5-C4	4.27	1.47	1.39
2	2	680	OMG	C5-C4	3.22	1.47	1.38
2	2	657	OMG	C5-C4	3.15	1.47	1.38
1	1	2992	4AC	C5-C4	3.10	1.47	1.40
1	1	2147	OMG	C5-C4	3.08	1.47	1.38
2	2	471	OMG	C5-C4	3.02	1.47	1.38
1	1	2138	OMG	C5-C4	2.99	1.47	1.38
2	2	751	4AC	C5-C4	2.99	1.47	1.40
1	1	2495	4AC	C5-C4	2.98	1.47	1.40
1	1	2144	OMG	C5-C4	2.98	1.47	1.38
2	2	873	OMG	C5-C4	2.97	1.47	1.38
2	2	913	OMG	C5-C4	2.96	1.47	1.38
2	2	1505	5MC	C6-C5	2.96	1.39	1.34
2	2	467	OMG	C5-C4	2.96	1.47	1.38
1	1	2642	4AC	C5-C4	2.96	1.47	1.40
2	2	1069	OMG	C5-C4	2.95	1.47	1.38
2	2	1184	4AC	C5-C4	2.95	1.47	1.40
2	2	934	OMG	C5-C4	2.95	1.47	1.38
2	2	851	4AC	C5-C4	2.95	1.47	1.40
2	2	379	4AC	C5-C4	2.94	1.47	1.40
1	1	2083	4AC	C5-C4	2.94	1.47	1.40
1	1	829	4AC	C5-C4	2.94	1.47	1.40
1	1	314	4AC	C5-C4	2.94	1.47	1.40
2	2	511	4AC	C5-C4	2.93	1.47	1.40
1	1	1938	4AC	C5-C4	2.93	1.47	1.40
1	1	1867	4AC	C5-C4	2.93	1.47	1.40
2	2	1239	4AC	C5-C4	2.93	1.47	1.40
1	1	2545	4AC	C5-C4	2.93	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	328	OMG	C5-C4	2.92	1.46	1.38
2	2	519	OMG	C5-C4	2.92	1.46	1.38
2	2	718	4AC	C5-C4	2.92	1.47	1.40
2	2	546	4AC	C5-C4	2.92	1.47	1.40
2	2	636	4AC	C5-C4	2.92	1.47	1.40
1	1	641	4AC	C5-C4	2.92	1.47	1.40
1	1	789	OMG	C5-C4	2.91	1.46	1.38
2	2	590	4AC	C5-C4	2.91	1.47	1.40
1	1	2548	4AC	C5-C4	2.91	1.47	1.40
2	2	703	4AC	C5-C4	2.91	1.47	1.40
1	1	22	4AC	C5-C4	2.91	1.47	1.40
2	2	1233	4AC	C5-C4	2.90	1.47	1.40
1	1	1293	4AC	C5-C4	2.90	1.47	1.40
1	1	451	4AC	C5-C4	2.90	1.47	1.40
1	1	1765	4AC	C5-C4	2.90	1.47	1.40
2	2	828	4AC	C5-C4	2.90	1.47	1.40
1	1	2136	4AC	C5-C4	2.90	1.47	1.40
2	2	626	4AC	C5-C4	2.90	1.47	1.40
2	2	1028	4AC	C5-C4	2.90	1.47	1.40
1	1	1621	4AC	C5-C4	2.89	1.47	1.40
1	1	211	4AC	C5-C4	2.89	1.47	1.40
1	1	1695	4AC	C5-C4	2.89	1.47	1.40
1	1	3004	4AC	C5-C4	2.89	1.47	1.40
1	1	229	4AC	C5-C4	2.88	1.47	1.40
1	1	136	4AC	C5-C4	2.88	1.47	1.40
1	1	2570	4AC	C5-C4	2.88	1.47	1.40
2	2	479	4AC	C5-C4	2.88	1.47	1.40
1	1	60	4AC	C5-C4	2.88	1.47	1.40
3	3	32	4AC	C5-C4	2.88	1.47	1.40
1	1	243	4AC	C5-C4	2.88	1.47	1.40
2	2	868	4AC	C5-C4	2.87	1.47	1.40
2	2	957	4AC	C5-C4	2.87	1.47	1.40
2	2	20	OMU	C4-N3	-2.87	1.33	1.38
2	2	286	4AC	C5-C4	2.87	1.47	1.40
1	1	341	4AC	C5-C4	2.87	1.47	1.40
1	1	835	4AC	C5-C4	2.87	1.47	1.40
1	1	2865	4AC	C5-C4	2.86	1.47	1.40
2	2	53	4AC	C5-C4	2.86	1.47	1.40
2	2	17	4AC	C5-C4	2.86	1.47	1.40
2	2	303	4AC	C5-C4	2.86	1.47	1.40
1	1	357	4AC	C5-C4	2.86	1.46	1.40
1	1	1048	4AC	C5-C4	2.85	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2966	4AC	C5-C4	2.85	1.46	1.40
2	2	1487	MA6	C5-C6	2.85	1.49	1.41
1	1	2718	4AC	C5-C4	2.85	1.46	1.40
1	1	2925	4AC	C5-C4	2.85	1.46	1.40
1	1	1873	4AC	C5-C4	2.85	1.46	1.40
1	1	1068	4AC	C5-C4	2.85	1.46	1.40
2	2	731	4AC	C5-C4	2.85	1.46	1.40
1	1	694	4AC	C5-C4	2.85	1.46	1.40
2	2	839	4AC	C5-C4	2.85	1.46	1.40
1	1	1222	4AC	C5-C4	2.85	1.46	1.40
1	1	161	4AC	C5-C4	2.85	1.46	1.40
1	1	2678	OMG	C5-C4	2.85	1.46	1.38
1	1	2249	4AC	C5-C4	2.84	1.46	1.40
1	1	2960	4AC	C5-C4	2.84	1.46	1.40
1	1	458	4AC	C5-C4	2.84	1.46	1.40
1	1	533	4AC	C5-C4	2.84	1.46	1.40
1	1	1962	4AC	C5-C4	2.84	1.46	1.40
1	1	2329	4AC	C5-C4	2.84	1.46	1.40
1	1	1243	4AC	C5-C4	2.84	1.46	1.40
2	2	1147	4AC	C5-C4	2.84	1.46	1.40
1	1	2908	4AC	C5-C4	2.83	1.46	1.40
1	1	923	OMG	C5-C4	2.83	1.46	1.38
2	2	319	4AC	C5-C4	2.83	1.46	1.40
1	1	1667	4AC	C5-C4	2.83	1.46	1.40
1	1	1594	4AC	C5-C4	2.83	1.46	1.40
1	1	1554	4AC	C5-C4	2.83	1.46	1.40
2	2	848	4AC	C5-C4	2.82	1.46	1.40
1	1	2733	5MC	C6-C5	2.82	1.39	1.34
1	1	1550	4AC	C5-C4	2.82	1.46	1.40
1	1	922	4AC	C5-C4	2.82	1.46	1.40
1	1	1557	4AC	C5-C4	2.82	1.46	1.40
2	2	1479	4AC	C5-C4	2.80	1.46	1.40
1	1	2027	4AC	C5-C4	2.80	1.46	1.40
1	1	91	4AC	C5-C4	2.79	1.46	1.40
1	1	1885	4AC	C5-C4	2.79	1.46	1.40
1	1	1065	4AC	C5-C4	2.79	1.46	1.40
1	1	2062	4AC	C5-C4	2.79	1.46	1.40
2	2	394	4AC	C5-C4	2.79	1.46	1.40
1	1	2937	4AC	C5-C4	2.79	1.46	1.40
1	1	1934	4AC	C5-C4	2.78	1.46	1.40
2	2	1488	MA6	C5-C6	2.78	1.48	1.41
2	2	1380	OMU	C4-N3	-2.78	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1662	4AC	C5-C4	2.77	1.46	1.40
1	1	981	4AC	C5-C4	2.77	1.46	1.40
1	1	1460	4AC	C5-C4	2.77	1.46	1.40
2	2	787	OMU	C4-N3	-2.76	1.33	1.38
1	1	789	OMG	C6-N1	-2.76	1.33	1.38
1	1	1755	4AC	C5-C4	2.76	1.46	1.40
1	1	923	OMG	C6-N1	-2.75	1.33	1.38
1	1	1617	4AC	C5-C4	2.75	1.46	1.40
1	1	1878	4AC	C5-C4	2.75	1.46	1.40
1	1	802	4AC	C5-C4	2.73	1.46	1.40
2	2	1469	6MZ	C5-C6	2.73	1.49	1.41
2	2	471	OMG	C6-N1	-2.73	1.33	1.38
2	2	1202	5MC	C6-C5	2.72	1.39	1.34
1	1	328	OMG	C6-N1	-2.72	1.33	1.38
1	1	2287	4AC	C5-C4	2.71	1.46	1.40
1	1	2585	4AC	C4-N3	-2.71	1.28	1.32
1	1	2144	OMG	C6-N1	-2.71	1.33	1.38
2	2	830	OMU	C4-N3	-2.71	1.33	1.38
1	1	2678	OMG	C6-N1	-2.70	1.33	1.38
1	1	1780	4AC	C5-C4	2.70	1.46	1.40
2	2	873	OMG	C6-N1	-2.69	1.33	1.38
1	1	2138	OMG	C6-N1	-2.68	1.33	1.38
2	2	467	OMG	C6-N1	-2.68	1.33	1.38
2	2	657	OMG	C6-N1	-2.67	1.33	1.38
2	2	519	OMG	C6-N1	-2.65	1.33	1.38
2	2	934	OMG	C6-N1	-2.65	1.33	1.38
2	2	1177	OMU	C4-N3	-2.63	1.33	1.38
1	1	2203	5MC	C6-C5	2.62	1.38	1.34
2	2	913	OMG	C6-N1	-2.62	1.34	1.38
1	1	2163	5MC	C6-C5	2.62	1.38	1.34
1	1	2183	5MC	C6-C5	2.62	1.38	1.34
1	1	2784	OMU	C4-N3	-2.60	1.33	1.38
1	1	2162	5MC	C6-C5	2.60	1.38	1.34
1	1	229	4AC	C4-N3	-2.59	1.28	1.32
2	2	1069	OMG	C6-N1	-2.59	1.34	1.38
1	1	2093	5MC	C6-C5	2.58	1.38	1.34
2	2	680	OMG	C6-N1	-2.58	1.34	1.38
2	2	1025	5MC	C6-C5	2.57	1.38	1.34
2	2	693	5MC	C6-C5	2.57	1.38	1.34
1	1	2608	4AC	C5-C4	2.56	1.46	1.40
2	2	64	OMU	C4-N3	-2.56	1.34	1.38
2	2	373	A2M	C5-C6	2.56	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2173	A2M	C5-C6	2.56	1.48	1.41
1	1	2001	4AC	C5-C4	2.55	1.46	1.40
1	1	2585	4AC	C5-C4	2.53	1.46	1.40
2	2	1498	5MC	C6-C5	2.53	1.38	1.34
1	1	2608	4AC	C4-N3	-2.53	1.28	1.32
1	1	2147	OMG	C6-N1	-2.53	1.34	1.38
2	2	1374	5MC	C6-C5	2.52	1.38	1.34
2	2	1496	5MC	C6-N1	-2.52	1.33	1.38
2	2	535	5MC	C6-N1	-2.52	1.33	1.38
2	2	875	5MC	C6-C5	2.51	1.38	1.34
1	1	1055	A2M	C5-C6	2.51	1.48	1.41
2	2	875	5MC	C6-N1	-2.50	1.33	1.38
1	1	1621	4AC	C4-N3	-2.49	1.28	1.32
2	2	774	OMU	C4-N3	-2.49	1.34	1.38
1	1	789	OMG	C5-N7	-2.48	1.34	1.39
2	2	20	OMU	C2-N3	-2.48	1.33	1.38
1	1	922	4AC	C4-N3	-2.48	1.28	1.32
2	2	1496	5MC	C6-C5	2.47	1.38	1.34
1	1	1048	4AC	C4-N3	-2.47	1.28	1.32
1	1	2083	4AC	C4-N3	-2.46	1.28	1.32
1	1	2093	5MC	C6-N1	-2.45	1.33	1.38
2	2	787	OMU	C2-N3	-2.45	1.33	1.38
1	1	2249	4AC	C4-N3	-2.44	1.28	1.32
1	1	2198	5MC	C6-N1	-2.44	1.33	1.38
1	1	923	OMG	C5-N7	-2.43	1.34	1.39
1	1	1885	4AC	C4-N3	-2.43	1.28	1.32
1	1	2001	4AC	C4-N3	-2.43	1.28	1.32
2	2	1498	5MC	C6-N1	-2.42	1.33	1.38
2	2	535	5MC	C6-C5	2.42	1.38	1.34
1	1	1873	4AC	C4-N3	-2.42	1.28	1.32
2	2	680	OMG	C5-N7	-2.42	1.34	1.39
1	1	1938	4AC	C4-N3	-2.41	1.28	1.32
1	1	829	4AC	C4-N3	-2.41	1.28	1.32
1	1	3004	4AC	C4-N3	-2.41	1.28	1.32
1	1	2183	5MC	C6-N1	-2.41	1.33	1.38
1	1	2203	5MC	C6-N1	-2.41	1.33	1.38
2	2	1380	OMU	C2-N3	-2.41	1.33	1.38
1	1	22	4AC	C4-N3	-2.41	1.28	1.32
1	1	1557	4AC	C4-N3	-2.41	1.28	1.32
1	1	1055	A2M	C5-N7	-2.40	1.34	1.39
1	1	981	4AC	C4-N3	-2.40	1.28	1.32
2	2	1374	5MC	C6-N1	-2.40	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2784	OMU	C2-N3	-2.40	1.33	1.38
1	1	314	4AC	C4-N3	-2.40	1.28	1.32
1	1	2198	5MC	C6-C5	2.40	1.38	1.34
1	1	1068	4AC	C4-N3	-2.40	1.28	1.32
2	2	1025	5MC	C6-N1	-2.39	1.34	1.38
1	1	2495	4AC	C4-N3	-2.39	1.28	1.32
2	2	693	5MC	C6-N1	-2.38	1.34	1.38
2	2	1202	5MC	C6-N1	-2.38	1.34	1.38
1	1	2162	5MC	C6-N1	-2.38	1.34	1.38
1	1	835	4AC	C4-N3	-2.37	1.28	1.32
1	1	1243	4AC	C4-N3	-2.37	1.28	1.32
1	1	2173	A2M	C5-N7	-2.37	1.34	1.39
1	1	1934	4AC	C4-N3	-2.36	1.28	1.32
1	1	2062	4AC	C4-N3	-2.36	1.28	1.32
2	2	657	OMG	C5-N7	-2.36	1.34	1.39
1	1	1554	4AC	C4-N3	-2.36	1.28	1.32
2	2	17	4AC	C4-N3	-2.36	1.28	1.32
1	1	1594	4AC	C4-N3	-2.35	1.28	1.32
2	2	373	A2M	C5-N7	-2.34	1.34	1.39
1	1	2678	OMG	C5-N7	-2.34	1.34	1.39
1	1	2163	5MC	C6-N1	-2.34	1.34	1.38
1	1	2925	4AC	C4-N3	-2.34	1.28	1.32
1	1	328	OMG	C5-N7	-2.34	1.34	1.39
1	1	1667	4AC	C4-N3	-2.33	1.28	1.32
1	1	1878	4AC	C4-N3	-2.33	1.28	1.32
2	2	373	A2M	C8-N7	2.33	1.36	1.31
1	1	641	4AC	C4-N3	-2.33	1.28	1.32
1	1	136	4AC	C4-N3	-2.32	1.28	1.32
1	1	2992	4AC	C4-N3	-2.32	1.28	1.32
1	1	2733	5MC	C6-N1	-2.32	1.34	1.38
2	2	471	OMG	C5-N7	-2.32	1.34	1.39
1	1	1962	4AC	C4-N3	-2.32	1.28	1.32
1	1	2966	4AC	C4-N3	-2.31	1.28	1.32
1	1	341	4AC	C4-N3	-2.31	1.28	1.32
1	1	1617	4AC	C4-N3	-2.31	1.28	1.32
1	1	2865	4AC	C4-N3	-2.31	1.28	1.32
1	1	1222	4AC	C4-N3	-2.31	1.28	1.32
1	1	2908	4AC	C4-N3	-2.31	1.28	1.32
1	1	2138	OMG	C5-N7	-2.30	1.34	1.39
1	1	694	4AC	C4-N3	-2.30	1.28	1.32
1	1	2718	4AC	C4-N3	-2.30	1.28	1.32
1	1	2136	4AC	C4-N3	-2.30	1.28	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	533	4AC	C4-N3	-2.30	1.28	1.32
2	2	851	4AC	C4-N3	-2.30	1.28	1.32
1	1	802	4AC	C4-N3	-2.30	1.28	1.32
2	2	1040	OMC	C6-N1	-2.30	1.32	1.38
2	2	873	OMG	C5-N7	-2.30	1.34	1.39
1	1	2027	4AC	C4-N3	-2.29	1.28	1.32
1	1	357	4AC	C4-N3	-2.29	1.28	1.32
1	1	161	4AC	C4-N3	-2.29	1.28	1.32
1	1	2144	OMG	C5-N7	-2.29	1.34	1.39
1	1	2642	4AC	C4-N3	-2.28	1.28	1.32
2	2	830	OMU	C2-N3	-2.28	1.33	1.38
1	1	243	4AC	C4-N3	-2.28	1.28	1.32
2	2	868	4AC	C4-N3	-2.27	1.28	1.32
1	1	2570	4AC	C4-N3	-2.27	1.28	1.32
2	2	511	4AC	C4-N3	-2.27	1.28	1.32
1	1	451	4AC	C4-N3	-2.27	1.28	1.32
1	1	1765	4AC	C4-N3	-2.27	1.28	1.32
1	1	1460	4AC	C4-N3	-2.27	1.28	1.32
1	1	2329	4AC	C4-N3	-2.26	1.28	1.32
1	1	211	4AC	C4-N3	-2.26	1.28	1.32
1	1	2960	4AC	C4-N3	-2.26	1.28	1.32
2	2	1479	4AC	C4-N3	-2.26	1.28	1.32
1	1	2548	4AC	C4-N3	-2.26	1.28	1.32
2	2	64	OMU	C2-N3	-2.25	1.33	1.38
2	2	839	4AC	C4-N3	-2.25	1.28	1.32
1	1	91	4AC	C4-N3	-2.25	1.28	1.32
1	1	1550	4AC	C4-N3	-2.25	1.28	1.32
2	2	1177	OMU	C2-N3	-2.25	1.34	1.38
2	2	303	4AC	C4-N3	-2.24	1.28	1.32
1	1	2937	4AC	C4-N3	-2.24	1.28	1.32
1	1	2147	OMG	C5-N7	-2.24	1.34	1.39
2	2	1469	6MZ	C5-N7	-2.24	1.34	1.39
1	1	1867	4AC	C4-N3	-2.24	1.28	1.32
1	1	2173	A2M	C8-N7	2.24	1.35	1.31
2	2	1487	MA6	C8-N7	2.24	1.35	1.31
2	2	286	4AC	C4-N3	-2.23	1.28	1.32
2	2	319	4AC	C4-N3	-2.23	1.28	1.32
1	1	2287	4AC	C4-N3	-2.22	1.28	1.32
2	2	718	4AC	C4-N3	-2.22	1.28	1.32
2	2	1069	OMG	C5-N7	-2.22	1.34	1.39
2	2	467	OMG	C5-N7	-2.22	1.34	1.39
2	2	519	OMG	C5-N7	-2.22	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	934	OMG	C5-N7	-2.22	1.34	1.39
2	2	590	4AC	C4-N3	-2.21	1.29	1.32
1	1	1065	4AC	C4-N3	-2.21	1.29	1.32
2	2	774	OMU	C2-N3	-2.21	1.34	1.38
2	2	848	4AC	C4-N3	-2.20	1.29	1.32
1	1	2545	4AC	C4-N3	-2.20	1.29	1.32
1	1	1055	A2M	C8-N7	2.20	1.35	1.31
2	2	1028	4AC	C4-N3	-2.20	1.29	1.32
2	2	1469	6MZ	C8-N7	2.19	1.35	1.31
2	2	1488	MA6	C5-N7	-2.19	1.34	1.39
2	2	828	4AC	C4-N3	-2.19	1.29	1.32
1	1	1293	4AC	C4-N3	-2.19	1.29	1.32
1	1	1695	4AC	C4-N3	-2.18	1.29	1.32
1	1	1662	4AC	C4-N3	-2.17	1.29	1.32
2	2	913	OMG	C5-N7	-2.16	1.34	1.39
2	2	1147	4AC	C4-N3	-2.16	1.29	1.32
3	3	32	4AC	C4-N3	-2.16	1.29	1.32
2	2	957	4AC	C4-N3	-2.15	1.29	1.32
2	2	1184	4AC	C4-N3	-2.15	1.29	1.32
1	1	458	4AC	C4-N3	-2.15	1.29	1.32
1	1	1780	4AC	C4-N3	-2.13	1.29	1.32
2	2	53	4AC	C4-N3	-2.13	1.29	1.32
2	2	1040	OMC	C5-C4	-2.13	1.38	1.42
2	2	1380	OMU	C2-N1	2.13	1.41	1.38
2	2	1488	MA6	C8-N7	2.13	1.35	1.31
1	1	2784	OMU	C5-C4	-2.13	1.38	1.43
2	2	379	4AC	C4-N3	-2.09	1.29	1.32
2	2	1233	4AC	C4-N3	-2.09	1.29	1.32
2	2	1239	4AC	C4-N3	-2.09	1.29	1.32
2	2	1487	MA6	C5-N7	-2.08	1.35	1.39
2	2	830	OMU	C5-C4	-2.08	1.39	1.43
2	2	546	4AC	C4-N3	-2.08	1.29	1.32
2	2	1177	OMU	C5-C4	-2.08	1.39	1.43
2	2	1505	5MC	C6-N1	-2.08	1.34	1.38
2	2	731	4AC	C4-N3	-2.07	1.29	1.32
1	1	60	4AC	C4-N3	-2.07	1.29	1.32
2	2	479	4AC	C4-N3	-2.07	1.29	1.32
2	2	751	4AC	C4-N3	-2.06	1.29	1.32
2	2	394	4AC	C4-N3	-2.04	1.29	1.32
2	2	20	OMU	C5-C4	-2.03	1.39	1.43
1	1	1755	4AC	C4-N3	-2.03	1.29	1.32
2	2	64	OMU	C5-C4	-2.02	1.39	1.43

All (637) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	680	OMG	C5-C4-N3	-6.70	117.59	128.46
2	2	657	OMG	C5-C4-N3	-6.41	118.06	128.46
2	2	373	A2M	C5-C4-N3	-6.32	118.51	126.75
1	1	2173	A2M	C5-C4-N3	-6.32	118.51	126.75
1	1	1055	A2M	C5-C4-N3	-6.28	118.56	126.75
1	1	2147	OMG	C5-C4-N3	-6.22	118.37	128.46
2	2	471	OMG	C5-C4-N3	-6.19	118.41	128.46
1	1	328	OMG	C5-C4-N3	-6.13	118.51	128.46
1	1	2144	OMG	C5-C4-N3	-6.08	118.60	128.46
2	2	467	OMG	C5-C4-N3	-6.07	118.61	128.46
2	2	873	OMG	C5-C4-N3	-6.06	118.63	128.46
1	1	789	OMG	C5-C4-N3	-6.05	118.64	128.46
1	1	2138	OMG	C5-C4-N3	-6.05	118.64	128.46
2	2	1469	6MZ	C5-C4-N3	-6.02	118.90	126.75
2	2	934	OMG	C5-C4-N3	-6.00	118.72	128.46
2	2	1488	MA6	C5-C4-N3	-5.99	118.94	126.75
1	1	2678	OMG	C5-C4-N3	-5.97	118.78	128.46
2	2	1069	OMG	C5-C4-N3	-5.93	118.85	128.46
2	2	519	OMG	C5-C4-N3	-5.86	118.95	128.46
2	2	913	OMG	C5-C4-N3	-5.86	118.95	128.46
1	1	923	OMG	C5-C4-N3	-5.86	118.96	128.46
2	2	1467	UR3	C4-N3-C2	-5.72	119.18	124.56
2	2	1487	MA6	C5-C4-N3	-5.62	119.42	126.75
1	1	2001	4AC	O7-C7-N4	5.40	130.56	121.82
1	1	1755	4AC	O7-C7-N4	5.27	130.35	121.82
2	2	680	OMG	N9-C4-N3	5.22	136.41	125.94
1	1	1780	4AC	O7-C7-N4	5.13	130.13	121.82
2	2	680	OMG	C2-N3-C4	4.96	121.14	112.30
2	2	787	OMU	C4-N3-C2	-4.94	120.06	126.58
1	1	1878	4AC	O7-C7-N4	4.93	129.80	121.82
1	1	1055	A2M	N3-C4-N9	4.87	135.10	127.08
1	1	2937	4AC	C5-C4-N4	-4.84	114.51	122.92
1	1	2678	OMG	C2-N3-C4	4.84	120.93	112.30
1	1	2144	OMG	C2-N3-C4	4.84	120.93	112.30
1	1	2147	OMG	C2-N3-C4	4.84	120.93	112.30
1	1	2173	A2M	N3-C4-N9	4.83	135.05	127.08
2	2	934	OMG	C2-N3-C4	4.83	120.91	112.30
1	1	789	OMG	C2-N3-C4	4.83	120.90	112.30
2	2	373	A2M	N3-C4-N9	4.82	135.02	127.08
2	2	1069	OMG	C2-N3-C4	4.82	120.88	112.30
2	2	467	OMG	C2-N3-C4	4.82	120.88	112.30
2	2	471	OMG	C2-N3-C4	4.81	120.87	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	20	OMU	C4-N3-C2	-4.80	120.24	126.58
2	2	657	OMG	N9-C4-N3	4.80	135.57	125.94
1	1	923	OMG	C2-N3-C4	4.79	120.84	112.30
2	2	657	OMG	C2-N3-C4	4.79	120.84	112.30
2	2	873	OMG	C2-N3-C4	4.79	120.83	112.30
2	2	913	OMG	C2-N3-C4	4.78	120.82	112.30
1	1	2138	OMG	C2-N3-C4	4.78	120.81	112.30
1	1	328	OMG	C2-N3-C4	4.77	120.80	112.30
1	1	2608	4AC	N4-C4-N3	4.75	121.82	113.85
2	2	519	OMG	C2-N3-C4	4.74	120.74	112.30
1	1	2147	OMG	N9-C4-N3	4.72	135.42	125.94
1	1	2937	4AC	N4-C4-N3	4.69	121.73	113.85
2	2	471	OMG	N9-C4-N3	4.68	135.33	125.94
1	1	1934	4AC	O7-C7-N4	4.62	129.30	121.82
2	2	873	OMG	N9-C4-N3	4.61	135.20	125.94
2	2	626	4AC	O7-C7-N4	4.61	129.27	121.82
1	1	328	OMG	N9-C4-N3	4.61	135.19	125.94
2	2	731	4AC	O7-C7-N4	4.60	129.26	121.82
1	1	1065	4AC	O7-C7-N4	4.59	129.24	121.82
1	1	2144	OMG	N9-C4-N3	4.58	135.14	125.94
1	1	1460	4AC	O7-C7-N4	4.58	129.23	121.82
2	2	17	4AC	O7-C7-N4	4.58	129.22	121.82
1	1	2608	4AC	C5-C4-N4	-4.57	114.98	122.92
2	2	774	OMU	C4-N3-C2	-4.56	120.57	126.58
1	1	789	OMG	N9-C4-N3	4.56	135.09	125.94
1	1	1617	4AC	O7-C7-N4	4.56	129.19	121.82
1	1	2249	4AC	O7-C7-N4	4.56	129.19	121.82
1	1	922	4AC	O7-C7-N4	4.55	129.18	121.82
1	1	91	4AC	O7-C7-N4	4.55	129.18	121.82
1	1	1048	4AC	O7-C7-N4	4.55	129.18	121.82
1	1	1662	4AC	O7-C7-N4	4.54	129.16	121.82
1	1	1243	4AC	O7-C7-N4	4.54	129.16	121.82
1	1	1962	4AC	O7-C7-N4	4.53	129.15	121.82
2	2	1147	4AC	O7-C7-N4	4.52	129.14	121.82
1	1	1068	4AC	O7-C7-N4	4.52	129.14	121.82
2	2	1028	4AC	O7-C7-N4	4.52	129.14	121.82
2	2	1487	MA6	C2-N1-C6	4.51	122.41	111.75
2	2	636	4AC	O7-C7-N4	4.51	129.12	121.82
1	1	2138	OMG	N9-C4-N3	4.51	135.00	125.94
3	3	32	4AC	O7-C7-N4	4.51	129.12	121.82
2	2	839	4AC	O7-C7-N4	4.51	129.11	121.82
2	2	848	4AC	O7-C7-N4	4.51	129.11	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1554	4AC	O7-C7-N4	4.50	129.11	121.82
2	2	467	OMG	N9-C4-N3	4.50	134.98	125.94
1	1	458	4AC	O7-C7-N4	4.50	129.10	121.82
2	2	319	4AC	O7-C7-N4	4.50	129.10	121.82
1	1	1938	4AC	O7-C7-N4	4.50	129.10	121.82
1	1	641	4AC	O7-C7-N4	4.50	129.10	121.82
2	2	703	4AC	O7-C7-N4	4.50	129.10	121.82
1	1	229	4AC	O7-C7-N4	4.50	129.10	121.82
1	1	1594	4AC	O7-C7-N4	4.49	129.09	121.82
1	1	2287	4AC	O7-C7-N4	4.49	129.09	121.82
2	2	303	4AC	O7-C7-N4	4.49	129.09	121.82
1	1	2718	4AC	O7-C7-N4	4.49	129.09	121.82
1	1	2784	OMU	C4-N3-C2	-4.49	120.66	126.58
2	2	379	4AC	O7-C7-N4	4.49	129.08	121.82
2	2	1233	4AC	O7-C7-N4	4.49	129.08	121.82
1	1	2136	4AC	O7-C7-N4	4.49	129.08	121.82
1	1	2329	4AC	O7-C7-N4	4.49	129.08	121.82
1	1	2925	4AC	O7-C7-N4	4.48	129.07	121.82
2	2	1380	OMU	C4-N3-C2	-4.48	120.67	126.58
2	2	53	4AC	O7-C7-N4	4.48	129.07	121.82
1	1	2585	4AC	N4-C4-N3	4.48	121.37	113.85
1	1	341	4AC	O7-C7-N4	4.48	129.07	121.82
1	1	2678	OMG	N9-C4-N3	4.48	134.93	125.94
1	1	1293	4AC	O7-C7-N4	4.47	129.06	121.82
1	1	1765	4AC	O7-C7-N4	4.47	129.06	121.82
1	1	802	4AC	O7-C7-N4	4.47	129.05	121.82
2	2	511	4AC	O7-C7-N4	4.47	129.04	121.82
1	1	1873	4AC	O7-C7-N4	4.46	129.04	121.82
2	2	1488	MA6	C2-N1-C6	4.46	122.30	111.75
1	1	243	4AC	O7-C7-N4	4.46	129.03	121.82
2	2	1488	MA6	N3-C4-N9	4.46	134.43	127.08
2	2	1069	OMG	N9-C4-N3	4.45	134.88	125.94
1	1	533	4AC	O7-C7-N4	4.45	129.02	121.82
1	1	1867	4AC	O7-C7-N4	4.45	129.02	121.82
1	1	2027	4AC	O7-C7-N4	4.44	129.01	121.82
2	2	479	4AC	O7-C7-N4	4.44	129.01	121.82
2	2	957	4AC	O7-C7-N4	4.44	129.01	121.82
1	1	2966	4AC	O7-C7-N4	4.44	129.01	121.82
1	1	1667	4AC	O7-C7-N4	4.44	129.01	121.82
2	2	546	4AC	O7-C7-N4	4.44	129.01	121.82
1	1	2545	4AC	O7-C7-N4	4.44	129.00	121.82
2	2	394	4AC	O7-C7-N4	4.44	129.00	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1621	4AC	O7-C7-N4	4.43	128.99	121.82
1	1	211	4AC	O7-C7-N4	4.43	128.99	121.82
1	1	694	4AC	O7-C7-N4	4.43	128.99	121.82
2	2	934	OMG	N9-C4-N3	4.43	134.83	125.94
1	1	451	4AC	O7-C7-N4	4.43	128.99	121.82
1	1	1222	4AC	O7-C7-N4	4.43	128.98	121.82
1	1	2570	4AC	O7-C7-N4	4.43	128.98	121.82
1	1	2548	4AC	O7-C7-N4	4.43	128.98	121.82
1	1	357	4AC	O7-C7-N4	4.42	128.97	121.82
1	1	1695	4AC	O7-C7-N4	4.41	128.96	121.82
1	1	2865	4AC	O7-C7-N4	4.41	128.96	121.82
1	1	2960	4AC	O7-C7-N4	4.41	128.95	121.82
2	2	751	4AC	O7-C7-N4	4.41	128.95	121.82
2	2	1177	OMU	C4-N3-C2	-4.40	120.77	126.58
1	1	22	4AC	O7-C7-N4	4.40	128.94	121.82
1	1	1557	4AC	O7-C7-N4	4.40	128.94	121.82
2	2	828	4AC	O7-C7-N4	4.39	128.93	121.82
1	1	161	4AC	O7-C7-N4	4.39	128.93	121.82
2	2	718	4AC	O7-C7-N4	4.39	128.92	121.82
2	2	1479	4AC	O7-C7-N4	4.39	128.92	121.82
1	1	60	4AC	O7-C7-N4	4.39	128.92	121.82
1	1	2495	4AC	O7-C7-N4	4.38	128.91	121.82
1	1	981	4AC	O7-C7-N4	4.38	128.91	121.82
1	1	2062	4AC	O7-C7-N4	4.38	128.91	121.82
2	2	590	4AC	O7-C7-N4	4.38	128.90	121.82
2	2	830	OMU	C4-N3-C2	-4.38	120.81	126.58
1	1	2642	4AC	O7-C7-N4	4.38	128.90	121.82
2	2	64	OMU	C4-N3-C2	-4.38	120.81	126.58
1	1	3004	4AC	O7-C7-N4	4.38	128.90	121.82
2	2	1469	6MZ	N3-C4-N9	4.37	134.29	127.08
1	1	1550	4AC	O7-C7-N4	4.37	128.89	121.82
2	2	787	OMU	N3-C2-N1	4.37	120.69	114.89
1	1	835	4AC	O7-C7-N4	4.37	128.88	121.82
1	1	314	4AC	O7-C7-N4	4.36	128.88	121.82
2	2	286	4AC	O7-C7-N4	4.36	128.87	121.82
2	2	1184	4AC	O7-C7-N4	4.36	128.87	121.82
2	2	1469	6MZ	C6-C5-N7	4.36	137.10	132.39
1	1	1885	4AC	O7-C7-N4	4.35	128.87	121.82
1	1	2908	4AC	O7-C7-N4	4.35	128.86	121.82
1	1	923	OMG	N9-C4-N3	4.35	134.67	125.94
2	2	20	OMU	N3-C2-N1	4.33	120.64	114.89
2	2	519	OMG	N9-C4-N3	4.32	134.62	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	913	OMG	N9-C4-N3	4.32	134.61	125.94
2	2	1380	OMU	N3-C2-N1	4.29	120.59	114.89
1	1	829	4AC	O7-C7-N4	4.29	128.77	121.82
2	2	1239	4AC	O7-C7-N4	4.29	128.77	121.82
1	1	136	4AC	O7-C7-N4	4.29	128.75	121.82
2	2	1487	MA6	N3-C4-N9	4.26	134.11	127.08
1	1	2083	4AC	O7-C7-N4	4.25	128.70	121.82
2	2	851	4AC	O7-C7-N4	4.23	128.67	121.82
1	1	2585	4AC	C5-C4-N4	-4.21	115.61	122.92
2	2	868	4AC	O7-C7-N4	4.19	128.59	121.82
1	1	2784	OMU	N3-C2-N1	4.16	120.41	114.89
2	2	774	OMU	N3-C2-N1	4.15	120.40	114.89
2	2	830	OMU	N3-C2-N1	4.15	120.40	114.89
2	2	1177	OMU	N3-C2-N1	4.08	120.31	114.89
2	2	64	OMU	N3-C2-N1	4.04	120.25	114.89
1	1	1755	4AC	C5-C4-N4	-4.03	115.92	122.92
1	1	2173	A2M	C2-N3-C4	3.92	121.02	111.75
2	2	1469	6MZ	C4-C5-N7	-3.91	105.86	110.62
2	2	1469	6MZ	C2-N3-C4	3.89	120.95	111.75
1	1	1055	A2M	C2-N3-C4	3.86	120.87	111.75
2	2	1488	MA6	C2-N3-C4	3.86	120.86	111.75
2	2	373	A2M	C2-N3-C4	3.85	120.85	111.75
2	2	787	OMU	C5-C4-N3	3.81	120.54	114.84
2	2	1487	MA6	C4-C5-N7	-3.78	106.02	110.62
2	2	1487	MA6	C2-N3-C4	3.78	120.67	111.75
2	2	1488	MA6	C4-C5-N7	-3.74	106.07	110.62
2	2	20	OMU	C5-C4-N3	3.73	120.43	114.84
1	1	2183	5MC	C5-C6-N1	-3.66	119.57	123.34
1	1	2093	5MC	C5-C6-N1	-3.66	119.57	123.34
1	1	1755	4AC	N4-C4-N3	3.65	119.97	113.85
2	2	1025	5MC	C5-C6-N1	-3.63	119.60	123.34
1	1	2784	OMU	C5-C4-N3	3.61	120.24	114.84
1	1	2198	5MC	C5-C6-N1	-3.60	119.63	123.34
2	2	64	OMU	C5-C4-N3	3.60	120.23	114.84
2	2	1202	5MC	C5-C6-N1	-3.59	119.65	123.34
2	2	875	5MC	C5-C6-N1	-3.58	119.66	123.34
2	2	774	OMU	C5-C4-N3	3.57	120.18	114.84
2	2	703	4AC	N4-C4-N3	3.57	119.84	113.85
2	2	1374	5MC	C5-C6-N1	-3.56	119.67	123.34
1	1	2733	5MC	C5-C6-N1	-3.56	119.67	123.34
2	2	535	5MC	C5-C6-N1	-3.56	119.68	123.34
2	2	1177	OMU	C5-C4-N3	3.55	120.16	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	830	OMU	C5-C4-N3	3.55	120.15	114.84
2	2	1496	5MC	C5-C6-N1	-3.55	119.69	123.34
2	2	693	5MC	C5-C6-N1	-3.54	119.69	123.34
1	1	2203	5MC	C5-C6-N1	-3.54	119.70	123.34
2	2	1380	OMU	C5-C4-N3	3.52	120.10	114.84
1	1	1780	4AC	C5-C4-N4	-3.50	116.84	122.92
1	1	2937	4AC	O7-C7-N4	3.47	127.43	121.82
1	1	2585	4AC	O2-C2-N3	-3.45	116.72	122.33
1	1	2001	4AC	CM7-C7-N4	-3.45	109.33	115.29
2	2	626	4AC	N4-C4-N3	3.44	119.62	113.85
1	1	1878	4AC	CM7-C7-N4	-3.42	109.37	115.29
1	1	2585	4AC	O7-C7-N4	3.40	127.32	121.82
2	2	913	OMG	C6-C5-N7	3.39	136.55	130.25
1	1	2162	5MC	C5-C6-N1	-3.37	119.87	123.34
1	1	923	OMG	C6-C5-N7	3.33	136.44	130.25
2	2	1487	MA6	N1-C2-N3	-3.32	123.42	128.60
2	2	519	OMG	C6-C5-N7	3.31	136.40	130.25
2	2	546	4AC	N4-C4-N3	3.31	119.40	113.85
2	2	934	OMG	C6-C5-N7	3.31	136.40	130.25
1	1	2608	4AC	O7-C7-N4	3.30	127.16	121.82
2	2	1069	OMG	C6-C5-N7	3.27	136.34	130.25
1	1	2163	5MC	C5-C6-N1	-3.27	119.97	123.34
1	1	60	4AC	N4-C4-N3	3.27	119.33	113.85
2	2	1469	6MZ	N1-C2-N3	-3.26	123.50	128.60
2	2	1488	MA6	N1-C2-N3	-3.26	123.51	128.60
2	2	373	A2M	C4-C5-N7	-3.25	106.66	110.62
1	1	2287	4AC	N4-C4-N3	3.24	119.30	113.85
2	2	703	4AC	C5-C4-N4	-3.23	117.32	122.92
2	2	394	4AC	N4-C4-N3	3.22	119.26	113.85
1	1	2678	OMG	C6-C5-N7	3.22	136.23	130.25
2	2	626	4AC	C5-C4-N4	-3.21	117.35	122.92
2	2	1184	4AC	N4-C4-N3	3.20	119.23	113.85
2	2	731	4AC	N4-C4-N3	3.19	119.21	113.85
1	1	1055	A2M	C4-C5-N7	-3.19	106.74	110.62
1	1	1780	4AC	N4-C4-N3	3.18	119.18	113.85
1	1	1662	4AC	N4-C4-N3	3.17	119.18	113.85
2	2	1505	5MC	C5-C6-N1	-3.17	120.08	123.34
1	1	2138	OMG	C6-C5-N7	3.16	136.12	130.25
1	1	2173	A2M	C4-C5-N7	-3.16	106.78	110.62
2	2	1233	4AC	N4-C4-N3	3.15	119.13	113.85
2	2	731	4AC	C5-C4-N4	-3.14	117.46	122.92
2	2	467	OMG	C6-C5-N7	3.14	136.08	130.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2173	A2M	N3-C2-N1	-3.13	123.71	128.60
1	1	922	4AC	N4-C4-N3	3.13	119.11	113.85
1	1	789	OMG	C6-C5-N7	3.11	136.03	130.25
1	1	2608	4AC	O2-C2-N3	-3.11	117.27	122.33
2	2	636	4AC	N4-C4-N3	3.11	119.07	113.85
1	1	1065	4AC	N4-C4-N3	3.11	119.07	113.85
2	2	479	4AC	N4-C4-N3	3.11	119.07	113.85
1	1	229	4AC	CM7-C7-N4	-3.10	109.93	115.29
1	1	328	OMG	C6-C5-N7	3.10	136.01	130.25
2	2	1487	MA6	C5-N7-C8	3.10	107.91	103.51
1	1	2144	OMG	C6-C5-N7	3.09	135.99	130.25
2	2	546	4AC	C5-C4-N4	-3.08	117.57	122.92
3	3	32	4AC	N4-C4-N3	3.07	119.00	113.85
2	2	1177	OMU	O4-C4-C5	-3.05	119.79	125.16
2	2	1469	6MZ	C5-N7-C8	3.05	107.85	103.51
1	1	91	4AC	N4-C4-N3	3.05	118.97	113.85
1	1	1055	A2M	N3-C2-N1	-3.05	123.83	128.60
2	2	873	OMG	C6-C5-N7	3.05	135.92	130.25
2	2	636	4AC	C5-C4-N4	-3.04	117.63	122.92
2	2	731	4AC	CM7-C7-N4	-3.04	110.03	115.29
1	1	1878	4AC	C5-C4-N4	-3.04	117.63	122.92
2	2	1498	5MC	C5-C6-N1	-3.04	120.21	123.34
1	1	1617	4AC	N4-C4-N3	3.04	118.96	113.85
2	2	1184	4AC	C5-C4-N4	-3.04	117.64	122.92
2	2	379	4AC	N4-C4-N3	3.03	118.94	113.85
2	2	17	4AC	CM7-C7-N4	-3.03	110.06	115.29
2	2	373	A2M	N3-C2-N1	-3.02	123.88	128.60
2	2	53	4AC	N4-C4-N3	3.02	118.92	113.85
1	1	802	4AC	N4-C4-N3	3.02	118.92	113.85
1	1	2718	4AC	N4-C4-N3	3.01	118.91	113.85
2	2	1233	4AC	C5-C4-N4	-3.01	117.69	122.92
2	2	1147	4AC	N4-C4-N3	3.01	118.90	113.85
2	2	64	OMU	O4-C4-C5	-3.00	119.88	125.16
2	2	1028	4AC	N4-C4-N3	3.00	118.89	113.85
1	1	2784	OMU	O4-C4-C5	-3.00	119.88	125.16
2	2	636	4AC	CM7-C7-N4	-3.00	110.11	115.29
1	1	1938	4AC	CM7-C7-N4	-3.00	110.11	115.29
1	1	641	4AC	CM7-C7-N4	-2.99	110.11	115.29
1	1	2147	OMG	C6-C5-N7	2.99	135.82	130.25
2	2	479	4AC	C5-C4-N4	-2.99	117.72	122.92
1	1	1662	4AC	C5-C4-N4	-2.99	117.72	122.92
1	1	458	4AC	N4-C4-N3	2.99	118.87	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	511	4AC	CM7-C7-N4	-2.98	110.14	115.29
2	2	319	4AC	N4-C4-N3	2.98	118.86	113.85
1	1	1048	4AC	CM7-C7-N4	-2.98	110.14	115.29
2	2	839	4AC	CM7-C7-N4	-2.98	110.14	115.29
2	2	1488	MA6	C5-N7-C8	2.98	107.74	103.51
1	1	2249	4AC	CM7-C7-N4	-2.97	110.16	115.29
2	2	471	OMG	C6-C5-N7	2.97	135.77	130.25
1	1	1460	4AC	N4-C4-N3	2.96	118.82	113.85
1	1	1934	4AC	N4-C4-N3	2.96	118.82	113.85
1	1	22	4AC	CM7-C7-N4	-2.96	110.18	115.29
1	1	1293	4AC	CM7-C7-N4	-2.96	110.18	115.29
2	2	774	OMU	O4-C4-C5	-2.96	119.96	125.16
1	1	1243	4AC	CM7-C7-N4	-2.95	110.18	115.29
1	1	2136	4AC	CM7-C7-N4	-2.95	110.19	115.29
1	1	2966	4AC	CM7-C7-N4	-2.95	110.19	115.29
1	1	357	4AC	N4-C4-N3	2.95	118.80	113.85
2	2	957	4AC	N4-C4-N3	2.95	118.80	113.85
2	2	379	4AC	C5-C4-N4	-2.95	117.80	122.92
1	1	2925	4AC	CM7-C7-N4	-2.94	110.21	115.29
1	1	211	4AC	CM7-C7-N4	-2.94	110.21	115.29
1	1	1873	4AC	CM7-C7-N4	-2.94	110.22	115.29
1	1	1293	4AC	N4-C4-N3	2.94	118.78	113.85
2	2	848	4AC	CM7-C7-N4	-2.94	110.22	115.29
2	2	828	4AC	N4-C4-N3	2.94	118.78	113.85
1	1	60	4AC	C5-C4-N4	-2.93	117.82	122.92
2	2	1147	4AC	CM7-C7-N4	-2.93	110.22	115.29
2	2	1487	MA6	C4-N9-C8	2.93	108.90	105.73
1	1	1962	4AC	CM7-C7-N4	-2.93	110.23	115.29
2	2	394	4AC	C5-C4-N4	-2.93	117.84	122.92
1	1	533	4AC	N4-C4-N3	2.92	118.76	113.85
1	1	1617	4AC	C5-C4-N4	-2.92	117.84	122.92
2	2	751	4AC	N4-C4-N3	2.92	118.76	113.85
1	1	2329	4AC	N4-C4-N3	2.92	118.76	113.85
2	2	1239	4AC	N4-C4-N3	2.92	118.75	113.85
1	1	1878	4AC	N4-C4-N3	2.92	118.75	113.85
2	2	303	4AC	N4-C4-N3	2.91	118.74	113.85
1	1	2545	4AC	CM7-C7-N4	-2.91	110.26	115.29
1	1	2960	4AC	N4-C4-N3	2.91	118.73	113.85
1	1	1695	4AC	CM7-C7-N4	-2.91	110.26	115.29
1	1	2062	4AC	CM7-C7-N4	-2.91	110.27	115.29
1	1	1068	4AC	CM7-C7-N4	-2.91	110.27	115.29
2	2	848	4AC	N4-C4-N3	2.91	118.73	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	53	4AC	CM7-C7-N4	-2.90	110.27	115.29
2	2	751	4AC	CM7-C7-N4	-2.90	110.27	115.29
1	1	2287	4AC	C5-C4-N4	-2.90	117.88	122.92
1	1	1621	4AC	CM7-C7-N4	-2.90	110.28	115.29
1	1	1550	4AC	N4-C4-N3	2.90	118.72	113.85
1	1	161	4AC	N4-C4-N3	2.90	118.72	113.85
1	1	2865	4AC	CM7-C7-N4	-2.90	110.28	115.29
2	2	1028	4AC	CM7-C7-N4	-2.89	110.29	115.29
3	3	32	4AC	C5-C4-N4	-2.89	117.90	122.92
1	1	458	4AC	C5-C4-N4	-2.89	117.90	122.92
1	1	2027	4AC	N4-C4-N3	2.89	118.70	113.85
2	2	1028	4AC	C5-C4-N4	-2.89	117.90	122.92
2	2	20	OMU	O4-C4-C5	-2.89	120.09	125.16
1	1	1934	4AC	CM7-C7-N4	-2.88	110.31	115.29
1	1	91	4AC	C5-C4-N4	-2.88	117.91	122.92
1	1	981	4AC	CM7-C7-N4	-2.88	110.31	115.29
1	1	2083	4AC	CM7-C7-N4	-2.88	110.31	115.29
2	2	839	4AC	N4-C4-N3	2.88	118.69	113.85
1	1	2733	5MC	C5-C4-N3	-2.87	118.57	121.67
1	1	1068	4AC	N4-C4-N3	2.87	118.68	113.85
1	1	2001	4AC	C5-C4-N4	-2.87	117.93	122.92
1	1	694	4AC	N4-C4-N3	2.87	118.68	113.85
1	1	1460	4AC	CM7-C7-N4	-2.87	110.33	115.29
1	1	341	4AC	N4-C4-N3	2.87	118.67	113.85
1	1	1554	4AC	CM7-C7-N4	-2.87	110.33	115.29
2	2	848	4AC	C5-C4-N4	-2.86	117.94	122.92
2	2	53	4AC	C5-C4-N4	-2.86	117.95	122.92
1	1	1222	4AC	N4-C4-N3	2.86	118.65	113.85
2	2	1505	5MC	C5-C4-N3	-2.86	118.59	121.67
1	1	1667	4AC	CM7-C7-N4	-2.85	110.36	115.29
1	1	1867	4AC	CM7-C7-N4	-2.85	110.37	115.29
1	1	1065	4AC	C5-C4-N4	-2.85	117.97	122.92
2	2	319	4AC	C5-C4-N4	-2.84	117.98	122.92
1	1	458	4AC	CM7-C7-N4	-2.84	110.38	115.29
1	1	2027	4AC	CM7-C7-N4	-2.84	110.39	115.29
1	1	1594	4AC	N4-C4-N3	2.84	118.62	113.85
1	1	451	4AC	N4-C4-N3	2.84	118.61	113.85
1	1	1594	4AC	CM7-C7-N4	-2.84	110.39	115.29
1	1	91	4AC	CM7-C7-N4	-2.84	110.39	115.29
1	1	2718	4AC	C5-C4-N4	-2.84	117.99	122.92
2	2	303	4AC	CM7-C7-N4	-2.84	110.39	115.29
1	1	1962	4AC	N4-C4-N3	2.83	118.61	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	590	4AC	N4-C4-N3	2.83	118.61	113.85
2	2	830	OMU	O4-C4-C5	-2.83	120.18	125.16
2	2	1479	4AC	N4-C4-N3	2.83	118.61	113.85
2	2	319	4AC	CM7-C7-N4	-2.83	110.40	115.29
2	2	657	OMG	C6-C5-N7	2.83	135.51	130.25
1	1	1934	4AC	C5-C4-N4	-2.83	118.00	122.92
2	2	828	4AC	C5-C4-N4	-2.83	118.00	122.92
1	1	314	4AC	CM7-C7-N4	-2.83	110.40	115.29
2	2	479	4AC	CM7-C7-N4	-2.83	110.40	115.29
1	1	2966	4AC	N4-C4-N3	2.83	118.60	113.85
1	1	2908	4AC	N4-C4-N3	2.82	118.59	113.85
2	2	751	4AC	C5-C4-N4	-2.82	118.01	122.92
1	1	2570	4AC	N4-C4-N3	2.82	118.59	113.85
1	1	243	4AC	CM7-C7-N4	-2.82	110.41	115.29
1	1	2545	4AC	N4-C4-N3	2.82	118.59	113.85
1	1	1885	4AC	CM7-C7-N4	-2.82	110.41	115.29
1	1	2495	4AC	CM7-C7-N4	-2.82	110.41	115.29
2	2	286	4AC	N4-C4-N3	2.82	118.59	113.85
1	1	243	4AC	N4-C4-N3	2.82	118.59	113.85
1	1	1867	4AC	N4-C4-N3	2.82	118.59	113.85
1	1	341	4AC	CM7-C7-N4	-2.82	110.42	115.29
2	2	379	4AC	CM7-C7-N4	-2.82	110.42	115.29
1	1	1695	4AC	N4-C4-N3	2.82	118.58	113.85
1	1	1765	4AC	N4-C4-N3	2.82	118.58	113.85
1	1	802	4AC	C5-C4-N4	-2.82	118.03	122.92
3	3	32	4AC	CM7-C7-N4	-2.81	110.43	115.29
1	1	1765	4AC	CM7-C7-N4	-2.81	110.43	115.29
2	2	626	4AC	CM7-C7-N4	-2.81	110.43	115.29
1	1	1293	4AC	C5-C4-N4	-2.81	118.04	122.92
1	1	2136	4AC	N4-C4-N3	2.81	118.57	113.85
2	2	17	4AC	N4-C4-N3	2.81	118.57	113.85
1	1	922	4AC	C5-C4-N4	-2.81	118.04	122.92
1	1	161	4AC	CM7-C7-N4	-2.81	110.44	115.29
1	1	2548	4AC	CM7-C7-N4	-2.81	110.44	115.29
1	1	2062	4AC	N4-C4-N3	2.81	118.56	113.85
1	1	2642	4AC	N4-C4-N3	2.81	118.56	113.85
1	1	1065	4AC	CM7-C7-N4	-2.81	110.44	115.29
1	1	1617	4AC	CM7-C7-N4	-2.80	110.45	115.29
2	2	590	4AC	CM7-C7-N4	-2.80	110.45	115.29
1	1	835	4AC	CM7-C7-N4	-2.80	110.46	115.29
1	1	2718	4AC	CM7-C7-N4	-2.80	110.46	115.29
1	1	1667	4AC	N4-C4-N3	2.80	118.55	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1662	4AC	CM7-C7-N4	-2.80	110.46	115.29
2	2	394	4AC	CM7-C7-N4	-2.79	110.47	115.29
2	2	1147	4AC	C5-C4-N4	-2.79	118.07	122.92
2	2	957	4AC	C5-C4-N4	-2.79	118.07	122.92
1	1	829	4AC	CM7-C7-N4	-2.79	110.47	115.29
1	1	1554	4AC	N4-C4-N3	2.79	118.53	113.85
1	1	1962	4AC	C5-C4-N4	-2.79	118.08	122.92
1	1	1460	4AC	C5-C4-N4	-2.79	118.08	122.92
2	2	303	4AC	C5-C4-N4	-2.78	118.09	122.92
1	1	1222	4AC	CM7-C7-N4	-2.78	110.48	115.29
1	1	357	4AC	CM7-C7-N4	-2.78	110.49	115.29
1	1	2865	4AC	N4-C4-N3	2.78	118.51	113.85
1	1	2329	4AC	CM7-C7-N4	-2.78	110.49	115.29
2	2	718	4AC	N4-C4-N3	2.78	118.51	113.85
2	2	787	OMU	O4-C4-C5	-2.77	120.28	125.16
1	1	2966	4AC	C5-C4-N4	-2.77	118.11	122.92
1	1	2585	4AC	C1'-N1-C2	2.77	124.60	118.42
1	1	2548	4AC	N4-C4-N3	2.77	118.50	113.85
2	2	1233	4AC	CM7-C7-N4	-2.77	110.51	115.29
1	1	451	4AC	CM7-C7-N4	-2.77	110.51	115.29
2	2	1380	OMU	O4-C4-C5	-2.77	120.30	125.16
2	2	957	4AC	CM7-C7-N4	-2.77	110.51	115.29
1	1	136	4AC	N4-C4-N3	2.77	118.50	113.85
1	1	694	4AC	CM7-C7-N4	-2.76	110.51	115.29
1	1	211	4AC	N4-C4-N3	2.76	118.49	113.85
2	2	868	4AC	N4-C4-N3	2.76	118.48	113.85
1	1	2960	4AC	C5-C4-N4	-2.76	118.13	122.92
1	1	2570	4AC	CM7-C7-N4	-2.75	110.53	115.29
1	1	802	4AC	CM7-C7-N4	-2.75	110.53	115.29
2	2	828	4AC	CM7-C7-N4	-2.75	110.53	115.29
2	2	511	4AC	N4-C4-N3	2.75	118.47	113.85
1	1	2545	4AC	C5-C4-N4	-2.75	118.14	122.92
1	1	3004	4AC	CM7-C7-N4	-2.75	110.54	115.29
2	2	286	4AC	C5-C4-N4	-2.75	118.15	122.92
1	1	1557	4AC	N4-C4-N3	2.74	118.46	113.85
1	1	1765	4AC	C5-C4-N4	-2.74	118.15	122.92
1	1	1695	4AC	C5-C4-N4	-2.74	118.16	122.92
1	1	1243	4AC	N4-C4-N3	2.74	118.45	113.85
2	2	17	4AC	C5-C4-N4	-2.74	118.16	122.92
1	1	533	4AC	C5-C4-N4	-2.74	118.17	122.92
1	1	641	4AC	N4-C4-N3	2.73	118.44	113.85
1	1	1867	4AC	C5-C4-N4	-2.73	118.17	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	839	4AC	C5-C4-N4	-2.73	118.18	122.92
1	1	2908	4AC	CM7-C7-N4	-2.73	110.57	115.29
1	1	2136	4AC	C5-C4-N4	-2.73	118.18	122.92
1	1	2027	4AC	C5-C4-N4	-2.73	118.18	122.92
1	1	1594	4AC	C5-C4-N4	-2.72	118.19	122.92
1	1	2329	4AC	C5-C4-N4	-2.72	118.19	122.92
1	1	60	4AC	CM7-C7-N4	-2.72	110.59	115.29
1	1	835	4AC	N4-C4-N3	2.72	118.42	113.85
1	1	1554	4AC	C5-C4-N4	-2.72	118.20	122.92
1	1	243	4AC	C5-C4-N4	-2.71	118.20	122.92
2	2	286	4AC	CM7-C7-N4	-2.71	110.60	115.29
1	1	694	4AC	C5-C4-N4	-2.71	118.21	122.92
1	1	1667	4AC	C5-C4-N4	-2.71	118.22	122.92
1	1	2570	4AC	C5-C4-N4	-2.71	118.22	122.92
1	1	161	4AC	C5-C4-N4	-2.70	118.23	122.92
1	1	451	4AC	C5-C4-N4	-2.70	118.23	122.92
1	1	1557	4AC	CM7-C7-N4	-2.70	110.62	115.29
2	2	718	4AC	CM7-C7-N4	-2.70	110.63	115.29
2	2	703	4AC	CM7-C7-N4	-2.70	110.63	115.29
1	1	533	4AC	CM7-C7-N4	-2.69	110.64	115.29
2	2	718	4AC	C5-C4-N4	-2.69	118.25	122.92
1	1	1243	4AC	C5-C4-N4	-2.69	118.25	122.92
2	2	546	4AC	CM7-C7-N4	-2.69	110.65	115.29
2	2	868	4AC	CM7-C7-N4	-2.69	110.65	115.29
2	2	934	OMG	C4-C5-N7	-2.68	106.48	110.72
1	1	2642	4AC	C5-C4-N4	-2.68	118.27	122.92
1	1	2249	4AC	C5-C4-N4	-2.67	118.28	122.92
1	1	2960	4AC	CM7-C7-N4	-2.67	110.67	115.29
2	2	590	4AC	C5-C4-N4	-2.67	118.29	122.92
2	2	913	OMG	C4-C5-N7	-2.66	106.50	110.72
2	2	851	4AC	CM7-C7-N4	-2.66	110.69	115.29
1	1	2198	5MC	C5-C4-N3	-2.66	118.81	121.67
1	1	1938	4AC	N4-C4-N3	2.65	118.31	113.85
2	2	875	5MC	C5-C4-N3	-2.65	118.81	121.67
1	1	1621	4AC	N4-C4-N3	2.65	118.30	113.85
1	1	922	4AC	CM7-C7-N4	-2.65	110.71	115.29
1	1	1068	4AC	C5-C4-N4	-2.65	118.32	122.92
1	1	1222	4AC	C5-C4-N4	-2.65	118.32	122.92
1	1	2249	4AC	N4-C4-N3	2.65	118.30	113.85
1	1	2062	4AC	C5-C4-N4	-2.65	118.32	122.92
1	1	341	4AC	C5-C4-N4	-2.64	118.33	122.92
2	2	1498	5MC	O2-C2-N3	-2.64	118.03	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2865	4AC	C5-C4-N4	-2.64	118.33	122.92
1	1	2642	4AC	CM7-C7-N4	-2.64	110.73	115.29
2	2	373	A2M	C5-N7-C8	2.64	107.26	103.51
2	2	511	4AC	C5-C4-N4	-2.64	118.34	122.92
2	2	519	OMG	C4-C5-N7	-2.64	106.55	110.72
1	1	1780	4AC	CM7-C7-N4	-2.64	110.73	115.29
1	1	641	4AC	C5-C4-N4	-2.63	118.34	122.92
1	1	2908	4AC	C5-C4-N4	-2.63	118.35	122.92
1	1	1550	4AC	C5-C4-N4	-2.63	118.35	122.92
1	1	314	4AC	N4-C4-N3	2.62	118.26	113.85
2	2	1202	5MC	C5-C4-N3	-2.62	118.84	121.67
1	1	1055	A2M	C5-N7-C8	2.62	107.23	103.51
1	1	136	4AC	CM7-C7-N4	-2.62	110.76	115.29
1	1	2925	4AC	N4-C4-N3	2.62	118.24	113.85
1	1	328	OMG	C4-C5-N7	-2.61	106.58	110.72
1	1	2608	4AC	C1'-N1-C2	2.61	124.25	118.42
1	1	1048	4AC	N4-C4-N3	2.61	118.24	113.85
2	2	1239	4AC	C5-C4-N4	-2.61	118.39	122.92
1	1	2203	5MC	C5-C4-N3	-2.61	118.86	121.67
2	2	693	5MC	C5-C4-N3	-2.60	118.86	121.67
2	2	1479	4AC	CM7-C7-N4	-2.60	110.79	115.29
1	1	211	4AC	C5-C4-N4	-2.60	118.40	122.92
1	1	829	4AC	N4-C4-N3	2.60	118.21	113.85
1	1	1550	4AC	CM7-C7-N4	-2.60	110.80	115.29
2	2	1239	4AC	CM7-C7-N4	-2.59	110.81	115.29
1	1	2287	4AC	CM7-C7-N4	-2.59	110.81	115.29
1	1	2138	OMG	C4-C5-N7	-2.59	106.62	110.72
1	1	981	4AC	N4-C4-N3	2.58	118.18	113.85
1	1	2548	4AC	C5-C4-N4	-2.58	118.44	122.92
2	2	1069	OMG	C4-C5-N7	-2.58	106.64	110.72
1	1	2001	4AC	N4-C4-N3	2.58	118.18	113.85
2	2	467	OMG	C4-C5-N7	-2.57	106.65	110.72
1	1	1885	4AC	N4-C4-N3	2.57	118.17	113.85
1	1	1048	4AC	C5-C4-N4	-2.57	118.46	122.92
2	2	1498	5MC	C5-C4-N3	-2.57	118.91	121.67
1	1	357	4AC	C5-C4-N4	-2.56	118.47	122.92
1	1	2147	OMG	C4-C5-N7	-2.55	106.68	110.72
1	1	2093	5MC	C5-C4-N3	-2.55	118.92	121.67
1	1	1557	4AC	C5-C4-N4	-2.54	118.50	122.92
2	2	535	5MC	C5-C4-N3	-2.54	118.93	121.67
1	1	2733	5MC	O2-C2-N3	-2.54	118.20	122.33
2	2	851	4AC	N4-C4-N3	2.54	118.11	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2173	A2M	C5-N7-C8	2.54	107.11	103.51
2	2	657	OMG	C4-C5-N7	-2.53	106.71	110.72
1	1	2678	OMG	C4-C5-N7	-2.53	106.72	110.72
1	1	923	OMG	C4-C5-N7	-2.53	106.72	110.72
1	1	1938	4AC	C5-C4-N4	-2.53	118.53	122.92
1	1	2162	5MC	C5-C4-N3	-2.52	118.95	121.67
1	1	835	4AC	C5-C4-N4	-2.52	118.54	122.92
1	1	2495	4AC	N4-C4-N3	2.52	118.08	113.85
1	1	789	OMG	C4-C5-N7	-2.51	106.74	110.72
1	1	2183	5MC	C5-C4-N3	-2.51	118.96	121.67
2	2	787	OMU	O2-C2-N1	-2.51	119.45	122.79
2	2	1025	5MC	C5-C4-N3	-2.50	118.98	121.67
2	2	1496	5MC	C5-C4-N3	-2.50	118.98	121.67
1	1	3004	4AC	C5-C4-N4	-2.50	118.58	122.92
2	2	1479	4AC	C5-C4-N4	-2.50	118.58	122.92
1	1	3004	4AC	N4-C4-N3	2.49	118.04	113.85
1	1	2144	OMG	C4-C5-N7	-2.49	106.78	110.72
1	1	1621	4AC	C5-C4-N4	-2.49	118.60	122.92
1	1	829	4AC	C5-C4-N4	-2.48	118.61	122.92
1	1	981	4AC	C5-C4-N4	-2.48	118.61	122.92
2	2	873	OMG	C4-C5-N7	-2.47	106.81	110.72
2	2	1374	5MC	C5-C4-N3	-2.46	119.02	121.67
1	1	1885	4AC	C5-C4-N4	-2.45	118.66	122.92
2	2	471	OMG	C4-C5-N7	-2.45	106.84	110.72
1	1	2925	4AC	C5-C4-N4	-2.45	118.67	122.92
1	1	22	4AC	N4-C4-N3	2.44	117.94	113.85
1	1	136	4AC	C5-C4-N4	-2.43	118.69	122.92
1	1	2162	5MC	O2-C2-N3	-2.43	118.38	122.33
1	1	2992	4AC	CM7-C7-N4	2.43	119.49	115.29
1	1	2163	5MC	C5-C4-N3	-2.42	119.07	121.67
1	1	314	4AC	C5-C4-N4	-2.42	118.72	122.92
1	1	2083	4AC	N4-C4-N3	2.41	117.90	113.85
2	2	680	OMG	C6-C5-N7	2.41	134.73	130.25
1	1	2495	4AC	C5-C4-N4	-2.41	118.74	122.92
1	1	1055	A2M	C4-N9-C8	2.40	108.33	105.73
2	2	868	4AC	C5-C4-N4	-2.40	118.75	122.92
2	2	1184	4AC	CM7-C7-N4	-2.39	111.16	115.29
1	1	1873	4AC	N4-C4-N3	2.38	117.84	113.85
1	1	1873	4AC	C5-C4-N4	-2.36	118.82	122.92
2	2	1487	MA6	C6-C5-N7	2.35	137.24	133.28
2	2	1487	MA6	N9-C8-N7	-2.35	110.70	113.91
2	2	20	OMU	O2-C2-N1	-2.34	119.67	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1498	5MC	C1'-N1-C6	-2.33	117.25	121.12
2	2	851	4AC	C5-C4-N4	-2.31	118.91	122.92
1	1	229	4AC	N4-C4-N3	2.30	117.72	113.85
2	2	1488	MA6	C4-N9-C8	2.30	108.22	105.73
2	2	680	OMG	O6-C6-C5	-2.29	120.51	126.60
2	2	373	A2M	C4-N9-C8	2.29	108.21	105.73
1	1	2083	4AC	C5-C4-N4	-2.28	118.96	122.92
2	2	1469	6MZ	C4-N9-C8	2.27	108.19	105.73
1	1	2784	OMU	O2-C2-N1	-2.26	119.79	122.79
2	2	680	OMG	C4-C5-N7	-2.25	107.16	110.72
1	1	2173	A2M	C4-N9-C8	2.24	108.16	105.73
1	1	1755	4AC	CM7-C7-N4	-2.22	111.45	115.29
1	1	2937	4AC	CM7-C7-N4	-2.22	111.45	115.29
1	1	2163	5MC	O2-C2-N3	-2.22	118.73	122.33
1	1	22	4AC	C5-C4-N4	-2.21	119.08	122.92
2	2	1202	5MC	O2-C2-N3	-2.20	118.75	122.33
2	2	1505	5MC	O2-C2-N3	-2.19	118.77	122.33
2	2	693	5MC	O2-C2-N3	-2.19	118.78	122.33
1	1	1055	A2M	C2'-C1'-N9	-2.18	109.85	113.53
1	1	229	4AC	C5-C4-N4	-2.18	119.13	122.92
1	1	2678	OMG	O6-C6-C5	-2.17	120.85	126.60
2	2	875	5MC	O2-C2-N3	-2.17	118.81	122.33
1	1	923	OMG	O6-C6-C5	-2.16	120.88	126.60
2	2	774	OMU	O2-C2-N1	-2.14	119.94	122.79
2	2	1488	MA6	C6-C5-N7	2.14	136.87	133.28
2	2	873	OMG	O6-C6-C5	-2.14	120.93	126.60
1	1	2144	OMG	O6-C6-C5	-2.13	120.95	126.60
2	2	1469	6MZ	C2-N1-C6	2.13	122.40	115.25
2	2	471	OMG	O6-C6-C5	-2.12	120.98	126.60
1	1	2147	OMG	O6-C6-C5	-2.11	120.99	126.60
2	2	1025	5MC	O2-C2-N3	-2.10	118.91	122.33
2	2	373	A2M	C2'-C1'-N9	-2.10	110.00	113.53
2	2	467	OMG	O6-C6-C5	-2.09	121.05	126.60
1	1	328	OMG	O6-C6-C5	-2.09	121.05	126.60
2	2	934	OMG	O6-C6-C5	-2.09	121.06	126.60
1	1	2173	A2M	C6-C5-N7	2.08	135.90	132.02
1	1	2138	OMG	O6-C6-C5	-2.08	121.08	126.60
2	2	1069	OMG	O6-C6-C5	-2.08	121.09	126.60
1	1	1755	4AC	O7-C7-CM7	-2.08	118.20	122.06
2	2	373	A2M	C6-C5-N7	2.07	135.87	132.02
1	1	1055	A2M	C6-C5-N7	2.07	135.87	132.02
2	2	913	OMG	O6-C6-C5	-2.06	121.14	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1496	5MC	O2-C2-N3	-2.05	119.00	122.33
2	2	519	OMG	O6-C6-C5	-2.04	121.18	126.60
1	1	789	OMG	O6-C6-C5	-2.04	121.20	126.60
2	2	1177	OMU	O2-C2-N1	-2.02	120.10	122.79
1	1	2992	4AC	O7-C7-CM7	-2.02	118.31	122.06
2	2	1467	UR3	C1'-N1-C2	2.00	120.37	116.99
1	1	615	OMC	O2-C2-N3	-2.00	119.07	122.33

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	1505	5MC	C2'-C1'-N1-C2
2	2	1505	5MC	C2'-C1'-N1-C6
1	1	2147	OMG	O4'-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	2733	5MC	C2'-C1'-N1-C6
1	1	2733	5MC	C2'-C1'-N1-C2
1	1	789	OMG	C3'-C4'-C5'-O5'
1	1	789	OMG	O4'-C4'-C5'-O5'
1	1	2147	OMG	C3'-C4'-C5'-O5'
2	2	20	OMU	C2'-C1'-N1-C6
2	2	934	OMG	O4'-C4'-C5'-O5'
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	787	OMU	C2'-C1'-N1-C6
2	2	20	OMU	O4'-C1'-N1-C6
2	2	1498	5MC	O4'-C1'-N1-C6
1	1	789	OMG	C3'-C2'-O2'-CM2
2	2	1505	5MC	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	1498	5MC	O4'-C1'-N1-C2
2	2	787	OMU	O4'-C1'-N1-C6
1	1	2733	5MC	O4'-C1'-N1-C6
2	2	20	OMU	C2'-C1'-N1-C2
1	1	2733	5MC	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
2	2	873	OMG	C4'-C5'-O5'-P
2	2	1488	MA6	C4'-C5'-O5'-P
2	2	20	OMU	O4'-C1'-N1-C2
2	2	20	OMU	C3'-C4'-C5'-O5'
2	2	1505	5MC	O4'-C1'-N1-C2
2	2	938	B8H	O4'-C1'-C5-C4
2	2	680	OMG	C3'-C2'-O2'-CM2
2	2	1069	OMG	C3'-C2'-O2'-CM2
2	2	787	OMU	O4'-C1'-N1-C2
2	2	934	OMG	C3'-C4'-C5'-O5'
1	1	1755	4AC	C3'-C4'-C5'-O5'
2	2	64	OMU	C1'-C2'-O2'-CM2
2	2	787	OMU	C2'-C1'-N1-C2
2	2	1498	5MC	O4'-C4'-C5'-O5'
2	2	64	OMU	C3'-C2'-O2'-CM2
1	1	923	OMG	C3'-C2'-O2'-CM2
1	1	2144	OMG	C3'-C2'-O2'-CM2
1	1	1755	4AC	O4'-C4'-C5'-O5'
2	2	1498	5MC	C2'-C1'-N1-C2

There are no ring outliers.

89 monomers are involved in 134 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	1177	OMU	2	0
2	2	636	4AC	1	0
2	2	286	4AC	1	0
2	2	1147	4AC	2	0
1	1	922	4AC	1	0
2	2	319	4AC	2	0
2	2	848	4AC	1	0
1	1	789	OMG	3	0
2	2	1184	4AC	1	0
1	1	458	4AC	1	0
2	2	546	4AC	2	0
1	1	2163	5MC	3	0
2	2	479	4AC	2	0
2	2	718	4AC	2	0
1	1	211	4AC	1	0
1	1	1055	A2M	1	0
2	2	53	4AC	1	0
2	2	751	4AC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	626	4AC	3	0
2	2	774	OMU	1	0
1	1	341	4AC	1	0
1	1	835	4AC	1	0
1	1	2162	5MC	2	0
2	2	868	4AC	1	0
1	1	1885	4AC	1	0
1	1	829	4AC	1	0
1	1	2585	4AC	3	0
2	2	1025	5MC	1	0
1	1	1617	4AC	3	0
1	1	2608	4AC	3	0
2	2	519	OMG	2	0
1	1	2144	OMG	1	0
2	2	1202	5MC	1	0
1	1	229	4AC	1	0
1	1	2198	5MC	1	0
1	1	451	4AC	3	0
2	2	1467	UR3	1	0
2	2	680	OMG	3	0
2	2	1233	4AC	1	0
1	1	2249	4AC	1	0
1	1	1594	4AC	1	0
1	1	802	4AC	2	0
2	2	693	5MC	1	0
2	2	703	4AC	5	0
1	1	1878	4AC	2	0
1	1	1867	4AC	1	0
1	1	2960	4AC	1	0
2	2	17	4AC	1	0
1	1	161	4AC	1	0
2	2	1380	OMU	2	0
1	1	1667	4AC	4	0
1	1	2718	4AC	1	0
2	2	731	4AC	2	0
1	1	1550	4AC	1	0
2	2	873	OMG	1	0
2	2	1376	OMC	2	0
1	1	91	4AC	2	0
1	1	2136	4AC	1	0
1	1	1662	4AC	1	0
2	2	1028	4AC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	830	OMU	1	0
1	1	1755	4AC	3	0
1	1	2287	4AC	2	0
1	1	1934	4AC	2	0
2	2	657	OMG	1	0
1	1	1065	4AC	2	0
2	2	828	4AC	1	0
2	2	394	4AC	2	0
2	2	1487	MA6	2	0
1	1	1765	4AC	1	0
1	1	1048	4AC	1	0
2	2	1488	MA6	1	0
1	1	1780	4AC	1	0
1	1	60	4AC	1	0
2	2	839	4AC	1	0
2	2	1479	4AC	1	0
1	1	1460	4AC	1	0
2	2	373	A2M	2	0
1	1	1068	4AC	1	0
1	1	2992	4AC	1	0
2	2	471	OMG	3	0
2	2	957	4AC	1	0
1	1	22	4AC	1	0
1	1	2908	4AC	1	0
3	3	32	4AC	1	0
2	2	511	4AC	3	0
2	2	303	4AC	1	0
2	2	851	4AC	1	0
2	2	1069	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 254 ligands modelled in this entry, 254 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

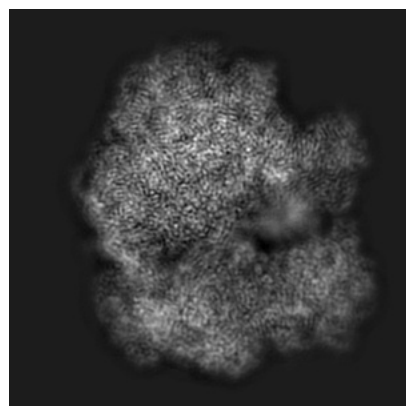
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55636. These allow visual inspection of the internal detail of the map and identification of artifacts.

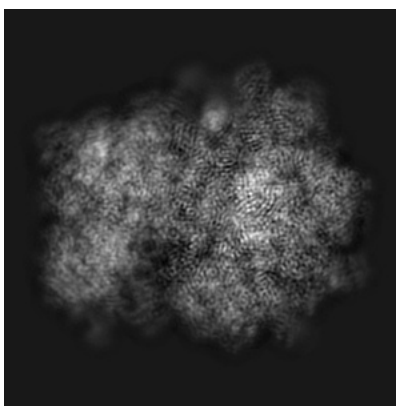
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

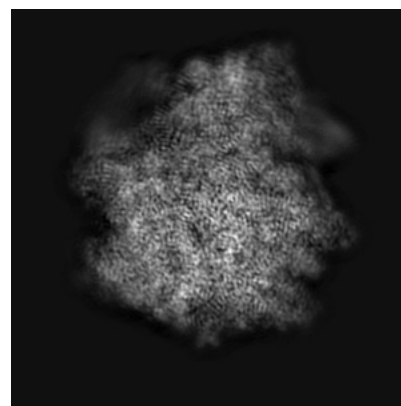
6.1.1 Primary map



X

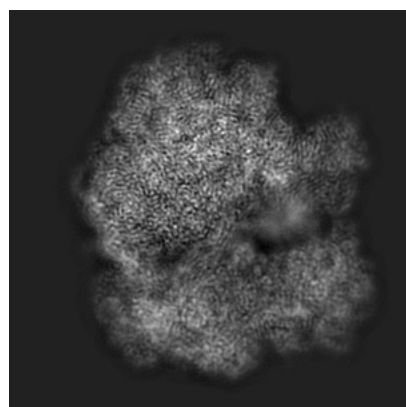


Y

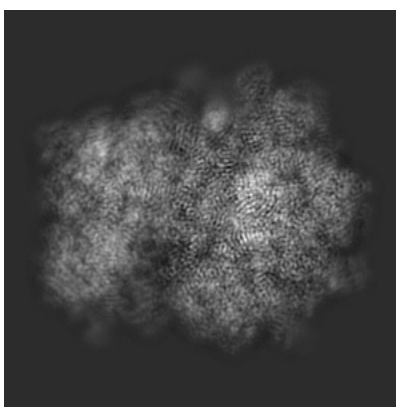


Z

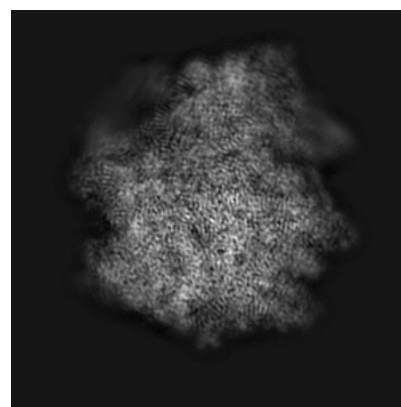
6.1.2 Raw map



X



Y

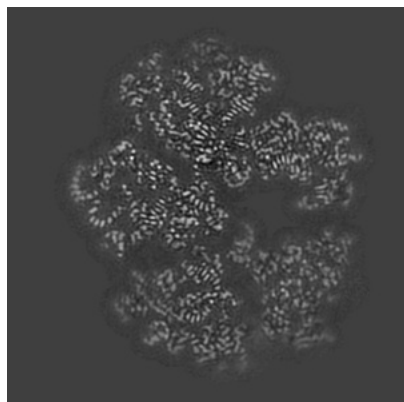


Z

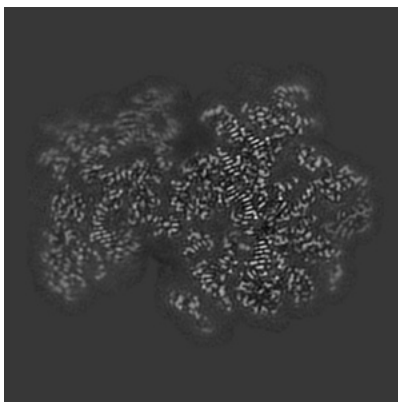
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

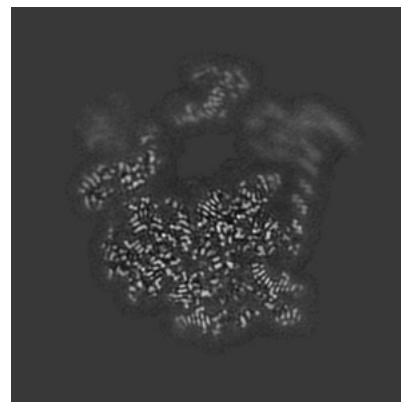
6.2.1 Primary map



X Index: 180

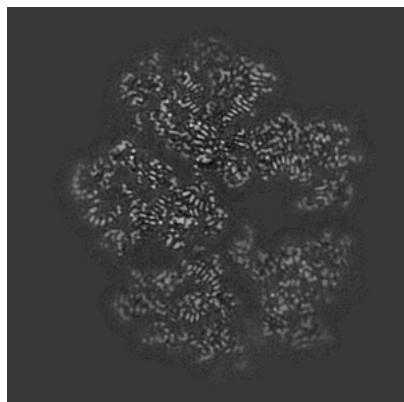


Y Index: 180

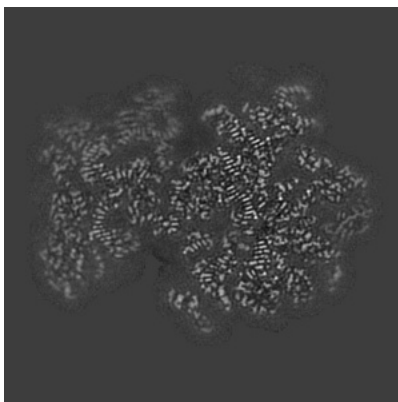


Z Index: 180

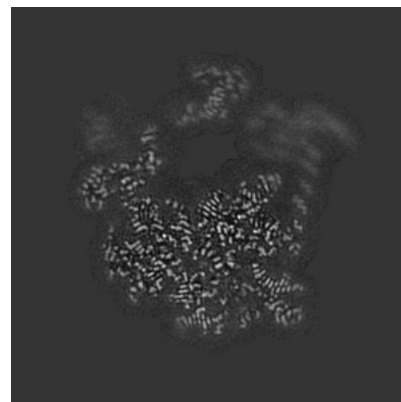
6.2.2 Raw map



X Index: 180



Y Index: 180

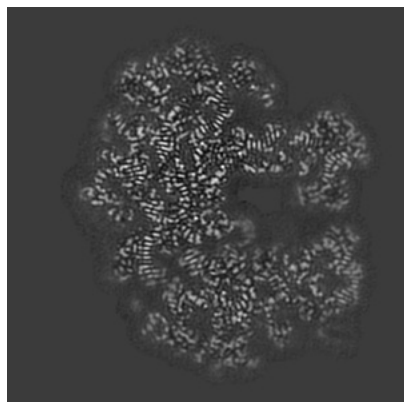


Z Index: 180

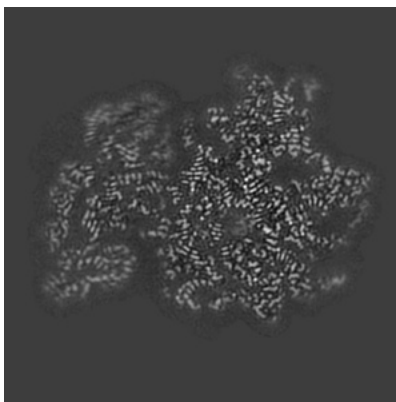
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

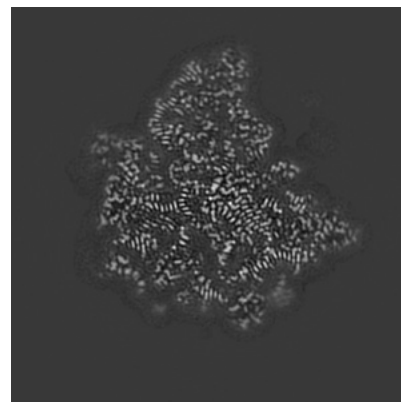
6.3.1 Primary map



X Index: 195

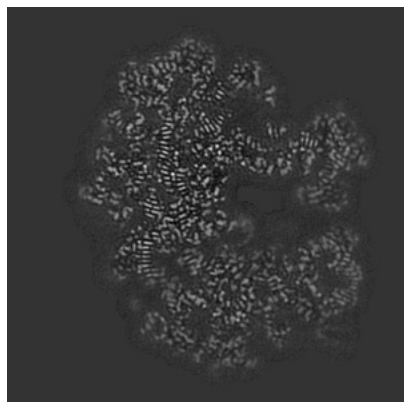


Y Index: 170

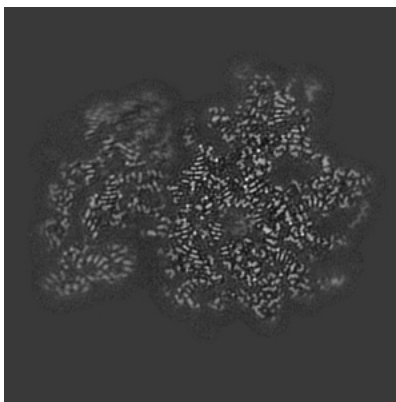


Z Index: 232

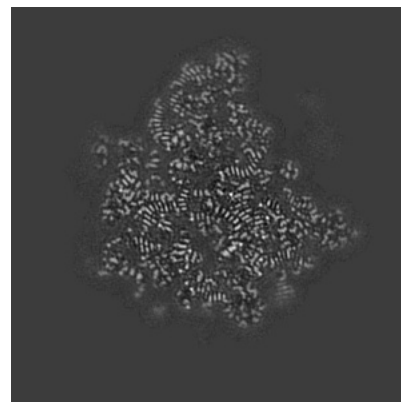
6.3.2 Raw map



X Index: 197



Y Index: 170

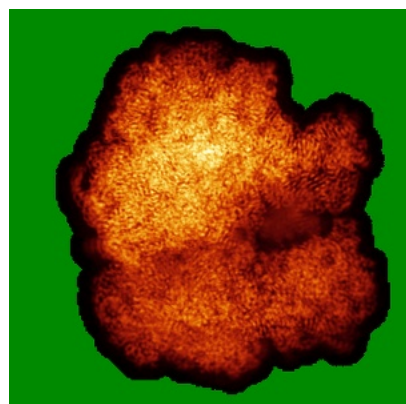


Z Index: 229

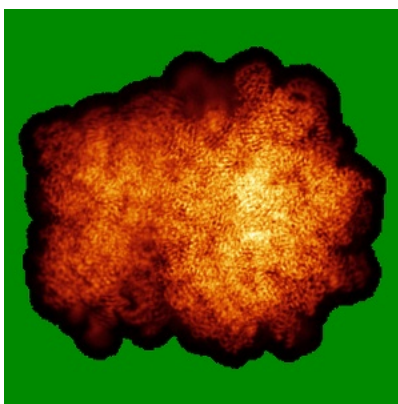
The images above show the largest variance slices of the map in three orthogonal directions.

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

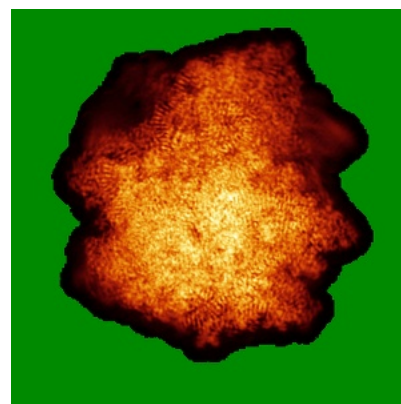
6.4.1 Primary map



X

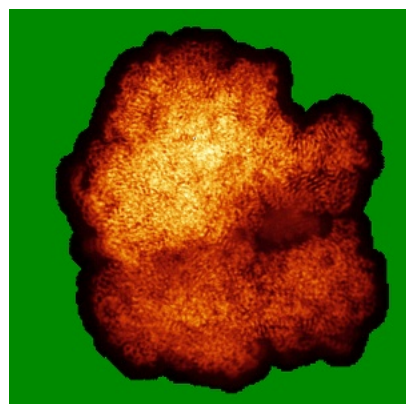


Y

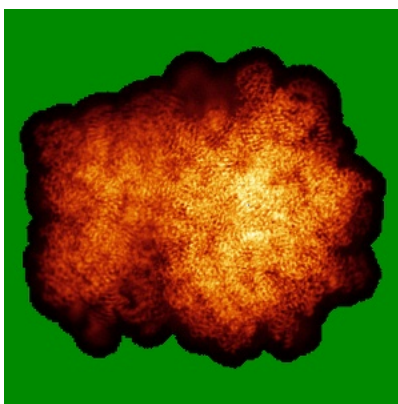


Z

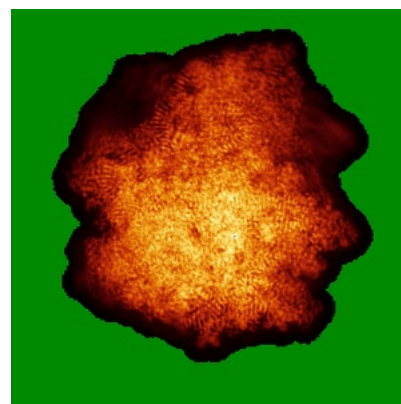
6.4.2 Raw map



X



Y

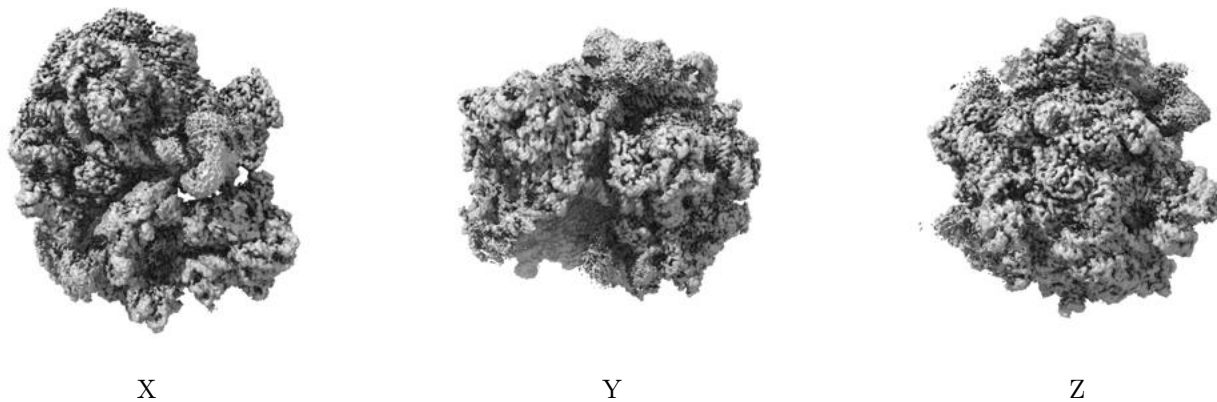


Z

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

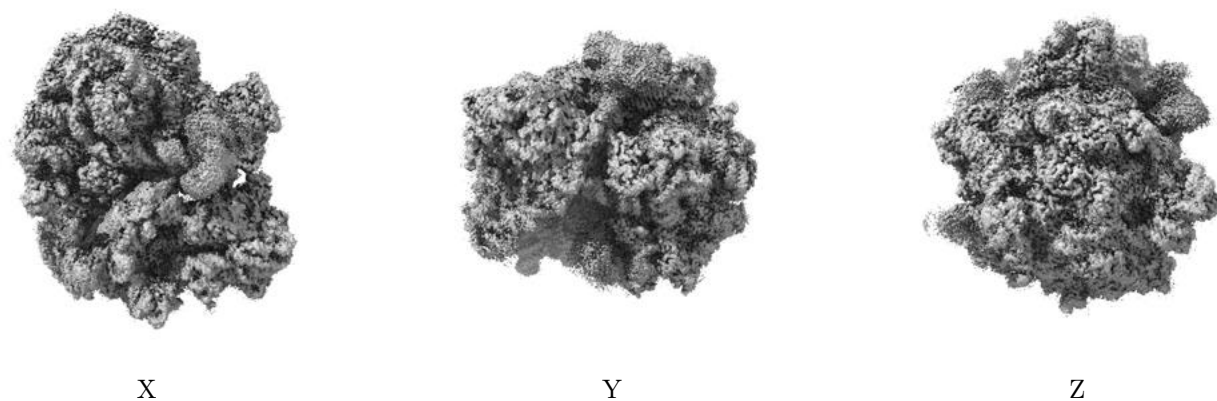
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

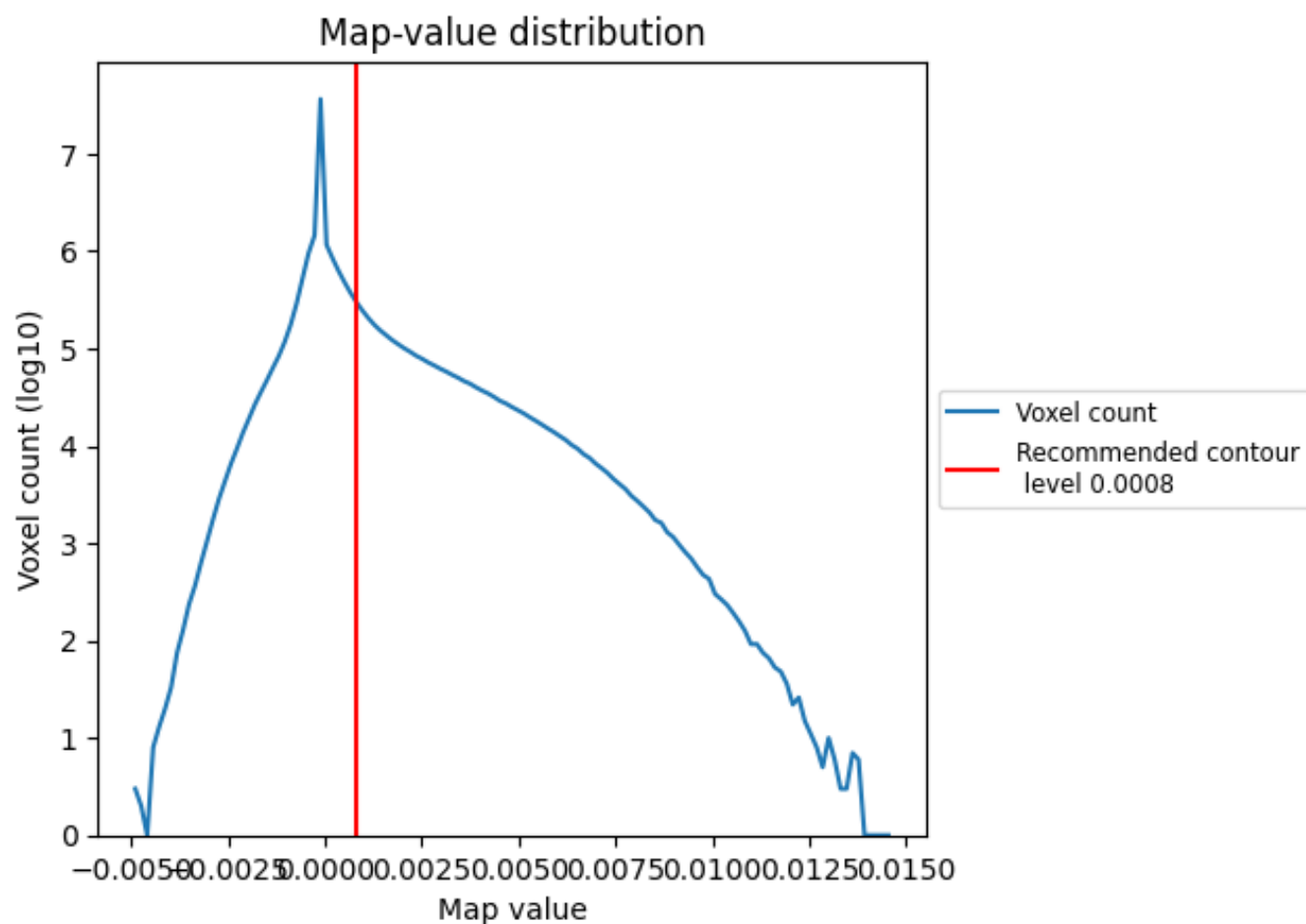
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

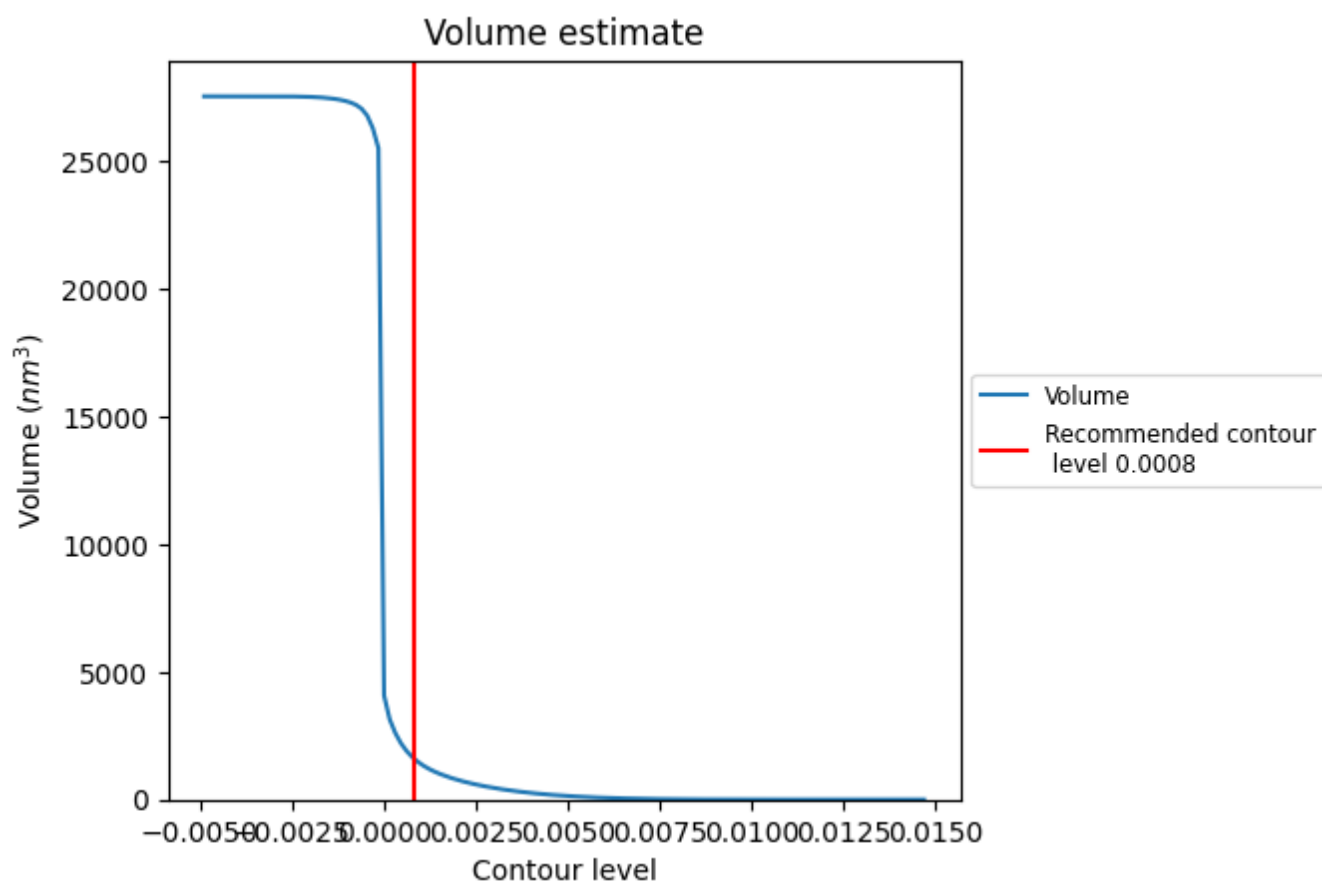
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

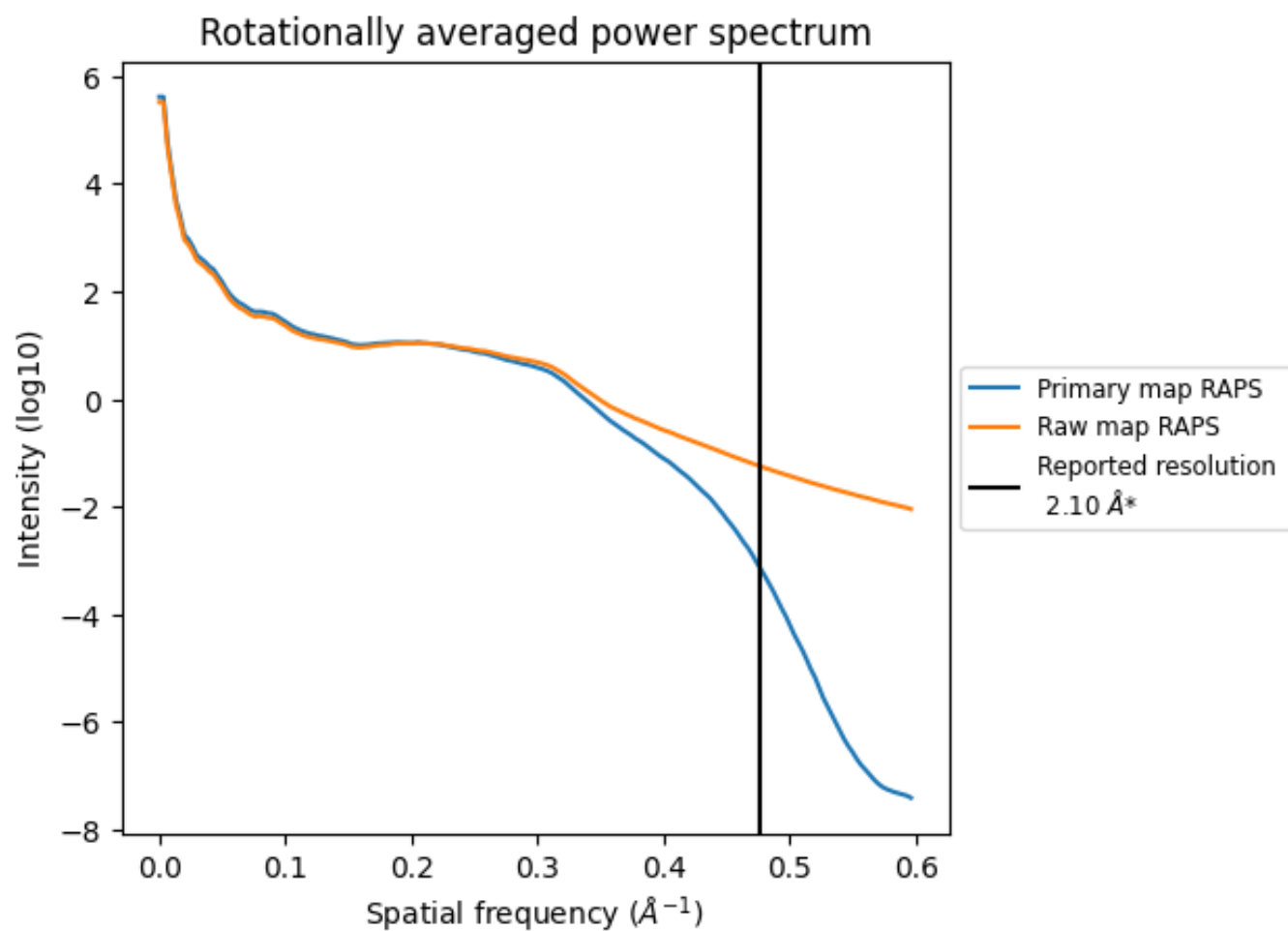
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1631 nm^3 ; this corresponds to an approximate mass of 1474 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 ⓘ

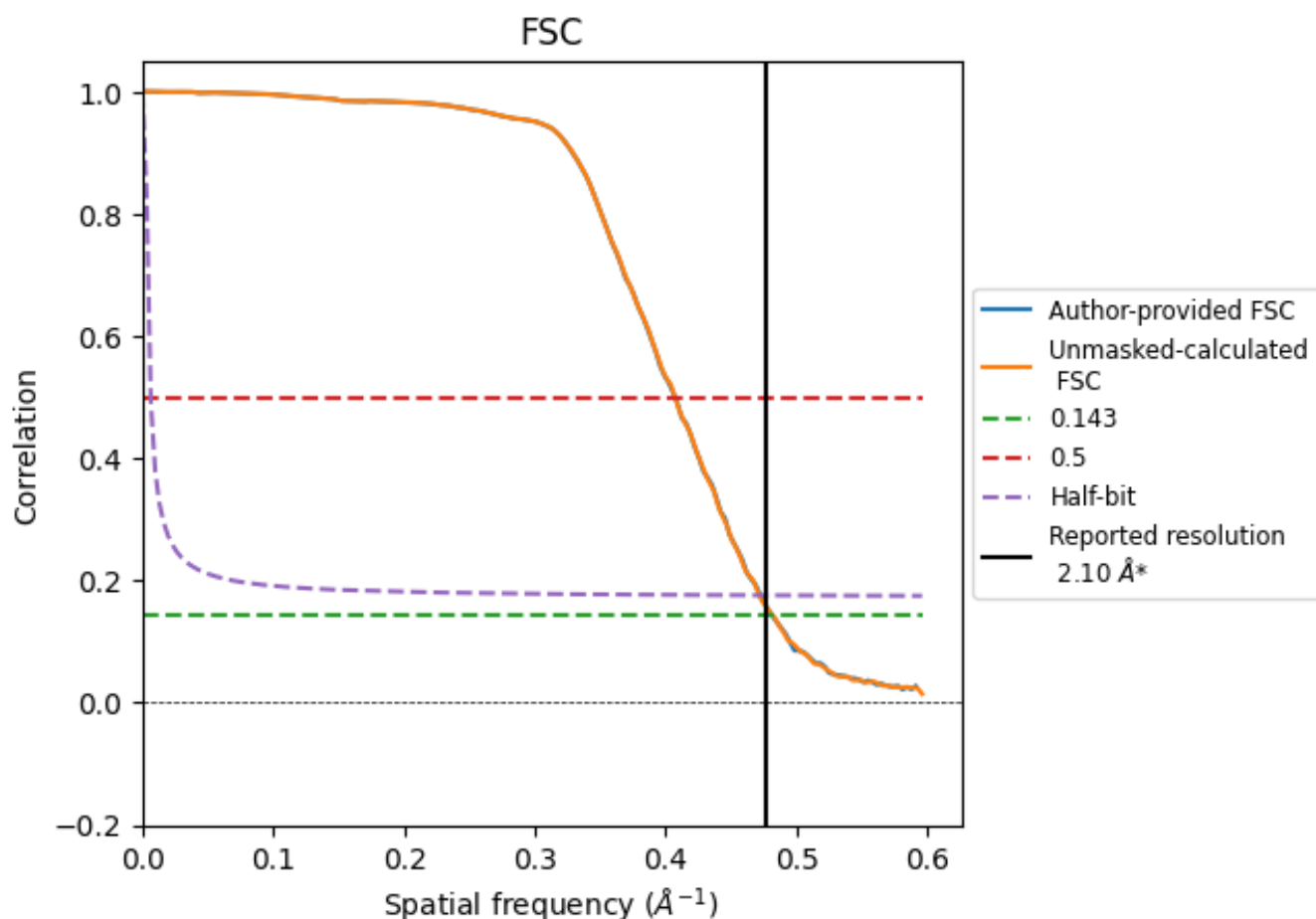


*Reported resolution corresponds to spatial frequency of 0.476 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.476 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

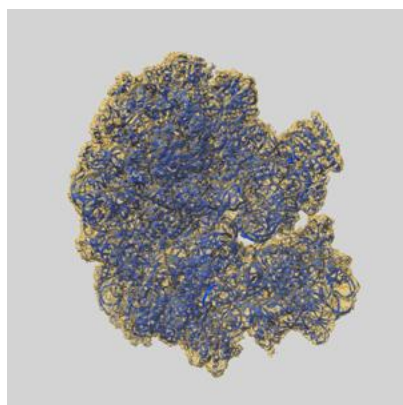
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.08	2.46	2.12
Unmasked-calculated*	2.08	2.46	2.12

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

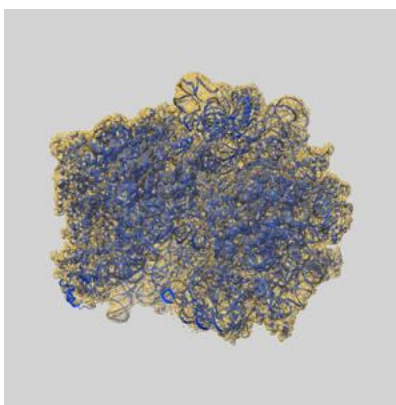
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55636 and PDB model 9T7H. Per-residue inclusion information can be found in section [3](#) on page [17](#).

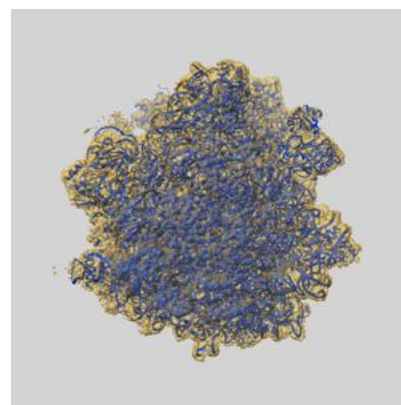
9.1 Map-model overlay [i](#)



X



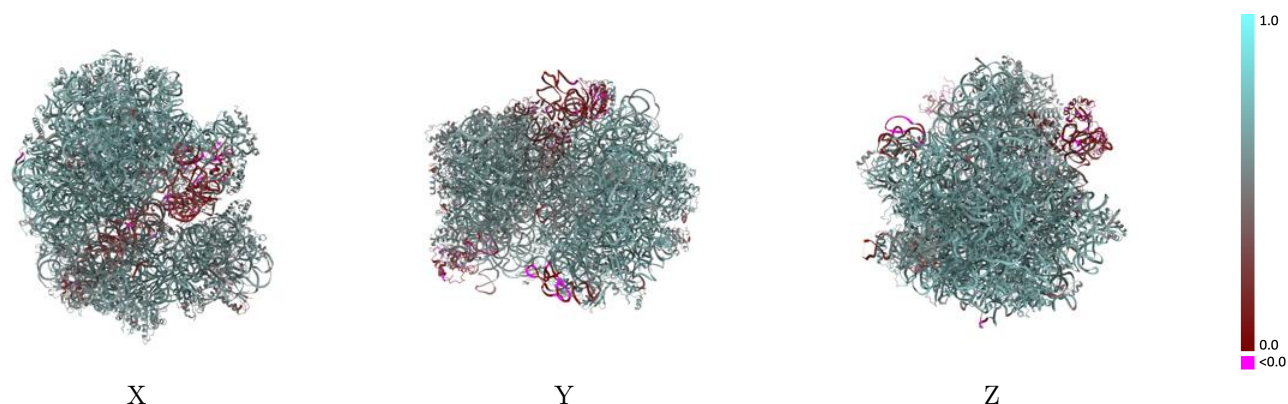
Y



Z

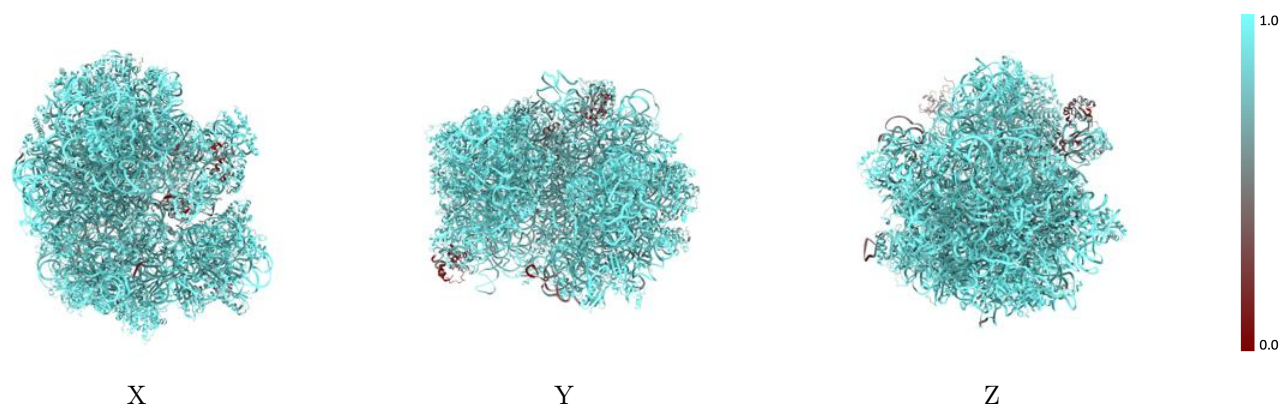
The images above show the 3D surface view of the map at the recommended contour level 0.0008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



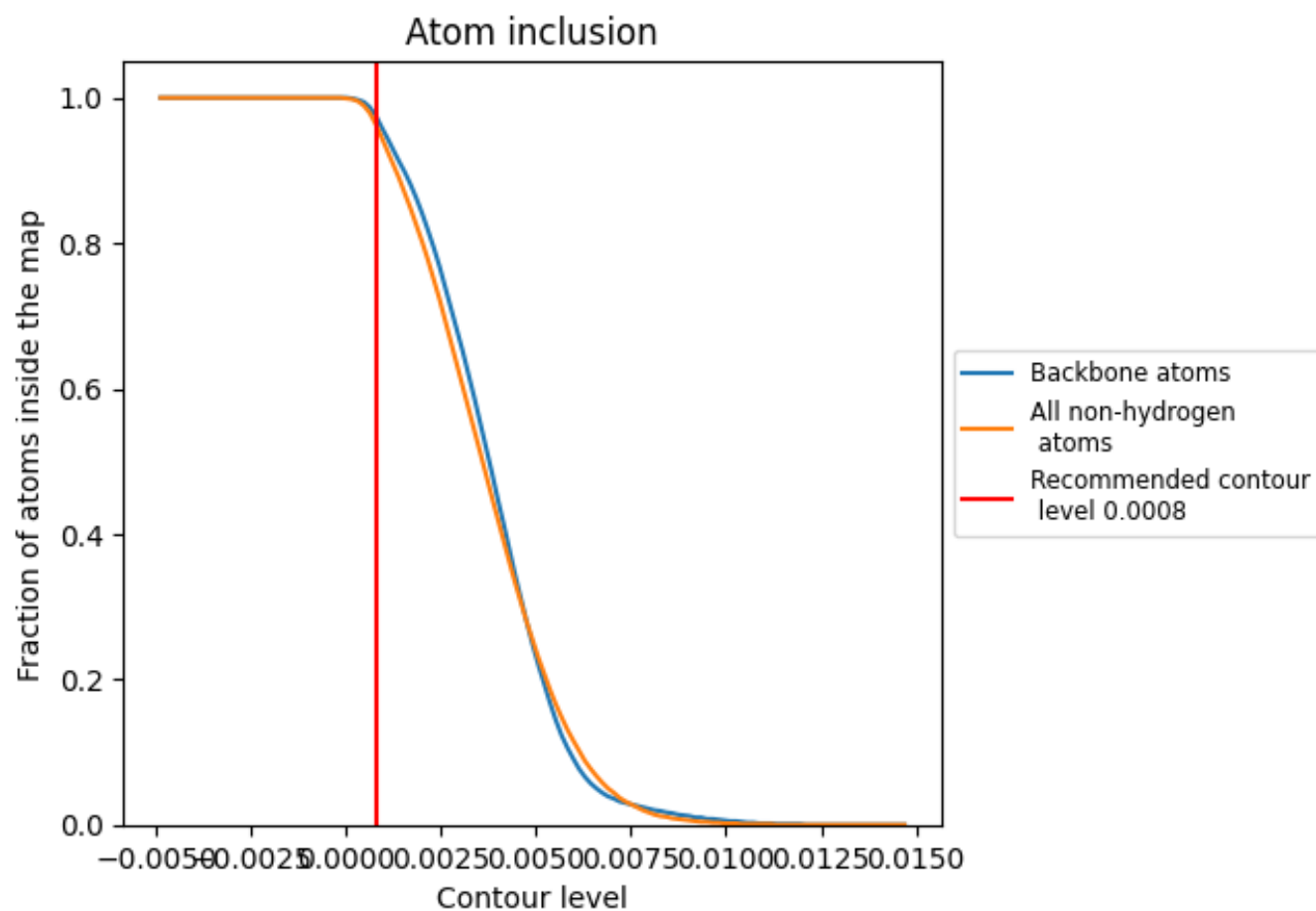
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0008).

9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 96% 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 (0.0008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9610	 0.5880
1	 0.9810	 0.6170
2	 0.9880	 0.5750
3	 0.9990	 0.6260
A0	 0.9590	 0.6450
A3	 0.3360	 0.1760
AA	 0.8060	 0.3140
AB	 0.9640	 0.5600
AC	 0.9710	 0.5850
AD	 0.9740	 0.5880
AE	 0.9820	 0.5840
AF	 0.9770	 0.6080
AG	 0.9120	 0.5450
AH	 0.9710	 0.5790
AI	 0.9790	 0.6040
AJ	 0.9720	 0.6140
AK	 0.9770	 0.5800
AL	 0.8960	 0.4860
AM	 0.8820	 0.4380
AN	 0.9640	 0.5860
AO	 0.9420	 0.5510
AP	 0.9520	 0.5840
AQ	 0.9170	 0.4170
AR	 0.9710	 0.5930
AS	 0.9700	 0.5350
AT	 0.9390	 0.5330
AU	 0.9790	 0.5740
AV	 0.9680	 0.5040
AW	 0.9540	 0.3650
AX	 0.9590	 0.5500
AY	 0.3810	 0.1020
AZ	 0.9120	 0.5200
B4	 0.8390	 0.4420
B5	 0.9950	 0.6030
B6	 0.8530	 0.6070



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Chain	Atom inclusion	Q-score
BA	 0.5150	 0.1550
BB	 0.9830	 0.6640
BC	 0.9790	 0.6580
BD	 0.9880	 0.6580
BE	 0.9510	 0.5540
BF	 0.9710	 0.6110
BG	 0.9730	 0.6170
BI	 0.9800	 0.6640
BJ	 0.9720	 0.6580
BK	 0.9760	 0.5840
BL	 0.9680	 0.6280
BM	 0.9940	 0.6810
BN	 0.9580	 0.6330
BO	 0.9780	 0.5970
BP	 0.9880	 0.6560
BQ	 0.9740	 0.6450
BR	 0.9840	 0.6600
BS	 0.9880	 0.6700
BT	 0.9770	 0.6450
BU	 0.9890	 0.6390
BV	 0.9710	 0.6570
BW	 0.9260	 0.5940
BY	 0.9880	 0.6560
BZ	 0.9580	 0.5760
Ba	 0.9630	 0.6300
Bb	 0.9770	 0.6580
Bc	 0.9810	 0.6560
Bd	 0.9790	 0.6450
Be	 1.0000	 0.6770
Bf	 0.9950	 0.6650
Bg	 0.9970	 0.6400
Bi	 0.9730	 0.6590
Bj	 0.9680	 0.6540
Bk	 0.9710	 0.6310
Bl	 0.9720	 0.6050
H	 0.6720	 0.3420