Full wwPDB EM Validation Report (i)

Aug 3, 2026 – 01:01 pm BST

PDB ID	:	9SRD / pdb_00009srd
EMDB ID	:	EMD-55138
Title	:	Cryo-EM structure of P. abyssi 70S ribosome in complex with hibernation factor HibA (HibA-uL5 conformation)
Authors	:	Madru, C.; Bourgeois, G.; Mechulam, Y.; Schmitt, E.
Deposited on	:	2025-09-24
Resolution	:	2.10 Å(reported)
Based on initial model	:	.

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 (i) 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 (1)) were used in the production of this report:

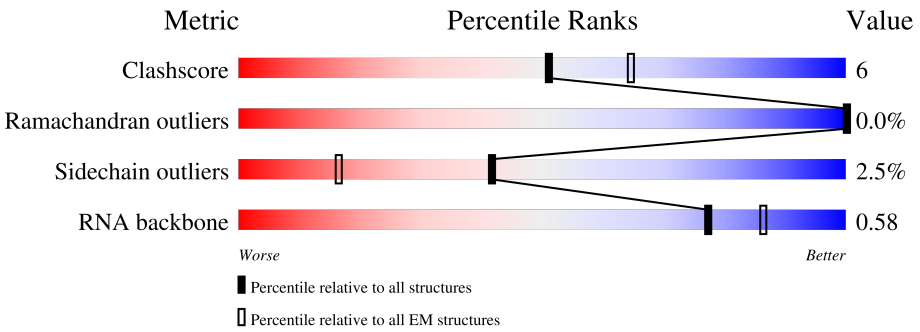
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal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

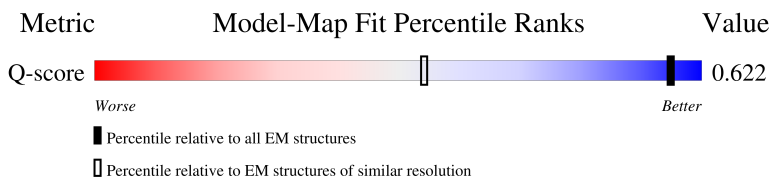
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	3018	6% 66% 28% 6%
2	2	1512	• 63% 30% 6% •
3	3	128	77% 18% • •

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Mol	Chain	Length	Quality of chain
4	AA	199	75% 19% 6%
5	AB	202	85% 11%
6	AC	63	75% 16% 10%
7	AD	180	86% 10%
8	AE	243	82% 17%
9	AF	236	85% 11%
10	AG	125	82% 16%
11	AH	215	83% 16%
12	AI	130	86% 13%
13	AJ	127	85% 13%
14	AK	135	84% 16%
15	AL	102	12% 72% 24%
16	AM	137	82% 9% 7%
17	AN	147	85% 14%
18	AP	56	82% 14%
19	AQ	158	87% 11%
20	AR	113	77% 17% 5%
21	AS	67	67% 27%
22	AU	150	87% 12%
23	AV	99	76% 20%
23	B6	99	12% 86% 9% 5%
24	AW	65	69% 22% 6%
25	AX	71	63% 27% 8%
26	AY	51	41% 39% 18% 43%
27	AZ	210	72% 20% 7%

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Mol	Chain	Length	Quality of chain
28	A0	37	89% 8%
29	A3	123	95% 60% 37%
29	B4	123	21% 66% 32%
29	BG	123	92% 7%
30	AT	132	80% 18%
31	AO	148	74% 20% 7%
32	BB	239	90% 9%
33	BY	155	90% 9%
34	BO	203	80% 17%
35	BC	361	89% 10%
36	B5	82	73% 23%
36	BK	82	84% 13%
37	BL	147	88% 11%
38	Bf	51	80% 18%
39	BU	121	85% 15%
40	Bb	130	94% 5%
41	Be	62	84% 15%
42	BE	188	76% 21%
43	Ba	94	80% 19%
44	BT	86	87% 12%
45	BW	68	10% 88% 12%
46	Bi	83	90% 8%
47	BI	142	88% 12%
48	BR	97	85% 14%
49	BQ	151	81% 18%

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Mol	Chain	Length	Quality of chain
50	BV	67	87% 7% 6%
51	Bj	94	97%
52	BD	255	87% 12%
53	BF	184	85% 14%
54	BZ	99	86% 13%
55	BP	120	87% 13%
56	BM	194	91% 9%
57	BS	155	87% 12%
58	Bd	91	92% 8%
59	BN	181	5% 77% 19%
60	Bg	51	84% 10% 6%
61	Bc	87	86% 13%
62	BJ	141	90% 9%
63	Bl	77	77% 22%
64	Bk	65	89% 8%
65	H	392	42% 63% 31%

2 Entry composition (i)

There are 67 unique types of molecules in this entry. The entry contains 170227 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
			Total	C	N	O	P		
1	1	3018	65181	29055	12094	21014	3018	0	0

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

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

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

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

- Molecule 4 is a protein called 30S ribosomal protein S3Ae.

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

- Molecule 5 is a protein called 30S ribosomal protein S2.

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

- Molecule 6 is a protein called Zn-ribbon RNA-binding protein involved in translation.

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

- Molecule 7 is a protein called 30S ribosomal protein S4.

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

- Molecule 8 is a protein called 30S ribosomal protein S4e.

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

- Molecule 9 is a protein called 30S ribosomal protein S5.

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

- Molecule 10 is a protein called 30S ribosomal protein S6e.

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

- Molecule 11 is a protein called 30S ribosomal protein S7.

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

- Molecule 12 is a protein called 30S ribosomal protein S8.

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

- Molecule 13 is a protein called 30S ribosomal protein S8e.

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

- Molecule 14 is a protein called 30S ribosomal protein S9.

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

- Molecule 15 is a protein called 30S ribosomal protein S10.

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

- Molecule 16 is a protein called 30S ribosomal protein S11.

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

- Molecule 17 is a protein called 30S ribosomal protein S12.

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

- Molecule 18 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 19 is a protein called 30S ribosomal protein S15.

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

- Molecule 20 is a protein called 30S ribosomal protein S17.

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

- Molecule 21 is a protein called 30S ribosomal protein S17e.

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

- Molecule 22 is a protein called 30S ribosomal protein S19e.

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

- Molecule 23 is a protein called 30S ribosomal protein S24e.

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

- Molecule 24 is a protein called 30S ribosomal protein S27e.

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

- Molecule 25 is a protein called 30S ribosomal protein S28e.

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

- Molecule 26 is a protein called 30S ribosomal protein S27ae.

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

- Molecule 27 is a protein called 30S ribosomal protein S3.

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

- Molecule 28 is a protein called Small ribosomal subunit protein eS32.

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

- Molecule 29 is a protein called 50S ribosomal protein L7Ae.

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

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

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

- Molecule 31 is a protein called 30S ribosomal protein S13.

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

- Molecule 32 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 36 is a protein called Large ribosomal subunit protein eL14.

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

- Molecule 37 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 38 is a protein called Large ribosomal subunit protein eL39.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 40 is a protein called Large ribosomal subunit protein eL32.

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

- Molecule 41 is a protein called Large ribosomal subunit protein eL37.

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

- Molecule 42 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 43 is a protein called Large ribosomal subunit protein eL31.

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

- Molecule 44 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 46 is a protein called Large ribosomal subunit protein eL43.

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

- Molecule 47 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 48 is a protein called Large ribosomal subunit protein eL21.

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

- Molecule 49 is a protein called Large ribosomal subunit protein eL19.

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

- Molecule 50 is a protein called Large ribosomal subunit protein eL24.

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

- Molecule 51 is a protein called Large ribosomal subunit protein eL42.

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

- Molecule 52 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 53 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 54 is a protein called Large ribosomal subunit protein eL30.

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

- Molecule 55 is a protein called Large ribosomal subunit protein eL18.

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

- Molecule 56 is a protein called Large ribosomal subunit protein eL15.

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

- Molecule 57 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 58 is a protein called Large ribosomal subunit protein eL34.

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

- Molecule 59 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 60 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 61 is a protein called Large ribosomal subunit protein eL33.

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

- Molecule 62 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 63 is a protein called Large ribosomal subunit protein eL20.

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

- Molecule 64 is a protein called C2H2-type domain-containing protein.

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

- Molecule 65 is a protein called Dehydrogenase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	H	377	3009	1922	525	552	10	0	0

- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
66	1	167	167	167	0
66	2	69	69	69	0
66	3	1	1	1	0
66	AK	1	1	1	0
66	AN	1	1	1	0
66	BB	1	1	1	0
66	Bb	1	1	1	0
66	BD	1	1	1	0
66	BM	1	1	1	0
66	BS	1	1	1	0

- Molecule 67 is ZINC ION (CCD ID: ZN) (formula: Zn).

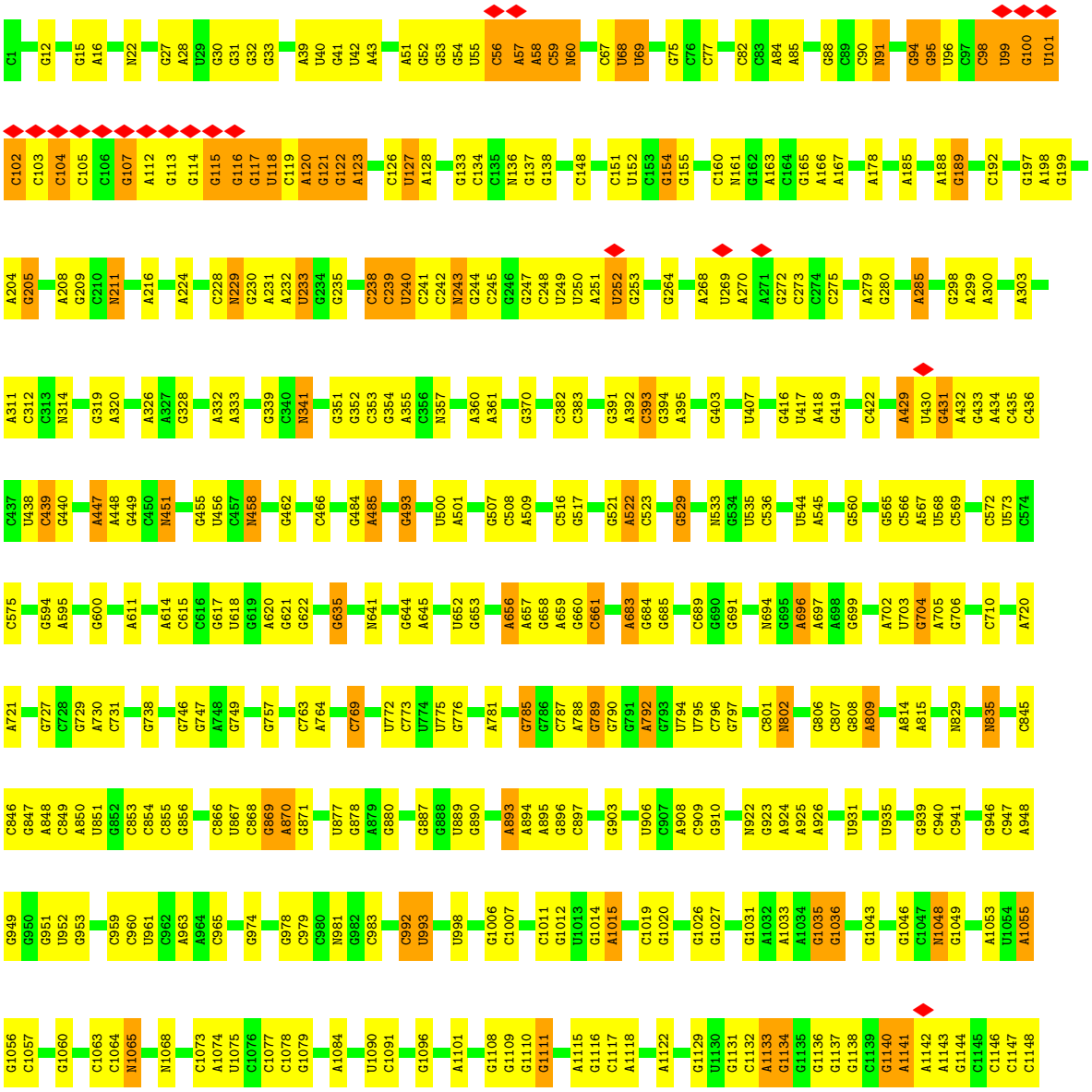
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
67	AC	2	2	2	0
67	AF	1	1	1	0
67	AP	1	1	1	0
67	AR	1	1	1	0
67	AW	1	1	1	0
67	Be	1	1	1	0
67	Bi	1	1	1	0
67	BV	1	1	1	0
67	Bj	1	1	1	0
67	Bd	1	1	1	0
67	Bg	1	1	1	0
67	Bk	1	1	1	0

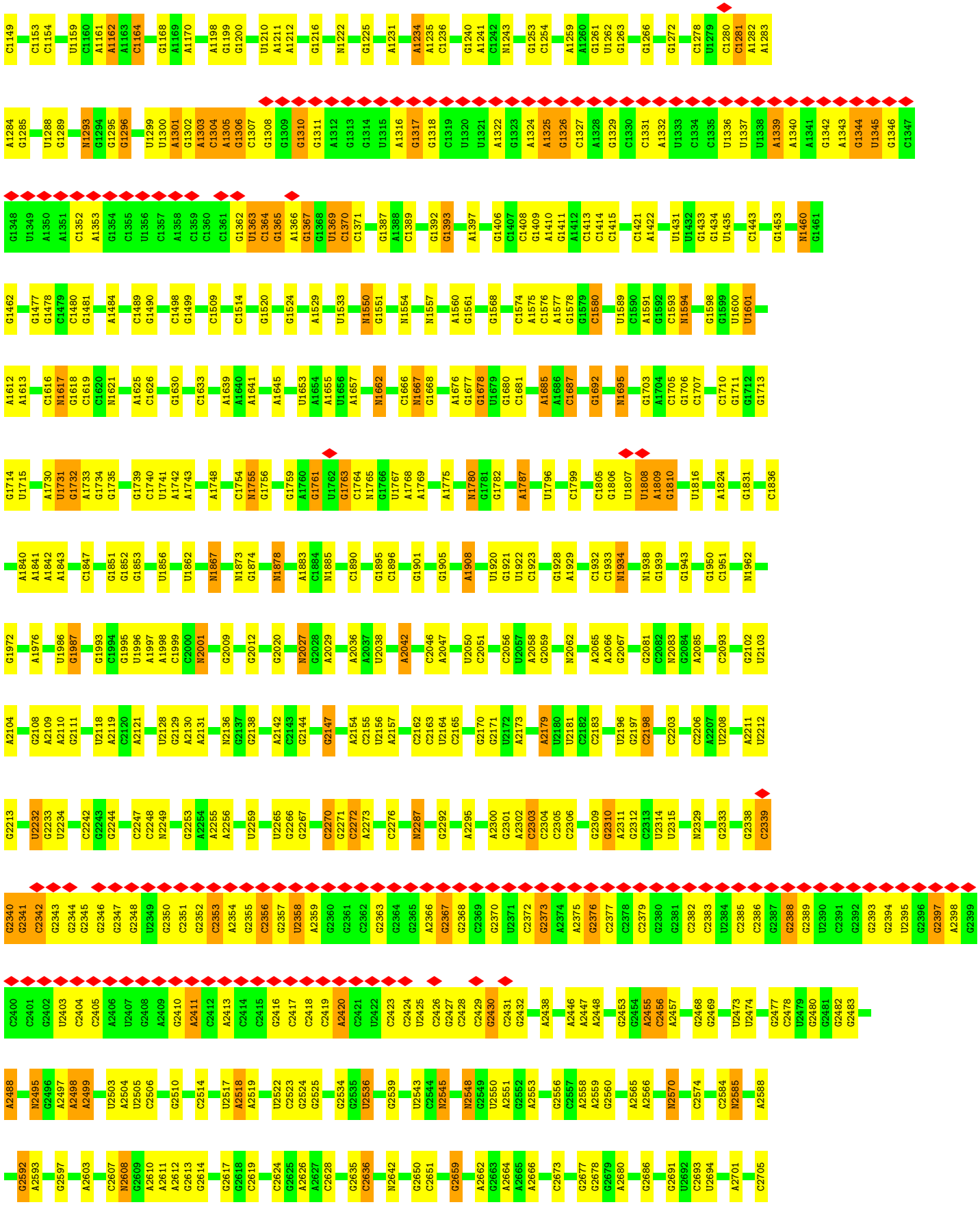
3 Residue-property plots (i)

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

- Molecule 1: rRNA 23S

Chain 1:

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A1284 G1285 U1288 G1289 N1293 G1294 G1295 G1296 U1299 U1300 A1301 G1302 A1303 C1304 A1305 G1306 C1307 G1308 G1309 G1310 G1311 A1312 G1313 G1314 U1315 A1316 G1317 G1318 C1319 U1320 U1321 A1322 G1323 A1324 A1325 G1326 C1327 A1328 G1329 C1330 C1331 A1332 U1333 C1334 C1335 U1336 U1337 U1338 A1339 A1340 A1341 G1342 A1343 G1344 U1345 G1346 C1347
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G1714 U1715 A1730 U1731 G1732 A1733 G1734 G1735 G1739 C1740 U1741 A1742 A1743 A1748 C1754 N1755 G1756 G1759 A1760 G1761 U1762 G1763 C1764 N1765 G1766 U1767 A1768 A1769 A1775 N1780 G1781 G1782 A1787 U1796 C1799 C1805 G1806 U1807 U1808 A1809 G1810 U1816 A1824 G1831 C1836
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G2340 G2341 C2342 G2343 G2344 G2345 G2346 G2347 G2348 U2349 G2350 C2351 G2352 C2353 A2354 G2355 C2356 G2357 U2358 A2359 G2360 G2361 C2362 G2363 G2364 G2365 A2366 G2367 G2368 C2369 G2370 U2371 C2372 G2373 A2374 A2375 G2376 C2377 C2378 C2379 G2380 G2381 C2382 C2383 U2384 C2385 C2386 G2387 G2388 G2389 U2390 C2391 G2392 G2393 G2394 U2395 G2396 G2397 A2398 G2399
C2400 C2401 G2402 U2403 C2404 C2405 A2406 U2407 G2408 A2409 G2410 A2411 C2412 A2413 C2414 C2415 G2416 C2417 C2418 C2419 A2420 C2421 U2422 C2423 C2424 U2425 C2426 G2427 C2428 C2429 G2430 C2431 G2432 A2438 A2446 A2447 A2448 G2453 G2454 A2455 C2456 A2457 G2468 G2469 U2473 U2474 G2477 C2478 U2479 G2480 G2481 G2482 G2483
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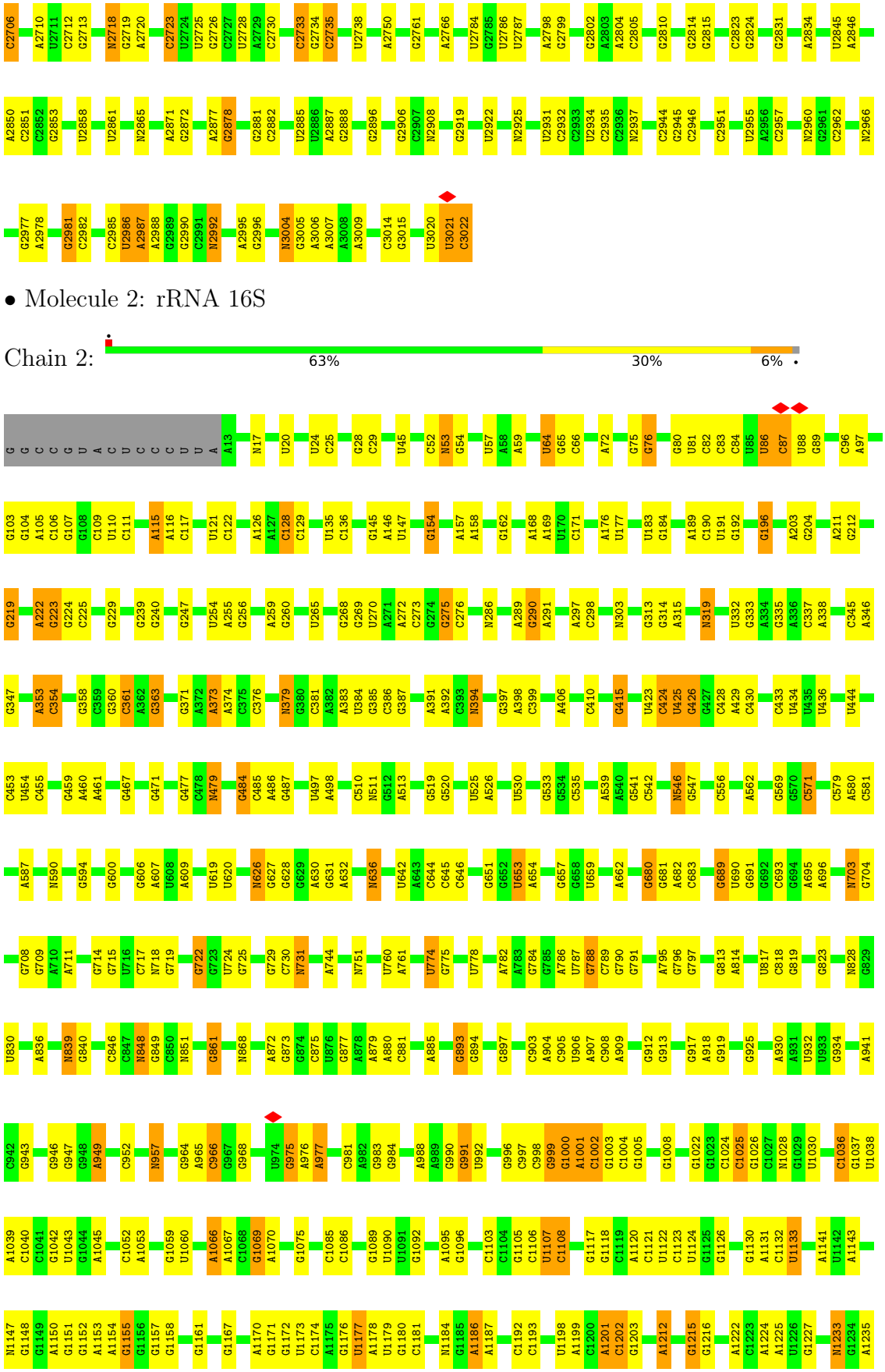
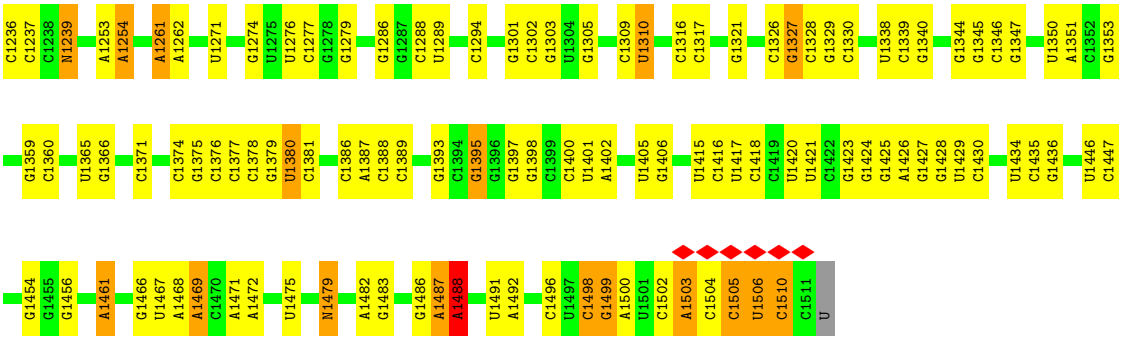


- Molecule 2: rRNA 16S

Chain 2:

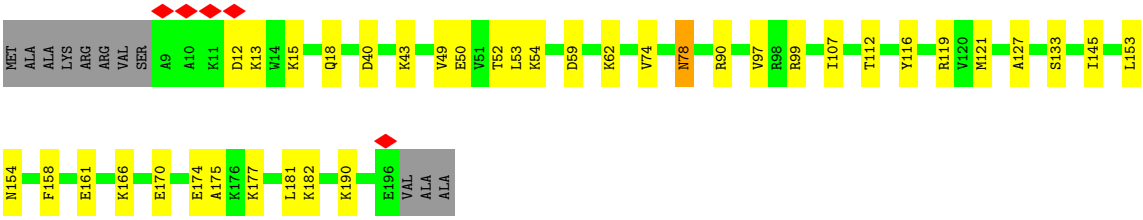


- Molecule 3: rRNA 5S

Chain 3:

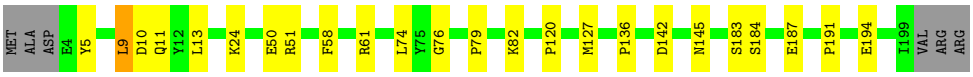
- Molecule 4: 30S ribosomal protein S3Ae

Chain AA:



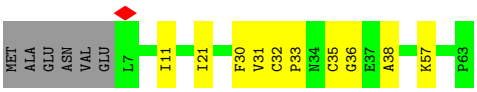
- Molecule 5: 30S ribosomal protein S2

Chain AB:



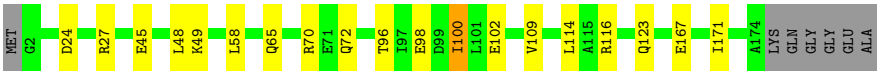
- Molecule 6: Zn-ribbon RNA-binding protein involved in translation

Chain AC:



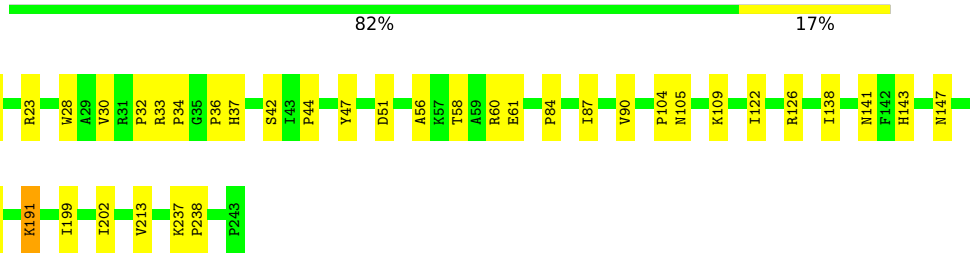
- Molecule 7: 30S ribosomal protein S4

Chain AD:



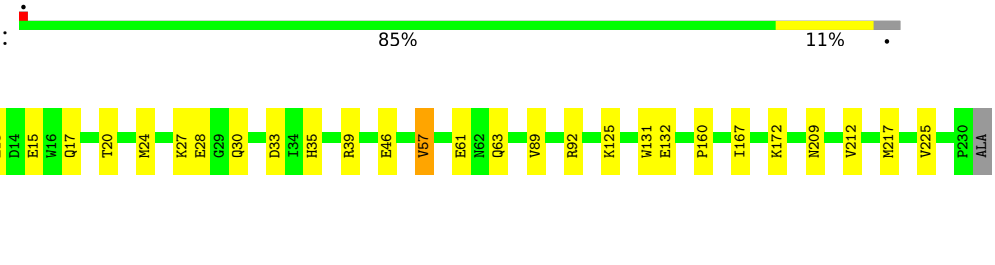
- Molecule 8: 30S ribosomal protein S4e

Chain AE:



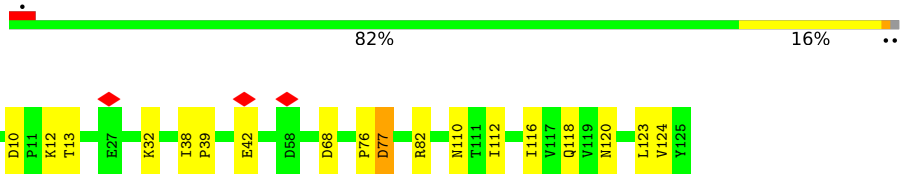
- Molecule 9: 30S ribosomal protein S5

Chain AF:



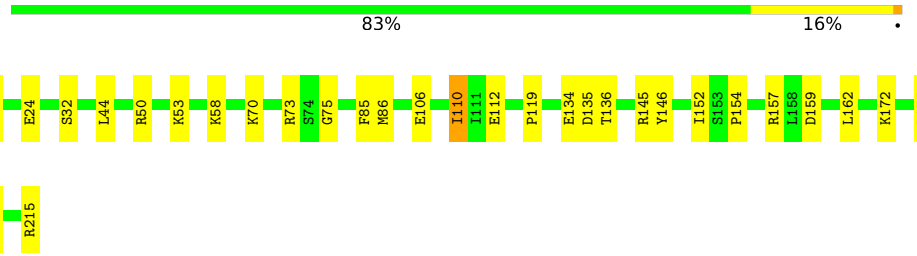
- Molecule 10: 30S ribosomal protein S6e

Chain AG:



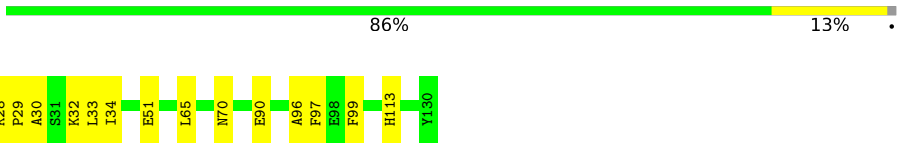
- Molecule 11: 30S ribosomal protein S7

Chain AH:



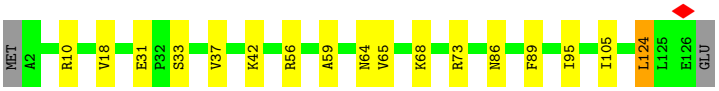
- Molecule 12: 30S ribosomal protein S8

Chain AI:



- Molecule 13: 30S ribosomal protein S8e

Chain AJ:

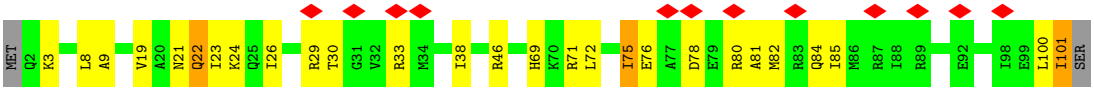


• Molecule 14: 30S ribosomal protein S9

Chain AK:

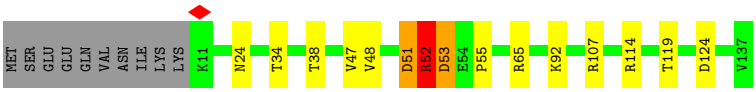
• Molecule 15: 30S ribosomal protein S10

Chain AL:



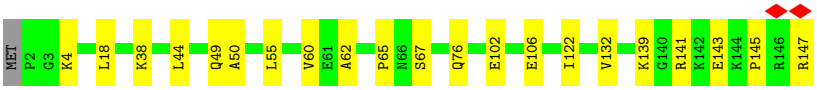
• Molecule 16: 30S ribosomal protein S11

Chain AM:



• Molecule 17: 30S ribosomal protein S12

Chain AN:

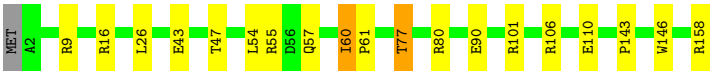


• Molecule 18: 30S ribosomal protein S14 type Z

Chain AP:

• Molecule 19: 30S ribosomal protein S15

Chain AQ:



• Molecule 20: 30S ribosomal protein S17

Chain AR: 77% 17% • 5%

MET VAL R3 C16 K20 V38 P43 T46 V47 T48 V49 E50 R66 R67 N74 C77 A80 K81 V82 G83 D84 K96 V105 L106 E107 R108 A109 GLU GLU ARG ARG

• Molecule 21: 30S ribosomal protein S17e

Chain AS: 67% 27% • •

MET G2 K3 I4 R5 Q6 I9 K10 F17 E23 F24 T25 R26 D27 H30 K34 L38 T39 N40 V41 K44 K45 R49 V58 R59 M60 K65 ILE LEU

• Molecule 22: 30S ribosomal protein S19e

Chain AU: 87% 12% •

MET A2 V7 R15 E22 E25 P45 R72 L73 R74 A93 I98 D130 T134 E135 L136 K137 E141 E142 I143 I144 P145 E146 Y150

• Molecule 23: 30S ribosomal protein S24e

Chain AV: • 76% 20% • •

M1 E2 I3 I23 Y24 H25 P29 T30 P31 S32 R33 K37 G38 K39 L40 V41 D45 L46 N47 P48 T51 V52 I53 I56 Y71 Y72 E82 I92 I93 K96 GLU GLY GLU

• Molecule 23: 30S ribosomal protein S24e

Chain B6: 12% 86% 9% 5%

M1 E2 E7 E10 K17 I23 P31 V41 D45 P48 E49 T50 Y71 Y72 Y73 D74 K75 D76 D90 G91 I92 I93 E94 LYS LYS GLU GLY GLU

• Molecule 24: 30S ribosomal protein S27e

Chain AW: • 69% 22% • 6%

MET ALA LEU PRO R5 N6 V7 I8 K19 D22 G23 G24 V29 H32 R36 V37 R38 T45 L46 V47 E48 K53 R57 L61 L64 E65

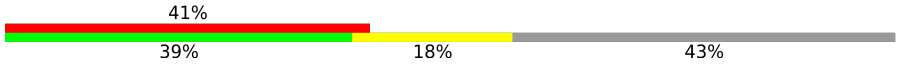
• Molecule 25: 30S ribosomal protein S28e

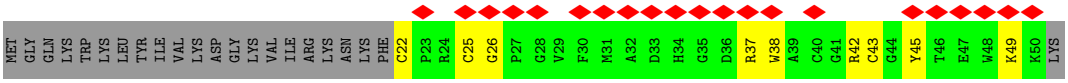
Chain AX: • 63% 27% • 8%

MET ALA GLU D4 A9 E10 E13 I14 I15 K28 V29 R30 I31 L32 E33 G34 R35 D36 K37 G38 R39 R42 R50 D53 I54 L55 T60 E61 R62 E66 I67 K68 SER ARG ARG

• Molecule 26: 30S ribosomal protein S27ae

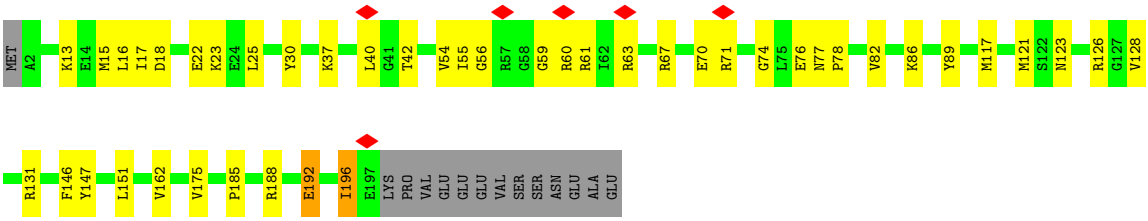
Chain AY:





• Molecule 27: 30S ribosomal protein S3

Chain AZ:

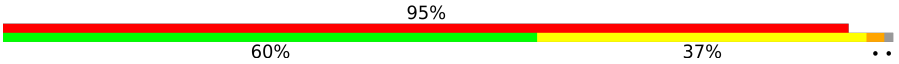


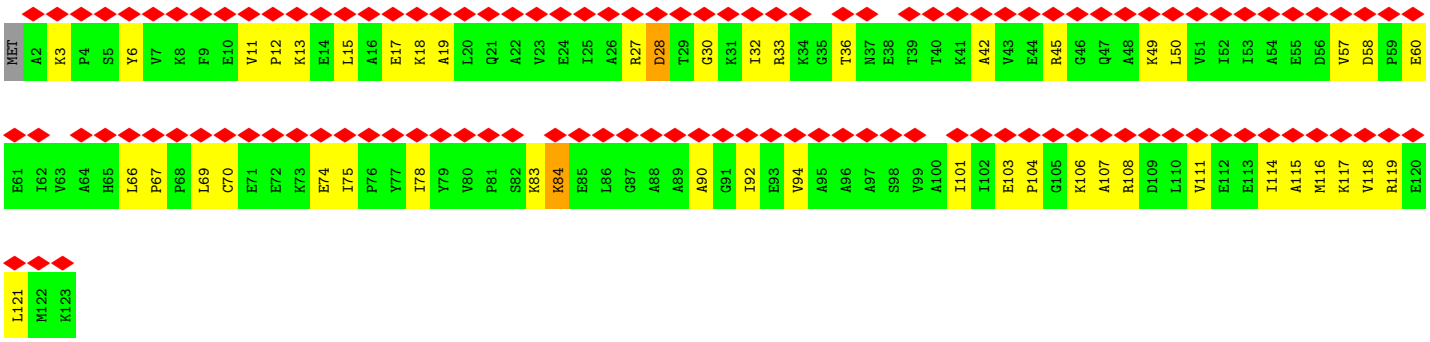
• Molecule 28: Small ribosomal subunit protein eS32

Chain A0:

• Molecule 29: 50S ribosomal protein L7Ae

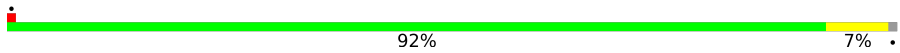
Chain A3:

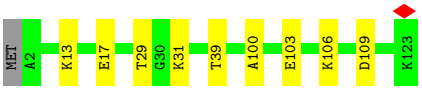




• Molecule 29: 50S ribosomal protein L7Ae

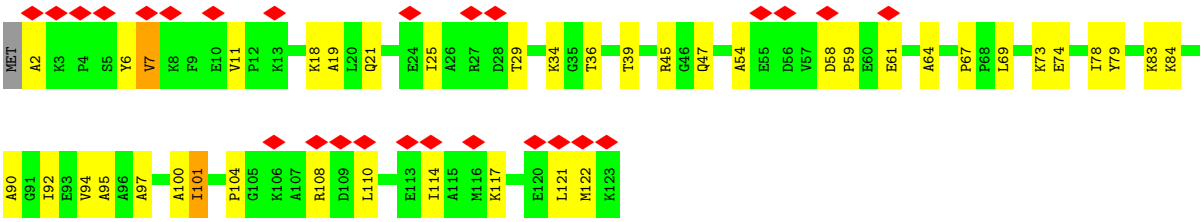
Chain BG:





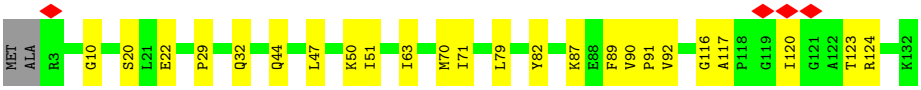
• Molecule 29: 50S ribosomal protein L7Ae

Chain B4:



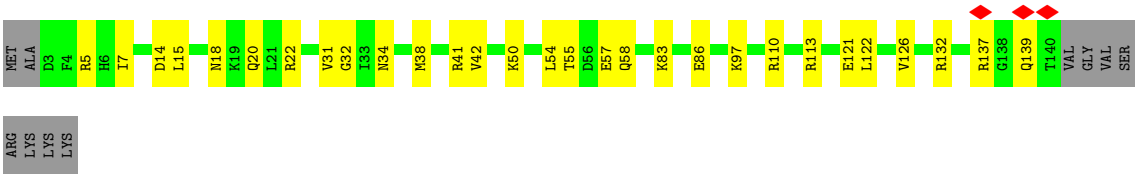
• Molecule 30: 30S ribosomal protein S19

Chain AT:



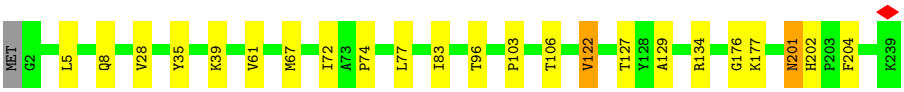
• Molecule 31: 30S ribosomal protein S13

Chain AO:



• Molecule 32: Large ribosomal subunit protein uL2

Chain BB:



• Molecule 33: Large ribosomal subunit protein uL30

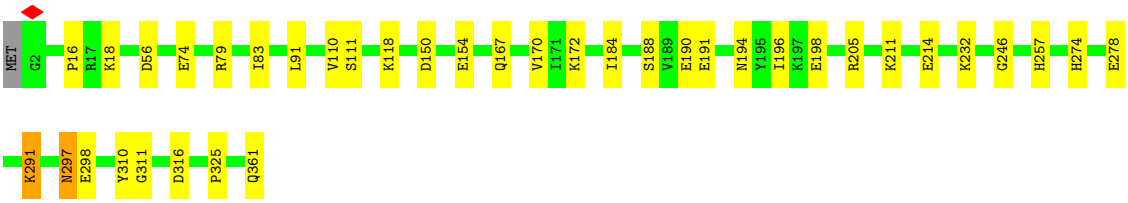
Chain BY:

• Molecule 34: Large ribosomal subunit protein uL18

Chain BO:

• Molecule 35: Large ribosomal subunit protein uL3

Chain BC: 89% 10%

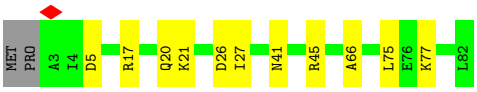


• Molecule 36: Large ribosomal subunit protein eL14

Chain B5: 73% 23%

• Molecule 36: Large ribosomal subunit protein eL14

Chain BK: 84% 13%



• Molecule 37: Large ribosomal subunit protein uL15

Chain BL: 88% 11%

• Molecule 38: Large ribosomal subunit protein eL39

Chain Bf: 80% 18%

• Molecule 39: Large ribosomal subunit protein uL24

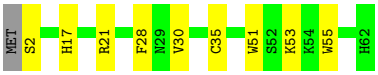
Chain BU: 85% 15%

• Molecule 40: Large ribosomal subunit protein eL32

Chain Bb: 94% 5%

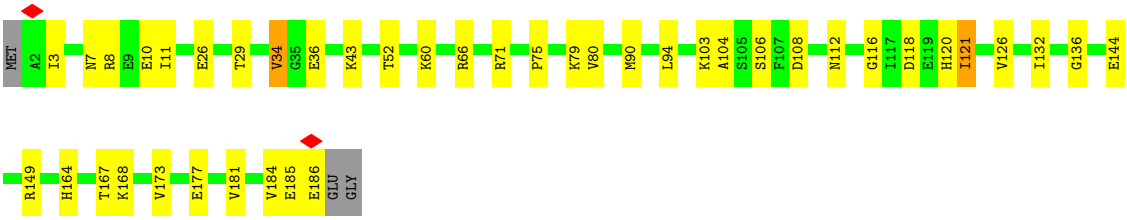
• Molecule 41: Large ribosomal subunit protein eL37

Chain Be:



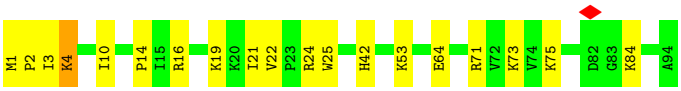
• Molecule 42: Large ribosomal subunit protein uL5

Chain BE:



• Molecule 43: Large ribosomal subunit protein eL31

Chain Ba:

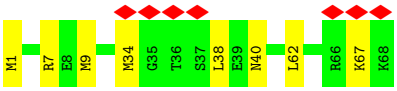


• Molecule 44: Large ribosomal subunit protein uL23

Chain BT:

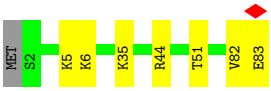
• Molecule 45: Large ribosomal subunit protein uL29

Chain BW:



• Molecule 46: Large ribosomal subunit protein eL43

Chain Bi:

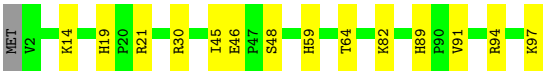


• Molecule 47: Large ribosomal subunit protein uL13

Chain BI:

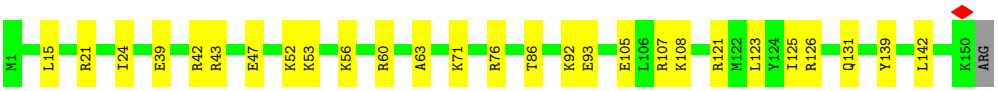
• Molecule 48: Large ribosomal subunit protein eL21

Chain BR:



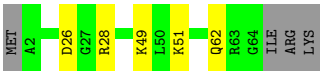
• Molecule 49: Large ribosomal subunit protein eL19

Chain BQ:



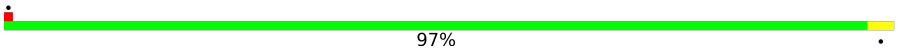
• Molecule 50: Large ribosomal subunit protein eL24

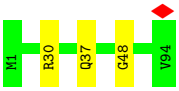
Chain BV:



• Molecule 51: Large ribosomal subunit protein eL42

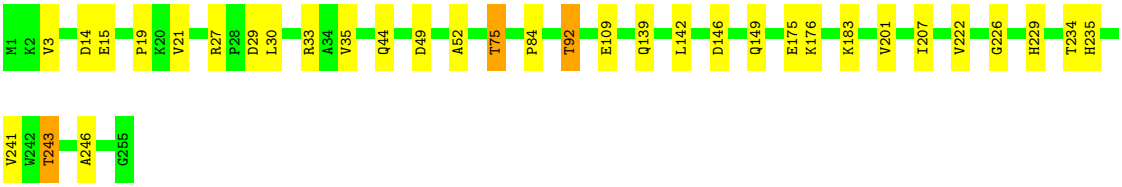
Chain Bj:





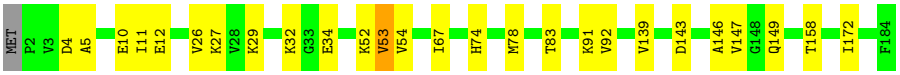
• Molecule 52: Large ribosomal subunit protein uL4

Chain BD:



• Molecule 53: Large ribosomal subunit protein uL6

Chain BF:

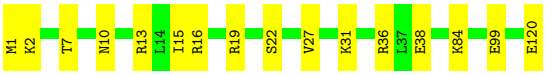


• Molecule 54: Large ribosomal subunit protein eL30

Chain BZ:

• Molecule 55: Large ribosomal subunit protein eL18

Chain BP:

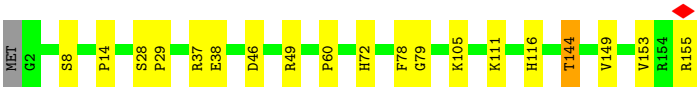


• Molecule 56: Large ribosomal subunit protein eL15

Chain BM:

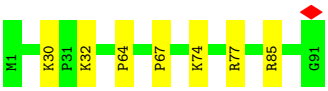
• Molecule 57: Large ribosomal subunit protein uL22

Chain BS:



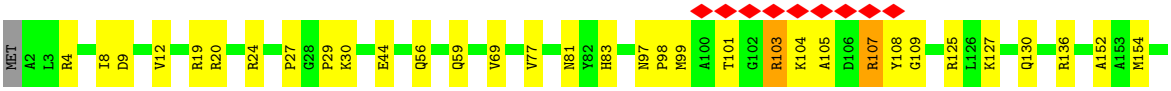
• Molecule 58: Large ribosomal subunit protein eL34

Chain Bd:



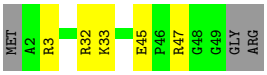
• Molecule 59: Large ribosomal subunit protein uL16

Chain BN:



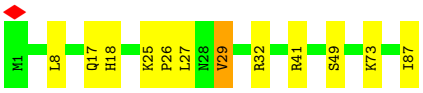
- Molecule 60: Large ribosomal subunit protein eL40

Chain Bg: 84% 10% 6%



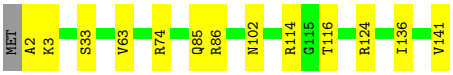
- Molecule 61: Large ribosomal subunit protein eL33

Chain Bc: 86% 13%



- Molecule 62: Large ribosomal subunit protein uL14

Chain BJ: 90% 9%



- Molecule 63: Large ribosomal subunit protein eL20

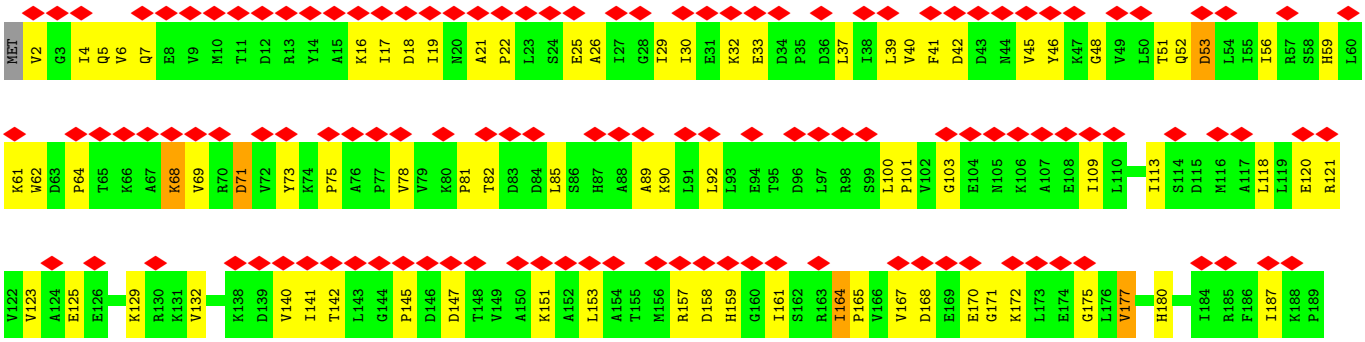
Chain Bl: 77% 22%

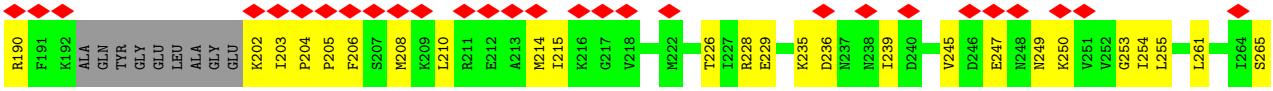
- Molecule 64: C2H2-type domain-containing protein

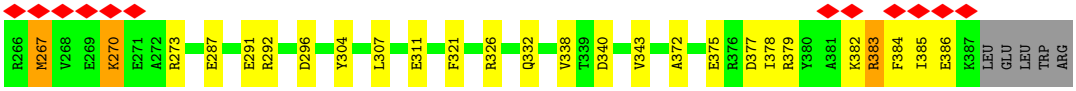
Chain Bk: 89% 8%

- Molecule 65: Dehydrogenase

Chain H: 42% 63% 31%




R190
F191
K192
ALA
GLN
TYR
GLY
GLU
LEU
ALA
GLY
GLU
K202
I203
P204
P205
F206
S207
M208
K209
L210
R211
E212
A213
M214
I215
K216
G217
V218
M222
T226
I227
R228
E229
K235
D236
N237
N238
I239
D240
V245
D246
E247
N248
N249
K250
V251
V252
C253
I254
L255
L261
I264
S265


R266
M267
V268
E269
K270
E271
A272
R273
E287
E291
R292
D296
Y304
L307
E311
F321
R326
Q332
V338
T339
D340
V343
A372
E375
R376
D377
I378
R379
Y380
A381
K382
R383
F384
I385
E386
K387
LEU
GLU
LEU
TRP
ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	207000	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.016	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00125	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 (i)

5.1 Standard geometry (i)

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

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	0.26	1/70601 (0.0%)	0.32	4/110066 (0.0%)
2	2	0.23	1/34435 (0.0%)	0.27	0/53681
3	3	0.20	0/2995	0.25	0/4669
4	AA	0.14	0/1557	0.25	0/2087
5	AB	0.15	0/1602	0.26	0/2165
6	AC	0.16	0/463	0.27	0/628
7	AD	0.15	0/1476	0.21	0/1980
8	AE	0.16	0/2032	0.27	0/2742
9	AF	0.18	0/1838	0.27	0/2478
10	AG	0.13	0/993	0.29	0/1329
11	AH	0.14	0/1762	0.26	0/2366
12	AI	0.18	0/1055	0.27	0/1415
13	AJ	0.15	0/995	0.23	0/1327
14	AK	0.16	0/1089	0.28	0/1459
15	AL	0.16	0/817	0.29	0/1097
16	AM	0.16	0/973	0.34	1/1311 (0.1%)
17	AN	0.17	0/1165	0.26	0/1547
18	AP	0.18	0/465	0.31	0/613
19	AQ	0.15	0/1333	0.24	0/1791
20	AR	0.16	0/907	0.31	0/1225
21	AS	0.15	0/548	0.25	0/725
22	AU	0.15	0/1253	0.25	0/1689
23	AV	0.14	0/826	0.23	0/1108
23	B6	0.11	0/808	0.24	0/1086
24	AW	0.15	0/476	0.25	0/641
25	AX	0.19	0/518	0.33	0/694
26	AY	0.10	0/235	0.27	0/315
27	AZ	0.14	0/1563	0.26	0/2099
28	A0	0.20	0/349	0.27	0/451
29	A3	0.12	0/945	0.30	0/1274
29	B4	0.14	0/945	0.32	0/1274
29	BG	0.16	0/944	0.27	0/1274

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
30	AT	0.14	0/1077	0.26	0/1439
31	AO	0.14	0/1135	0.26	0/1526
32	BB	0.22	0/1882	0.32	0/2538
33	BY	0.19	0/1254	0.27	0/1677
34	BO	0.15	0/1645	0.25	0/2209
35	BC	0.21	0/2933	0.29	0/3943
36	B5	0.16	0/619	0.29	0/830
36	BK	0.16	0/611	0.28	0/819
37	BL	0.19	0/1167	0.32	0/1552
38	Bf	0.21	0/443	0.27	0/589
39	BU	0.18	0/1027	0.27	0/1368
40	Bb	0.20	0/1120	0.27	0/1494
41	Be	0.22	0/514	0.29	0/676
42	BE	0.15	0/1509	0.28	0/2022
43	Ba	0.19	0/793	0.27	0/1064
44	BT	0.18	0/705	0.26	0/945
45	BW	0.16	0/566	0.23	0/747
46	Bi	0.19	0/630	0.31	0/839
47	BI	0.20	0/1166	0.26	0/1559
48	BR	0.20	0/819	0.29	0/1098
49	BQ	0.20	0/1281	0.27	0/1689
50	BV	0.20	0/547	0.25	0/729
51	Bj	0.18	0/807	0.26	0/1070
52	BD	0.20	0/2069	0.30	0/2787
53	BF	0.17	0/1485	0.27	0/2003
54	BZ	0.17	0/759	0.28	0/1023
55	BP	0.19	0/984	0.26	0/1314
56	BM	0.23	0/1627	0.30	0/2170
57	BS	0.20	0/1275	0.31	0/1715
58	Bd	0.19	0/778	0.28	0/1036
59	BN	0.18	0/1483	0.28	0/1992
60	Bg	0.16	0/396	0.25	0/526
61	Bc	0.19	0/693	0.30	0/926
62	BJ	0.20	0/1080	0.28	0/1456
63	Bl	0.16	0/669	0.27	0/886
64	Bk	0.22	0/538	0.28	0/709
65	H	0.16	0/3053	0.39	3/4117 (0.1%)
All	All	0.22	2/179102 (0.0%)	0.30	8/263688 (0.0%)

All (2) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1036	C	O3'-P	-7.02	1.50	1.61
1	1	96	U	C1'-N1	5.75	1.57	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	126	C	P-O3'-C3'	-15.70	96.65	120.20
1	1	126	C	OP1-P-O3'	-8.35	82.94	108.00
65	H	383	ARG	N-CA-C	6.30	120.58	113.01
16	AM	52	ARG	N-CA-C	5.98	117.79	111.28
65	H	377	ASP	CA-C-N	-5.92	115.08	122.48
65	H	377	ASP	C-N-CA	-5.92	115.08	122.48
1	1	126	C	O3'-P-O5'	5.68	112.52	104.00
1	1	126	C	OP2-P-O3'	5.40	124.20	108.00

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	32948	579	0
2	2	32291	0	16342	301	0
3	3	2703	0	1375	17	0
4	AA	1531	0	1623	24	0
5	AB	1571	0	1630	16	0
6	AC	449	0	435	7	0
7	AD	1452	0	1521	13	0
8	AE	1983	0	2060	25	0
9	AF	1808	0	1879	20	0
10	AG	977	0	1037	14	0
11	AH	1725	0	1780	28	0
12	AI	1034	0	1069	14	0
13	AJ	986	0	1070	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	AK	1073	0	1133	14	0
15	AL	809	0	859	18	0
16	AM	955	0	981	15	0
17	AN	1148	0	1248	12	0
18	AP	455	0	475	7	0
19	AQ	1305	0	1388	16	0
20	AR	884	0	906	11	0
21	AS	541	0	573	15	0
22	AU	1223	0	1263	12	0
23	AV	808	0	832	15	0
23	B6	790	0	806	5	0
24	AW	470	0	495	8	0
25	AX	516	0	544	13	0
26	AY	227	0	207	7	0
27	AZ	1541	0	1624	32	0
28	A0	343	0	407	1	0
29	A3	933	0	982	38	0
29	B4	933	0	982	25	0
29	BG	932	0	982	5	0
30	AT	1057	0	1131	15	0
31	AO	1116	0	1152	19	0
32	BB	1838	0	1903	17	0
33	BY	1235	0	1314	10	0
34	BO	1607	0	1638	24	0
35	BC	2870	0	3021	21	0
36	B5	614	0	671	15	0
36	BK	607	0	663	8	0
37	BL	1149	0	1218	16	0
38	Bf	435	0	494	8	0
39	BU	1011	0	1078	13	0
40	Bb	1095	0	1190	4	0
41	Be	503	0	533	8	0
42	BE	1485	0	1539	27	0
43	Ba	778	0	851	13	0
44	BT	696	0	758	8	0
45	BW	565	0	628	6	0
46	Bi	620	0	668	4	0
47	BI	1148	0	1237	13	0
48	BR	797	0	835	11	0
49	BQ	1265	0	1392	21	0
50	BV	532	0	523	4	0
51	Bj	789	0	842	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	BD	2026	0	2131	23	0
53	BF	1456	0	1514	16	0
54	BZ	749	0	796	8	0
55	BP	971	0	1039	10	0
56	BM	1588	0	1683	12	0
57	BS	1247	0	1280	10	0
58	Bd	759	0	825	7	0
59	BN	1452	0	1491	26	0
60	Bg	387	0	397	3	0
61	Bc	684	0	748	8	0
62	BJ	1066	0	1133	9	0
63	Bl	659	0	702	10	0
64	Bk	528	0	575	3	0
65	H	3009	0	3133	92	0
66	1	167	0	0	0	0
66	2	69	0	0	0	0
66	3	1	0	0	0	0
66	AK	1	0	0	0	0
66	AN	1	0	0	0	0
66	BB	1	0	0	0	0
66	BD	1	0	0	0	0
66	BM	1	0	0	0	0
66	BS	1	0	0	0	0
66	Bb	1	0	0	0	0
67	AC	2	0	0	0	0
67	AF	1	0	0	0	0
67	AP	1	0	0	0	0
67	AR	1	0	0	0	0
67	AW	1	0	0	0	0
67	BV	1	0	0	0	0
67	Bd	1	0	0	0	0
67	Be	1	0	0	0	0
67	Bg	1	0	0	0	0
67	Bi	1	0	0	0	0
67	Bj	1	0	0	0	0
67	Bk	1	0	0	0	0
All	All	170227	0	124182	1619	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1619) 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
1:1:100:G:N2	1:1:119:C:O2	1.82	1.12
1:1:117:G:O2'	1:1:118:U:OP1	1.67	1.12
1:1:2585:4AC:H5	1:1:2597:G:H1	1.12	1.09
1:1:2608:4AC:H5	1:1:2613:G:H1	1.17	1.07
1:1:2887:A:HO2'	62:BJ:2:ALA:N	1.57	1.01
1:1:102:C:N4	1:1:117:G:O6	1.97	0.97
2:2:977:A:H62	2:2:999:G:H21	1.16	0.91
1:1:235:G:H1	1:1:242:C:H5	1.21	0.89
1:1:2346:G:N2	1:1:2423:C:O2	2.10	0.83
2:2:631:G:H22	2:2:708:G:H1	1.26	0.83
1:1:1713:G:H21	1:1:1787:A:H8	1.26	0.82
1:1:931:U:H3	1:1:1046:G:H1	1.27	0.82
9:AF:212:VAL:H	12:AI:70:ASN:HD21	1.26	0.80
37:BL:1:MET:HE1	52:BD:30:LEU:HD12	1.64	0.79
1:1:2346:G:N1	1:1:2423:C:N3	2.29	0.79
29:A3:27:ARG:HH11	29:A3:32:ILE:HG12	1.48	0.79
65:H:48:GLY:HA3	65:H:75:PRO:HA	1.65	0.79
16:AM:53:ASP:OD1	16:AM:53:ASP:N	2.08	0.77
2:2:1321:G:OP2	11:AH:53:LYS:NZ	2.18	0.77
48:BR:19:HIS:HD2	48:BR:21:ARG:H	1.31	0.77
23:AV:33:ARG:NH2	23:AV:53:ILE:O	2.19	0.76
2:2:96:C:H2'	2:2:97:A:C8	2.21	0.75
29:A3:18:LYS:HE3	29:A3:111:VAL:HA	1.67	0.75
65:H:71:ASP:N	65:H:71:ASP:OD1	2.17	0.75
2:2:415:G:H21	7:AD:123:GLN:HE22	1.34	0.75
32:BB:122:VAL:HG13	32:BB:127:THR:HG22	1.69	0.75
65:H:4:ILE:HG12	65:H:121:ARG:HD2	1.68	0.74
1:1:792:A:H62	1:1:1509:C:H5	1.31	0.74
19:AQ:77:THR:HG22	19:AQ:80:ARG:H	1.51	0.74
26:AY:25:CYS:HB3	29:A3:45:ARG:HH22	1.50	0.74
65:H:19:ILE:O	65:H:68:LYS:NZ	2.19	0.74
29:B4:101:ILE:HD11	29:B4:104:PRO:HA	1.70	0.74
1:1:2608:4AC:H5	1:1:2613:G:N1	2.00	0.73
1:1:103:C:H2'	1:1:104:C:C6	2.23	0.73
2:2:627:G:H2'	2:2:628:G:C8	2.23	0.73
1:1:117:G:O2'	1:1:118:U:P	2.47	0.72
1:1:1299:U:H4'	1:1:1303:A:H5"	1.69	0.72
1:1:205:G:N7	38:Bf:34:ARG:NH2	2.36	0.72
1:1:2344:G:H1	1:1:2425:U:H3	1.37	0.72
21:AS:23:GLU:OE2	21:AS:34:LYS:NZ	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BC:291:LYS:HG2	35:BC:298:GLU:HG2	1.71	0.72
1:1:102:C:C4	1:1:103:C:C4	2.78	0.72
47:BI:17:ARG:NH1	47:BI:117:GLU:OE2	2.22	0.72
1:1:103:C:H2'	1:1:104:C:H6	1.55	0.72
36:BK:21:LYS:O	36:BK:41:ASN:ND2	2.22	0.71
54:BZ:22:GLU:OE1	54:BZ:25:ARG:NH2	2.23	0.71
1:1:117:G:HO2'	1:1:118:U:P	2.12	0.71
1:1:102:C:N4	1:1:103:C:N4	2.38	0.71
29:B4:83:LYS:HG2	29:B4:95:ALA:HB1	1.73	0.71
1:1:2536:U:H5"	42:BE:116:GLY:HA3	1.73	0.71
1:1:2585:4AC:H5	1:1:2597:G:N1	1.97	0.71
1:1:112:A:H3'	1:1:113:G:C8	2.26	0.71
1:1:1601:U:O4	44:BT:15:LYS:NZ	2.23	0.71
2:2:1130:G:N7	21:AS:44:LYS:NZ	2.34	0.71
32:BB:5:LEU:H	32:BB:8:GLN:HE21	1.39	0.71
1:1:1653:U:OP2	49:BQ:42:ARG:NH2	2.23	0.70
2:2:1379:G:H2'	2:2:1380:OMU:H6	1.73	0.70
36:BK:45:ARG:NH2	36:BK:66:ALA:O	2.23	0.70
1:1:1140:G:O2'	1:1:1143:A:N6	2.22	0.70
2:2:717:C:OP2	19:AQ:16:ARG:NH2	2.23	0.70
2:2:651:G:H21	16:AM:38:THR:HG21	1.56	0.70
2:2:1395:G:OP1	62:BJ:74:ARG:NH2	2.24	0.70
22:AU:2:ALA:HB3	22:AU:134:THR:HG22	1.72	0.70
34:BO:63:HIS:HD2	34:BO:65:ARG:H	1.40	0.70
9:AF:61:GLU:O	9:AF:92:ARG:NH1	2.24	0.70
1:1:1739:G:HO2'	1:1:1816:U:HO2'	1.33	0.70
59:BN:56:GLN:HE21	59:BN:125:ARG:HE	1.39	0.69
2:2:908:C:H2'	2:2:909:A:H8	1.58	0.69
43:Ba:16:ARG:HA	43:Ba:19:LYS:HG3	1.75	0.69
2:2:717:C:H4'	19:AQ:47:THR:HG22	1.75	0.69
12:AI:96:ALA:HB3	12:AI:99:PHE:HB2	1.75	0.68
2:2:1022:G:H22	2:2:1177:OMU:HN3	1.39	0.68
48:BR:45:ILE:H	48:BR:59:HIS:HD2	1.42	0.68
65:H:378:ILE:HG13	65:H:378:ILE:O	1.93	0.68
1:1:3007:A:H2	1:1:3009:A:H62	1.42	0.68
65:H:68:LYS:HD2	65:H:69:VAL:H	1.58	0.68
1:1:2426:C:H2'	1:1:2427:G:C8	2.29	0.68
2:2:636:4AC:HM73	2:2:703:4AC:HM73	1.75	0.68
1:1:2701:A:N6	1:1:2713:G:O2'	2.27	0.68
1:1:102:C:C4	1:1:103:C:C5	2.81	0.68
21:AS:25:THR:HG23	21:AS:27:ASP:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:428:C:H2'	2:2:429:A:H8	1.58	0.67
27:AZ:37:LYS:NZ	27:AZ:76:GLU:OE2	2.27	0.67
54:BZ:30:GLY:HA2	54:BZ:58:ILE:HD11	1.76	0.67
1:1:117:G:C2	1:1:118:U:C6	2.83	0.67
32:BB:202:HIS:HD2	32:BB:204:PHE:H	1.40	0.67
20:AR:74:ASN:HD21	20:AR:80:ALA:H	1.42	0.67
1:1:113:G:H2'	1:1:114:G:H8	1.59	0.67
53:BF:10:GLU:HB3	53:BF:52:LYS:HD3	1.77	0.67
16:AM:107:ARG:NH2	25:AX:36:ASP:OD2	2.24	0.67
1:1:189:G:H22	1:1:224:A:H2	1.43	0.67
2:2:714:G:O2'	19:AQ:55:ARG:NH1	2.28	0.67
2:2:1089:G:N2	2:2:1090:U:O4	2.28	0.67
59:BN:105:ALA:O	59:BN:109:GLY:N	2.28	0.67
2:2:1177:OMU:HM22	2:2:1178:A:H5'	1.77	0.66
1:1:869:G:O2'	1:1:870:A:O5'	2.13	0.66
1:1:710:C:O2	1:1:747:G:N2	2.17	0.66
22:AU:137:LYS:NZ	22:AU:141:GLU:OE2	2.28	0.66
8:AE:15:ALA:O	8:AE:23:ARG:NH2	2.28	0.66
39:BU:28:ALA:HA	39:BU:45:PRO:HA	1.77	0.66
23:B6:23:ILE:HG21	23:B6:31:PRO:HG3	1.75	0.66
1:1:1108:G:OP1	48:BR:97:LYS:NZ	2.28	0.66
24:AW:19:LYS:NZ	24:AW:24:GLY:O	2.29	0.66
1:1:163:A:H2	1:1:233:U:H3	1.43	0.66
35:BC:278:GLU:HG3	35:BC:325:PRO:HD3	1.78	0.66
2:2:689:G:OP1	4:AA:99:ARG:NH1	2.28	0.66
24:AW:45:THR:O	24:AW:57:ARG:NH1	2.29	0.66
1:1:2388:G:H2'	1:1:2389:G:H8	1.61	0.65
1:1:894:A:H2'	1:1:895:A:C8	2.32	0.65
15:AL:30:THR:HB	15:AL:80:ARG:HE	1.62	0.65
2:2:965:A:H5"	2:2:966:C:H5	1.62	0.65
42:BE:66:ARG:HB3	65:H:229:GLU:HG3	1.78	0.65
2:2:977:A:H62	2:2:999:G:N2	1.89	0.65
29:B4:6:TYR:OH	29:B4:54:ALA:O	2.13	0.65
2:2:918:A:H2'	2:2:919:G:C8	2.32	0.65
1:1:1317:G:H2'	1:1:1318:G:H8	1.62	0.65
1:1:764:A:O2'	61:Bc:17:GLN:NE2	2.27	0.65
65:H:226:THR:OG1	65:H:229:GLU:OE1	2.15	0.65
2:2:1036:C:H2'	2:2:1037:G:H8	1.62	0.64
11:AH:215:ARG:OXT	25:AX:62:ARG:NH1	2.30	0.64
22:AU:143:ILE:HG13	22:AU:144:ILE:HG13	1.78	0.64
1:1:1905:G:N1	1:1:1908:A:OP2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AL:33:ARG:HH12	15:AL:75:ILE:HA	1.61	0.64
1:1:116:G:H2'	1:1:117:G:H8	1.62	0.64
49:BQ:126:ARG:HH11	49:BQ:131:GLN:HE22	1.46	0.64
2:2:484:G:N2	17:AN:65:PRO:O	2.31	0.64
20:AR:43:PRO:HB2	20:AR:46:THR:HB	1.78	0.64
1:1:102:C:C2	1:1:103:C:C6	2.86	0.64
3:3:10:G:O6	34:BO:12:ARG:NH1	2.30	0.64
65:H:382:LYS:HD2	65:H:382:LYS:N	2.12	0.64
57:BS:46:ASP:OD1	57:BS:49:ARG:NH2	2.31	0.64
1:1:2001:4AC:OP2	49:BQ:76:ARG:NH1	2.31	0.63
33:BY:123:ARG:NH1	33:BY:155:LEU:O	2.30	0.63
1:1:1715:U:H5	1:1:1824:A:N7	1.96	0.63
26:AY:42:ARG:NH1	26:AY:43:CYS:SG	2.72	0.63
27:AZ:60:ARG:HH21	27:AZ:63:ARG:HD2	1.64	0.63
65:H:92:LEU:HD23	65:H:100:LEU:HD13	1.81	0.63
1:1:1676:A:N1	1:1:1692:G:O2'	2.31	0.63
2:2:154:G:H21	10:AG:118:GLN:HE22	1.46	0.63
52:BD:49:ASP:HB3	52:BD:52:ALA:HB2	1.81	0.63
59:BN:97:ASN:HD22	59:BN:98:PRO:HD2	1.64	0.63
30:AT:116:GLY:HA2	30:AT:124:ARG:HH11	1.64	0.63
1:1:230:G:OP1	41:Be:21:ARG:NH1	2.31	0.63
60:Bg:32:ARG:HG3	60:Bg:33:LYS:HD2	1.80	0.63
1:1:2311:A:H2'	1:1:2312:G:C8	2.33	0.63
15:AL:33:ARG:O	15:AL:33:ARG:NH1	2.30	0.63
19:AQ:77:THR:HB	19:AQ:80:ARG:HD2	1.81	0.63
1:1:2242:C:O2'	43:Ba:24:ARG:NH2	2.32	0.63
1:1:2498:A:H2	1:1:2503:U:H3	1.46	0.63
1:1:1787:A:OP1	58:Bd:30:LYS:NZ	2.28	0.62
1:1:2388:G:H2'	1:1:2389:G:C8	2.33	0.62
2:2:975:G:N2	2:2:1000:G:O2'	2.30	0.62
2:2:1321:G:O6	14:AK:10:ARG:NH2	2.31	0.62
33:BY:60:ASN:H	33:BY:148:ASN:HD21	1.47	0.62
1:1:67:C:OP2	1:1:68:U:O2'	2.17	0.62
1:1:112:A:H3'	1:1:113:G:H8	1.63	0.62
1:1:710:C:N3	1:1:747:G:N1	2.35	0.62
29:A3:83:LYS:HG2	29:A3:84:LYS:HD2	1.80	0.62
1:1:418:A:H2'	1:1:419:G:C8	2.35	0.62
1:1:1283:A:H2'	1:1:1284:A:C8	2.34	0.62
1:1:2990:G:H21	53:BF:149:GLN:HE22	1.47	0.62
29:B4:92:ILE:HG22	29:B4:94:VAL:H	1.63	0.62
1:1:2887:A:O2'	62:BJ:2:ALA:N	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2103:U:O2'	1:1:2104:A:N7	2.25	0.62
1:1:2109:A:H2'	1:1:2110:A:C8	2.35	0.62
1:1:2559:A:H2'	1:1:2560:G:C8	2.35	0.62
2:2:912:G:OP1	11:AH:73:ARG:NH1	2.32	0.62
29:B4:39:THR:HG23	29:B4:100:ALA:HB2	1.82	0.62
2:2:1036:C:H2'	2:2:1037:G:C8	2.35	0.62
65:H:147:ASP:OD2	65:H:151:LYS:NZ	2.29	0.62
1:1:209:G:O2'	45:BW:40:ASN:ND2	2.32	0.62
31:AO:55:THR:H	31:AO:58:GLN:HE21	1.45	0.62
29:B4:45:ARG:HB3	29:B4:47:GLN:HE22	1.65	0.61
1:1:2341:G:HO2'	1:1:2342:C:H6	1.48	0.61
36:B5:6:VAL:O	36:B5:59:LYS:NZ	2.32	0.61
54:BZ:40:ASN:HB2	54:BZ:66:THR:HA	1.82	0.61
2:2:75:G:H2'	2:2:76:G:C8	2.34	0.61
55:BP:36:ARG:NH1	55:BP:120:GLU:OE2	2.27	0.61
16:AM:51:ASP:OD1	16:AM:51:ASP:N	2.31	0.61
1:1:1031:G:H1	32:BB:201:ASN:HD21	1.48	0.61
52:BD:226:GLY:H	52:BD:229:HIS:HD2	1.49	0.61
2:2:1227:G:OP1	15:AL:46:ARG:NH2	2.33	0.61
5:AB:120:PRO:HB3	5:AB:127:MET:HE1	1.83	0.61
13:AJ:73:ARG:HH21	13:AJ:105:ILE:HD12	1.66	0.61
1:1:2377:C:H42	1:1:2394:G:H1	1.49	0.60
3:3:9:G:OP1	34:BO:24:ARG:NH1	2.34	0.60
1:1:595:A:O2'	52:BD:44:GLN:NE2	2.32	0.60
1:1:3022:C:H2'	1:1:3022:C:O2	2.00	0.60
27:AZ:89:TYR:HB2	27:AZ:123:ASN:HD22	1.66	0.60
36:BK:20:GLN:NE2	36:BK:41:ASN:O	2.34	0.60
2:2:977:A:N6	2:2:999:G:H21	1.95	0.60
2:2:1502:C:C4	2:2:1503:A:H1'	2.36	0.60
65:H:21:ALA:HB1	65:H:25:GLU:HG2	1.84	0.60
14:AK:36:VAL:O	14:AK:42:ARG:NH1	2.34	0.60
2:2:976:A:N6	2:2:1001:A:O4'	2.34	0.60
52:BD:175:GLU:OE1	52:BD:176:LYS:NZ	2.34	0.60
52:BD:243:THR:HG22	52:BD:246:ALA:H	1.66	0.60
32:BB:28:VAL:HG11	32:BB:72:ILE:HG13	1.82	0.60
34:BO:48:ILE:HG21	34:BO:99:ILE:HD13	1.84	0.60
1:1:31:G:H4'	43:Ba:14:PRO:HG3	1.84	0.60
1:1:113:G:H2'	1:1:114:G:C8	2.36	0.60
1:1:1406:G:OP2	33:BY:127:ARG:NH2	2.31	0.60
1:1:2302:A:H2	1:1:2735:C:H42	1.50	0.60
1:1:2036:A:HO2'	41:Be:2:SER:N	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:918:A:H2'	2:2:919:G:H8	1.65	0.60
2:2:1201:A:H4'	31:AO:139:GLN:HA	1.84	0.60
21:AS:39:THR:HG22	21:AS:41:VAL:H	1.65	0.60
1:1:806:G:OP1	52:BD:27:ARG:NH2	2.35	0.59
65:H:30:ILE:HG13	65:H:52:GLN:HE22	1.66	0.59
65:H:140:VAL:HB	65:H:253:GLY:HA2	1.84	0.59
8:AE:58:THR:HG22	8:AE:60:ARG:H	1.68	0.59
29:A3:28:ASP:OD1	29:A3:28:ASP:N	2.34	0.59
30:AT:82:TYR:HB3	30:AT:89:PHE:HB3	1.84	0.59
1:1:2356:C:H42	1:1:2411:A:H61	1.48	0.59
5:AB:183:SER:N	5:AB:187:GLU:OE2	2.35	0.59
8:AE:105:ASN:N	8:AE:109:LYS:O	2.36	0.59
36:BK:45:ARG:NH1	63:Bl:1:MET:O	2.34	0.59
52:BD:33:ARG:NH1	52:BD:109:GLU:OE2	2.35	0.59
2:2:778:U:O2'	2:2:872:A:N1	2.31	0.59
11:AH:112:GLU:HB3	11:AH:119:PRO:HG3	1.83	0.59
34:BO:177:ASP:HB3	34:BO:180:LYS:HG2	1.83	0.59
1:1:653:G:N1	1:1:656:A:OP2	2.36	0.59
2:2:680:OMG:H2'	2:2:681:G:C8	2.38	0.59
2:2:1380:OMU:HM22	2:2:1381:C:H5'	1.85	0.59
1:1:2376:G:H1	1:1:2395:U:H3	1.50	0.59
10:AG:10:ASP:HB3	10:AG:123:LEU:HD12	1.85	0.59
22:AU:45:PRO:O	31:AO:41:ARG:NH2	2.36	0.59
29:BG:109:ASP:OD1	29:BG:109:ASP:N	2.36	0.59
1:1:462:G:H21	1:1:485:A:H62	1.51	0.59
29:A3:27:ARG:O	29:A3:27:ARG:NE	2.36	0.58
14:AK:19:ILE:HG13	14:AK:62:ILE:HG12	1.84	0.58
1:1:2878:G:OP2	1:1:2962:C:O2'	2.19	0.58
1:1:772:U:H2'	1:1:773:C:C6	2.37	0.58
1:1:848:A:HO2'	1:1:887:G:HO2'	1.51	0.58
1:1:1806:G:OP2	1:1:1806:G:N2	2.31	0.58
15:AL:81:ALA:HA	15:AL:84:GLN:HE21	1.66	0.58
34:BO:112:VAL:HG22	34:BO:115:SER:HB2	1.85	0.58
5:AB:142:ASP:H	5:AB:145:ASN:HD22	1.51	0.58
1:1:447:A:N7	1:1:500:U:O2'	2.37	0.58
1:1:1310:G:O2'	1:1:1339:A:N6	2.37	0.58
1:1:720:A:H2'	1:1:721:A:H8	1.68	0.58
2:2:790:G:HO2'	12:AI:2:THR:N	2.01	0.58
59:BN:107:ARG:NH1	59:BN:108:TYR:OH	2.36	0.58
1:1:1317:G:H2'	1:1:1318:G:C8	2.38	0.58
1:1:1756:G:OP1	58:Bd:77:ARG:NH1	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:H:132:VAL:HG13	65:H:255:LEU:HD22	1.86	0.58
1:1:1327:C:N4	1:1:1352:C:O3'	2.34	0.58
8:AE:2:ALA:HB2	8:AE:7:LYS:HG2	1.84	0.58
1:1:1421:C:H2'	1:1:1422:A:C8	2.38	0.58
33:BY:55:THR:HG21	33:BY:143:ARG:HH21	1.69	0.57
65:H:205:PRO:HG2	65:H:208:MET:HB3	1.85	0.57
53:BF:4:ASP:OD1	53:BF:5:ALA:N	2.35	0.57
65:H:53:ASP:OD1	65:H:53:ASP:N	2.37	0.57
1:1:229:4AC:O2'	41:Be:21:ARG:HG2	2.05	0.57
12:AI:90:GLU:OE2	12:AI:113:HIS:NE2	2.30	0.57
15:AL:3:LYS:HA	15:AL:76:GLU:HA	1.86	0.57
42:BE:8:ARG:NH1	42:BE:177:GLU:OE2	2.37	0.57
63:Bl:72:ARG:NH1	63:Bl:76:GLU:OE1	2.36	0.57
1:1:116:G:H2'	1:1:117:G:C8	2.40	0.57
1:1:600:G:H2'	52:BD:183:LYS:HE3	1.86	0.57
1:1:1415:C:OP2	33:BY:118:ARG:NH2	2.36	0.57
2:2:893:G:H2'	2:2:894:G:C8	2.39	0.57
19:AQ:26:LEU:HD11	19:AQ:60:ILE:HG22	1.85	0.57
63:Bl:67:ASP:HB3	63:Bl:70:VAL:HG22	1.86	0.57
1:1:2314:U:H2'	1:1:2315:U:C6	2.40	0.57
27:AZ:126:ARG:HG3	27:AZ:185:PRO:HA	1.86	0.57
65:H:90:LYS:HE3	65:H:265:SER:HB3	1.86	0.57
31:AO:113:ARG:NH1	31:AO:121:GLU:OE2	2.33	0.57
63:Bl:10:GLY:HA2	63:Bl:55:LYS:HG2	1.87	0.57
65:H:190:ARG:NH2	65:H:204:PRO:O	2.37	0.57
29:A3:70:CYS:HA	29:A3:75:ILE:HD12	1.85	0.57
24:AW:36:ARG:NH2	24:AW:48:GLU:OE2	2.37	0.57
51:Bj:30:ARG:HH11	51:Bj:37:GLN:HE22	1.53	0.57
8:AE:36:PRO:HD2	8:AE:84:PRO:HG2	1.87	0.57
1:1:1301:A:H4'	1:1:1302:G:H5'	1.85	0.56
2:2:219:G:H21	2:2:222:A:H8	1.51	0.56
16:AM:52:ARG:HB2	65:H:382:LYS:HB2	1.86	0.56
65:H:62:TRP:CH2	65:H:71:ASP:HB2	2.41	0.56
65:H:385:ILE:O	65:H:385:ILE:HG13	2.05	0.56
1:1:100:G:O2'	1:1:101:U:H5'	2.05	0.56
1:1:192:C:OP1	45:BW:7:ARG:NH2	2.38	0.56
2:2:223:G:H2'	2:2:224:G:H8	1.70	0.56
25:AX:15:ILE:HD11	25:AX:28:LYS:HG2	1.87	0.56
1:1:2426:C:H2'	1:1:2427:G:H8	1.68	0.56
2:2:453:C:H2'	2:2:454:U:H6	1.71	0.56
10:AG:68:ASP:HA	10:AG:116:ILE:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AM:24:ASN:HD22	65:H:383:ARG:HD2	1.69	0.56
1:1:2118:U:N3	1:1:2121:A:OP2	2.31	0.56
1:1:2367:G:H21	1:1:2413:A:H1'	1.71	0.56
21:AS:5:ARG:HB2	21:AS:10:LYS:HD2	1.88	0.56
48:BR:45:ILE:H	48:BR:59:HIS:CD2	2.21	0.56
1:1:720:A:OP1	61:Bc:32:ARG:NH2	2.37	0.56
1:1:658:G:H5"	1:1:661:C:H1'	1.88	0.56
1:1:850:A:N6	37:BL:117:LYS:O	2.33	0.56
1:1:2050:U:H2'	1:1:2051:C:H6	1.70	0.56
2:2:1176:G:N2	18:AP:45:GLU:OE2	2.39	0.56
8:AE:87:ILE:HD12	8:AE:104:PRO:HD3	1.86	0.56
1:1:1164:C:OP1	59:BN:19:ARG:NH1	2.39	0.56
2:2:24:U:H2'	2:2:25:C:C6	2.41	0.56
2:2:121:U:H2'	2:2:122:C:C6	2.41	0.56
17:AN:49:GLN:HG2	17:AN:106:GLU:HG2	1.88	0.56
19:AQ:158:ARG:NH2	54:BZ:12:GLU:OE2	2.39	0.56
42:BE:10:GLU:OE1	42:BE:10:GLU:N	2.35	0.56
1:1:1084:A:H62	1:1:1198:A:H2	1.54	0.56
2:2:183:U:H2'	2:2:184:G:H8	1.71	0.56
4:AA:175:ALA:HB3	4:AA:181:LEU:HD11	1.88	0.56
65:H:125:GLU:OE1	65:H:125:GLU:N	2.39	0.56
1:1:360:A:H2'	1:1:361:A:C8	2.40	0.55
9:AF:33:ASP:OD2	9:AF:35:HIS:ND1	2.27	0.55
1:1:431:G:OP2	1:1:431:G:H8	1.90	0.55
2:2:398:A:H3'	2:2:399:C:H6	1.71	0.55
12:AI:18:GLU:HG2	12:AI:65:LEU:HD13	1.88	0.55
2:2:1499:G:H2'	2:2:1500:A:C8	2.42	0.55
37:BL:36:MET:HE3	37:BL:39:THR:HG21	1.89	0.55
65:H:56:ILE:HD13	65:H:180:HIS:CD2	2.42	0.55
1:1:2419:C:H2'	1:1:2420:A:H8	1.72	0.55
30:AT:50:LYS:HE3	30:AT:63:ILE:HG23	1.88	0.55
1:1:107:G:N2	1:1:112:A:H8	1.93	0.55
1:1:127:U:H2'	1:1:128:A:H8	1.72	0.55
1:1:264:G:OP1	1:1:403:G:O2'	2.24	0.55
1:1:2304:C:H2'	1:1:2305:C:C6	2.41	0.55
2:2:1365:U:H2'	2:2:1366:G:C8	2.42	0.55
44:BT:21:GLU:N	44:BT:21:GLU:OE1	2.39	0.55
47:BI:56:ARG:HA	47:BI:65:PRO:HD2	1.88	0.55
64:Bk:4:LEU:HD13	64:Bk:37:VAL:HG13	1.87	0.55
1:1:2108:G:N1	1:1:2130:A:OP2	2.33	0.55
2:2:145:G:H2'	2:2:146:A:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1049:G:OP1	41:Be:53:LYS:NZ	2.38	0.55
5:AB:191:PRO:HG2	5:AB:194:GLU:HB2	1.89	0.55
22:AU:25:GLU:N	22:AU:25:GLU:OE1	2.40	0.55
29:A3:27:ARG:NH1	29:A3:32:ILE:HG12	2.21	0.55
38:Bf:21:ARG:O	38:Bf:38:HIS:HE1	1.89	0.55
1:1:1006:G:H2'	1:1:1007:C:C6	2.42	0.55
1:1:2305:C:H2'	1:1:2306:C:H6	1.71	0.55
1:1:94:G:C2	1:1:3020:U:C6	2.95	0.55
1:1:974:G:OP1	49:BQ:92:LYS:NZ	2.36	0.55
1:1:1612:A:H2'	1:1:1613:A:C8	2.42	0.55
2:2:1415:U:H4'	50:BV:62:GLN:O	2.05	0.55
1:1:1575:A:H2'	1:1:1576:C:C6	2.41	0.55
1:1:2305:C:H2'	1:1:2306:C:C6	2.42	0.55
2:2:1271:U:HO2'	11:AH:177:LYS:HZ1	1.52	0.55
3:3:30:C:H5'	42:BE:149:ARG:HD3	1.88	0.55
23:AV:92:ILE:HG22	23:AV:93:ILE:HG23	1.89	0.55
32:BB:122:VAL:HG21	32:BB:129:ALA:HB2	1.89	0.55
46:Bi:82:VAL:HG12	46:Bi:83:GLU:HG3	1.89	0.55
47:BI:115:ILE:HG22	47:BI:117:GLU:HG2	1.88	0.55
1:1:94:G:C2	1:1:3020:U:C5	2.95	0.54
1:1:238:C:H4'	1:1:239:C:O5'	2.07	0.54
1:1:1703:G:OP2	58:Bd:32:LYS:NZ	2.39	0.54
1:1:2373:G:N2	1:1:2397:G:N3	2.54	0.54
29:A3:114:ILE:HD12	29:A3:117:LYS:HE3	1.88	0.54
49:BQ:43:ARG:O	49:BQ:47:GLU:HG2	2.07	0.54
2:2:791:G:OP2	19:AQ:9:ARG:NH2	2.39	0.54
9:AF:125:LYS:HG2	9:AF:225:VAL:HG22	1.88	0.54
61:Bc:8:LEU:HD11	61:Bc:25:LYS:HB2	1.88	0.54
65:H:147:ASP:HB3	65:H:151:LYS:HD3	1.88	0.54
65:H:235:LYS:NZ	65:H:236:ASP:OD1	2.40	0.54
1:1:102:C:N3	1:1:103:C:C5	2.74	0.54
1:1:382:C:H2'	1:1:383:C:H6	1.71	0.54
1:1:567:A:H1'	1:1:2121:A:C2	2.41	0.54
31:AO:20:GLN:HE22	31:AO:22:ARG:HH21	1.54	0.54
42:BE:66:ARG:NH1	65:H:236:ASP:OD2	2.41	0.54
49:BQ:105:GLU:OE2	49:BQ:139:TYR:OH	2.24	0.54
1:1:1568:G:N7	38:Bf:3:ARG:NH2	2.56	0.54
2:2:1502:C:H2'	2:2:1503:A:H4'	1.90	0.54
39:BU:84:ARG:NH1	39:BU:90:GLU:OE2	2.40	0.54
1:1:889:U:H2'	1:1:890:G:C8	2.42	0.54
1:1:2455:A:H4'	1:1:2456:C:O5'	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:695:A:H2'	2:2:696:A:C8	2.42	0.54
8:AE:183:ALA:HB3	8:AE:199:ILE:HD12	1.90	0.54
20:AR:105:VAL:HG11	20:AR:108:ARG:HD2	1.89	0.54
52:BD:14:ASP:OD1	52:BD:15:GLU:N	2.37	0.54
1:1:32:G:H2'	1:1:33:G:C8	2.43	0.54
1:1:1116:G:H2'	1:1:1117:C:C6	2.42	0.54
2:2:1095:A:H2'	2:2:1096:G:C8	2.43	0.54
59:BN:166:ASP:OD2	59:BN:170:ASN:ND2	2.39	0.54
29:B4:19:ALA:HB2	29:B4:78:ILE:HD13	1.89	0.54
1:1:353:C:OP2	1:1:2628:C:O2'	2.25	0.54
2:2:709:G:OP1	19:AQ:101:ARG:NH2	2.40	0.54
29:BG:29:THR:HG21	29:BG:106:LYS:HG3	1.88	0.54
1:1:1266:G:N2	63:Bl:43:SER:HB2	2.23	0.54
2:2:681:G:H2'	2:2:682:A:H8	1.72	0.54
25:AX:28:LYS:HD3	25:AX:42:ARG:HB3	1.90	0.54
52:BD:149:GLN:HA	52:BD:207:ILE:HB	1.89	0.54
1:1:1331:C:H2'	1:1:1332:A:C8	2.42	0.54
11:AH:70:LYS:HG3	11:AH:162:LEU:HB3	1.90	0.54
12:AI:28:LYS:HB3	12:AI:29:PRO:HD3	1.90	0.54
1:1:382:C:H2'	1:1:383:C:C6	2.41	0.54
1:1:1524:G:N7	57:BS:28:SER:OG	2.36	0.54
2:2:594:G:O2'	7:AD:65:GLN:NE2	2.39	0.54
2:2:1506:U:H2'	2:2:1510:C:C6	2.43	0.54
4:AA:145:ILE:HD13	4:AA:170:GLU:HG3	1.90	0.54
36:B5:58:GLU:N	36:B5:58:GLU:OE1	2.40	0.54
1:1:1303:A:H61	1:1:1367:G:H1'	1.73	0.53
2:2:247:G:OP1	20:AR:66:ARG:NH1	2.36	0.53
2:2:569:G:P	8:AE:191:LYS:HZ1	2.31	0.53
2:2:1350:U:H2'	2:2:1351:A:H8	1.73	0.53
8:AE:237:LYS:HD2	8:AE:238:PRO:HD2	1.90	0.53
10:AG:112:ILE:HA	10:AG:116:ILE:HD12	1.91	0.53
59:BN:127:LYS:H	59:BN:130:GLN:NE2	2.06	0.53
29:B4:108:ARG:HA	29:B4:108:ARG:HH11	1.73	0.53
1:1:1393:G:OP2	47:BI:52:ARG:NH2	2.30	0.53
9:AF:167:ILE:O	9:AF:172:LYS:NZ	2.30	0.53
13:AJ:33:SER:HB3	13:AJ:56:ARG:HD3	1.89	0.53
37:BL:47:TRP:CZ2	37:BL:51:ILE:HD11	2.43	0.53
1:1:1755:4AC:O7	1:1:1755:4AC:H5	2.08	0.53
2:2:1261:A:H2'	2:2:1262:A:C8	2.43	0.53
1:1:910:G:H21	55:BP:1:MET:HE1	1.74	0.53
2:2:579:C:H2'	2:2:580:A:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:52:A:H62	34:BO:42:ASN:HD21	1.55	0.53
15:AL:38:ILE:HB	15:AL:72:LEU:HB3	1.90	0.53
18:AP:53:ARG:NH2	18:AP:55:TYR:OH	2.42	0.53
29:A3:12:PRO:HG2	29:A3:15:LEU:HD22	1.91	0.53
36:B5:9:ILE:HG12	36:B5:23:VAL:HG12	1.89	0.53
49:BQ:56:LYS:O	49:BQ:56:LYS:HG2	2.09	0.53
29:BG:13:LYS:NZ	29:BG:17:GLU:OE2	2.42	0.53
65:H:56:ILE:HD13	65:H:180:HIS:HD2	1.73	0.53
1:1:1300:U:H5	1:1:1302:G:H5"	1.73	0.53
1:1:163:A:H2	1:1:233:U:N3	2.07	0.53
4:AA:53:LEU:HD23	4:AA:62:LYS:HB3	1.91	0.53
7:AD:24:ASP:OD1	7:AD:27:ARG:NH2	2.42	0.53
23:AV:23:ILE:HG21	23:AV:31:PRO:HG2	1.90	0.53
33:BY:66:LYS:NZ	33:BY:152:GLU:OE2	2.34	0.53
1:1:102:C:C2	1:1:103:C:C5	2.97	0.53
2:2:444:U:O2'	23:AV:56:ILE:O	2.26	0.53
2:2:861:G:O2'	2:2:877:G:O6	2.23	0.53
17:AN:143:GLU:HG3	17:AN:147:ARG:HE	1.74	0.53
25:AX:13:GLU:HG2	25:AX:28:LYS:HB2	1.90	0.53
65:H:5:GLN:OE1	65:H:7:GLN:N	2.30	0.53
2:2:1201:A:C8	30:AT:123:THR:HA	2.43	0.53
3:3:97:G:H2'	3:3:98:G:H8	1.73	0.53
54:BZ:28:LYS:HE3	54:BZ:52:TYR:CZ	2.44	0.53
65:H:142:THR:HG22	65:H:165:PRO:HG2	1.91	0.53
1:1:1342:G:N2	1:1:1345:U:O4	2.42	0.53
1:1:1763:G:H2'	1:1:1764:C:C6	2.44	0.53
2:2:1487:MA6:H93	2:2:1488:MA6:H92	1.91	0.53
32:BB:202:HIS:CD2	32:BB:204:PHE:H	2.25	0.53
47:BI:42:ARG:NH2	47:BI:133:GLU:OE1	2.42	0.53
65:H:175:GLY:HA3	65:H:214:MET:HE3	1.91	0.53
17:AN:62:ALA:O	65:H:326:ARG:NH2	2.38	0.52
23:AV:41:VAL:HG11	23:AV:48:PRO:HB3	1.90	0.52
24:AW:22:ASP:OD1	24:AW:22:ASP:N	2.32	0.52
1:1:1283:A:H2'	1:1:1284:A:H8	1.74	0.52
1:1:1754:C:H5'	58:Bd:74:LYS:HE2	1.91	0.52
2:2:1309:C:O2'	11:AH:175:ARG:NH1	2.41	0.52
8:AE:126:ARG:H	8:AE:143:HIS:HD2	1.56	0.52
29:A3:107:ALA:H	29:A3:108:ARG:HE	1.58	0.52
1:1:493:G:H5'	39:BU:1:MET:HG2	1.90	0.52
1:1:1742:A:H2'	1:1:1743:A:C8	2.45	0.52
11:AH:50:ARG:NH1	14:AK:110:ASP:OD2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:BU:5:SER:O	39:BU:11:GLN:NE2	2.40	0.52
2:2:907:A:H2'	2:2:908:C:C6	2.45	0.52
1:1:1393:G:H5'	47:BI:78:THR:HG23	1.92	0.52
1:1:1842:A:H2'	1:1:1843:A:C8	2.45	0.52
2:2:410:C:O2'	2:2:587:A:N3	2.39	0.52
4:AA:52:THR:HG22	4:AA:54:LYS:H	1.74	0.52
8:AE:172:GLU:N	8:AE:172:GLU:OE1	2.42	0.52
2:2:703:4AC:H2'	2:2:704:G:H8	1.75	0.52
2:2:703:4AC:H5	2:2:703:4AC:O7	2.10	0.52
15:AL:78:ASP:O	15:AL:82:MET:HG2	2.10	0.52
35:BC:91:LEU:O	47:BI:141:LYS:NZ	2.42	0.52
65:H:29:ILE:HG12	65:H:32:LYS:HZ1	1.75	0.52
65:H:61:LYS:C	65:H:62:TRP:HD1	2.17	0.52
1:1:1142:A:H4'	1:1:1143:A:C8	2.44	0.52
1:1:2951:C:O2'	35:BC:361:GLN:O	2.19	0.52
1:1:3021:U:H3'	1:1:3021:U:OP2	2.10	0.52
63:Bl:64:GLU:OE1	63:Bl:64:GLU:N	2.41	0.52
29:B4:121:LEU:HD23	29:B4:122:MET:H	1.74	0.52
1:1:617:G:N2	1:1:620:A:OP2	2.36	0.52
1:1:2009:G:N2	1:1:2012:G:OP2	2.40	0.52
2:2:724:U:H2'	2:2:725:G:O4'	2.10	0.52
42:BE:104:ALA:O	42:BE:168:LYS:NZ	2.43	0.52
1:1:2944:C:O2'	1:1:2946:C:OP2	2.18	0.52
2:2:386:C:H2'	2:2:387:G:H8	1.75	0.52
2:2:662:A:OP1	16:AM:52:ARG:HD2	2.10	0.52
7:AD:116:ARG:HG3	7:AD:171:ILE:HA	1.91	0.52
19:AQ:43:GLU:OE1	19:AQ:43:GLU:N	2.43	0.52
34:BO:63:HIS:CD2	34:BO:65:ARG:H	2.24	0.52
1:1:1035:G:H5'	1:1:1036:G:OP1	2.10	0.52
1:1:2065:A:H2'	1:1:2066:A:C8	2.45	0.52
1:1:2725:U:H4'	59:BN:103:ARG:HG2	1.92	0.52
2:2:681:G:H2'	2:2:682:A:C8	2.45	0.52
2:2:724:U:OP1	2:2:789:C:O2'	2.27	0.52
2:2:1434:U:H2'	2:2:1435:C:C6	2.45	0.52
15:AL:33:ARG:H	15:AL:33:ARG:HD3	1.75	0.52
34:BO:145:ARG:NH1	34:BO:147:GLU:OE2	2.41	0.52
37:BL:1:MET:HE2	52:BD:33:ARG:HD2	1.91	0.52
53:BF:10:GLU:HG2	53:BF:54:VAL:HG22	1.91	0.52
1:1:351:G:OP2	1:1:353:C:N4	2.36	0.51
2:2:1416:C:H2'	2:2:1417:U:C6	2.45	0.51
1:1:789:OMG:HM22	1:1:790:G:H5'	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1775:A:N1	54:BZ:67:SER:OG	2.31	0.51
57:BS:37:ARG:NH1	57:BS:38:GLU:OE2	2.42	0.51
65:H:157:ARG:NH2	65:H:158:ASP:OD1	2.43	0.51
1:1:418:A:H2'	1:1:419:G:H8	1.74	0.51
2:2:86:U:H3'	2:2:87:C:H5"	1.93	0.51
2:2:813:G:O2'	4:AA:177:LYS:O	2.24	0.51
11:AH:75:GLY:HA3	11:AH:86:MET:HE3	1.91	0.51
29:B4:18:LYS:HG2	29:B4:110:LEU:HD11	1.92	0.51
1:1:1278:C:OP1	1:1:1281:C:N4	2.44	0.51
1:1:1769:A:N1	1:1:1831:G:O2'	2.41	0.51
32:BB:61:VAL:HG11	32:BB:83:ILE:HD11	1.92	0.51
32:BB:74:PRO:HD2	32:BB:77:LEU:HD22	1.93	0.51
42:BE:43:LYS:HB3	42:BE:132:ILE:HG22	1.92	0.51
55:BP:22:SER:OG	55:BP:27:VAL:O	2.25	0.51
65:H:270:LYS:H	65:H:270:LYS:HD3	1.75	0.51
1:1:2344:G:O6	1:1:2426:C:N4	2.43	0.51
16:AM:55:PRO:HG3	65:H:383:ARG:HG2	1.93	0.51
27:AZ:86:LYS:H	27:AZ:86:LYS:HD2	1.75	0.51
29:A3:18:LYS:HD2	29:A3:114:ILE:HG21	1.93	0.51
53:BF:32:LYS:NZ	53:BF:83:THR:O	2.43	0.51
57:BS:60:PRO:HG2	57:BS:78:PHE:CZ	2.45	0.51
1:1:451:4AC:H5"	39:BU:119:ARG:HG2	1.92	0.51
1:1:1998:A:H2'	1:1:1999:C:C6	2.45	0.51
1:1:1998:A:OP2	49:BQ:71:LYS:HE2	2.10	0.51
1:1:2706:C:N4	60:Bg:47:ARG:O	2.43	0.51
2:2:453:C:H2'	2:2:454:U:C6	2.46	0.51
8:AE:33:ARG:HG3	8:AE:34:PRO:HD2	1.93	0.51
19:AQ:54:LEU:HD23	19:AQ:60:ILE:HD11	1.92	0.51
34:BO:139:PRO:HG2	34:BO:144:ILE:HD11	1.93	0.51
53:BF:11:ILE:HB	53:BF:53:VAL:HG13	1.92	0.51
1:1:122:G:H2'	1:1:123:A:C8	2.45	0.51
1:1:691:G:OP1	61:Bc:49:SER:OG	2.24	0.51
1:1:1015:A:H5'	32:BB:176:GLY:HA2	1.93	0.51
1:1:1685:A:N3	1:1:1755:4AC:O2'	2.41	0.51
2:2:1069:OMG:HM22	2:2:1070:A:H5'	1.92	0.51
11:AH:172:LYS:HB3	11:AH:183:ALA:HB1	1.92	0.51
29:A3:32:ILE:HD11	29:A3:90:ALA:HB1	1.92	0.51
55:BP:19:ARG:NH2	55:BP:38:GLU:OE1	2.38	0.51
65:H:59:HIS:CD2	65:H:64:PRO:HG3	2.46	0.51
1:1:115:G:N3	1:1:115:G:H2'	2.26	0.51
1:1:1706:G:H2'	1:1:1707:C:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:683:C:O2'	16:AM:124:ASP:OD2	2.28	0.51
2:2:1092:G:H5'	2:2:1254:A:O2'	2.10	0.51
16:AM:52:ARG:HG3	65:H:382:LYS:HG2	1.92	0.51
56:BM:76:TRP:CD1	56:BM:76:TRP:H	2.27	0.51
1:1:133:G:H2'	1:1:134:C:C6	2.46	0.51
1:1:508:C:H2'	1:1:509:A:C8	2.46	0.51
1:1:951:G:OP1	49:BQ:86:THR:HG23	2.10	0.51
1:1:1667:4AC:H2'	1:1:1668:G:H8	1.76	0.51
1:1:1706:G:H2'	1:1:1707:C:H6	1.76	0.51
1:1:2341:G:O2'	1:1:2342:C:H6	1.94	0.51
1:1:2888:G:OP2	62:BJ:3:LYS:NZ	2.38	0.51
2:2:952:C:O2	18:AP:17:GLY:N	2.38	0.51
2:2:1089:G:O4'	15:AL:38:ILE:HD11	2.10	0.51
29:A3:3:LYS:HD2	29:A3:60:GLU:HG2	1.91	0.51
36:B5:61:ASP:OD1	36:B5:61:ASP:N	2.40	0.51
1:1:703:U:H3'	1:1:704:G:H5'	1.92	0.51
1:1:2477:G:H2'	1:1:2478:C:H6	1.76	0.51
37:BL:97:GLU:HB3	37:BL:102:ILE:HD13	1.93	0.51
36:BK:5:ASP:OD1	36:BK:5:ASP:N	2.44	0.51
52:BD:142:LEU:HD23	52:BD:241:VAL:HG22	1.92	0.51
1:1:1133:A:O2'	1:1:1134:G:H5'	2.11	0.50
1:1:1841:A:H2'	1:1:1842:A:C8	2.45	0.50
2:2:115:A:OP2	2:2:297:A:N6	2.40	0.50
59:BN:20:ARG:NH2	59:BN:27:PRO:O	2.27	0.50
1:1:703:U:H5'	29:B4:36:THR:HG22	1.92	0.50
2:2:579:C:H2'	2:2:580:A:H8	1.76	0.50
17:AN:60:VAL:HG21	17:AN:122:ILE:HD11	1.92	0.50
1:1:855:C:H2'	1:1:856:G:O4'	2.11	0.50
1:1:1305:A:C6	1:1:1306:G:C6	2.99	0.50
2:2:1126:G:OP1	15:AL:69:HIS:ND1	2.43	0.50
59:BN:30:LYS:H	59:BN:59:GLN:NE2	2.08	0.50
1:1:1110:G:N3	1:1:2499:A:H2'	2.26	0.50
1:1:1295:G:N1	1:1:1296:G:N7	2.59	0.50
1:1:2823:C:H2'	1:1:2824:G:C8	2.46	0.50
2:2:730:C:H2'	2:2:731:4AC:H6	1.93	0.50
35:BC:205:ARG:NH1	35:BC:316:ASP:OD2	2.45	0.50
1:1:53:G:H2'	1:1:54:G:O4'	2.10	0.50
1:1:720:A:H2'	1:1:721:A:C8	2.45	0.50
1:1:978:G:O2'	1:1:1014:G:H4'	2.11	0.50
2:2:1132:C:H5'	21:AS:49:ARG:HE	1.75	0.50
2:2:1416:C:H2'	2:2:1417:U:H6	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AG:39:PRO:HG2	10:AG:42:GLU:HB3	1.94	0.50
10:AG:76:PRO:C	10:AG:110:ASN:HD21	2.18	0.50
27:AZ:121:MET:HE3	27:AZ:128:VAL:HG12	1.92	0.50
35:BC:79:ARG:HH21	35:BC:167:GLN:HE22	1.58	0.50
65:H:48:GLY:O	65:H:73:TYR:OH	2.16	0.50
1:1:993:U:OP2	1:1:1951:C:O2'	2.29	0.50
2:2:28:G:H2'	2:2:29:C:C6	2.47	0.50
2:2:386:C:H2'	2:2:387:G:C8	2.46	0.50
27:AZ:18:ASP:OD1	27:AZ:30:TYR:OH	2.20	0.50
1:1:394:G:H2'	1:1:395:A:C8	2.46	0.50
1:1:795:U:H2'	1:1:796:C:C6	2.47	0.50
1:1:2338:G:H2'	1:1:2339:C:C6	2.47	0.50
1:1:2428:C:H2'	1:1:2429:C:C2	2.47	0.50
2:2:520:G:OP1	17:AN:38:LYS:NZ	2.44	0.50
2:2:630:A:OP1	4:AA:133:SER:OG	2.18	0.50
2:2:1174:C:O2'	2:2:1179:U:O4	2.29	0.50
7:AD:98:GLU:O	7:AD:102:GLU:HG2	2.11	0.50
17:AN:139:LYS:HB3	17:AN:141:ARG:HE	1.76	0.50
1:1:568:U:H2'	1:1:569:C:C6	2.46	0.50
1:1:705:A:H2'	1:1:706:G:C8	2.47	0.50
2:2:965:A:H5"	2:2:966:C:C5	2.44	0.50
42:BE:7:ASN:N	42:BE:7:ASN:OD1	2.43	0.50
65:H:168:ASP:OD1	65:H:172:LYS:N	2.39	0.50
1:1:118:U:H2'	1:1:118:U:O2	2.12	0.50
1:1:299:A:H5"	37:BL:37:ALA:HB2	1.92	0.50
1:1:757:G:O2'	1:1:1478:G:OP1	2.29	0.50
1:1:2850:A:H2'	1:1:2851:C:C6	2.47	0.50
1:1:2473:U:H2'	1:1:2474:U:C6	2.47	0.49
1:1:2723:C:H5'	1:1:2802:G:H5"	1.94	0.49
2:2:644:C:H2'	2:2:645:C:C6	2.47	0.49
2:2:659:U:O4	65:H:383:ARG:HD3	2.12	0.49
2:2:836:A:H5'	2:2:1043:U:C5	2.46	0.49
3:3:98:G:H2'	3:3:99:G:C8	2.47	0.49
27:AZ:40:LEU:O	27:AZ:77:ASN:ND2	2.35	0.49
42:BE:60:LYS:HA	42:BE:75:PRO:HA	1.94	0.49
1:1:107:G:C2	1:1:112:A:N7	2.75	0.49
1:1:2358:U:H3	1:1:2388:G:H1'	1.77	0.49
9:AF:57:VAL:HG22	9:AF:89:VAL:HB	1.94	0.49
1:1:1210:U:H4'	59:BN:8:ILE:HG23	1.94	0.49
2:2:191:U:H2'	2:2:192:G:O4'	2.12	0.49
2:2:653:U:OP2	4:AA:13:LYS:NZ	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:AX:36:ASP:O	25:AX:39:ARG:HG2	2.13	0.49
27:AZ:54:VAL:HG11	27:AZ:82:VAL:HG11	1.93	0.49
1:1:84:A:OP1	43:Ba:2:PRO:HD2	2.13	0.49
1:1:434:A:H2'	1:1:435:C:C6	2.47	0.49
1:1:1303:A:H1'	1:1:1304:C:H5'	1.94	0.49
1:1:2066:A:H2'	1:1:2067:G:O4'	2.12	0.49
1:1:3014:C:H2'	1:1:3015:G:C8	2.48	0.49
49:BQ:39:GLU:OE1	49:BQ:42:ARG:NH1	2.45	0.49
29:B4:58:ASP:HB2	29:B4:59:PRO:HD3	1.93	0.49
1:1:1939:G:O2'	1:1:2919:G:H4'	2.12	0.49
2:2:1066:A:H4'	2:2:1067:A:O5'	2.13	0.49
55:BP:15:ILE:HD13	55:BP:38:GLU:HG3	1.93	0.49
65:H:22:PRO:O	65:H:25:GLU:HG3	2.12	0.49
1:1:1713:G:N2	1:1:1787:A:H8	2.04	0.49
2:2:423:U:OP2	2:2:424:C:N4	2.46	0.49
2:2:988:A:OP1	30:AT:50:LYS:NZ	2.46	0.49
21:AS:27:ASP:OD2	21:AS:30:HIS:N	2.40	0.49
65:H:62:TRP:CZ3	65:H:71:ASP:HB2	2.48	0.49
1:1:2858:U:H3	1:1:3007:A:H62	1.60	0.49
2:2:510:C:OP1	7:AD:27:ARG:NH1	2.45	0.49
2:2:1201:A:H4'	31:AO:139:GLN:HG2	1.94	0.49
4:AA:107:ILE:HG12	4:AA:121:MET:HG3	1.92	0.49
14:AK:52:ALA:HB1	14:AK:56:ILE:HD11	1.95	0.49
44:BT:78:GLU:O	44:BT:82:ARG:N	2.41	0.49
1:1:895:A:H2'	1:1:896:G:O4'	2.13	0.49
2:2:345:C:H2'	2:2:346:A:H8	1.76	0.49
2:2:391:A:H2'	2:2:392:A:C8	2.47	0.49
2:2:1024:C:O3'	18:AP:44:ARG:NH2	2.46	0.49
21:AS:38:LEU:HA	27:AZ:196:ILE:HD11	1.94	0.49
1:1:1055:A2M:HM'2	1:1:1057:C:C6	2.47	0.49
2:2:223:G:H2'	2:2:224:G:C8	2.47	0.49
2:2:1103:C:O2'	22:AU:130:ASP:OD2	2.28	0.49
2:2:1401:U:H2'	2:2:1402:A:C8	2.47	0.49
44:BT:12:ILE:HG13	45:BW:34:MET:HB3	1.95	0.49
65:H:78:VAL:HG22	65:H:101:PRO:HG2	1.95	0.49
65:H:287:GLU:O	65:H:291:GLU:HG2	2.13	0.49
1:1:32:G:H2'	1:1:33:G:H8	1.75	0.49
1:1:252:U:OP2	44:BT:41:ARG:NH2	2.46	0.49
1:1:1453:G:OP1	55:BP:2:LYS:NZ	2.37	0.49
36:BK:26:ASP:OD1	36:BK:27:ILE:N	2.45	0.49
49:BQ:123:LEU:HD11	49:BQ:142:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:BN:56:GLN:NE2	59:BN:125:ARG:HH21	2.11	0.49
1:1:197:G:OP2	39:BU:118:ARG:NH2	2.46	0.48
1:1:1296:G:H1'	59:BN:178:SER:HB3	1.95	0.48
5:AB:184:SER:N	5:AB:187:GLU:OE2	2.45	0.48
31:AO:20:GLN:NE2	31:AO:22:ARG:HE	2.11	0.48
59:BN:4:ARG:NH2	59:BN:9:ASP:OD1	2.43	0.48
1:1:814:A:H2'	1:1:815:A:C8	2.48	0.48
1:1:952:U:H2'	1:1:953:G:O4'	2.13	0.48
1:1:1598:G:O2'	1:1:1655:A:N1	2.45	0.48
1:1:2346:G:O6	1:1:2423:C:N4	2.36	0.48
2:2:444:U:H5"	23:AV:33:ARG:HG3	1.94	0.48
2:2:908:C:C2	2:2:909:A:C8	3.01	0.48
2:2:1401:U:H2'	2:2:1402:A:H8	1.77	0.48
10:AG:12:LYS:H	10:AG:12:LYS:HD3	1.78	0.48
1:1:90:C:H2'	1:1:91:4AC:H6	1.95	0.48
1:1:407:U:H4'	56:BM:3:MET:HE1	1.94	0.48
1:1:521:G:H4'	1:1:522:A:N7	2.28	0.48
1:1:2130:A:H2'	1:1:2131:A:C8	2.49	0.48
1:1:2344:G:H22	1:1:2425:U:H3	1.61	0.48
1:1:2584:C:H2'	1:1:2585:4AC:O2	2.13	0.48
55:BP:10:ASN:HD22	55:BP:13:ARG:HH12	1.60	0.48
1:1:360:A:H2'	1:1:361:A:H8	1.79	0.48
1:1:1161:A:H2'	1:1:1164:C:C5	2.48	0.48
1:1:1300:U:C5	1:1:1302:G:H5"	2.49	0.48
1:1:1591:A:H2'	1:1:1593:C:C5	2.48	0.48
1:1:2565:A:N6	34:BO:19:THR:O	2.43	0.48
26:AY:26:GLY:H	29:A3:45:ARG:NH1	2.11	0.48
65:H:85:LEU:HB3	65:H:118:LEU:HD21	1.96	0.48
1:1:792:A:N1	1:1:1060:G:O2'	2.42	0.48
1:1:1734:G:H2'	1:1:1735:G:H8	1.78	0.48
1:1:2624:C:N4	1:1:2659:G:O6	2.44	0.48
3:3:7:G:O2'	34:BO:47:GLN:NE2	2.47	0.48
4:AA:153:LEU:HD23	4:AA:158:PHE:HA	1.96	0.48
20:AR:38:VAL:HG22	20:AR:82:VAL:HA	1.94	0.48
65:H:5:GLN:NE2	65:H:82:THR:HA	2.29	0.48
1:1:1084:A:N6	1:1:1198:A:H2	2.11	0.48
1:1:2611:A:H2'	1:1:2612:A:C8	2.49	0.48
2:2:459:G:O2'	2:2:461:A:H1'	2.13	0.48
13:AJ:37:VAL:HG22	13:AJ:95:ILE:HD11	1.95	0.48
25:AX:36:ASP:HB3	25:AX:39:ARG:HD3	1.96	0.48
47:BI:43:GLU:CD	47:BI:43:GLU:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:BD:146:ASP:O	52:BD:149:GLN:HG2	2.12	0.48
65:H:39:LEU:HB3	65:H:41:PHE:HE1	1.79	0.48
1:1:729:G:H2'	1:1:730:A:C8	2.48	0.48
1:1:2558:A:H2'	1:1:2559:A:C8	2.48	0.48
43:Ba:25:TRP:HA	43:Ba:64:GLU:HG2	1.94	0.48
62:BJ:85:GLN:HA	62:BJ:102:ASN:HD22	1.78	0.48
1:1:56:C:H5'	1:1:57:A:C4	2.49	0.48
1:1:117:G:N3	1:1:118:U:C6	2.82	0.48
1:1:298:G:H4'	37:BL:34:ARG:HD3	1.95	0.48
1:1:1064:C:H2'	1:1:1065:4AC:H6	1.96	0.48
1:1:1687:C:H5"	58:Bd:64:PRO:HB3	1.95	0.48
2:2:1042:G:N2	2:2:1045:A:OP2	2.40	0.48
2:2:1286:G:OP1	31:AO:83:LYS:NZ	2.38	0.48
5:AB:61:ARG:NH1	6:AC:32:CYS:O	2.46	0.48
15:AL:3:LYS:HE3	15:AL:101:ILE:HG12	1.96	0.48
62:BJ:116:THR:C	62:BJ:136:ILE:HD11	2.39	0.48
1:1:2931:U:H2'	1:1:2932:C:C6	2.48	0.48
2:2:1429:U:P	10:AG:82:ARG:HH22	2.37	0.48
29:A3:74:GLU:HG2	29:A3:75:ILE:N	2.28	0.48
48:BR:19:HIS:CD2	48:BR:21:ARG:H	2.22	0.48
1:1:98:C:H5"	1:1:98:C:H6	1.78	0.48
1:1:2986:U:H1'	1:1:2987:A:H5"	1.95	0.48
2:2:157:A:H2'	2:2:158:A:O4'	2.14	0.48
2:2:204:G:O2'	13:AJ:64:ASN:ND2	2.47	0.48
2:2:964:G:H22	2:2:1186:A:P	2.37	0.48
2:2:1310:U:O2'	11:AH:85:PHE:O	2.27	0.48
65:H:141:ILE:HD13	65:H:159:HIS:ND1	2.28	0.48
1:1:102:C:C4	1:1:103:C:N4	2.81	0.47
1:1:102:C:N3	1:1:103:C:C4	2.81	0.47
8:AE:37:HIS:HB2	8:AE:42:SER:HB3	1.96	0.47
38:Bf:20:ASN:ND2	38:Bf:42:ARG:H	2.12	0.47
53:BF:139:VAL:HG12	53:BF:147:VAL:HG13	1.95	0.47
29:B4:2:ALA:HA	29:B4:7:VAL:HG11	1.96	0.47
65:H:101:PRO:HB2	65:H:109:ILE:HD12	1.96	0.47
1:1:1211:A:H2'	1:1:1212:A:C8	2.49	0.47
2:2:82:C:H2'	2:2:83:C:C6	2.48	0.47
2:2:146:A:H2'	2:2:147:U:C6	2.49	0.47
2:2:925:G:N7	31:AO:132:ARG:NH2	2.56	0.47
9:AF:63:GLN:HG2	9:AF:89:VAL:HG12	1.95	0.47
9:AF:132:GLU:HG3	9:AF:160:PRO:HG3	1.96	0.47
29:A3:13:LYS:O	29:A3:17:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AT:20:SER:OG	30:AT:22:GLU:OE2	2.25	0.47
43:Ba:10:ILE:HD13	43:Ba:73:LYS:HB3	1.95	0.47
1:1:785:G:H5"	1:1:2259:U:H5"	1.96	0.47
1:1:2050:U:H2'	1:1:2051:C:C6	2.50	0.47
1:1:2265:U:H2'	1:1:2266:G:C8	2.49	0.47
2:2:1329:G:H2'	2:2:1330:C:C6	2.50	0.47
37:BL:77:THR:HB	37:BL:115:THR:HG23	1.95	0.47
1:1:54:G:O2'	1:1:58:A:N6	2.48	0.47
1:1:208:A:H2'	1:1:209:G:O4'	2.15	0.47
1:1:228:C:O2'	1:1:240:U:O2'	2.31	0.47
1:1:394:G:H2'	1:1:395:A:H8	1.80	0.47
1:1:801:C:H2'	1:1:802:4AC:H6	1.97	0.47
1:1:1806:G:O2'	1:1:1808:U:OP1	2.22	0.47
1:1:1847:C:OP1	1:1:1862:U:H5	1.97	0.47
1:1:2988:A:N1	53:BF:74:HIS:HE1	2.12	0.47
2:2:1236:C:H2'	2:2:1237:C:H6	1.80	0.47
10:AG:12:LYS:HG2	10:AG:13:THR:HG23	1.95	0.47
27:AZ:25:LEU:HD22	27:AZ:54:VAL:HG23	1.96	0.47
33:BY:83:GLU:OE1	33:BY:83:GLU:N	2.36	0.47
47:BI:57:THR:H	47:BI:64:GLY:HA3	1.80	0.47
1:1:113:G:C4	1:1:114:G:C8	3.03	0.47
1:1:1011:C:H2'	1:1:1012:G:O4'	2.14	0.47
1:1:2712:C:H2'	1:1:2713:G:O4'	2.15	0.47
2:2:991:G:H2'	2:2:992:U:C6	2.50	0.47
2:2:1141:A:O2'	2:2:1143:A:N7	2.45	0.47
2:2:1339:C:H2'	2:2:1340:G:C8	2.50	0.47
18:AP:22:ILE:HG13	18:AP:37:MET:O	2.14	0.47
35:BC:184:ILE:HG13	35:BC:196:ILE:HD11	1.97	0.47
42:BE:118:ASP:OD1	42:BE:118:ASP:N	2.38	0.47
57:BS:29:PRO:HG3	57:BS:144:THR:HG22	1.96	0.47
59:BN:99:MET:HG3	59:BN:101:THR:HG23	1.96	0.47
60:Bg:3:ARG:NH1	60:Bg:45:GLU:OE2	2.47	0.47
1:1:59:C:H2'	1:1:60:4AC:H6	1.97	0.47
1:1:102:C:OP2	1:1:102:C:H6	1.96	0.47
1:1:1667:4AC:H2'	1:1:1668:G:C8	2.50	0.47
2:2:1167:G:OP2	27:AZ:131:ARG:NH2	2.47	0.47
13:AJ:86:ASN:HB3	13:AJ:89:PHE:CG	2.50	0.47
17:AN:132:VAL:HG21	17:AN:145:PRO:HD3	1.96	0.47
27:AZ:56:GLY:HA3	27:AZ:61:ARG:HB3	1.97	0.47
29:B4:73:LYS:C	29:B4:74:GLU:HG3	2.40	0.47
29:B4:84:LYS:HD2	29:B4:95:ALA:HB2	1.94	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
1:1:889:U:H2'	1:1:890:G:H8	1.77	0.47
1:1:1780:4AC:O7	1:1:1780:4AC:H5	2.14	0.47
1:1:2310:G:H2'	1:1:2311:A:C8	2.50	0.47
8:AE:122:ILE:HD11	8:AE:165:LEU:HB3	1.95	0.47
9:AF:15:GLU:O	9:AF:17:GLN:NE2	2.47	0.47
11:AH:18:MET:O	11:AH:20:ARG:NH1	2.47	0.47
22:AU:15:ARG:HH21	22:AU:135:GLU:CD	2.22	0.47
24:AW:29:VAL:HG11	24:AW:47:VAL:HG21	1.96	0.47
26:AY:22:CYS:HB2	26:AY:25:CYS:HB2	1.97	0.47
30:AT:117:ALA:HB3	30:AT:120:ILE:HB	1.97	0.47
31:AO:18:ASN:O	31:AO:50:LYS:NZ	2.43	0.47
35:BC:188:SER:HB3	35:BC:191:GLU:HB2	1.96	0.47
36:B5:31:ASN:HD21	54:BZ:25:ARG:HH11	1.63	0.47
37:BL:47:TRP:CH2	37:BL:51:ILE:HD11	2.50	0.47
48:BR:89:HIS:HD2	48:BR:91:VAL:H	1.63	0.47
29:B4:61:GLU:CD	29:B4:61:GLU:H	2.23	0.47
65:H:250:LYS:HE2	65:H:250:LYS:HB2	1.72	0.47
2:2:1415:U:H2'	2:2:1416:C:C6	2.49	0.47
4:AA:59:ASP:OD1	4:AA:59:ASP:N	2.48	0.47
11:AH:58:LYS:NZ	11:AH:159:ASP:OD2	2.46	0.47
13:AJ:68:LYS:HE2	13:AJ:68:LYS:HB2	1.68	0.47
29:A3:33:ARG:HH22	29:A3:42:ALA:HB2	1.79	0.47
53:BF:143:ASP:HB3	53:BF:146:ALA:HB3	1.97	0.47
23:B6:74:ASP:OD1	23:B6:74:ASP:N	2.47	0.47
65:H:229:GLU:OE1	65:H:229:GLU:N	2.44	0.47
1:1:120:A:C8	1:1:120:A:H5"	2.49	0.47
1:1:727:G:N7	36:BK:17:ARG:NH2	2.63	0.47
1:1:2304:C:H2'	1:1:2305:C:H6	1.80	0.47
1:1:2480:G:O2'	1:1:2728:U:OP1	2.22	0.47
2:2:1386:C:H2'	2:2:1387:A:C8	2.50	0.47
4:AA:161:GLU:OE1	4:AA:166:LYS:HB2	2.15	0.47
42:BE:11:ILE:HG21	42:BE:173:VAL:HG11	1.97	0.47
23:B6:50:THR:OG1	23:B6:72:TYR:O	2.31	0.47
1:1:659:A:H5"	1:1:660:G:H3'	1.97	0.47
2:2:485:C:H2'	2:2:486:A:O4'	2.14	0.47
2:2:1316:C:H2'	2:2:1317:C:C6	2.50	0.47
26:AY:38:TRP:HE3	26:AY:45:TYR:HB2	1.80	0.47
65:H:338:VAL:HG13	65:H:343:VAL:HG22	1.97	0.47
2:2:203:A:H2'	2:2:204:G:C8	2.49	0.46
2:2:353:A:H3'	2:2:354:C:H6	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:204:A:H1'	38:Bf:30:LYS:HE2	1.96	0.46
1:1:1048:4AC:O2'	41:Be:51:TRP:O	2.31	0.46
1:1:1305:A:H2'	1:1:1306:G:C8	2.50	0.46
1:1:2498:A:N3	1:1:2498:A:H2'	2.30	0.46
2:2:729:G:H2'	2:2:730:C:C6	2.51	0.46
29:A3:107:ALA:H	29:A3:108:ARG:HH21	1.63	0.46
53:BF:92:VAL:HG22	53:BF:172:ILE:HG12	1.97	0.46
1:1:42:U:H4'	1:1:43:A:H5'	1.97	0.46
1:1:102:C:N3	1:1:117:G:N1	2.37	0.46
1:1:763:C:H2'	1:1:764:A:C8	2.51	0.46
1:1:808:G:N7	55:BP:84:LYS:NZ	2.63	0.46
1:1:939:G:H2'	1:1:940:C:C6	2.50	0.46
1:1:1421:C:H2'	1:1:1422:A:H8	1.77	0.46
1:1:2522:U:H2'	1:1:2523:C:C6	2.50	0.46
1:1:2693:C:H2'	1:1:2694:U:C6	2.50	0.46
2:2:255:A:C2	2:2:291:A:C5	3.03	0.46
2:2:1117:G:H2'	2:2:1118:G:H8	1.79	0.46
20:AR:16:CYS:HB3	20:AR:77:CYS:HB3	1.97	0.46
26:AY:38:TRP:CE3	26:AY:45:TYR:HB2	2.50	0.46
41:Be:28:PHE:HA	41:Be:35:CYS:HA	1.97	0.46
1:1:529:G:OP2	56:BM:44:ARG:NH1	2.46	0.46
1:1:877:U:H2'	1:1:878:G:O4'	2.15	0.46
1:1:1077:C:H5'	1:1:2662:A:O2'	2.15	0.46
1:1:2255:A:H2'	1:1:2256:A:C8	2.51	0.46
1:1:2272:C:OP1	1:1:2686:G:O2'	2.28	0.46
2:2:83:C:H2'	2:2:84:C:C6	2.50	0.46
2:2:1303:G:H5"	31:AO:32:GLY:H	1.79	0.46
18:AP:22:ILE:HD13	27:AZ:16:LEU:HD21	1.98	0.46
27:AZ:17:ILE:HG13	27:AZ:18:ASP:N	2.30	0.46
29:A3:111:VAL:O	29:A3:114:ILE:HG22	2.16	0.46
43:Ba:53:LYS:HE2	43:Ba:53:LYS:HB3	1.74	0.46
53:BF:27:LYS:HD3	53:BF:34:GLU:OE2	2.15	0.46
65:H:42:ASP:O	65:H:45:VAL:HG12	2.15	0.46
1:1:1680:G:OP1	36:B5:42:LYS:NZ	2.32	0.46
1:1:2042:A:H1'	1:1:2179:A:N6	2.30	0.46
2:2:1025:5MC:H2'	2:2:1026:G:H8	1.79	0.46
2:2:1107:U:O2'	2:2:1108:C:H5"	2.16	0.46
2:2:1123:C:H2'	2:2:1124:U:C6	2.50	0.46
21:AS:45:LYS:O	21:AS:49:ARG:HG2	2.16	0.46
27:AZ:40:LEU:HD23	27:AZ:40:LEU:H	1.80	0.46
1:1:120:A:C8	1:1:120:A:C5'	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:311:A:H2'	1:1:312:C:O4'	2.16	0.46
2:2:1212:A:H5'	11:AH:175:ARG:HG2	1.97	0.46
11:AH:32:SER:HB2	11:AH:154:PRO:HB3	1.97	0.46
1:1:107:G:C2	1:1:113:G:C6	3.04	0.46
1:1:1710:C:H2'	1:1:1711:G:H8	1.81	0.46
2:2:425:U:H3'	2:2:426:G:H8	1.80	0.46
2:2:1428:G:O3'	10:AG:82:ARG:NH2	2.48	0.46
21:AS:6:GLN:HG3	21:AS:9:ILE:HD12	1.97	0.46
21:AS:25:THR:HG22	21:AS:30:HIS:CD2	2.51	0.46
29:A3:104:PRO:HG2	29:A3:108:ARG:HH22	1.81	0.46
35:BC:16:PRO:HD3	47:BI:62:ARG:NH2	2.30	0.46
56:BM:73:ARG:HD2	56:BM:90:TYR:CD1	2.51	0.46
63:Bl:34:LYS:HE3	63:Bl:34:LYS:HB2	1.78	0.46
1:1:1616:C:H2'	1:1:1617:4AC:H6	1.97	0.46
1:1:2955:U:OP1	35:BC:232:LYS:NZ	2.40	0.46
2:2:636:4AC:CM7	2:2:703:4AC:HM73	2.44	0.46
2:2:849:G:OP2	17:AN:4:LYS:NZ	2.43	0.46
3:3:115:G:H2'	3:3:116:C:C6	2.50	0.46
24:AW:32:HIS:CE1	24:AW:53:LYS:HG3	2.50	0.46
27:AZ:55:ILE:HG22	27:AZ:59:GLY:H	1.80	0.46
34:BO:173:GLU:OE1	34:BO:173:GLU:N	2.49	0.46
42:BE:185:GLU:CD	42:BE:186:GLU:HG2	2.41	0.46
1:1:16:A:N1	1:1:2287:4AC:O2'	2.46	0.46
1:1:117:G:C6	1:1:118:U:C5	3.04	0.46
1:1:635:G:O2'	1:1:659:A:N1	2.47	0.46
1:1:776:G:H2'	1:1:2270:C:C5	2.51	0.46
1:1:1653:U:P	49:BQ:42:ARG:HH22	2.37	0.46
1:1:2375:A:C4	1:1:2376:G:C8	3.04	0.46
1:1:2593:A:H2	1:1:2662:A:H61	1.63	0.46
1:1:2934:U:H2'	1:1:2935:C:H6	1.80	0.46
2:2:196:G:N3	2:2:196:G:H2'	2.31	0.46
2:2:1212:A:H2	2:2:1215:G:N3	2.13	0.46
4:AA:50:GLU:OE2	16:AM:114:ARG:NH1	2.49	0.46
8:AE:184:TYR:CE1	8:AE:238:PRO:HG3	2.51	0.46
23:AV:1:MET:HE2	23:AV:39:LYS:HD3	1.98	0.46
35:BC:194:ASN:O	35:BC:198:GLU:HG2	2.16	0.46
36:B5:69:GLU:OE1	36:B5:69:GLU:N	2.43	0.46
49:BQ:15:LEU:HD13	49:BQ:52:LYS:HB2	1.98	0.46
56:BM:157:ARG:HB2	56:BM:162:LEU:HB2	1.96	0.46
1:1:2504:A:H2'	1:1:2505:U:C6	2.51	0.46
2:2:1224:A:H2'	2:2:1225:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AB:24:LYS:HE3	5:AB:24:LYS:HB3	1.71	0.46
8:AE:202:ILE:HG12	8:AE:213:VAL:HG12	1.96	0.46
16:AM:47:VAL:HG23	16:AM:48:VAL:HG13	1.98	0.46
19:AQ:60:ILE:HD12	19:AQ:61:PRO:O	2.16	0.46
29:A3:66:LEU:HB3	29:A3:67:PRO:HD3	1.98	0.46
30:AT:82:TYR:CE2	30:AT:91:PRO:HB3	2.50	0.46
31:AO:7:ILE:HG23	31:AO:14:ASP:OD1	2.15	0.46
1:1:197:G:P	39:BU:118:ARG:HH22	2.38	0.45
1:1:704:G:H8	1:1:704:G:OP2	1.99	0.45
1:1:1146:C:H2'	1:1:1147:C:C6	2.51	0.45
3:3:97:G:H2'	3:3:98:G:C8	2.50	0.45
4:AA:18:GLN:N	4:AA:18:GLN:OE1	2.50	0.45
5:AB:136:PRO:HG3	6:AC:30:PHE:HB3	1.97	0.45
11:AH:187:GLU:OE2	11:AH:199:TYR:N	2.49	0.45
31:AO:5:ARG:NH2	31:AO:54:LEU:O	2.41	0.45
35:BC:297:ASN:N	35:BC:297:ASN:OD1	2.48	0.45
45:BW:1:MET:HE1	45:BW:9:MET:HE1	1.99	0.45
29:B4:11:VAL:HG21	29:B4:79:TYR:HB2	1.98	0.45
1:1:845:C:H2'	1:1:846:C:C6	2.52	0.45
2:2:879:A:H2'	2:2:880:A:C8	2.51	0.45
28:A0:9:LYS:O	28:A0:13:ARG:NH1	2.38	0.45
34:BO:34:ARG:NH1	34:BO:105:ASP:OD2	2.45	0.45
34:BO:75:GLY:HA2	34:BO:171:TYR:HE1	1.81	0.45
29:BG:31:LYS:HB2	29:BG:103:GLU:HB2	1.98	0.45
59:BN:77:VAL:HG12	59:BN:81:ASN:HB2	1.98	0.45
1:1:1324:A:H4'	1:1:1325:A:H5"	1.97	0.45
1:1:1324:A:O2'	1:1:1329:G:O6	2.32	0.45
2:2:332:U:H2'	2:2:333:G:O4'	2.15	0.45
2:2:1328:C:H2'	2:2:1329:G:H8	1.82	0.45
4:AA:12:ASP:HA	4:AA:15:LYS:HG2	1.98	0.45
23:AV:46:LEU:HD13	23:AV:51:THR:HG21	1.96	0.45
23:AV:72:TYR:OH	23:AV:82:GLU:OE1	2.22	0.45
37:BL:44:LYS:HG3	37:BL:47:TRP:HB2	1.98	0.45
1:1:1392:G:OP1	47:BI:52:ARG:NH2	2.49	0.45
1:1:1434:G:H2'	1:1:1435:U:C6	2.51	0.45
1:1:2339:C:N4	1:1:2340:G:O6	2.49	0.45
2:2:818:C:H2'	2:2:819:G:H8	1.81	0.45
65:H:18:ASP:OD1	65:H:19:ILE:N	2.43	0.45
65:H:383:ARG:CZ	65:H:383:ARG:HB2	2.44	0.45
65:H:384:PHE:O	65:H:384:PHE:CD1	2.69	0.45
1:1:429:A:H1'	1:1:431:G:N7	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:566:C:H2'	1:1:567:A:H8	1.82	0.45
2:2:1037:G:H2'	2:2:1038:U:C6	2.51	0.45
29:A3:49:LYS:HD3	29:A3:103:GLU:H	1.81	0.45
30:AT:51:ILE:HG23	30:AT:79:LEU:HD22	1.98	0.45
53:BF:12:GLU:OE1	53:BF:12:GLU:N	2.35	0.45
61:Bc:41:ARG:HE	61:Bc:87:ILE:C	2.25	0.45
1:1:57:A:H4'	1:1:58:A:O4'	2.17	0.45
1:1:252:U:O2'	44:BT:2:ASP:N	2.49	0.45
1:1:794:U:H2'	1:1:795:U:C6	2.52	0.45
2:2:1038:U:C2	2:2:1039:A:C8	3.05	0.45
18:AP:49:LYS:NZ	27:AZ:15:MET:HA	2.32	0.45
29:A3:106:LYS:HD2	29:A3:106:LYS:N	2.31	0.45
34:BO:40:SER:OG	34:BO:41:LEU:N	2.49	0.45
56:BM:33:GLU:O	56:BM:65:ARG:NH2	2.50	0.45
63:Bl:4:LYS:HD2	63:Bl:59:GLU:OE2	2.17	0.45
1:1:438:U:O2'	1:1:440:G:N7	2.48	0.45
1:1:809:A:N7	1:1:903:G:O2'	2.42	0.45
1:1:1019:C:H2'	1:1:1020:G:C8	2.52	0.45
1:1:1625:A:H2'	1:1:1626:C:C6	2.52	0.45
1:1:2353:C:N4	1:1:2359:A:H62	2.14	0.45
1:1:3004:4AC:H2'	1:1:3005:G:O4'	2.17	0.45
59:BN:83:HIS:HD2	59:BN:136:ARG:HE	1.65	0.45
1:1:77:C:H4'	35:BC:311:GLY:HA2	1.98	0.45
1:1:1733:A:C2	1:1:1734:G:H1'	2.51	0.45
1:1:1842:A:H2'	1:1:1843:A:H8	1.81	0.45
2:2:1405:U:H2'	2:2:1406:G:O4'	2.16	0.45
15:AL:19:VAL:HA	15:AL:22:GLN:HG2	1.98	0.45
24:AW:7:VAL:HG13	24:AW:8:ILE:HD12	1.98	0.45
1:1:1170:A:H5"	3:3:102:G:O2'	2.16	0.45
1:1:1303:A:N6	1:1:1367:G:H1'	2.31	0.45
1:1:1810:G:OP2	49:BQ:43:ARG:NH1	2.50	0.45
1:1:2592:G:OP1	48:BR:82:LYS:NZ	2.36	0.45
2:2:80:G:H2'	2:2:81:U:C6	2.52	0.45
2:2:109:C:H2'	2:2:110:U:C6	2.52	0.45
2:2:797:G:H5"	5:AB:24:LYS:O	2.16	0.45
11:AH:44:LEU:HD11	14:AK:40:ILE:HG13	1.97	0.45
11:AH:135:ASP:HB2	11:AH:152:ILE:HD11	1.99	0.45
29:A3:15:LEU:HG	29:A3:114:ILE:HD11	1.98	0.45
35:BC:150:ASP:O	35:BC:154:GLU:HG2	2.16	0.45
45:BW:38:LEU:HD23	45:BW:38:LEU:H	1.82	0.45
52:BD:35:VAL:HB	52:BD:234:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:H:321:PHE:HE2	65:H:332:GLN:HB2	1.82	0.45
1:1:154:G:C5	1:1:155:G:C8	3.04	0.45
1:1:279:A:H2'	1:1:280:G:C8	2.52	0.45
1:1:2001:4AC:O7	1:1:2001:4AC:H5	2.16	0.45
1:1:2302:A:H2'	1:1:2303:C:H5'	1.99	0.45
1:1:2881:G:H2'	1:1:2882:C:C6	2.52	0.45
2:2:949:A:N6	2:2:1198:U:O5'	2.50	0.45
11:AH:32:SER:OG	11:AH:157:ARG:NH2	2.42	0.45
11:AH:134:GLU:HG2	11:AH:211:ALA:HB1	1.98	0.45
34:BO:52:ASP:HB3	34:BO:55:GLY:O	2.17	0.45
29:B4:25:ILE:O	29:B4:29:THR:OG1	2.32	0.45
1:1:1618:G:H2'	1:1:1619:C:H6	1.83	0.44
1:1:1733:A:H2'	1:1:1734:G:O4'	2.17	0.44
1:1:2477:G:H2'	1:1:2478:C:C6	2.52	0.44
2:2:424:C:H4'	2:2:425:U:C5	2.52	0.44
2:2:645:C:H2'	2:2:646:C:C6	2.51	0.44
2:2:1052:C:H2'	2:2:1053:A:C8	2.53	0.44
4:AA:49:VAL:HG12	16:AM:34:THR:HG22	1.99	0.44
15:AL:26:ILE:HG12	15:AL:29:ARG:NH2	2.32	0.44
29:A3:50:LEU:HD23	29:A3:101:ILE:HB	1.98	0.44
35:BC:74:GLU:OE1	35:BC:310:TYR:OH	2.21	0.44
23:B6:17:LYS:HB3	23:B6:71:TYR:HB3	1.99	0.44
59:BN:24:ARG:HA	59:BN:24:ARG:HD3	1.75	0.44
61:Bc:73:LYS:HB3	61:Bc:73:LYS:HE2	1.84	0.44
65:H:129:LYS:HZ2	65:H:228:ARG:HH22	1.65	0.44
1:1:2081:G:OP1	32:BB:202:HIS:HE1	2.00	0.44
1:1:2128:U:H2'	1:1:2129:G:O4'	2.17	0.44
1:1:2393:G:H2'	1:1:2394:G:H8	1.83	0.44
1:1:2522:U:OP1	1:1:2614:G:O2'	2.35	0.44
1:1:2559:A:H2'	1:1:2560:G:H8	1.79	0.44
1:1:2650:G:H2'	1:1:2651:C:H6	1.83	0.44
2:2:1375:G:H2'	2:2:1376:OMC:O4'	2.18	0.44
8:AE:9:HIS:HB3	8:AE:28:TRP:CZ3	2.52	0.44
57:BS:111:LYS:O	57:BS:153:VAL:HG22	2.17	0.44
59:BN:175:LYS:NZ	59:BN:179:GLN:HE22	2.15	0.44
65:H:304:TYR:HD1	65:H:307:LEU:HD12	1.82	0.44
65:H:372:ALA:O	65:H:375:GLU:HG3	2.18	0.44
1:1:1761:G:O4'	1:1:1763:G:H1'	2.17	0.44
1:1:2394:G:H2'	1:1:2395:U:H6	1.83	0.44
1:1:2523:C:H2'	1:1:2524:G:C8	2.52	0.44
2:2:135:U:H2'	2:2:136:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1235:A:H4'	22:AU:72:ARG:NH1	2.33	0.44
2:2:1346:C:H2'	2:2:1347:G:O4'	2.16	0.44
22:AU:146:GLU:OE1	22:AU:146:GLU:N	2.44	0.44
25:AX:50:ARG:O	25:AX:53:ASP:HB2	2.17	0.44
49:BQ:126:ARG:HD3	49:BQ:131:GLN:HE22	1.81	0.44
1:1:703:U:OP1	29:B4:97:ALA:N	2.47	0.44
1:1:880:G:H22	1:1:1096:G:P	2.40	0.44
1:1:2197:G:C8	1:1:2198:5MC:HM52	2.52	0.44
1:1:2524:G:H2'	1:1:2525:G:H8	1.83	0.44
7:AD:45:GLU:HG2	7:AD:49:LYS:HE2	1.98	0.44
29:A3:27:ARG:NH2	29:A3:30:GLY:O	2.51	0.44
42:BE:120:HIS:O	42:BE:126:VAL:HG11	2.17	0.44
1:1:1285:G:H5"	59:BN:154:MET:HE1	1.99	0.44
1:1:1986:U:H2'	1:1:1987:G:O4'	2.17	0.44
1:1:2046:C:H2'	1:1:2047:A:C5	2.52	0.44
1:1:2164:U:H2'	1:1:2165:C:C6	2.53	0.44
1:1:2534:G:O3'	42:BE:106:SER:HA	2.17	0.44
2:2:259:A:OP1	13:AJ:10:ARG:NH2	2.50	0.44
2:2:546:4AC:H2'	2:2:547:G:O4'	2.17	0.44
2:2:1180:G:H2'	2:2:1181:C:H6	1.82	0.44
8:AE:141:ASN:ND2	8:AE:147:ASN:OD1	2.49	0.44
13:AJ:42:LYS:HB3	13:AJ:59:ALA:HB3	1.99	0.44
14:AK:47:GLU:HG3	14:AK:79:ARG:NH2	2.33	0.44
34:BO:137:ILE:H	34:BO:137:ILE:HG13	1.61	0.44
37:BL:44:LYS:HG3	37:BL:47:TRP:CB	2.47	0.44
29:BG:39:THR:HG23	29:BG:100:ALA:HB2	2.00	0.44
52:BD:84:PRO:HB3	52:BD:92:THR:HG22	1.98	0.44
23:B6:41:VAL:HG11	23:B6:48:PRO:HG3	2.00	0.44
1:1:120:A:C5'	1:1:120:A:H8	2.31	0.44
1:1:1162:A:N3	1:1:2495:4AC:O2'	2.46	0.44
1:1:2382:C:H2'	1:1:2383:C:C6	2.53	0.44
1:1:2429:C:H3'	1:1:2430:G:H5"	1.99	0.44
2:2:110:U:H2'	2:2:111:C:C6	2.52	0.44
2:2:1150:A:H3'	2:2:1151:G:H8	1.83	0.44
52:BD:19:PRO:HB2	52:BD:21:VAL:HG12	1.99	0.44
1:1:431:G:H2'	1:1:432:A:C8	2.53	0.44
1:1:1943:G:O2'	1:1:2232:U:O4	2.29	0.44
2:2:373:A2M:HM'2	2:2:374:A:C5	2.52	0.44
7:AD:48:LEU:HB2	7:AD:100:ILE:HD13	2.00	0.44
8:AE:32:PRO:HB3	8:AE:44:PRO:HG3	2.00	0.44
9:AF:131:TRP:NE1	12:AI:97:PHE:HA	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AH:135:ASP:OD1	11:AH:136:THR:N	2.47	0.44
11:AH:145:ARG:NH1	65:H:378:ILE:HB	2.33	0.44
12:AI:30:ALA:O	12:AI:34:ILE:HB	2.18	0.44
47:BI:72:ASP:N	47:BI:72:ASP:OD1	2.49	0.44
65:H:37:LEU:HD12	65:H:37:LEU:HA	1.82	0.44
1:1:189:G:H2'	1:1:189:G:N3	2.33	0.44
1:1:614:A:H2'	1:1:615:OMC:O4'	2.17	0.44
1:1:618:U:O2'	41:Be:17:HIS:HD2	2.00	0.44
1:1:2517:U:H4'	1:1:2518:A:O4'	2.18	0.44
2:2:1161:G:O5'	14:AK:118:LYS:HE3	2.18	0.44
9:AF:20:THR:OG1	9:AF:46:GLU:OE1	2.33	0.44
27:AZ:117:MET:SD	27:AZ:146:PHE:HB3	2.58	0.44
33:BY:59:ILE:HA	33:BY:148:ASN:HD21	1.81	0.44
42:BE:26:GLU:HB2	42:BE:144:GLU:HG2	2.00	0.44
42:BE:52:THR:HG22	42:BE:90:MET:HE3	1.98	0.44
1:1:102:C:OP2	1:1:102:C:C6	2.71	0.44
1:1:622:G:N3	52:BD:75:THR:HG21	2.33	0.44
1:1:908:A:N3	52:BD:33:ARG:NH2	2.56	0.44
1:1:1253:G:H2'	1:1:1254:C:C6	2.53	0.44
1:1:1295:G:C2	1:1:1296:G:C8	3.05	0.44
1:1:1302:G:H8	1:1:1365:G:C2	2.35	0.44
1:1:2247:C:H2'	1:1:2248:C:C6	2.53	0.44
2:2:1301:G:H2'	2:2:1302:C:C6	2.53	0.44
3:3:93:G:H2'	3:3:94:A:C8	2.53	0.44
15:AL:9:ALA:HA	15:AL:69:HIS:O	2.18	0.44
27:AZ:13:LYS:HZ1	27:AZ:74:GLY:H	1.65	0.44
27:AZ:42:THR:O	27:AZ:78:PRO:HA	2.18	0.44
65:H:2:VAL:HG21	65:H:85:LEU:HD12	2.00	0.44
65:H:19:ILE:HG13	65:H:40:VAL:HG12	2.00	0.44
1:1:354:G:H2'	1:1:355:A:C8	2.53	0.43
2:2:556:C:H5"	12:AI:32:LYS:HD3	2.00	0.43
52:BD:201:VAL:HG11	52:BD:207:ILE:HG21	2.00	0.43
1:1:40:U:H2'	1:1:41:G:O4'	2.19	0.43
1:1:137:G:H1'	57:BS:8:SER:HB3	2.00	0.43
1:1:1019:C:H2'	1:1:1020:G:H8	1.83	0.43
2:2:168:A:H2'	2:2:169:A:C8	2.53	0.43
2:2:190:C:H2'	2:2:191:U:C6	2.52	0.43
2:2:1491:U:H2'	2:2:1492:A:H8	1.84	0.43
13:AJ:31:GLU:H	13:AJ:31:GLU:CD	2.26	0.43
25:AX:33:GLU:HA	25:AX:37:LYS:HE2	2.00	0.43
31:AO:14:ASP:OD1	31:AO:15:LEU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:H:16:LYS:HE2	65:H:41:PHE:HB2	1.99	0.43
1:1:68:U:H4'	1:1:69:U:O5'	2.18	0.43
1:1:773:C:H5'	37:BL:22:LYS:HE2	1.98	0.43
1:1:2804:A:OP2	35:BC:257:HIS:HD2	2.01	0.43
2:2:1417:U:H2'	2:2:1418:C:C6	2.54	0.43
2:2:1435:C:H2'	2:2:1436:G:O4'	2.18	0.43
4:AA:119:ARG:HB3	4:AA:190:LYS:HG3	2.01	0.43
5:AB:82:LYS:HZ2	5:AB:194:GLU:HG3	1.83	0.43
27:AZ:117:MET:HE2	27:AZ:117:MET:HB3	1.94	0.43
36:B5:67:SER:O	36:B5:71:VAL:HG12	2.18	0.43
40:Bb:124:LYS:HE3	40:Bb:124:LYS:HB2	1.79	0.43
48:BR:14:LYS:HA	48:BR:14:LYS:HE2	2.00	0.43
48:BR:46:GLU:OE1	48:BR:48:SER:OG	2.31	0.43
51:Bj:48:GLY:HA2	56:BM:83:SER:HA	2.00	0.43
55:BP:31:LYS:HE3	55:BP:31:LYS:HB2	1.78	0.43
29:B4:114:ILE:HA	29:B4:117:LYS:HG2	2.01	0.43
65:H:37:LEU:HD11	65:H:51:THR:HG22	2.00	0.43
65:H:210:LEU:O	65:H:214:MET:HG3	2.19	0.43
65:H:245:VAL:HB	65:H:249:ASN:HA	2.01	0.43
65:H:340:ASP:OD1	65:H:340:ASP:N	2.49	0.43
1:1:99:U:O4	1:1:120:A:N1	2.51	0.43
1:1:1574:C:H2'	1:1:1575:A:C8	2.53	0.43
1:1:2109:A:H2'	1:1:2110:A:H8	1.82	0.43
2:2:541:G:O2'	2:2:788:G:H5'	2.18	0.43
2:2:579:C:O2'	7:AD:72:GLN:NE2	2.51	0.43
2:2:839:4AC:H2'	2:2:840:G:O4'	2.18	0.43
2:2:1152:G:N2	2:2:1155:G:OP2	2.51	0.43
2:2:1378:C:H2'	2:2:1379:G:C8	2.54	0.43
2:2:1491:U:H2'	2:2:1492:A:C8	2.53	0.43
4:AA:112:THR:OG1	4:AA:116:TYR:HB2	2.18	0.43
27:AZ:22:GLU:HG2	27:AZ:30:TYR:CE2	2.54	0.43
36:B5:76:GLU:OE1	36:B5:76:GLU:N	2.51	0.43
1:1:30:G:H21	43:Ba:42:HIS:HE1	1.66	0.43
1:1:114:G:N3	1:1:115:G:C8	2.86	0.43
1:1:893:A:N1	1:1:2603:A:O2'	2.50	0.43
1:1:2058:A:H2'	1:1:2059:G:C8	2.53	0.43
1:1:2342:C:N4	1:1:2343:G:O6	2.50	0.43
1:1:2523:C:H2'	1:1:2524:G:H8	1.84	0.43
2:2:106:C:H2'	2:2:107:G:O4'	2.19	0.43
2:2:917:G:C2	2:2:918:A:C8	3.07	0.43
2:2:1133:U:H5"	21:AS:3:LYS:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1339:C:H2'	2:2:1340:G:H8	1.83	0.43
4:AA:40:ASP:HB3	4:AA:43:LYS:HG3	1.99	0.43
4:AA:174:GLU:N	4:AA:174:GLU:OE1	2.52	0.43
6:AC:21:ILE:O	9:AF:39:ARG:NH1	2.46	0.43
7:AD:109:VAL:HG13	7:AD:114:LEU:HB2	1.99	0.43
32:BB:103:PRO:HA	32:BB:134:ARG:NH1	2.33	0.43
35:BC:190:GLU:OE1	35:BC:190:GLU:N	2.42	0.43
46:Bi:5:LYS:HE2	46:Bi:5:LYS:HB3	1.80	0.43
56:BM:126:LYS:HG2	56:BM:128:PHE:CE2	2.53	0.43
1:1:1311:G:H4'	1:1:1340:A:H2	1.83	0.43
2:2:1202:5MC:H2'	2:2:1203:G:C8	2.53	0.43
3:3:121:G:H2'	3:3:122:G:H8	1.82	0.43
6:AC:38:ALA:HB2	6:AC:57:LYS:HG2	2.00	0.43
9:AF:131:TRP:CE2	12:AI:97:PHE:HA	2.53	0.43
14:AK:116:PRO:O	14:AK:118:LYS:NZ	2.51	0.43
19:AQ:143:PRO:HG2	19:AQ:146:TRP:HB2	2.00	0.43
32:BB:39:LYS:HE3	32:BB:39:LYS:HB3	1.89	0.43
34:BO:73:TRP:HE3	34:BO:188:VAL:HG21	1.83	0.43
36:B5:18:ALA:HB3	58:Bd:67:PRO:HG2	2.01	0.43
1:1:1413:C:H2'	1:1:1414:C:H6	1.84	0.43
2:2:645:C:H2'	2:2:646:C:H6	1.83	0.43
2:2:1482:A:H2'	2:2:1483:G:C8	2.53	0.43
5:AB:142:ASP:H	5:AB:145:ASN:ND2	2.13	0.43
9:AF:28:GLU:HG3	9:AF:30:GLN:OE1	2.18	0.43
22:AU:74:ARG:HG2	22:AU:98:ILE:HD12	2.00	0.43
65:H:164:ILE:HB	65:H:177:VAL:HG13	2.00	0.43
1:1:99:U:H3	1:1:120:A:H2	1.66	0.43
1:1:117:G:N2	1:1:118:U:H1'	2.34	0.43
1:1:391:G:O6	1:1:393:C:H5'	2.19	0.43
1:1:869:G:H4'	1:1:870:A:OP1	2.19	0.43
1:1:894:A:H2'	1:1:895:A:H8	1.84	0.43
1:1:2102:G:H2'	1:1:2103:U:O4'	2.17	0.43
2:2:53:4AC:O7	2:2:53:4AC:H5	2.18	0.43
2:2:425:U:H3'	2:2:426:G:C8	2.53	0.43
2:2:907:A:H2'	2:2:908:C:H6	1.84	0.43
5:AB:10:ASP:OD1	5:AB:11:GLN:N	2.52	0.43
10:AG:77:ASP:OD1	10:AG:77:ASP:N	2.51	0.43
29:A3:58:ASP:OD1	29:A3:58:ASP:N	2.51	0.43
29:A3:84:LYS:HB3	29:A3:84:LYS:HE3	1.74	0.43
36:B5:8:ARG:HB3	36:B5:24:ILE:HD12	2.00	0.43
42:BE:34:VAL:HG22	42:BE:36:GLU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BF:29:LYS:HE3	53:BF:29:LYS:HB2	1.82	0.43
54:BZ:55:LEU:HD23	54:BZ:55:LEU:HA	1.88	0.43
1:1:1031:G:H1	32:BB:201:ASN:ND2	2.14	0.43
1:1:1431:U:O2	55:BP:7:THR:HG23	2.19	0.43
1:1:1878:4AC:O7	1:1:1878:4AC:H5	2.18	0.43
1:1:2593:A:H4'	37:BL:51:ILE:HG22	2.00	0.43
1:1:2607:C:H2'	1:1:2608:4AC:O2	2.19	0.43
2:2:64:OMU:HM22	2:2:65:G:O4'	2.18	0.43
2:2:162:G:O2'	10:AG:120:ASN:ND2	2.51	0.43
2:2:265:U:OP2	20:AR:20:LYS:NZ	2.52	0.43
2:2:722:G:O2'	12:AI:2:THR:HG21	2.19	0.43
2:2:1345:G:O3'	14:AK:70:GLY:HA3	2.18	0.43
2:2:1429:U:H2'	2:2:1430:C:C6	2.54	0.43
2:2:1479:4AC:H5	2:2:1479:4AC:O7	2.18	0.43
5:AB:5:TYR:CZ	5:AB:9:LEU:HD21	2.54	0.43
23:AV:41:VAL:HA	23:AV:46:LEU:HD12	2.01	0.43
23:AV:51:THR:HG22	23:AV:71:TYR:HD1	1.83	0.43
42:BE:43:LYS:HD3	42:BE:132:ILE:HA	2.00	0.43
61:Bc:26:PRO:HB2	61:Bc:29:VAL:HG13	2.00	0.43
1:1:775:U:O2'	1:1:1234:A:N1	2.48	0.43
1:1:960:C:H2'	1:1:961:U:H6	1.84	0.43
1:1:1363:U:O2'	1:1:1364:C:OP1	2.30	0.43
1:1:1836:C:OP1	32:BB:177:LYS:NZ	2.50	0.43
1:1:2416:G:H2'	1:1:2417:C:C6	2.54	0.43
1:1:2738:U:H3	1:1:2815:G:H1	1.67	0.43
2:2:1120:A:H2	14:AK:5:GLN:HE22	1.67	0.43
2:2:1326:C:H2'	2:2:1327:G:C8	2.54	0.43
8:AE:138:ILE:HB	8:AE:150:ILE:HG13	1.99	0.43
19:AQ:106:ARG:O	19:AQ:110:GLU:HG3	2.19	0.43
27:AZ:23:LYS:HE2	27:AZ:23:LYS:HB3	1.79	0.43
33:BY:105:MET:HB2	33:BY:109:ASP:OD2	2.18	0.43
36:B5:67:SER:OG	36:B5:70:GLU:OE1	2.20	0.43
44:BT:50:LYS:HA	44:BT:50:LYS:HD3	1.88	0.43
65:H:29:ILE:HA	65:H:32:LYS:HG2	2.01	0.43
1:1:566:C:H2'	1:1:567:A:C8	2.53	0.42
1:1:835:4AC:O2'	1:1:906:U:OP1	2.29	0.42
1:1:1618:G:H2'	1:1:1619:C:C6	2.54	0.42
1:1:3022:C:O2	1:1:3022:C:C2'	2.67	0.42
2:2:268:G:H2'	2:2:269:G:C8	2.54	0.42
2:2:289:A:H3'	2:2:290:G:H5'	2.01	0.42
2:2:1052:C:H2'	2:2:1053:A:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1212:A:C8	2:2:1277:C:H1'	2.53	0.42
23:AV:25:HIS:O	23:AV:25:HIS:ND1	2.52	0.42
25:AX:35:ARG:HG3	25:AX:36:ASP:OD1	2.19	0.42
27:AZ:196:ILE:H	27:AZ:196:ILE:HG13	1.56	0.42
65:H:29:ILE:HG12	65:H:32:LYS:NZ	2.32	0.42
1:1:151:C:H2'	1:1:152:U:C6	2.54	0.42
1:1:948:A:H2'	1:1:949:G:O4'	2.20	0.42
1:1:1115:A:H2'	1:1:1116:G:C8	2.54	0.42
1:1:1932:C:H2'	1:1:1933:C:H6	1.85	0.42
2:2:626:4AC:H5	2:2:626:4AC:O7	2.18	0.42
2:2:795:A:H2'	2:2:796:G:O4'	2.19	0.42
23:AV:37:LYS:HE3	23:AV:37:LYS:HB2	1.90	0.42
29:A3:116:MET:SD	29:A3:119:ARG:NH2	2.92	0.42
39:BU:34:GLU:OE1	39:BU:34:GLU:N	2.44	0.42
56:BM:65:ARG:HG3	56:BM:127:TRP:CE2	2.54	0.42
65:H:267:MET:HE2	65:H:267:MET:HB2	1.74	0.42
1:1:15:G:H2'	1:1:16:A:H5"	2.01	0.42
1:1:27:G:OP2	35:BC:111:SER:OG	2.27	0.42
1:1:103:C:C2	1:1:117:G:C2	3.08	0.42
1:1:1410:A:OP1	61:Bc:18:HIS:HE1	2.02	0.42
2:2:397:G:H4'	2:2:399:C:H41	1.83	0.42
49:BQ:21:ARG:HD2	49:BQ:53:LYS:O	2.19	0.42
59:BN:97:ASN:HD22	59:BN:98:PRO:CD	2.30	0.42
1:1:439:C:H2'	1:1:440:G:H5'	2.01	0.42
1:1:572:C:H2'	1:1:573:U:H6	1.83	0.42
1:1:1763:G:H2'	1:1:1764:C:H6	1.84	0.42
1:1:2488:A:C4	1:1:2506:C:H5'	2.54	0.42
2:2:433:C:H2'	2:2:434:U:C6	2.54	0.42
2:2:817:U:H2'	2:2:818:C:C6	2.54	0.42
19:AQ:57:GLN:HE22	24:AW:38:ARG:HG3	1.85	0.42
25:AX:9:ALA:N	25:AX:55:LEU:O	2.51	0.42
29:A3:114:ILE:HA	29:A3:117:LYS:HE3	2.01	0.42
39:BU:31:LEU:HD23	39:BU:102:ILE:HB	2.01	0.42
57:BS:116:HIS:HB3	57:BS:149:VAL:HB	2.02	0.42
1:1:94:G:H3'	1:1:95:G:H5'	2.01	0.42
1:1:702:A:C6	29:B4:92:ILE:HD12	2.55	0.42
1:1:853:C:H2'	1:1:854:C:H6	1.85	0.42
1:1:908:A:H2'	1:1:909:C:C6	2.54	0.42
1:1:1369:U:H2'	1:1:1370:C:C6	2.54	0.42
1:1:2705:C:H2'	1:1:2705:C:O2	2.19	0.42
2:2:711:A:H4'	2:2:823:G:O2'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1180:G:H2'	2:2:1181:C:C6	2.55	0.42
2:2:1502:C:N3	2:2:1503:A:H1'	2.34	0.42
6:AC:35:CYS:SG	6:AC:36:GLY:N	2.93	0.42
8:AE:56:ALA:HB1	8:AE:61:GLU:HG3	2.01	0.42
15:AL:21:ASN:O	15:AL:24:LYS:HG2	2.18	0.42
29:A3:115:ALA:HA	29:A3:118:VAL:HG22	2.02	0.42
1:1:1731:U:H4'	1:1:1732:G:O5'	2.18	0.42
1:1:2719:G:H2'	1:1:2720:A:H8	1.84	0.42
2:2:122:C:OP1	2:2:571:C:O2'	2.29	0.42
2:2:145:G:H2'	2:2:146:A:H8	1.83	0.42
2:2:313:G:H2'	2:2:314:G:O4'	2.18	0.42
2:2:619:U:O4	2:2:719:G:O2'	2.32	0.42
2:2:636:4AC:O7	2:2:636:4AC:H5	2.19	0.42
2:2:1085:C:H2'	2:2:1086:C:H6	1.83	0.42
4:AA:121:MET:SD	4:AA:121:MET:N	2.93	0.42
45:BW:67:LYS:HB3	45:BW:67:LYS:HE3	1.83	0.42
36:BK:77:LYS:HE3	36:BK:77:LYS:HB3	1.93	0.42
49:BQ:93:GLU:CD	49:BQ:93:GLU:H	2.27	0.42
62:BJ:124:ARG:N	62:BJ:141:VAL:O	2.49	0.42
65:H:26:ALA:O	65:H:30:ILE:HG12	2.20	0.42
1:1:652:U:H2'	1:1:653:G:O4'	2.19	0.42
1:1:806:G:H2'	1:1:807:C:C6	2.55	0.42
1:1:1216:G:H21	1:1:2498:A:H62	1.66	0.42
1:1:1364:C:H4'	1:1:1365:G:OP1	2.20	0.42
1:1:1498:C:H2'	1:1:1499:G:H8	1.84	0.42
1:1:1580:C:C5	1:1:1589:U:H5"	2.55	0.42
1:1:1666:C:H2'	1:1:1667:4AC:H6	2.02	0.42
1:1:2524:G:H2'	1:1:2525:G:C8	2.55	0.42
1:1:2977:G:O6	1:1:2985:C:H5"	2.20	0.42
1:1:2992:4AC:H5	1:1:2992:4AC:CM7	2.49	0.42
2:2:96:C:H2'	2:2:97:A:H8	1.77	0.42
2:2:903:C:H2'	2:2:904:A:C8	2.55	0.42
6:AC:11:ILE:HG23	9:AF:39:ARG:HD3	2.01	0.42
7:AD:96:THR:HG22	7:AD:98:GLU:H	1.84	0.42
10:AG:5:LYS:HE3	10:AG:5:LYS:HB2	1.91	0.42
21:AS:30:HIS:O	21:AS:34:LYS:HG2	2.20	0.42
30:AT:10:GLY:N	31:AO:86:GLU:O	2.52	0.42
33:BY:3:LYS:HD3	33:BY:3:LYS:HA	1.90	0.42
57:BS:14:PRO:O	57:BS:105:LYS:HD3	2.20	0.42
29:B4:64:ALA:O	29:B4:67:PRO:HD2	2.19	0.42
65:H:4:ILE:HG21	65:H:121:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:H:147:ASP:O	65:H:210:LEU:HD22	2.20	0.42
1:1:696:A:H2'	1:1:697:A:C8	2.55	0.42
1:1:1137:G:H2'	1:1:1138:G:C8	2.55	0.42
1:1:2536:U:C2	42:BE:136:GLY:HA3	2.55	0.42
2:2:479:4AC:H5	2:2:479:4AC:O7	2.20	0.42
2:2:880:A:H2'	2:2:881:C:O4'	2.19	0.42
5:AB:76:GLY:C	5:AB:79:PRO:HD2	2.44	0.42
9:AF:13:LEU:O	9:AF:27:LYS:NZ	2.43	0.42
17:AN:55:LEU:HD11	17:AN:76:GLN:HB2	2.01	0.42
27:AZ:42:THR:HG22	27:AZ:76:GLU:O	2.19	0.42
32:BB:35:TYR:CD2	32:BB:67:MET:HE1	2.55	0.42
38:Bf:20:ASN:HD21	38:Bf:42:ARG:H	1.66	0.42
63:Bl:34:LYS:HD3	63:Bl:54:ILE:HD12	2.01	0.42
1:1:431:G:H8	1:1:431:G:P	2.43	0.42
1:1:1111:G:O2'	1:1:1168:G:O6	2.33	0.42
1:1:1336:U:H2'	1:1:1337:U:C6	2.54	0.42
1:1:2393:G:H2'	1:1:2394:G:C8	2.55	0.42
1:1:3014:C:H2'	1:1:3015:G:H8	1.83	0.42
2:2:957:4AC:O7	2:2:957:4AC:H5	2.20	0.42
2:2:1172:G:H2'	2:2:1173:U:C6	2.54	0.42
2:2:1192:C:H2'	2:2:1193:C:H6	1.85	0.42
2:2:1239:4AC:O7	2:2:1239:4AC:H5	2.20	0.42
8:AE:126:ARG:H	8:AE:143:HIS:CD2	2.36	0.42
25:AX:10:GLU:N	25:AX:30:ARG:O	2.32	0.42
31:AO:97:LYS:HB2	31:AO:97:LYS:HE2	1.80	0.42
32:BB:74:PRO:HG2	32:BB:77:LEU:HB2	2.01	0.42
49:BQ:60:ARG:HG2	49:BQ:63:ALA:HB3	2.01	0.42
29:B4:90:ALA:O	29:B4:92:ILE:HG12	2.19	0.42
1:1:60:4AC:O7	1:1:60:4AC:H5	2.20	0.42
1:1:279:A:H2'	1:1:280:G:H8	1.85	0.42
1:1:796:C:H2'	1:1:797:G:H8	1.85	0.42
1:1:1662:4AC:H5	1:1:1662:4AC:O7	2.20	0.42
1:1:2981:G:H5"	1:1:2982:C:H5	1.85	0.42
2:2:319:4AC:O7	2:2:319:4AC:H5	2.20	0.42
2:2:379:4AC:H5	2:2:379:4AC:O7	2.20	0.42
4:AA:127:ALA:HB2	4:AA:182:LYS:HB2	2.01	0.42
11:AH:75:GLY:O	11:AH:86:MET:HB2	2.19	0.42
13:AJ:65:VAL:HG11	13:AJ:124:LEU:HD23	2.02	0.42
16:AM:52:ARG:HH21	65:H:382:LYS:HE2	1.85	0.42
31:AO:57:GLU:H	31:AO:57:GLU:CD	2.26	0.42
34:BO:36:VAL:HG22	34:BO:47:GLN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:BN:44:GLU:OE1	59:BN:44:GLU:N	2.38	0.42
65:H:89:ALA:HB1	65:H:261:LEU:HD22	2.01	0.42
1:1:594:G:OP2	39:BU:10:LYS:NZ	2.48	0.41
1:1:960:C:H2'	1:1:961:U:C6	2.54	0.41
1:1:1806:G:H2'	1:1:1807:U:H5"	2.02	0.41
1:1:1933:C:H2'	1:1:1934:4AC:H6	2.02	0.41
1:1:2340:G:C2	1:1:2341:G:C6	3.07	0.41
2:2:128:C:H2'	2:2:129:OMC:C6	2.55	0.41
2:2:484:G:H1'	17:AN:67:SER:OG	2.19	0.41
2:2:703:4AC:H2'	2:2:704:G:C8	2.55	0.41
2:2:848:4AC:O7	2:2:848:4AC:H5	2.20	0.41
2:2:1350:U:OP2	11:AH:58:LYS:HD3	2.19	0.41
4:AA:90:ARG:NH2	16:AM:119:THR:O	2.45	0.41
11:AH:14:GLU:N	11:AH:14:GLU:OE1	2.53	0.41
21:AS:17:PHE:CE1	21:AS:58:VAL:HG12	2.55	0.41
53:BF:91:LYS:HE3	53:BF:91:LYS:HB2	1.84	0.41
56:BM:93:LYS:HD3	56:BM:93:LYS:HA	1.90	0.41
1:1:341:4AC:O7	1:1:341:4AC:H5	2.21	0.41
1:1:974:G:OP1	1:1:1768:A:O2'	2.34	0.41
1:1:1006:G:H2'	1:1:1007:C:H6	1.85	0.41
1:1:1551:G:H5'	49:BQ:24:ILE:O	2.20	0.41
1:1:2610:A:H4'	34:BO:134:SER:HB2	2.02	0.41
2:2:398:A:H3'	2:2:399:C:C6	2.55	0.41
2:2:606:G:O6	2:2:607:A:N6	2.53	0.41
2:2:976:A:N7	2:2:1002:C:O2'	2.39	0.41
2:2:1468:A:H2'	2:2:1469:6MZ:H8	2.02	0.41
5:AB:51:ARG:HD3	5:AB:51:ARG:HA	1.88	0.41
11:AH:24:GLU:OE1	11:AH:24:GLU:N	2.52	0.41
31:AO:34:ASN:O	31:AO:38:MET:HG3	2.20	0.41
48:BR:89:HIS:CD2	48:BR:91:VAL:H	2.38	0.41
59:BN:29:PRO:HA	59:BN:59:GLN:HE22	1.85	0.41
29:B4:34:LYS:HE3	29:B4:34:LYS:HB2	1.87	0.41
65:H:21:ALA:O	65:H:69:VAL:HG23	2.20	0.41
1:1:946:G:H2'	1:1:947:C:C6	2.55	0.41
1:1:1550:4AC:O7	1:1:1550:4AC:H5	2.19	0.41
1:1:2247:C:H2'	1:1:2248:C:H6	1.86	0.41
1:1:2447:A:H2'	1:1:2448:A:C8	2.54	0.41
1:1:2725:U:H2'	1:1:2726:G:O4'	2.20	0.41
1:1:2871:A:H2'	1:1:2872:G:O4'	2.20	0.41
2:2:270:U:P	13:AJ:56:ARG:HH22	2.41	0.41
2:2:1121:C:O2	14:AK:16:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1215:G:H2'	2:2:1216:G:C8	2.54	0.41
2:2:1425:G:H2'	2:2:1426:A:C8	2.55	0.41
2:2:1499:G:H2'	2:2:1500:A:H8	1.84	0.41
17:AN:44:LEU:HG	17:AN:50:ALA:HB2	2.02	0.41
22:AU:130:ASP:O	22:AU:134:THR:HG23	2.20	0.41
25:AX:61:GLU:N	25:AX:61:GLU:OE1	2.53	0.41
27:AZ:117:MET:HE1	27:AZ:147:TYR:C	2.45	0.41
37:BL:12:ARG:HG3	37:BL:12:ARG:HH11	1.85	0.41
39:BU:114:LYS:HB3	39:BU:114:LYS:HE2	1.72	0.41
42:BE:66:ARG:NH1	42:BE:71:ARG:HH12	2.19	0.41
42:BE:108:ASP:OD2	42:BE:112:ASN:HB2	2.19	0.41
62:BJ:86:ARG:H	62:BJ:102:ASN:ND2	2.19	0.41
1:1:458:4AC:O7	1:1:458:4AC:H5	2.20	0.41
1:1:940:C:H2'	1:1:941:C:H6	1.86	0.41
1:1:1161:A:H2'	1:1:1164:C:H5	1.84	0.41
1:1:1677:G:H2'	1:1:1678:G:H5"	2.01	0.41
1:1:1874:G:O2'	38:Bf:3:ARG:O	2.38	0.41
2:2:103:G:H2'	2:2:104:G:O4'	2.21	0.41
2:2:1359:G:H2'	2:2:1360:C:H6	1.85	0.41
3:3:57:A:O2'	42:BE:164:HIS:HD2	2.04	0.41
27:AZ:25:LEU:HB2	27:AZ:30:TYR:HB2	2.03	0.41
27:AZ:67:ARG:HD3	27:AZ:71:ARG:HH11	1.86	0.41
29:A3:18:LYS:HD3	29:A3:18:LYS:C	2.45	0.41
34:BO:36:VAL:HG12	34:BO:105:ASP:HB3	2.02	0.41
53:BF:74:HIS:O	53:BF:78:MET:HG3	2.21	0.41
1:1:1153:C:H2'	1:1:1154:C:H6	1.85	0.41
1:1:1695:4AC:H5	1:1:1695:4AC:O7	2.21	0.41
1:1:1767:U:P	49:BQ:107:ARG:HH22	2.42	0.41
2:2:774:OMU:HM22	2:2:775:G:H5'	2.02	0.41
5:AB:58:PHE:HB2	6:AC:33:PRO:HB3	2.03	0.41
19:AQ:90:GLU:H	19:AQ:90:GLU:CD	2.28	0.41
30:AT:44:GLN:NE2	30:AT:70:MET:SD	2.69	0.41
38:Bf:38:HIS:HD2	38:Bf:40:LYS:H	1.69	0.41
39:BU:51:LYS:HB3	39:BU:104:GLU:HB3	2.02	0.41
65:H:273:ARG:NH2	65:H:311:GLU:OE1	2.46	0.41
1:1:113:G:H8	1:1:113:G:O5'	2.03	0.41
1:1:166:A:H2'	1:1:167:A:C8	2.56	0.41
1:1:243:4AC:H5	1:1:243:4AC:O7	2.21	0.41
1:1:455:G:OP2	39:BU:42:ARG:NH1	2.45	0.41
1:1:644:G:H2'	1:1:645:A:C8	2.55	0.41
1:1:776:G:H2'	1:1:2270:C:C4	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:992:C:H3'	1:1:993:U:H4'	2.01	0.41
1:1:1806:G:H1'	1:1:1809:A:C8	2.56	0.41
1:1:1867:4AC:O7	1:1:1867:4AC:H5	2.21	0.41
1:1:2118:U:O2'	1:1:2121:A:N7	2.52	0.41
1:1:2423:C:H2'	1:1:2424:C:C6	2.55	0.41
2:2:580:A:H2'	2:2:581:C:C6	2.55	0.41
2:2:846:OMC:H1'	12:AI:16:ASN:HD21	1.86	0.41
2:2:930:A:C5	30:AT:87:LYS:HD2	2.56	0.41
2:2:1288:C:H2'	2:2:1289:U:C6	2.56	0.41
10:AG:32:LYS:HE3	10:AG:32:LYS:HB3	1.88	0.41
11:AH:172:LYS:HE2	11:AH:172:LYS:HB2	1.95	0.41
14:AK:98:LYS:O	14:AK:101:LYS:HG2	2.21	0.41
30:AT:116:GLY:HA2	30:AT:124:ARG:HD2	2.03	0.41
35:BC:18:LYS:O	35:BC:274:HIS:HD2	2.04	0.41
42:BE:103:LYS:HA	42:BE:184:VAL:HG22	2.03	0.41
50:BV:26:ASP:OD1	50:BV:28:ARG:HG3	2.19	0.41
50:BV:49:LYS:HB3	50:BV:49:LYS:HE2	1.83	0.41
59:BN:104:LYS:HG3	59:BN:107:ARG:HG3	2.02	0.41
65:H:202:LYS:HD3	65:H:203:ILE:N	2.35	0.41
1:1:163:A:C2	1:1:233:U:N3	2.81	0.41
1:1:198:A:C2	1:1:216:A:C5	3.08	0.41
1:1:392:A:O2'	1:1:393:C:H5"	2.20	0.41
1:1:435:C:H2'	1:1:436:C:H6	1.86	0.41
1:1:535:U:H2'	1:1:536:C:C6	2.55	0.41
1:1:802:4AC:O7	1:1:802:4AC:H5	2.21	0.41
1:1:1408:C:H2'	1:1:1409:G:O4'	2.20	0.41
1:1:1481:G:N2	1:1:1484:A:OP2	2.48	0.41
1:1:2110:A:H2'	1:1:2111:G:O4'	2.20	0.41
1:1:2429:C:C4	1:1:2430:G:C8	3.09	0.41
2:2:1153:A:H2'	2:2:1154:A:O4'	2.21	0.41
4:AA:78:ASN:HD22	4:AA:78:ASN:N	2.19	0.41
9:AF:24:MET:O	9:AF:28:GLU:HG2	2.19	0.41
9:AF:39:ARG:HH22	9:AF:209:ASN:ND2	2.18	0.41
20:AR:84:ASP:HB2	20:AR:107:GLU:O	2.21	0.41
1:1:103:C:O2'	1:1:104:C:H5'	2.21	0.41
1:1:163:A:H5"	1:1:165:G:O4'	2.21	0.41
1:1:796:C:H2'	1:1:797:G:C8	2.55	0.41
1:1:1529:A:N3	1:1:2244:G:O2'	2.51	0.41
1:1:2570:4AC:H5	1:1:2570:4AC:O7	2.20	0.41
1:1:2635:G:O2'	1:1:2636:C:O5'	2.33	0.41
11:AH:106:GLU:O	11:AH:110:ILE:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AK:43:PHE:O	14:AK:47:GLU:HG2	2.20	0.41
36:B5:45:ARG:NH2	36:B5:66:ALA:O	2.46	0.41
36:B5:54:GLU:OE2	58:Bd:85:ARG:NE	2.47	0.41
42:BE:3:ILE:HG21	42:BE:185:GLU:HB3	2.03	0.41
42:BE:79:LYS:HG2	42:BE:80:VAL:N	2.35	0.41
42:BE:121:ILE:H	42:BE:121:ILE:HG13	1.56	0.41
43:Ba:4:LYS:HE3	43:Ba:4:LYS:HB3	1.90	0.41
47:BI:17:ARG:O	47:BI:21:MET:HG3	2.21	0.41
49:BQ:121:ARG:O	49:BQ:125:ILE:HG12	2.20	0.41
53:BF:67:ILE:HD13	53:BF:67:ILE:HA	1.87	0.41
57:BS:72:HIS:HA	57:BS:79:GLY:O	2.20	0.41
62:BJ:33:SER:HB3	62:BJ:114:ARG:O	2.21	0.41
65:H:292:ARG:NH1	65:H:296:ASP:OD1	2.53	0.41
1:1:91:4AC:O7	1:1:91:4AC:H5	2.20	0.41
1:1:120:A:H2'	1:1:121:G:C8	2.56	0.41
1:1:285:A:H5"	41:Be:55:TRP:HZ3	1.86	0.41
1:1:959:C:H2'	1:1:960:C:H6	1.86	0.41
1:1:1090:U:H2'	1:1:1091:C:C6	2.55	0.41
1:1:1734:G:H2'	1:1:1735:G:C8	2.56	0.41
1:1:1993:G:N2	1:1:1995:G:H3'	2.36	0.41
1:1:2612:A:O3'	34:BO:30:SER:HB3	2.21	0.41
1:1:2650:G:H2'	1:1:2651:C:C6	2.56	0.41
1:1:2881:G:H2'	1:1:2882:C:H6	1.86	0.41
2:2:176:A:H2'	2:2:177:U:C6	2.56	0.41
2:2:203:A:H2'	2:2:204:G:H8	1.86	0.41
2:2:272:A:H2'	2:2:273:C:C6	2.56	0.41
2:2:998:C:H2'	2:2:999:G:C8	2.56	0.41
2:2:1376:OMC:H2'	2:2:1377:C:O4'	2.21	0.41
2:2:1461:A:C8	65:H:326:ARG:HG3	2.56	0.41
3:3:28:C:H2'	3:3:29:A:O4'	2.21	0.41
3:3:98:G:H5"	63:Bl:51:LYS:HE3	2.03	0.41
9:AF:131:TRP:HA	12:AI:97:PHE:HB3	2.03	0.41
9:AF:217:MET:HE1	12:AI:99:PHE:CZ	2.56	0.41
15:AL:8:LEU:HB2	15:AL:71:ARG:HB2	2.03	0.41
20:AR:50:GLU:OE2	20:AR:67:ARG:HD2	2.20	0.41
22:AU:74:ARG:NH1	22:AU:93:ALA:O	2.54	0.41
27:AZ:70:GLU:OE1	27:AZ:78:PRO:HD3	2.21	0.41
27:AZ:188:ARG:HG3	27:AZ:192:GLU:HG3	2.03	0.41
29:A3:12:PRO:HB2	29:A3:15:LEU:HB2	2.03	0.41
29:A3:19:ALA:HB1	29:A3:78:ILE:HD13	2.03	0.41
30:AT:29:PRO:HG2	30:AT:32:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:BD:29:ASP:OD1	52:BD:29:ASP:N	2.54	0.41
64:Bk:31:LYS:HE3	64:Bk:31:LYS:HB3	1.92	0.41
65:H:17:ILE:HD12	65:H:17:ILE:HA	1.99	0.41
1:1:117:G:C4	1:1:118:U:C6	3.09	0.41
1:1:846:C:H2'	1:1:847:G:O4'	2.21	0.41
1:1:1489:C:H2'	1:1:1490:G:C8	2.56	0.41
1:1:2027:4AC:H5	1:1:2027:4AC:O7	2.21	0.41
1:1:2287:4AC:O7	1:1:2287:4AC:H5	2.20	0.41
1:1:2456:C:H2'	1:1:2457:A:O4'	2.21	0.41
1:1:2823:C:H2'	1:1:2824:G:H8	1.86	0.41
2:2:346:A:H2'	2:2:347:G:C8	2.56	0.41
2:2:383:A:C6	2:2:384:U:C4	3.09	0.41
2:2:384:U:O2'	8:AE:28:TRP:O	2.39	0.41
2:2:385:G:H5'	8:AE:30:VAL:HG22	2.03	0.41
2:2:1107:U:O2'	2:2:1108:C:H6	2.04	0.41
2:2:1122:U:H2'	2:2:1123:C:O4'	2.20	0.41
2:2:1150:A:H3'	2:2:1151:G:C8	2.55	0.41
7:AD:58:LEU:HD13	7:AD:70:ARG:HA	2.02	0.41
23:AV:3:ILE:HG12	23:AV:23:ILE:HG12	2.03	0.41
26:AY:37:ARG:HA	26:AY:49:LYS:HG2	2.02	0.41
35:BC:211:LYS:O	35:BC:214:GLU:HG2	2.21	0.41
37:BL:72:GLU:CD	37:BL:72:GLU:H	2.29	0.41
43:Ba:10:ILE:HG21	43:Ba:71:ARG:NH2	2.36	0.41
56:BM:152:LYS:HG3	64:Bk:12:ARG:HA	2.03	0.41
65:H:81:PRO:HD3	65:H:103:GLY:C	2.46	0.41
1:1:42:U:C4	50:BV:51:LYS:HB2	2.56	0.40
1:1:787:C:H2'	1:1:788:A:C8	2.56	0.40
1:1:1293:4AC:O7	1:1:1293:4AC:H5	2.20	0.40
1:1:1460:4AC:O7	1:1:1460:4AC:H5	2.21	0.40
1:1:1594:4AC:O7	1:1:1594:4AC:H5	2.21	0.40
1:1:1617:4AC:O7	1:1:1617:4AC:H5	2.21	0.40
1:1:2718:4AC:O7	1:1:2718:4AC:H5	2.21	0.40
2:2:275:G:H3'	20:AR:96:LYS:HB2	2.03	0.40
2:2:1085:C:H2'	2:2:1086:C:C6	2.56	0.40
7:AD:167:GLU:O	7:AD:171:ILE:HG12	2.21	0.40
8:AE:47:TYR:HD1	8:AE:51:ASP:OD2	2.04	0.40
40:Bb:7:LYS:HE2	40:Bb:7:LYS:HB2	1.84	0.40
43:Ba:21:ILE:HG13	43:Ba:22:VAL:HG13	2.02	0.40
1:1:683:A:O2'	1:1:769:C:H5"	2.21	0.40
1:1:1074:A:H2'	1:1:1075:U:C6	2.56	0.40
1:1:1109:G:O2'	1:1:1110:G:H5'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1600:U:C4	44:BT:60:PRO:HG3	2.57	0.40
1:1:1852:G:C2	1:1:1853:G:C8	3.09	0.40
1:1:2705:C:C2	1:1:2706:C:O2	2.74	0.40
1:1:2786:U:H2'	1:1:2787:U:C6	2.57	0.40
2:2:105:A:C6	2:2:335:G:C6	3.09	0.40
2:2:361:C:H4'	2:2:363:G:OP1	2.21	0.40
2:2:394:4AC:O7	2:2:394:4AC:H5	2.21	0.40
2:2:1388:C:H2'	2:2:1389:C:H6	1.85	0.40
29:A3:32:ILE:HD13	29:A3:32:ILE:HA	1.93	0.40
30:AT:32:GLN:HG3	30:AT:71:ILE:HD13	2.03	0.40
43:Ba:84:LYS:HD2	43:Ba:84:LYS:HA	1.87	0.40
48:BR:30:ARG:NH2	48:BR:94:ARG:HD2	2.36	0.40
52:BD:3:VAL:HB	52:BD:139:GLN:HE22	1.86	0.40
29:B4:84:LYS:HE3	29:B4:84:LYS:HB3	1.87	0.40
65:H:167:VAL:HB	65:H:171:GLY:HA2	2.02	0.40
1:1:896:G:H2'	1:1:897:C:C6	2.56	0.40
1:1:1141:A:H4'	31:AO:110:ARG:HH21	1.87	0.40
1:1:1326:G:N2	1:1:1344:G:O2'	2.54	0.40
1:1:1462:G:O2'	52:BD:235:HIS:HD2	2.03	0.40
1:1:1480:C:H5'	40:Bb:76:PRO:HD3	2.03	0.40
1:1:1681:C:OP2	36:B5:42:LYS:NZ	2.40	0.40
1:1:2482:G:H2'	1:1:2483:G:H8	1.86	0.40
1:1:2548:4AC:O7	1:1:2548:4AC:H5	2.21	0.40
2:2:525:U:H4'	2:2:526:A:H3'	2.03	0.40
2:2:1233:4AC:O7	2:2:1233:4AC:H5	2.20	0.40
2:2:1420:U:O2'	2:2:1423:G:O6	2.24	0.40
3:3:52:A:H5"	34:BO:170:GLY:H	1.86	0.40
3:3:98:G:H2'	3:3:99:G:H8	1.85	0.40
15:AL:22:GLN:HG3	15:AL:23:ILE:N	2.36	0.40
29:A3:3:LYS:HG2	29:A3:6:TYR:HB2	2.02	0.40
29:A3:92:ILE:HG13	29:A3:94:VAL:HG22	2.02	0.40
40:Bb:127:ASN:OD1	40:Bb:127:ASN:N	2.53	0.40
1:1:1153:C:H2'	1:1:1154:C:C6	2.56	0.40
1:1:2545:4AC:O7	1:1:2545:4AC:H5	2.20	0.40
2:2:239:G:H2'	2:2:240:G:O4'	2.22	0.40
2:2:644:C:H2'	2:2:645:C:H6	1.85	0.40
2:2:983:G:C2	2:2:984:G:C8	3.10	0.40
2:2:1236:C:H2'	2:2:1237:C:C6	2.57	0.40
43:Ba:75:LYS:HB3	43:Ba:75:LYS:HE3	1.90	0.40
59:BN:12:VAL:HG12	59:BN:56:GLN:HG3	2.02	0.40
59:BN:69:VAL:HG21	59:BN:152:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:H:145:PRO:HA	65:H:210:LEU:HD21	2.03	0.40
1:1:211:4AC:O7	1:1:211:4AC:H5	2.21	0.40
1:1:1302:G:H1'	1:1:1303:A:C2	2.56	0.40
1:1:1740:C:O2'	1:1:1741:U:H5'	2.22	0.40
1:1:1809:A:C5	1:1:1810:G:H1'	2.56	0.40
1:1:1933:C:H5"	35:BC:246:GLY:HA3	2.02	0.40
2:2:455:C:H1'	23:AV:29:PRO:HB3	2.03	0.40
2:2:546:4AC:O7	2:2:546:4AC:H5	2.21	0.40
2:2:703:4AC:H6	2:2:703:4AC:O5'	2.21	0.40
2:2:998:C:N4	2:2:999:G:O6	2.55	0.40
2:2:1075:G:O2'	21:AS:6:GLN:NE2	2.54	0.40
2:2:1446:U:H2'	2:2:1447:C:C6	2.57	0.40
20:AR:81:LYS:HA	20:AR:81:LYS:HD3	1.97	0.40
27:AZ:188:ARG:HD3	27:AZ:188:ARG:HA	1.87	0.40
46:Bi:5:LYS:HB3	46:Bi:6:LYS:HG3	2.03	0.40
46:Bi:35:LYS:HB3	46:Bi:44:ARG:HG2	2.02	0.40
56:BM:111:LEU:HB2	56:BM:132:MET:HE2	2.03	0.40
65:H:41:PHE:CE2	65:H:46:TYR:HB3	2.56	0.40
65:H:62:TRP:HH2	65:H:71:ASP:HB2	1.86	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	AA	186/199 (94%)	182 (98%)	4 (2%)	0	100	100
5	AB	194/202 (96%)	192 (99%)	2 (1%)	0	100	100
6	AC	55/63 (87%)	53 (96%)	2 (4%)	0	100	100
7	AD	171/180 (95%)	169 (99%)	2 (1%)	0	100	100
8	AE	240/243 (99%)	234 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AF	227/236 (96%)	222 (98%)	5 (2%)	0	100	100
10	AG	122/125 (98%)	117 (96%)	5 (4%)	0	100	100
11	AH	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
12	AI	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
13	AJ	123/127 (97%)	121 (98%)	2 (2%)	0	100	100
14	AK	133/135 (98%)	129 (97%)	4 (3%)	0	100	100
15	AL	98/102 (96%)	95 (97%)	3 (3%)	0	100	100
16	AM	125/137 (91%)	122 (98%)	3 (2%)	0	100	100
17	AN	144/147 (98%)	144 (100%)	0	0	100	100
18	AP	53/56 (95%)	53 (100%)	0	0	100	100
19	AQ	155/158 (98%)	152 (98%)	3 (2%)	0	100	100
20	AR	105/113 (93%)	103 (98%)	2 (2%)	0	100	100
21	AS	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
22	AU	147/150 (98%)	145 (99%)	2 (1%)	0	100	100
23	AV	94/99 (95%)	92 (98%)	2 (2%)	0	100	100
23	B6	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
24	AW	59/65 (91%)	55 (93%)	4 (7%)	0	100	100
25	AX	63/71 (89%)	62 (98%)	1 (2%)	0	100	100
26	AY	27/51 (53%)	23 (85%)	4 (15%)	0	100	100
27	AZ	194/210 (92%)	184 (95%)	10 (5%)	0	100	100
28	A0	34/37 (92%)	34 (100%)	0	0	100	100
29	A3	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
29	B4	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
29	BG	120/123 (98%)	120 (100%)	0	0	100	100
30	AT	128/132 (97%)	128 (100%)	0	0	100	100
31	AO	136/148 (92%)	127 (93%)	9 (7%)	0	100	100
32	BB	236/239 (99%)	229 (97%)	6 (2%)	1 (0%)	30	28
33	BY	152/155 (98%)	151 (99%)	1 (1%)	0	100	100
34	BO	196/203 (97%)	195 (100%)	1 (0%)	0	100	100
35	BC	358/361 (99%)	348 (97%)	10 (3%)	0	100	100
36	B5	79/82 (96%)	77 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BK	78/82 (95%)	74 (95%)	4 (5%)	0	100	100
37	BL	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
38	Bf	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
39	BU	119/121 (98%)	119 (100%)	0	0	100	100
40	Bb	127/130 (98%)	127 (100%)	0	0	100	100
41	Be	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
42	BE	183/188 (97%)	180 (98%)	3 (2%)	0	100	100
43	Ba	92/94 (98%)	92 (100%)	0	0	100	100
44	BT	84/86 (98%)	84 (100%)	0	0	100	100
45	BW	66/68 (97%)	66 (100%)	0	0	100	100
46	Bi	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
47	BI	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
48	BR	94/97 (97%)	94 (100%)	0	0	100	100
49	BQ	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
50	BV	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
51	Bj	92/94 (98%)	92 (100%)	0	0	100	100
52	BD	253/255 (99%)	249 (98%)	4 (2%)	0	100	100
53	BF	181/184 (98%)	180 (99%)	1 (1%)	0	100	100
54	BZ	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
55	BP	118/120 (98%)	118 (100%)	0	0	100	100
56	BM	191/194 (98%)	188 (98%)	3 (2%)	0	100	100
57	BS	152/155 (98%)	148 (97%)	4 (3%)	0	100	100
58	Bd	89/91 (98%)	89 (100%)	0	0	100	100
59	BN	176/181 (97%)	172 (98%)	4 (2%)	0	100	100
60	Bg	46/51 (90%)	46 (100%)	0	0	100	100
61	Bc	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
62	BJ	138/141 (98%)	138 (100%)	0	0	100	100
63	Bl	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
64	Bk	61/65 (94%)	60 (98%)	1 (2%)	0	100	100
65	H	373/392 (95%)	349 (94%)	23 (6%)	1 (0%)	36	36
All	All	8537/8861 (96%)	8347 (98%)	188 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
65	H	206	PHE
32	BB	122	VAL

5.3.2 Protein sidechains (i)

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	AA	160/167 (96%)	156 (98%)	4 (2%)	42	48
5	AB	168/173 (97%)	164 (98%)	4 (2%)	43	49
6	AC	50/55 (91%)	49 (98%)	1 (2%)	48	56
7	AD	156/160 (98%)	155 (99%)	1 (1%)	78	86
8	AE	213/214 (100%)	211 (99%)	2 (1%)	70	78
9	AF	192/198 (97%)	190 (99%)	2 (1%)	68	76
10	AG	107/108 (99%)	102 (95%)	5 (5%)	23	24
11	AH	183/184 (100%)	180 (98%)	3 (2%)	55	64
12	AI	106/107 (99%)	104 (98%)	2 (2%)	50	58
13	AJ	101/103 (98%)	99 (98%)	2 (2%)	48	56
14	AK	111/111 (100%)	107 (96%)	4 (4%)	31	34
15	AL	89/91 (98%)	84 (94%)	5 (6%)	19	18
16	AM	94/104 (90%)	89 (95%)	5 (5%)	20	19
17	AN	120/121 (99%)	118 (98%)	2 (2%)	53	62
18	AP	45/46 (98%)	43 (96%)	2 (4%)	25	26
19	AQ	142/143 (99%)	140 (99%)	2 (1%)	59	67
20	AR	96/102 (94%)	93 (97%)	3 (3%)	35	39
21	AS	58/61 (95%)	56 (97%)	2 (3%)	32	35
22	AU	126/127 (99%)	124 (98%)	2 (2%)	55	64
23	AV	88/90 (98%)	86 (98%)	2 (2%)	44	51
23	B6	86/90 (96%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	AW	53/56 (95%)	49 (92%)	4 (8%)	12	10
25	AX	55/60 (92%)	51 (93%)	4 (7%)	13	10
26	AY	22/42 (52%)	22 (100%)	0	100	100
27	AZ	155/168 (92%)	150 (97%)	5 (3%)	34	38
28	A0	34/35 (97%)	33 (97%)	1 (3%)	37	42
29	A3	98/99 (99%)	91 (93%)	7 (7%)	13	11
29	B4	98/99 (99%)	94 (96%)	4 (4%)	27	29
29	BG	98/99 (99%)	98 (100%)	0	100	100
30	AT	113/114 (99%)	110 (97%)	3 (3%)	39	45
31	AO	115/123 (94%)	110 (96%)	5 (4%)	26	27
32	BB	188/189 (100%)	185 (98%)	3 (2%)	55	64
33	BY	132/133 (99%)	131 (99%)	1 (1%)	73	81
34	BO	167/170 (98%)	162 (97%)	5 (3%)	36	41
35	BC	306/307 (100%)	298 (97%)	8 (3%)	40	46
36	B5	65/66 (98%)	61 (94%)	4 (6%)	16	14
36	BK	64/66 (97%)	63 (98%)	1 (2%)	55	64
37	BL	118/118 (100%)	116 (98%)	2 (2%)	53	62
38	Bf	46/47 (98%)	45 (98%)	1 (2%)	45	53
39	BU	109/109 (100%)	108 (99%)	1 (1%)	70	78
40	Bb	117/118 (99%)	114 (97%)	3 (3%)	40	46
41	Be	52/53 (98%)	51 (98%)	1 (2%)	50	58
42	BE	158/160 (99%)	152 (96%)	6 (4%)	29	32
43	Ba	84/84 (100%)	81 (96%)	3 (4%)	31	34
44	BT	77/77 (100%)	74 (96%)	3 (4%)	28	31
45	BW	63/63 (100%)	62 (98%)	1 (2%)	55	64
46	Bi	61/62 (98%)	60 (98%)	1 (2%)	55	64
47	BI	122/122 (100%)	121 (99%)	1 (1%)	73	81
48	BR	86/87 (99%)	85 (99%)	1 (1%)	63	72
49	BQ	132/133 (99%)	131 (99%)	1 (1%)	73	81
50	BV	54/58 (93%)	54 (100%)	0	100	100
51	Bj	83/84 (99%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	BD	212/212 (100%)	208 (98%)	4 (2%)	50	58
53	BF	156/157 (99%)	153 (98%)	3 (2%)	50	58
54	BZ	79/80 (99%)	77 (98%)	2 (2%)	42	48
55	BP	102/102 (100%)	100 (98%)	2 (2%)	48	56
56	BM	160/161 (99%)	160 (100%)	0	100	100
57	BS	130/131 (99%)	128 (98%)	2 (2%)	57	65
58	Bd	82/82 (100%)	82 (100%)	0	100	100
59	BN	149/151 (99%)	146 (98%)	3 (2%)	48	56
60	Bg	37/39 (95%)	37 (100%)	0	100	100
61	Bc	74/74 (100%)	72 (97%)	2 (3%)	39	45
62	BJ	108/109 (99%)	107 (99%)	1 (1%)	70	78
63	Bl	72/72 (100%)	67 (93%)	5 (7%)	14	12
64	Bk	55/57 (96%)	54 (98%)	1 (2%)	51	60
65	H	327/338 (97%)	305 (93%)	22 (7%)	15	12
All	All	7359/7521 (98%)	7177 (98%)	182 (2%)	42	48

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	AA	74	VAL
4	AA	78	ASN
4	AA	97	VAL
4	AA	154	ASN
5	AB	9	LEU
5	AB	13	LEU
5	AB	50	GLU
5	AB	74	LEU
6	AC	31	VAL
7	AD	100	ILE
8	AE	90	VAL
8	AE	191	LYS
9	AF	10	LYS
9	AF	57	VAL
10	AG	3	THR
10	AG	7	VAL
10	AG	38	ILE
10	AG	77	ASP

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Mol	Chain	Res	Type
10	AG	124	VAL
11	AH	18	MET
11	AH	110	ILE
11	AH	146	TYR
12	AI	33	LEU
12	AI	51	GLU
13	AJ	18	VAL
13	AJ	124	LEU
14	AK	18	VAL
14	AK	56	ILE
14	AK	76	GLU
14	AK	96	LYS
15	AL	22	GLN
15	AL	75	ILE
15	AL	85	ILE
15	AL	100	LEU
15	AL	101	ILE
16	AM	51	ASP
16	AM	52	ARG
16	AM	53	ASP
16	AM	65	ARG
16	AM	92	LYS
17	AN	18	LEU
17	AN	102	GLU
18	AP	46	VAL
18	AP	49	LYS
19	AQ	60	ILE
19	AQ	77	THR
20	AR	38	VAL
20	AR	48	THR
20	AR	106	LEU
21	AS	39	THR
21	AS	60	MET
22	AU	7	VAL
22	AU	22	GLU
23	AV	45	ASP
23	AV	46	LEU
24	AW	22	ASP
24	AW	29	VAL
24	AW	61	LEU
24	AW	64	LEU
25	AX	32	LEU

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Mol	Chain	Res	Type
25	AX	53	ASP
25	AX	60	THR
25	AX	67	ILE
27	AZ	151	LEU
27	AZ	162	VAL
27	AZ	175	VAL
27	AZ	192	GLU
27	AZ	196	ILE
28	A0	36	LEU
29	A3	11	VAL
29	A3	28	ASP
29	A3	36	THR
29	A3	57	VAL
29	A3	69	LEU
29	A3	84	LYS
29	A3	121	LEU
30	AT	47	LEU
30	AT	90	VAL
30	AT	92	VAL
31	AO	31	VAL
31	AO	42	VAL
31	AO	122	LEU
31	AO	126	VAL
31	AO	137	ARG
32	BB	96	THR
32	BB	106	THR
32	BB	201	ASN
33	BY	55	THR
34	BO	64	THR
34	BO	112	VAL
34	BO	137	ILE
34	BO	159	GLN
34	BO	172	LEU
35	BC	56	ASP
35	BC	83	ILE
35	BC	110	VAL
35	BC	118	LYS
35	BC	170	VAL
35	BC	172	LYS
35	BC	291	LYS
35	BC	297	ASN
36	B5	23	VAL

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Mol	Chain	Res	Type
36	B5	33	VAL
36	B5	60	ILE
36	B5	71	VAL
37	BL	69	VAL
37	BL	115	THR
38	Bf	47	THR
39	BU	79	GLU
40	Bb	80	GLU
40	Bb	84	ILE
40	Bb	91	GLU
41	Be	30	VAL
42	BE	29	THR
42	BE	34	VAL
42	BE	94	LEU
42	BE	121	ILE
42	BE	167	THR
42	BE	181	VAL
43	Ba	1	MET
43	Ba	3	ILE
43	Ba	4	LYS
44	BT	12	ILE
44	BT	27	THR
44	BT	75	SER
45	BW	62	LEU
46	Bi	51	THR
47	BI	1	MET
48	BR	64	THR
36	BK	75	LEU
49	BQ	108	LYS
52	BD	75	THR
52	BD	92	THR
52	BD	222	VAL
52	BD	243	THR
53	BF	26	VAL
53	BF	53	VAL
53	BF	158	THR
54	BZ	79	VAL
54	BZ	96	LEU
55	BP	16	ARG
55	BP	99	GLU
57	BS	144	THR
57	BS	155	ARG

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Mol	Chain	Res	Type
59	BN	103	ARG
59	BN	107	ARG
59	BN	170	ASN
61	Bc	27	LEU
61	Bc	29	VAL
62	BJ	63	VAL
63	Bl	2	ASN
63	Bl	8	VAL
63	Bl	46	LYS
63	Bl	58	LYS
63	Bl	59	GLU
29	B4	7	VAL
29	B4	21	GLN
29	B4	69	LEU
29	B4	101	ILE
64	Bk	16	GLU
65	H	6	VAL
65	H	33	GLU
65	H	53	ASP
65	H	68	LYS
65	H	71	ASP
65	H	113	ILE
65	H	120	GLU
65	H	123	VAL
65	H	153	LEU
65	H	161	ILE
65	H	164	ILE
65	H	170	GLU
65	H	177	VAL
65	H	187	ILE
65	H	215	ILE
65	H	239	ILE
65	H	247	GLU
65	H	254	ILE
65	H	267	MET
65	H	270	LYS
65	H	379	ARG
65	H	386	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (161) such sidechains are listed below:

Mol	Chain	Res	Type
4	AA	70	GLN
4	AA	77	GLN
5	AB	11	GLN
5	AB	23	GLN
5	AB	145	ASN
5	AB	178	ASN
7	AD	47	GLN
7	AD	50	ASN
7	AD	65	GLN
7	AD	72	GLN
7	AD	123	GLN
7	AD	135	GLN
8	AE	143	HIS
8	AE	148	HIS
9	AF	17	GLN
9	AF	58	ASN
9	AF	186	GLN
9	AF	209	ASN
10	AG	110	ASN
10	AG	118	GLN
10	AG	120	ASN
11	AH	55	HIS
11	AH	69	ASN
11	AH	84	HIS
11	AH	90	HIS
11	AH	147	HIS
11	AH	193	ASN
12	AI	9	ASN
12	AI	16	ASN
12	AI	70	ASN
13	AJ	40	GLN
13	AJ	64	ASN
13	AJ	121	ASN
14	AK	5	GLN
14	AK	67	GLN
15	AL	12	ASN
16	AM	24	ASN
16	AM	99	GLN
17	AN	66	ASN
17	AN	76	GLN
19	AQ	5	HIS
19	AQ	57	GLN
19	AQ	123	GLN

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Mol	Chain	Res	Type
19	AQ	152	GLN
20	AR	52	GLN
20	AR	55	HIS
20	AR	74	ASN
20	AR	79	ASN
21	AS	6	GLN
21	AS	18	ASN
21	AS	30	HIS
25	AX	26	GLN
27	AZ	95	GLN
27	AZ	123	ASN
28	A0	29	GLN
29	A3	37	ASN
29	A3	65	HIS
30	AT	15	GLN
31	AO	20	GLN
31	AO	58	GLN
31	AO	72	HIS
32	BB	8	GLN
32	BB	34	ASN
32	BB	50	HIS
32	BB	154	ASN
32	BB	201	ASN
32	BB	202	HIS
32	BB	229	HIS
33	BY	14	ASN
33	BY	48	GLN
33	BY	98	GLN
33	BY	148	ASN
34	BO	42	ASN
34	BO	47	GLN
34	BO	63	HIS
34	BO	76	HIS
35	BC	167	GLN
35	BC	241	HIS
35	BC	257	HIS
35	BC	270	GLN
35	BC	274	HIS
35	BC	280	ASN
35	BC	309	HIS
35	BC	348	GLN
35	BC	351	GLN

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Mol	Chain	Res	Type
36	B5	31	ASN
37	BL	57	HIS
37	BL	70	GLN
37	BL	84	ASN
38	Bf	19	GLN
38	Bf	20	ASN
38	Bf	38	HIS
39	BU	7	GLN
39	BU	96	HIS
40	Bb	26	GLN
40	Bb	119	GLN
41	Be	17	HIS
42	BE	164	HIS
43	Ba	42	HIS
45	BW	40	ASN
47	BI	51	GLN
47	BI	119	HIS
48	BR	19	HIS
48	BR	42	HIS
48	BR	59	HIS
48	BR	89	HIS
48	BR	96	GLN
36	BK	20	GLN
36	BK	31	ASN
49	BQ	58	GLN
49	BQ	67	HIS
49	BQ	75	HIS
49	BQ	131	GLN
49	BQ	136	HIS
50	BV	57	GLN
51	Bj	6	GLN
51	Bj	37	GLN
52	BD	44	GLN
52	BD	93	HIS
52	BD	139	GLN
52	BD	213	ASN
52	BD	214	HIS
52	BD	229	HIS
52	BD	235	HIS
53	BF	24	ASN
53	BF	74	HIS
53	BF	135	GLN

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Mol	Chain	Res	Type
53	BF	149	GLN
54	BZ	21	ASN
23	B6	25	HIS
55	BP	10	ASN
55	BP	23	ASN
55	BP	110	ASN
56	BM	87	GLN
56	BM	97	GLN
56	BM	154	HIS
56	BM	174	ASN
56	BM	189	ASN
57	BS	70	GLN
57	BS	97	ASN
58	Bd	35	HIS
58	Bd	70	HIS
59	BN	38	ASN
59	BN	56	GLN
59	BN	59	GLN
59	BN	70	ASN
59	BN	76	ASN
59	BN	83	HIS
59	BN	97	ASN
59	BN	130	GLN
59	BN	170	ASN
59	BN	179	GLN
61	Bc	17	GLN
61	Bc	18	HIS
61	Bc	28	ASN
62	BJ	47	HIS
62	BJ	102	ASN
65	H	20	ASN
65	H	52	GLN
65	H	180	HIS
65	H	355	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3016/3018 (99%)	444 (14%)	22 (0%)
2	2	1495/1512 (98%)	176 (11%)	2 (0%)
3	3	125/128 (97%)	12 (9%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4636/4658 (99%)	632 (13%)	24 (0%)

All (632) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	12	G
1	1	28	A
1	1	39	A
1	1	51	A
1	1	52	G
1	1	55	U
1	1	56	C
1	1	57	A
1	1	58	A
1	1	59	C
1	1	68	U
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	127	U
1	1	138	G
1	1	148	C
1	1	154	G

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Mol	Chain	Res	Type
1	1	160	C
1	1	178	A
1	1	185	A
1	1	188	A
1	1	189	G
1	1	199	G
1	1	205	G
1	1	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	268	A
1	1	269	U
1	1	270	A
1	1	272	G
1	1	273	C
1	1	275	C
1	1	285	A
1	1	300	A
1	1	303	A
1	1	319	G
1	1	320	A
1	1	326	A
1	1	332	A
1	1	333	A
1	1	339	G
1	1	352	G
1	1	370	G
1	1	393	C
1	1	416	G

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Mol	Chain	Res	Type
1	1	417	U
1	1	422	C
1	1	429	A
1	1	430	U
1	1	431	G
1	1	433	G
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	523	C
1	1	529	G
1	1	544	U
1	1	545	A
1	1	560	G
1	1	565	G
1	1	575	C
1	1	611	A
1	1	621	G
1	1	635	G
1	1	657	A
1	1	661	C
1	1	683	A
1	1	684	G
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

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Mol	Chain	Res	Type
1	1	749	G
1	1	769	C
1	1	781	A
1	1	785	G
1	1	792	A
1	1	809	A
1	1	849	C
1	1	851	U
1	1	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	979	C
1	1	983	C
1	1	993	U
1	1	998	U
1	1	1015	A
1	1	1026	G
1	1	1027	G
1	1	1033	A
1	1	1035	G
1	1	1036	G
1	1	1043	G
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	1101	A
1	1	1111	G
1	1	1118	A
1	1	1122	A

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Mol	Chain	Res	Type
1	1	1129	G
1	1	1131	G
1	1	1132	C
1	1	1133	A
1	1	1134	G
1	1	1136	G
1	1	1140	G
1	1	1141	A
1	1	1144	G
1	1	1148	C
1	1	1149	C
1	1	1159	U
1	1	1162	A
1	1	1164	C
1	1	1199	G
1	1	1200	G
1	1	1225	G
1	1	1231	A
1	1	1234	A
1	1	1235	A
1	1	1236	C
1	1	1240	G
1	1	1241	A
1	1	1259	A
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	1296	G
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	1362	G
1	1	1363	U
1	1	1364	C
1	1	1365	G
1	1	1366	A
1	1	1367	G
1	1	1369	U
1	1	1370	C
1	1	1371	C
1	1	1387	G
1	1	1389	C
1	1	1393	G
1	1	1397	A
1	1	1411	G
1	1	1433	G
1	1	1443	C
1	1	1477	G
1	1	1514	C
1	1	1520	G
1	1	1533	U
1	1	1560	A
1	1	1561	G
1	1	1577	A
1	1	1578	G
1	1	1580	C
1	1	1601	U
1	1	1630	G
1	1	1633	C
1	1	1639	A
1	1	1641	A
1	1	1645	A

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Mol	Chain	Res	Type
1	1	1657	A
1	1	1678	G
1	1	1685	A
1	1	1687	C
1	1	1692	G
1	1	1705	C
1	1	1714	G
1	1	1730	A
1	1	1731	U
1	1	1732	G
1	1	1748	A
1	1	1759	G
1	1	1761	G
1	1	1763	G
1	1	1782	G
1	1	1787	A
1	1	1796	U
1	1	1799	C
1	1	1805	C
1	1	1808	U
1	1	1809	A
1	1	1810	G
1	1	1840	A
1	1	1851	G
1	1	1856	U
1	1	1883	A
1	1	1890	C
1	1	1895	G
1	1	1896	C
1	1	1901	G
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

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Mol	Chain	Res	Type
1	1	1997	A
1	1	2020	G
1	1	2029	A
1	1	2038	U
1	1	2042	A
1	1	2056	C
1	1	2085	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	2179	A
1	1	2181	U
1	1	2196	U
1	1	2206	C
1	1	2208	U
1	1	2211	A
1	1	2212	U
1	1	2213	G
1	1	2232	U
1	1	2233	G
1	1	2234	U
1	1	2253	G
1	1	2267	G
1	1	2270	C
1	1	2271	G
1	1	2272	C
1	1	2273	A
1	1	2276	C
1	1	2292	G
1	1	2295	A
1	1	2300	A
1	1	2301	G
1	1	2303	C
1	1	2309	G
1	1	2310	G
1	1	2333	G

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Mol	Chain	Res	Type
1	1	2339	C
1	1	2340	G
1	1	2341	G
1	1	2342	C
1	1	2345	G
1	1	2347	G
1	1	2348	G
1	1	2350	G
1	1	2351	C
1	1	2352	G
1	1	2353	C
1	1	2354	A
1	1	2355	G
1	1	2356	C
1	1	2357	G
1	1	2358	U
1	1	2363	G
1	1	2366	A
1	1	2368	G
1	1	2370	G
1	1	2372	C
1	1	2373	G
1	1	2376	G
1	1	2379	C
1	1	2385	C
1	1	2386	C
1	1	2388	G
1	1	2397	G
1	1	2398	A
1	1	2403	U
1	1	2404	C
1	1	2405	C
1	1	2410	G
1	1	2411	A
1	1	2418	C
1	1	2420	A
1	1	2430	G
1	1	2431	C
1	1	2432	G
1	1	2438	A
1	1	2446	A
1	1	2453	G

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Mol	Chain	Res	Type
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	2543	U
1	1	2550	U
1	1	2551	A
1	1	2553	A
1	1	2556	G
1	1	2566	A
1	1	2574	C
1	1	2588	A
1	1	2592	G
1	1	2617	G
1	1	2619	C
1	1	2626	A
1	1	2636	C
1	1	2659	G
1	1	2664	A
1	1	2666	A
1	1	2673	C
1	1	2677	G
1	1	2680	A
1	1	2691	G
1	1	2706	C
1	1	2710	A
1	1	2723	C
1	1	2730	C
1	1	2733	5MC
1	1	2734	G
1	1	2735	C
1	1	2750	A

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Mol	Chain	Res	Type
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	2853	G
1	1	2861	U
1	1	2877	A
1	1	2878	G
1	1	2885	U
1	1	2896	G
1	1	2906	G
1	1	2922	U
1	1	2945	G
1	1	2957	C
1	1	2978	A
1	1	2981	G
1	1	2987	A
1	1	2995	A
1	1	2996	G
1	1	3006	A
1	1	3021	U
1	1	3022	C
2	2	45	U
2	2	52	C
2	2	54	G
2	2	57	U
2	2	59	A
2	2	66	C
2	2	72	A
2	2	76	G
2	2	86	U
2	2	87	C
2	2	88	U
2	2	89	G
2	2	115	A

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Mol	Chain	Res	Type
2	2	116	A
2	2	117	C
2	2	126	A
2	2	128	C
2	2	154	G
2	2	171	C
2	2	189	A
2	2	196	G
2	2	211	A
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	275	G
2	2	276	C
2	2	290	G
2	2	298	C
2	2	315	A
2	2	337	C
2	2	338	A
2	2	353	A
2	2	354	C
2	2	358	G
2	2	360	G
2	2	361	C
2	2	363	G
2	2	371	G
2	2	376	C
2	2	381	C
2	2	406	A
2	2	415	G
2	2	424	C
2	2	425	U
2	2	426	G
2	2	430	C
2	2	436	U
2	2	460	A

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Mol	Chain	Res	Type
2	2	477	G
2	2	484	G
2	2	487	G
2	2	497	U
2	2	498	A
2	2	513	A
2	2	530	U
2	2	533	G
2	2	539	A
2	2	542	C
2	2	562	A
2	2	571	C
2	2	600	G
2	2	609	A
2	2	620	U
2	2	632	A
2	2	642	U
2	2	654	A
2	2	689	G
2	2	690	U
2	2	691	G
2	2	715	G
2	2	722	G
2	2	744	A
2	2	760	U
2	2	761	A
2	2	782	A
2	2	784	G
2	2	786	A
2	2	788	G
2	2	814	A
2	2	861	G
2	2	885	A
2	2	893	G
2	2	897	G
2	2	905	C
2	2	906	U
2	2	932	U
2	2	941	A
2	2	943	G
2	2	946	G
2	2	947	G

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Mol	Chain	Res	Type
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	1002	C
2	2	1003	G
2	2	1004	C
2	2	1005	G
2	2	1008	G
2	2	1030	U
2	2	1059	G
2	2	1060	U
2	2	1066	A
2	2	1105	G
2	2	1106	C
2	2	1107	U
2	2	1108	C
2	2	1131	A
2	2	1133	U
2	2	1148	G
2	2	1155	G
2	2	1157	G
2	2	1158	G
2	2	1170	A
2	2	1171	G
2	2	1186	A
2	2	1187	A
2	2	1199	A
2	2	1201	A
2	2	1212	A
2	2	1215	G
2	2	1222	A
2	2	1253	A

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Mol	Chain	Res	Type
2	2	1254	A
2	2	1261	A
2	2	1274	G
2	2	1276	U
2	2	1279	G
2	2	1294	C
2	2	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	1395	G
2	2	1397	G
2	2	1398	G
2	2	1400	C
2	2	1421	U
2	2	1424	G
2	2	1427	G
2	2	1454	G
2	2	1456	G
2	2	1461	A
2	2	1466	G
2	2	1471	A
2	2	1472	A
2	2	1475	U
2	2	1486	G
2	2	1488	MA6
2	2	1498	5MC
2	2	1499	G
2	2	1503	A
2	2	1504	C
2	2	1505	5MC
2	2	1506	U
2	2	1510	C
3	3	5	C
3	3	9	G
3	3	25	C
3	3	30	C
3	3	53	A

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Mol	Chain	Res	Type
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	115	G

All (24) 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	870	A
1	1	992	C
1	1	1035	G
1	1	1303	A
1	1	1363	U
1	1	1364	C
1	1	1731	U
1	1	2341	G
1	1	2367	G
1	1	2455	A
1	1	2733	5MC
1	1	2986	U
1	1	3021	U
2	2	653	U
2	2	1106	C

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	$\#\|Z\| > 2$
1	4AC	1	2545	1	21,24,25	1.03	2 (9%)	29,34,37	1.33	4 (13%)
2	4AC	2	751	2	21,24,25	1.03	2 (9%)	29,34,37	1.28	4 (13%)
1	OMG	1	789	1	23,26,27	1.25	3 (13%)	33,38,41	1.97	6 (18%)
2	4AC	2	839	2	21,24,25	1.03	2 (9%)	29,34,37	1.31	4 (13%)
1	4AC	1	533	1	21,24,25	1.01	2 (9%)	29,34,37	1.32	4 (13%)
1	A2M	1	2173	1	22,25,26	1.43	4 (18%)	31,36,39	2.07	8 (25%)
2	OMG	2	467	2	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
2	5MC	2	875	2	18,22,23	0.93	2 (11%)	26,32,35	1.17	3 (11%)
1	OMG	1	2138	1	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
1	OMU	1	2784	1	19,22,23	1.23	3 (15%)	26,31,34	1.74	5 (19%)
1	4AC	1	1293	1	21,24,25	1.03	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	1	1873	1	21,24,25	1.07	2 (9%)	29,34,37	1.32	4 (13%)
1	OMG	1	2678	1	23,26,27	1.21	3 (13%)	33,38,41	1.93	7 (21%)
1	4AC	1	2925	1	21,24,25	1.04	2 (9%)	29,34,37	1.33	4 (13%)
2	4AC	2	590	2	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
2	5MC	2	1498	2	18,22,23	0.92	2 (11%)	26,32,35	1.25	4 (15%)
1	5MC	1	2162	1	18,22,23	0.93	2 (11%)	26,32,35	1.14	3 (11%)
1	4AC	1	1885	1	21,24,25	1.04	2 (9%)	29,34,37	1.23	4 (13%)
1	LHH	1	616	1	22,25,26	0.31	0	29,35,38	0.46	0
2	4AC	2	626	2	21,24,25	1.02	2 (9%)	29,34,37	1.37	4 (13%)
2	4AC	2	319	2	21,24,25	1.03	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	1780	1	21,24,25	1.04	2 (9%)	29,34,37	1.60	4 (13%)
1	5MC	1	2093	1	18,22,23	0.94	2 (11%)	26,32,35	1.11	2 (7%)
1	4AC	1	1554	1	21,24,25	1.02	2 (9%)	29,34,37	1.30	4 (13%)
1	4AC	1	229	1	21,24,25	1.06	2 (9%)	29,34,37	1.30	3 (10%)
1	4AC	1	314	1	21,24,25	1.05	2 (9%)	29,34,37	1.26	4 (13%)
1	4AC	1	2001	1	21,24,25	1.07	2 (9%)	29,34,37	1.50	4 (13%)
1	4AC	1	2642	1	21,24,25	1.02	2 (9%)	29,34,37	1.30	4 (13%)
2	OMU	2	1380	2	19,22,23	1.30	3 (15%)	26,31,34	1.75	4 (15%)
1	5MC	1	2198	1	18,22,23	0.93	2 (11%)	26,32,35	1.11	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	4AC	1	2992	1	21,24,25	1.04	2 (9%)	29,34,37	0.88	1 (3%)
2	4AC	2	546	2	21,24,25	1.01	2 (9%)	29,34,37	1.31	4 (13%)
2	4AC	2	1239	2	21,24,25	1.02	2 (9%)	29,34,37	1.37	4 (13%)
1	OMG	1	2144	1	23,26,27	1.22	3 (13%)	33,38,41	1.94	6 (18%)
2	OMC	2	846	2	19,22,23	0.81	0	26,31,34	0.80	0
2	4AC	2	851	2	21,24,25	1.06	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	1065	1	21,24,25	1.03	2 (9%)	29,34,37	1.34	4 (13%)
1	5MC	1	2183	1	18,22,23	0.94	2 (11%)	26,32,35	1.12	2 (7%)
1	OMG	1	923	1,66	23,26,27	1.21	3 (13%)	33,38,41	1.98	7 (21%)
1	5MC	1	2163	1	18,22,23	0.93	2 (11%)	26,32,35	1.11	2 (7%)
2	4AC	2	1233	2	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
2	OMG	2	657	2	23,26,27	1.24	3 (13%)	33,38,41	1.97	6 (18%)
2	OMU	2	1177	2	19,22,23	1.24	3 (15%)	26,31,34	1.71	4 (15%)
2	UR3	2	1467	2	19,22,23	0.94	0	26,32,35	1.45	2 (7%)
1	4AC	1	1594	1,66	21,24,25	1.03	2 (9%)	29,34,37	1.32	4 (13%)
2	5MC	2	535	2	18,22,23	0.93	2 (11%)	26,32,35	1.14	2 (7%)
1	4AC	1	1938	1	21,24,25	1.06	2 (9%)	29,34,37	1.31	4 (13%)
2	LHH	2	1041	2	22,25,26	0.31	0	29,35,38	0.49	0
2	OMG	2	680	2	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
1	4AC	1	3004	1	21,24,25	1.05	2 (9%)	29,34,37	1.27	4 (13%)
2	4AC	2	394	2	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
2	4AC	2	1147	2	21,24,25	1.02	2 (9%)	29,34,37	1.44	4 (13%)
1	4AC	1	2960	1	21,24,25	1.03	2 (9%)	29,34,37	1.30	4 (13%)
1	4AC	1	2495	1	21,24,25	1.05	2 (9%)	29,34,37	1.29	4 (13%)
2	LHH	2	250	2	22,25,26	0.31	0	29,35,38	0.49	0
1	4AC	1	1222	1,66	21,24,25	1.04	2 (9%)	29,34,37	1.26	4 (13%)
2	5MC	2	1505	2	18,22,23	0.94	2 (11%)	26,32,35	1.59	5 (19%)
1	4AC	1	2570	1	21,24,25	1.01	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	829	1	21,24,25	1.04	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	161	1	21,24,25	1.04	2 (9%)	29,34,37	1.30	4 (13%)
1	4AC	1	1617	1	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
1	OMC	1	1948	1	19,22,23	0.81	0	26,31,34	0.77	0
2	OMU	2	787	2	19,22,23	1.25	3 (15%)	26,31,34	1.85	5 (19%)
1	4AC	1	1068	1	21,24,25	1.04	2 (9%)	29,34,37	1.33	4 (13%)
2	5MC	2	1025	2	18,22,23	0.95	2 (11%)	26,32,35	1.15	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	4AC	1	1755	1	21,24,25	1.04	2 (9%)	29,34,37	1.67	5 (17%)
1	4AC	1	1550	1	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	2062	1	21,24,25	1.03	2 (9%)	29,34,37	1.27	4 (13%)
1	4AC	1	91	1	21,24,25	1.01	2 (9%)	29,34,37	1.40	4 (13%)
2	OMG	2	873	2	23,26,27	1.22	3 (13%)	33,38,41	1.92	6 (18%)
1	4AC	1	1048	1	21,24,25	1.06	2 (9%)	29,34,37	1.33	4 (13%)
2	4AC	2	17	2	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
2	OMU	2	64	2	19,22,23	1.24	3 (15%)	26,31,34	1.70	5 (19%)
2	4AC	2	479	2	21,24,25	1.01	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	243	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
2	OMG	2	519	2	23,26,27	1.21	3 (13%)	33,38,41	1.98	6 (18%)
1	4AC	1	1460	1	21,24,25	1.03	2 (9%)	29,34,37	1.33	4 (13%)
2	4AC	2	1184	2	21,24,25	1.03	2 (9%)	29,34,37	1.30	4 (13%)
2	OMU	2	774	2	19,22,23	1.23	3 (15%)	26,31,34	1.71	5 (19%)
2	4AC	2	703	2	21,24,25	1.01	2 (9%)	29,34,37	1.58	4 (13%)
2	OMU	2	830	2	19,22,23	1.27	3 (15%)	26,31,34	1.72	5 (19%)
2	4AC	2	303	2	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	2937	1,66	21,24,25	1.02	2 (9%)	29,34,37	1.52	4 (13%)
2	4AC	2	379	2	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	1	835	1	21,24,25	1.05	2 (9%)	29,34,37	1.30	4 (13%)
2	OMC	2	1376	2	19,22,23	0.81	0	26,31,34	0.77	0
1	4AC	1	1667	1	21,24,25	1.03	2 (9%)	29,34,37	1.32	4 (13%)
1	4AC	1	2966	1	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	2548	1	21,24,25	1.02	2 (9%)	29,34,37	1.31	4 (13%)
1	4AC	1	2585	1	21,24,25	1.08	2 (9%)	29,34,37	1.76	6 (20%)
2	B8H	2	938	2	19,22,23	0.57	0	22,32,35	0.62	0
1	4AC	1	2136	1	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	1934	1	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	2608	1	21,24,25	1.07	2 (9%)	29,34,37	1.80	6 (20%)
1	4AC	1	1878	1	21,24,25	1.04	2 (9%)	29,34,37	1.50	4 (13%)
1	4AC	1	1621	1	21,24,25	1.04	2 (9%)	29,34,37	1.24	4 (13%)
2	4AC	2	511	2	21,24,25	1.04	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	1	694	1	21,24,25	1.01	2 (9%)	29,34,37	1.27	4 (13%)
2	4AC	2	286	2	21,24,25	1.02	2 (9%)	29,34,37	1.31	4 (13%)
2	4AC	2	718	2	21,24,25	1.02	2 (9%)	29,34,37	1.28	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	4AC	1	451	1	21,24,25	1.02	2 (9%)	29,34,37	1.32	4 (13%)
2	5MC	2	1202	2	18,22,23	0.96	2 (11%)	26,32,35	1.28	4 (15%)
1	4AC	1	1695	1	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
2	MA6	2	1487	2	23,26,27	1.45	5 (21%)	34,38,41	2.11	10 (29%)
1	4AC	1	641	1	21,24,25	1.03	2 (9%)	29,34,37	1.32	4 (13%)
1	4AC	1	1962	1	21,24,25	1.03	2 (9%)	29,34,37	1.36	4 (13%)
2	5MC	2	1496	2	18,22,23	0.92	2 (11%)	26,32,35	1.13	3 (11%)
1	4AC	1	2865	1	21,24,25	1.03	2 (9%)	29,34,37	1.31	4 (13%)
1	4AC	1	2908	1	21,24,25	1.04	2 (9%)	29,34,37	1.30	4 (13%)
1	4AC	1	1662	1	21,24,25	1.01	2 (9%)	29,34,37	1.37	4 (13%)
2	OMU	2	20	2	19,22,23	1.27	3 (15%)	26,31,34	1.83	5 (19%)
2	4AC	2	848	2	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
2	4AC	2	53	2	21,24,25	1.02	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	802	1	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	1765	1	21,24,25	1.04	2 (9%)	29,34,37	1.32	4 (13%)
2	OMC	2	1040	2	19,22,23	0.83	0	26,31,34	0.90	1 (3%)
1	4AC	1	22	1	21,24,25	1.04	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	1557	1	21,24,25	1.02	2 (9%)	29,34,37	1.27	4 (13%)
1	4AC	1	136	1	21,24,25	1.03	2 (9%)	29,34,37	1.30	4 (13%)
2	4AC	2	636	2	21,24,25	1.03	2 (9%)	29,34,37	1.47	4 (13%)
2	OMG	2	934	2	23,26,27	1.20	3 (13%)	33,38,41	1.99	6 (18%)
1	4AC	1	341	1	21,24,25	1.03	2 (9%)	29,34,37	1.32	4 (13%)
1	4AC	1	2718	1	21,24,25	1.03	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	211	1	21,24,25	1.03	2 (9%)	29,34,37	1.32	4 (13%)
3	4AC	3	32	3	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
2	6MZ	2	1469	2,66	22,25,26	1.47	4 (18%)	30,36,39	2.20	9 (30%)
1	OMG	1	2147	1	23,26,27	1.21	3 (13%)	33,38,41	1.91	6 (18%)
1	4AC	1	458	1	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
2	A2M	2	373	2	22,25,26	1.45	4 (18%)	31,36,39	2.06	8 (25%)
1	4AC	1	2249	1	21,24,25	1.06	2 (9%)	29,34,37	1.34	4 (13%)
2	4AC	2	731	2	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	981	1	21,24,25	1.04	2 (9%)	29,34,37	1.23	4 (13%)
2	4AC	2	1479	2	21,24,25	1.01	2 (9%)	29,34,37	1.30	4 (13%)
1	4AC	1	2027	1	21,24,25	1.04	2 (9%)	29,34,37	1.30	4 (13%)
1	4AC	1	1243	1	21,24,25	1.05	2 (9%)	29,34,37	1.29	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	4AC	1	2329	1	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
2	OMC	2	129	2	19,22,23	0.83	0	26,31,34	0.84	0
2	OMC	2	773	2	19,22,23	0.82	0	26,31,34	0.77	0
1	4AC	1	60	1	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
2	4AC	2	828	2	21,24,25	1.02	2 (9%)	29,34,37	1.31	4 (13%)
1	OMC	1	615	1	19,22,23	0.80	0	26,31,34	0.76	0
1	4AC	1	2083	1	21,24,25	1.09	2 (9%)	29,34,37	1.25	3 (10%)
2	5MC	2	1374	2	18,22,23	0.93	2 (11%)	26,32,35	1.11	2 (7%)
1	A2M	1	1055	1	22,25,26	1.44	4 (18%)	31,36,39	2.10	8 (25%)
2	4AC	2	868	2	21,24,25	1.03	2 (9%)	29,34,37	1.28	4 (13%)
1	4AC	1	357	1	21,24,25	1.01	2 (9%)	29,34,37	1.29	5 (17%)
2	OMG	2	913	2	23,26,27	1.22	3 (13%)	33,38,41	1.95	6 (18%)
2	4AC	2	1028	2	21,24,25	1.02	2 (9%)	29,34,37	1.32	4 (13%)
1	5MC	1	2733	1	18,22,23	0.97	2 (11%)	26,32,35	1.25	4 (15%)
1	4AC	1	2287	1	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
2	5MC	2	693	2	18,22,23	0.92	2 (11%)	26,32,35	1.15	3 (11%)
1	5MC	1	2203	1	18,22,23	0.93	2 (11%)	26,32,35	1.11	2 (7%)
1	4AC	1	922	1	21,24,25	1.06	2 (9%)	29,34,37	1.39	4 (13%)
1	4AC	1	1867	1	21,24,25	1.03	2 (9%)	29,34,37	1.34	4 (13%)
1	OMG	1	328	1	23,26,27	1.22	3 (13%)	33,38,41	1.99	6 (18%)
2	OMG	2	1069	2	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
2	OMG	2	471	2	23,26,27	1.23	3 (13%)	33,38,41	1.94	6 (18%)
2	4AC	2	957	2	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
2	MA6	2	1488	2	23,26,27	1.44	5 (21%)	34,38,41	2.13	10 (29%)

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
1	4AC	1	2545	1	-	0/11/29/30	0/2/2/2
2	4AC	2	751	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	839	2	-	0/11/29/30	0/2/2/2
1	4AC	1	533	1	-	0/11/29/30	0/2/2/2
1	A2M	1	2173	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	2	467	2	-	0/9/27/28	0/3/3/3
2	5MC	2	875	2	-	0/7/25/26	0/2/2/2
1	OMG	1	2138	1	-	0/9/27/28	0/3/3/3
1	OMU	1	2784	1	-	0/9/27/28	0/2/2/2
1	4AC	1	1293	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1873	1	-	0/11/29/30	0/2/2/2
1	OMG	1	2678	1	-	0/9/27/28	0/3/3/3
1	4AC	1	2925	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	1498	2	-	4/7/25/26	0/2/2/2
1	5MC	1	2162	1	-	0/7/25/26	0/2/2/2
1	4AC	1	1885	1	-	0/11/29/30	0/2/2/2
1	LHH	1	616	1	-	0/13/31/32	0/2/2/2
2	4AC	2	626	2	-	0/11/29/30	0/2/2/2
2	4AC	2	319	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1780	1	-	0/11/29/30	0/2/2/2
1	5MC	1	2093	1	-	0/7/25/26	0/2/2/2
1	4AC	1	1554	1	-	0/11/29/30	0/2/2/2
1	4AC	1	229	1	-	0/11/29/30	0/2/2/2
1	4AC	1	314	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2001	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2642	1	-	0/11/29/30	0/2/2/2
2	OMU	2	1380	2	-	0/9/27/28	0/2/2/2
1	5MC	1	2198	1	-	0/7/25/26	0/2/2/2
1	4AC	1	2992	1	-	3/11/29/30	0/2/2/2
2	4AC	2	546	2	-	0/11/29/30	0/2/2/2
2	4AC	2	1239	2	-	0/11/29/30	0/2/2/2
1	OMG	1	2144	1	-	1/9/27/28	0/3/3/3
2	OMC	2	846	2	-	0/9/27/28	0/2/2/2
2	4AC	2	851	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1065	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	923	1,66	-	0/9/27/28	0/3/3/3
1	5MC	1	2163	1	-	0/7/25/26	0/2/2/2
2	4AC	2	1233	2	-	0/11/29/30	0/2/2/2
2	OMG	2	657	2	-	0/9/27/28	0/3/3/3
2	OMU	2	1177	2	-	1/9/27/28	0/2/2/2
2	UR3	2	1467	2	-	0/7/25/26	0/2/2/2
1	4AC	1	1594	1,66	-	0/11/29/30	0/2/2/2
2	5MC	2	535	2	-	0/7/25/26	0/2/2/2
1	4AC	1	1938	1	-	0/11/29/30	0/2/2/2
2	LHH	2	1041	2	-	0/13/31/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	2	680	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	394	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	2960	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2495	1	-	0/11/29/30	0/2/2/2
2	LHH	2	250	2	-	0/13/31/32	0/2/2/2
1	4AC	1	1222	1,66	-	0/11/29/30	0/2/2/2
2	5MC	2	1505	2	-	4/7/25/26	0/2/2/2
1	4AC	1	2570	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	161	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1617	1	-	0/11/29/30	0/2/2/2
1	OMC	1	1948	1	-	0/9/27/28	0/2/2/2
2	OMU	2	787	2	-	2/9/27/28	0/2/2/2
1	4AC	1	1068	1	-	0/11/29/30	0/2/2/2
2	5MC	2	1025	2	-	0/7/25/26	0/2/2/2
1	4AC	1	1755	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1550	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2062	1	-	0/11/29/30	0/2/2/2
1	4AC	1	91	1	-	0/11/29/30	0/2/2/2
2	OMG	2	873	2	-	1/9/27/28	0/3/3/3
1	4AC	1	1048	1	-	0/11/29/30	0/2/2/2
2	4AC	2	17	2	-	0/11/29/30	0/2/2/2
2	OMU	2	64	2	-	0/9/27/28	0/2/2/2
2	4AC	2	479	2	-	0/11/29/30	0/2/2/2
1	4AC	1	243	1	-	0/11/29/30	0/2/2/2
2	OMG	2	519	2	-	0/9/27/28	0/3/3/3
1	4AC	1	1460	1	-	0/11/29/30	0/2/2/2
2	4AC	2	1184	2	-	0/11/29/30	0/2/2/2
2	OMU	2	774	2	-	0/9/27/28	0/2/2/2
2	4AC	2	703	2	-	0/11/29/30	0/2/2/2
2	OMU	2	830	2	-	0/9/27/28	0/2/2/2
2	4AC	2	303	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2937	1,66	-	1/11/29/30	0/2/2/2
2	4AC	2	379	2	-	0/11/29/30	0/2/2/2
1	4AC	1	835	1	-	0/11/29/30	0/2/2/2
2	OMC	2	1376	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	2966	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2548	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2585	1	-	3/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B8H	2	938	2	-	0/7/25/26	0/2/2/2
1	4AC	1	2136	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1934	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2608	1	-	3/11/29/30	0/2/2/2
1	4AC	1	1878	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1621	1	-	0/11/29/30	0/2/2/2
2	4AC	2	511	2	-	0/11/29/30	0/2/2/2
1	4AC	1	694	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	718	2	-	0/11/29/30	0/2/2/2
1	4AC	1	451	1	-	0/11/29/30	0/2/2/2
2	5MC	2	1202	2	-	2/7/25/26	0/2/2/2
1	4AC	1	1695	1	-	0/11/29/30	0/2/2/2
2	MA6	2	1487	2	-	0/11/29/30	0/3/3/3
1	4AC	1	641	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1962	1	-	0/11/29/30	0/2/2/2
2	5MC	2	1496	2	-	0/7/25/26	0/2/2/2
1	4AC	1	2865	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2908	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1662	1	-	0/11/29/30	0/2/2/2
2	OMU	2	20	2	-	5/9/27/28	0/2/2/2
2	4AC	2	848	2	-	0/11/29/30	0/2/2/2
2	4AC	2	53	2	-	0/11/29/30	0/2/2/2
1	4AC	1	802	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1765	1	-	0/11/29/30	0/2/2/2
2	OMC	2	1040	2	-	0/9/27/28	0/2/2/2
1	4AC	1	22	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1557	1	-	0/11/29/30	0/2/2/2
1	4AC	1	136	1	-	0/11/29/30	0/2/2/2
2	4AC	2	636	2	-	0/11/29/30	0/2/2/2
2	OMG	2	934	2	-	2/9/27/28	0/3/3/3
1	4AC	1	341	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2718	1	-	0/11/29/30	0/2/2/2
1	4AC	1	211	1	-	0/11/29/30	0/2/2/2
3	4AC	3	32	3	-	0/11/29/30	0/2/2/2
2	6MZ	2	1469	2,66	-	0/9/27/28	0/3/3/3
1	OMG	1	2147	1	-	3/9/27/28	0/3/3/3
1	4AC	1	458	1	-	0/11/29/30	0/2/2/2
2	A2M	2	373	2	-	0/9/27/28	0/3/3/3
1	4AC	1	2249	1	-	0/11/29/30	0/2/2/2
2	4AC	2	731	2	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	1	981	1	-	0/11/29/30	0/2/2/2
2	4AC	2	1479	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2027	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1243	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2329	1	-	0/11/29/30	0/2/2/2
2	OMC	2	129	2	-	0/9/27/28	0/2/2/2
2	OMC	2	773	2	-	0/9/27/28	0/2/2/2
1	4AC	1	60	1	-	0/11/29/30	0/2/2/2
2	4AC	2	828	2	-	0/11/29/30	0/2/2/2
1	OMC	1	615	1	-	0/9/27/28	0/2/2/2
1	4AC	1	2083	1	-	0/11/29/30	0/2/2/2
2	5MC	2	1374	2	-	0/7/25/26	0/2/2/2
1	A2M	1	1055	1	-	0/9/27/28	0/3/3/3
2	4AC	2	868	2	-	0/11/29/30	0/2/2/2
1	4AC	1	357	1	-	0/11/29/30	0/2/2/2
2	OMG	2	913	2	-	1/9/27/28	0/3/3/3
2	4AC	2	1028	2	-	0/11/29/30	0/2/2/2
1	5MC	1	2733	1	-	4/7/25/26	0/2/2/2
1	4AC	1	2287	1	-	0/11/29/30	0/2/2/2
2	5MC	2	693	2	-	0/7/25/26	0/2/2/2
1	5MC	1	2203	1	-	0/7/25/26	0/2/2/2
1	4AC	1	922	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1867	1	-	0/11/29/30	0/2/2/2
1	OMG	1	328	1	-	0/9/27/28	0/3/3/3
2	OMG	2	1069	2	-	2/9/27/28	0/3/3/3
2	OMG	2	471	2	-	0/9/27/28	0/3/3/3
2	4AC	2	957	2	-	0/11/29/30	0/2/2/2
2	MA6	2	1488	2	-	2/11/29/30	0/3/3/3

All (332) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1469	6MZ	C5-C4	4.50	1.47	1.39
2	2	1487	MA6	C5-C4	4.30	1.47	1.39
2	2	373	A2M	C5-C4	4.28	1.47	1.39
1	1	2173	A2M	C5-C4	4.28	1.47	1.39
2	2	1488	MA6	C5-C4	4.23	1.46	1.39
1	1	1055	A2M	C5-C4	4.20	1.46	1.39
1	1	2992	4AC	C5-C4	3.06	1.47	1.40
2	2	657	OMG	C5-C4	3.03	1.47	1.38
2	2	680	OMG	C5-C4	2.98	1.47	1.38
1	1	2083	4AC	C5-C4	2.97	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1873	4AC	C5-C4	2.96	1.47	1.40
1	1	229	4AC	C5-C4	2.96	1.47	1.40
2	2	1184	4AC	C5-C4	2.95	1.47	1.40
2	2	751	4AC	C5-C4	2.95	1.47	1.40
1	1	2147	OMG	C5-C4	2.95	1.46	1.38
1	1	1243	4AC	C5-C4	2.94	1.47	1.40
2	2	471	OMG	C5-C4	2.93	1.46	1.38
1	1	2642	4AC	C5-C4	2.93	1.47	1.40
1	1	314	4AC	C5-C4	2.92	1.47	1.40
1	1	1938	4AC	C5-C4	2.92	1.47	1.40
2	2	1380	OMU	C4-N3	-2.92	1.33	1.38
1	1	2545	4AC	C5-C4	2.92	1.47	1.40
2	2	1239	4AC	C5-C4	2.92	1.47	1.40
1	1	1695	4AC	C5-C4	2.92	1.47	1.40
1	1	211	4AC	C5-C4	2.91	1.47	1.40
2	2	511	4AC	C5-C4	2.91	1.47	1.40
2	2	851	4AC	C5-C4	2.91	1.47	1.40
1	1	1765	4AC	C5-C4	2.91	1.47	1.40
1	1	2960	4AC	C5-C4	2.90	1.47	1.40
3	3	32	4AC	C5-C4	2.90	1.47	1.40
1	1	2548	4AC	C5-C4	2.89	1.47	1.40
1	1	1867	4AC	C5-C4	2.89	1.47	1.40
1	1	835	4AC	C5-C4	2.89	1.47	1.40
1	1	641	4AC	C5-C4	2.89	1.47	1.40
2	2	590	4AC	C5-C4	2.89	1.47	1.40
2	2	479	4AC	C5-C4	2.88	1.47	1.40
1	1	1962	4AC	C5-C4	2.88	1.47	1.40
2	2	1069	OMG	C5-C4	2.88	1.46	1.38
1	1	1621	4AC	C5-C4	2.88	1.47	1.40
1	1	2138	OMG	C5-C4	2.88	1.46	1.38
2	2	934	OMG	C5-C4	2.87	1.46	1.38
2	2	20	OMU	C4-N3	-2.87	1.33	1.38
1	1	2249	4AC	C5-C4	2.87	1.47	1.40
2	2	787	OMU	C4-N3	-2.87	1.33	1.38
2	2	828	4AC	C5-C4	2.87	1.47	1.40
1	1	2908	4AC	C5-C4	2.87	1.47	1.40
1	1	2495	4AC	C5-C4	2.87	1.47	1.40
1	1	136	4AC	C5-C4	2.87	1.47	1.40
1	1	1222	4AC	C5-C4	2.87	1.47	1.40
1	1	451	4AC	C5-C4	2.87	1.47	1.40
1	1	3004	4AC	C5-C4	2.87	1.47	1.40
2	2	839	4AC	C5-C4	2.87	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2570	4AC	C5-C4	2.86	1.47	1.40
1	1	60	4AC	C5-C4	2.86	1.47	1.40
1	1	1667	4AC	C5-C4	2.86	1.47	1.40
1	1	22	4AC	C5-C4	2.86	1.47	1.40
2	2	1147	4AC	C5-C4	2.86	1.47	1.40
1	1	2144	OMG	C5-C4	2.86	1.46	1.38
2	2	379	4AC	C5-C4	2.86	1.47	1.40
2	2	868	4AC	C5-C4	2.86	1.47	1.40
1	1	829	4AC	C5-C4	2.86	1.46	1.40
1	1	922	4AC	C5-C4	2.86	1.46	1.40
1	1	2925	4AC	C5-C4	2.86	1.46	1.40
2	2	636	4AC	C5-C4	2.85	1.46	1.40
1	1	2027	4AC	C5-C4	2.85	1.46	1.40
2	2	913	OMG	C5-C4	2.85	1.46	1.38
2	2	286	4AC	C5-C4	2.85	1.46	1.40
1	1	981	4AC	C5-C4	2.84	1.46	1.40
1	1	1065	4AC	C5-C4	2.84	1.46	1.40
1	1	2136	4AC	C5-C4	2.84	1.46	1.40
2	2	17	4AC	C5-C4	2.84	1.46	1.40
2	2	394	4AC	C5-C4	2.84	1.46	1.40
2	2	957	4AC	C5-C4	2.84	1.46	1.40
1	1	458	4AC	C5-C4	2.84	1.46	1.40
1	1	243	4AC	C5-C4	2.84	1.46	1.40
2	2	626	4AC	C5-C4	2.84	1.46	1.40
2	2	718	4AC	C5-C4	2.84	1.46	1.40
2	2	1233	4AC	C5-C4	2.84	1.46	1.40
1	1	2733	5MC	C6-C5	2.84	1.39	1.34
1	1	1068	4AC	C5-C4	2.84	1.46	1.40
1	1	1293	4AC	C5-C4	2.84	1.46	1.40
1	1	1048	4AC	C5-C4	2.84	1.46	1.40
2	2	1028	4AC	C5-C4	2.83	1.46	1.40
2	2	467	OMG	C5-C4	2.83	1.46	1.38
2	2	873	OMG	C5-C4	2.83	1.46	1.38
1	1	161	4AC	C5-C4	2.82	1.46	1.40
1	1	341	4AC	C5-C4	2.82	1.46	1.40
1	1	1554	4AC	C5-C4	2.82	1.46	1.40
1	1	328	OMG	C5-C4	2.82	1.46	1.38
2	2	53	4AC	C5-C4	2.82	1.46	1.40
1	1	2144	OMG	C6-N1	-2.82	1.33	1.38
1	1	2865	4AC	C5-C4	2.82	1.46	1.40
2	2	546	4AC	C5-C4	2.82	1.46	1.40
1	1	2585	4AC	C4-N3	-2.82	1.27	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	533	4AC	C5-C4	2.81	1.46	1.40
1	1	2678	OMG	C5-C4	2.81	1.46	1.38
2	2	519	OMG	C5-C4	2.81	1.46	1.38
1	1	2966	4AC	C5-C4	2.81	1.46	1.40
1	1	357	4AC	C5-C4	2.81	1.46	1.40
1	1	1617	4AC	C5-C4	2.81	1.46	1.40
2	2	319	4AC	C5-C4	2.80	1.46	1.40
1	1	694	4AC	C5-C4	2.80	1.46	1.40
1	1	1460	4AC	C5-C4	2.80	1.46	1.40
2	2	731	4AC	C5-C4	2.80	1.46	1.40
1	1	2784	OMU	C4-N3	-2.80	1.33	1.38
2	2	848	4AC	C5-C4	2.79	1.46	1.40
1	1	2718	4AC	C5-C4	2.79	1.46	1.40
1	1	1594	4AC	C5-C4	2.79	1.46	1.40
2	2	303	4AC	C5-C4	2.79	1.46	1.40
1	1	2062	4AC	C5-C4	2.78	1.46	1.40
2	2	1488	MA6	C5-C6	2.78	1.48	1.41
1	1	923	OMG	C5-C4	2.78	1.46	1.38
1	1	1885	4AC	C5-C4	2.78	1.46	1.40
1	1	923	OMG	C6-N1	-2.78	1.33	1.38
1	1	1550	4AC	C5-C4	2.78	1.46	1.40
2	2	471	OMG	C6-N1	-2.78	1.33	1.38
2	2	873	OMG	C6-N1	-2.78	1.33	1.38
1	1	2329	4AC	C5-C4	2.78	1.46	1.40
1	1	802	4AC	C5-C4	2.77	1.46	1.40
2	2	830	OMU	C4-N3	-2.77	1.33	1.38
2	2	657	OMG	C6-N1	-2.77	1.33	1.38
1	1	789	OMG	C5-C4	2.77	1.46	1.38
1	1	2937	4AC	C5-C4	2.77	1.46	1.40
2	2	1479	4AC	C5-C4	2.74	1.46	1.40
1	1	328	OMG	C6-N1	-2.73	1.33	1.38
1	1	91	4AC	C5-C4	2.73	1.46	1.40
1	1	1557	4AC	C5-C4	2.73	1.46	1.40
2	2	1487	MA6	C5-C6	2.73	1.48	1.41
1	1	1934	4AC	C5-C4	2.73	1.46	1.40
1	1	2678	OMG	C6-N1	-2.71	1.33	1.38
1	1	2138	OMG	C6-N1	-2.71	1.33	1.38
2	2	1177	OMU	C4-N3	-2.71	1.33	1.38
1	1	1662	4AC	C5-C4	2.70	1.46	1.40
1	1	2083	4AC	C4-N3	-2.70	1.28	1.32
1	1	789	OMG	C6-N1	-2.70	1.33	1.38
1	1	229	4AC	C4-N3	-2.69	1.28	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	519	OMG	C6-N1	-2.69	1.33	1.38
1	1	2287	4AC	C5-C4	2.68	1.46	1.40
2	2	913	OMG	C6-N1	-2.68	1.33	1.38
2	2	1469	6MZ	C5-C6	2.67	1.48	1.41
2	2	934	OMG	C6-N1	-2.67	1.33	1.38
1	1	1878	4AC	C5-C4	2.67	1.46	1.40
2	2	774	OMU	C4-N3	-2.67	1.33	1.38
1	1	1780	4AC	C5-C4	2.67	1.46	1.40
2	2	703	4AC	C5-C4	2.66	1.46	1.40
2	2	64	OMU	C4-N3	-2.66	1.33	1.38
2	2	1069	OMG	C6-N1	-2.64	1.33	1.38
1	1	2163	5MC	C6-C5	2.63	1.38	1.34
2	2	467	OMG	C6-N1	-2.63	1.34	1.38
2	2	680	OMG	C6-N1	-2.63	1.34	1.38
1	1	3004	4AC	C4-N3	-2.62	1.28	1.32
1	1	1621	4AC	C4-N3	-2.61	1.28	1.32
2	2	20	OMU	C2-N3	-2.61	1.33	1.38
1	1	1873	4AC	C4-N3	-2.61	1.28	1.32
2	2	1202	5MC	C6-C5	2.60	1.38	1.34
1	1	2147	OMG	C6-N1	-2.60	1.34	1.38
1	1	2183	5MC	C6-C5	2.60	1.38	1.34
1	1	2249	4AC	C4-N3	-2.60	1.28	1.32
1	1	2162	5MC	C6-C5	2.60	1.38	1.34
1	1	981	4AC	C4-N3	-2.60	1.28	1.32
1	1	1755	4AC	C5-C4	2.59	1.46	1.40
2	2	373	A2M	C5-C6	2.59	1.48	1.41
1	1	2608	4AC	C4-N3	-2.58	1.28	1.32
2	2	1374	5MC	C6-C5	2.58	1.38	1.34
1	1	1048	4AC	C4-N3	-2.58	1.28	1.32
1	1	2001	4AC	C4-N3	-2.58	1.28	1.32
2	2	1025	5MC	C6-C5	2.58	1.38	1.34
1	1	2908	4AC	C4-N3	-2.57	1.28	1.32
1	1	2001	4AC	C5-C4	2.56	1.46	1.40
2	2	851	4AC	C4-N3	-2.56	1.28	1.32
1	1	2203	5MC	C6-C5	2.56	1.38	1.34
1	1	2198	5MC	C6-N1	-2.55	1.33	1.38
2	2	787	OMU	C2-N3	-2.55	1.33	1.38
1	1	1885	4AC	C4-N3	-2.55	1.28	1.32
1	1	161	4AC	C4-N3	-2.55	1.28	1.32
1	1	2608	4AC	C5-C4	2.55	1.46	1.40
1	1	1055	A2M	C5-C6	2.54	1.48	1.41
1	1	314	4AC	C4-N3	-2.54	1.28	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	829	4AC	C4-N3	-2.54	1.28	1.32
2	2	1505	5MC	C6-N1	-2.54	1.33	1.38
2	2	875	5MC	C6-N1	-2.53	1.33	1.38
1	1	2585	4AC	C5-C4	2.53	1.46	1.40
2	2	535	5MC	C6-N1	-2.53	1.33	1.38
1	1	2027	4AC	C4-N3	-2.52	1.28	1.32
1	1	2062	4AC	C4-N3	-2.52	1.28	1.32
1	1	1938	4AC	C4-N3	-2.52	1.28	1.32
2	2	1380	OMU	C2-N3	-2.51	1.33	1.38
2	2	1496	5MC	C6-N1	-2.51	1.33	1.38
1	1	2495	4AC	C4-N3	-2.50	1.28	1.32
1	1	2093	5MC	C6-N1	-2.50	1.33	1.38
1	1	835	4AC	C4-N3	-2.50	1.28	1.32
1	1	2173	A2M	C5-C6	2.49	1.48	1.41
1	1	922	4AC	C4-N3	-2.49	1.28	1.32
1	1	2784	OMU	C2-N3	-2.48	1.33	1.38
1	1	789	OMG	C5-N7	-2.48	1.34	1.39
1	1	1243	4AC	C4-N3	-2.48	1.28	1.32
1	1	1594	4AC	C4-N3	-2.47	1.28	1.32
1	1	1222	4AC	C4-N3	-2.46	1.28	1.32
2	2	535	5MC	C6-C5	2.46	1.38	1.34
2	2	693	5MC	C6-N1	-2.46	1.33	1.38
2	2	657	OMG	C5-N7	-2.46	1.34	1.39
2	2	1374	5MC	C6-N1	-2.45	1.33	1.38
1	1	1068	4AC	C4-N3	-2.45	1.28	1.32
1	1	22	4AC	C4-N3	-2.45	1.28	1.32
2	2	1025	5MC	C6-N1	-2.45	1.33	1.38
1	1	2183	5MC	C6-N1	-2.45	1.33	1.38
1	1	1557	4AC	C4-N3	-2.45	1.28	1.32
2	2	1498	5MC	C6-N1	-2.45	1.33	1.38
2	2	875	5MC	C6-C5	2.44	1.38	1.34
1	1	2093	5MC	C6-C5	2.44	1.38	1.34
2	2	731	4AC	C4-N3	-2.44	1.28	1.32
1	1	2865	4AC	C4-N3	-2.44	1.28	1.32
1	1	1055	A2M	C5-N7	-2.44	1.34	1.39
2	2	1496	5MC	C6-C5	2.43	1.38	1.34
2	2	1498	5MC	C6-C5	2.43	1.38	1.34
1	1	2925	4AC	C4-N3	-2.43	1.28	1.32
2	2	868	4AC	C4-N3	-2.43	1.28	1.32
1	1	1554	4AC	C4-N3	-2.42	1.28	1.32
1	1	1878	4AC	C4-N3	-2.42	1.28	1.32
1	1	2203	5MC	C6-N1	-2.42	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	848	4AC	C4-N3	-2.42	1.28	1.32
1	1	357	4AC	C4-N3	-2.42	1.28	1.32
1	1	2718	4AC	C4-N3	-2.42	1.28	1.32
1	1	2678	OMG	C5-N7	-2.41	1.34	1.39
1	1	1460	4AC	C4-N3	-2.41	1.28	1.32
1	1	2198	5MC	C6-C5	2.41	1.38	1.34
1	1	2966	4AC	C4-N3	-2.41	1.28	1.32
1	1	1617	4AC	C4-N3	-2.40	1.28	1.32
1	1	1765	4AC	C4-N3	-2.40	1.28	1.32
2	2	873	OMG	C5-N7	-2.40	1.34	1.39
1	1	136	4AC	C4-N3	-2.40	1.28	1.32
2	2	1202	5MC	C6-N1	-2.40	1.34	1.38
1	1	1962	4AC	C4-N3	-2.39	1.28	1.32
1	1	1065	4AC	C4-N3	-2.39	1.28	1.32
1	1	1667	4AC	C4-N3	-2.39	1.28	1.32
1	1	2173	A2M	C5-N7	-2.39	1.34	1.39
1	1	923	OMG	C5-N7	-2.39	1.34	1.39
2	2	373	A2M	C5-N7	-2.39	1.34	1.39
2	2	839	4AC	C4-N3	-2.38	1.28	1.32
2	2	286	4AC	C4-N3	-2.38	1.28	1.32
1	1	2960	4AC	C4-N3	-2.38	1.28	1.32
2	2	693	5MC	C6-C5	2.38	1.38	1.34
1	1	2329	4AC	C4-N3	-2.38	1.28	1.32
2	2	319	4AC	C4-N3	-2.38	1.28	1.32
1	1	694	4AC	C4-N3	-2.38	1.28	1.32
1	1	451	4AC	C4-N3	-2.38	1.28	1.32
1	1	1780	4AC	C4-N3	-2.38	1.28	1.32
2	2	511	4AC	C4-N3	-2.37	1.28	1.32
1	1	328	OMG	C5-N7	-2.37	1.34	1.39
2	2	471	OMG	C5-N7	-2.37	1.34	1.39
2	2	774	OMU	C2-N3	-2.36	1.33	1.38
2	2	718	4AC	C4-N3	-2.36	1.28	1.32
2	2	828	4AC	C4-N3	-2.36	1.28	1.32
2	2	17	4AC	C4-N3	-2.36	1.28	1.32
1	1	2144	OMG	C5-N7	-2.36	1.34	1.39
2	2	751	4AC	C4-N3	-2.36	1.28	1.32
1	1	2162	5MC	C6-N1	-2.35	1.34	1.38
2	2	64	OMU	C2-N3	-2.35	1.33	1.38
1	1	2287	4AC	C4-N3	-2.35	1.28	1.32
1	1	641	4AC	C4-N3	-2.35	1.28	1.32
1	1	1867	4AC	C4-N3	-2.35	1.28	1.32
1	1	2992	4AC	C4-N3	-2.35	1.28	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2138	OMG	C5-N7	-2.35	1.34	1.39
2	2	680	OMG	C5-N7	-2.35	1.34	1.39
1	1	1662	4AC	C4-N3	-2.34	1.28	1.32
2	2	1028	4AC	C4-N3	-2.34	1.28	1.32
2	2	913	OMG	C5-N7	-2.34	1.34	1.39
1	1	1934	4AC	C4-N3	-2.34	1.28	1.32
1	1	243	4AC	C4-N3	-2.34	1.28	1.32
1	1	341	4AC	C4-N3	-2.33	1.28	1.32
2	2	1469	6MZ	C5-N7	-2.33	1.34	1.39
1	1	2136	4AC	C4-N3	-2.33	1.28	1.32
2	2	1177	OMU	C2-N3	-2.33	1.33	1.38
1	1	2642	4AC	C4-N3	-2.32	1.28	1.32
1	1	802	4AC	C4-N3	-2.32	1.28	1.32
2	2	1479	4AC	C4-N3	-2.32	1.28	1.32
1	1	533	4AC	C4-N3	-2.31	1.28	1.32
2	2	1184	4AC	C4-N3	-2.31	1.28	1.32
2	2	303	4AC	C4-N3	-2.31	1.28	1.32
1	1	2548	4AC	C4-N3	-2.31	1.28	1.32
1	1	2163	5MC	C6-N1	-2.31	1.34	1.38
1	1	2545	4AC	C4-N3	-2.31	1.28	1.32
2	2	519	OMG	C5-N7	-2.30	1.34	1.39
2	2	546	4AC	C4-N3	-2.30	1.28	1.32
2	2	830	OMU	C2-N3	-2.30	1.33	1.38
1	1	211	4AC	C4-N3	-2.29	1.28	1.32
2	2	1147	4AC	C4-N3	-2.29	1.28	1.32
2	2	379	4AC	C4-N3	-2.29	1.28	1.32
1	1	2733	5MC	C6-N1	-2.28	1.34	1.38
2	2	373	A2M	C8-N7	2.28	1.35	1.31
1	1	91	4AC	C4-N3	-2.28	1.28	1.32
2	2	53	4AC	C4-N3	-2.28	1.28	1.32
2	2	467	OMG	C5-N7	-2.27	1.34	1.39
2	2	957	4AC	C4-N3	-2.27	1.28	1.32
2	2	590	4AC	C4-N3	-2.27	1.28	1.32
1	1	1550	4AC	C4-N3	-2.27	1.28	1.32
1	1	1293	4AC	C4-N3	-2.27	1.28	1.32
2	2	1069	OMG	C5-N7	-2.26	1.34	1.39
1	1	1695	4AC	C4-N3	-2.25	1.28	1.32
1	1	2147	OMG	C5-N7	-2.24	1.34	1.39
2	2	636	4AC	C4-N3	-2.24	1.28	1.32
1	1	2937	4AC	C4-N3	-2.24	1.28	1.32
2	2	394	4AC	C4-N3	-2.23	1.28	1.32
1	1	2570	4AC	C4-N3	-2.23	1.28	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	458	4AC	C4-N3	-2.23	1.28	1.32
2	2	1233	4AC	C4-N3	-2.22	1.29	1.32
2	2	626	4AC	C4-N3	-2.22	1.29	1.32
3	3	32	4AC	C4-N3	-2.22	1.29	1.32
2	2	934	OMG	C5-N7	-2.21	1.34	1.39
2	2	1487	MA6	C5-N7	-2.20	1.34	1.39
2	2	1488	MA6	C5-N7	-2.20	1.34	1.39
1	1	60	4AC	C4-N3	-2.19	1.29	1.32
2	2	1488	MA6	C8-N7	2.19	1.35	1.31
2	2	830	OMU	C5-C4	-2.18	1.38	1.43
1	1	1055	A2M	C8-N7	2.17	1.35	1.31
2	2	1177	OMU	C5-C4	-2.16	1.38	1.43
2	2	479	4AC	C4-N3	-2.15	1.29	1.32
2	2	1239	4AC	C4-N3	-2.13	1.29	1.32
2	2	774	OMU	C5-C4	-2.13	1.38	1.43
1	1	1755	4AC	C4-N3	-2.13	1.29	1.32
1	1	2784	OMU	C5-C4	-2.13	1.38	1.43
2	2	1487	MA6	C8-N7	2.12	1.35	1.31
2	2	64	OMU	C5-C4	-2.10	1.39	1.43
2	2	1505	5MC	C6-C5	2.10	1.38	1.34
2	2	1380	OMU	C5-C4	-2.09	1.39	1.43
2	2	20	OMU	C5-C4	-2.09	1.39	1.43
1	1	2173	A2M	C8-N7	2.08	1.35	1.31
2	2	1487	MA6	C4-N9	-2.08	1.33	1.37
2	2	1488	MA6	C4-N9	-2.07	1.33	1.37
2	2	1469	6MZ	C8-N7	2.07	1.35	1.31
2	2	787	OMU	C5-C4	-2.01	1.39	1.43
2	2	703	4AC	C4-N3	-2.01	1.29	1.32

All (643) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	657	OMG	C5-C4-N3	-6.46	117.99	128.46
1	1	1055	A2M	C5-C4-N3	-6.34	118.48	126.75
1	1	2173	A2M	C5-C4-N3	-6.28	118.56	126.75
2	2	373	A2M	C5-C4-N3	-6.25	118.60	126.75
2	2	471	OMG	C5-C4-N3	-6.23	118.36	128.46
2	2	680	OMG	C5-C4-N3	-6.22	118.36	128.46
1	1	328	OMG	C5-C4-N3	-6.17	118.45	128.46
2	2	1469	6MZ	C5-C4-N3	-6.11	118.78	126.75
1	1	789	OMG	C5-C4-N3	-6.07	118.61	128.46
1	1	2144	OMG	C5-C4-N3	-6.07	118.61	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2138	OMG	C5-C4-N3	-6.06	118.63	128.46
2	2	934	OMG	C5-C4-N3	-6.02	118.69	128.46
1	1	923	OMG	C5-C4-N3	-5.96	118.79	128.46
1	1	2678	OMG	C5-C4-N3	-5.95	118.81	128.46
2	2	519	OMG	C5-C4-N3	-5.94	118.83	128.46
2	2	913	OMG	C5-C4-N3	-5.94	118.83	128.46
2	2	467	OMG	C5-C4-N3	-5.93	118.83	128.46
1	1	2147	OMG	C5-C4-N3	-5.93	118.84	128.46
2	2	1069	OMG	C5-C4-N3	-5.85	118.97	128.46
2	2	873	OMG	C5-C4-N3	-5.84	118.98	128.46
2	2	1467	UR3	C4-N3-C2	-5.69	119.20	124.56
2	2	1487	MA6	C5-C4-N3	-5.69	119.33	126.75
2	2	1488	MA6	C5-C4-N3	-5.67	119.36	126.75
1	1	2001	4AC	O7-C7-N4	5.61	130.90	121.82
1	1	1780	4AC	O7-C7-N4	5.29	130.38	121.82
1	1	1755	4AC	O7-C7-N4	5.06	130.00	121.82
2	2	787	OMU	C4-N3-C2	-5.02	119.95	126.58
1	1	1878	4AC	O7-C7-N4	5.01	129.93	121.82
1	1	789	OMG	C2-N3-C4	5.00	121.20	112.30
2	2	680	OMG	C2-N3-C4	4.98	121.17	112.30
1	1	923	OMG	C2-N3-C4	4.97	121.16	112.30
1	1	2608	4AC	N4-C4-N3	4.94	122.14	113.85
2	2	657	OMG	C2-N3-C4	4.94	121.10	112.30
2	2	20	OMU	C4-N3-C2	-4.94	120.07	126.58
2	2	636	4AC	O7-C7-N4	4.93	129.80	121.82
2	2	471	OMG	C2-N3-C4	4.91	121.05	112.30
1	1	2138	OMG	C2-N3-C4	4.91	121.04	112.30
2	2	519	OMG	C2-N3-C4	4.91	121.04	112.30
2	2	467	OMG	C2-N3-C4	4.91	121.04	112.30
2	2	657	OMG	N9-C4-N3	4.90	135.78	125.94
2	2	934	OMG	C2-N3-C4	4.89	121.02	112.30
1	1	2678	OMG	C2-N3-C4	4.88	121.00	112.30
1	1	328	OMG	C2-N3-C4	4.88	121.00	112.30
1	1	2173	A2M	N3-C4-N9	4.87	135.11	127.08
2	2	913	OMG	C2-N3-C4	4.87	120.97	112.30
1	1	2144	OMG	C2-N3-C4	4.84	120.92	112.30
2	2	703	4AC	O7-C7-N4	4.83	129.63	121.82
1	1	1055	A2M	N3-C4-N9	4.81	135.01	127.08
2	2	1069	OMG	C2-N3-C4	4.81	120.87	112.30
1	1	2608	4AC	C5-C4-N4	-4.79	114.61	122.92
1	1	2147	OMG	C2-N3-C4	4.78	120.82	112.30
2	2	873	OMG	C2-N3-C4	4.74	120.75	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2937	4AC	C5-C4-N4	-4.70	114.76	122.92
2	2	373	A2M	N3-C4-N9	4.68	134.80	127.08
1	1	328	OMG	N9-C4-N3	4.68	135.34	125.94
2	2	680	OMG	N9-C4-N3	4.66	135.31	125.94
1	1	2144	OMG	N9-C4-N3	4.63	135.23	125.94
1	1	2784	OMU	C4-N3-C2	-4.62	120.48	126.58
2	2	471	OMG	N9-C4-N3	4.62	135.21	125.94
2	2	1380	OMU	C4-N3-C2	-4.56	120.56	126.58
1	1	91	4AC	O7-C7-N4	4.55	129.19	121.82
2	2	873	OMG	N9-C4-N3	4.54	135.06	125.94
2	2	303	4AC	O7-C7-N4	4.53	129.15	121.82
2	2	1487	MA6	C2-N1-C6	4.52	122.44	111.75
1	1	789	OMG	N9-C4-N3	4.52	135.02	125.94
1	1	1934	4AC	O7-C7-N4	4.52	129.13	121.82
1	1	1962	4AC	O7-C7-N4	4.52	129.13	121.82
1	1	2937	4AC	N4-C4-N3	4.51	121.42	113.85
2	2	1488	MA6	C2-N1-C6	4.49	122.37	111.75
1	1	1065	4AC	O7-C7-N4	4.49	129.09	121.82
1	1	1293	4AC	O7-C7-N4	4.49	129.08	121.82
1	1	923	OMG	N9-C4-N3	4.48	134.94	125.94
2	2	1177	OMU	C4-N3-C2	-4.48	120.67	126.58
2	2	774	OMU	C4-N3-C2	-4.48	120.67	126.58
1	1	243	4AC	O7-C7-N4	4.48	129.07	121.82
1	1	2718	4AC	O7-C7-N4	4.48	129.07	121.82
2	2	20	OMU	N3-C2-N1	4.48	120.83	114.89
2	2	934	OMG	N9-C4-N3	4.48	134.93	125.94
3	3	32	4AC	O7-C7-N4	4.47	129.06	121.82
1	1	2136	4AC	O7-C7-N4	4.47	129.04	121.82
2	2	1233	4AC	O7-C7-N4	4.46	129.04	121.82
2	2	53	4AC	O7-C7-N4	4.46	129.04	121.82
1	1	2138	OMG	N9-C4-N3	4.46	134.90	125.94
1	1	2570	4AC	O7-C7-N4	4.46	129.03	121.82
1	1	2678	OMG	N9-C4-N3	4.45	134.88	125.94
1	1	2147	OMG	N9-C4-N3	4.45	134.87	125.94
1	1	2966	4AC	O7-C7-N4	4.45	129.01	121.82
2	2	957	4AC	O7-C7-N4	4.44	129.01	121.82
1	1	1617	4AC	O7-C7-N4	4.44	129.01	121.82
2	2	590	4AC	O7-C7-N4	4.44	129.00	121.82
2	2	830	OMU	C4-N3-C2	-4.44	120.73	126.58
1	1	1662	4AC	O7-C7-N4	4.43	128.99	121.82
2	2	1469	6MZ	N3-C4-N9	4.43	134.38	127.08
1	1	1667	4AC	O7-C7-N4	4.43	128.98	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1873	4AC	O7-C7-N4	4.42	128.98	121.82
2	2	1147	4AC	O7-C7-N4	4.42	128.98	121.82
1	1	1460	4AC	O7-C7-N4	4.42	128.97	121.82
2	2	626	4AC	O7-C7-N4	4.41	128.96	121.82
2	2	379	4AC	O7-C7-N4	4.41	128.96	121.82
1	1	1550	4AC	O7-C7-N4	4.41	128.96	121.82
1	1	2249	4AC	O7-C7-N4	4.41	128.95	121.82
2	2	479	4AC	O7-C7-N4	4.41	128.95	121.82
1	1	1048	4AC	O7-C7-N4	4.40	128.94	121.82
1	1	229	4AC	O7-C7-N4	4.40	128.94	121.82
2	2	787	OMU	N3-C2-N1	4.40	120.73	114.89
2	2	511	4AC	O7-C7-N4	4.40	128.94	121.82
1	1	2585	4AC	N4-C4-N3	4.40	121.23	113.85
1	1	22	4AC	O7-C7-N4	4.39	128.92	121.82
2	2	848	4AC	O7-C7-N4	4.39	128.92	121.82
2	2	467	OMG	N9-C4-N3	4.38	134.74	125.94
2	2	17	4AC	O7-C7-N4	4.38	128.91	121.82
2	2	394	4AC	O7-C7-N4	4.38	128.91	121.82
1	1	2287	4AC	O7-C7-N4	4.38	128.91	121.82
1	1	1695	4AC	O7-C7-N4	4.38	128.91	121.82
1	1	533	4AC	O7-C7-N4	4.38	128.91	121.82
2	2	1028	4AC	O7-C7-N4	4.38	128.90	121.82
2	2	286	4AC	O7-C7-N4	4.37	128.90	121.82
1	1	2329	4AC	O7-C7-N4	4.37	128.90	121.82
2	2	839	4AC	O7-C7-N4	4.37	128.89	121.82
1	1	60	4AC	O7-C7-N4	4.37	128.89	121.82
2	2	519	OMG	N9-C4-N3	4.36	134.70	125.94
2	2	1069	OMG	N9-C4-N3	4.36	134.70	125.94
1	1	1554	4AC	O7-C7-N4	4.36	128.88	121.82
2	2	731	4AC	O7-C7-N4	4.36	128.88	121.82
1	1	2925	4AC	O7-C7-N4	4.36	128.87	121.82
1	1	2062	4AC	O7-C7-N4	4.36	128.87	121.82
1	1	802	4AC	O7-C7-N4	4.36	128.87	121.82
1	1	1068	4AC	O7-C7-N4	4.36	128.87	121.82
2	2	913	OMG	N9-C4-N3	4.36	134.68	125.94
1	1	458	4AC	O7-C7-N4	4.35	128.86	121.82
1	1	2545	4AC	O7-C7-N4	4.35	128.85	121.82
1	1	2908	4AC	O7-C7-N4	4.35	128.85	121.82
1	1	1594	4AC	O7-C7-N4	4.34	128.85	121.82
2	2	64	OMU	C4-N3-C2	-4.34	120.85	126.58
1	1	1867	4AC	O7-C7-N4	4.34	128.85	121.82
1	1	2960	4AC	O7-C7-N4	4.34	128.84	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	451	4AC	O7-C7-N4	4.34	128.84	121.82
1	1	1765	4AC	O7-C7-N4	4.33	128.83	121.82
1	1	211	4AC	O7-C7-N4	4.33	128.83	121.82
1	1	2784	OMU	N3-C2-N1	4.33	120.63	114.89
1	1	641	4AC	O7-C7-N4	4.33	128.82	121.82
1	1	2548	4AC	O7-C7-N4	4.32	128.81	121.82
2	2	828	4AC	O7-C7-N4	4.32	128.81	121.82
2	2	1380	OMU	N3-C2-N1	4.32	120.62	114.89
1	1	829	4AC	O7-C7-N4	4.31	128.80	121.82
1	1	922	4AC	O7-C7-N4	4.31	128.80	121.82
1	1	2495	4AC	O7-C7-N4	4.31	128.79	121.82
1	1	3004	4AC	O7-C7-N4	4.31	128.79	121.82
2	2	546	4AC	O7-C7-N4	4.30	128.78	121.82
1	1	341	4AC	O7-C7-N4	4.30	128.78	121.82
1	1	357	4AC	O7-C7-N4	4.30	128.77	121.82
1	1	1243	4AC	O7-C7-N4	4.30	128.77	121.82
2	2	1184	4AC	O7-C7-N4	4.29	128.76	121.82
1	1	2642	4AC	O7-C7-N4	4.28	128.75	121.82
2	2	851	4AC	O7-C7-N4	4.28	128.75	121.82
1	1	1938	4AC	O7-C7-N4	4.28	128.75	121.82
1	1	1557	4AC	O7-C7-N4	4.28	128.74	121.82
2	2	1487	MA6	N3-C4-N9	4.27	134.12	127.08
2	2	1469	6MZ	C6-C5-N7	4.27	137.01	132.39
2	2	1239	4AC	O7-C7-N4	4.26	128.71	121.82
1	1	136	4AC	O7-C7-N4	4.26	128.71	121.82
2	2	718	4AC	O7-C7-N4	4.25	128.70	121.82
1	1	1222	4AC	O7-C7-N4	4.25	128.70	121.82
1	1	694	4AC	O7-C7-N4	4.25	128.70	121.82
2	2	751	4AC	O7-C7-N4	4.25	128.69	121.82
1	1	2865	4AC	O7-C7-N4	4.24	128.69	121.82
1	1	314	4AC	O7-C7-N4	4.23	128.66	121.82
2	2	319	4AC	O7-C7-N4	4.23	128.66	121.82
1	1	161	4AC	O7-C7-N4	4.21	128.63	121.82
2	2	830	OMU	N3-C2-N1	4.21	120.47	114.89
1	1	981	4AC	O7-C7-N4	4.20	128.61	121.82
1	1	2027	4AC	O7-C7-N4	4.19	128.60	121.82
1	1	1621	4AC	O7-C7-N4	4.18	128.59	121.82
2	2	1479	4AC	O7-C7-N4	4.18	128.58	121.82
1	1	835	4AC	O7-C7-N4	4.18	128.58	121.82
2	2	868	4AC	O7-C7-N4	4.14	128.51	121.82
2	2	774	OMU	N3-C2-N1	4.13	120.38	114.89
1	1	2585	4AC	C5-C4-N4	-4.12	115.76	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1488	MA6	N3-C4-N9	4.12	133.87	127.08
1	1	2083	4AC	O7-C7-N4	4.09	128.44	121.82
1	1	1755	4AC	N4-C4-N3	4.07	120.69	113.85
2	2	703	4AC	N4-C4-N3	4.05	120.65	113.85
2	2	1177	OMU	N3-C2-N1	4.05	120.26	114.89
1	1	1885	4AC	O7-C7-N4	4.04	128.36	121.82
2	2	64	OMU	N3-C2-N1	4.04	120.25	114.89
2	2	1488	MA6	C4-C5-N7	-3.98	105.77	110.62
1	1	1755	4AC	C5-C4-N4	-3.96	116.04	122.92
2	2	1469	6MZ	C4-C5-N7	-3.92	105.84	110.62
2	2	373	A2M	C2-N3-C4	3.92	121.02	111.75
1	1	1055	A2M	C2-N3-C4	3.92	121.01	111.75
2	2	1469	6MZ	C2-N3-C4	3.90	120.97	111.75
2	2	703	4AC	C5-C4-N4	-3.89	116.16	122.92
1	1	2173	A2M	C2-N3-C4	3.89	120.94	111.75
2	2	1487	MA6	C4-C5-N7	-3.85	105.93	110.62
2	2	1488	MA6	C2-N3-C4	3.83	120.80	111.75
2	2	535	5MC	C5-C6-N1	-3.83	119.40	123.34
2	2	787	OMU	C5-C4-N3	3.83	120.57	114.84
2	2	1487	MA6	C2-N3-C4	3.76	120.64	111.75
2	2	20	OMU	C5-C4-N3	3.75	120.45	114.84
2	2	1374	5MC	C5-C6-N1	-3.73	119.50	123.34
2	2	875	5MC	C5-C6-N1	-3.68	119.56	123.34
1	1	1780	4AC	C5-C4-N4	-3.66	116.57	122.92
1	1	2784	OMU	C5-C4-N3	3.65	120.30	114.84
2	2	1025	5MC	C5-C6-N1	-3.64	119.59	123.34
2	2	1380	OMU	C5-C4-N3	3.62	120.26	114.84
2	2	1177	OMU	C5-C4-N3	3.62	120.25	114.84
1	1	2203	5MC	C5-C6-N1	-3.61	119.62	123.34
2	2	774	OMU	C5-C4-N3	3.60	120.23	114.84
1	1	2183	5MC	C5-C6-N1	-3.59	119.65	123.34
2	2	64	OMU	C5-C4-N3	3.58	120.20	114.84
1	1	2585	4AC	O2-C2-N3	-3.56	116.54	122.33
1	1	2162	5MC	C5-C6-N1	-3.55	119.68	123.34
2	2	830	OMU	C5-C4-N3	3.53	120.12	114.84
1	1	2733	5MC	C5-C6-N1	-3.52	119.72	123.34
1	1	2093	5MC	C5-C6-N1	-3.48	119.75	123.34
1	1	2198	5MC	C5-C6-N1	-3.46	119.78	123.34
1	1	2163	5MC	C5-C6-N1	-3.45	119.79	123.34
1	1	2608	4AC	O7-C7-N4	3.45	127.40	121.82
1	1	2585	4AC	O7-C7-N4	3.44	127.39	121.82
1	1	2937	4AC	O7-C7-N4	3.43	127.37	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1878	4AC	CM7-C7-N4	-3.43	109.37	115.29
1	1	1780	4AC	N4-C4-N3	3.41	119.58	113.85
2	2	519	OMG	C6-C5-N7	3.39	136.56	130.25
1	1	923	OMG	C6-C5-N7	3.39	136.56	130.25
2	2	373	A2M	C4-C5-N7	-3.38	106.50	110.62
2	2	467	OMG	C6-C5-N7	3.38	136.53	130.25
1	1	1055	A2M	C4-C5-N7	-3.37	106.51	110.62
2	2	693	5MC	C5-C6-N1	-3.35	119.89	123.34
2	2	913	OMG	C6-C5-N7	3.35	136.48	130.25
2	2	1239	4AC	N4-C4-N3	3.33	119.45	113.85
2	2	934	OMG	C6-C5-N7	3.33	136.45	130.25
2	2	1069	OMG	C6-C5-N7	3.33	136.44	130.25
2	2	1488	MA6	N1-C2-N3	-3.33	123.40	128.60
1	1	1780	4AC	CM7-C7-N4	-3.32	109.56	115.29
2	2	1496	5MC	C5-C6-N1	-3.29	119.95	123.34
1	1	2678	OMG	C6-C5-N7	3.29	136.37	130.25
2	2	1469	6MZ	N1-C2-N3	-3.28	123.47	128.60
2	2	1487	MA6	N1-C2-N3	-3.27	123.48	128.60
1	1	2138	OMG	C6-C5-N7	3.27	136.33	130.25
2	2	636	4AC	CM7-C7-N4	-3.25	109.66	115.29
1	1	1878	4AC	C5-C4-N4	-3.25	117.27	122.92
1	1	2173	A2M	C4-C5-N7	-3.24	106.67	110.62
1	1	789	OMG	C6-C5-N7	3.24	136.27	130.25
2	2	1488	MA6	C5-N7-C8	3.23	108.10	103.51
1	1	229	4AC	CM7-C7-N4	-3.21	109.74	115.29
1	1	2147	OMG	C6-C5-N7	3.21	136.21	130.25
2	2	636	4AC	C5-C4-N4	-3.18	117.40	122.92
2	2	626	4AC	N4-C4-N3	3.18	119.18	113.85
2	2	1487	MA6	C5-N7-C8	3.15	107.99	103.51
2	2	1505	5MC	O4'-C1'-N1	3.15	115.56	108.36
1	1	1055	A2M	N3-C2-N1	-3.14	123.69	128.60
2	2	680	OMG	C6-C5-N7	3.14	136.08	130.25
2	2	471	OMG	C6-C5-N7	3.14	136.08	130.25
2	2	373	A2M	N3-C2-N1	-3.13	123.70	128.60
2	2	1469	6MZ	C5-N7-C8	3.13	107.96	103.51
2	2	873	OMG	C6-C5-N7	3.13	136.07	130.25
1	1	1873	4AC	CM7-C7-N4	-3.13	109.88	115.29
1	1	2173	A2M	N3-C2-N1	-3.12	123.72	128.60
1	1	2144	OMG	C6-C5-N7	3.12	136.05	130.25
1	1	328	OMG	C6-C5-N7	3.10	136.01	130.25
2	2	53	4AC	N4-C4-N3	3.10	119.05	113.85
1	1	2001	4AC	CM7-C7-N4	-3.09	109.96	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	626	4AC	C5-C4-N4	-3.08	117.57	122.92
1	1	1550	4AC	N4-C4-N3	3.08	119.02	113.85
1	1	22	4AC	CM7-C7-N4	-3.06	110.00	115.29
2	2	1479	4AC	N4-C4-N3	3.05	118.98	113.85
1	1	91	4AC	N4-C4-N3	3.05	118.97	113.85
2	2	479	4AC	N4-C4-N3	3.05	118.97	113.85
1	1	2608	4AC	O2-C2-N3	-3.05	117.37	122.33
2	2	64	OMU	O4-C4-C5	-3.03	119.83	125.16
2	2	774	OMU	O4-C4-C5	-3.03	119.84	125.16
1	1	2062	4AC	CM7-C7-N4	-3.03	110.06	115.29
2	2	1498	5MC	C5-C6-N1	-3.01	120.24	123.34
1	1	2001	4AC	N4-C4-N3	3.01	118.91	113.85
1	1	91	4AC	C5-C4-N4	-3.01	117.69	122.92
2	2	511	4AC	CM7-C7-N4	-3.00	110.10	115.29
1	1	2966	4AC	CM7-C7-N4	-3.00	110.11	115.29
1	1	1293	4AC	CM7-C7-N4	-2.99	110.12	115.29
2	2	303	4AC	CM7-C7-N4	-2.98	110.14	115.29
2	2	1202	5MC	C5-C6-N1	-2.98	120.28	123.34
1	1	1962	4AC	CM7-C7-N4	-2.98	110.15	115.29
2	2	1177	OMU	O4-C4-C5	-2.98	119.93	125.16
1	1	2908	4AC	CM7-C7-N4	-2.98	110.15	115.29
1	1	2287	4AC	N4-C4-N3	2.97	118.84	113.85
2	2	53	4AC	C5-C4-N4	-2.97	117.76	122.92
2	2	286	4AC	CM7-C7-N4	-2.97	110.16	115.29
1	1	2495	4AC	CM7-C7-N4	-2.96	110.17	115.29
1	1	1550	4AC	C5-C4-N4	-2.96	117.77	122.92
2	2	394	4AC	N4-C4-N3	2.96	118.82	113.85
2	2	839	4AC	CM7-C7-N4	-2.96	110.17	115.29
1	1	2865	4AC	CM7-C7-N4	-2.96	110.18	115.29
2	2	319	4AC	N4-C4-N3	2.95	118.81	113.85
2	2	1233	4AC	N4-C4-N3	2.95	118.81	113.85
3	3	32	4AC	CM7-C7-N4	-2.95	110.20	115.29
2	2	828	4AC	CM7-C7-N4	-2.95	110.20	115.29
2	2	1233	4AC	C5-C4-N4	-2.94	117.81	122.92
1	1	1667	4AC	CM7-C7-N4	-2.94	110.20	115.29
2	2	479	4AC	C5-C4-N4	-2.94	117.81	122.92
1	1	60	4AC	N4-C4-N3	2.94	118.79	113.85
2	2	1239	4AC	C5-C4-N4	-2.94	117.81	122.92
1	1	1662	4AC	CM7-C7-N4	-2.94	110.21	115.29
1	1	2570	4AC	CM7-C7-N4	-2.94	110.21	115.29
1	1	1878	4AC	N4-C4-N3	2.94	118.78	113.85
2	2	1505	5MC	C5-C6-N1	-2.94	120.32	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1938	4AC	CM7-C7-N4	-2.93	110.22	115.29
2	2	1147	4AC	CM7-C7-N4	-2.93	110.22	115.29
1	1	1934	4AC	N4-C4-N3	2.93	118.77	113.85
2	2	379	4AC	N4-C4-N3	2.93	118.76	113.85
1	1	1617	4AC	CM7-C7-N4	-2.92	110.24	115.29
2	2	848	4AC	CM7-C7-N4	-2.92	110.24	115.29
2	2	957	4AC	N4-C4-N3	2.92	118.75	113.85
1	1	2784	OMU	O4-C4-C5	-2.92	120.03	125.16
1	1	802	4AC	N4-C4-N3	2.92	118.75	113.85
2	2	787	OMU	O4-C4-C5	-2.91	120.04	125.16
1	1	829	4AC	CM7-C7-N4	-2.91	110.27	115.29
1	1	458	4AC	N4-C4-N3	2.91	118.73	113.85
1	1	1765	4AC	CM7-C7-N4	-2.91	110.27	115.29
1	1	1662	4AC	C5-C4-N4	-2.90	117.87	122.92
2	2	546	4AC	N4-C4-N3	2.90	118.72	113.85
1	1	161	4AC	CM7-C7-N4	-2.90	110.28	115.29
2	2	379	4AC	C5-C4-N4	-2.90	117.89	122.92
1	1	1048	4AC	CM7-C7-N4	-2.90	110.28	115.29
2	2	1487	MA6	C4-N9-C8	2.89	108.86	105.73
1	1	1867	4AC	CM7-C7-N4	-2.89	110.29	115.29
1	1	1695	4AC	CM7-C7-N4	-2.89	110.30	115.29
1	1	243	4AC	N4-C4-N3	2.89	118.70	113.85
2	2	636	4AC	N4-C4-N3	2.89	118.70	113.85
1	1	2083	4AC	CM7-C7-N4	-2.88	110.31	115.29
1	1	2570	4AC	C5-C4-N4	-2.88	117.92	122.92
2	2	1233	4AC	CM7-C7-N4	-2.88	110.32	115.29
1	1	341	4AC	N4-C4-N3	2.88	118.68	113.85
1	1	2718	4AC	CM7-C7-N4	-2.87	110.32	115.29
2	2	17	4AC	CM7-C7-N4	-2.87	110.33	115.29
1	1	2570	4AC	N4-C4-N3	2.87	118.67	113.85
1	1	243	4AC	CM7-C7-N4	-2.87	110.33	115.29
1	1	91	4AC	CM7-C7-N4	-2.87	110.33	115.29
1	1	1243	4AC	CM7-C7-N4	-2.86	110.34	115.29
1	1	1065	4AC	N4-C4-N3	2.86	118.66	113.85
2	2	1147	4AC	N4-C4-N3	2.86	118.66	113.85
1	1	2287	4AC	C5-C4-N4	-2.86	117.95	122.92
3	3	32	4AC	N4-C4-N3	2.86	118.65	113.85
1	1	922	4AC	N4-C4-N3	2.86	118.65	113.85
1	1	1662	4AC	N4-C4-N3	2.86	118.65	113.85
1	1	2733	5MC	C5-C4-N3	-2.86	118.59	121.67
1	1	1068	4AC	CM7-C7-N4	-2.86	110.35	115.29
1	1	211	4AC	CM7-C7-N4	-2.86	110.35	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1293	4AC	C5-C4-N4	-2.86	117.96	122.92
2	2	957	4AC	C5-C4-N4	-2.86	117.96	122.92
2	2	1028	4AC	N4-C4-N3	2.85	118.64	113.85
1	1	60	4AC	C5-C4-N4	-2.85	117.97	122.92
1	1	1293	4AC	N4-C4-N3	2.85	118.64	113.85
1	1	1617	4AC	N4-C4-N3	2.85	118.63	113.85
1	1	802	4AC	CM7-C7-N4	-2.85	110.37	115.29
1	1	981	4AC	CM7-C7-N4	-2.85	110.37	115.29
1	1	1934	4AC	CM7-C7-N4	-2.85	110.37	115.29
1	1	2545	4AC	CM7-C7-N4	-2.84	110.39	115.29
1	1	314	4AC	CM7-C7-N4	-2.84	110.39	115.29
2	2	751	4AC	CM7-C7-N4	-2.84	110.39	115.29
2	2	1202	5MC	O2-C2-N3	-2.83	117.72	122.33
1	1	3004	4AC	CM7-C7-N4	-2.83	110.39	115.29
1	1	2136	4AC	C5-C4-N4	-2.83	118.00	122.92
1	1	2136	4AC	N4-C4-N3	2.83	118.60	113.85
2	2	394	4AC	CM7-C7-N4	-2.83	110.40	115.29
2	2	590	4AC	CM7-C7-N4	-2.83	110.40	115.29
1	1	1554	4AC	CM7-C7-N4	-2.83	110.40	115.29
2	2	657	OMG	C6-C5-N7	2.83	135.51	130.25
2	2	1147	4AC	C5-C4-N4	-2.83	118.01	122.92
1	1	2329	4AC	N4-C4-N3	2.83	118.60	113.85
2	2	20	OMU	O4-C4-C5	-2.82	120.19	125.16
1	1	2545	4AC	N4-C4-N3	2.82	118.59	113.85
2	2	830	OMU	O4-C4-C5	-2.82	120.20	125.16
1	1	357	4AC	CM7-C7-N4	-2.82	110.42	115.29
1	1	2136	4AC	CM7-C7-N4	-2.82	110.42	115.29
1	1	533	4AC	N4-C4-N3	2.81	118.58	113.85
3	3	32	4AC	C5-C4-N4	-2.81	118.03	122.92
1	1	1695	4AC	C5-C4-N4	-2.81	118.04	122.92
1	1	458	4AC	C5-C4-N4	-2.81	118.04	122.92
2	2	957	4AC	CM7-C7-N4	-2.81	110.44	115.29
1	1	802	4AC	C5-C4-N4	-2.81	118.05	122.92
1	1	1065	4AC	CM7-C7-N4	-2.81	110.44	115.29
1	1	1617	4AC	C5-C4-N4	-2.80	118.05	122.92
1	1	1695	4AC	N4-C4-N3	2.80	118.56	113.85
1	1	2545	4AC	C5-C4-N4	-2.80	118.05	122.92
1	1	2925	4AC	CM7-C7-N4	-2.80	110.45	115.29
1	1	2718	4AC	N4-C4-N3	2.80	118.56	113.85
2	2	479	4AC	CM7-C7-N4	-2.80	110.45	115.29
2	2	394	4AC	C5-C4-N4	-2.80	118.06	122.92
1	1	451	4AC	CM7-C7-N4	-2.80	110.45	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1594	4AC	CM7-C7-N4	-2.80	110.45	115.29
1	1	1055	A2M	C5-N7-C8	2.80	107.48	103.51
1	1	243	4AC	C5-C4-N4	-2.80	118.06	122.92
1	1	2249	4AC	CM7-C7-N4	-2.80	110.46	115.29
1	1	2585	4AC	C1'-N1-C2	2.80	124.66	118.42
1	1	533	4AC	CM7-C7-N4	-2.79	110.46	115.29
2	2	1488	MA6	C4-N9-C8	2.79	108.75	105.73
1	1	2329	4AC	CM7-C7-N4	-2.79	110.46	115.29
1	1	641	4AC	CM7-C7-N4	-2.79	110.47	115.29
2	2	731	4AC	CM7-C7-N4	-2.79	110.47	115.29
1	1	1621	4AC	CM7-C7-N4	-2.79	110.48	115.29
1	1	1934	4AC	C5-C4-N4	-2.78	118.09	122.92
1	1	1460	4AC	CM7-C7-N4	-2.78	110.49	115.29
1	1	835	4AC	CM7-C7-N4	-2.77	110.50	115.29
1	1	2548	4AC	N4-C4-N3	2.77	118.50	113.85
2	2	53	4AC	CM7-C7-N4	-2.77	110.51	115.29
2	2	1028	4AC	C5-C4-N4	-2.77	118.11	122.92
2	2	379	4AC	CM7-C7-N4	-2.77	110.51	115.29
2	2	373	A2M	C5-N7-C8	2.77	107.44	103.51
2	2	1479	4AC	C5-C4-N4	-2.76	118.12	122.92
1	1	1867	4AC	C5-C4-N4	-2.76	118.12	122.92
1	1	2718	4AC	C5-C4-N4	-2.76	118.12	122.92
1	1	694	4AC	CM7-C7-N4	-2.76	110.52	115.29
1	1	2329	4AC	C5-C4-N4	-2.76	118.13	122.92
2	2	319	4AC	C5-C4-N4	-2.75	118.14	122.92
1	1	211	4AC	N4-C4-N3	2.75	118.47	113.85
1	1	1460	4AC	N4-C4-N3	2.75	118.47	113.85
1	1	2027	4AC	CM7-C7-N4	-2.75	110.54	115.29
2	2	546	4AC	C5-C4-N4	-2.75	118.14	122.92
2	2	590	4AC	N4-C4-N3	2.75	118.47	113.85
2	2	1380	OMU	O4-C4-C5	-2.75	120.33	125.16
1	1	641	4AC	N4-C4-N3	2.74	118.46	113.85
2	2	1202	5MC	C5-C4-N3	-2.74	118.71	121.67
1	1	2548	4AC	CM7-C7-N4	-2.74	110.55	115.29
1	1	2642	4AC	CM7-C7-N4	-2.74	110.55	115.29
2	2	303	4AC	N4-C4-N3	2.74	118.45	113.85
1	1	641	4AC	C5-C4-N4	-2.74	118.16	122.92
2	2	1028	4AC	CM7-C7-N4	-2.74	110.56	115.29
1	1	451	4AC	N4-C4-N3	2.73	118.44	113.85
2	2	731	4AC	N4-C4-N3	2.73	118.44	113.85
1	1	60	4AC	CM7-C7-N4	-2.73	110.57	115.29
2	2	303	4AC	C5-C4-N4	-2.73	118.19	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	546	4AC	CM7-C7-N4	-2.72	110.58	115.29
2	2	718	4AC	CM7-C7-N4	-2.72	110.59	115.29
1	1	136	4AC	CM7-C7-N4	-2.72	110.59	115.29
1	1	2027	4AC	N4-C4-N3	2.72	118.41	113.85
1	1	458	4AC	CM7-C7-N4	-2.71	110.61	115.29
1	1	211	4AC	C5-C4-N4	-2.71	118.21	122.92
1	1	1460	4AC	C5-C4-N4	-2.71	118.21	122.92
1	1	1557	4AC	CM7-C7-N4	-2.70	110.62	115.29
2	2	851	4AC	CM7-C7-N4	-2.70	110.62	115.29
1	1	22	4AC	C5-C4-N4	-2.70	118.23	122.92
1	1	533	4AC	C5-C4-N4	-2.69	118.24	122.92
1	1	1962	4AC	C5-C4-N4	-2.69	118.24	122.92
1	1	2608	4AC	C1'-N1-C2	2.69	124.43	118.42
1	1	2287	4AC	CM7-C7-N4	-2.69	110.64	115.29
2	2	519	OMG	C4-C5-N7	-2.69	106.47	110.72
1	1	2173	A2M	C5-N7-C8	2.68	107.32	103.51
1	1	1867	4AC	N4-C4-N3	2.68	118.36	113.85
2	2	17	4AC	C5-C4-N4	-2.68	118.27	122.92
1	1	2925	4AC	N4-C4-N3	2.68	118.34	113.85
1	1	341	4AC	C5-C4-N4	-2.68	118.27	122.92
1	1	1065	4AC	C5-C4-N4	-2.68	118.27	122.92
2	2	848	4AC	N4-C4-N3	2.67	118.34	113.85
2	2	848	4AC	C5-C4-N4	-2.67	118.28	122.92
2	2	913	OMG	C4-C5-N7	-2.67	106.50	110.72
1	1	2960	4AC	N4-C4-N3	2.67	118.33	113.85
2	2	934	OMG	C4-C5-N7	-2.67	106.50	110.72
2	2	731	4AC	C5-C4-N4	-2.66	118.29	122.92
1	1	22	4AC	N4-C4-N3	2.66	118.32	113.85
1	1	1550	4AC	CM7-C7-N4	-2.66	110.70	115.29
1	1	1068	4AC	N4-C4-N3	2.66	118.31	113.85
2	2	17	4AC	N4-C4-N3	2.66	118.31	113.85
1	1	1222	4AC	CM7-C7-N4	-2.65	110.71	115.29
1	1	1885	4AC	CM7-C7-N4	-2.65	110.71	115.29
2	2	868	4AC	N4-C4-N3	2.65	118.30	113.85
1	1	1594	4AC	N4-C4-N3	2.65	118.30	113.85
2	2	590	4AC	C5-C4-N4	-2.65	118.32	122.92
1	1	1962	4AC	N4-C4-N3	2.65	118.29	113.85
1	1	2966	4AC	C5-C4-N4	-2.64	118.33	122.92
1	1	2138	OMG	C4-C5-N7	-2.64	106.54	110.72
1	1	922	4AC	C5-C4-N4	-2.64	118.34	122.92
2	2	828	4AC	N4-C4-N3	2.64	118.28	113.85
2	2	839	4AC	N4-C4-N3	2.64	118.28	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1667	4AC	C5-C4-N4	-2.63	118.35	122.92
1	1	1554	4AC	C5-C4-N4	-2.63	118.36	122.92
1	1	1594	4AC	C5-C4-N4	-2.63	118.36	122.92
1	1	2027	4AC	C5-C4-N4	-2.63	118.36	122.92
2	2	467	OMG	C4-C5-N7	-2.63	106.56	110.72
1	1	451	4AC	C5-C4-N4	-2.63	118.36	122.92
1	1	2925	4AC	C5-C4-N4	-2.62	118.37	122.92
2	2	1498	5MC	O2-C2-N3	-2.62	118.07	122.33
2	2	1505	5MC	C5-C4-N3	-2.62	118.85	121.67
1	1	2960	4AC	CM7-C7-N4	-2.61	110.77	115.29
2	2	471	OMG	C4-C5-N7	-2.61	106.58	110.72
1	1	136	4AC	N4-C4-N3	2.61	118.24	113.85
1	1	2966	4AC	N4-C4-N3	2.61	118.24	113.85
1	1	1554	4AC	N4-C4-N3	2.61	118.23	113.85
1	1	2548	4AC	C5-C4-N4	-2.61	118.39	122.92
2	2	1184	4AC	N4-C4-N3	2.60	118.22	113.85
1	1	2198	5MC	C5-C4-N3	-2.60	118.87	121.67
2	2	1184	4AC	CM7-C7-N4	-2.60	110.80	115.29
1	1	1667	4AC	N4-C4-N3	2.59	118.20	113.85
1	1	2733	5MC	O2-C2-N3	-2.59	118.12	122.33
1	1	341	4AC	CM7-C7-N4	-2.59	110.82	115.29
1	1	2001	4AC	C5-C4-N4	-2.59	118.42	122.92
2	2	751	4AC	N4-C4-N3	2.59	118.19	113.85
2	2	511	4AC	N4-C4-N3	2.59	118.19	113.85
1	1	1557	4AC	N4-C4-N3	2.59	118.19	113.85
2	2	1498	5MC	C5-C4-N3	-2.59	118.88	121.67
1	1	789	OMG	C4-C5-N7	-2.58	106.63	110.72
2	2	1184	4AC	C5-C4-N4	-2.58	118.43	122.92
2	2	1496	5MC	C5-C4-N3	-2.58	118.89	121.67
2	2	1069	OMG	C4-C5-N7	-2.58	106.63	110.72
1	1	923	OMG	C4-C5-N7	-2.58	106.64	110.72
2	2	828	4AC	C5-C4-N4	-2.58	118.44	122.92
1	1	328	OMG	C4-C5-N7	-2.58	106.64	110.72
2	2	718	4AC	C5-C4-N4	-2.57	118.45	122.92
2	2	693	5MC	C5-C4-N3	-2.57	118.90	121.67
2	2	1505	5MC	CM5-C5-C6	-2.57	119.41	122.85
2	2	787	OMU	O2-C2-N1	-2.57	119.38	122.79
1	1	2960	4AC	C5-C4-N4	-2.56	118.47	122.92
1	1	694	4AC	C5-C4-N4	-2.56	118.47	122.92
2	2	680	OMG	C4-C5-N7	-2.56	106.67	110.72
1	1	2865	4AC	C5-C4-N4	-2.56	118.47	122.92
2	2	1488	MA6	C6-C5-N7	2.56	137.57	133.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	626	4AC	CM7-C7-N4	-2.55	110.88	115.29
2	2	319	4AC	CM7-C7-N4	-2.55	110.88	115.29
1	1	922	4AC	CM7-C7-N4	-2.55	110.88	115.29
2	2	511	4AC	C5-C4-N4	-2.55	118.50	122.92
1	1	2147	OMG	C4-C5-N7	-2.54	106.69	110.72
1	1	2678	OMG	C4-C5-N7	-2.54	106.69	110.72
1	1	1765	4AC	N4-C4-N3	2.54	118.12	113.85
1	1	694	4AC	N4-C4-N3	2.54	118.12	113.85
2	2	286	4AC	C5-C4-N4	-2.54	118.51	122.92
1	1	1222	4AC	N4-C4-N3	2.54	118.11	113.85
2	2	851	4AC	N4-C4-N3	2.53	118.10	113.85
2	2	851	4AC	C5-C4-N4	-2.53	118.53	122.92
1	1	829	4AC	C5-C4-N4	-2.53	118.53	122.92
2	2	718	4AC	N4-C4-N3	2.52	118.09	113.85
2	2	20	OMU	O2-C2-N1	-2.52	119.43	122.79
2	2	839	4AC	C5-C4-N4	-2.52	118.54	122.92
1	1	2865	4AC	N4-C4-N3	2.52	118.08	113.85
1	1	2642	4AC	N4-C4-N3	2.51	118.07	113.85
2	2	1505	5MC	O2'-C2'-C3'	2.51	119.94	111.82
2	2	751	4AC	C5-C4-N4	-2.51	118.57	122.92
2	2	1025	5MC	C5-C4-N3	-2.51	118.97	121.67
2	2	868	4AC	C5-C4-N4	-2.50	118.58	122.92
1	1	1765	4AC	C5-C4-N4	-2.50	118.58	122.92
1	1	2093	5MC	C5-C4-N3	-2.50	118.98	121.67
1	1	1068	4AC	C5-C4-N4	-2.49	118.59	122.92
2	2	286	4AC	N4-C4-N3	2.49	118.03	113.85
1	1	357	4AC	N4-C4-N3	2.49	118.03	113.85
1	1	2203	5MC	C5-C4-N3	-2.49	118.99	121.67
1	1	2144	OMG	C4-C5-N7	-2.48	106.79	110.72
1	1	2062	4AC	N4-C4-N3	2.48	118.02	113.85
1	1	2249	4AC	C5-C4-N4	-2.48	118.61	122.92
2	2	657	OMG	C4-C5-N7	-2.48	106.80	110.72
1	1	829	4AC	N4-C4-N3	2.47	118.00	113.85
1	1	161	4AC	N4-C4-N3	2.47	118.00	113.85
1	1	1557	4AC	C5-C4-N4	-2.47	118.63	122.92
1	1	136	4AC	C5-C4-N4	-2.47	118.63	122.92
1	1	2162	5MC	C5-C4-N3	-2.46	119.02	121.67
1	1	2249	4AC	N4-C4-N3	2.46	117.98	113.85
2	2	875	5MC	C5-C4-N3	-2.45	119.03	121.67
1	1	2784	OMU	O2-C2-N1	-2.45	119.54	122.79
1	1	2183	5MC	C5-C4-N3	-2.44	119.04	121.67
1	1	161	4AC	C5-C4-N4	-2.44	118.69	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1488	MA6	N9-C8-N7	-2.43	110.59	113.91
1	1	1222	4AC	C5-C4-N4	-2.43	118.70	122.92
1	1	1938	4AC	N4-C4-N3	2.43	117.93	113.85
1	1	2163	5MC	C5-C4-N3	-2.42	119.06	121.67
2	2	703	4AC	CM7-C7-N4	-2.41	111.12	115.29
1	1	2642	4AC	C5-C4-N4	-2.41	118.73	122.92
1	1	835	4AC	N4-C4-N3	2.41	117.90	113.85
1	1	1755	4AC	CM7-C7-N4	-2.41	111.12	115.29
1	1	2173	A2M	C4-N9-C8	2.40	108.33	105.73
1	1	3004	4AC	C5-C4-N4	-2.40	118.74	122.92
2	2	873	OMG	C4-C5-N7	-2.40	106.93	110.72
2	2	868	4AC	CM7-C7-N4	-2.40	111.15	115.29
1	1	2992	4AC	CM7-C7-N4	2.39	119.44	115.29
1	1	314	4AC	N4-C4-N3	2.39	117.86	113.85
1	1	1885	4AC	N4-C4-N3	2.39	117.86	113.85
2	2	1239	4AC	CM7-C7-N4	-2.38	111.17	115.29
2	2	1479	4AC	CM7-C7-N4	-2.38	111.18	115.29
2	2	1487	MA6	N9-C8-N7	-2.37	110.67	113.91
1	1	1243	4AC	C5-C4-N4	-2.36	118.82	122.92
1	1	1048	4AC	C5-C4-N4	-2.36	118.82	122.92
1	1	1243	4AC	N4-C4-N3	2.36	117.81	113.85
2	2	830	OMU	C1'-N1-C2	2.36	121.83	117.57
2	2	1374	5MC	C5-C4-N3	-2.35	119.14	121.67
1	1	1938	4AC	C5-C4-N4	-2.35	118.84	122.92
1	1	2062	4AC	C5-C4-N4	-2.34	118.85	122.92
2	2	1487	MA6	C6-C5-N7	2.34	137.21	133.28
2	2	535	5MC	C5-C4-N3	-2.32	119.17	121.67
1	1	357	4AC	C5-C4-N4	-2.32	118.88	122.92
1	1	835	4AC	C5-C4-N4	-2.31	118.91	122.92
1	1	1055	A2M	C4-N9-C8	2.30	108.23	105.73
1	1	1885	4AC	C5-C4-N4	-2.30	118.92	122.92
1	1	1873	4AC	C5-C4-N4	-2.29	118.93	122.92
2	2	373	A2M	C6-C5-N7	2.29	136.29	132.02
1	1	314	4AC	C5-C4-N4	-2.28	118.96	122.92
1	1	1048	4AC	N4-C4-N3	2.28	117.68	113.85
2	2	373	A2M	C4-N9-C8	2.26	108.17	105.73
1	1	328	OMG	O6-C6-C5	-2.25	120.62	126.60
1	1	2908	4AC	N4-C4-N3	2.25	117.63	113.85
1	1	3004	4AC	N4-C4-N3	2.25	117.63	113.85
1	1	923	OMG	O6-C6-C5	-2.24	120.66	126.60
2	2	1498	5MC	C1'-N1-C6	-2.23	117.42	121.12
1	1	1873	4AC	N4-C4-N3	2.22	117.58	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	873	OMG	O6-C6-C5	-2.22	120.71	126.60
1	1	2908	4AC	C5-C4-N4	-2.21	119.07	122.92
1	1	2608	4AC	CM7-C7-N4	-2.21	111.47	115.29
1	1	2495	4AC	N4-C4-N3	2.21	117.57	113.85
1	1	1055	A2M	C6-C5-N7	2.20	136.12	132.02
2	2	1202	5MC	C1'-N1-C6	-2.20	117.47	121.12
2	2	1467	UR3	C1'-N1-C2	2.20	120.70	116.99
1	1	981	4AC	C5-C4-N4	-2.19	119.11	122.92
1	1	2144	OMG	O6-C6-C5	-2.19	120.78	126.60
1	1	2083	4AC	O2-C2-N3	-2.18	118.78	122.33
2	2	1040	OMC	O2-C2-N3	-2.18	118.79	122.33
1	1	1621	4AC	C5-C4-N4	-2.17	119.14	122.92
1	1	2495	4AC	C5-C4-N4	-2.17	119.14	122.92
1	1	2678	OMG	O6-C6-C5	-2.17	120.85	126.60
2	2	1469	6MZ	C4-N9-C8	2.16	108.07	105.73
2	2	1025	5MC	O2-C2-N3	-2.16	118.81	122.33
1	1	789	OMG	O6-C6-C5	-2.16	120.88	126.60
2	2	1469	6MZ	C2-N1-C6	2.15	122.48	115.25
1	1	2138	OMG	O6-C6-C5	-2.15	120.89	126.60
2	2	913	OMG	O6-C6-C5	-2.15	120.90	126.60
1	1	981	4AC	N4-C4-N3	2.15	117.46	113.85
2	2	680	OMG	O6-C6-C5	-2.15	120.91	126.60
2	2	467	OMG	O6-C6-C5	-2.14	120.91	126.60
1	1	2173	A2M	C6-C5-N7	2.14	136.01	132.02
2	2	1069	OMG	O6-C6-C5	-2.14	120.94	126.60
2	2	471	OMG	O6-C6-C5	-2.13	120.94	126.60
1	1	2147	OMG	O6-C6-C5	-2.13	120.95	126.60
2	2	519	OMG	O6-C6-C5	-2.13	120.96	126.60
2	2	875	5MC	O2-C2-N3	-2.12	118.88	122.33
1	1	1621	4AC	N4-C4-N3	2.12	117.42	113.85
2	2	693	5MC	O2-C2-N3	-2.11	118.89	122.33
2	2	934	OMG	O6-C6-C5	-2.11	120.99	126.60
2	2	657	OMG	O6-C6-C5	-2.11	121.01	126.60
1	1	357	4AC	O2-C2-N3	-2.10	118.92	122.33
1	1	2937	4AC	CM7-C7-N4	-2.09	111.68	115.29
2	2	64	OMU	C1'-N1-C2	2.08	121.34	117.57
1	1	1755	4AC	C1'-N1-C2	2.08	123.05	118.42
1	1	923	OMG	C5-C6-N1	2.07	118.44	113.19
1	1	2585	4AC	CM7-C7-N4	-2.04	111.76	115.29
1	1	229	4AC	C5-C4-N4	-2.03	119.39	122.92
1	1	2162	5MC	O2-C2-N3	-2.02	119.04	122.33
2	2	1496	5MC	O2-C2-N3	-2.02	119.05	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	774	OMU	O2-C2-N1	-2.01	120.11	122.79
1	1	2733	5MC	N1-C2-N3	2.01	122.47	118.81
1	1	2678	OMG	C5-C6-N1	2.00	118.28	113.19

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	2147	OMG	O4'-C4'-C5'-O5'
1	1	2147	OMG	C3'-C4'-C5'-O5'
1	1	2585	4AC	O4'-C1'-N1-C2
1	1	2585	4AC	O4'-C1'-N1-C6
1	1	2608	4AC	O4'-C1'-N1-C2
1	1	2608	4AC	O4'-C1'-N1-C6
1	1	2733	5MC	C2'-C1'-N1-C6
2	2	1505	5MC	C2'-C1'-N1-C2
2	2	1505	5MC	C2'-C1'-N1-C6
1	1	789	OMG	C3'-C4'-C5'-O5'
2	2	1488	MA6	O4'-C4'-C5'-O5'
1	1	789	OMG	O4'-C4'-C5'-O5'
1	1	2733	5MC	C2'-C1'-N1-C2
2	2	20	OMU	C2'-C1'-N1-C6
2	2	1488	MA6	C3'-C4'-C5'-O5'
2	2	934	OMG	O4'-C4'-C5'-O5'
1	1	2992	4AC	O7-C7-N4-C4
1	1	2992	4AC	CM7-C7-N4-C4
2	2	1069	OMG	C1'-C2'-O2'-CM2
2	2	20	OMU	O4'-C1'-N1-C6
2	2	1498	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
1	1	2733	5MC	O4'-C1'-N1-C2
2	2	1498	5MC	O4'-C1'-N1-C2
2	2	1202	5MC	O4'-C4'-C5'-O5'
1	1	2733	5MC	O4'-C1'-N1-C6
1	1	789	OMG	C3'-C2'-O2'-CM2
1	1	2147	OMG	C3'-C2'-O2'-CM2
2	2	913	OMG	C3'-C2'-O2'-CM2
2	2	1177	OMU	C3'-C2'-O2'-CM2
2	2	1505	5MC	O4'-C1'-N1-C6
2	2	20	OMU	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
2	2	20	OMU	O4'-C1'-N1-C2
2	2	1069	OMG	C3'-C2'-O2'-CM2
2	2	787	OMU	C2'-C1'-N1-C6
2	2	934	OMG	C3'-C4'-C5'-O5'
2	2	787	OMU	O4'-C1'-N1-C6
1	1	2992	4AC	O4'-C4'-C5'-O5'
2	2	20	OMU	O4'-C4'-C5'-O5'
2	2	1505	5MC	O4'-C1'-N1-C2
1	1	2144	OMG	C3'-C2'-O2'-CM2
2	2	1498	5MC	O4'-C4'-C5'-O5'
2	2	1202	5MC	C2'-C1'-N1-C2
2	2	1498	5MC	C2'-C1'-N1-C2
2	2	873	OMG	C4'-C5'-O5'-P

There are no ring outliers.

72 monomers are involved in 93 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	2545	4AC	1	0
1	1	789	OMG	1	0
2	2	839	4AC	1	0
1	1	1293	4AC	1	0
2	2	626	4AC	1	0
2	2	319	4AC	1	0
1	1	1780	4AC	1	0
1	1	229	4AC	1	0
1	1	2001	4AC	2	0
2	2	1380	OMU	2	0
1	1	2198	5MC	1	0
1	1	2992	4AC	1	0
2	2	546	4AC	2	0
2	2	1239	4AC	1	0
2	2	846	OMC	1	0
1	1	1065	4AC	1	0
2	2	1233	4AC	1	0
2	2	1177	OMU	2	0
1	1	1594	4AC	1	0
2	2	680	OMG	1	0
1	1	3004	4AC	1	0
2	2	394	4AC	1	0
1	1	2495	4AC	1	0
1	1	2570	4AC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	1617	4AC	2	0
2	2	1025	5MC	1	0
1	1	1755	4AC	2	0
1	1	1550	4AC	1	0
1	1	91	4AC	2	0
1	1	1048	4AC	1	0
2	2	64	OMU	1	0
2	2	479	4AC	1	0
1	1	243	4AC	1	0
1	1	1460	4AC	1	0
2	2	774	OMU	1	0
2	2	703	4AC	6	0
2	2	379	4AC	1	0
1	1	835	4AC	1	0
2	2	1376	OMC	2	0
1	1	1667	4AC	3	0
1	1	2548	4AC	1	0
1	1	2585	4AC	3	0
1	1	1934	4AC	1	0
1	1	2608	4AC	3	0
1	1	1878	4AC	1	0
1	1	451	4AC	1	0
2	2	1202	5MC	1	0
1	1	1695	4AC	1	0
2	2	1487	MA6	1	0
1	1	1662	4AC	1	0
2	2	848	4AC	1	0
2	2	53	4AC	1	0
1	1	802	4AC	2	0
2	2	636	4AC	3	0
1	1	341	4AC	1	0
1	1	2718	4AC	1	0
1	1	211	4AC	1	0
2	2	1469	6MZ	1	0
1	1	458	4AC	1	0
2	2	373	A2M	1	0
2	2	731	4AC	1	0
2	2	1479	4AC	1	0
1	1	2027	4AC	1	0
2	2	129	OMC	1	0
1	1	60	4AC	2	0
1	1	615	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	1055	A2M	1	0
1	1	2287	4AC	2	0
1	1	1867	4AC	1	0
2	2	1069	OMG	1	0
2	2	957	4AC	1	0
2	2	1488	MA6	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 257 ligands modelled in this entry, 257 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	107:G	O3'	112:A	P	11.57

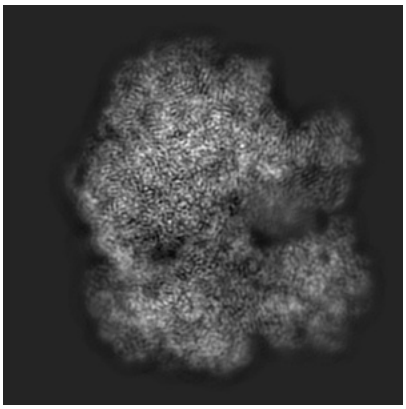
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-55138. These allow visual inspection of the internal detail of the map and identification of artifacts.

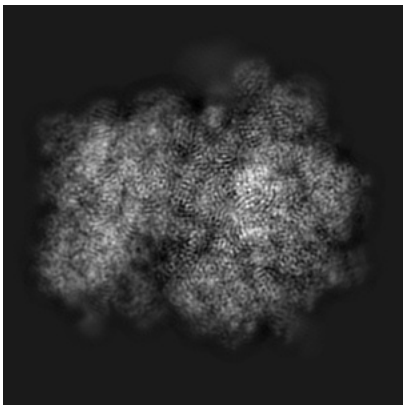
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

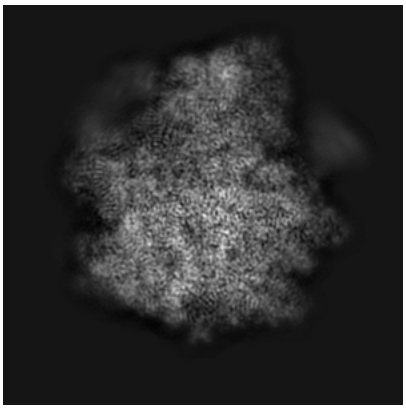
6.1.1 Primary map



X

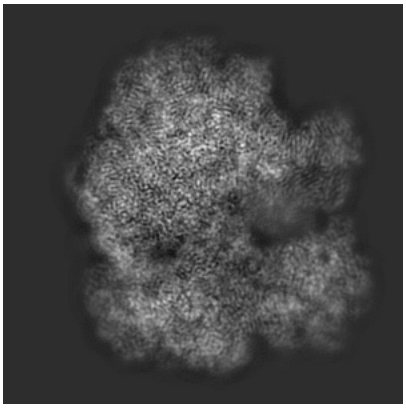


Y

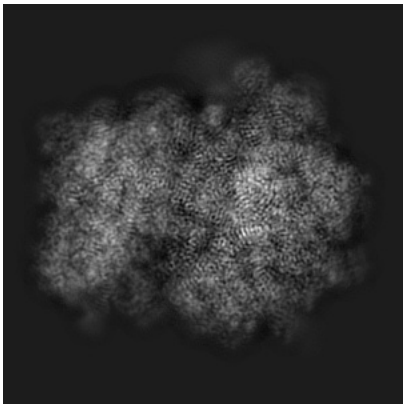


Z

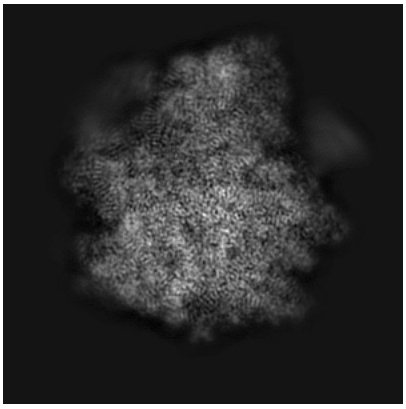
6.1.2 Raw map



X



Y

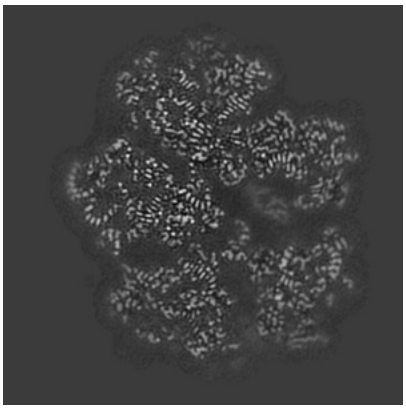


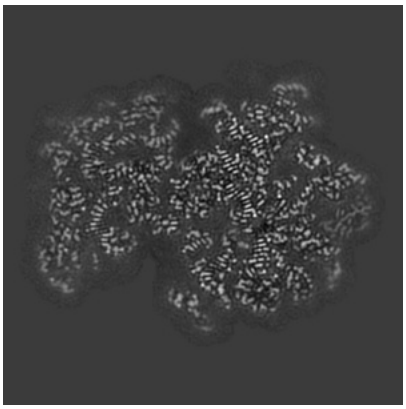
Z

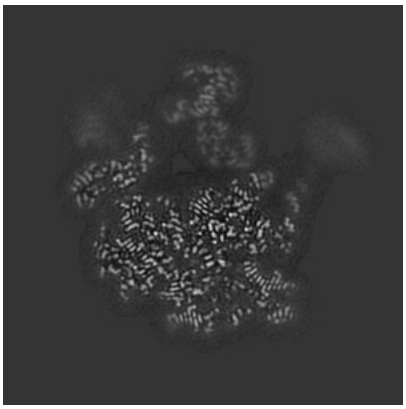
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

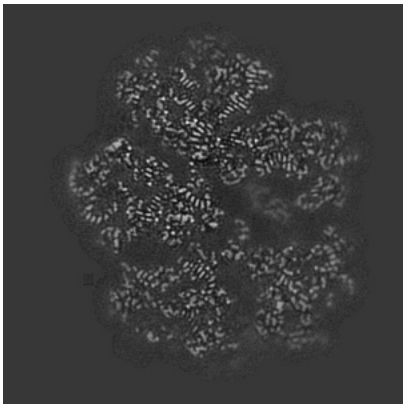
6.2.1 Primary map

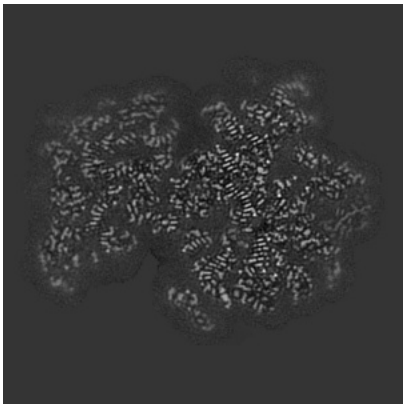

X Index: 180

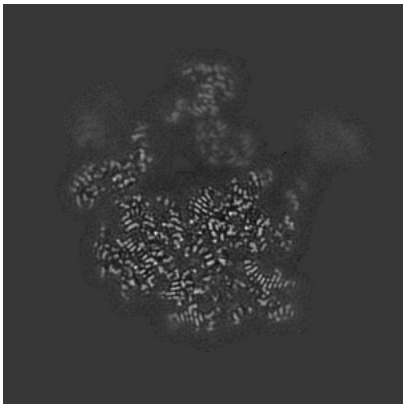

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

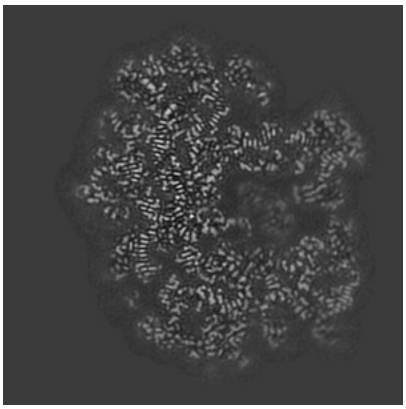

Y Index: 180


Z Index: 180

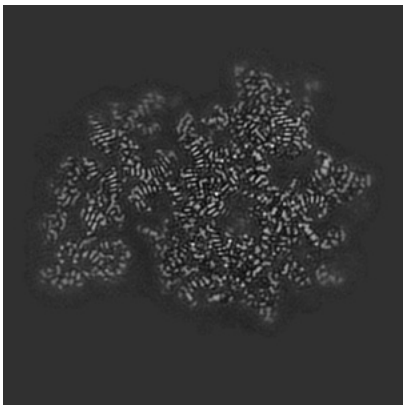
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

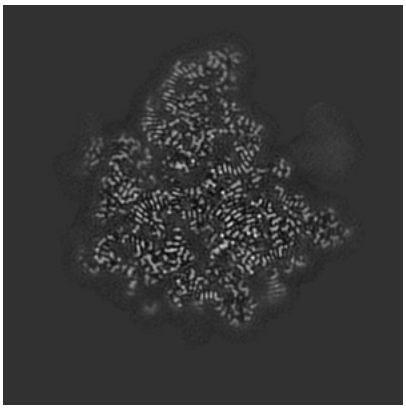
6.3.1 Primary map



X Index: 195

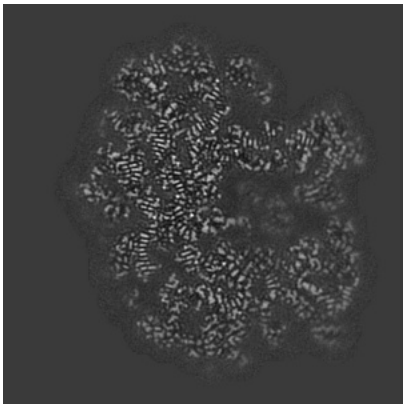


Y Index: 166

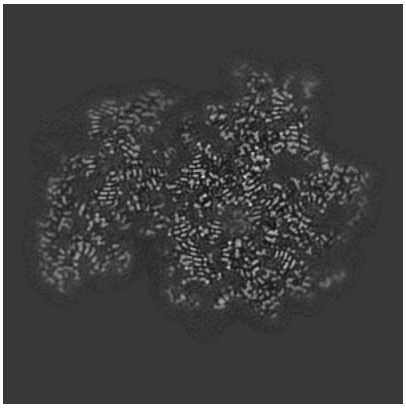


Z Index: 228

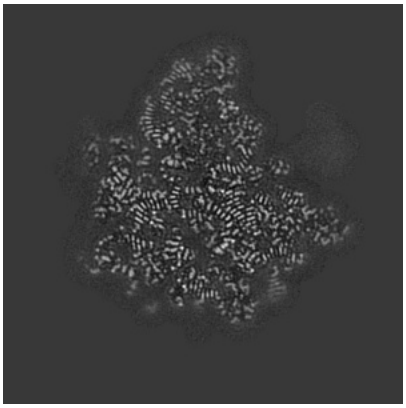
6.3.2 Raw map



X Index: 195



Y Index: 171

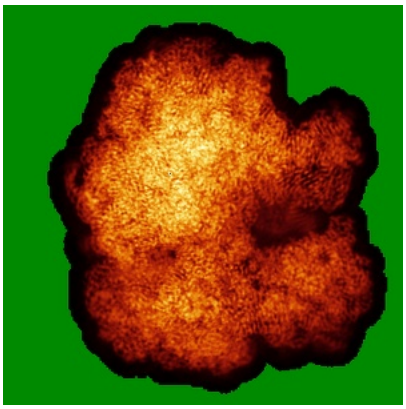


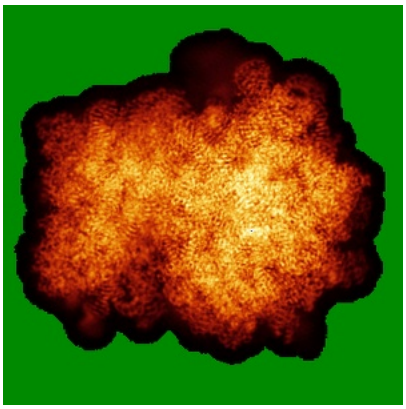
Z Index: 229

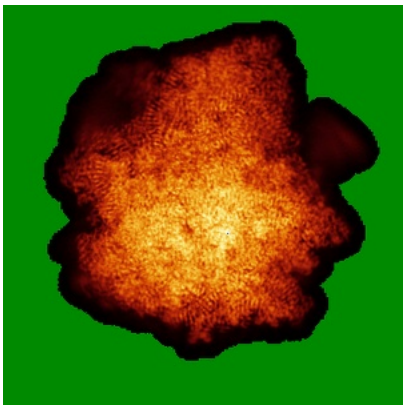
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

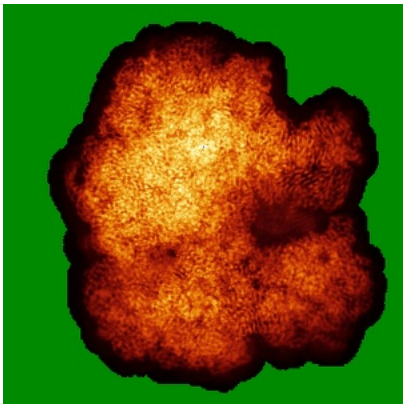
6.4.1 Primary map

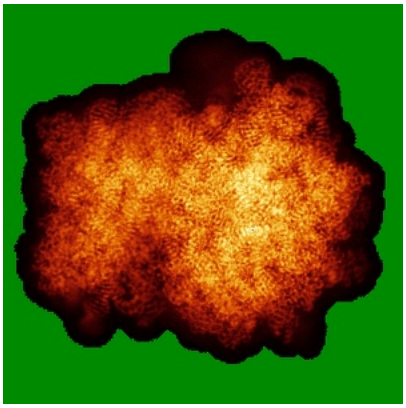

X

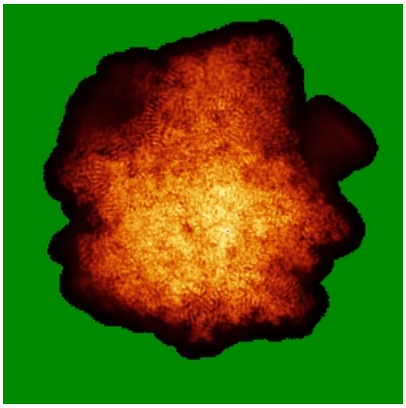

Y


Z

6.4.2 Raw map


X

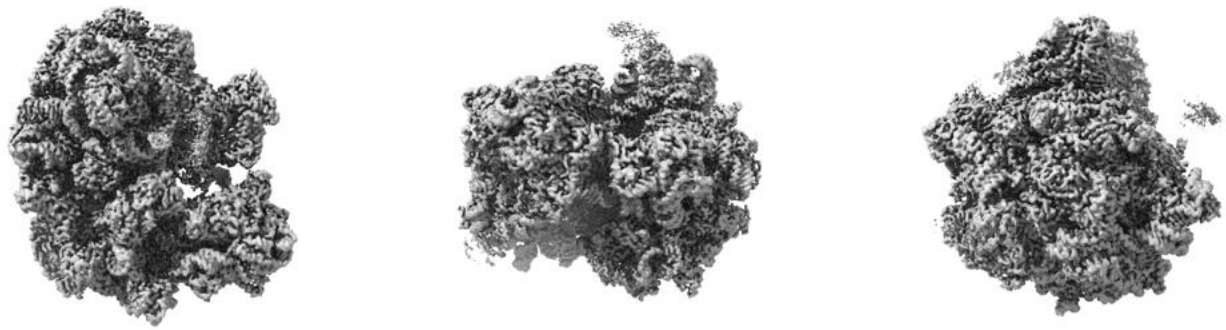

Y


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)

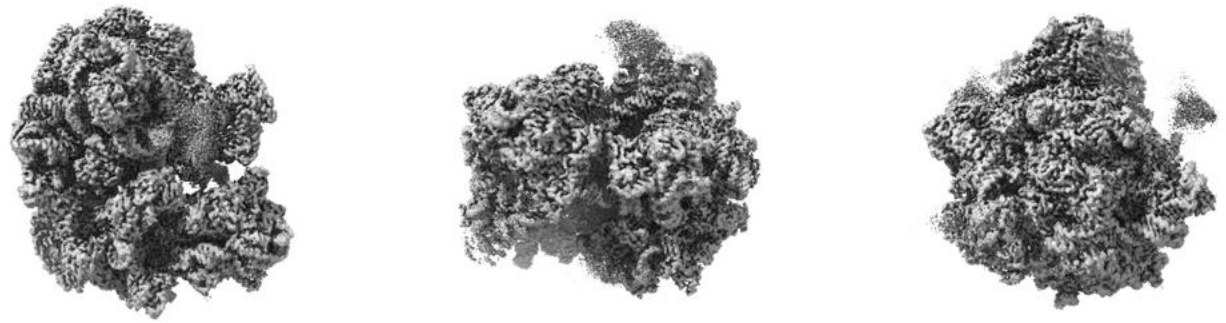
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

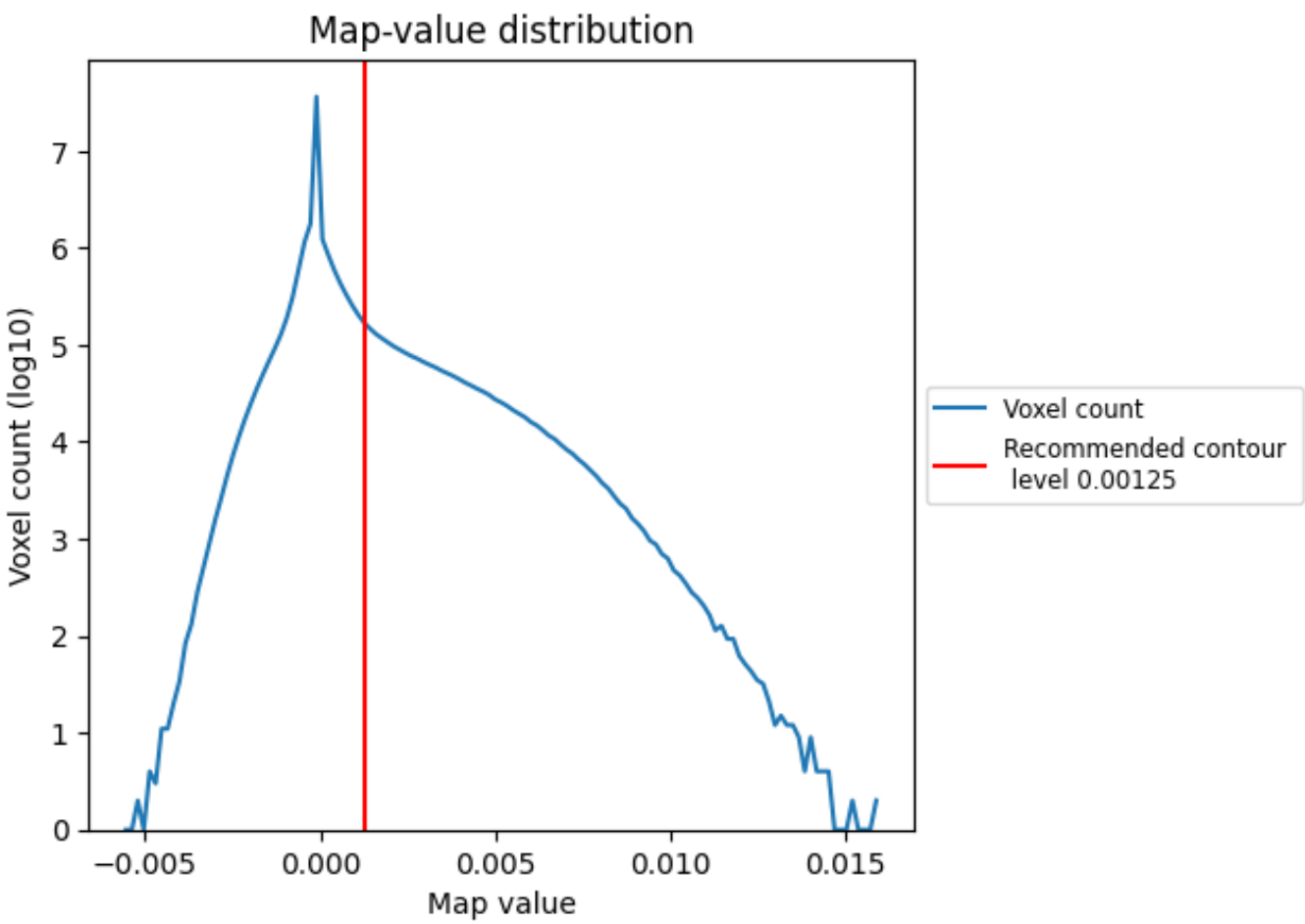
6.6 Mask visualisation (i)

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

7 Map analysis (i)

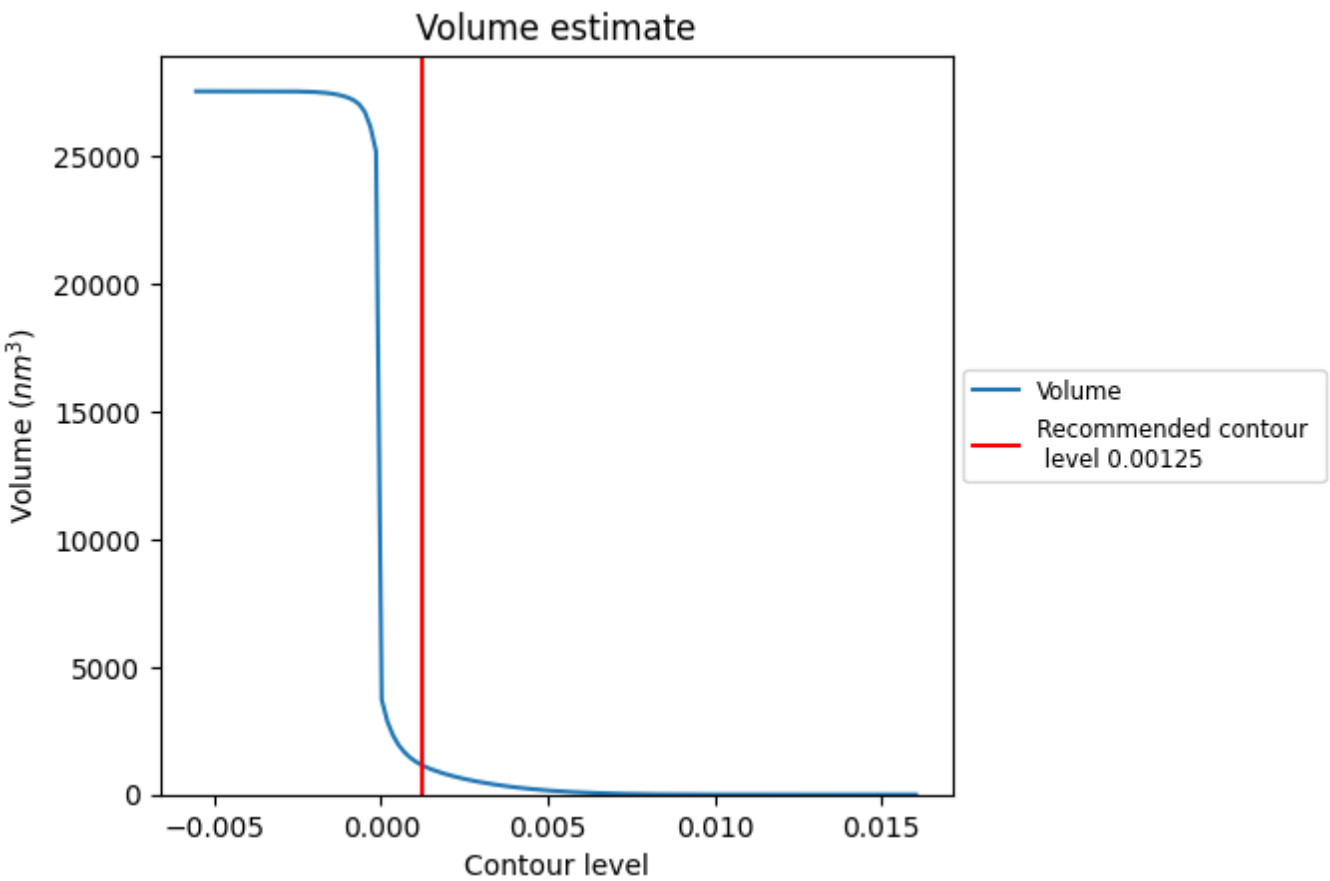
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

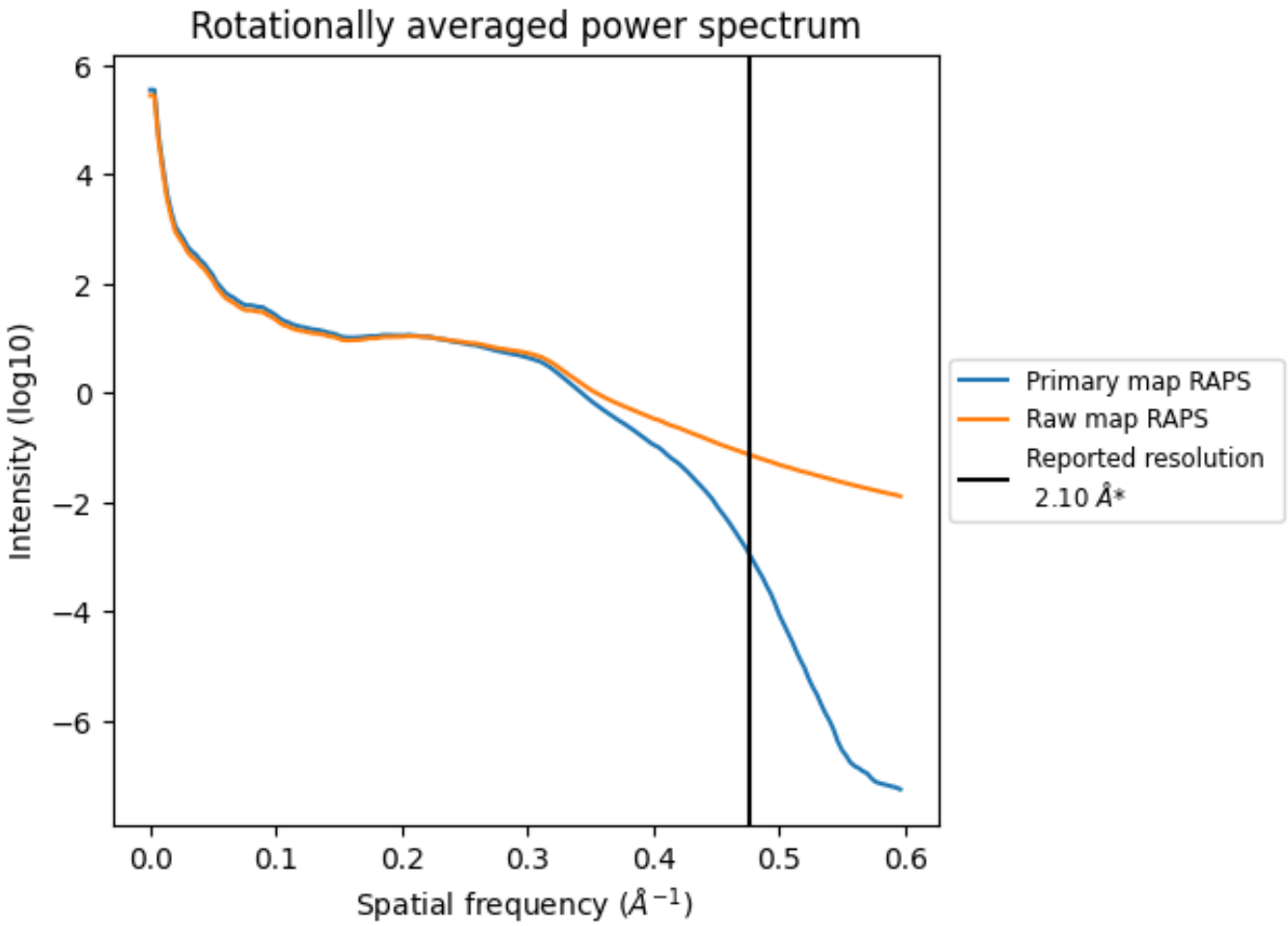
7.2 Volume estimate (i)



The volume at the recommended contour level is 1139 nm^3; this corresponds to an approximate mass of 1029 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 (i)

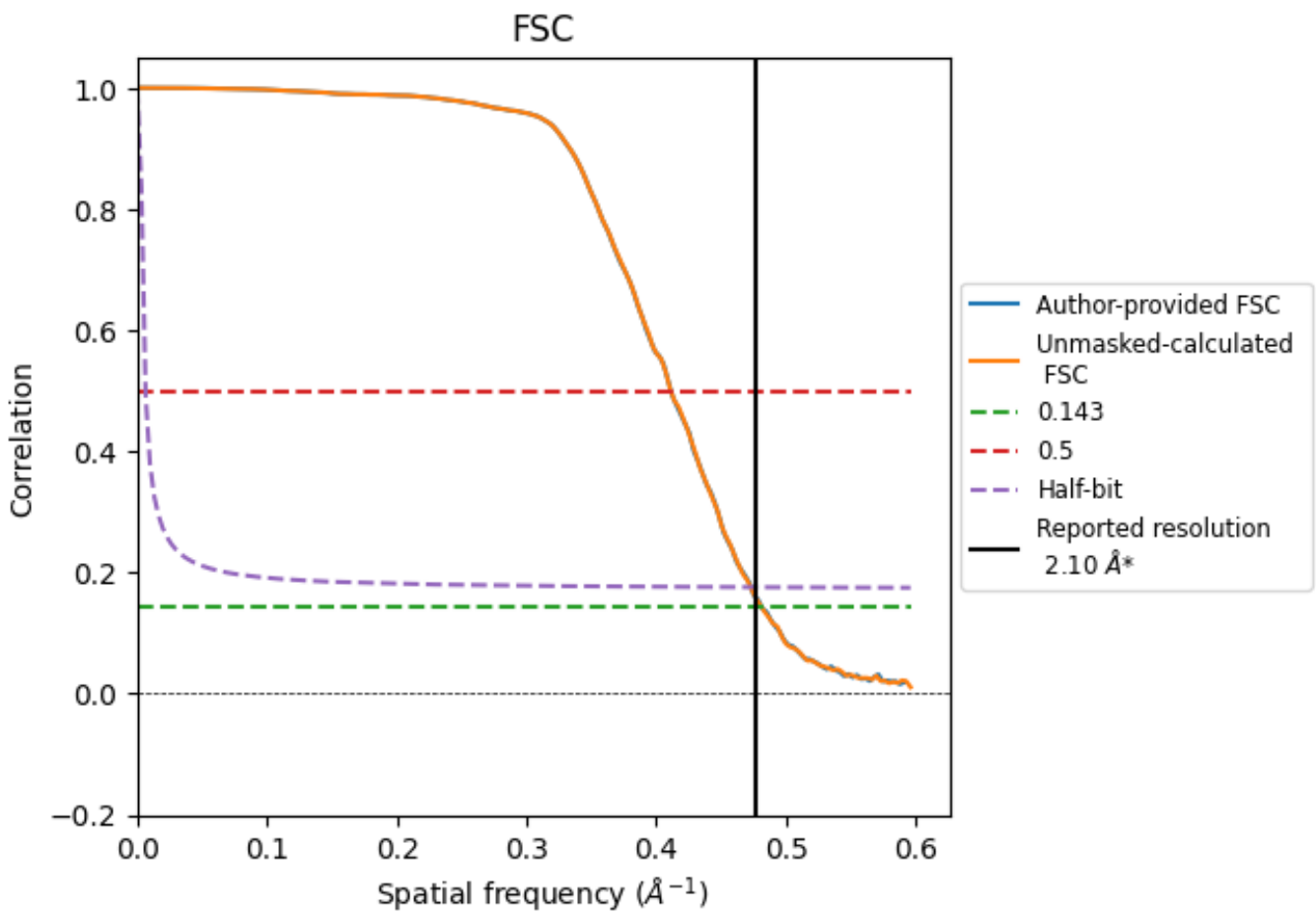


*Reported resolution corresponds to spatial frequency of 0.476 Å^{-1}

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 Å^{-1}

8.2 Resolution estimates (i)

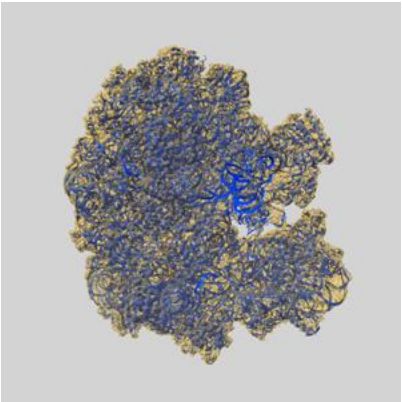
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.08	2.43	2.11
Unmasked-calculated*	2.08	2.43	2.12

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

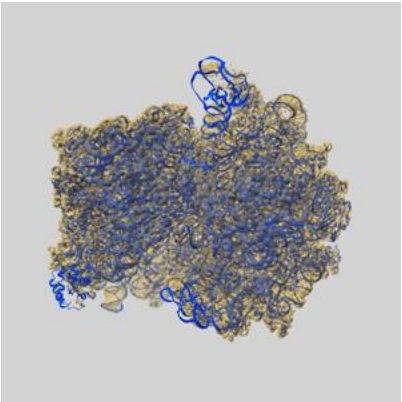
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-55138 and PDB model 9SRD. Per-residue inclusion information can be found in section 3 on page 17.

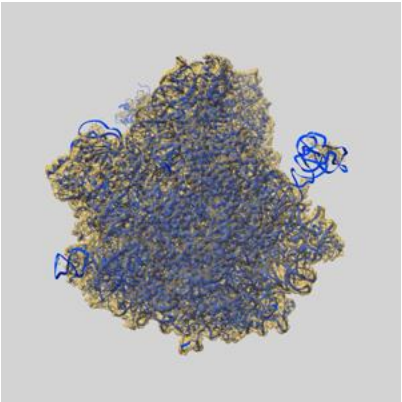
9.1 Map-model overlay (i)



X



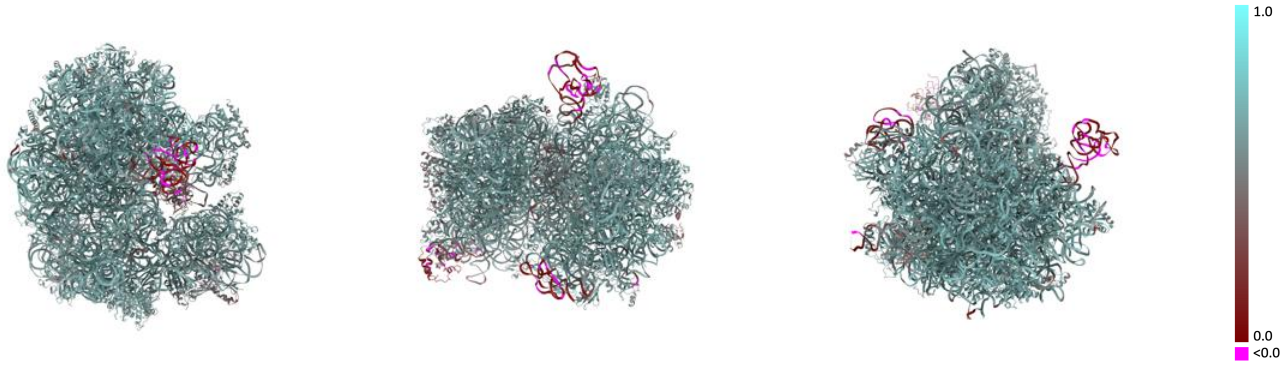
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00125 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.

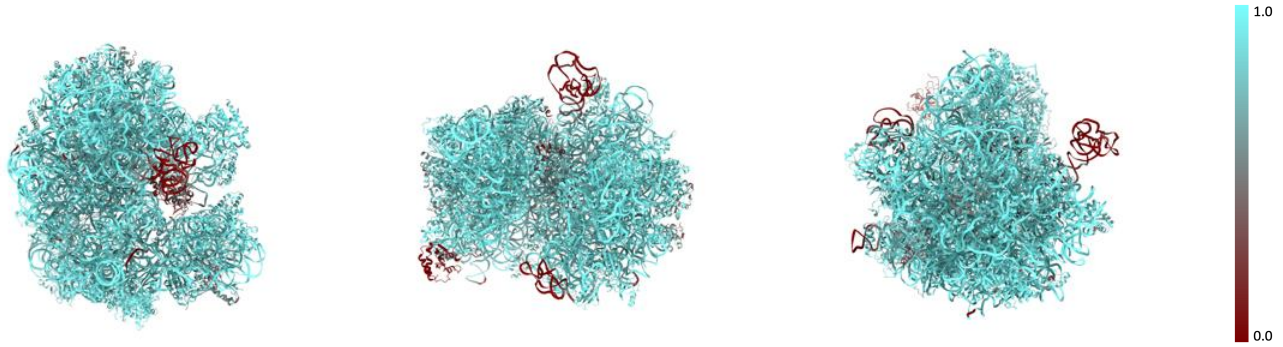
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

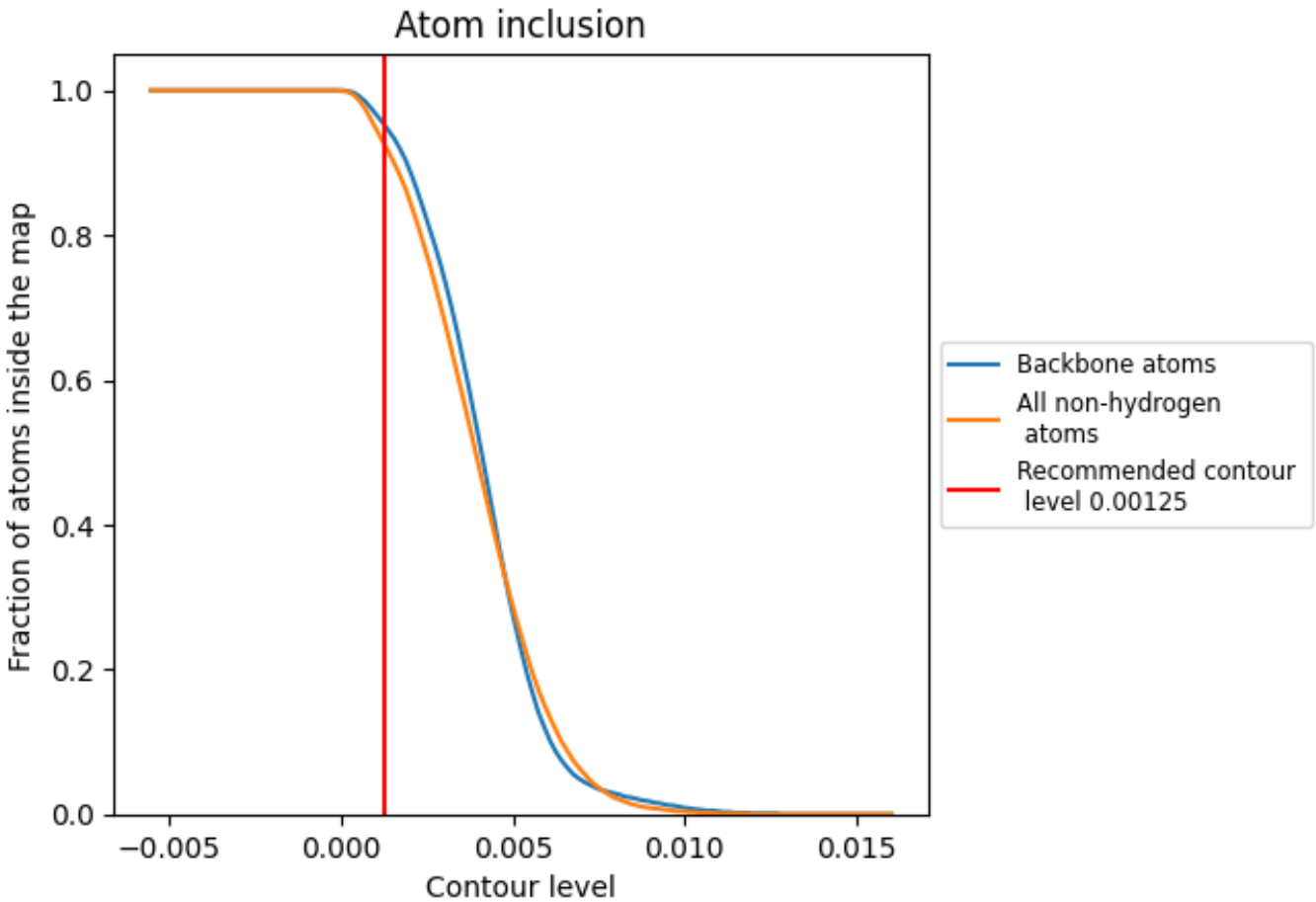
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.00125).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.00125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9260	0.6220
1	0.9380	0.6260
2	0.9820	0.6300
3	0.9930	0.6230
A0	0.9370	0.6750
A3	0.0610	0.1700
AA	0.8560	0.5930
AB	0.9310	0.6050
AC	0.9230	0.6260
AD	0.9430	0.6360
AE	0.9420	0.6230
AF	0.9300	0.6310
AG	0.8190	0.5470
AH	0.9060	0.6020
AI	0.9550	0.6530
AJ	0.9170	0.6330
AK	0.9210	0.5980
AL	0.7630	0.5090
AM	0.9140	0.6230
AN	0.9220	0.6420
AO	0.9110	0.5930
AP	0.8940	0.5950
AQ	0.9210	0.6270
AR	0.9360	0.6450
AS	0.8820	0.5560
AT	0.8750	0.5810
AU	0.9380	0.6170
AV	0.9070	0.6030
AW	0.8910	0.5760
AX	0.8480	0.5710
AY	0.1880	0.1240
AZ	0.8230	0.5440
B4	0.5690	0.4650
B5	0.9400	0.6200
B6	0.6350	0.6090

Continued on next page...

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Chain	Atom inclusion	Q-score
BB	0.9680	0.6850
BC	0.9590	0.6760
BD	0.9720	0.6730
BE	0.8700	0.5700
BF	0.9160	0.6180
BG	0.9150	0.6260
BI	0.9550	0.6700
BJ	0.9570	0.6790
BK	0.9190	0.5900
BL	0.9220	0.6350
BM	0.9860	0.6940
BN	0.9140	0.6360
BO	0.9290	0.6120
BP	0.9620	0.6620
BQ	0.9390	0.6610
BR	0.9620	0.6690
BS	0.9680	0.6740
BT	0.9490	0.6500
BU	0.9540	0.6490
BV	0.9530	0.6680
BW	0.8530	0.5920
BY	0.9600	0.6650
BZ	0.9060	0.6070
Ba	0.9120	0.6390
Bb	0.9570	0.6770
Bc	0.9440	0.6640
Bd	0.9610	0.6540
Be	0.9920	0.6890
Bf	0.9880	0.6720
Bg	0.9650	0.6490
Bi	0.9430	0.6790
Bj	0.9350	0.6550
Bk	0.9330	0.6450
Bl	0.8920	0.6140
H	0.5110	0.4780