



## wwPDB EM Map/Model Validation Report ⓘ

May 19, 2016 – 03:50 PM EDT

PDB ID : 5AJ4  
EMDB ID: : EMD-2914  
Title : Structure of the 55S mammalian mitoribosome.  
Authors : Greber, B.J.; Bieri, P.; Leibundgut, M.; Leitner, A.; Aebersold, R.; Boehringer, D.; Ban, N.  
Deposited on : 2015-02-20  
Resolution : 3.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

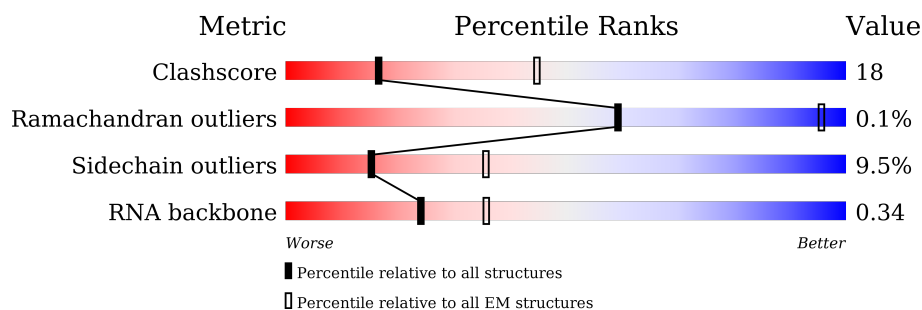
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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.











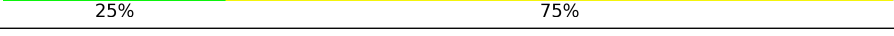

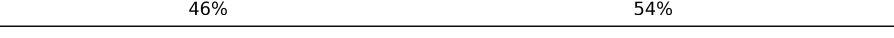
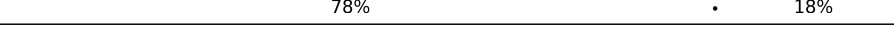

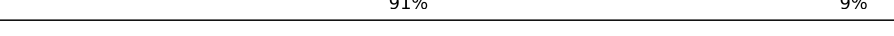
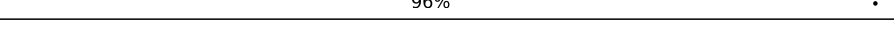
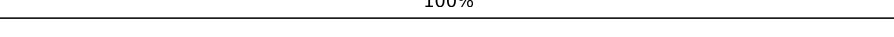
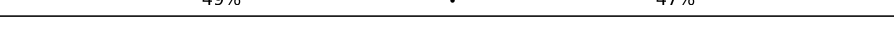

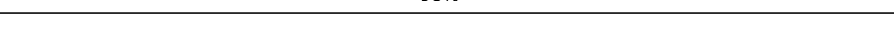






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	AA	962	42% (green) 43% (yellow) 15% (orange)
2	AB	220	72% (green) 25% (yellow) . (orange)
3	AC	132	64% (green) 33% (yellow) . (orange)
4	AE	328	59% (green) 37% (yellow) . (orange)
5	AF	124	69% (green) 27% (yellow) . . (orange)
6	AG	208	69% (green) 28% (yellow) . (orange)
7	AI	311	67% (green) 31% (yellow) . (orange)
8	AJ	201	38% (green) 24% (yellow) . (orange) 36% (grey)

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Mol	Chain	Length	Quality of chain
9	AK	136	
10	AL	109	
11	AN	128	
12	AO	239	
13	AP	117	
14	AQ	109	
15	AR	97	
16	AU	86	
17	AV	69	
17	AY	69	
18	AX	13	
19	Aa	356	
20	Ab	190	
21	Ac	169	
22	Ad	177	
23	Ae	336	
24	Af	188	
25	Ag	397	
26	Ah	103	
27	Ai	99	
28	Aj	218	
29	Ak	275	
30	Am	116	
31	An	72	
32	Ao	530	






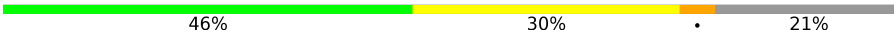



















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Mol	Chain	Length	Quality of chain
33	Ap	188	
34	As	16	
35	Az	17	
36	B0	148	
37	B1	256	
38	B2	252	
39	B3	161	
40	B4	126	
41	B5	188	
42	B6	65	
43	B7	95	
44	B8	188	
45	B9	100	
46	BA	1570	
47	BB	51	
48	BD	306	
49	BE	348	
50	BF	294	
51	BI	268	
52	BJ	262	
53	BK	192	
54	BN	178	
55	BO	145	
56	BP	296	
57	BQ	251	

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Mol	Chain	Length	Quality of chain
58	BR	169	
59	BS	180	
60	BT	292	
61	BU	149	
62	BV	209	
63	BW	210	
64	BX	150	
65	BY	216	
66	Ba	423	
67	Bb	380	
68	Bc	334	
69	Bd	206	
70	Be	135	
71	Bf	142	
72	Bg	159	
73	Bh	332	
74	Bi	312	
75	Bj	279	
76	Bk	212	
77	Bl	166	
78	Bm	159	
79	Bn	128	
80	Bo	124	
81	Bp	112	
82	Bq	138	

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Mol	Chain	Length	Quality of chain
83	Bt	102	 78%14%8%
84	Bu	205	 70%26%
85	Bv	222	 56%41%
86	Bw	433	 79%10%11%
87	Bx	196	 75%8%17%
88	Bz	94	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	Y5P	AV	55	-	-	X	-
17	Y5P	AY	55	-	-	X	-
17	Y5P	AY	58	-	-	X	-

## 2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 167915 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 MITORIBOSOMAL 12S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	960	Total	C	N	O	P	0	0
			20411	9162	3708	6581	960		

- Molecule 2 is a protein called MITORIBOSOMAL PROTEIN US2M, MRPS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	220	Total	C	N	O	S	0	0
			1762	1126	326	304	6		

- Molecule 3 is a protein called MITORIBOSOMAL PROTEIN US3M, MRPS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	132	Total	C	N	O	S	0	0
			1075	695	195	181	4		

- Molecule 4 is a protein called MITORIBOSOMAL PROTEIN US5M, MRPS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AE	328	Total	C	N	O	S	0	0
			2621	1641	498	471	11		

- Molecule 5 is a protein called MITORIBOSOMAL PROTEIN BS6M, MRPS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AF	123	Total	C	N	O	S	0	0
			990	626	180	178	6		

- Molecule 6 is a protein called MITORIBOSOMAL PROTEIN US7M, MRPS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AG	208	Total	C	N	O	S	0	0
			1721	1097	314	299	11		

- Molecule 7 is a protein called MITORIBOSOMAL PROTEIN US9M, MRPS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AI	311	Total	C	N	O	S	0	0
			2498	1586	450	449	13		

- Molecule 8 is a protein called MITORIBOSOMAL PROTEIN US10M, MRPS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AJ	129	Total	C	N	O	S	0	0
			1067	690	182	192	3		

- Molecule 9 is a protein called MITORIBOSOMAL PROTEIN US11M, MRPS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AK	136	Total	C	N	O	S	0	0
			1001	628	192	178	3		

- Molecule 10 is a protein called MITORIBOSOMAL PROTEIN US12M, MRPS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AL	109	Total	C	N	O	S	0	0
			840	524	172	138	6		

- Molecule 11 is a protein called MITORIBOSOMAL PROTEIN US14M, MRPS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AN	101	Total	C	N	O	S	0	0
			858	534	174	144	6		

- Molecule 12 is a protein called MITORIBOSOMAL PROTEIN US15M, MRPS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AO	175	Total	C	N	O	S	0	0
			1448	919	272	248	9		

- Molecule 13 is a protein called MITORIBOSOMAL PROTEIN BS16M, MRPS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AP	117	Total	C	N	O	S	0	0
			932	588	184	155	5		

- Molecule 14 is a protein called MITORIBOSOMAL PROTEIN US17M, MRPS17.



Mol	Chain	Residues	Atoms					AltConf	Trace
14	AQ	109	Total	C	N	O	S	0	0
			853	555	150	145	3		

- Molecule 15 is a protein called MITORIBOSOMAL PROTEIN BS18M, MRPS18C.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AR	97	Total	C	N	O	S	0	0
			784	507	132	138	7		

- Molecule 16 is a protein called MITORIBOSOMAL PROTEIN BS21M, MRPS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AU	86	Total	C	N	O	S	0	0
			734	453	148	125	8		

- Molecule 17 is a RNA chain called P-SITE AND A-SITE TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AV	69	Total	C	N	O	P	0	0
			1251	625	146	412	68		
17	AY	69	Total	C	N	O	P	0	0
			1251	625	146	412	68		

- Molecule 18 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AX	13	Total	C	N	O	P	0	0
			231	117	26	76	12		

- Molecule 19 is a protein called MITORIBOSOMAL PROTEIN MS22, MRPS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Aa	292	Total	C	N	O	S	0	0
			2296	1476	394	417	9		

- Molecule 20 is a protein called MITORIBOSOMAL PROTEIN MS23, MRPS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Ab	135	Total	C	N	O	S	0	0
			1101	709	199	192	1		

- Molecule 21 is a protein called MITORIBOSOMAL PROTEIN MS25, MRPS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Ac	169	Total	C	N	O	S	0	0
			1367	876	236	245	10		

- Molecule 22 is a protein called MITORIBOSOMAL PROTEIN MS26, MRPS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Ad	177	Total	C	N	O	S	0	0
			1467	904	288	273	2		

- Molecule 23 is a protein called MITORIBOSOMAL PROTEIN MS27, MRPS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Ae	336	Total	C	N	O	S	0	0
			2016	1344	336	336			

- Molecule 24 is a protein called MITORIBOSOMAL PROTEIN MS28, MRPS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Af	99	Total	C	N	O	S	0	0
			778	494	134	146	4		

- Molecule 25 is a protein called MITORIBOSOMAL PROTEIN MS29, MRPS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ag	346	Total	C	N	O	S	0	0
			2774	1786	489	489	10		

- Molecule 26 is a protein called MITORIBOSOMAL PROTEIN MS31, MRPS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Ah	103	Total	C	N	O	S	0	0
			876	569	145	159	3		

- Molecule 27 is a protein called MITORIBOSOMAL PROTEIN MS33, MRPS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Ai	99	Total	C	N	O	S	0	0
			824	522	156	143	3		

- Molecule 28 is a protein called MITORIBOSOMAL PROTEIN MS34, MRPS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Aj	213	Total	C	N	O	S	0	0
			1777	1123	339	308	7		

- Molecule 29 is a protein called MITORIBOSOMAL PROTEIN MS35, MRPS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Ak	275	Total	C	N	O	S	0	0
			2222	1414	380	419	9		

- Molecule 30 is a protein called MITORIBOSOMAL PROTEIN MS37, MRPS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Am	116	Total	C	N	O	S	0	0
			930	577	185	160	8		

- Molecule 31 is a protein called MITORIBOSOMAL PROTEIN MS38, MRPS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	An	72	Total	C	N	O	S	0	0
			639	407	139	92	1		

- Molecule 32 is a protein called MITORIBOSOMAL PROTEIN MS39, MRPS39.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ao	476	Total	C	N	O	S	0	0
			3028	2007	500	519	2		

- Molecule 33 is a protein called 28S RIBOSOMAL PROTEIN S18B, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ap	188	Total	C	N	O	S	0	0
			1551	983	290	270	8		

- Molecule 34 is a protein called UNASSIGNED HELICES.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	As	16	Total	C	N	O	0	0
			96	64	16	16		

- Molecule 35 is a protein called UNASSIGNED HELICES.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	Az	17	Total	C	N	O	0	0
			102	68	17	17		

- Molecule 36 is a protein called MITORIBOSOMAL PROTEIN BL27M, MRPL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B0	114	Total	C	N	O	S	0	0
			878	564	160	151	3		

- Molecule 37 is a protein called MITORIBOSOMAL PROTEIN BL28M, MRPL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	B1	244	Total	C	N	O	S	0	0
			2036	1315	363	353	5		

- Molecule 38 is a protein called MITORIBOSOMAL PROTEIN UL29M, MRPL47.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	B2	178	Total	C	N	O	S	0	0
			1544	990	289	259	6		

- Molecule 39 is a protein called MITORIBOSOMAL PROTEIN UL30M, MRPL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	B3	118	Total	C	N	O	S	0	0
			968	622	178	165	3		

- Molecule 40 is a protein called MITORIBOSOMAL PROTEIN BL31M, MRPL55.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	B4	45	Total	C	N	O	S	0	0
			381	239	77	62	3		

- Molecule 41 is a protein called MITORIBOSOMAL PROTEIN BL32M, MRPL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	B5	110	Total	C	N	O	S	0	0
			902	553	181	162	6		

- Molecule 42 is a protein called MITORIBOSOMAL PROTEIN BL33M, MRPL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	B6	48	Total	C	N	O	S	0	0
			391	253	70	66	2		

- Molecule 43 is a protein called MITORIBOSOMAL PROTEIN BL34M, MRPL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	B7	46	Total	C	N	O	S	0	0
			387	239	89	58	1		

- Molecule 44 is a protein called MITORIBOSOMAL PROTEIN BL35M, MRPL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	B8	95	Total	C	N	O	S	0	0
			833	539	163	129	2		

- Molecule 45 is a protein called MITORIBOSOMAL PROTEIN BL36M, MRPL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	B9	38	Total	C	N	O	S	0	0
			335	214	70	47	4		

- Molecule 46 is a RNA chain called MITORIBOSOMAL 16S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BA	1515	Total	C	N	O	P	0	0
			32233	14473	5860	10385	1515		

- Molecule 47 is a RNA chain called MITORIBOSOMAL CP TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BB	51	Total	C	N	O	P	0	0
			1008	489	162	306	51		

- Molecule 48 is a protein called MITORIBOSOMAL PROTEIN UL2M, MRPL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BD	240	Total	C	N	O	S	0	0
			1860	1160	371	319	10		

- Molecule 49 is a protein called MITORIBOSOMAL PROTEIN UL3M, MRPL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BE	307	Total	C	N	O	S	0	0
			2420	1554	426	430	10		

- Molecule 50 is a protein called MITORIBOSOMAL PROTEIN UL4M, MRPL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BF	250	Total	C	N	O	S	0	0
			2011	1294	367	344	6		

- Molecule 51 is a protein called MITORIBOSOMAL PROTEIN BL9M, MRPL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BI	98	Total	C	N	O	S	0	0
			805	509	155	141			

- Molecule 52 is a protein called MITORIBOSOMAL PROTEIN UL10M, MRPL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BJ	168	Total	C	N	O	S	0	0
			1361	879	248	226	8		

- Molecule 53 is a protein called MITORIBOSOMAL PROTEIN UL11M, MRPL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BK	142	Total	C	N	O	S	0	0
			1081	690	197	192	2		

- Molecule 54 is a protein called MITORIBOSOMAL PROTEIN UL13M, MRPL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BN	177	Total	C	N	O	S	0	0
			1444	926	258	253	7		

- Molecule 55 is a protein called MITORIBOSOMAL PROTEIN UL14M, MRPL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BO	115	Total	C	N	O	S	0	0
			896	562	176	154	4		

- Molecule 56 is a protein called MITORIBOSOMAL PROTEIN UL15M, MRPL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BP	288	Total	C	N	O	S	0	0
			2312	1473	430	403	6		

- Molecule 57 is a protein called MITORIBOSOMAL PROTEIN UL16M, MRPL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BQ	221	Total	C	N	O	S	0	0
			1792	1147	330	305	10		

- Molecule 58 is a protein called MITORIBOSOMAL PROTEIN BL17M, MRPL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BR	153	Total	C	N	O	S	0	0
			1240	777	236	222	5		

- Molecule 59 is a protein called MITORIBOSOMAL PROTEIN UL18M, MRPL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BS	143	Total	C	N	O	S	0	0
			1168	733	227	204	4		

- Molecule 60 is a protein called MITORIBOSOMAL PROTEIN BL19M, MRPL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BT	239	Total	C	N	O	S	0	0
			1950	1249	339	353	9		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	54	UNK	PHE	CONFLICT	UNP I3LNJ0
BT	55	UNK	GLN	CONFLICT	UNP I3LNJ0
BT	56	UNK	PRO	CONFLICT	UNP I3LNJ0
BT	57	UNK	PRO	CONFLICT	UNP I3LNJ0
BT	58	UNK	PRO	CONFLICT	UNP I3LNJ0
BT	59	UNK	LYS	CONFLICT	UNP I3LNJ0
BT	60	UNK	PRO	CONFLICT	UNP I3LNJ0
BT	61	UNK	VAL	CONFLICT	UNP I3LNJ0
BT	62	UNK	ILE	CONFLICT	UNP I3LNJ0
BT	63	UNK	VAL	CONFLICT	UNP I3LNJ0
BT	64	UNK	ASP	CONFLICT	UNP I3LNJ0
BT	65	UNK	LYS	CONFLICT	UNP I3LNJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
BT	66	UNK	ARG	CONFLICT	UNP I3LNJ0
BT	67	UNK	ARG	CONFLICT	UNP I3LNJ0
BT	68	UNK	PRO	CONFLICT	UNP I3LNJ0

- Molecule 61 is a protein called MITORIBOSOMAL PROTEIN BL20M, MRPL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BU	140	Total	C	N	O	S	0	0
			1159	732	239	185	3		

- Molecule 62 is a protein called MITORIBOSOMAL PROTEIN BL21M, MRPL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	BV	155	Total	C	N	O	S	0	0
			1231	789	219	219	4		

- Molecule 63 is a protein called MITORIBOSOMAL PROTEIN UL22M, MRPL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BW	166	Total	C	N	O	S	0	0
			1374	876	258	234	6		

- Molecule 64 is a protein called MITORIBOSOMAL PROTEIN UL23M, MRPL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	BX	134	Total	C	N	O	S	0	0
			1120	715	217	186	2		

- Molecule 65 is a protein called MITORIBOSOMAL PROTEIN UL24M, MRPL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	BY	204	Total	C	N	O	S	0	0
			1663	1047	305	306	5		

- Molecule 66 is a protein called MITORIBOSOMAL PROTEIN ML37, MRPL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Ba	393	Total	C	N	O	S	0	0
			3173	2040	556	565	12		

- Molecule 67 is a protein called MITORIBOSOMAL PROTEIN ML38, MRPL38.



Mol	Chain	Residues	Atoms					AltConf	Trace
67	Bb	354	Total	C	N	O	S	0	0
			2952	1876	542	525	9		

- Molecule 68 is a protein called MITORIBOSOMAL PROTEIN ML39, MRPL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Bc	295	Total	C	N	O	S	0	0
			2408	1541	410	441	16		

- Molecule 69 is a protein called MITORIBOSOMAL PROTEIN ML40, MRPL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Bd	99	Total	C	N	O	S	0	0
			832	528	148	155	1		

- Molecule 70 is a protein called MITORIBOSOMAL PROTEIN ML41, MRPL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Be	121	Total	C	N	O	S	0	0
			968	626	167	172	3		

- Molecule 71 is a protein called MITORIBOSOMAL PROTEIN ML42, MRPL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Bf	108	Total	C	N	O	S	0	0
			852	544	154	150	4		

- Molecule 72 is a protein called MITORIBOSOMAL PROTEIN ML43, MRPL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bg	148	Total	C	N	O	S	0	0
			1167	727	225	212	3		

- Molecule 73 is a protein called MITORIBOSOMAL PROTEIN ML44, MRPL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Bh	289	Total	C	N	O	S	0	0
			2319	1486	399	426	8		

- Molecule 74 is a protein called MITORIBOSOMAL PROTEIN ML45, MRPL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bi	242	Total	C	N	O	S	0	0
			1979	1266	352	351	10		

- Molecule 75 is a protein called MITORIBOSOMAL PROTEIN ML46, MRPL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Bj	217	Total	C	N	O	S	0	0
			1775	1137	311	321	6		

- Molecule 76 is a protein called MITORIBOSOMAL PROTEIN ML48, MRPL48.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Bk	136	Total	C	N	O	S	0	0
			1087	692	185	205	5		

- Molecule 77 is a protein called MITORIBOSOMAL PROTEIN ML49, MRPL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Bl	133	Total	C	N	O	S	0	0
			1097	709	192	194	2		

- Molecule 78 is a protein called MITORIBOSOMAL PROTEIN ML50, MRPL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Bm	109	Total	C	N	O	S	0	0
			893	568	160	162	3		

- Molecule 79 is a protein called MITORIBOSOMAL PROTEIN ML51, MRPL51.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Bn	97	Total	C	N	O	S	0	0
			837	539	166	128	4		

- Molecule 80 is a protein called MITORIBOSOMAL PROTEIN ML52, MRPL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Bo	94	Total	C	N	O	S	0	0
			747	466	143	136	2		

- Molecule 81 is a protein called MITORIBOSOMAL PROTEIN ML53, MRPL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Bp	97	Total	C	N	O	S	0	0
			742	459	143	134	6		

- Molecule 82 is a protein called MITORIBOSOMAL PROTEIN ML54, MRPL54.

Mol	Chain	Residues	Atoms				AltConf	Trace
82	Bq	37	Total	C	N	O	0	0
			336	214	69	53		

- Molecule 83 is a protein called MITORIBOSOMAL PROTEIN ML63, MRPL57.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Bt	94	Total	C	N	O	S	0	0
			780	485	168	126	1		

- Molecule 84 is a protein called MITORIBOSOMAL PROTEIN ML62, MRPL58.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Bu	151	Total	C	N	O	S	0	0
			1208	748	233	222	5		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bu	164	UNK	ALA	CONFLICT	UNP W5IDC0
Bu	165	UNK	LYS	CONFLICT	UNP W5IDC0
Bu	166	UNK	GLU	CONFLICT	UNP W5IDC0
Bu	167	UNK	PRO	CONFLICT	UNP W5IDC0
Bu	168	UNK	SER	CONFLICT	UNP W5IDC0
Bu	169	UNK	ARG	CONFLICT	UNP W5IDC0
Bu	170	UNK	GLU	CONFLICT	UNP W5IDC0
Bu	171	UNK	ASP	CONFLICT	UNP W5IDC0
Bu	172	UNK	ALA	CONFLICT	UNP W5IDC0
Bu	173	UNK	GLU	CONFLICT	UNP W5IDC0

- Molecule 85 is a protein called MITORIBOSOMAL PROTEIN ML64, MRPL59.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Bv	131	Total	C	N	O	S	0	0
			1068	662	206	195	5		

- Molecule 86 is a protein called MITORIBOSOMAL PROTEIN ML65, MRPS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Bw	387	Total	C	N	O	S	0	0
			3126	2011	548	555	12		

- Molecule 87 is a protein called MITORIBOSOMAL PROTEIN ML66, MRPS18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	Bx	162	Total	C	N	O	S	0	0
			1325	845	249	224	7		

- Molecule 88 is a protein called UNASSIGNED SECONDARY STRUCTURE ELEMENTS.

Mol	Chain	Residues	Atoms				AltConf	Trace
88	Bz	94	Total	C	N	O	0	0
			564	376	94	94		

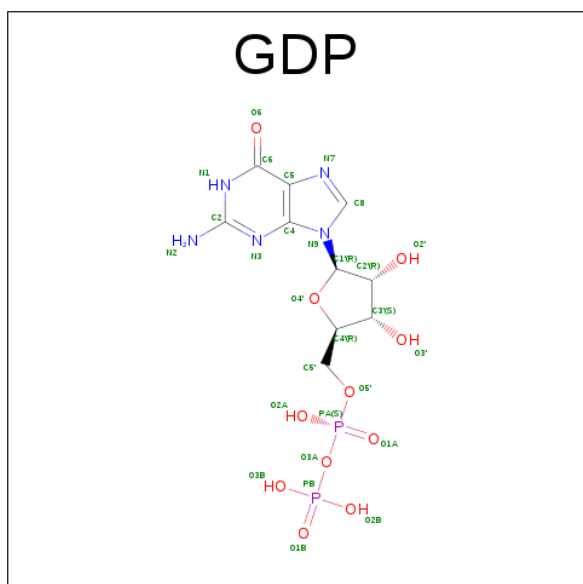
- Molecule 89 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	Ag	1	Total	Mg	0
			1	1	
89	BA	195	Total	Mg	0
			195	195	
89	BR	2	Total	Mg	0
			2	2	
89	BP	1	Total	Mg	0
			1	1	
89	AA	146	Total	Mg	0
			146	146	
89	BX	1	Total	Mg	0
			1	1	
89	BE	1	Total	Mg	0
			1	1	
89	B2	1	Total	Mg	0
			1	1	
89	BD	2	Total	Mg	0
			2	2	
89	B0	1	Total	Mg	0
			1	1	

- Molecule 90 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
90	Ap	1	Total	Zn	0
			1	1	
90	B5	1	Total	Zn	0
			1	1	
90	B9	1	Total	Zn	0
			1	1	
90	Ac	1	Total	Zn	0
			1	1	
90	Bx	1	Total	Zn	0
			1	1	
90	AR	1	Total	Zn	0
			1	1	

- Molecule 91 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
91	Ag	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 92 is water.

Mol	Chain	Residues	Atoms		AltConf
92	AA	114	Total	O	0
			114	114	
92	Ag	4	Total	O	0
			4	4	

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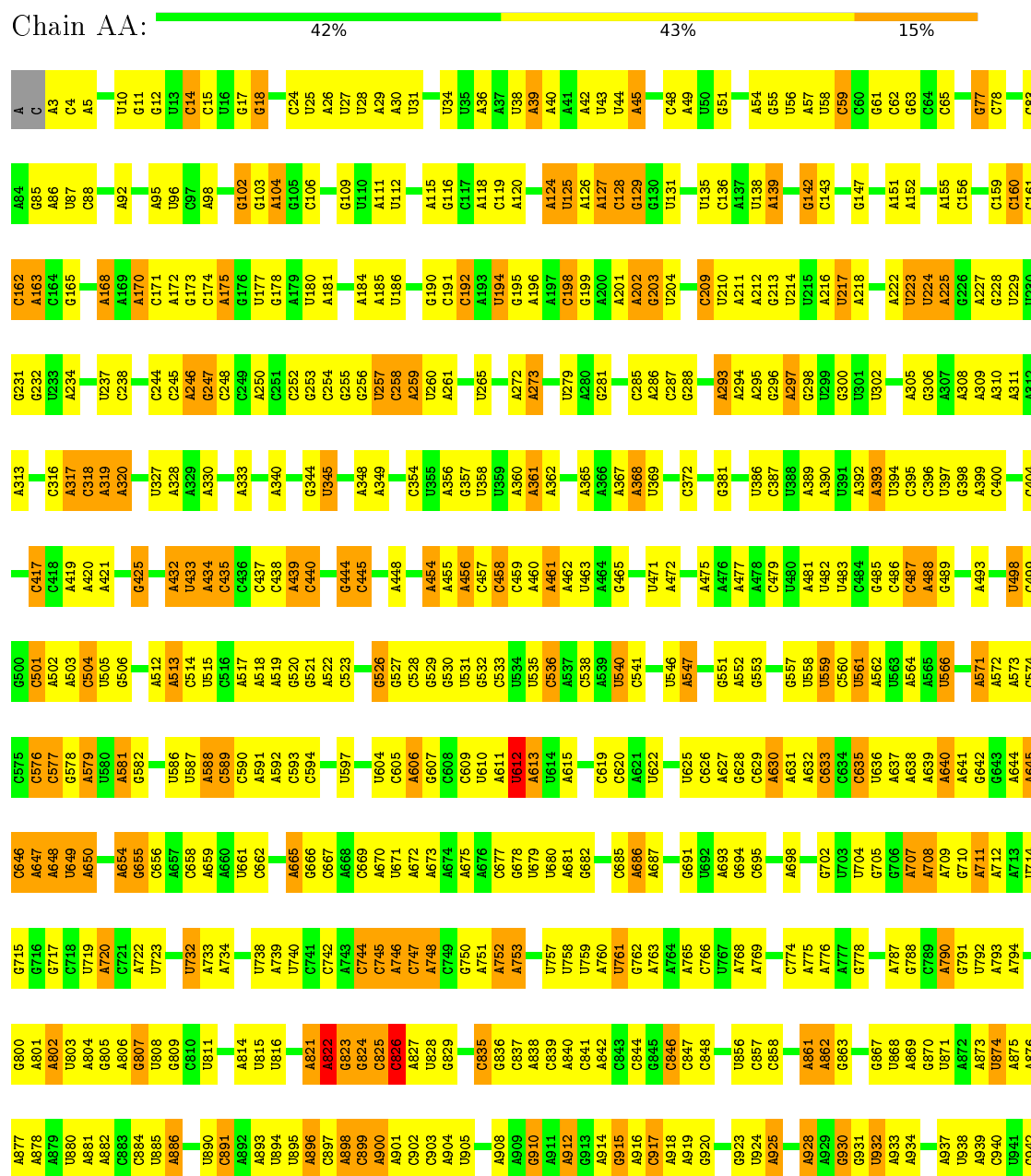
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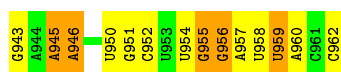
Mol	Chain	Residues	Atoms		AltConf
92	B0	3	Total 3	O 3	0
92	B7	2	Total 2	O 2	0
92	B8	1	Total 1	O 1	0
92	BA	196	Total 196	O 196	0
92	BD	3	Total 3	O 3	0
92	BF	4	Total 4	O 4	0
92	BI	1	Total 1	O 1	0
92	BO	2	Total 2	O 2	0
92	BP	3	Total 3	O 3	0
92	BR	2	Total 2	O 2	0
92	BU	1	Total 1	O 1	0
92	BW	4	Total 4	O 4	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

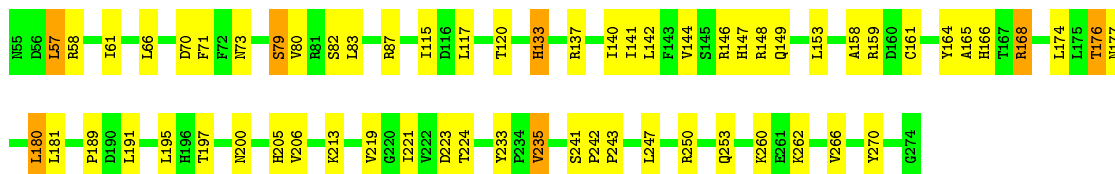
- Molecule 1: MITORIBOSOMAL 12S RRNA



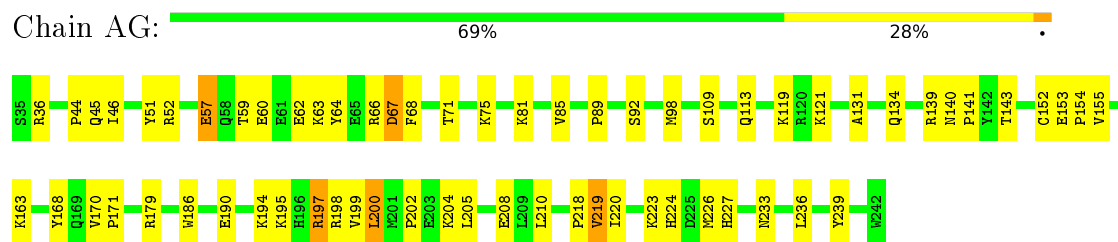


- Molecule 2: MITORIBOSOMAL PROTEIN US2M, MRPS2

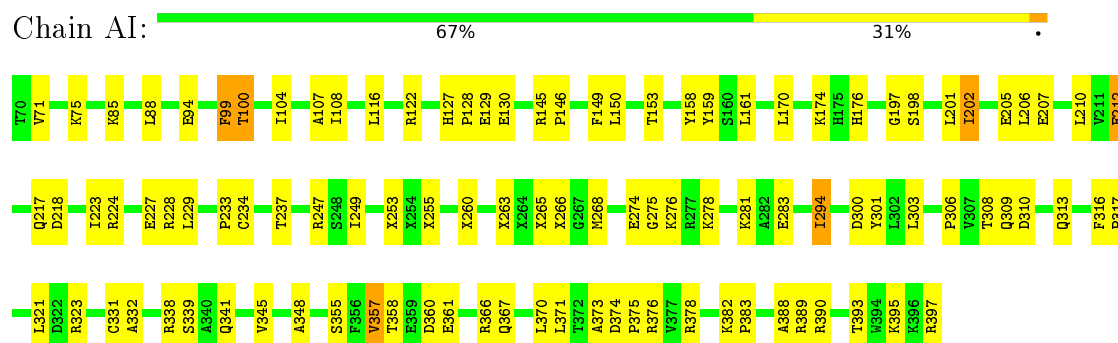
Chain AB: 72% 25%



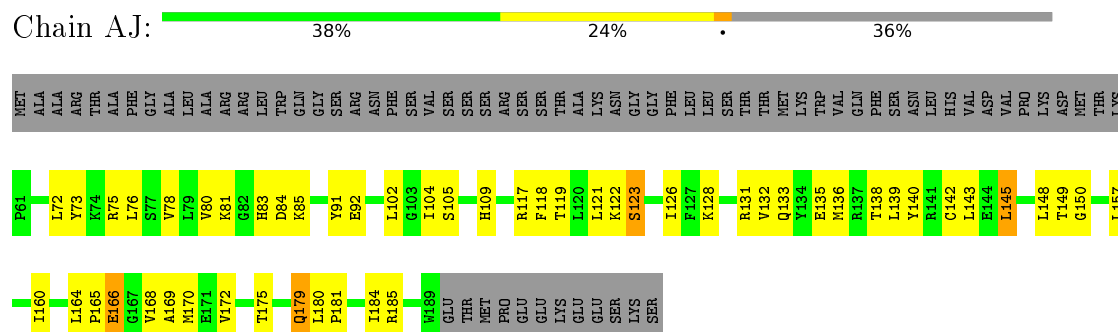




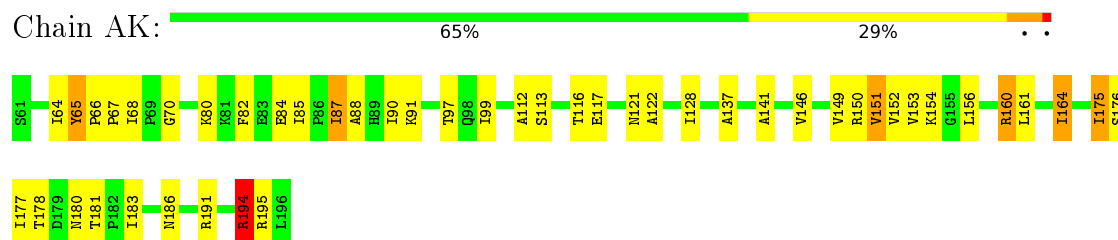
• Molecule 7: MITORIBOSOMAL PROTEIN US9M, MRPS9



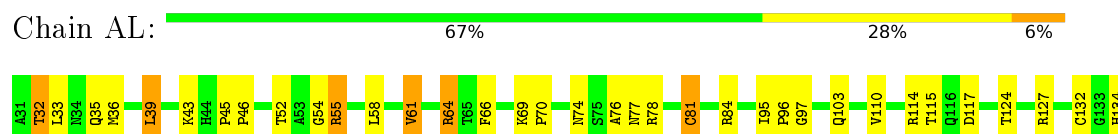
• Molecule 8: MITORIBOSOMAL PROTEIN US10M, MRPS10



• Molecule 9: MITORIBOSOMAL PROTEIN US11M, MRPS11



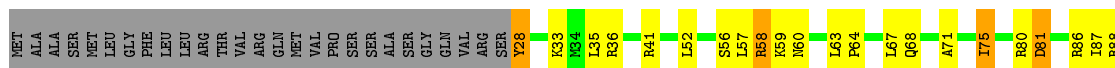
• Molecule 10: MITORIBOSOMAL PROTEIN US12M, MRPS12





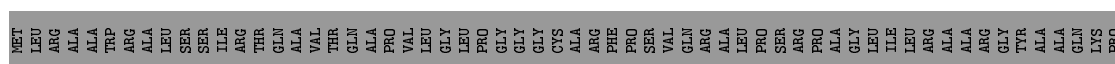
- Molecule 11: MITORIBOSOMAL PROTEIN US14M, MRPS14

Chain AN: 48% 23% 8% 21%



- Molecule 12: MITORIBOSOMAL PROTEIN US15M, MRPS15

Chain AO: 56% 16% 27%



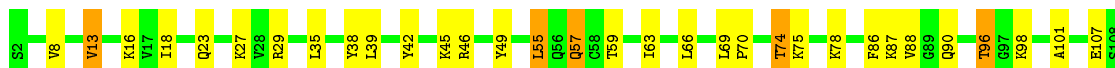
- Molecule 13: MITORIBOSOMAL PROTEIN BS16M, MRPS16

Chain AP: 72% 27% 1%



- Molecule 14: MITORIBOSOMAL PROTEIN US17M, MRPS17

Chain AQ: 70% 26% 5%

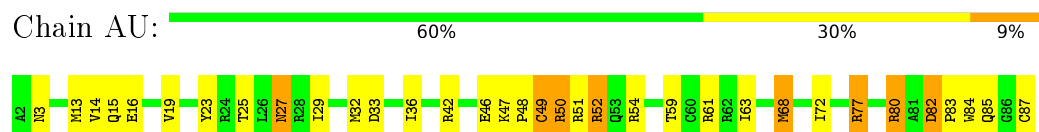


- Molecule 15: MITORIBOSOMAL PROTEIN BS18M, MRPS18C

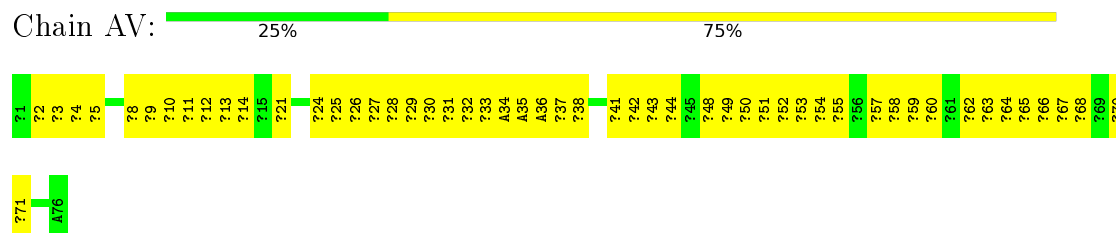
Chain AR: 70% 26% 4%



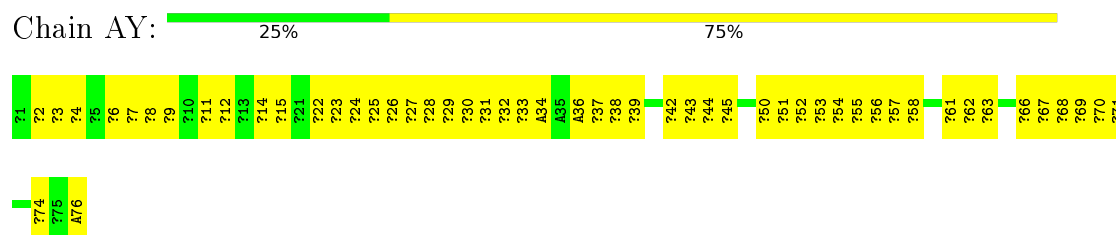
- Molecule 16: MITORIBOSOMAL PROTEIN BS21M, MRPS21



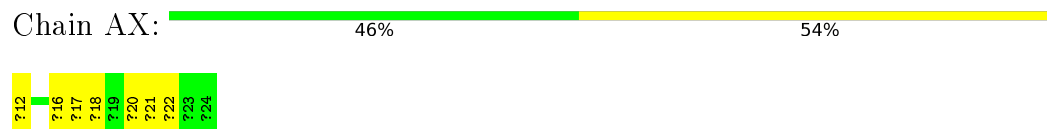
- Molecule 17: P-SITE AND A-SITE TRNA



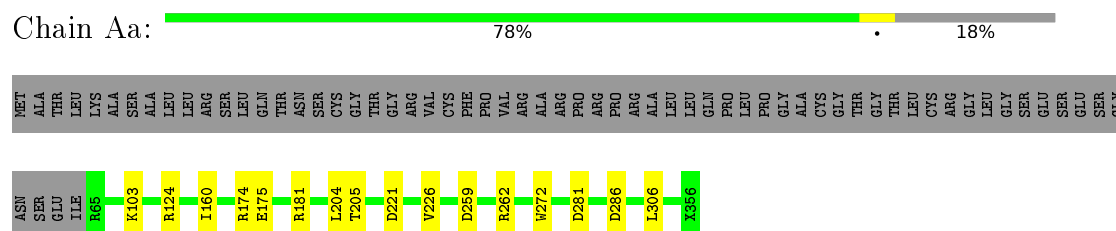
- Molecule 17: P-SITE AND A-SITE TRNA



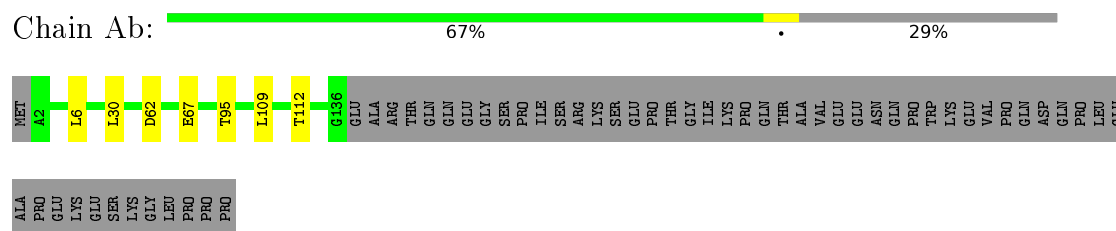
- Molecule 18: MRNA



- Molecule 19: MITORIBOSOMAL PROTEIN MS22, MRPS22



- Molecule 20: MITORIBOSOMAL PROTEIN MS23, MRPS23



- Molecule 21: MITORIBOSOMAL PROTEIN MS25, MRPS25

Chain Ac:  91% 9%



- Molecule 22: MITORIBOSOMAL PROTEIN MS26, MRPS26

Chain Ad:  96%



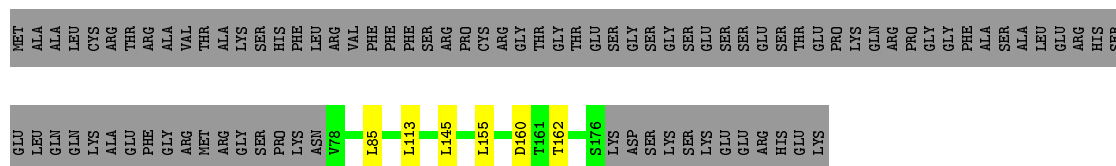
- Molecule 23: MITORIBOSOMAL PROTEIN MS27, MRPS27

Chain Ae:  100%


There are no outlier residues recorded for this chain.

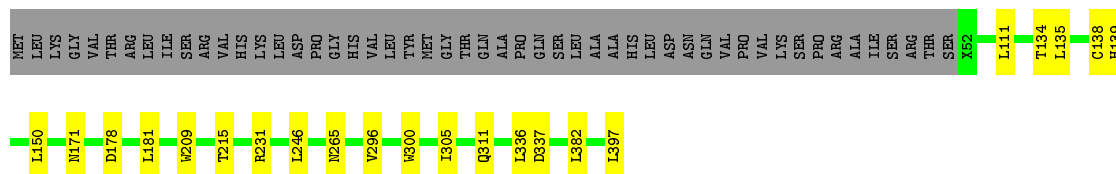
- Molecule 24: MITORIBOSOMAL PROTEIN MS28, MRPS28

Chain Af:  49% 47%



- Molecule 25: MITORIBOSOMAL PROTEIN MS29, MRPS29

Chain Ag:  82% 6% 13%



- Molecule 26: MITORIBOSOMAL PROTEIN MS31, MRPS31

Chain Ah:  98%



- Molecule 27: MITORIBOSOMAL PROTEIN MS33, MRPS33

Chain Ai:  94% 6%



- Molecule 28: MITORIBOSOMAL PROTEIN MS34, MRPS34

Chain Aj:  93% 5%



- Molecule 29: MITORIBOSOMAL PROTEIN MS35, MRPS35

Chain Ak:  92% 8%



- Molecule 30: MITORIBOSOMAL PROTEIN MS37, MRPS37

Chain Am:  91% 9%



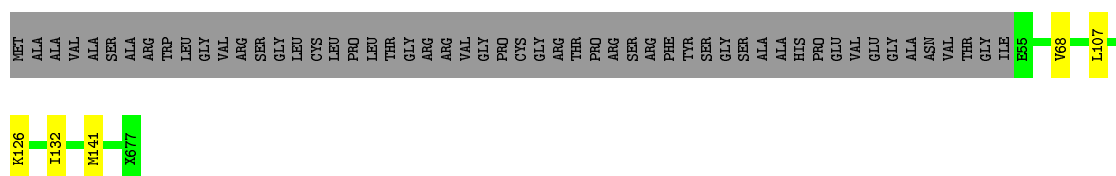
- Molecule 31: MITORIBOSOMAL PROTEIN MS38, MRPS38

Chain An:  88% 13%



- Molecule 32: MITORIBOSOMAL PROTEIN MS39, MRPS39

Chain Ao:  89% 10%



- Molecule 33: 28S RIBOSOMAL PROTEIN S18B, MITOCHONDRIAL

Chain Ap:  91% 9%



- Molecule 34: UNASSIGNED HELICES

Chain As:  100%

There are no outlier residues recorded for this chain.

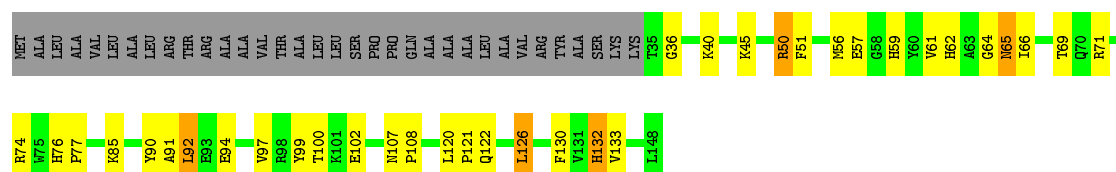
- Molecule 35: UNASSIGNED HELICES

Chain Az:  100%

There are no outlier residues recorded for this chain.

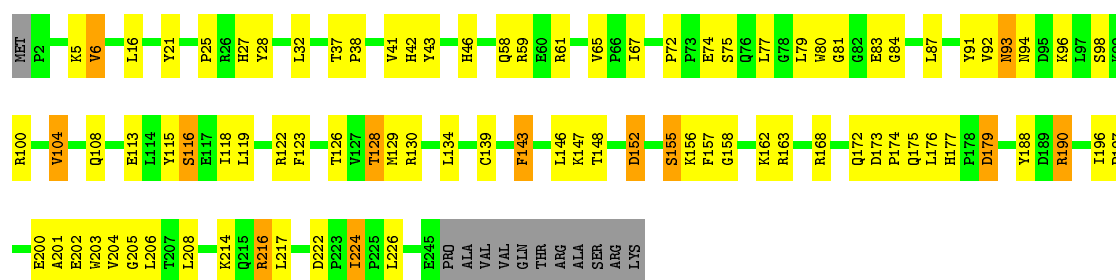
- Molecule 36: MITORIBOSOMAL PROTEIN BL27M, MRPL27

Chain B0:  53% 21% 0% 23%



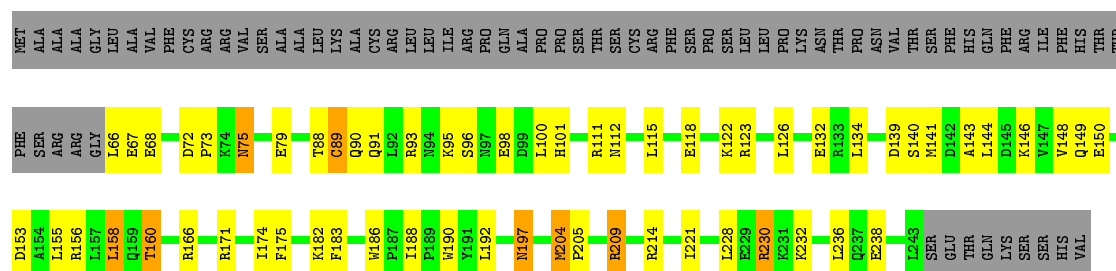
- Molecule 37: MITORIBOSOMAL PROTEIN BL28M, MRPL28

Chain B1: 



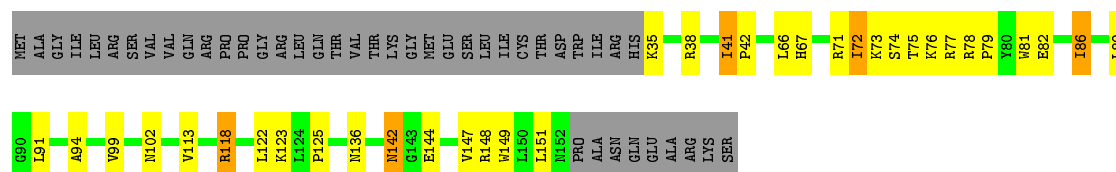
- Molecule 38: MITORIBOSOMAL PROTEIN UL29M, MRPL47

Chain B2: 

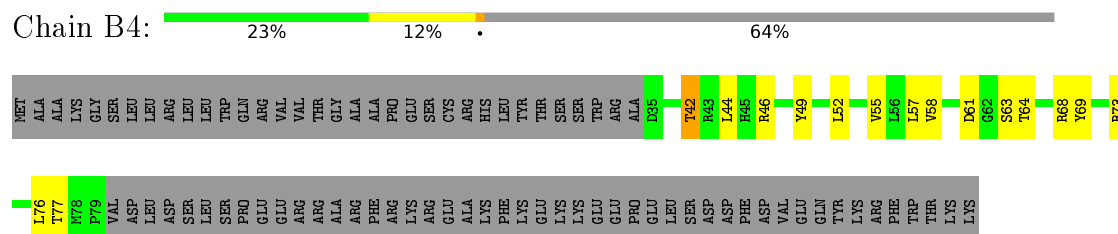


- Molecule 39: MITORIBOSOMAL PROTEIN UL30M, MRPL30

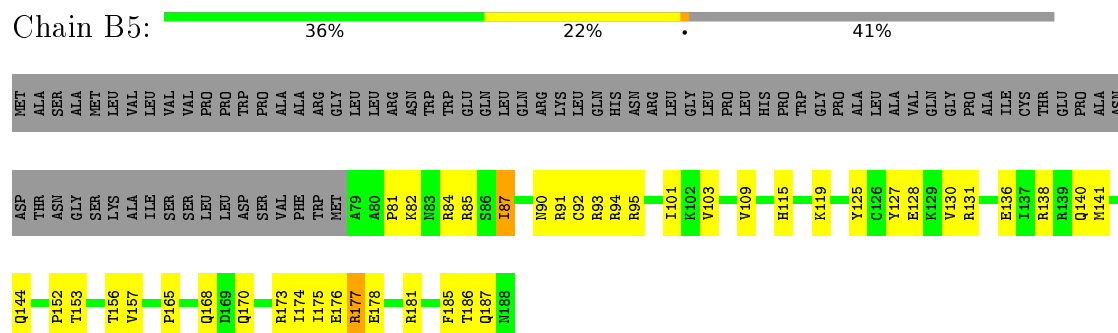
Chain B3: 



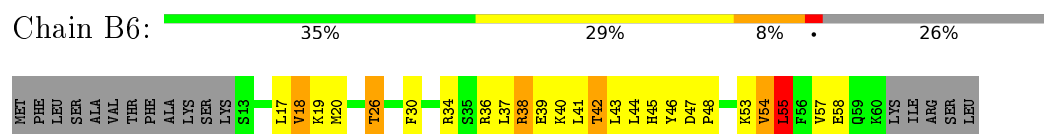
- Molecule 40: MITORIBOSOMAL PROTEIN BL31M, MRPL55



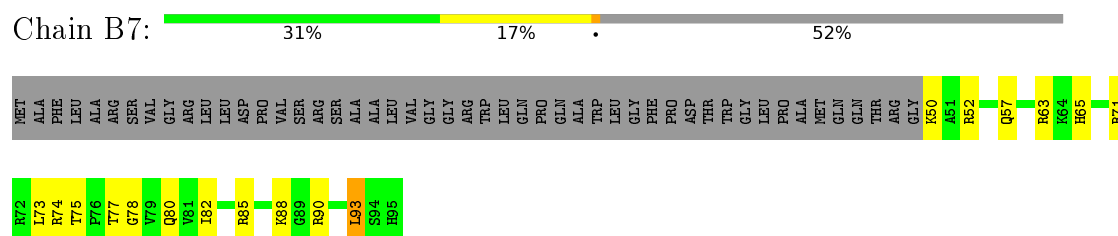
- Molecule 41: MITORIBOSOMAL PROTEIN BL32M, MRPL32



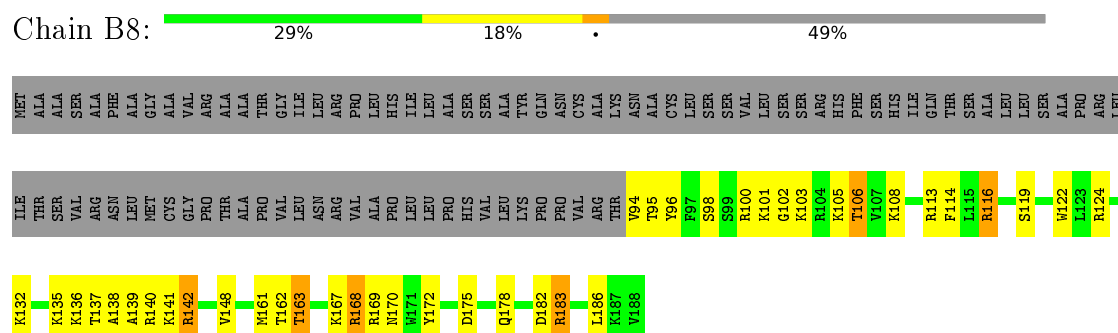
- Molecule 42: MITORIBOSOMAL PROTEIN BL33M, MRPL33



- Molecule 43: MITORIBOSOMAL PROTEIN BL34M, MRPL34



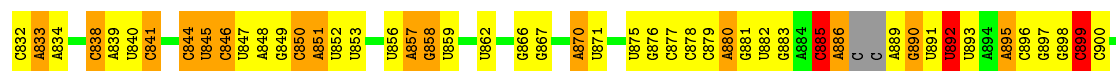
- Molecule 44: MITORIBOSOMAL PROTEIN BL35M, MRPL35



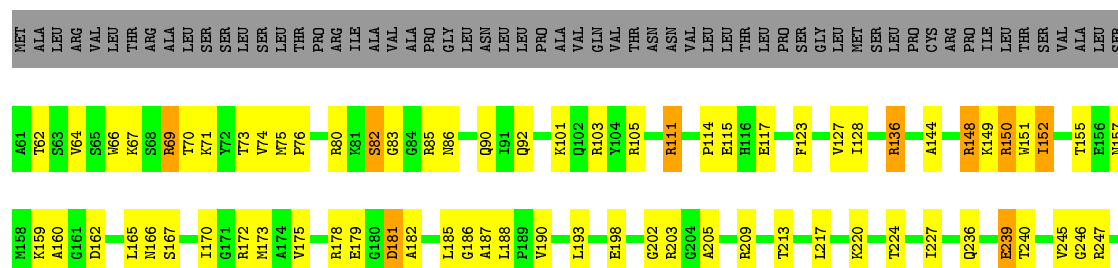
- Molecule 45: MITORIBOSOMAL PROTEIN BL36M, MRPL36



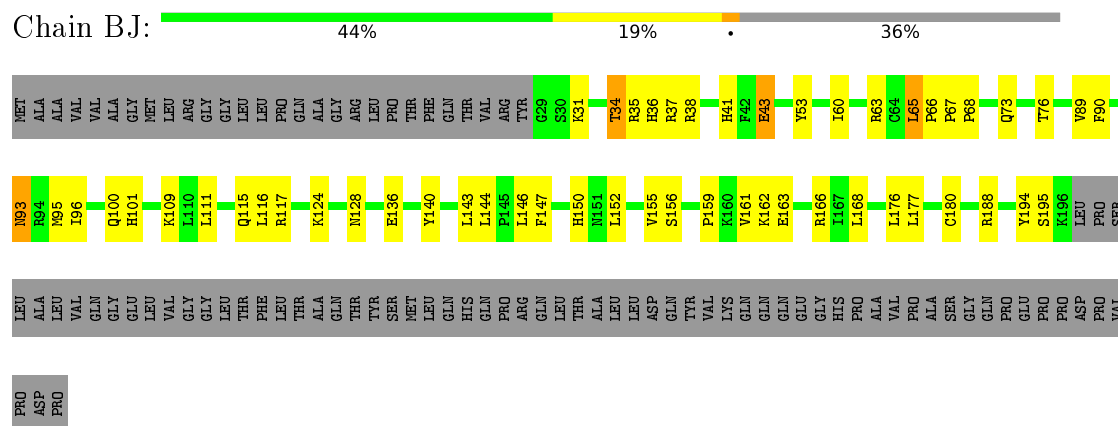
- Molecule 46: MITORIBOSOMAL 16S RRNA



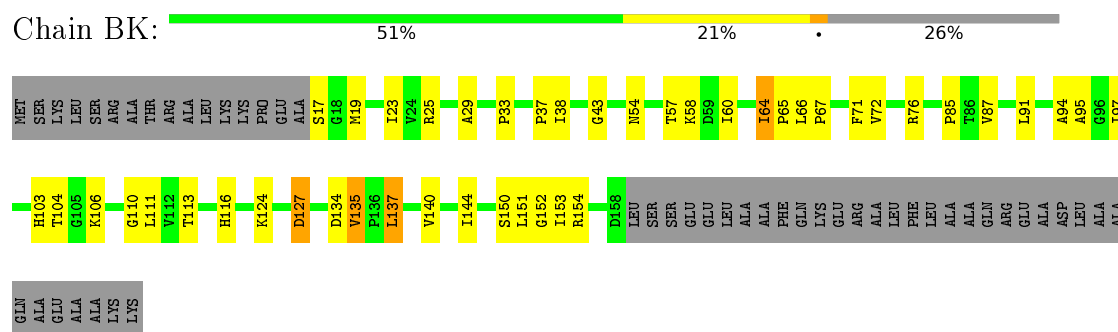




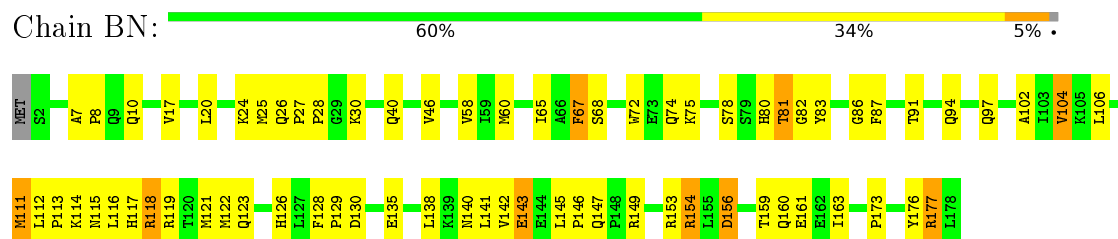




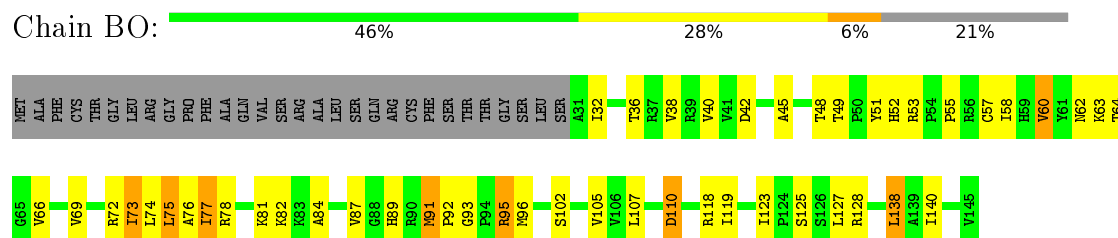
- Molecule 53: MITORIBOSOMAL PROTEIN UL11M, MRPL11



- Molecule 54: MITORIBOSOMAL PROTEIN UL13M, MRPL13

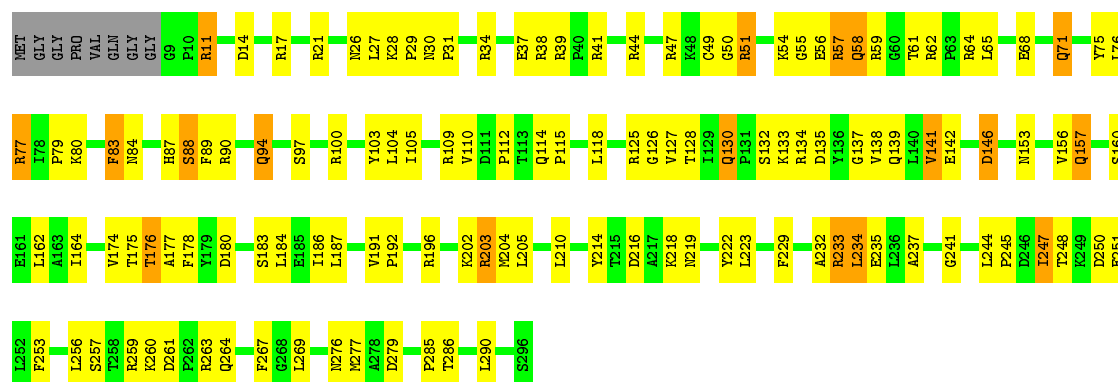


- Molecule 55: MITORIBOSOMAL PROTEIN UL14M, MRPL14



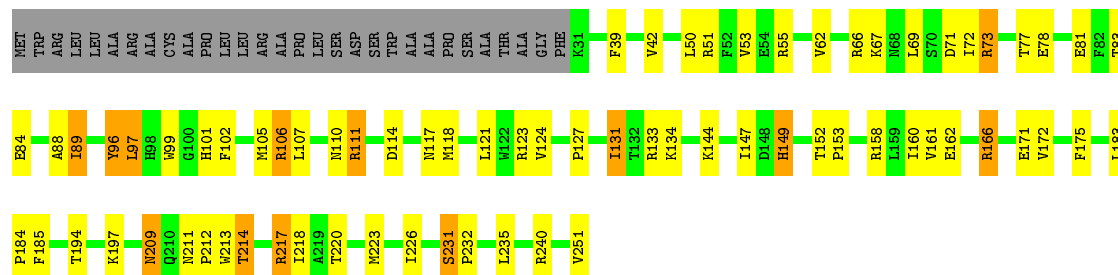
- Molecule 56: MITORIBOSOMAL PROTEIN UL15M, MRPL15





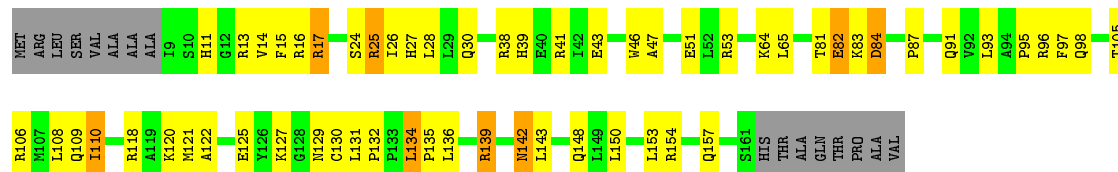
- Molecule 57: MITORIBOSOMAL PROTEIN UL16M, MRPL16

Chain BQ: 59% 24% 5% 12%



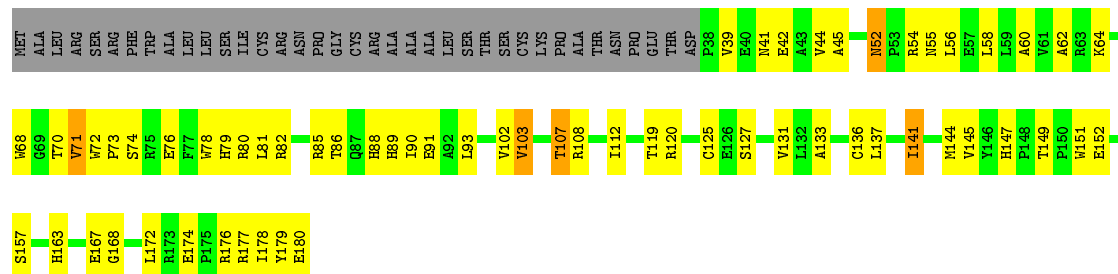
- Molecule 58: MITORIBOSOMAL PROTEIN BL17M, MRPL17

Chain BR: 56% 30% 5% 9%



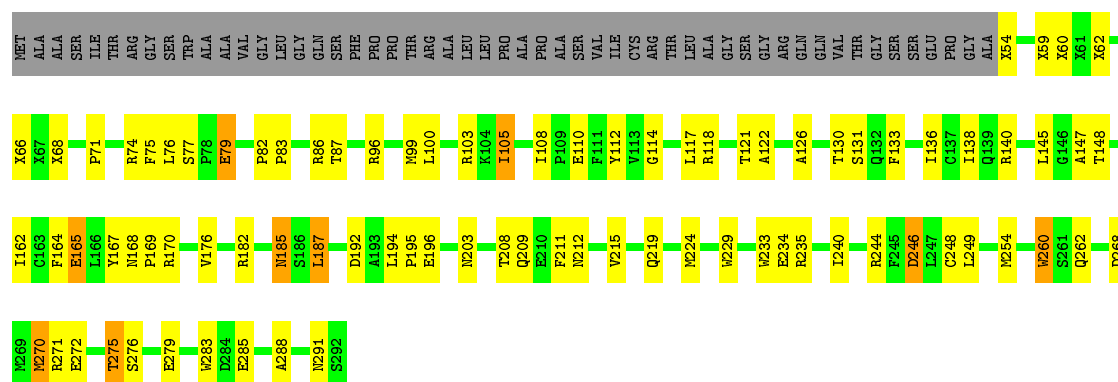
- Molecule 59: MITORIBOSOMAL PROTEIN UL18M, MRPL18

Chain BS: 44% 32% 21% 3%



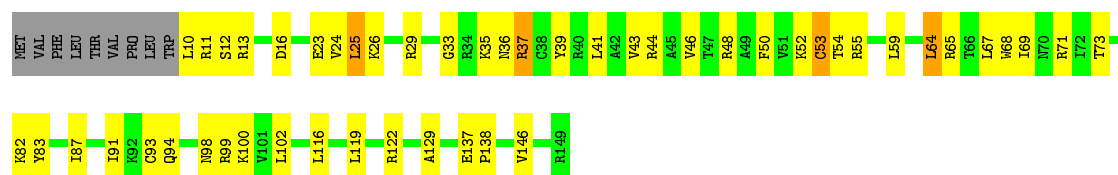
- Molecule 60: MITORIBOSOMAL PROTEIN BL19M, MRPL19

Chain BT: 53% 26% 18% 3%



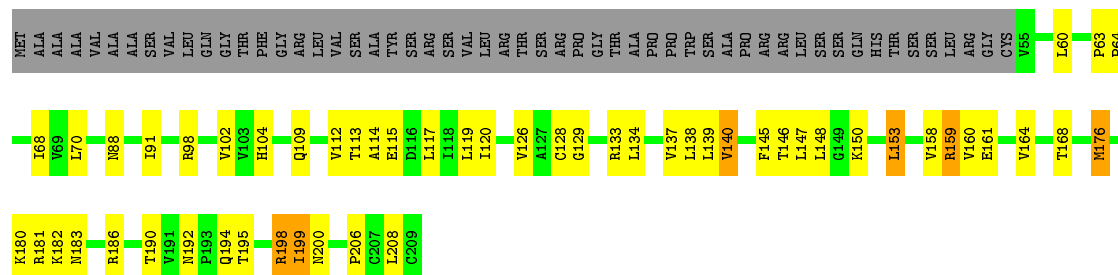
- Molecule 61: MITORIBOSOMAL PROTEIN BL20M, MRPL20

Chain BU: 60% 31% 6%



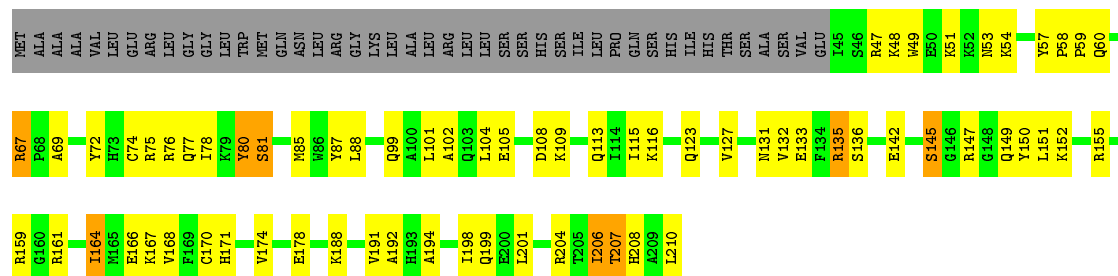
- Molecule 62: MITORIBOSOMAL PROTEIN BL21M, MRPL21

Chain BV: 48% 23% 26%



- Molecule 63: MITORIBOSOMAL PROTEIN UL22M, MRPL22

Chain BW: 46% 30% 21%

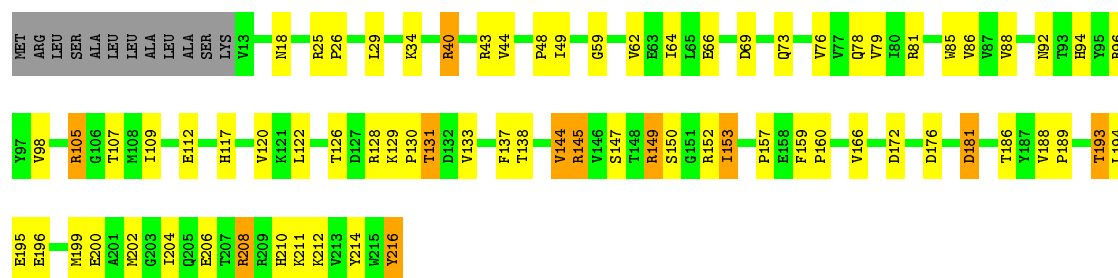


- Molecule 64: MITORIBOSOMAL PROTEIN UL23M, MRPL23


Chain BX: 51% 33% 5% 11%

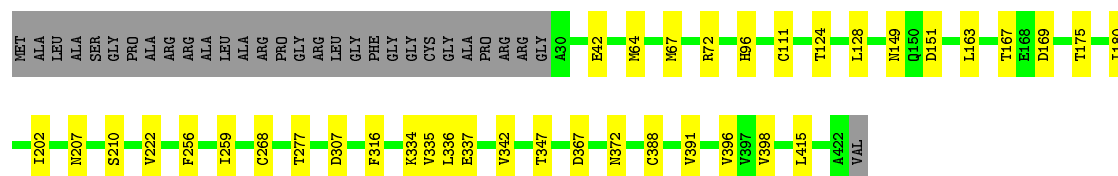
- Molecule 65: MITORIBOSOMAL PROTEIN UL24M, MRPL24

Chain BY: 

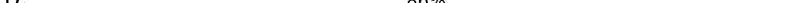


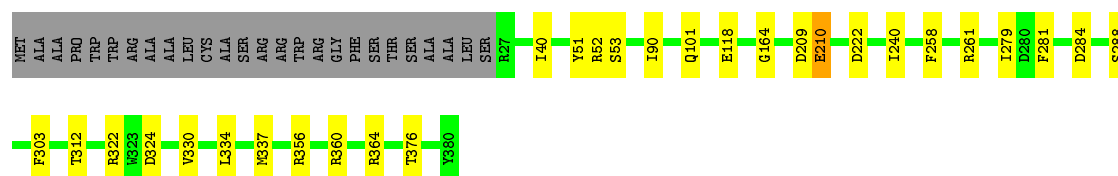
- Molecule 66: MITORIBOSOMAL PROTEIN ML37, MRPL37

Chain Ba:  84% 9% 7%

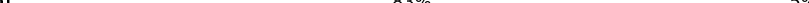


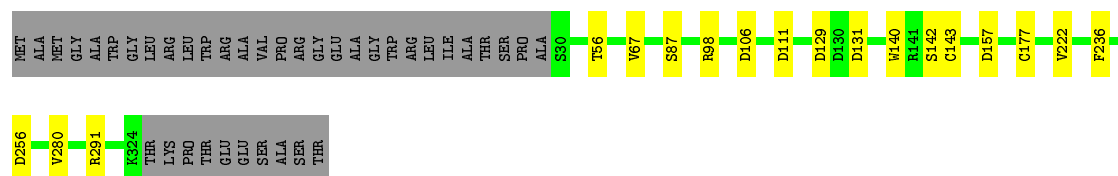
- Molecule 67: MITORIBOSOMAL PROTEIN ML38, MRPL38

Chain Bb:  86% 7% 7%




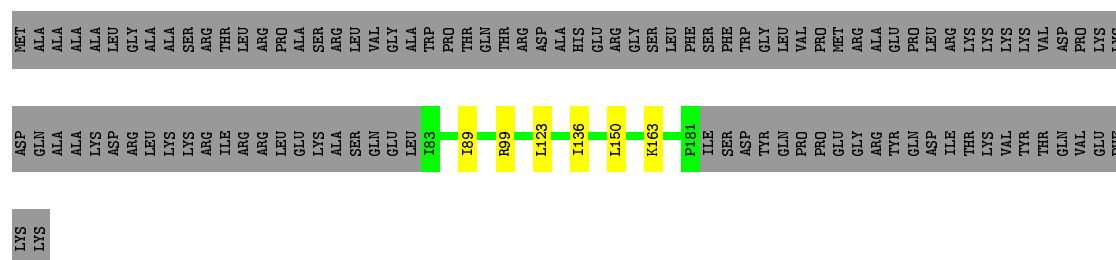
- Molecule 68: MITORIBOSOMAL PROTEIN ML39, MRPL39

Chain Bc:  83% 5% 12%




- Molecule 69: MITORIBOSOMAL PROTEIN ML40, MRPL40

Chain Bd:  45% 52%



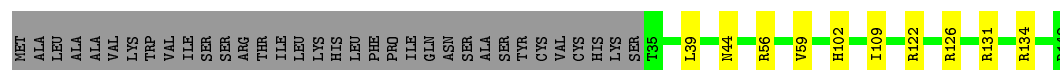
- Molecule 70: MITORIBOSOMAL PROTEIN ML41, MRPL41

Chain Be:  81% 8% 10%




- Molecule 71: MITORIBOSOMAL PROTEIN ML42, MRPL42

Chain Bf:  69% 7% 24%




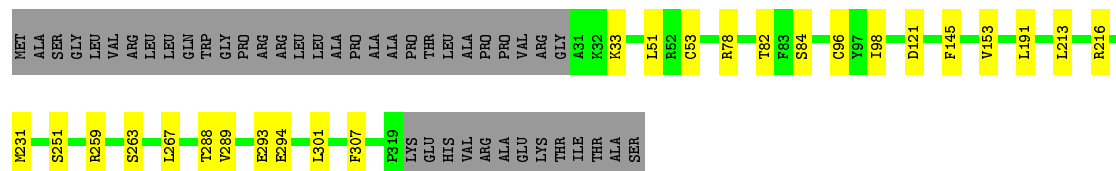
- Molecule 72: MITORIBOSOMAL PROTEIN ML43, MRPL43

Chain Bg:  82% 11% 7%



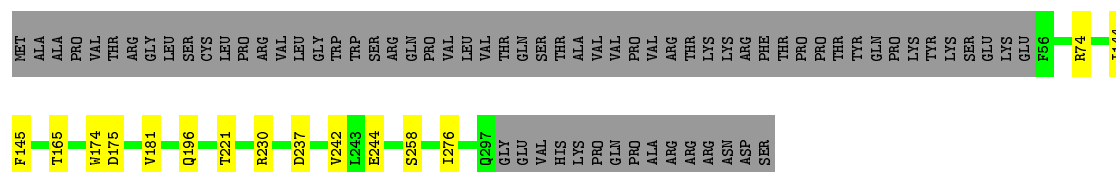
- Molecule 73: MITORIBOSOMAL PROTEIN ML44, MRPL44

Chain Bh:  80% 8% 13%

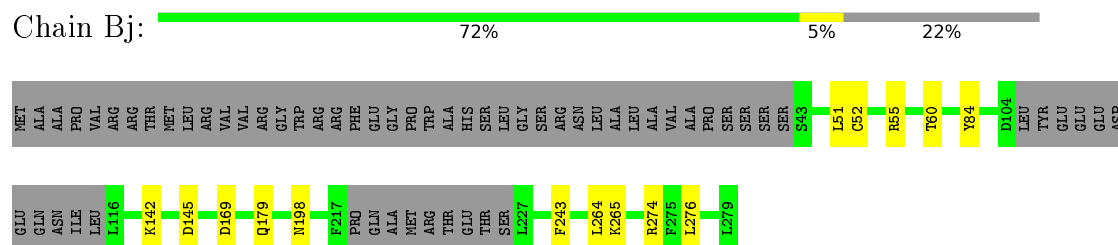


- Molecule 74: MITORIBOSOMAL PROTEIN ML45, MRPL45

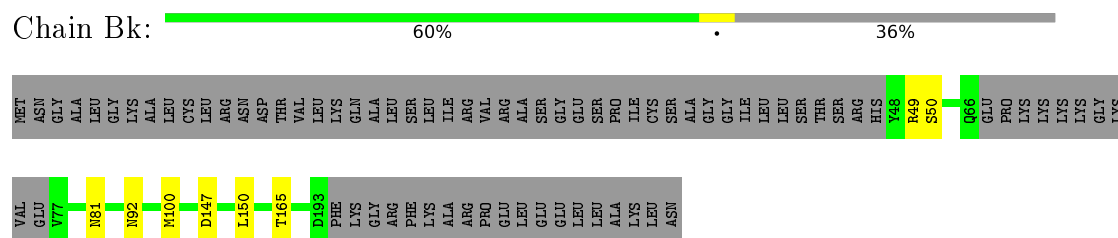
Chain Bi:  73% 5% 22%



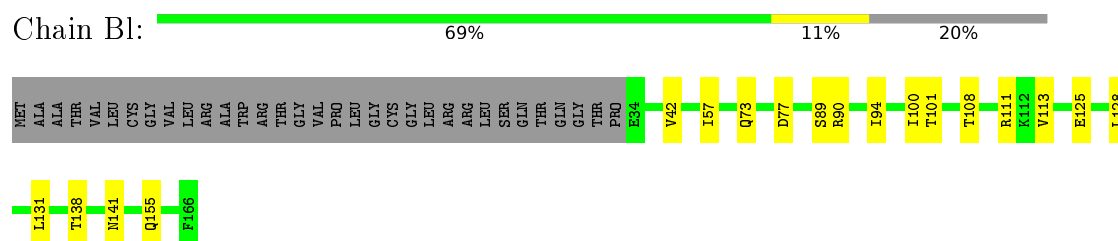
- Molecule 75: MITORIBOSOMAL PROTEIN ML46, MRPL46



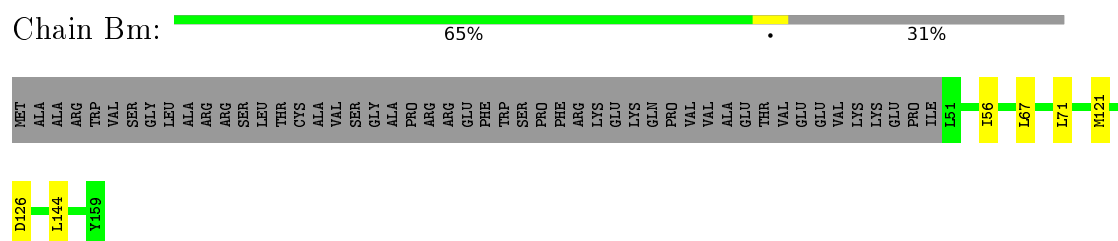
- Molecule 76: MITORIBOSOMAL PROTEIN ML48, MRPL48



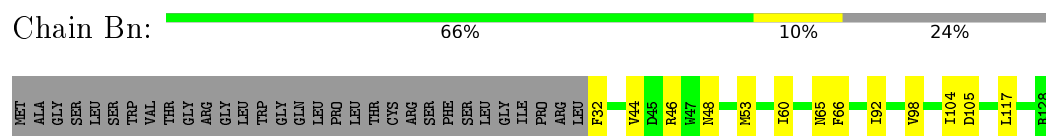
- Molecule 77: MITORIBOSOMAL PROTEIN ML49, MRPL49



- Molecule 78: MITORIBOSOMAL PROTEIN ML50, MRPL50



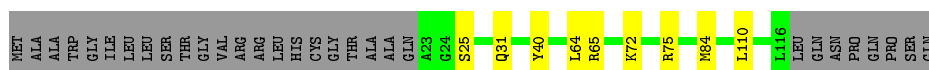
- Molecule 79: MITORIBOSOMAL PROTEIN ML51, MRPL51



- Molecule 80: MITORIBOSOMAL PROTEIN ML52, MRPL52

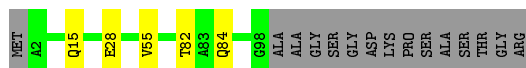






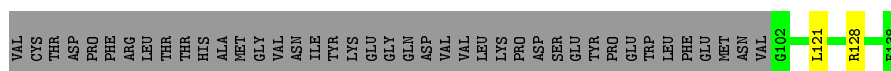
- Molecule 81: MITORIBOSOMAL PROTEIN ML53, MRPL53

Chain Bp: 82% 13%



- Molecule 82: MITORIBOSOMAL PROTEIN ML54, MRPL54

Chain Bq: 25% 73%



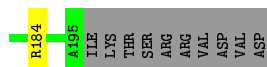
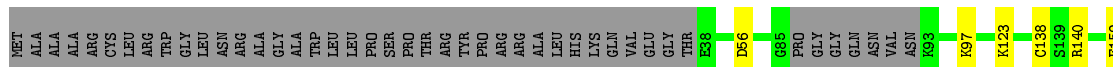
- Molecule 83: MITORIBOSOMAL PROTEIN ML63, MRPL57

Chain Bt: 78% 14% 8%



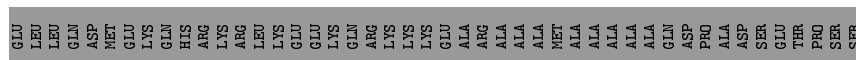
- Molecule 84: MITORIBOSOMAL PROTEIN ML62, MRPL58

Chain Bu: 70% 26%



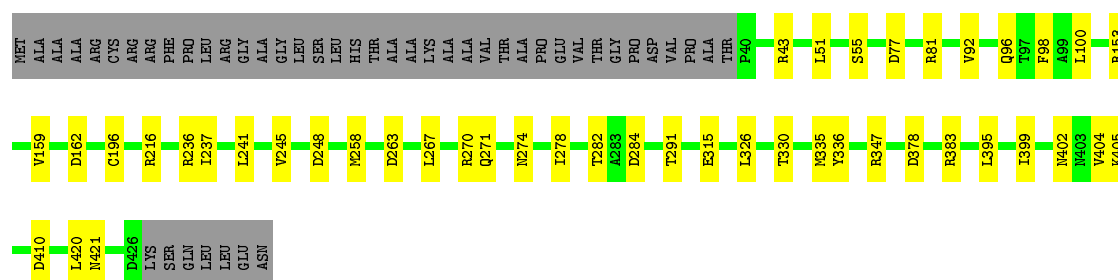
- Molecule 85: MITORIBOSOMAL PROTEIN ML64, MRPL59

Chain Bv: 56% 41%



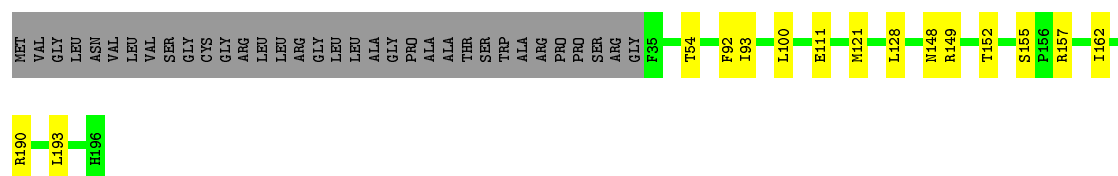
- Molecule 86: MITORIBOSOMAL PROTEIN ML65, MRPS30

Chain Bw: 79% 10% 11%



- Molecule 87: MITORIBOSOMAL PROTEIN ML66, MRPS18A

Chain Bx: 75% 8% 17%



- Molecule 88: UNASSIGNED SECONDARY STRUCTURE ELEMENTS

Chain Bz: 100%

There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PER DETECTOR FRAME	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, Y5P, ZN, P5P, MG

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  > 2$	RMSZ	# $ Z  > 2$
1	AA	0.47	2/22852 (0.0%)	1.00	23/35580 (0.1%)
10	AL	0.31	0/858	0.53	0/1152
11	AN	0.30	0/874	0.46	0/1171
12	AO	0.37	0/1473	0.51	0/1970
13	AP	0.33	0/954	0.49	0/1284
14	AQ	0.34	0/871	0.57	0/1181
15	AR	0.41	1/802 (0.1%)	0.58	0/1079
16	AU	0.37	0/745	0.52	0/993
19	Aa	0.32	0/2052	0.48	0/2774
2	AB	0.35	0/1804	0.52	0/2445
20	Ab	0.33	0/1126	0.48	0/1514
21	Ac	0.33	0/1399	0.53	0/1881
22	Ad	0.35	0/1490	0.46	0/2005
24	Af	0.33	0/790	0.54	0/1064
25	Ag	0.33	0/2731	0.50	0/3696
26	Ah	0.30	0/903	0.46	0/1215
27	Ai	0.30	0/841	0.48	0/1121
28	Aj	0.30	0/1779	0.53	0/2404
29	Ak	0.31	0/2268	0.49	0/3069
3	AC	0.32	0/1105	0.53	0/1496
30	Am	0.35	0/947	0.54	0/1268
31	An	0.46	0/650	0.58	0/858
32	Ao	0.31	0/726	0.51	0/988
33	Ap	0.30	0/1602	0.52	0/2175
36	B0	0.54	0/901	0.67	1/1217 (0.1%)
37	B1	0.40	0/2093	0.53	0/2835
38	B2	0.42	0/1582	0.56	0/2118
39	B3	0.49	0/993	0.66	0/1341
4	AE	0.34	0/2673	0.52	0/3591
40	B4	0.29	0/388	0.61	0/523
41	B5	0.45	0/917	0.57	0/1227
42	B6	0.36	0/396	0.62	1/526 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
43	B7	0.57	0/395	0.70	0/524
44	B8	0.55	0/853	0.67	0/1136
45	B9	0.59	0/342	0.58	0/450
46	BA	0.81	19/36094 (0.1%)	1.28	247/56186 (0.4%)
48	BD	0.50	0/1898	0.65	0/2555
49	BE	0.46	0/2493	0.66	0/3387
5	AF	0.36	0/1008	0.59	0/1358
50	BF	0.52	0/2069	0.65	0/2816
51	BI	0.40	0/819	0.58	0/1101
52	BJ	0.36	0/1392	0.56	0/1881
53	BK	0.34	0/1099	0.51	0/1480
54	BN	0.48	0/1487	0.62	0/2017
55	BO	0.49	0/912	0.66	0/1231
56	BP	0.46	0/2368	0.62	0/3198
57	BQ	0.48	0/1838	0.64	1/2475 (0.0%)
58	BR	0.47	0/1262	0.59	0/1700
59	BS	0.42	0/1197	0.59	0/1624
6	AG	0.34	0/1763	0.49	0/2368
60	BT	0.44	0/1903	0.62	0/2567
61	BU	0.54	0/1179	0.65	0/1578
62	BV	0.51	0/1256	0.65	0/1706
63	BW	0.52	0/1407	0.64	0/1891
64	BX	0.43	0/1149	0.60	0/1554
65	BY	0.34	0/1704	0.56	0/2310
66	Ba	0.39	0/3267	0.58	0/4455
67	Bb	0.39	0/3047	0.59	0/4139
68	Bc	0.36	0/2464	0.54	0/3330
69	Bd	0.32	0/853	0.53	0/1153
7	AI	0.32	0/2455	0.45	0/3291
70	Be	0.42	0/996	0.60	0/1340
71	Bf	0.42	0/731	0.60	0/990
72	Bg	0.47	0/1191	0.64	0/1614
73	Bh	0.42	0/2372	0.58	0/3211
74	Bi	0.35	0/2034	0.53	0/2759
75	Bj	0.31	0/1811	0.52	0/2436
76	Bk	0.39	0/1108	0.58	0/1499
77	Bl	0.43	0/1135	0.60	0/1549
78	Bm	0.33	0/917	0.52	0/1248
79	Bn	0.57	0/860	0.72	1/1150 (0.1%)
8	AJ	0.36	0/1091	0.56	0/1474
80	Bo	0.45	0/762	0.59	0/1022
81	Bp	0.32	0/752	0.54	0/1013
82	Bq	0.32	0/346	0.44	0/463

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
83	Bt	0.49	0/798	0.67	0/1073
84	Bu	0.32	0/1163	0.50	0/1557
85	Bv	0.37	0/1022	0.45	0/1382
86	Bw	0.44	0/3206	0.61	0/4354
87	Bx	0.43	0/1364	0.63	0/1849
9	AK	0.35	0/1021	0.60	0/1381
All	All	0.53	22/166238 (0.0%)	0.86	274/236586 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
49	BE	0	1
57	BQ	0	1
60	BT	0	1
67	Bb	0	2
79	Bn	0	1
83	Bt	0	1
9	AK	0	1
All	All	0	8

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	BA	1255	A	N9-C4	-8.31	1.32	1.37
46	BA	1410	A	N9-C4	-7.55	1.33	1.37
46	BA	52	A	N9-C4	-7.33	1.33	1.37
46	BA	85	A	N9-C4	-6.79	1.33	1.37
46	BA	1047	A	N9-C4	-6.50	1.33	1.37
46	BA	889	A	N9-C4	6.07	1.41	1.37
46	BA	367	A	N9-C4	6.06	1.41	1.37
46	BA	1274	A	N9-C4	-5.95	1.34	1.37
46	BA	1053	A	N9-C4	-5.88	1.34	1.37
46	BA	730	A	N9-C4	-5.77	1.34	1.37
46	BA	478	A	N9-C4	-5.63	1.34	1.37
46	BA	1045	A	N9-C4	-5.49	1.34	1.37
1	AA	822	A	N9-C4	5.48	1.41	1.37
46	BA	1047	A	N3-C4	-5.39	1.31	1.34
46	BA	483	A	N9-C4	-5.36	1.34	1.37
46	BA	1423	A	N9-C4	5.34	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	862	A	N9-C4	-5.33	1.34	1.37
46	BA	627	A	N9-C4	-5.33	1.34	1.37
46	BA	256	A	N9-C4	-5.29	1.34	1.37
46	BA	52	A	N3-C4	-5.22	1.31	1.34
46	BA	558	A	N9-C4	5.18	1.41	1.37
15	AR	69	CYS	CB-SG	5.14	1.91	1.82

All (274) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	BA	374	U	N3-C2-O2	-11.16	114.39	122.20
1	AA	846	C	C6-N1-C2	-9.81	116.38	120.30
46	BA	374	U	N1-C2-O2	9.67	129.57	122.80
46	BA	12	C	C6-N1-C2	-9.04	116.68	120.30
46	BA	81	G	N3-C4-C5	-9.01	124.09	128.60
46	BA	598	C	C6-N1-C2	8.48	123.69	120.30
1	AA	848	C	C6-N1-C2	-8.19	117.03	120.30
46	BA	467	A	O4'-C1'-N9	8.12	114.70	108.20
46	BA	52	A	C2-N3-C4	-8.10	106.55	110.60
46	BA	1255	A	C2-N3-C4	-8.10	106.55	110.60
1	AA	440	C	C6-N1-C2	-8.08	117.07	120.30
46	BA	1249	C	C6-N1-C2	-7.89	117.14	120.30
46	BA	823	C	C6-N1-C2	-7.84	117.16	120.30
46	BA	82	G	C8-N9-C4	7.79	109.52	106.40
46	BA	66	U	C2-N1-C1'	7.72	126.97	117.70
46	BA	1340	C	C6-N1-C2	7.70	123.38	120.30
46	BA	850	C	C6-N1-C2	7.65	123.36	120.30
46	BA	1255	A	C5-N7-C8	-7.47	100.16	103.90
46	BA	246	C	C6-N1-C2	-7.43	117.33	120.30
46	BA	823	C	N3-C2-O2	-7.35	116.75	121.90
46	BA	68	A	P-O3'-C3'	7.34	128.51	119.70
46	BA	812	C	N1-C2-O2	7.34	123.30	118.90
46	BA	688	U	C2-N1-C1'	7.26	126.42	117.70
46	BA	1340	C	C5-C6-N1	-7.22	117.39	121.00
46	BA	113	G	N3-C4-N9	7.17	130.30	126.00
46	BA	104	C	C2-N1-C1'	7.01	126.52	118.80
1	AA	24	C	C6-N1-C2	-7.01	117.50	120.30
46	BA	512	A	P-O3'-C3'	7.01	128.11	119.70
46	BA	632	G	C4-C5-N7	6.99	113.59	110.80
46	BA	1205	C	C6-N1-C2	-6.96	117.52	120.30
46	BA	48	U	N3-C2-O2	-6.95	117.34	122.20
46	BA	1070	A	C8-N9-C4	-6.91	103.04	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	BA	81	G	C4-N9-C1'	6.89	135.46	126.50
46	BA	593	C	N1-C2-O2	6.83	123.00	118.90
46	BA	688	U	C5-C6-N1	6.83	126.12	122.70
46	BA	931	A	P-O3'-C3'	6.80	127.87	119.70
79	Bn	117	LEU	CA-CB-CG	-6.78	99.72	115.30
46	BA	1020	G	N3-C4-C5	-6.72	125.24	128.60
46	BA	593	C	N3-C2-O2	-6.64	117.25	121.90
46	BA	846	C	C2-N1-C1'	6.61	126.07	118.80
46	BA	802	A	N1-C2-N3	6.61	132.60	129.30
46	BA	1433	C	N1-C2-O2	6.60	122.86	118.90
46	BA	113	G	N1-C2-N2	-6.59	110.27	116.20
46	BA	1264	U	N1-C2-N3	6.58	118.85	114.90
46	BA	329	A	N1-C6-N6	-6.53	114.68	118.60
46	BA	1433	C	C2-N1-C1'	6.53	125.98	118.80
46	BA	374	U	C2-N1-C1'	6.52	125.52	117.70
46	BA	632	G	C5-N7-C8	-6.50	101.05	104.30
46	BA	113	G	N3-C4-C5	-6.48	125.36	128.60
46	BA	841	C	C6-N1-C2	6.44	122.88	120.30
46	BA	969	A	C8-N9-C4	6.41	108.36	105.80
46	BA	472	G	C2-N3-C4	6.40	115.10	111.90
46	BA	899	C	N1-C2-O2	6.39	122.74	118.90
46	BA	558	A	C8-N9-C4	-6.36	103.25	105.80
46	BA	32	C	C2-N1-C1'	6.35	125.79	118.80
46	BA	1014	C	C4-C5-C6	6.35	120.58	117.40
46	BA	980	U	N1-C2-O2	6.31	127.22	122.80
46	BA	242	A	N1-C2-N3	6.29	132.44	129.30
46	BA	355	G	C4-N9-C1'	6.26	134.64	126.50
46	BA	81	G	N3-C4-N9	6.25	129.75	126.00
46	BA	447	G	O5'-P-OP2	-6.25	100.08	105.70
46	BA	1055	A	C4-C5-C6	-6.24	113.88	117.00
46	BA	619	U	C5-C6-N1	6.22	125.81	122.70
46	BA	1149	G	C4-N9-C1'	6.20	134.56	126.50
46	BA	1010	U	C5-C6-N1	-6.19	119.60	122.70
46	BA	802	A	C6-N1-C2	-6.18	114.89	118.60
46	BA	1246	C	C2-N1-C1'	-6.14	112.04	118.80
36	B0	92	LEU	CA-CB-CG	-6.14	101.19	115.30
46	BA	991	U	C5-C6-N1	-6.13	119.63	122.70
46	BA	1490	C	C6-N1-C2	6.13	122.75	120.30
46	BA	598	C	C5-C6-N1	-6.11	117.94	121.00
46	BA	943	C	C6-N1-C2	-6.11	117.86	120.30
46	BA	1014	C	C5-C6-N1	-6.09	117.96	121.00
46	BA	370	A	C8-N9-C4	-6.08	103.37	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	BA	453	U	C5-C6-N1	-6.08	119.66	122.70
46	BA	1053	A	C8-N9-C4	6.07	108.23	105.80
46	BA	48	U	P-O3'-C3'	6.05	126.96	119.70
46	BA	586	C	C6-N1-C2	-6.05	117.88	120.30
46	BA	1381	G	C8-N9-C4	-6.04	103.98	106.40
46	BA	88	G	C8-N9-C4	6.02	108.81	106.40
46	BA	396	C	C6-N1-C2	-6.02	117.89	120.30
46	BA	997	C	N3-C2-O2	-6.01	117.69	121.90
46	BA	640	G	N3-C4-C5	-5.97	125.61	128.60
1	AA	404	C	N1-C2-O2	5.96	122.47	118.90
46	BA	85	A	C8-N9-C4	5.96	108.18	105.80
46	BA	85	A	N7-C8-N9	-5.95	110.83	113.80
46	BA	812	C	N3-C2-O2	-5.94	117.74	121.90
46	BA	808	C	C6-N1-C2	-5.93	117.93	120.30
46	BA	969	A	N7-C8-N9	-5.93	110.84	113.80
46	BA	456	A	C6-N1-C2	-5.92	115.05	118.60
46	BA	997	C	C6-N1-C2	-5.92	117.93	120.30
46	BA	323	G	N3-C4-C5	-5.90	125.65	128.60
46	BA	396	C	N3-C2-O2	-5.88	117.78	121.90
46	BA	1431	U	P-O3'-C3'	5.88	126.76	119.70
46	BA	183	U	C2-N1-C1'	-5.88	110.65	117.70
46	BA	1266	G	C8-N9-C4	-5.86	104.06	106.40
46	BA	68	A	O4'-C1'-N9	5.86	112.89	108.20
46	BA	1003	G	N3-C4-N9	5.85	129.51	126.00
46	BA	1149	G	C8-N9-C1'	-5.83	119.41	127.00
46	BA	113	G	C4-N9-C1'	5.83	134.08	126.50
46	BA	319	U	C5-C6-N1	-5.83	119.79	122.70
46	BA	1003	G	C4-N9-C1'	5.81	134.06	126.50
46	BA	1255	A	C4-C5-N7	5.81	113.61	110.70
1	AA	432	A	O4'-C1'-N9	5.81	112.85	108.20
46	BA	1316	C	C6-N1-C2	5.79	122.61	120.30
46	BA	1055	A	C8-N9-C4	5.79	108.11	105.80
46	BA	355	G	C8-N9-C1'	-5.78	119.48	127.00
46	BA	1020	G	N3-C4-N9	5.77	129.46	126.00
1	AA	826	C	C6-N1-C2	-5.76	118.00	120.30
46	BA	1026	A	C6-N1-C2	-5.75	115.15	118.60
46	BA	640	G	N3-C4-N9	5.75	129.45	126.00
46	BA	169	U	C2-N1-C1'	5.74	124.59	117.70
46	BA	184	U	C5-C6-N1	-5.73	119.83	122.70
46	BA	574	U	O5'-P-OP1	-5.73	100.54	105.70
46	BA	1069	U	C5-C6-N1	-5.72	119.84	122.70
46	BA	465	C	C6-N1-C2	5.72	122.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	BA	330	A	N9-C4-C5	-5.71	103.52	105.80
46	BA	446	A	C8-N9-C4	-5.71	103.52	105.80
46	BA	1255	A	N3-C4-C5	5.71	130.79	126.80
46	BA	658	C	C6-N1-C2	-5.68	118.03	120.30
46	BA	840	U	C5-C6-N1	-5.68	119.86	122.70
46	BA	178	U	C5-C6-N1	-5.67	119.86	122.70
1	AA	501	C	C6-N1-C2	-5.66	118.03	120.30
46	BA	5	A	C8-N9-C4	-5.66	103.54	105.80
46	BA	12	C	N3-C2-O2	-5.65	117.94	121.90
46	BA	32	C	N1-C2-O2	5.65	122.29	118.90
46	BA	192	U	C2-N3-C4	-5.64	123.61	127.00
46	BA	485	A	C8-N9-C4	5.64	108.06	105.80
46	BA	1255	A	N1-C6-N6	5.63	121.98	118.60
46	BA	558	A	P-O3'-C3'	5.63	126.45	119.70
46	BA	1229	U	C2-N1-C1'	5.62	124.45	117.70
46	BA	172	C	N1-C2-O2	5.62	122.27	118.90
46	BA	330	A	N9-C1'-C2'	-5.62	105.82	112.00
46	BA	66	U	C5-C6-N1	5.59	125.50	122.70
46	BA	794	U	C5-C6-N1	-5.59	119.91	122.70
46	BA	113	G	C8-N9-C1'	-5.58	119.75	127.00
46	BA	277	A	N7-C8-N9	5.57	116.58	113.80
46	BA	980	U	C2-N1-C1'	5.56	124.37	117.70
1	AA	252	C	C6-N1-C2	-5.55	118.08	120.30
46	BA	1003	G	N3-C4-C5	-5.54	125.83	128.60
1	AA	612	U	C2-N1-C1'	5.54	124.34	117.70
46	BA	160	A	P-O3'-C3'	5.53	126.34	119.70
46	BA	572	A	P-O3'-C3'	5.53	126.33	119.70
46	BA	1020	G	C4-N9-C1'	5.53	133.68	126.50
46	BA	825	U	C5-C6-N1	-5.50	119.95	122.70
46	BA	474	C	C2-N1-C1'	5.50	124.85	118.80
46	BA	64	C	N3-C2-O2	-5.50	118.05	121.90
46	BA	1255	A	C5-C6-N1	-5.50	114.95	117.70
46	BA	222	A	C8-N9-C4	5.50	108.00	105.80
46	BA	1394	C	C6-N1-C2	-5.50	118.10	120.30
46	BA	1262	C	C6-N1-C2	5.50	122.50	120.30
46	BA	559	C	N3-C2-O2	-5.49	118.06	121.90
46	BA	941	C	C6-N1-C2	-5.47	118.11	120.30
46	BA	82	G	N9-C4-C5	-5.47	103.21	105.40
46	BA	1433	C	C6-N1-C1'	-5.47	114.23	120.80
46	BA	844	C	N1-C2-O2	5.46	122.18	118.90
46	BA	1246	C	N3-C4-N4	-5.45	114.19	118.00
57	BQ	97	LEU	CA-CB-CG	5.45	127.83	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	BA	257	C	C6-N1-C2	5.44	122.47	120.30
46	BA	66	U	N1-C2-O2	5.43	126.60	122.80
46	BA	1071	A	C8-N9-C4	-5.43	103.63	105.80
46	BA	181	C	C6-N1-C2	5.42	122.47	120.30
46	BA	823	C	C2-N1-C1'	5.42	124.76	118.80
46	BA	1244	A	C8-N9-C4	5.42	107.97	105.80
46	BA	643	U	C2-N1-C1'	5.41	124.20	117.70
46	BA	124	A	C8-N9-C4	5.39	107.96	105.80
46	BA	1026	A	N1-C2-N3	5.38	131.99	129.30
46	BA	112	A	P-O3'-C3'	5.38	126.16	119.70
46	BA	478	A	C8-N9-C4	5.38	107.95	105.80
1	AA	903	C	N1-C2-O2	5.37	122.12	118.90
46	BA	81	G	C8-N9-C1'	-5.37	120.02	127.00
46	BA	512	A	OP2-P-O3'	5.36	116.99	105.20
46	BA	1518	U	P-O3'-C3'	5.36	126.13	119.70
46	BA	68	A	C3'-C2'-C1'	-5.35	97.22	101.50
46	BA	1205	C	C5-C6-N1	5.35	123.67	121.00
46	BA	695	C	C5-C6-N1	5.34	123.67	121.00
46	BA	433	U	C2-N3-C4	-5.34	123.80	127.00
46	BA	170	A	C8-N9-C4	5.34	107.94	105.80
46	BA	573	C	C2-N1-C1'	5.32	124.65	118.80
46	BA	1534	U	N3-C2-O2	-5.30	118.49	122.20
46	BA	78	A	C8-N9-C4	5.30	107.92	105.80
46	BA	104	C	C6-N1-C2	-5.30	118.18	120.30
46	BA	885	C	C5-C6-N1	5.30	123.65	121.00
46	BA	806	G	C8-N9-C4	-5.29	104.28	106.40
46	BA	706	C	C5-C6-N1	5.28	123.64	121.00
46	BA	642	G	C8-N9-C4	5.28	108.51	106.40
46	BA	339	A	N9-C4-C5	-5.28	103.69	105.80
46	BA	619	U	C6-N1-C2	-5.27	117.84	121.00
46	BA	352	C	C5-C6-N1	-5.26	118.37	121.00
46	BA	971	A	C8-N9-C4	-5.26	103.69	105.80
46	BA	823	C	N1-C2-O2	5.26	122.06	118.90
42	B6	55	LEU	CA-CB-CG	5.25	127.39	115.30
46	BA	1322	C	OP2-P-O3'	5.25	116.75	105.20
46	BA	1055	A	N9-C4-C5	-5.24	103.70	105.80
46	BA	277	A	C5-N7-C8	-5.23	101.28	103.90
46	BA	1266	G	N3-C4-C5	-5.23	125.98	128.60
46	BA	962	A	C8-N9-C4	-5.23	103.71	105.80
46	BA	369	A	C5-C6-N1	5.22	120.31	117.70
46	BA	1392	U	C5-C6-N1	-5.22	120.09	122.70
1	AA	136	C	C6-N1-C2	-5.22	118.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	BA	587	C	C6-N1-C2	-5.21	118.22	120.30
46	BA	1394	C	C5-C6-N1	5.20	123.60	121.00
46	BA	1384	U	N3-C2-O2	-5.20	118.56	122.20
46	BA	125	A	C8-N9-C4	5.20	107.88	105.80
46	BA	1268	G	C8-N9-C4	5.20	108.48	106.40
46	BA	573	C	N1-C2-O2	5.19	122.01	118.90
46	BA	634	U	C5-C6-N1	-5.19	120.11	122.70
46	BA	85	A	N1-C6-N6	-5.19	115.49	118.60
1	AA	425	G	N3-C4-C5	-5.18	126.01	128.60
46	BA	1534	U	N1-C2-O2	5.18	126.42	122.80
46	BA	67	A	C8-N9-C4	-5.17	103.73	105.80
46	BA	761	C	C6-N1-C2	5.17	122.37	120.30
46	BA	1149	G	N3-C4-N9	5.17	129.10	126.00
46	BA	640	G	N1-C2-N2	-5.17	111.55	116.20
46	BA	54	A	N1-C2-N3	5.17	131.89	129.30
1	AA	425	G	N3-C4-N9	5.17	129.10	126.00
46	BA	77	U	C5-C6-N1	-5.17	120.12	122.70
46	BA	1552	G	C8-N9-C4	-5.17	104.33	106.40
1	AA	209	C	C6-N1-C2	-5.16	118.23	120.30
46	BA	250	C	C5-C6-N1	-5.16	118.42	121.00
46	BA	1057	C	N1-C2-O2	-5.16	115.81	118.90
46	BA	64	C	N1-C2-O2	5.15	121.99	118.90
1	AA	440	C	C5-C6-N1	5.15	123.58	121.00
46	BA	666	A	C8-N9-C4	5.15	107.86	105.80
46	BA	277	A	C8-N9-C4	-5.15	103.74	105.80
1	AA	112	U	C6-N1-C2	5.14	124.08	121.00
1	AA	435	C	C6-N1-C2	5.13	122.35	120.30
46	BA	69	C	N3-C4-C5	5.13	123.95	121.90
46	BA	1149	G	C6-C5-N7	-5.13	127.32	130.40
46	BA	1434	U	C5-C6-N1	-5.13	120.13	122.70
46	BA	593	C	C2-N1-C1'	5.13	124.44	118.80
46	BA	851	A	C2-N3-C4	5.12	113.16	110.60
46	BA	631	U	C2-N1-C1'	-5.12	111.56	117.70
46	BA	846	C	C6-N1-C1'	-5.12	114.66	120.80
46	BA	867	G	C4-C5-N7	5.12	112.85	110.80
46	BA	1437	C	C5-C6-N1	-5.12	118.44	121.00
46	BA	1330	G	C4-C5-N7	5.11	112.84	110.80
46	BA	162	C	N3-C2-O2	-5.11	118.32	121.90
1	AA	822	A	C2-N3-C4	5.10	113.15	110.60
46	BA	113	G	N1-C2-N3	5.10	126.96	123.90
46	BA	943	C	C5-C6-N1	5.10	123.55	121.00
46	BA	323	G	N1-C6-O6	-5.10	116.84	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	BA	356	U	C5-C6-N1	5.09	125.25	122.70
1	AA	119	C	C2-N1-C1'	5.09	124.40	118.80
46	BA	453	U	C6-N1-C2	5.09	124.05	121.00
46	BA	784	U	C6-N1-C2	-5.09	117.95	121.00
1	AA	514	C	C6-N1-C2	-5.08	118.27	120.30
1	AA	774	C	C6-N1-C2	-5.08	118.27	120.30
46	BA	1149	G	C4-C5-N7	5.08	112.83	110.80
46	BA	558	A	C4-N9-C1'	5.08	135.44	126.30
46	BA	1021	U	N3-C4-C5	-5.07	111.56	114.60
46	BA	584	C	C2-N1-C1'	5.07	124.38	118.80
46	BA	256	A	N1-C2-N3	5.07	131.83	129.30
46	BA	81	G	C8-N9-C4	-5.07	104.37	106.40
46	BA	187	C	C5-C6-N1	-5.07	118.47	121.00
46	BA	1156	C	C6-N1-C2	5.07	122.33	120.30
46	BA	1330	G	C6-C5-N7	-5.07	127.36	130.40
46	BA	747	C	O4'-C1'-N1	5.06	112.25	108.20
46	BA	845	U	C5-C6-N1	5.06	125.23	122.70
46	BA	1053	A	C2-N3-C4	-5.06	108.07	110.60
46	BA	382	C	C6-N1-C2	-5.06	118.28	120.30
46	BA	892	U	N3-C2-O2	-5.06	118.66	122.20
46	BA	1060	A	C6-N1-C2	-5.06	115.57	118.60
46	BA	646	C	C6-N1-C2	5.05	122.32	120.30
46	BA	1054	G	N3-C4-N9	5.05	129.03	126.00
46	BA	5	A	N7-C8-N9	5.04	116.32	113.80
46	BA	66	U	C6-N1-C2	-5.04	117.98	121.00
46	BA	183	U	C5-C6-N1	-5.04	120.18	122.70
46	BA	991	U	C6-N1-C2	5.03	124.02	121.00
46	BA	1053	A	N9-C4-C5	-5.03	103.79	105.80
1	AA	59	C	C6-N1-C2	-5.02	118.29	120.30
46	BA	639	U	N3-C2-O2	-5.02	118.69	122.20
46	BA	323	G	N3-C4-N9	5.00	129.00	126.00
46	BA	567	C	C6-N1-C2	5.00	122.30	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	AK	194	ARG	Peptide
49	BE	316	PHE	Peptide
57	BQ	149	HIS	Peptide
60	BT	275	THR	Peptide
67	Bb	164	GLY	Peptide

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Mol	Chain	Res	Type	Group
67	Bb	210	GLU	Peptide
79	Bn	65	ASN	Peptide
83	Bt	62	HIS	Peptide

## 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	AA	20411	0	10345	323	0
2	AB	1762	0	1774	43	0
3	AC	1075	0	1087	33	0
4	AE	2621	0	2640	91	0
5	AF	990	0	1025	36	0
6	AG	1721	0	1747	41	0
7	AI	2498	0	2473	79	0
8	AJ	1067	0	1101	42	0
9	AK	1001	0	1037	39	0
10	AL	840	0	890	26	0
11	AN	858	0	883	41	0
12	AO	1448	0	1536	29	0
13	AP	932	0	951	25	0
14	AQ	853	0	913	35	0
15	AR	784	0	813	29	0
16	AU	734	0	745	28	0
17	AV	1251	0	823	70	0
17	AY	1251	0	824	78	0
18	AX	231	0	157	7	0
19	Aa	2296	0	2317	0	0
20	Ab	1101	0	1118	0	0
21	Ac	1367	0	1385	0	0
22	Ad	1467	0	1466	0	0
23	Ae	2016	0	2028	0	0
24	Af	778	0	791	0	0
25	Ag	2774	0	2810	0	0
26	Ah	876	0	832	0	0
27	Ai	824	0	842	0	0
28	Aj	1777	0	1788	0	0
29	Ak	2222	0	2270	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	Am	930	0	959	0	0
31	An	639	0	709	0	0
32	Ao	3028	0	3081	0	0
33	Ap	1551	0	1519	0	0
34	As	96	0	98	0	0
35	Az	102	0	104	0	0
36	B0	878	0	896	31	0
37	B1	2036	0	2058	57	0
38	B2	1544	0	1580	46	0
39	B3	968	0	1018	29	0
40	B4	381	0	400	8	0
41	B5	902	0	916	37	0
42	B6	391	0	429	23	0
43	B7	387	0	413	14	0
44	B8	833	0	883	38	0
45	B9	335	0	359	16	0
46	BA	32233	0	16311	642	0
47	BB	1008	0	555	29	0
48	BD	1860	0	1923	69	0
49	BE	2420	0	2418	108	0
50	BF	2011	0	2049	82	0
51	BI	805	0	845	26	0
52	BJ	1361	0	1448	37	0
53	BK	1081	0	1146	35	0
54	BN	1444	0	1437	50	0
55	BO	896	0	946	39	0
56	BP	2312	0	2373	112	0
57	BQ	1792	0	1832	51	0
58	BR	1240	0	1260	46	0
59	BS	1168	0	1159	50	0
60	BT	1950	0	1969	62	0
61	BU	1159	0	1228	49	0
62	BV	1231	0	1278	43	0
63	BW	1374	0	1405	47	0
64	BX	1120	0	1133	48	0
65	BY	1663	0	1665	57	0
66	Ba	3173	0	3153	0	0
67	Bb	2952	0	2840	0	0
68	Bc	2408	0	2415	0	0
69	Bd	832	0	828	0	0
70	Be	968	0	968	0	0
71	Bf	852	0	834	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	Bg	1167	0	1173	0	0
73	Bh	2319	0	2332	0	0
74	Bi	1979	0	1974	0	0
75	Bj	1775	0	1797	0	0
76	Bk	1087	0	1080	0	0
77	Bl	1097	0	1080	0	0
78	Bm	893	0	878	0	0
79	Bn	837	0	860	0	0
80	Bo	747	0	748	0	0
81	Bp	742	0	749	0	0
82	Bq	336	0	342	0	0
83	Bt	780	0	792	0	0
84	Bu	1208	0	1227	0	0
85	Bv	1068	0	1032	0	0
86	Bw	3126	0	3153	0	0
87	Bx	1325	0	1354	0	0
88	Bz	564	0	574	0	0
89	AA	146	0	0	0	0
89	Ag	1	0	0	0	0
89	B0	1	0	0	0	0
89	B2	1	0	0	0	0
89	BA	195	0	0	0	0
89	BD	2	0	0	0	0
89	BE	1	0	0	0	0
89	BP	1	0	0	0	0
89	BR	2	0	0	0	0
89	BX	1	0	0	0	0
90	AR	1	0	0	0	0
90	Ac	1	0	0	0	0
90	Ap	1	0	0	0	0
90	B5	1	0	0	0	0
90	B9	1	0	0	0	0
90	Bx	1	0	0	0	0
91	Ag	28	0	12	0	0
92	AA	114	0	0	7	0
92	Ag	4	0	0	0	0
92	B0	3	0	0	0	0
92	B7	2	0	0	0	0
92	B8	1	0	0	0	0
92	BA	196	0	0	12	0
92	BD	3	0	0	0	0
92	BF	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	BI	1	0	0	0	0
92	BO	2	0	0	0	0
92	BP	3	0	0	2	0
92	BR	2	0	0	0	0
92	BU	1	0	0	0	0
92	BW	4	0	0	0	0
All	All	167915	0	141408	2642	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 18.

All (2642) 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)
17:AV:54:Y5P:N3	17:AV:58:Y5P:H5	1.56	1.20
92:AA:8117:HOH:O	17:AV:29:Y5P:H4A	1.44	1.17
44:B8:142:ARG:NH1	46:BA:1191:C:OP2	1.90	1.05
53:BK:124:LYS:NZ	53:BK:127:ASP:OD2	1.89	1.05
55:BO:72:ARG:HH11	55:BO:72:ARG:HB2	1.22	1.02
1:AA:209:C:H4'	13:AP:43:ARG:HH12	1.19	1.01
17:AY:6:Y5P:H4A	17:AY:7:Y5P:H4	1.40	0.99
17:AV:55:Y5P:C2'	17:AV:57:Y5P:H5	1.93	0.99
48:BD:263:ARG:HB2	48:BD:263:ARG:HH11	1.24	0.99
17:AY:70:Y5P:H4A	17:AY:71:Y5P:H4	1.45	0.99
47:BB:65:Y5P:H2'	47:BB:66:P5P:H8	1.45	0.99
17:AY:25:Y5P:H4A	17:AY:26:Y5P:H4	1.43	0.98
46:BA:62:C:OP1	51:BI:76:ARG:NH1	1.99	0.96
61:BU:54:THR:HG21	62:BV:176:MET:H	1.27	0.96
1:AA:393:A:OP1	12:AO:136:LYS:NZ	1.99	0.96
46:BA:79:U:O2'	51:BI:61:LYS:NZ	1.98	0.96
44:B8:132:LYS:HE3	46:BA:1230:G:H5'	1.48	0.95
7:AI:255:UNK:HG1	7:AI:371:LEU:HD13	1.48	0.95
46:BA:346:U:H4'	46:BA:347:G:H5'	1.49	0.95
50:BF:257:GLN:O	56:BP:21:ARG:NH1	2.00	0.95
1:AA:59:C:H42	8:AJ:133:GLN:HG2	149.01	0.94
17:AV:37:Y5P:H4A	17:AV:38:Y5P:H4	1.48	0.94
17:AY:54:Y5P:N3	17:AY:58:Y5P:C5	2.31	0.94
49:BE:341:GLY:HA2	60:BT:105:ILE:HD11	1.49	0.93
6:AG:197:ARG:HB3	6:AG:197:ARG:HH11	1.33	0.93
16:AU:52:ARG:HH11	16:AU:52:ARG:HB2	1.34	0.92
3:AC:93:ARG:NH1	3:AC:108:LEU:O	2.03	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BF:59:ARG:HH11	50:BF:59:ARG:HG2	1.36	0.91
7:AI:253:UNK:HG3	7:AI:366:ARG:HH12	1.35	0.91
17:AY:54:Y5P:N3	17:AY:58:Y5P:H5	1.86	0.91
46:BA:618:A:HO2'	46:BA:619:U:H6	0.95	0.91
56:BP:137:GLY:HA3	56:BP:157:GLN:HG3	1.52	0.91
60:BT:66:UNK:HG3	60:BT:66:UNK:O	1.72	0.89
41:B5:152:PRO:HG3	41:B5:173:ARG:NH1	1.88	0.89
46:BA:1230:G:O2'	46:BA:1246:C:N4	2.05	0.89
48:BD:111:ARG:NH1	48:BD:182:ALA:HB2	1.88	0.88
46:BA:100:C:O2'	54:BN:75:LYS:NZ	106.03	0.87
56:BP:11:ARG:HG2	56:BP:11:ARG:HH11	1.38	0.87
38:B2:182:LYS:NZ	46:BA:28:A:OP2	2.06	0.87
48:BD:111:ARG:HH11	48:BD:182:ALA:HB2	1.37	0.86
17:AV:54:Y5P:N3	17:AV:58:Y5P:C5	2.39	0.86
59:BS:86:THR:HG22	59:BS:88:HIS:H	1.38	0.86
46:BA:948:U:O4	46:BA:1377:C:N4	2.09	0.86
17:AV:8:Y5P:N3	17:AV:14:Y5P:H5	1.92	0.85
17:AY:32:Y5P:H4A	17:AY:33:Y5P:H4	1.59	0.85
49:BE:96:ARG:NH1	49:BE:301:ASP:OD2	2.09	0.85
64:BX:71:ARG:NH1	64:BX:96:TYR:OH	2.10	0.85
50:BF:83:HIS:HD2	50:BF:85:ASP:H	1.24	0.84
2:AB:219:VAL:HG22	2:AB:233:TYR:HB2	1.60	0.84
41:B5:85:ARG:NH1	46:BA:640:G:OP1	2.11	0.84
48:BD:115:GLU:OE1	48:BD:148:ARG:NH1	2.11	0.83
17:AV:42:Y5P:H4A	17:AV:43:Y5P:H4	1.59	0.83
17:AY:68:Y5P:H2'	17:AY:69:Y5P:H6	1.59	0.83
59:BS:107:THR:HG21	59:BS:119:THR:HG23	1.61	0.83
55:BO:72:ARG:HB2	55:BO:72:ARG:NH1	1.92	0.83
1:AA:209:C:H4'	13:AP:43:ARG:NH1	1.93	0.82
17:AV:37:Y5P:H4A	17:AV:38:Y5P:C4	2.09	0.82
17:AY:23:Y5P:H4A	17:AY:24:Y5P:H4	1.59	0.82
17:AY:55:Y5P:C5	17:AY:58:Y5P:H5	2.09	0.82
46:BA:68:A:O2'	46:BA:69:C:O4'	1.95	0.82
58:BR:41:ARG:NH1	58:BR:134:LEU:HD13	1.94	0.82
1:AA:475:A:OP2	5:AF:123:ARG:NH2	2.11	0.82
14:AQ:13:VAL:HG23	14:AQ:66:LEU:HB2	1.61	0.82
61:BU:65:ARG:HH12	61:BU:99:ARG:NH1	1.76	0.82
17:AY:28:Y5P:H4A	17:AY:29:Y5P:H4	1.59	0.82
46:BA:134:G:O6	65:BY:34:LYS:NZ	2.11	0.82
17:AV:55:Y5P:C1'	17:AV:57:Y5P:H5	2.10	0.81
17:AY:9:Y5P:H4A	17:AY:22:Y5P:H4A	1.59	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AF:9:ILE:HB	5:AF:89:ILE:HG22	1.63	0.81
41:B5:181:ARG:HH11	41:B5:187:GLN:HG2	1.44	0.80
1:AA:103:G:OP1	14:AQ:78:LYS:NZ	2.13	0.80
50:BF:85:ASP:HB3	50:BF:274:LEU:HD21	1.61	0.80
4:AE:284:ARG:NH1	4:AE:328:GLY:O	2.14	0.80
17:AV:66:Y5P:H4A	17:AV:67:Y5P:H4	1.63	0.80
17:AV:11:Y5P:H4A	17:AV:12:Y5P:H4	1.64	0.80
42:B6:38:ARG:NH2	46:BA:1185:U:OP2	2.15	0.80
92:AA:8113:HOH:O	17:AV:30:Y5P:H4A	1.81	0.80
1:AA:106:C:OP2	14:AQ:45:LYS:NZ	2.15	0.80
41:B5:81:PRO:HA	46:BA:1436:U:C2	2.17	0.79
17:AY:9:Y5P:H4A	17:AY:22:Y5P:C4	2.12	0.79
46:BA:442:G:O6	52:BJ:31:LYS:NZ	2.16	0.79
64:BX:50:ARG:NH1	64:BX:69:ARG:HA	1.95	0.79
46:BA:996:C:OP1	92:BA:1852:HOH:O	2.00	0.79
6:AG:195:LYS:HB3	6:AG:204:LYS:HZ2	1.47	0.79
17:AV:59:Y5P:H4A	17:AV:60:Y5P:H4	1.63	0.79
46:BA:911:G:O2'	46:BA:913:C:N4	2.15	0.79
47:BB:28:P5P:H2'	47:BB:29:P5P:H8	1.65	0.79
50:BF:205:GLU:HG2	50:BF:208:ARG:HH12	1.48	0.78
1:AA:707:A:H3'	1:AA:708:A:H5''	1.64	0.78
45:B9:83:GLY:H	46:BA:1525:U:H5'	1.47	0.78
7:AI:260:UNK:HG3	7:AI:355:SER:HB3	1.66	0.78
1:AA:579:A:OP2	11:AN:96:ARG:NH1	2.15	0.78
1:AA:633:C:OP1	4:AE:269:ARG:NH1	2.17	0.78
59:BS:86:THR:O	59:BS:120:ARG:NH1	2.17	0.78
47:BB:29:P5P:H2'	47:BB:30:P5P:H8	1.65	0.78
1:AA:103:G:H4'	14:AQ:8:VAL:HG13	1.66	0.77
36:B0:100:THR:HB	36:B0:132:HIS:HE2	1.48	0.77
39:B3:71:ARG:NH2	46:BA:472:G:OP1	2.17	0.77
48:BD:86:ASN:HD21	48:BD:90:GLN:HB2	1.50	0.77
53:BK:43:GLY:HA3	53:BK:76:ARG:HH11	1.50	0.77
46:BA:497:C:O2	46:BA:548:A:N6	2.15	0.77
1:AA:576:C:HO2'	1:AA:809:G:HO2'	1.26	0.76
38:B2:188:ILE:O	65:BY:216:TYR:OH	2.03	0.76
42:B6:38:ARG:HE	46:BA:1184:U:H3'	1.51	0.76
52:BJ:162:LYS:HG3	52:BJ:195:SER:HB2	1.65	0.76
64:BX:44:ILE:HD12	64:BX:48:MET:HG2	1.68	0.76
46:BA:163:A:HO2'	46:BA:1014:C:H5	1.32	0.76
54:BN:156:ASP:N	54:BN:156:ASP:OD1	2.19	0.76
17:AV:55:Y5P:O2'	17:AV:57:Y5P:H5	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B0:50:ARG:NH1	46:BA:1198:A:OP1	2.17	0.76
50:BF:74:GLN:O	50:BF:210:ARG:NH2	2.18	0.76
2:AB:79:SER:H	2:AB:82:SER:HB3	1.51	0.76
1:AA:437:C:OP1	9:AK:191:ARG:NH2	2.18	0.76
1:AA:631:A:H5'	3:AC:46:LYS:HE3	1.66	0.76
7:AI:253:UNK:CG	7:AI:366:ARG:HH12	1.98	0.75
46:BA:1481:C:H5'	49:BE:290:PRO:HA	1.68	0.75
17:AV:54:Y5P:C4	17:AV:58:Y5P:H5	2.15	0.75
64:BX:68:VAL:HG22	64:BX:97:VAL:HG12	1.67	0.75
55:BO:74:LEU:HD11	55:BO:81:LYS:HB3	1.69	0.75
1:AA:566:U:O2	1:AA:686:A:N6	2.19	0.75
50:BF:262:THR:HG22	50:BF:264:PRO:HD2	1.69	0.75
46:BA:276:A:H2'	46:BA:277:A:H5''	1.68	0.75
40:B4:58:VAL:HG22	40:B4:64:THR:HG22	1.66	0.75
17:AY:55:Y5P:H6	17:AY:57:Y5P:H5	1.67	0.74
49:BE:113:ASP:OD1	49:BE:113:ASP:N	2.18	0.74
50:BF:59:ARG:NH1	50:BF:59:ARG:HG2	1.97	0.74
52:BJ:161:VAL:HG21	52:BJ:194:TYR:HB3	1.69	0.74
8:AJ:128:LYS:HG2	8:AJ:131:ARG:HH21	1.50	0.74
1:AA:458:C:O2'	1:AA:460:A:OP2	2.05	0.74
61:BU:94:GLN:HB2	62:BV:150:LYS:HG2	1.70	0.74
17:AV:24:Y5P:H4A	17:AV:25:Y5P:H4	1.69	0.74
17:AY:67:Y5P:H4A	17:AY:68:Y5P:H4	1.68	0.74
46:BA:293:G:H5'	63:BW:159:ARG:HD2	1.68	0.74
46:BA:163:A:OP2	61:BU:48:ARG:NH1	2.20	0.74
46:BA:162:C:H5	46:BA:1011:A:H61	1.36	0.74
7:AI:228:ARG:HD2	16:AU:85:GLN:HE21	1.51	0.73
56:BP:14:ASP:OD1	56:BP:17:ARG:NH1	2.21	0.73
5:AF:3:ARG:NH1	5:AF:4:TYR:HE1	1.86	0.73
1:AA:361:A:N6	92:AA:8120:HOH:O	2.16	0.73
9:AK:160:ARG:NH1	16:AU:23:TYR:OH	2.21	0.73
7:AI:382:LYS:NZ	7:AI:388:ALA:O	2.16	0.73
65:BY:130:PRO:O	65:BY:149:ARG:NH1	2.22	0.73
48:BD:136:ARG:HH11	48:BD:136:ARG:HG2	1.53	0.73
4:AE:160:ARG:NH1	4:AE:165:GLN:OE1	2.21	0.73
46:BA:658:C:H4'	58:BR:81:THR:HG21	1.69	0.73
1:AA:12:G:H5'	4:AE:229:PHE:HD2	1.52	0.73
6:AG:64:TYR:HA	6:AG:67:ASP:HB2	1.70	0.73
54:BN:114:LYS:HA	54:BN:118:ARG:NH1	2.04	0.73
54:BN:27:PRO:HG2	54:BN:30:LYS:HB2	1.70	0.73
11:AN:41:ARG:HD3	11:AN:87:ILE:HD13	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:BJ:93:ASN:HD22	52:BJ:96:ILE:HG12	1.53	0.73
57:BQ:209:ASN:ND2	57:BQ:211:ASN:OD1	2.21	0.73
9:AK:65:TYR:HB3	16:AU:13:MET:H	1.53	0.72
1:AA:858:C:H42	1:AA:912:A:H61	1.36	0.72
46:BA:213:A:O3'	50:BF:92:ARG:NH2	2.21	0.72
1:AA:56:U:O2'	1:AA:198:C:O2	2.08	0.72
48:BD:258:ILE:HG23	48:BD:263:ARG:HB3	1.71	0.72
62:BV:159:ARG:NH1	62:BV:161:GLU:OE2	2.22	0.72
1:AA:744:C:H3'	1:AA:745:C:H4'	1.71	0.72
17:AV:67:Y5P:H4A	17:AV:68:Y5P:H4	1.70	0.72
46:BA:786:A:C5	58:BR:17:ARG:HD2	2.24	0.72
50:BF:292:ASP:N	50:BF:292:ASP:OD1	2.22	0.72
44:B8:137:THR:HG22	44:B8:139:ALA:H	1.54	0.72
54:BN:114:LYS:HA	54:BN:118:ARG:HH12	1.54	0.72
65:BY:133:VAL:HG13	65:BY:145:ARG:HB3	1.72	0.72
47:BB:62:Y5P:H4A	47:BB:63:Y5P:H4	1.72	0.71
46:BA:598:C:H5''	56:BP:50:GLY:HA2	1.72	0.71
41:B5:130:VAL:HG21	58:BR:135:PRO:HD3	1.72	0.71
46:BA:1048:C:H2'	46:BA:1325:U:H4'	1.71	0.71
50:BF:167:MET:HA	50:BF:170:ARG:HH21	1.55	0.71
56:BP:130:GLN:NE2	92:BP:401:HOH:O	2.23	0.71
1:AA:645:A:H5'	1:AA:646:C:H5	1.55	0.71
16:AU:49:CYS:SG	16:AU:50:ARG:N	2.63	0.71
17:AY:30:Y5P:H4A	17:AY:31:Y5P:H4	1.71	0.71
46:BA:684:C:OP2	92:BA:1930:HOH:O	2.08	0.71
1:AA:811:U:H5'	8:AJ:131:ARG:HH12	1.55	0.71
58:BR:41:ARG:HB2	58:BR:125:GLU:HG3	1.73	0.71
64:BX:45:PRO:HD2	64:BX:48:MET:HE2	1.73	0.71
17:AY:55:Y5P:C6	17:AY:58:Y5P:H5	2.19	0.71
59:BS:88:HIS:HB3	59:BS:89:HIS:HD2	1.55	0.71
1:AA:361:A:OP1	5:AF:57:ARG:NH1	2.24	0.71
46:BA:819:C:O2'	46:BA:951:G:OP1	2.09	0.71
1:AA:512:A:H2'	1:AA:513:A:H8	1.56	0.71
46:BA:741:U:H3'	46:BA:742:A:H5''	1.73	0.71
46:BA:875:U:O2'	46:BA:963:A:OP2	2.08	0.71
50:BF:205:GLU:HG2	50:BF:208:ARG:NH1	2.06	0.71
1:AA:648:A:OP2	2:AB:200:ASN:ND2	2.24	0.70
1:AA:670:A:N3	6:AG:36:ARG:NH1	2.40	0.70
62:BV:102:VAL:HB	62:BV:139:LEU:HB3	1.72	0.70
17:AY:3:Y5P:H4A	17:AY:4:Y5P:H4	1.71	0.70
46:BA:618:A:O2'	46:BA:619:U:H6	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:52:THR:HG22	3:AC:54:GLU:H	1.56	0.70
4:AE:198:TRP:HB2	4:AE:225:VAL:HG11	1.74	0.70
42:B6:37:LEU:HD11	42:B6:40:LYS:HG3	1.74	0.70
46:BA:1250:G:N7	92:BA:1842:HOH:O	2.24	0.70
46:BA:512:A:O2'	46:BA:513:A:OP2	2.08	0.70
49:BE:165:TYR:CE2	49:BE:172:PRO:HA	2.27	0.70
56:BP:104:LEU:HD11	56:BP:126:GLY:HA3	1.73	0.70
11:AN:60:ASN:O	11:AN:68:GLN:NE2	2.24	0.70
5:AF:90:ARG:NH1	15:AR:117:ILE:O	2.25	0.70
48:BD:64:VAL:O	48:BD:80:ARG:NH2	2.21	0.70
1:AA:606:A:HO2'	11:AN:28:TYR:HH	1.40	0.69
17:AY:6:Y5P:C4	17:AY:7:Y5P:H4	2.17	0.69
60:BT:66:UNK:CG	60:BT:66:UNK:O	2.39	0.69
1:AA:647:A:H1'	2:AB:148:ARG:NH1	2.07	0.69
46:BA:428:G:OP1	56:BP:62:ARG:NH2	2.25	0.69
52:BJ:156:SER:HB3	52:BJ:159:PRO:HB3	1.74	0.69
37:B1:5:LYS:HG3	37:B1:6:VAL:HG12	1.73	0.69
55:BO:73:ILE:HG22	55:BO:84:ALA:HB3	1.74	0.69
17:AY:27:Y5P:H6	17:AY:27:Y5P:O5'	1.90	0.69
46:BA:1264:U:H2'	46:BA:1265:A:H8	1.57	0.69
1:AA:588:A:OP1	11:AN:33:LYS:NZ	2.26	0.69
17:AY:36:P5P:H2'	17:AY:37:Y5P:H6	1.73	0.69
48:BD:69:ARG:HB2	48:BD:69:ARG:HH11	1.57	0.69
38:B2:175:PHE:O	38:B2:214:ARG:NH2	2.25	0.69
61:BU:65:ARG:HH12	61:BU:99:ARG:HH11	1.39	0.69
1:AA:512:A:H2'	1:AA:513:A:C8	2.28	0.69
10:AL:32:THR:HG23	10:AL:35:GLN:HE21	1.57	0.69
17:AY:14:Y5P:H4A	17:AY:15:Y5P:H4	1.75	0.69
60:BT:99:MET:HB2	60:BT:167:TYR:CE1	2.28	0.69
45:B9:65:THR:HG23	45:B9:100:MET:HB3	1.75	0.69
56:BP:28:LYS:NZ	56:BP:31:PRO:HD3	2.07	0.69
46:BA:529:G:H1	46:BA:544:C:H42	1.40	0.68
10:AL:69:LYS:NZ	10:AL:77:ASN:HB3	2.07	0.68
17:AY:38:Y5P:H4A	17:AY:39:Y5P:H4	1.75	0.68
37:B1:96:LYS:O	46:BA:60:U:O2'	2.11	0.68
46:BA:147:A:H4'	46:BA:148:A:H5''	1.75	0.68
50:BF:92:ARG:NH1	50:BF:95:ILE:HD11	2.09	0.68
46:BA:136:A:H5''	65:BY:85:TRP:CH2	2.29	0.68
60:BT:192:ASP:OD2	60:BT:233:TRP:NE1	2.18	0.68
1:AA:826:C:H2'	1:AA:827:A:H8	1.58	0.68
10:AL:55:ARG:HD3	10:AL:58:LEU:HD21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:973:G:O2'	46:BA:975:G:OP2	2.11	0.68
2:AB:57:LEU:HB2	2:AB:270:TYR:HE2	1.58	0.68
17:AV:62:Y5P:H4A	17:AV:63:Y5P:H4	1.75	0.68
40:B4:61:ASP:HB3	40:B4:63:SER:H	1.57	0.68
50:BF:283:LEU:HB2	56:BP:125:ARG:HH12	1.59	0.68
46:BA:1416:G:N2	46:BA:1419:A:OP2	2.25	0.68
4:AE:160:ARG:HD2	4:AE:165:GLN:HE22	1.57	0.68
41:B5:93:ARG:NH1	46:BA:642:G:OP2	2.27	0.68
50:BF:279:ARG:NH1	50:BF:286:PHE:HE2	1.92	0.68
1:AA:702:G:H5'	11:AN:36:ARG:HD3	1.74	0.68
60:BT:246:ASP:OD1	60:BT:246:ASP:N	2.26	0.68
64:BX:28:LEU:HD11	64:BX:40:VAL:HG12	1.76	0.68
41:B5:156:THR:HG21	41:B5:173:ARG:NH1	2.08	0.68
7:AI:274:GLU:HG2	7:AI:283:GLU:HG2	1.75	0.68
14:AQ:69:LEU:HD12	14:AQ:70:PRO:HD2	1.76	0.68
17:AV:64:Y5P:H4A	17:AV:65:Y5P:H4	1.76	0.67
17:AV:4:Y5P:H4A	17:AV:5:Y5P:H4	1.74	0.67
6:AG:71:THR:HA	7:AI:253:UNK:HG1	1.76	0.67
17:AV:55:Y5P:HC	17:AV:57:Y5P:H5	1.76	0.67
41:B5:181:ARG:NH1	41:B5:187:GLN:HA	2.10	0.67
54:BN:65:ILE:HD11	54:BN:104:VAL:HG23	1.76	0.67
46:BA:68:A:O2'	46:BA:69:C:O5'	2.12	0.67
46:BA:925:A:H2'	46:BA:926:G:O4'	1.94	0.67
1:AA:835:C:H2'	1:AA:836:G:C8	2.30	0.67
60:BT:233:TRP:HB3	60:BT:240:ILE:HD12	1.75	0.67
65:BY:18:ASN:OD1	65:BY:43:ARG:NH1	2.28	0.67
11:AN:58:ARG:HH11	11:AN:58:ARG:HB3	1.59	0.67
37:B1:96:LYS:NZ	46:BA:82:G:OP1	2.27	0.67
7:AI:253:UNK:HG3	7:AI:366:ARG:NH1	2.10	0.67
41:B5:152:PRO:HG3	41:B5:173:ARG:HH11	1.59	0.67
17:AV:51:Y5P:H2'	17:AV:52:Y5P:C6	2.25	0.67
5:AF:53:ALA:HB1	5:AF:54:HIS:HD2	1.59	0.66
48:BD:114:PRO:HA	48:BD:123:PHE:CZ	2.30	0.66
17:AY:52:Y5P:H4A	17:AY:53:Y5P:H4	1.78	0.66
14:AQ:18:ILE:HG12	14:AQ:29:ARG:HB2	1.76	0.66
17:AV:54:Y5P:H4A	17:AV:55:Y5P:H4	1.77	0.66
60:BT:114:GLY:HA3	60:BT:182:ARG:HG3	1.78	0.66
1:AA:368:A:O2'	16:AU:42:ARG:NH2	2.29	0.66
92:AA:8139:HOH:O	17:AY:34:P5P:OP1	2.12	0.66
50:BF:130:GLN:HE22	50:BF:137:ARG:HD2	1.60	0.66
6:AG:233:ASN:HB3	6:AG:236:LEU:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:86:A:O2'	13:AP:13:ARG:O	2.13	0.66
42:B6:42:THR:HG23	42:B6:55:LEU:HD13	1.76	0.66
46:BA:1290:A:N6	46:BA:1302:G:O2'	2.29	0.66
55:BO:38:VAL:HG21	55:BO:75:LEU:HD11	1.76	0.66
57:BQ:124:VAL:HA	57:BQ:158:ARG:HH21	1.60	0.66
62:BV:180:LYS:HB3	62:BV:181:ARG:NH1	2.11	0.66
1:AA:747:C:H2'	1:AA:748:A:H5''	1.78	0.66
57:BQ:106:ARG:HB3	57:BQ:106:ARG:NH1	2.11	0.66
1:AA:300:G:N7	92:AA:8061:HOH:O	2.29	0.66
4:AE:365:LYS:HE3	4:AE:366:LYS:HE2	1.76	0.66
7:AI:374:ASP:OD1	7:AI:376:ARG:NH1	2.29	0.66
38:B2:88:THR:HB	38:B2:91:GLN:HG3	1.77	0.66
42:B6:30:PHE:HZ	46:BA:1240:U:C2	2.12	0.66
48:BD:111:ARG:HE	48:BD:152:ILE:HD12	1.61	0.66
58:BR:142:ASN:O	58:BR:148:GLN:NE2	2.28	0.66
59:BS:68:TRP:HB3	59:BS:71:VAL:HG23	1.76	0.66
48:BD:263:ARG:NH1	48:BD:263:ARG:HB2	2.06	0.66
11:AN:58:ARG:HH12	11:AN:59:LYS:HE2	1.60	0.66
49:BE:236:THR:HA	49:BE:239:ARG:HD2	1.77	0.65
64:BX:14:ASN:HD21	65:BY:211:LYS:H	1.42	0.65
46:BA:186:G:H2'	46:BA:1023:A:N7	2.11	0.65
59:BS:56:LEU:HB3	59:BS:62:ALA:HB2	1.77	0.65
64:BX:18:ARG:NH2	65:BY:206:GLU:OE1	2.29	0.65
46:BA:185:U:OP1	46:BA:431:A:O2'	2.14	0.65
46:BA:234:A:H4'	56:BP:34:ARG:HD3	1.77	0.65
64:BX:50:ARG:HH12	64:BX:69:ARG:HA	1.60	0.65
37:B1:91:TYR:CE2	51:BI:79:VAL:HG11	2.31	0.65
46:BA:226:U:O2'	46:BA:229:G:H4'	1.97	0.65
17:AY:25:Y5P:C4	17:AY:26:Y5P:H4	2.24	0.65
14:AQ:55:LEU:HB2	14:AQ:57:GLN:HB2	1.77	0.65
17:AV:26:Y5P:H4A	17:AV:27:Y5P:H4	1.77	0.65
46:BA:1449:U:O2'	55:BO:63:LYS:NZ	2.22	0.65
46:BA:112:A:N6	46:BA:115:U:OP2	2.23	0.65
46:BA:476:A:O2'	62:BV:192:ASN:ND2	2.29	0.65
46:BA:689:A:OP2	92:BA:1929:HOH:O	2.15	0.65
63:BW:123:GLN:HE21	63:BW:135:ARG:HB2	1.60	0.65
46:BA:1251:G:O6	56:BP:77:ARG:NH2	2.30	0.65
17:AV:34:P5P:H8	17:AV:34:P5P:OP2	1.96	0.65
59:BS:91:GLU:HG2	59:BS:93:LEU:HD21	1.79	0.65
63:BW:76:ARG:HA	63:BW:171:HIS:HD2	1.60	0.65
46:BA:690:A:H2'	46:BA:691:U:H5'	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AJ:91:TYR:OH	8:AJ:160:ILE:O	2.14	0.64
55:BO:93:GLY:O	55:BO:95:ARG:NH1	2.26	0.64
4:AE:371:VAL:HG22	4:AE:383:VAL:HG22	1.79	0.64
17:AV:9:Y5P:O2'	17:AV:10:Y5P:C5	2.45	0.64
46:BA:657:U:O2'	58:BR:82:GLU:OE2	2.14	0.64
46:BA:879:C:H4'	46:BA:880:A:H5'	1.78	0.64
4:AE:302:HIS:HB2	4:AE:337:SER:HB2	1.79	0.64
40:B4:58:VAL:HB	40:B4:77:THR:HG23	1.79	0.64
60:BT:60:UNK:HG2	60:BT:60:UNK:O	1.98	0.64
17:AV:9:Y5P:O2'	17:AV:10:Y5P:H5	1.97	0.64
17:AY:54:Y5P:H4A	17:AY:55:Y5P:H4A	1.78	0.64
46:BA:455:G:N7	92:BA:1861:HOH:O	2.30	0.64
46:BA:747:C:O2'	46:BA:748:A:H5''	1.97	0.64
2:AB:140:ILE:HB	2:AB:189:PRO:HA	1.80	0.64
17:AV:49:Y5P:H4A	17:AV:50:Y5P:H4	1.80	0.64
56:BP:229:PHE:O	56:BP:233:ARG:HB3	1.97	0.64
17:AV:66:Y5P:H4A	17:AV:67:Y5P:C4	2.27	0.64
46:BA:58:C:H2'	46:BA:59:A:H5''	1.79	0.64
49:BE:90:TRP:HA	49:BE:316:PHE:HE2	1.62	0.64
57:BQ:50:LEU:H	57:BQ:110:ASN:HD21	1.45	0.64
8:AJ:123:SER:O	11:AN:108:ARG:NH2	2.31	0.64
41:B5:90:ASN:O	41:B5:94:ARG:HG2	1.98	0.64
42:B6:44:LEU:HB3	42:B6:53:LYS:HE3	1.79	0.64
1:AA:571:A:H2'	1:AA:572:A:C8	2.32	0.64
37:B1:116:SER:HB3	37:B1:119:LEU:HB2	1.80	0.64
42:B6:34:ARG:HG3	42:B6:36:ARG:HG2	1.80	0.64
48:BD:73:THR:HG22	48:BD:75:MET:H	1.63	0.64
50:BF:240:PHE:O	50:BF:241:ASN:ND2	2.31	0.64
46:BA:658:C:N4	63:BW:54:LYS:HB3	60.48	0.63
1:AA:257:U:H4'	1:AA:258:C:H5'	1.79	0.63
46:BA:15:A:H2'	46:BA:16:A:H8	1.64	0.63
46:BA:575:A:OP1	61:BU:82:LYS:NZ	2.28	0.63
48:BD:263:ARG:HH11	48:BD:263:ARG:CB	2.05	0.63
49:BE:96:ARG:CB	49:BE:96:ARG:HH11	2.11	0.63
57:BQ:131:ILE:HB	57:BQ:149:HIS:HB2	1.79	0.63
1:AA:790:A:OP1	7:AI:389:ARG:NH1	2.29	0.63
46:BA:303:U:H2'	46:BA:304:G:O4'	1.99	0.63
65:BY:129:LYS:HD3	65:BY:149:ARG:HH21	1.63	0.63
17:AY:31:Y5P:H4A	17:AY:32:Y5P:H4	1.81	0.63
46:BA:694:A:H3'	46:BA:695:C:H5''	1.80	0.63
12:AO:172:ARG:HH12	14:AQ:88:VAL:HG21	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AO:74:LEU:HG	12:AO:94:LEU:O	1.98	0.63
17:AY:24:Y5P:H4A	17:AY:25:Y5P:H4	1.81	0.63
46:BA:1431:U:H4'	46:BA:1432:U:H5'	1.81	0.63
46:BA:32:C:O2'	46:BA:36:A:N6	2.31	0.63
46:BA:65:C:N4	92:BA:1924:HOH:O	2.15	0.63
65:BY:64:ILE:HD11	65:BY:88:VAL:HG21	1.81	0.63
3:AC:112:ARG:HB2	3:AC:112:ARG:HH11	1.62	0.63
42:B6:45:HIS:CD2	42:B6:46:TYR:H	2.16	0.63
45:B9:74:ARG:NH1	46:BA:543:U:O2'	2.32	0.63
48:BD:172:ARG:HB2	48:BD:173:MET:SD	2.39	0.63
50:BF:279:ARG:NH1	50:BF:286:PHE:CE2	2.67	0.63
56:BP:94:GLN:NE2	56:BP:128:THR:O	2.31	0.63
46:BA:658:C:H41	63:BW:54:LYS:HB3	60.72	0.63
17:AY:37:Y5P:HB	17:AY:38:Y5P:H6	1.81	0.63
17:AY:44:Y5P:H4A	17:AY:45:Y5P:H4	1.81	0.63
13:AP:54:TYR:HD1	13:AP:66:VAL:HG22	1.64	0.63
49:BE:95:SER:HB2	49:BE:303:LYS:NZ	2.13	0.63
55:BO:55:PRO:HB3	55:BO:77:ILE:HG23	1.81	0.63
62:BV:98:ARG:HH11	62:BV:113:THR:HG21	1.64	0.63
46:BA:1349:U:H2'	46:BA:1351:C:H5''	1.80	0.62
63:BW:88:LEU:HD21	63:BW:109:LYS:HG3	1.80	0.62
7:AI:383:PRO:HB2	8:AJ:131:ARG:HB2	1.81	0.62
46:BA:1440:U:H5''	49:BE:253:PRO:HA	1.81	0.62
48:BD:114:PRO:HA	48:BD:123:PHE:CE1	2.34	0.62
51:BI:59:TRP:HE1	51:BI:81:LYS:HB3	1.64	0.62
54:BN:142:VAL:HG12	54:BN:143:GLU:HB3	1.80	0.62
1:AA:552:A:H2'	1:AA:553:G:C8	2.34	0.62
46:BA:924:U:O2'	46:BA:925:A:H8	1.82	0.62
1:AA:513:A:N3	1:AA:857:C:O2'	2.31	0.62
1:AA:591:A:H61	1:AA:704:U:H3	1.45	0.62
40:B4:52:LEU:HG	40:B4:68:ARG:HB3	1.81	0.62
60:BT:59:UNK:O	60:BT:59:UNK:HG2	1.99	0.62
1:AA:654:A:H2'	1:AA:655:G:H5'	1.81	0.62
14:AQ:57:GLN:HE21	14:AQ:87:LYS:NZ	1.97	0.62
46:BA:48:U:C1'	51:BI:78:ARG:HH12	2.12	0.62
56:BP:55:GLY:O	56:BP:59:ARG:NH1	2.32	0.62
46:BA:1002:A:N6	92:BA:1815:HOH:O	2.33	0.62
54:BN:154:ARG:HH11	54:BN:154:ARG:HB2	1.65	0.62
57:BQ:124:VAL:HG22	57:BQ:158:ARG:HE	1.64	0.62
64:BX:24:PHE:HD2	64:BX:45:PRO:HG2	1.64	0.62
37:B1:92:VAL:HG23	37:B1:98:SER:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:BQ:67:LYS:HD2	57:BQ:69:LEU:HD21	1.82	0.62
4:AE:224:GLU:HB2	4:AE:342:MET:HG2	1.81	0.62
60:BT:68:UNK:HG2	60:BT:68:UNK:O	2.00	0.62
3:AC:62:ILE:HG12	3:AC:66:LYS:HD3	1.82	0.62
4:AE:304:LYS:NZ	4:AE:410:ASP:OD1	2.25	0.62
42:B6:17:LEU:HD22	46:BA:1242:U:H4'	1.82	0.62
48:BD:188:LEU:O	48:BD:220:LYS:NZ	2.33	0.62
46:BA:479:G:H4'	61:BU:98:ASN:HD21	1.64	0.61
3:AC:88:GLU:HG3	3:AC:147:TYR:CZ	2.36	0.61
46:BA:1258:U:H2'	46:BA:1259:U:C6	2.35	0.61
46:BA:185:U:O4'	46:BA:432:G:O2'	2.15	0.61
1:AA:671:U:H2'	1:AA:672:A:H8	1.64	0.61
52:BJ:100:GLN:HB2	52:BJ:177:LEU:HD11	1.83	0.61
60:BT:276:SER:HA	60:BT:279:GLU:HG3	1.82	0.61
8:AJ:78:VAL:HG22	8:AJ:172:VAL:HG22	1.82	0.61
39:B3:74:SER:HB2	46:BA:471:U:H5''	1.82	0.61
4:AE:160:ARG:NH1	4:AE:168:VAL:HG21	2.14	0.61
56:BP:54:LYS:O	56:BP:58:GLN:HB2	2.00	0.61
62:BV:117:LEU:HD13	62:BV:198:ARG:NH1	2.16	0.61
17:AY:55:Y5P:C5	17:AY:58:Y5P:C5	2.79	0.61
48:BD:74:VAL:HG13	48:BD:151:TRP:HE1	1.65	0.61
62:BV:134:LEU:HB2	62:BV:160:VAL:HG13	1.82	0.61
1:AA:131:U:O2'	14:AQ:23:GLN:NE2	2.33	0.61
17:AY:66:Y5P:H4A	17:AY:67:Y5P:H4	1.82	0.61
36:B0:57:GLU:OE1	36:B0:99:TYR:N	2.32	0.61
46:BA:446:A:H5'	46:BA:447:G:OP2	2.00	0.61
50:BF:71:GLY:H	50:BF:74:GLN:NE2	1.99	0.61
54:BN:117:HIS:O	54:BN:121:MET:HG2	2.01	0.61
46:BA:163:A:H2'	61:BU:35:LYS:NZ	2.15	0.61
2:AB:141:ILE:HG12	2:AB:191:LEU:HB3	1.83	0.61
46:BA:192:U:H2'	46:BA:193:G:C8	2.36	0.61
50:BF:230:VAL:O	50:BF:234:THR:OG1	2.17	0.61
1:AA:43:U:H2'	1:AA:44:U:O4'	2.00	0.61
17:AY:9:Y5P:H4A	17:AY:22:Y5P:C5	2.31	0.61
1:AA:356:A:H2'	1:AA:357:G:H8	1.66	0.60
1:AA:573:A:C8	1:AA:622:U:H4'	2.36	0.60
46:BA:1255:A:H8	46:BA:1255:A:H3'	1.66	0.60
46:BA:718:C:H5'	48:BD:75:MET:HG2	1.83	0.60
1:AA:356:A:H2'	1:AA:357:G:C8	2.36	0.60
44:B8:135:LYS:HD3	46:BA:1229:U:H5'	1.83	0.60
46:BA:276:A:C2'	46:BA:277:A:H5''	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B3:77:ARG:NH1	46:BA:456:A:H4'	2.15	0.60
46:BA:716:A:H5'	46:BA:717:C:OP2	2.01	0.60
49:BE:175:LYS:HD2	49:BE:296:LEU:HB3	1.82	0.60
60:BT:96:ARG:NH1	60:BT:285:GLU:OE1	2.34	0.60
1:AA:124:A:H1'	1:AA:125:U:C5	2.37	0.60
7:AI:265:UNK:HG2	7:AI:266:UNK:N	2.16	0.60
8:AJ:84:ASP:N	8:AJ:84:ASP:OD1	2.29	0.60
44:B8:101:LYS:HE3	46:BA:75:A:H2	1.65	0.60
38:B2:232:LYS:NZ	46:BA:10:A:OP1	2.35	0.60
46:BA:187:C:H3'	62:BV:181:ARG:NH2	2.15	0.60
58:BR:106:ARG:HE	58:BR:127:LYS:HE2	1.66	0.60
17:AV:30:Y5P:H2'	17:AV:31:Y5P:H6	1.82	0.60
46:BA:1334:A:H2'	46:BA:1335:G:C8	2.35	0.60
51:BI:91:LYS:NZ	51:BI:116:LYS:HB2	2.16	0.60
16:AU:15:GLN:HG2	16:AU:16:GLU:HG3	1.82	0.60
36:B0:56:MET:H	36:B0:59:HIS:HD2	1.48	0.60
49:BE:76:LYS:NZ	49:BE:168:LEU:HD12	2.16	0.60
56:BP:276:ASN:ND2	56:BP:279:ASP:OD2	2.34	0.60
10:AL:33:LEU:HD22	14:AQ:39:LEU:HD23	1.82	0.60
46:BA:1253:A:H2'	46:BA:1254:C:C6	2.37	0.60
46:BA:797:A:H61	46:BA:989:C:H42	1.50	0.60
61:BU:11:ARG:NH1	61:BU:13:ARG:HD2	2.16	0.60
65:BY:105:ARG:HD3	65:BY:105:ARG:H	1.67	0.60
1:AA:223:U:O2'	1:AA:224:U:OP1	2.17	0.60
8:AJ:73:TYR:HE2	8:AJ:150:GLY:HA2	1.66	0.60
15:AR:83:GLN:NE2	15:AR:134:PRO:HG2	2.17	0.60
38:B2:66:LEU:N	38:B2:68:GLU:OE1	2.35	0.60
1:AA:17:G:H2'	1:AA:18:G:C8	2.37	0.60
56:BP:11:ARG:HG2	56:BP:11:ARG:NH1	2.15	0.60
1:AA:645:A:H5'	1:AA:646:C:C5	2.37	0.60
17:AV:43:Y5P:H4A	17:AV:44:Y5P:H4	1.82	0.60
17:AY:9:Y5P:C4	17:AY:22:Y5P:H5	2.31	0.60
47:BB:61:Y5P:H4A	47:BB:62:Y5P:H4	1.84	0.60
5:AF:53:ALA:HB1	5:AF:54:HIS:CD2	2.37	0.59
9:AK:65:TYR:O	9:AK:67:PRO:HD3	2.02	0.59
65:BY:131:THR:HG23	65:BY:149:ARG:HD2	1.83	0.59
1:AA:389:A:O2'	12:AO:143:HIS:ND1	2.30	0.59
11:AN:58:ARG:NH1	11:AN:58:ARG:HB3	2.16	0.59
17:AY:55:Y5P:H5	17:AY:58:Y5P:C5	2.32	0.59
65:BY:145:ARG:HH12	65:BY:157:PRO:HD3	1.66	0.59
46:BA:1230:G:H4'	46:BA:1230:G:OP1	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:1269:A:HO2'	46:BA:1270:U:H5	1.50	0.59
46:BA:58:C:C2'	46:BA:59:A:H5''	2.33	0.59
49:BE:128:HIS:CD2	49:BE:173:LYS:NZ	2.70	0.59
55:BO:64:THR:HG22	55:BO:66:VAL:H	1.66	0.59
60:BT:79:GLU:HG2	60:BT:147:ALA:HB1	1.84	0.59
1:AA:444:G:H5'	1:AA:445:C:OP2	2.03	0.59
38:B2:100:LEU:HB3	38:B2:144:LEU:HD11	1.85	0.59
46:BA:747:C:N3	64:BX:54:ARG:HD3	2.17	0.59
49:BE:210:THR:OG1	49:BE:262:GLY:O	2.12	0.59
56:BP:56:GLU:HG2	56:BP:62:ARG:HA	1.84	0.59
44:B8:113:ARG:NH1	56:BP:76:LEU:HA	2.18	0.59
39:B3:38:ARG:HB2	46:BA:409:U:OP1	2.03	0.59
46:BA:275:G:O4'	48:BD:260:LYS:NZ	2.28	0.59
56:BP:138:VAL:O	56:BP:157:GLN:HG2	2.03	0.59
56:BP:261:ASP:HB2	56:BP:264:GLN:HB2	1.84	0.59
1:AA:77:G:H8	1:AA:77:G:OP1	1.84	0.59
7:AI:207:GLU:HG3	7:AI:212:GLU:O	2.03	0.59
46:BA:622:A:P	56:BP:34:ARG:HH22	2.25	0.59
55:BO:52:HIS:CD2	55:BO:53:ARG:HG3	2.38	0.59
46:BA:1306:A:H5'	57:BQ:184:PRO:HA	1.83	0.59
62:BV:104:HIS:HB2	62:BV:138:LEU:HD11	1.84	0.59
4:AE:308:GLN:HG3	4:AE:312:TYR:CD1	2.38	0.59
12:AO:153:HIS:HA	12:AO:156:PHE:HD2	1.67	0.59
17:AV:55:Y5P:O2'	17:AV:57:Y5P:C5	2.51	0.59
44:B8:168:ARG:NE	46:BA:225:U:OP1	2.21	0.59
57:BQ:106:ARG:HB3	57:BQ:106:ARG:HH11	1.67	0.59
5:AF:10:LEU:HD23	5:AF:88:VAL:HA	1.84	0.59
46:BA:329:A:N3	46:BA:329:A:H2'	2.17	0.59
56:BP:183:SER:HA	56:BP:186:ILE:HD12	1.85	0.59
60:BT:138:ILE:HA	60:BT:187:LEU:HD12	1.84	0.59
60:BT:79:GLU:OE2	60:BT:140:ARG:NH2	2.36	0.59
4:AE:162:LYS:O	4:AE:166:GLU:HG2	2.03	0.59
10:AL:127:ARG:HD2	10:AL:132:CYS:HB3	1.85	0.59
11:AN:33:LYS:HB3	11:AN:90:ARG:CZ	2.33	0.59
13:AP:34:ILE:HG22	13:AP:51:LEU:HB2	1.83	0.59
56:BP:216:ASP:HB3	56:BP:218:LYS:HB2	1.85	0.59
62:BV:117:LEU:HD13	62:BV:198:ARG:HH11	1.67	0.59
17:AV:59:Y5P:H4A	17:AV:60:Y5P:C4	2.31	0.58
46:BA:1255:A:C8	46:BA:1255:A:H3'	2.38	0.58
45:B9:96:LYS:NZ	46:BA:1511:U:OP1	2.33	0.58
49:BE:197:HIS:CD2	49:BE:318:THR:HG22	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AE:358:THR:HG22	4:AE:360:GLN:H	1.67	0.58
7:AI:276:LYS:HG3	7:AI:281:LYS:HG2	1.85	0.58
46:BA:101:U:O2'	46:BA:102:G:O4'	2.20	0.58
65:BY:126:THR:HB	65:BY:152:ARG:NH1	2.18	0.58
12:AO:174:THR:HB	14:AQ:101:ALA:HB1	1.86	0.58
46:BA:1161:A:H5''	46:BA:1162:G:OP2	2.04	0.58
46:BA:1205:C:H5'	46:BA:1206:A:OP2	2.03	0.58
46:BA:704:A:OP1	64:BX:50:ARG:NH2	2.28	0.58
49:BE:95:SER:HB2	49:BE:303:LYS:HZ1	1.68	0.58
53:BK:19:MET:HG2	53:BK:71:PHE:HD1	1.68	0.58
54:BN:81:THR:HB	54:BN:83:TYR:HD2	1.69	0.58
46:BA:218:A:P	56:BP:109:ARG:HH22	2.27	0.58
2:AB:79:SER:OG	2:AB:80:VAL:N	2.35	0.58
46:BA:686:A:H3'	46:BA:687:A:H4'	1.86	0.58
46:BA:971:A:N3	92:BA:1958:HOH:O	2.32	0.58
53:BK:66:LEU:HA	53:BK:85:PRO:HA	1.85	0.58
54:BN:20:LEU:HB2	54:BN:141:LEU:HD22	1.84	0.58
46:BA:131:G:O2'	65:BY:40:ARG:O	2.16	0.58
42:B6:18:VAL:HG21	42:B6:58:GLU:HG3	1.84	0.58
1:AA:174:C:H2'	1:AA:175:A:O4'	2.04	0.58
10:AL:76:ALA:HB3	10:AL:78:ARG:HE	1.68	0.58
11:AN:52:LEU:O	11:AN:56:SER:OG	2.17	0.58
61:BU:23:GLU:HA	61:BU:26:LYS:HE3	1.84	0.58
1:AA:320:A:N6	1:AA:390:A:H1'	2.19	0.58
3:AC:72:HIS:HD2	3:AC:74:GLY:H	1.51	0.58
38:B2:123:ARG:HH22	64:BX:30:ARG:HG2	1.68	0.58
46:BA:841:C:OP1	48:BD:264:ASN:ND2	2.37	0.58
60:BT:165:GLU:HB2	60:BT:168:ASN:HB2	1.85	0.58
65:BY:195:GLU:N	65:BY:195:GLU:OE1	2.37	0.58
46:BA:664:G:H2'	46:BA:665:C:C6	2.37	0.58
49:BE:292:HIS:CE1	49:BE:295:CYS:HB3	2.39	0.58
63:BW:151:LEU:HB2	63:BW:167:LYS:HB2	1.86	0.58
1:AA:527:G:N2	1:AA:839:C:N3	2.52	0.58
46:BA:1025:G:OP2	46:BA:1276:C:H5'	2.04	0.58
64:BX:71:ARG:HH11	64:BX:71:ARG:HG2	1.68	0.58
1:AA:707:A:H3'	1:AA:708:A:C5'	2.31	0.58
7:AI:170:LEU:HD11	7:AI:174:LYS:HE3	1.84	0.58
12:AO:116:VAL:O	12:AO:181:LYS:NZ	2.28	0.58
49:BE:96:ARG:NH2	49:BE:197:HIS:O	2.37	0.58
46:BA:224:C:H5'	56:BP:133:LYS:HE3	1.84	0.58
46:BA:1546:A:H5'	46:BA:1547:A:OP2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:178:U:O2'	46:BA:188:A:O4'	2.18	0.57
48:BD:157:ASN:HB2	48:BD:179:GLU:OE2	2.04	0.57
49:BE:99:LEU:HD12	49:BE:198:PHE:HE1	1.68	0.57
56:BP:100:ARG:HH21	56:BP:126:GLY:HA2	1.69	0.57
1:AA:641:A:H2'	1:AA:642:G:H8	1.67	0.57
3:AC:100:PHE:HE2	3:AC:155:LEU:HD21	1.69	0.57
4:AE:286:GLU:HB3	4:AE:288:HIS:CE1	2.39	0.57
41:B5:140:GLN:NE2	41:B5:176:GLU:O	2.36	0.57
55:BO:87:VAL:HG13	55:BO:123:ILE:HG12	1.85	0.57
46:BA:1199:A:H61	56:BP:71:GLN:HE22	1.51	0.57
1:AA:641:A:H2'	1:AA:642:G:C8	2.39	0.57
4:AE:288:HIS:HD2	4:AE:289:THR:H	1.52	0.57
6:AG:152:CYS:SG	6:AG:219:VAL:HB	2.44	0.57
46:BA:1293:G:H2'	46:BA:1296:C:H42	1.68	0.57
46:BA:1546:A:C2	49:BE:176:VAL:HG21	2.39	0.57
54:BN:58:VAL:HG22	54:BN:126:HIS:HB2	1.85	0.57
65:BY:212:LYS:HZ3	65:BY:214:TYR:HE1	1.50	0.57
1:AA:630:A:H2'	1:AA:631:A:H8	1.68	0.57
3:AC:50:PRO:HB3	3:AC:167:ILE:HD11	1.86	0.57
4:AE:288:HIS:CD2	4:AE:289:THR:H	2.22	0.57
4:AE:292:HIS:HE1	4:AE:357:GLU:H	1.52	0.57
1:AA:62:C:O2'	1:AA:198:C:H5'	2.04	0.57
1:AA:196:A:P	13:AP:20:ARG:HH11	2.28	0.57
48:BD:198:GLU:OE2	48:BD:202:GLY:N	2.37	0.57
46:BA:1565:G:O5'	49:BE:174:GLN:NE2	2.38	0.57
47:BB:24:P5P:H4'	59:BS:108:ARG:HH11	1.69	0.57
59:BS:39:VAL:HG12	59:BS:41:ASN:H	1.69	0.57
41:B5:141:MET:HB2	41:B5:173:ARG:NH2	2.19	0.57
1:AA:561:U:H1'	1:AA:711:A:N6	2.19	0.57
3:AC:112:ARG:NH1	3:AC:112:ARG:HB2	2.20	0.57
4:AE:198:TRP:HB2	4:AE:225:VAL:CG1	2.35	0.57
1:AA:14:C:OP2	4:AE:226:ARG:NH2	2.37	0.57
7:AI:255:UNK:HG1	7:AI:371:LEU:CD1	2.31	0.57
46:BA:1074:A:H2'	46:BA:1075:A:C8	2.39	0.57
1:AA:956:G:H2'	1:AA:957:A:C8	2.40	0.57
4:AE:323:ILE:HD13	4:AE:350:PHE:CE1	2.39	0.57
9:AK:112:ALA:HB3	9:AK:137:ALA:HB2	1.85	0.57
18:AX:21:Y5P:H4A	18:AX:22:Y5P:H4	1.87	0.57
36:B0:100:THR:HG22	36:B0:102:GLU:HG3	1.85	0.57
53:BK:54:ASN:HB3	53:BK:58:LYS:HE3	1.85	0.57
4:AE:369:HIS:HE1	4:AE:391:LEU:HD22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AI:275:GLY:H	7:AI:348:ALA:HB2	1.70	0.57
38:B2:88:THR:HG22	38:B2:90:GLN:H	1.69	0.57
43:B7:75:THR:HG23	43:B7:78:GLY:H	1.70	0.57
45:B9:83:GLY:H	46:BA:1525:U:C5'	2.17	0.57
46:BA:341:C:H2'	46:BA:342:C:C6	2.39	0.57
46:BA:558:A:O2'	46:BA:559:C:OP1	2.20	0.57
46:BA:664:G:H5''	46:BA:777:G:O2'	2.04	0.57
56:BP:47:ARG:NH1	62:BV:183:ASN:HB2	2.20	0.57
1:AA:28:U:H2'	1:AA:29:A:H8	1.70	0.57
1:AA:344:G:H1	9:AK:121:ASN:HB2	1.70	0.57
36:B0:65:ASN:N	36:B0:65:ASN:OD1	2.37	0.57
46:BA:1476:U:H2'	46:BA:1477:G:H8	1.70	0.57
61:BU:93:CYS:O	62:BV:150:LYS:HE2	2.04	0.57
62:BV:98:ARG:HH11	62:BV:113:THR:CG2	2.18	0.57
65:BY:131:THR:HG21	65:BY:147:SER:HB3	1.87	0.57
4:AE:261:ALA:HB2	4:AE:270:LYS:NZ	2.20	0.56
13:AP:20:ARG:NH2	13:AP:38:HIS:O	2.38	0.56
15:AR:65:LYS:HD3	15:AR:69:CYS:HB3	1.88	0.56
15:AR:73:VAL:HG22	15:AR:80:LEU:HD21	1.87	0.56
16:AU:52:ARG:HH11	16:AU:52:ARG:CB	2.14	0.56
17:AY:67:Y5P:C4	17:AY:68:Y5P:H4	2.34	0.56
44:B8:172:TYR:HB2	44:B8:175:ASP:HB2	1.86	0.56
46:BA:1386:A:H5'	46:BA:1387:A:OP2	2.05	0.56
50:BF:244:PRO:HB2	50:BF:246:VAL:HG23	1.86	0.56
1:AA:15:C:O2'	1:AA:293:A:N1	2.29	0.56
9:AK:68:ILE:HG22	9:AK:70:GLY:H	1.71	0.56
64:BX:37:GLU:HB3	64:BX:104:THR:HG23	1.87	0.56
1:AA:891:C:H4'	1:AA:891:C:OP1	2.04	0.56
17:AY:36:P5P:C6	17:AY:37:Y5P:H4	2.34	0.56
17:AY:9:Y5P:H4	17:AY:22:Y5P:H5	1.87	0.56
37:B1:87:LEU:HD23	37:B1:104:VAL:HB	1.86	0.56
46:BA:39:A:H4'	46:BA:40:C:OP1	2.06	0.56
46:BA:664:G:H2'	46:BA:665:C:H6	1.70	0.56
46:BA:892:U:O2'	48:BD:285:ARG:O	2.20	0.56
55:BO:58:ILE:HD11	55:BO:76:ALA:HB2	1.87	0.56
1:AA:641:A:N7	4:AE:260:LYS:NZ	2.53	0.56
4:AE:290:ILE:HG13	4:AE:307:LYS:HB2	1.87	0.56
46:BA:472:G:H3'	46:BA:472:G:N3	2.20	0.56
46:BA:526:U:O2'	46:BA:527:G:O4'	2.21	0.56
52:BJ:101:HIS:CE1	52:BJ:109:LYS:NZ	2.73	0.56
60:BT:103:ARG:NH1	60:BT:108:ILE:HB	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AI:263:UNK:HG2	7:AI:265:UNK:HG3	1.86	0.56
1:AA:844:C:H5'	18:AX:18:Y5P:H4A	1.87	0.56
36:B0:90:TYR:HE1	36:B0:92:LEU:HD21	1.71	0.56
48:BD:111:ARG:HG3	48:BD:111:ARG:NH1	2.20	0.56
46:BA:174:C:OP1	54:BN:115:ASN:HB2	2.05	0.56
55:BO:77:ILE:HD11	55:BO:107:LEU:HD21	1.87	0.56
57:BQ:72:ILE:HD11	57:BQ:96:TYR:CE1	2.41	0.56
58:BR:139:ARG:HG3	58:BR:139:ARG:HH11	1.71	0.56
1:AA:327:U:O2'	1:AA:328:A:N7	2.35	0.56
37:B1:108:GLN:HB2	51:BI:87:LYS:HZ1	1.70	0.56
46:BA:115:U:H3'	46:BA:116:A:H5''	1.86	0.56
45:B9:98:ARG:HH12	46:BA:1360:U:H4'	1.70	0.56
46:BA:478:A:C2	63:BW:208:HIS:HA	2.40	0.56
50:BF:204:ILE:HD11	50:BF:237:LEU:HD21	1.87	0.56
50:BF:290:TYR:HB2	50:BF:293:PHE:HB3	1.87	0.56
61:BU:50:PHE:O	61:BU:53:CYS:HB3	2.05	0.56
63:BW:47:ARG:NH1	63:BW:76:ARG:HD2	2.20	0.56
1:AA:255:G:O6	10:AL:74:ASN:HB2	2.06	0.56
17:AV:31:Y5P:H4A	17:AV:32:Y5P:H4	1.87	0.56
47:BB:30:P5P:H2'	47:BB:31:Y5P:H6	1.87	0.56
6:AG:155:VAL:H	6:AG:227:HIS:CE1	2.23	0.56
17:AY:43:Y5P:HA	17:AY:43:Y5P:OP2	2.06	0.56
38:B2:209:ARG:HH11	38:B2:209:ARG:HG2	1.71	0.56
38:B2:209:ARG:NH1	38:B2:209:ARG:HG2	2.21	0.56
46:BA:513:A:N7	46:BA:539:A:H4'	2.21	0.56
50:BF:142:ARG:NH2	63:BW:210:LEU:HD21	73.88	0.56
7:AI:373:ALA:O	7:AI:375:PRO:HD3	2.06	0.56
38:B2:139:ASP:O	38:B2:143:ALA:N	2.31	0.56
49:BE:195:ALA:H	49:BE:281:ASN:ND2	2.04	0.56
56:BP:202:LYS:HZ1	56:BP:263:ARG:NH1	2.04	0.56
59:BS:163:HIS:O	59:BS:167:GLU:HG2	2.06	0.56
1:AA:248:C:OP1	10:AL:97:GLY:N	2.36	0.56
5:AF:97:PRO:HG3	15:AR:76:LYS:NZ	2.21	0.56
17:AV:2:Y5P:HA	36:B0:36:GLY:HA3	1.87	0.56
46:BA:478:A:OP1	46:BA:478:A:H8	1.89	0.56
48:BD:123:PHE:HB2	48:BD:166:ASN:HB2	1.87	0.56
59:BS:79:HIS:N	59:BS:174:GLU:OE2	2.37	0.56
63:BW:127:VAL:HG13	63:BW:132:VAL:O	2.06	0.56
41:B5:140:GLN:HE22	41:B5:176:GLU:C	2.08	0.56
49:BE:149:GLY:O	49:BE:173:LYS:HD2	2.06	0.56
1:AA:297:A:N6	1:AA:485:G:H4'	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AO:74:LEU:HB2	12:AO:77:TYR:HD2	1.70	0.55
17:AY:8:Y5P:N3	17:AY:14:Y5P:C5	2.69	0.55
17:AY:55:Y5P:H5	17:AY:58:Y5P:C6	2.36	0.55
46:BA:1546:A:H3'	46:BA:1547:A:H5'	1.88	0.55
46:BA:822:G:H5'	46:BA:823:C:OP2	2.06	0.55
46:BA:159:A:H61	54:BN:119:ARG:CB	2.19	0.55
56:BP:100:ARG:NH2	56:BP:126:GLY:HA2	2.21	0.55
4:AE:197:THR:HG22	4:AE:199:GLY:H	1.71	0.55
4:AE:284:ARG:HH11	4:AE:328:GLY:C	2.09	0.55
9:AK:191:ARG:HH21	9:AK:194:ARG:HD3	1.71	0.55
1:AA:386:U:H5''	15:AR:114:ARG:HE	1.71	0.55
37:B1:75:SER:HA	37:B1:80:TRP:CE2	2.41	0.55
43:B7:74:ARG:NH2	46:BA:31:A:O2'	2.39	0.55
46:BA:131:G:H8	46:BA:131:G:H5'	1.70	0.55
46:BA:277:A:H5'	46:BA:277:A:H8	1.71	0.55
50:BF:195:LEU:HD22	50:BF:202:TYR:HE2	1.71	0.55
46:BA:1519:U:H5	54:BN:177:ARG:HG3	1.71	0.55
56:BP:84:ASN:O	56:BP:87:HIS:HB3	2.07	0.55
1:AA:12:G:H5'	4:AE:229:PHE:CD2	2.38	0.55
1:AA:344:G:N1	9:AK:121:ASN:HB2	2.22	0.55
1:AA:44:U:H5'	1:AA:45:A:OP2	2.06	0.55
1:AA:487:C:H5'	1:AA:488:A:OP2	2.06	0.55
38:B2:156:ARG:O	38:B2:160:THR:N	2.38	0.55
52:BJ:89:VAL:HG22	52:BJ:124:LYS:NZ	2.21	0.55
54:BN:20:LEU:HD22	54:BN:141:LEU:HD13	1.88	0.55
55:BO:128:ARG:NH1	60:BT:126:ALA:HA	2.21	0.55
55:BO:69:VAL:HG23	55:BO:89:HIS:CE1	2.42	0.55
56:BP:54:LYS:HG2	56:BP:59:ARG:HH22	1.72	0.55
7:AI:294:ILE:HG12	7:AI:301:TYR:HB3	1.88	0.55
9:AK:80:LYS:HB3	9:AK:84:GLU:HB2	1.88	0.55
14:AQ:57:GLN:HE21	14:AQ:87:LYS:HZ3	1.53	0.55
46:BA:163:A:H2'	61:BU:35:LYS:HZ1	1.71	0.55
46:BA:168:U:H4'	63:BW:207:THR:HG21	1.87	0.55
6:AG:197:ARG:HH11	6:AG:197:ARG:CB	2.12	0.55
1:AA:196:A:OP1	13:AP:20:ARG:NH1	2.38	0.55
17:AV:37:Y5P:C4	17:AV:38:Y5P:H4	2.29	0.55
38:B2:230:ARG:HB3	38:B2:230:ARG:HH11	1.72	0.55
46:BA:342:C:H2'	46:BA:343:U:C6	2.42	0.55
46:BA:944:C:OP2	92:BA:1955:HOH:O	2.18	0.55
64:BX:64:PRO:HG2	64:BX:103:GLN:HE22	1.72	0.55
1:AA:287:C:N4	14:AQ:39:LEU:HA	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:632:A:OP1	4:AE:269:ARG:NH2	2.39	0.55
9:AK:156:LEU:HD21	16:AU:36:ILE:HG23	1.89	0.55
46:BA:478:A:N1	63:BW:208:HIS:HA	2.21	0.55
56:BP:203:ARG:NH1	56:BP:264:GLN:O	2.40	0.55
60:BT:235:ARG:NH1	60:BT:260:TRP:CE2	2.75	0.55
4:AE:365:LYS:HG3	4:AE:366:LYS:HG2	1.88	0.55
5:AF:8:LEU:HB2	5:AF:64:PHE:HB2	1.86	0.55
46:BA:128:A:C2	46:BA:129:A:C4	2.95	0.55
50:BF:97:HIS:CD2	56:BP:29:PRO:HB3	2.41	0.55
59:BS:151:TRP:CD1	59:BS:152:GLU:HG3	2.41	0.55
1:AA:560:C:H42	1:AA:710:G:H1	1.54	0.55
4:AE:150:ARG:HB2	4:AE:155:GLN:HE21	1.72	0.55
1:AA:811:U:H5'	8:AJ:131:ARG:NH1	2.21	0.55
17:AY:24:Y5P:C4	17:AY:25:Y5P:H4	2.37	0.55
46:BA:119:A:C6	46:BA:128:A:C8	2.95	0.55
59:BS:52:ASN:HD21	59:BS:54:ARG:HB3	1.72	0.55
60:BT:196:GLU:H	60:BT:196:GLU:CD	2.09	0.55
63:BW:77:GLN:H	63:BW:171:HIS:CD2	2.24	0.55
14:AQ:96:THR:HB	14:AQ:98:LYS:NZ	2.20	0.55
46:BA:1343:A:H2	46:BA:1364:A:N6	2.05	0.55
46:BA:1519:U:C5	54:BN:177:ARG:HG3	2.42	0.55
46:BA:545:A:H3'	46:BA:546:A:H5'	1.87	0.55
49:BE:96:ARG:HB3	49:BE:96:ARG:HH11	1.71	0.55
53:BK:67:PRO:HD2	53:BK:85:PRO:HA	1.88	0.55
65:BY:144:VAL:HG11	65:BY:153:ILE:HD12	1.89	0.55
4:AE:173:VAL:O	4:AE:177:GLU:HG2	2.07	0.55
5:AF:57:ARG:HH21	16:AU:3:ASN:HD22	1.55	0.55
37:B1:130:ARG:NH1	37:B1:134:LEU:HD11	2.22	0.55
46:BA:1141:U:H2'	46:BA:1142:U:H6	1.72	0.55
46:BA:1397:G:O2'	46:BA:1400:C:OP2	2.24	0.55
46:BA:228:A:H4'	46:BA:229:G:H5'	1.89	0.55
46:BA:29:A:H2'	46:BA:30:U:O4'	2.07	0.55
63:BW:81:SER:HA	63:BW:168:VAL:HG11	1.89	0.55
8:AJ:132:VAL:HG21	11:AN:112:ARG:CZ	2.37	0.54
38:B2:101:HIS:HB2	65:BY:194:LEU:HD11	1.89	0.54
46:BA:277:A:H5'	46:BA:277:A:C8	2.42	0.54
59:BS:89:HIS:CD2	59:BS:119:THR:HG21	2.42	0.54
63:BW:113:GLN:O	63:BW:116:LYS:HB3	2.07	0.54
38:B2:123:ARG:HH12	64:BX:30:ARG:HB3	1.71	0.54
1:AA:647:A:H3'	1:AA:648:A:C5'	2.36	0.54
4:AE:369:HIS:HA	4:AE:387:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AI:161:LEU:HD11	7:AI:210:LEU:HD21	1.88	0.54
1:AA:717:G:OP1	7:AI:393:THR:OG1	2.26	0.54
12:AO:69:PRO:HD2	12:AO:72:MET:SD	2.47	0.54
46:BA:338:G:N3	46:BA:1065:G:O2'	2.39	0.54
46:BA:786:A:C2	58:BR:17:ARG:NH1	2.76	0.54
49:BE:239:ARG:HB3	49:BE:240:PRO:HD2	1.88	0.54
56:BP:105:ILE:HG23	56:BP:112:PRO:HD3	1.90	0.54
56:BP:138:VAL:H	56:BP:157:GLN:HE21	1.55	0.54
56:BP:26:ASN:OD1	56:BP:26:ASN:N	2.39	0.54
46:BA:895:A:H2'	46:BA:896:C:H6	1.71	0.54
48:BD:247:ARG:HH12	48:BD:251:VAL:HG11	1.72	0.54
46:BA:479:G:O2'	61:BU:98:ASN:OD1	2.23	0.54
8:AJ:73:TYR:CE2	8:AJ:150:GLY:HA2	2.43	0.54
12:AO:144:MET:HE3	12:AO:153:HIS:HB2	1.89	0.54
17:AY:68:Y5P:H4A	17:AY:69:Y5P:H4	1.88	0.54
46:BA:122:G:H5'	46:BA:123:U:OP2	2.06	0.54
53:BK:95:ALA:HB1	53:BK:110:GLY:HA3	1.90	0.54
54:BN:80:HIS:HD2	54:BN:82:GLY:H	1.53	0.54
54:BN:91:THR:HB	54:BN:94:GLN:HG3	1.90	0.54
2:AB:223:ASP:OD1	2:AB:224:THR:N	2.37	0.54
4:AE:353:LEU:O	4:AE:356:GLN:HB2	2.07	0.54
10:AL:136:GLN:H	10:AL:136:GLN:CD	2.11	0.54
46:BA:130:A:O2'	46:BA:131:G:H5''	2.08	0.54
46:BA:241:G:H2'	46:BA:350:A:H61	1.72	0.54
46:BA:403:C:C2'	46:BA:404:C:H5'	2.38	0.54
46:BA:432:G:H22	46:BA:457:A:H2	1.55	0.54
46:BA:981:U:H5'	46:BA:982:A:OP2	2.07	0.54
1:AA:482:U:H2'	1:AA:483:U:O4'	2.07	0.54
1:AA:635:C:H5'	2:AB:176:THR:HG21	1.88	0.54
9:AK:67:PRO:HG2	9:AK:82:PHE:CD2	2.42	0.54
46:BA:1519:U:H3'	46:BA:1520:A:C5'	2.37	0.54
46:BA:498:C:N4	46:BA:544:C:OP2	2.39	0.54
56:BP:77:ARG:NH1	56:BP:77:ARG:HB3	2.22	0.54
61:BU:65:ARG:NH1	61:BU:99:ARG:NH1	2.51	0.54
56:BP:47:ARG:HH11	62:BV:183:ASN:HB2	1.73	0.54
12:AO:150:ASP:OD2	12:AO:153:HIS:HD2	1.91	0.54
13:AP:42:PRO:HG2	13:AP:45:GLY:HA3	1.90	0.54
15:AR:67:ILE:HD12	15:AR:136:VAL:HG13	1.90	0.54
41:B5:144:GLN:HE22	41:B5:175:ILE:HA	1.72	0.54
46:BA:374:U:H2'	46:BA:374:U:O2	2.07	0.54
46:BA:403:C:H2'	46:BA:404:C:H5'	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:60:U:C5	46:BA:61:U:H1'	2.43	0.54
52:BJ:168:LEU:HD13	52:BJ:176:LEU:HB2	1.88	0.54
6:AG:199:VAL:HG11	6:AG:204:LYS:HD3	1.90	0.54
16:AU:51:ARG:HG3	16:AU:54:ARG:HH12	1.73	0.54
17:AY:34:P5P:O5'	17:AY:34:P5P:H8	2.08	0.54
46:BA:615:A:H2'	46:BA:615:A:OP1	2.07	0.54
46:BA:661:C:C2	46:BA:778:G:N2	2.75	0.54
46:BA:790:G:H2'	46:BA:791:A:H8	1.72	0.54
57:BQ:117:ASN:HB3	57:BQ:166:ARG:HG3	1.90	0.54
60:BT:121:THR:HB	60:BT:131:SER:HB3	1.89	0.54
1:AA:3:A:H3'	4:AE:335:LYS:HE3	1.90	0.54
6:AG:44:PRO:HD3	6:AG:75:LYS:HB2	1.89	0.54
46:BA:99:C:H5	54:BN:75:LYS:HZ1	107.79	0.54
50:BF:127:PRO:HD3	50:BF:139:GLY:O	2.08	0.54
50:BF:99:VAL:HG22	50:BF:165:LEU:HD23	1.89	0.54
56:BP:177:ALA:HA	56:BP:222:TYR:CD1	2.42	0.54
2:AB:57:LEU:HB2	2:AB:270:TYR:CE2	2.40	0.54
7:AI:300:ASP:HB2	7:AI:303:LEU:HG	1.90	0.54
11:AN:91:CYS:SG	11:AN:94:THR:HG22	2.48	0.54
36:B0:76:HIS:HB2	36:B0:130:PHE:CE1	2.43	0.54
44:B8:124:ARG:NH2	46:BA:1202:A:OP1	2.41	0.54
46:BA:1053:A:OP2	50:BF:134:GLY:HA2	2.08	0.54
46:BA:899:C:H3'	46:BA:923:G:C8	2.43	0.54
60:BT:268:ASP:HB3	60:BT:271:ARG:HB2	1.89	0.54
56:BP:30:ASN:HD21	60:BT:86:ARG:HH12	111.61	0.54
1:AA:177:U:H2'	1:AA:178:G:H8	1.73	0.53
39:B3:148:ARG:HH21	39:B3:151:LEU:HD22	1.73	0.53
46:BA:721:A:H3'	46:BA:722:A:H5''	1.90	0.53
47:BB:11:Y5P:H4A	47:BB:12:Y5P:H4	1.88	0.53
49:BE:197:HIS:NE2	49:BE:318:THR:HG22	2.23	0.53
50:BF:49:ARG:NH1	50:BF:81:GLU:O	2.41	0.53
59:BS:149:THR:HG21	59:BS:151:TRP:CZ2	2.42	0.53
4:AE:124:LYS:HG3	4:AE:183:ARG:HH22	1.73	0.53
1:AA:577:C:O3'	8:AJ:128:LYS:HD2	2.08	0.53
10:AL:61:VAL:HG23	10:AL:84:ARG:HB2	1.90	0.53
13:AP:36:ALA:HB2	13:AP:51:LEU:HD11	1.90	0.53
46:BA:747:C:O2	64:BX:54:ARG:NH1	2.41	0.53
1:AA:180:U:H2'	1:AA:181:A:C8	2.43	0.53
4:AE:140:LEU:HD21	4:AE:160:ARG:HE	1.72	0.53
44:B8:113:ARG:HB3	56:BP:80:LYS:HA	1.91	0.53
46:BA:1017:C:H2'	46:BA:1018:C:H6	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:1230:G:H8	46:BA:1230:G:H5''	1.73	0.53
49:BE:317:PRO:HG2	49:BE:320:PHE:HE2	1.73	0.53
49:BE:49:TRP:CD1	49:BE:155:PHE:HB3	2.43	0.53
61:BU:52:LYS:HG2	61:BU:55:ARG:HH21	1.73	0.53
46:BA:2:C:OP1	63:BW:48:LYS:N	2.39	0.53
1:AA:714:U:H2'	1:AA:715:G:H8	1.74	0.53
3:AC:163:VAL:HG21	3:AC:167:ILE:HD12	1.89	0.53
17:AV:41:Y5P:H4A	17:AV:42:Y5P:C5	2.38	0.53
46:BA:195:U:O2'	46:BA:1012:A:OP1	2.25	0.53
46:BA:1139:A:H2'	46:BA:1140:U:C6	2.43	0.53
1:AA:578:G:H3'	1:AA:579:A:H5''	1.91	0.53
1:AA:279:U:O2'	10:AL:54:GLY:O	2.26	0.53
17:AV:28:Y5P:N3	17:AV:29:Y5P:C5	2.71	0.53
17:AV:36:P5P:C6	17:AV:37:Y5P:H4	2.38	0.53
44:B8:113:ARG:HH11	56:BP:76:LEU:HA	1.72	0.53
48:BD:111:ARG:HH11	48:BD:111:ARG:HG3	1.73	0.53
56:BP:88:SER:O	56:BP:134:ARG:HG3	2.09	0.53
62:BV:88:ASN:HD21	62:BV:208:LEU:H	1.56	0.53
1:AA:103:G:P	14:AQ:78:LYS:NZ	2.81	0.53
37:B1:163:ARG:HD3	37:B1:205:GLY:H	1.73	0.53
46:BA:415:U:H2'	46:BA:416:G:C8	2.43	0.53
46:BA:677:U:H2'	46:BA:678:C:C6	2.44	0.53
50:BF:283:LEU:HB2	56:BP:125:ARG:NH1	2.22	0.53
37:B1:58:GLN:HG3	56:BP:89:PHE:CE1	2.44	0.53
1:AA:38:U:H4'	3:AC:150:PRO:HB2	108.39	0.53
5:AF:3:ARG:HH11	5:AF:4:TYR:HE1	1.55	0.53
17:AY:55:Y5P:C6	17:AY:58:Y5P:C5	2.85	0.53
46:BA:160:A:OP2	46:BA:160:A:H3'	2.09	0.53
46:BA:366:A:C2	46:BA:432:G:C4	2.97	0.53
49:BE:316:PHE:CG	49:BE:316:PHE:O	2.62	0.53
54:BN:26:GLN:NE2	54:BN:147:GLN:OE1	2.42	0.53
58:BR:153:LEU:O	58:BR:157:GLN:HG2	2.09	0.53
60:BT:112:TYR:CE2	60:BT:215:VAL:HG11	2.44	0.53
1:AA:295:A:H1'	1:AA:487:C:H1'	1.90	0.53
1:AA:640:A:OP1	4:AE:242:ARG:NH1	2.42	0.53
46:BA:1189:A:H2'	46:BA:1190:U:H6	1.73	0.53
46:BA:175:U:H2'	46:BA:176:U:C6	2.44	0.53
46:BA:801:A:O2'	46:BA:807:G:N7	2.33	0.53
49:BE:67:ASP:HA	49:BE:70:LYS:HE3	1.91	0.53
52:BJ:36:HIS:O	52:BJ:37:ARG:HB3	2.09	0.53
1:AA:647:A:H1'	2:AB:148:ARG:CZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AE:149:MET:HG2	4:AE:154:VAL:H	1.74	0.53
6:AG:220:ILE:HG23	6:AG:223:LYS:HD3	1.90	0.53
1:AA:344:G:H1	9:AK:121:ASN:CB	2.21	0.53
10:AL:69:LYS:HZ2	10:AL:77:ASN:HB3	1.74	0.53
37:B1:42:HIS:O	51:BI:55:ILE:HA	2.09	0.53
38:B2:166:ARG:NH2	38:B2:183:PHE:O	2.42	0.53
39:B3:142:ASN:ND2	39:B3:142:ASN:H	2.07	0.53
46:BA:1334:A:H2'	46:BA:1335:G:H8	1.74	0.53
46:BA:96:U:H1'	46:BA:97:A:H5''	1.91	0.53
50:BF:195:LEU:HD22	50:BF:196:PRO:HD2	1.90	0.53
62:BV:139:LEU:HD12	62:BV:140:VAL:H	1.74	0.53
1:AA:225:A:N6	1:AA:273:A:O5'	2.38	0.53
1:AA:529:G:H2'	1:AA:531:U:H5	1.73	0.53
46:BA:390:A:O2'	46:BA:391:U:O4'	2.27	0.53
46:BA:806:G:H2'	46:BA:807:G:H5''	1.91	0.53
48:BD:198:GLU:OE2	48:BD:203:ARG:N	2.42	0.53
50:BF:120:VAL:HG11	50:BF:142:ARG:HD2	1.91	0.53
52:BJ:37:ARG:O	52:BJ:37:ARG:HG3	2.09	0.53
56:BP:11:ARG:CG	56:BP:11:ARG:HH11	2.15	0.53
56:BP:88:SER:OG	56:BP:134:ARG:NH2	2.41	0.53
61:BU:33:GLY:O	61:BU:36:ASN:ND2	2.42	0.53
46:BA:175:U:H2'	46:BA:176:U:H6	1.74	0.52
50:BF:174:LEU:HD23	50:BF:253:MET:HE1	1.90	0.52
56:BP:191:VAL:HB	56:BP:192:PRO:HD3	1.89	0.52
11:AN:103:ARG:HB3	11:AN:104:TRP:CE3	2.44	0.52
38:B2:89:CYS:O	38:B2:93:ARG:HG2	2.09	0.52
44:B8:113:ARG:NH1	56:BP:76:LEU:HD23	2.23	0.52
49:BE:199:ARG:HG3	49:BE:199:ARG:HH11	1.73	0.52
64:BX:28:LEU:HD11	64:BX:40:VAL:CG1	2.40	0.52
65:BY:49:ILE:HD11	65:BY:117:HIS:CE1	2.44	0.52
8:AJ:85:LYS:HG3	8:AJ:139:LEU:HD13	1.90	0.52
17:AV:54:Y5P:H4A	17:AV:55:Y5P:C4	2.37	0.52
54:BN:135:GLU:HA	54:BN:138:LEU:HB2	1.92	0.52
56:BP:153:ASN:HB2	56:BP:256:LEU:HD23	1.90	0.52
7:AI:266:UNK:HG2	7:AI:268:MET:HB3	1.90	0.52
7:AI:357:VAL:HG22	7:AI:361:GLU:OE1	2.09	0.52
11:AN:81:ASP:OD1	11:AN:81:ASP:N	2.42	0.52
46:BA:119:A:H5'	46:BA:120:C:OP2	2.09	0.52
49:BE:195:ALA:H	49:BE:281:ASN:HD22	1.57	0.52
46:BA:1129:U:O2'	51:BI:87:LYS:NZ	2.42	0.52
56:BP:28:LYS:HZ1	56:BP:31:PRO:HD3	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:BW:53:ASN:ND2	63:BW:72:TYR:O	2.41	0.52
3:AC:72:HIS:HB3	3:AC:112:ARG:HH11	1.73	0.52
3:AC:72:HIS:HB3	3:AC:112:ARG:NH1	2.24	0.52
4:AE:380:LEU:HD12	4:AE:381:PRO:HD2	1.91	0.52
8:AJ:119:THR:OG1	8:AJ:133:GLN:NE2	2.42	0.52
14:AQ:63:ILE:HB	14:AQ:86:PHE:HB2	1.90	0.52
17:AV:11:Y5P:H6	17:AV:11:Y5P:O5'	2.10	0.52
36:B0:51:PHE:HE2	36:B0:71:ARG:NH1	2.06	0.52
46:BA:528:A:H5'	46:BA:529:G:OP1	2.10	0.52
56:BP:248:THR:HA	56:BP:253:PHE:CD1	2.45	0.52
57:BQ:55:ARG:HA	57:BQ:99:TRP:CD1	2.44	0.52
4:AE:206:PRO:HG2	4:AE:215:TYR:HD2	1.73	0.52
46:BA:718:C:OP2	48:BD:149:LYS:NZ	2.30	0.52
47:BB:43:Y5P:H2'	47:BB:44:Y5P:HA1	1.92	0.52
52:BJ:143:LEU:HD23	52:BJ:146:LEU:HD12	1.92	0.52
55:BO:125:SER:OG	55:BO:128:ARG:NH2	2.30	0.52
56:BP:285:PRO:HB3	56:BP:290:LEU:HD23	1.92	0.52
58:BR:139:ARG:HG3	58:BR:139:ARG:NH1	2.24	0.52
60:BT:60:UNK:CG	60:BT:60:UNK:O	2.57	0.52
4:AE:408:TRP:NE1	4:AE:412:LYS:HE2	2.25	0.52
17:AY:50:Y5P:H4A	17:AY:51:Y5P:H4	1.91	0.52
17:AY:74:Y5P:H4	46:BA:1376:U:C2	2.44	0.52
46:BA:1379:A:H2'	46:BA:1380:C:O4'	2.09	0.52
46:BA:310:A:H5'	48:BD:262:GLY:HA2	1.92	0.52
49:BE:128:HIS:CD2	49:BE:173:LYS:HZ1	2.28	0.52
58:BR:46:TRP:HD1	58:BR:122:ALA:HB2	1.74	0.52
65:BY:81:ARG:HG2	65:BY:81:ARG:HH11	1.74	0.52
46:BA:931:A:H1'	46:BA:1426:U:O2'	2.10	0.52
48:BD:136:ARG:HG2	48:BD:136:ARG:NH1	2.17	0.52
54:BN:25:MET:O	54:BN:149:ARG:NH1	2.43	0.52
61:BU:98:ASN:H	62:BV:109:GLN:NE2	2.07	0.52
4:AE:289:THR:HG23	4:AE:331:ASP:O	2.09	0.52
1:AA:317:A:O2'	15:AR:103:LYS:N	2.43	0.52
17:AY:55:Y5P:H5	17:AY:58:Y5P:H5	1.90	0.52
55:BO:69:VAL:HG23	55:BO:89:HIS:ND1	2.24	0.52
62:BV:129:GLY:H	62:BV:164:VAL:HG13	1.73	0.52
63:BW:132:VAL:HG12	63:BW:133:GLU:O	2.10	0.52
38:B2:111:ARG:HG2	64:BX:25:PHE:CD1	2.45	0.52
64:BX:56:TYR:O	64:BX:60:ILE:HG12	2.10	0.52
65:BY:98:VAL:HG21	65:BY:109:ILE:HD12	1.92	0.52
1:AA:649:U:H3'	1:AA:650:A:H5''	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:62:ILE:HA	3:AC:66:LYS:HB3	1.92	0.52
7:AI:150:LEU:O	7:AI:153:THR:OG1	2.17	0.52
17:AY:3:Y5P:O5'	17:AY:3:Y5P:H6	2.10	0.52
46:BA:110:A:C4	46:BA:111:G:C8	2.97	0.52
46:BA:1240:U:O2'	46:BA:1241:U:OP2	2.28	0.52
46:BA:467:A:H5''	46:BA:468:C:H5	1.74	0.52
46:BA:486:U:H3'	46:BA:487:C:O4'	2.09	0.52
46:BA:654:C:H1'	46:BA:655:U:C2	2.45	0.52
48:BD:159:LYS:O	48:BD:162:ASP:HB2	2.10	0.52
61:BU:54:THR:HG21	62:BV:176:MET:N	2.11	0.52
63:BW:69:ALA:HB3	63:BW:178:GLU:HB3	1.92	0.52
1:AA:29:A:H2'	1:AA:30:A:C8	2.45	0.51
1:AA:954:U:H4'	1:AA:955:G:H5'	1.91	0.51
8:AJ:118:PHE:CD2	11:AN:101:LYS:NZ	2.79	0.51
46:BA:1210:U:H5'	46:BA:1211:A:OP2	2.09	0.51
51:BI:59:TRP:NE1	51:BI:81:LYS:HB3	2.23	0.51
54:BN:17:VAL:HG13	54:BN:142:VAL:HG21	1.92	0.51
50:BF:97:HIS:HB2	56:BP:27:LEU:HD22	1.92	0.51
60:BT:75:PHE:CD2	60:BT:110:GLU:HG3	2.44	0.51
1:AA:828:U:H2'	1:AA:829:G:C8	2.46	0.51
1:AA:828:U:H2'	1:AA:829:G:H8	1.75	0.51
1:AA:732:U:OP1	7:AI:306:PRO:HG2	2.10	0.51
13:AP:107:ALA:O	13:AP:111:ARG:HG3	2.08	0.51
36:B0:61:VAL:HG21	36:B0:97:VAL:HG23	1.91	0.51
63:BW:142:GLU:O	63:BW:174:VAL:HA	2.11	0.51
1:AA:589:C:H2'	1:AA:590:C:C6	2.45	0.51
1:AA:856:U:H2'	1:AA:857:C:C6	2.45	0.51
46:BA:319:U:O3'	48:BD:90:GLN:NE2	2.43	0.51
48:BD:170:ILE:HA	48:BD:187:ALA:HB2	1.93	0.51
51:BI:122:ARG:O	51:BI:126:GLN:NE2	2.42	0.51
55:BO:128:ARG:HA	55:BO:138:LEU:HD21	1.91	0.51
55:BO:74:LEU:HD12	55:BO:82:LYS:O	2.10	0.51
7:AI:85:LYS:HE2	7:AI:99:PHE:HB3	1.92	0.51
41:B5:156:THR:HG22	41:B5:173:ARG:HB3	1.93	0.51
43:B7:85:ARG:HH12	43:B7:90:ARG:HD2	1.76	0.51
46:BA:450:U:O2'	46:BA:1171:A:N3	2.36	0.51
55:BO:110:ASP:N	55:BO:110:ASP:OD1	2.36	0.51
63:BW:150:TYR:CE2	63:BW:168:VAL:HG13	2.46	0.51
1:AA:135:U:OP2	14:AQ:27:LYS:NZ	2.40	0.51
2:AB:70:ASP:O	2:AB:73:ASN:N	2.35	0.51
2:AB:71:PHE:CE2	2:AB:262:LYS:HG2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AE:314:LEU:H	4:AE:331:ASP:HA	1.75	0.51
46:BA:1529:C:H3'	46:BA:1530:U:H5''	1.92	0.51
46:BA:160:A:N6	46:BA:1034:A:H62	2.09	0.51
46:BA:198:A:H2'	46:BA:199:A:C8	2.46	0.51
41:B5:94:ARG:NH1	46:BA:642:G:OP2	2.43	0.51
49:BE:97:VAL:O	49:BE:197:HIS:HE1	1.94	0.51
52:BJ:111:LEU:O	52:BJ:115:GLN:HG2	2.10	0.51
56:BP:264:GLN:NE2	56:BP:269:LEU:O	2.23	0.51
61:BU:73:THR:HG23	61:BU:83:TYR:HB2	1.92	0.51
4:AE:225:VAL:HA	4:AE:243:VAL:HG12	1.92	0.51
17:AY:11:Y5P:H2'	17:AY:12:Y5P:H6	1.93	0.51
17:AY:25:Y5P:H2'	17:AY:26:Y5P:H6	1.91	0.51
17:AY:42:Y5P:HB	17:AY:43:Y5P:HB2	1.92	0.51
44:B8:138:ALA:HA	44:B8:141:LYS:HE3	1.93	0.51
46:BA:134:G:C6	65:BY:34:LYS:NZ	2.78	0.51
39:B3:73:LYS:NZ	46:BA:470:U:OP1	2.44	0.51
46:BA:503:U:H4'	46:BA:504:A:H5'	1.92	0.51
46:BA:658:C:H4'	58:BR:81:THR:CG2	2.39	0.51
49:BE:236:THR:O	49:BE:238:ARG:N	2.43	0.51
53:BK:23:ILE:HG12	53:BK:67:PRO:HB3	1.91	0.51
57:BQ:218:ILE:HG23	57:BQ:223:MET:HB2	1.93	0.51
7:AI:223:ILE:O	7:AI:227:GLU:HG2	2.11	0.51
39:B3:72:ILE:HD11	39:B3:118:ARG:HD3	1.93	0.51
44:B8:142:ARG:HH22	46:BA:1190:U:H5''	1.76	0.51
46:BA:219:G:H2'	46:BA:220:A:C8	2.46	0.51
46:BA:55:A:H3'	46:BA:56:A:H4'	1.93	0.51
48:BD:186:GLY:HA3	48:BD:239:GLU:HG3	1.93	0.51
50:BF:69:LEU:O	50:BF:202:TYR:OH	2.27	0.51
63:BW:150:TYR:CD2	63:BW:168:VAL:HA	2.45	0.51
7:AI:316:PHE:CD1	7:AI:370:LEU:HD21	2.46	0.51
12:AO:75:LEU:HD23	12:AO:106:LYS:HB3	1.92	0.51
17:AY:56:Y5P:O2'	17:AY:57:Y5P:O4'	2.29	0.51
45:B9:93:PRO:HB2	46:BA:1348:G:O3'	2.11	0.51
46:BA:624:G:O4'	50:BF:154:GLY:HA2	2.11	0.51
50:BF:49:ARG:HD2	50:BF:80:THR:HG23	1.92	0.51
37:B1:176:LEU:HD22	37:B1:188:TYR:CZ	2.46	0.51
43:B7:74:ARG:NH2	46:BA:32:C:OP2	2.44	0.51
46:BA:252:A:C2	46:BA:256:A:C6	2.99	0.51
54:BN:80:HIS:CD2	54:BN:82:GLY:H	2.29	0.51
57:BQ:232:PRO:O	57:BQ:235:LEU:HG	2.11	0.51
1:AA:586:U:H5''	11:AN:90:ARG:HH21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:611:A:H2'	1:AA:612:U:O4'	2.11	0.51
1:AA:814:A:OP2	7:AI:378:ARG:NH1	2.43	0.51
8:AJ:102:LEU:HB3	8:AJ:104:ILE:HG13	1.93	0.51
9:AK:151:VAL:HG12	9:AK:177:ILE:HA	1.93	0.51
44:B8:140:ARG:HD2	46:BA:1204:U:OP1	2.11	0.51
46:BA:229:G:H2'	46:BA:230:C:C6	2.46	0.51
49:BE:285:VAL:HG12	49:BE:286:ASN:H	1.76	0.51
49:BE:202:GLN:NE2	49:BE:301:ASP:OD1	2.43	0.51
57:BQ:72:ILE:HD11	57:BQ:96:TYR:CZ	2.45	0.51
1:AA:28:U:H2'	1:AA:29:A:C8	2.47	0.50
1:AA:648:A:OP2	2:AB:146:ARG:NH2	2.43	0.50
41:B5:95:ARG:NH1	46:BA:156:A:H5'	2.26	0.50
49:BE:129:VAL:HG23	49:BE:189:PRO:HA	1.92	0.50
62:BV:180:LYS:HD3	62:BV:181:ARG:HH12	1.76	0.50
6:AG:195:LYS:CB	6:AG:204:LYS:HZ2	2.23	0.50
7:AI:249:ILE:HG13	7:AI:249:ILE:O	2.11	0.50
36:B0:102:GLU:HB2	36:B0:130:PHE:CE2	2.47	0.50
46:BA:163:A:OP1	61:BU:52:LYS:NZ	2.43	0.50
49:BE:206:VAL:HG11	49:BE:289:VAL:HG13	1.92	0.50
50:BF:276:HIS:HA	50:BF:279:ARG:HG2	1.92	0.50
53:BK:140:VAL:O	53:BK:144:ILE:HG12	2.12	0.50
56:BP:233:ARG:HH21	56:BP:247:ILE:HG12	1.76	0.50
13:AP:117:GLU:HA	13:AP:120:LEU:HB2	1.93	0.50
17:AY:70:Y5P:C4	17:AY:71:Y5P:H4	2.29	0.50
46:BA:1011:A:H2'	46:BA:1012:A:O4'	2.11	0.50
46:BA:1351:C:OP2	46:BA:1356:G:N2	2.44	0.50
41:B5:91:ARG:NH2	46:BA:153:A:OP2	2.44	0.50
46:BA:350:A:H3'	46:BA:352:C:N4	2.26	0.50
46:BA:353:U:H2'	46:BA:354:G:H8	1.74	0.50
46:BA:562:A:N3	46:BA:1337:A:O2'	2.36	0.50
49:BE:164:PHE:HD1	49:BE:165:TYR:CD1	2.30	0.50
56:BP:248:THR:HA	56:BP:253:PHE:CE1	2.47	0.50
62:BV:168:THR:HG23	62:BV:194:GLN:HB2	1.93	0.50
7:AI:197:GLY:O	7:AI:249:ILE:HG12	2.11	0.50
7:AI:94:GLU:HB2	7:AI:99:PHE:HE2	1.76	0.50
17:AV:42:Y5P:H4A	17:AV:43:Y5P:C4	2.37	0.50
37:B1:115:TYR:HD1	37:B1:122:ARG:HG2	1.76	0.50
46:BA:1018:C:H2'	46:BA:1019:C:C6	2.46	0.50
46:BA:1141:U:H2'	46:BA:1142:U:C6	2.45	0.50
46:BA:1403:A:H2'	46:BA:1404:G:O4'	2.11	0.50
45:B9:85:TRP:HZ2	46:BA:492:U:HO2'	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:BB:36:P5P:H2'	47:BB:37:P5P:O4'	2.10	0.50
48:BD:111:ARG:NE	48:BD:152:ILE:HD12	2.26	0.50
53:BK:97:ILE:HD11	53:BK:153:ILE:HD11	1.93	0.50
56:BP:141:VAL:HG12	56:BP:142:GLU:H	1.77	0.50
1:AA:671:U:H2'	1:AA:672:A:C8	2.46	0.50
2:AB:58:ARG:O	2:AB:61:ILE:HG22	2.10	0.50
5:AF:22:LEU:HD22	5:AF:39:LEU:HD11	1.93	0.50
39:B3:79:PRO:HD2	39:B3:82:GLU:HG3	1.93	0.50
46:BA:41:A:H2'	46:BA:42:C:H4'	1.94	0.50
46:BA:602:A:H2'	46:BA:603:C:O4'	2.12	0.50
49:BE:212:GLY:O	58:BR:11:HIS:HE1	1.95	0.50
64:BX:66:ALA:HB2	64:BX:100:ALA:HA	1.93	0.50
2:AB:161:CYS:SG	2:AB:253:GLN:HA	2.51	0.50
17:AV:37:Y5P:C5	17:AV:38:Y5P:C5	2.89	0.50
37:B1:79:LEU:HD21	37:B1:157:PHE:HD1	1.77	0.50
41:B5:165:PRO:HB3	41:B5:174:ILE:HD11	1.93	0.50
46:BA:1078:A:H61	46:BA:1134:U:H3	1.58	0.50
46:BA:858:G:O5'	48:BD:136:ARG:NH2	2.44	0.50
56:BP:178:PHE:HB2	56:BP:214:TYR:CZ	2.46	0.50
1:AA:124:A:H5'	1:AA:125:U:OP1	2.11	0.50
3:AC:124:LEU:HD11	3:AC:160:SER:HA	1.94	0.50
46:BA:1417:C:H2'	46:BA:1418:A:O4'	2.12	0.50
46:BA:785:U:H2'	46:BA:786:A:O4'	2.12	0.50
49:BE:221:ARG:NH1	49:BE:259:GLY:HA3	2.27	0.50
49:BE:90:TRP:CH2	49:BE:92:PRO:HA	2.47	0.50
50:BF:61:PRO:HA	50:BF:84:PRO:HD3	1.93	0.50
55:BO:51:TYR:CE2	55:BO:78:ARG:HA	2.47	0.50
57:BQ:81:GLU:O	57:BQ:123:ARG:NH2	2.44	0.50
3:AC:93:ARG:HH11	3:AC:108:LEU:HB3	1.77	0.50
3:AC:73:THR:HG23	8:AJ:169:ALA:HB2	1.94	0.50
4:AE:370:VAL:HG22	4:AE:385:ALA:HB3	1.93	0.50
11:AN:60:ASN:HD22	11:AN:63:LEU:HG	1.76	0.50
17:AY:6:Y5P:O5'	17:AY:6:Y5P:H6	2.12	0.50
41:B5:125:TYR:O	41:B5:128:GLU:HB2	2.12	0.50
46:BA:1209:A:P	59:BS:176:ARG:HH22	2.34	0.50
46:BA:1343:A:H2	46:BA:1364:A:H61	1.59	0.50
46:BA:434:C:H1'	46:BA:467:A:C8	2.46	0.50
48:BD:69:ARG:CB	48:BD:69:ARG:HH11	2.24	0.50
51:BI:130:VAL:HB	51:BI:136:ASN:ND2	2.26	0.50
59:BS:89:HIS:CG	59:BS:119:THR:HG21	2.46	0.50
64:BX:71:ARG:HG2	64:BX:71:ARG:NH1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:BY:122:LEU:HD23	65:BY:133:VAL:HG21	1.94	0.50
1:AA:939:A:H2'	1:AA:940:C:H6	1.77	0.50
7:AI:260:UNK:CG	7:AI:355:SER:HB3	2.39	0.50
9:AK:113:SER:O	9:AK:117:GLU:HB2	2.11	0.50
10:AL:81:CYS:HB2	10:AL:95:ILE:HD11	1.94	0.50
12:AO:196:TYR:HB3	12:AO:198:ARG:HD2	1.93	0.50
14:AQ:35:LEU:HB2	14:AQ:42:TYR:CZ	2.47	0.50
15:AR:114:ARG:O	15:AR:118:LEU:HG	2.11	0.50
15:AR:65:LYS:HB3	15:AR:69:CYS:HB2	1.94	0.50
41:B5:127:TYR:OH	58:BR:43:GLU:OE1	2.29	0.50
46:BA:257:C:H2'	46:BA:258:C:O4'	2.11	0.50
46:BA:732:A:OP2	48:BD:105:ARG:NH2	2.45	0.50
48:BD:128:ILE:HD11	48:BD:144:ALA:HB3	1.93	0.50
48:BD:69:ARG:HB2	48:BD:69:ARG:NH1	2.25	0.50
1:AA:368:A:P	9:AK:186:ASN:HD22	2.35	0.49
1:AA:836:G:H2'	1:AA:837:C:C6	2.47	0.49
3:AC:75:ASN:HD21	11:AN:104:TRP:HE1	1.60	0.49
17:AY:2:Y5P:H4A	17:AY:3:Y5P:H4	1.93	0.49
37:B1:41:VAL:HG11	37:B1:83:GLU:HB3	1.93	0.49
46:BA:1194:G:H8	46:BA:1194:G:O5'	1.95	0.49
46:BA:1024:A:C6	46:BA:1319:C:H1'	2.47	0.49
46:BA:134:G:H1	65:BY:34:LYS:HZ3	1.59	0.49
46:BA:1395:G:H2'	46:BA:1396:U:O4'	2.12	0.49
46:BA:1483:A:H2'	46:BA:1484:A:C8	2.47	0.49
46:BA:878:C:O2'	46:BA:920:A:N3	2.39	0.49
46:BA:983:C:H2'	46:BA:984:U:C6	2.47	0.49
46:BA:859:U:H2'	48:BD:209:ARG:HD2	1.95	0.49
50:BF:175:LYS:NZ	50:BF:277:ASN:OD1	2.44	0.49
46:BA:437:A:O3'	57:BQ:231:SER:HB2	2.12	0.49
59:BS:90:ILE:O	59:BS:107:THR:OG1	2.30	0.49
61:BU:65:ARG:NH1	61:BU:99:ARG:HH11	2.10	0.49
46:BA:687:A:N1	63:BW:155:ARG:HG3	2.27	0.49
1:AA:194:U:H2'	1:AA:195:G:H8	1.75	0.49
17:AV:27:Y5P:H4A	17:AV:28:Y5P:H4	1.94	0.49
42:B6:41:LEU:HB3	42:B6:58:GLU:HB2	1.94	0.49
47:BB:13:Y5P:H4	47:BB:24:P5P:N1	2.26	0.49
52:BJ:128:ASN:ND2	52:BJ:147:PHE:O	2.43	0.49
54:BN:81:THR:OG1	54:BN:86:GLY:O	2.29	0.49
54:BN:94:GLN:O	54:BN:97:GLN:HB3	2.11	0.49
56:BP:260:LYS:HG3	56:BP:267:PHE:CE1	2.47	0.49
59:BS:149:THR:HG21	59:BS:151:TRP:CH2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:BY:199:MET:HG3	65:BY:204:ILE:HB	1.93	0.49
1:AA:551:G:H21	1:AA:778:G:H4'	1.77	0.49
1:AA:924:U:H4'	1:AA:945:A:H2	1.76	0.49
1:AA:675:A:OP1	3:AC:41:ARG:NH1	2.46	0.49
3:AC:42:VAL:HG13	3:AC:49:LYS:NZ	2.27	0.49
3:AC:84:GLU:HB2	3:AC:85:ARG:NH1	2.28	0.49
1:AA:102:G:O3'	14:AQ:78:LYS:NZ	2.45	0.49
17:AV:27:Y5P:H2'	17:AV:28:Y5P:C6	2.43	0.49
42:B6:34:ARG:NE	46:BA:1183:A:OP2	2.45	0.49
46:BA:1007:A:H2'	46:BA:1008:A:C8	2.47	0.49
46:BA:446:A:O2'	46:BA:1277:G:O2'	2.25	0.49
52:BJ:93:ASN:ND2	52:BJ:155:VAL:HG22	2.28	0.49
61:BU:24:VAL:HG12	61:BU:25:LEU:HD23	1.94	0.49
64:BX:15:PRO:HG3	65:BY:208:ARG:O	2.11	0.49
65:BY:92:ASN:O	65:BY:112:GLU:HA	2.13	0.49
1:AA:211:A:H2'	1:AA:212:A:O4'	2.12	0.49
1:AA:217:U:H2'	1:AA:218:A:C8	2.48	0.49
1:AA:320:A:H61	1:AA:390:A:H1'	1.76	0.49
1:AA:629:C:H2'	1:AA:630:A:C8	2.48	0.49
1:AA:807:G:O6	1:AA:809:G:N2	2.46	0.49
4:AE:160:ARG:HD2	4:AE:165:GLN:NE2	2.26	0.49
6:AG:57:GLU:HB2	6:AG:60:GLU:HB2	1.93	0.49
7:AI:94:GLU:HB2	7:AI:99:PHE:CE2	2.48	0.49
14:AQ:29:ARG:NH1	14:AQ:46:ARG:NH1	2.60	0.49
17:AV:35:P5P:O5'	17:AV:35:P5P:H8	2.13	0.49
17:AV:63:Y5P:H2'	17:AV:64:Y5P:H6	1.94	0.49
39:B3:71:ARG:HH12	39:B3:94:ALA:N	2.11	0.49
46:BA:786:A:C4	58:BR:17:ARG:HD2	2.47	0.49
47:BB:25:P5P:C6	47:BB:26:Y5P:H4	2.43	0.49
50:BF:97:HIS:CE1	56:BP:29:PRO:HD3	2.48	0.49
1:AA:397:U:H2'	1:AA:398:G:O4'	2.13	0.49
1:AA:821:A:H5'	1:AA:822:A:OP1	2.12	0.49
1:AA:904:A:H2'	1:AA:905:U:C6	2.47	0.49
7:AI:263:UNK:CG	7:AI:265:UNK:HG3	2.42	0.49
37:B1:168:ARG:HH21	37:B1:175:GLN:HG3	1.78	0.49
37:B1:93:ASN:O	37:B1:94:ASN:HB2	2.13	0.49
46:BA:275:G:C5	48:BD:260:LYS:HB2	2.47	0.49
60:BT:62:UNK:O	60:BT:62:UNK:HG2	2.12	0.49
1:AA:519:A:C2	1:AA:520:G:H1'	2.47	0.49
4:AE:282:ILE:HG23	4:AE:353:LEU:HB3	1.93	0.49
8:AJ:117:ARG:HG2	8:AJ:135:GLU:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:688:U:H1'	46:BA:1003:G:H21	1.78	0.49
46:BA:1197:A:H2'	46:BA:1198:A:O4'	2.12	0.49
46:BA:356:U:H6	46:BA:356:U:H5''	1.76	0.49
52:BJ:89:VAL:HG22	52:BJ:124:LYS:HZ2	1.76	0.49
60:BT:59:UNK:CG	60:BT:59:UNK:O	2.60	0.49
1:AA:124:A:H4'	1:AA:125:U:O5'	2.12	0.49
1:AA:719:U:H2'	1:AA:720:A:O4'	2.12	0.49
1:AA:750:G:H2'	1:AA:751:A:H5''	1.94	0.49
1:AA:846:C:H2'	1:AA:847:C:O4'	2.13	0.49
4:AE:309:PRO:HB3	4:AE:374:ARG:HH12	1.78	0.49
9:AK:64:ILE:HG22	9:AK:66:PRO:HD2	1.94	0.49
16:AU:48:PRO:O	16:AU:52:ARG:HD3	2.12	0.49
17:AV:28:Y5P:C2	17:AV:29:Y5P:C5	2.90	0.49
41:B5:92:CYS:HG	46:BA:156:A:HO2'	1.60	0.49
46:BA:1556:U:C2	49:BE:292:HIS:CD2	3.01	0.49
46:BA:462:A:H5''	46:BA:463:U:H5'	1.94	0.49
46:BA:560:A:N3	46:BA:560:A:H3'	2.28	0.49
47:BB:44:Y5P:H2'	47:BB:45:P5P:H8	1.95	0.49
48:BD:193:LEU:O	48:BD:246:GLY:N	2.45	0.49
49:BE:111:THR:HG22	49:BE:115:GLN:O	2.11	0.49
1:AA:138:U:H5''	1:AA:139:A:N7	2.27	0.49
1:AA:928:A:H5'	1:AA:930:G:N7	2.28	0.49
2:AB:66:LEU:HD23	2:AB:133:HIS:CE1	2.48	0.49
6:AG:140:ASN:HB3	6:AG:143:THR:HG22	1.95	0.49
17:AY:55:Y5P:H6	17:AY:58:Y5P:C5	2.43	0.49
46:BA:1238:A:O2'	46:BA:1239:U:O4'	2.26	0.49
46:BA:833:A:HO2'	46:BA:1428:G:HO2'	1.58	0.49
47:BB:38:P5P:H2'	47:BB:39:P5P:C8	2.43	0.49
49:BE:139:ASN:ND2	49:BE:141:ARG:HB2	2.28	0.49
52:BJ:101:HIS:CE1	52:BJ:109:LYS:HZ1	2.31	0.49
61:BU:122:ARG:NH1	62:BV:70:LEU:HG	2.28	0.49
1:AA:939:A:H2'	1:AA:940:C:C6	2.48	0.49
1:AA:349:A:OP2	9:AK:121:ASN:ND2	2.45	0.49
17:AY:8:Y5P:N3	17:AY:14:Y5P:H5	2.28	0.49
37:B1:113:GLU:HA	37:B1:123:PHE:O	2.12	0.49
46:BA:1354:C:H2'	46:BA:1355:C:O4'	2.13	0.49
46:BA:1399:U:C4	49:BE:242:ALA:HB2	2.48	0.49
46:BA:506:G:H4'	53:BK:151:LEU:HD13	1.94	0.49
46:BA:63:A:H3'	46:BA:64:C:O2	2.12	0.49
46:BA:974:A:H5''	46:BA:975:G:OP2	2.13	0.49
49:BE:200:PRO:HA	49:BE:273:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:524:A:O2'	53:BK:135:VAL:HG11	2.12	0.49
58:BR:129:ASN:ND2	58:BR:131:LEU:HB2	2.28	0.49
59:BS:102:VAL:HG12	59:BS:103:VAL:HG12	1.94	0.49
60:BT:229:TRP:CH2	60:BT:249:LEU:HD21	2.48	0.49
1:AA:546:U:H2'	1:AA:547:A:C8	2.48	0.49
1:AA:882:A:N3	1:AA:886:A:N6	2.59	0.49
2:AB:166:HIS:ND1	7:AI:153:THR:HA	2.28	0.49
11:AN:103:ARG:HB3	11:AN:104:TRP:CZ3	2.48	0.49
17:AY:76:P5P:N3	46:BA:1404:G:N2	2.58	0.49
37:B1:179:ASP:N	37:B1:179:ASP:OD1	2.44	0.49
46:BA:1161:A:H2'	46:BA:1161:A:N3	2.27	0.49
46:BA:1230:G:C2'	46:BA:1246:C:H41	2.26	0.49
54:BN:159:THR:HG22	54:BN:161:GLU:H	1.76	0.49
57:BQ:106:ARG:CB	57:BQ:106:ARG:HH11	2.26	0.49
49:BE:347:PHE:HD1	60:BT:122:ALA:HB1	1.76	0.49
38:B2:111:ARG:HG2	64:BX:25:PHE:CE1	2.47	0.49
1:AA:641:A:OP1	4:AE:230:ASN:HB2	2.12	0.48
1:AA:386:U:O2'	5:AF:93:ILE:O	2.31	0.48
12:AO:204:TRP:CZ2	12:AO:208:LYS:HD2	2.48	0.48
17:AV:28:Y5P:H2'	17:AV:29:Y5P:H6	1.95	0.48
46:BA:375:A:O2'	46:BA:376:G:H5'	2.12	0.48
64:BX:138:ASP:HB3	64:BX:141:ARG:HB2	1.94	0.48
1:AA:587:U:H5''	11:AN:33:LYS:NZ	2.28	0.48
6:AG:194:LYS:NZ	6:AG:218:PRO:HG2	2.29	0.48
1:AA:763:A:O3'	11:AN:58:ARG:NH2	2.46	0.48
39:B3:86:ILE:HD12	39:B3:113:VAL:HG11	1.95	0.48
39:B3:122:LEU:HD12	39:B3:123:LYS:H	1.78	0.48
46:BA:1020:G:C5	46:BA:1021:U:C5	3.01	0.48
46:BA:945:A:C6	46:BA:946:A:N1	2.81	0.48
52:BJ:117:ARG:HG3	53:BK:134:ASP:HB3	1.95	0.48
2:AB:133:HIS:O	2:AB:137:ARG:HG3	2.13	0.48
1:AA:738:U:H2'	6:AG:198:ARG:HE	1.78	0.48
6:AG:89:PRO:HA	6:AG:92:SER:HB3	1.94	0.48
9:AK:151:VAL:HG11	9:AK:164:ILE:HD11	1.95	0.48
15:AR:133:ASP:HB3	15:AR:134:PRO:HD2	1.94	0.48
46:BA:1006:A:H2'	46:BA:1006:A:N3	2.29	0.48
46:BA:175:U:P	54:BN:115:ASN:HD22	2.36	0.48
46:BA:733:A:H2'	46:BA:734:C:O4'	2.13	0.48
48:BD:115:GLU:H	48:BD:123:PHE:HZ	1.61	0.48
49:BE:205:ASP:OD2	49:BE:302:SER:HA	2.12	0.48
58:BR:53:ARG:HH21	58:BR:105:THR:HG22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:BS:54:ARG:O	59:BS:58:LEU:HG	2.13	0.48
60:BT:71:PRO:HG2	60:BT:212:ASN:ND2	2.29	0.48
64:BX:14:ASN:ND2	65:BY:210:HIS:HA	2.28	0.48
1:AA:109:G:H5''	10:AL:43:LYS:NZ	2.29	0.48
1:AA:159:C:H2'	1:AA:160:C:H5'	1.94	0.48
1:AA:787:A:H2'	1:AA:788:G:C8	2.49	0.48
3:AC:115:ASN:HD21	3:AC:150:PRO:HD2	1.79	0.48
4:AE:289:THR:HB	4:AE:307:LYS:HG3	1.95	0.48
14:AQ:57:GLN:O	14:AQ:57:GLN:NE2	2.46	0.48
14:AQ:74:THR:HG22	14:AQ:75:LYS:H	1.79	0.48
36:B0:77:PRO:HD2	59:BS:70:THR:OG1	2.12	0.48
46:BA:1399:U:O4	49:BE:242:ALA:HB2	2.13	0.48
46:BA:1550:C:H5'	46:BA:1551:A:OP1	2.13	0.48
46:BA:982:A:H2'	46:BA:983:C:O4'	2.14	0.48
49:BE:252:TRP:HE3	49:BE:253:PRO:HD2	1.78	0.48
56:BP:232:ALA:O	56:BP:235:GLU:HB3	2.13	0.48
38:B2:186:TRP:CD1	65:BY:216:TYR:CE2	3.02	0.48
1:AA:26:A:H2'	1:AA:27:U:C6	2.49	0.48
9:AK:87:ILE:H	9:AK:87:ILE:HG13	1.42	0.48
1:AA:254:C:H41	10:AL:74:ASN:HD22	1.61	0.48
36:B0:107:ASN:OD1	36:B0:108:PRO:HD2	2.14	0.48
46:BA:151:G:OP2	61:BU:37:ARG:NH1	2.35	0.48
46:BA:177:C:O2	61:BU:52:LYS:HD3	2.13	0.48
46:BA:1494:C:H5'	49:BE:220:ARG:HH12	1.78	0.48
52:BJ:136:GLU:HG2	52:BJ:144:LEU:HD11	1.95	0.48
53:BK:25:ARG:HA	53:BK:65:PRO:HB3	1.94	0.48
54:BN:80:HIS:CE1	54:BN:87:PHE:HB2	2.48	0.48
46:BA:378:U:O2'	56:BP:68:GLU:OE2	2.31	0.48
60:BT:168:ASN:OD1	60:BT:169:PRO:HD2	2.13	0.48
65:BY:212:LYS:NZ	65:BY:214:TYR:HE1	2.11	0.48
1:AA:185:A:H1'	1:AA:214:U:O2	2.13	0.48
1:AA:194:U:H5'	13:AP:86:PRO:HG3	1.96	0.48
1:AA:529:G:H2'	1:AA:531:U:C5	2.48	0.48
4:AE:320:ILE:HD13	4:AE:349:LEU:HD13	1.96	0.48
37:B1:224:ILE:H	37:B1:224:ILE:HG13	1.41	0.48
42:B6:26:THR:HB	46:BA:1239:U:H3'	1.96	0.48
46:BA:289:A:O2'	46:BA:792:A:OP1	2.32	0.48
46:BA:569:A:H3'	46:BA:570:A:H5''	1.96	0.48
46:BA:572:A:OP2	54:BN:68:SER:OG	2.27	0.48
46:BA:856:U:O4'	46:BA:858:G:H1'	2.13	0.48
46:BA:924:U:O2'	46:BA:925:A:O5'	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BF:216:VAL:HG22	50:BF:258:THR:HB	1.95	0.48
51:BI:57:GLU:HG2	51:BI:58:ARG:N	2.29	0.48
60:BT:74:ARG:HB3	60:BT:283:TRP:CZ2	2.48	0.48
1:AA:605:C:H2'	1:AA:606:A:O4'	2.13	0.48
5:AF:6:LEU:HB3	5:AF:66:VAL:HB	1.94	0.48
6:AG:52:ARG:NH1	7:AI:361:GLU:OE2	2.23	0.48
5:AF:97:PRO:HG3	15:AR:76:LYS:HZ2	1.77	0.48
17:AY:9:Y5P:C4	17:AY:22:Y5P:C5	2.92	0.48
36:B0:90:TYR:CZ	46:BA:1206:A:H4'	2.48	0.48
44:B8:98:SER:OG	44:B8:102:GLY:N	2.46	0.48
46:BA:501:A:H5'	46:BA:502:G:OP2	2.14	0.48
53:BK:17:SER:N	53:BK:72:VAL:O	2.46	0.48
1:AA:800:G:H2'	1:AA:801:A:C8	2.48	0.48
16:AU:83:PRO:HG2	16:AU:84:TRP:CD1	2.49	0.48
37:B1:156:LYS:NZ	37:B1:205:GLY:O	2.46	0.48
38:B2:143:ALA:O	38:B2:146:LYS:HB2	2.14	0.48
46:BA:1368:U:H2'	46:BA:1369:C:H6	1.79	0.48
41:B5:91:ARG:HD3	46:BA:156:A:H4'	1.93	0.48
46:BA:63:A:H2'	46:BA:63:A:N3	2.29	0.48
46:BA:674:A:H5'	46:BA:675:C:OP2	2.14	0.48
54:BN:111:MET:HB3	54:BN:111:MET:HE2	1.85	0.48
60:BT:148:THR:HG22	60:BT:165:GLU:HA	1.96	0.48
1:AA:201:A:H2'	1:AA:202:A:C8	2.49	0.48
1:AA:759:U:H2'	1:AA:760:A:H8	1.78	0.48
1:AA:768:A:H2'	1:AA:769:A:C8	2.49	0.48
1:AA:874:U:H3	1:AA:893:A:N6	2.12	0.48
6:AG:119:LYS:HG3	6:AG:141:PRO:HD3	1.96	0.48
9:AK:90:ILE:HG12	9:AK:99:ILE:HG12	1.96	0.48
11:AN:125:ARG:HH11	11:AN:125:ARG:HG2	1.78	0.48
18:AX:17:Y5P:H4A	18:AX:18:Y5P:H4	1.95	0.48
39:B3:76:LYS:HB2	39:B3:76:LYS:HE3	1.56	0.48
41:B5:90:ASN:OD1	41:B5:93:ARG:NH2	2.46	0.48
48:BD:80:ARG:HB2	48:BD:80:ARG:HE	1.37	0.48
49:BE:145:LEU:HA	49:BE:145:LEU:HD23	1.64	0.48
50:BF:166:PRO:HG2	50:BF:169:VAL:HG21	1.95	0.48
50:BF:190:VAL:HG11	50:BF:193:LEU:HD13	1.96	0.48
59:BS:54:ARG:HH12	59:BS:141:ILE:HG22	1.79	0.48
1:AA:194:U:H2'	1:AA:195:G:C8	2.49	0.48
1:AA:560:C:N4	1:AA:710:G:H1	2.11	0.48
39:B3:91:LEU:HA	39:B3:91:LEU:HD23	1.65	0.48
46:BA:1255:A:C8	46:BA:1255:A:C3'	2.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:420:U:H2'	46:BA:421:U:C6	2.49	0.48
46:BA:617:C:H2'	46:BA:618:A:C8	2.48	0.48
49:BE:202:GLN:HB3	49:BE:273:VAL:HG13	1.96	0.48
1:AA:744:C:O2'	1:AA:746:A:O2'	2.24	0.47
7:AI:104:ILE:O	7:AI:108:ILE:HG13	2.14	0.47
15:AR:55:MET:SD	15:AR:58:PRO:HG3	2.54	0.47
17:AY:55:Y5P:H5	17:AY:58:Y5P:H6	1.96	0.47
46:BA:164:A:H2'	46:BA:165:A:O4'	2.14	0.47
46:BA:624:G:C5	61:BU:11:ARG:HB2	2.49	0.47
56:BP:146:ASP:N	56:BP:146:ASP:OD1	2.44	0.47
58:BR:27:HIS:O	58:BR:30:GLN:HB2	2.14	0.47
59:BS:144:MET:O	59:BS:172:LEU:HA	2.14	0.47
63:BW:188:LYS:HB3	63:BW:192:ALA:HB3	1.95	0.47
5:AF:3:ARG:NH1	5:AF:4:TYR:CE1	2.76	0.47
1:AA:59:C:N4	8:AJ:133:GLN:HG2	148.61	0.47
17:AV:62:Y5P:C4	17:AV:63:Y5P:H4	2.43	0.47
41:B5:127:TYR:CE1	58:BR:110:ILE:HD11	2.49	0.47
44:B8:94:VAL:HG22	44:B8:161:MET:HG2	1.96	0.47
46:BA:1125:A:H2'	46:BA:1126:A:C8	2.49	0.47
46:BA:1264:U:H2'	46:BA:1265:A:C8	2.43	0.47
46:BA:1053:A:H3'	50:BF:131:LYS:NZ	2.30	0.47
50:BF:192:SER:OG	50:BF:193:LEU:N	2.44	0.47
46:BA:442:G:C6	52:BJ:31:LYS:NZ	2.80	0.47
46:BA:571:A:H4'	54:BN:30:LYS:HG3	1.96	0.47
46:BA:99:C:H5	54:BN:75:LYS:NZ	107.89	0.47
57:BQ:240:ARG:HG2	57:BQ:240:ARG:HH11	1.79	0.47
57:BQ:78:GLU:OE2	57:BQ:158:ARG:NH1	2.47	0.47
1:AA:116:G:OP1	12:AO:207:LYS:NZ	2.28	0.47
1:AA:647:A:H3'	1:AA:648:A:H5''	1.96	0.47
46:BA:1253:A:H2'	46:BA:1254:C:H6	1.79	0.47
46:BA:150:A:H8	46:BA:150:A:O5'	1.96	0.47
46:BA:355:G:C2	46:BA:356:U:C2	3.03	0.47
49:BE:194:TYR:HB3	49:BE:281:ASN:HD21	1.79	0.47
49:BE:215:PHE:CE2	49:BE:259:GLY:HA2	2.48	0.47
46:BA:14:C:O2'	50:BF:111:TYR:HB3	2.14	0.47
61:BU:83:TYR:CZ	61:BU:87:ILE:HG13	2.49	0.47
62:BV:140:VAL:O	62:BV:146:THR:HG23	2.14	0.47
1:AA:520:G:C2	1:AA:521:G:N7	2.83	0.47
1:AA:708:A:OP2	1:AA:708:A:H4'	2.15	0.47
12:AO:178:VAL:O	12:AO:182:ILE:HG12	2.15	0.47
14:AQ:16:LYS:O	14:AQ:29:ARG:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B0:76:HIS:CG	59:BS:70:THR:HG21	2.49	0.47
36:B0:92:LEU:HD23	36:B0:92:LEU:HA	1.53	0.47
45:B9:71:LYS:NZ	46:BA:494:C:H5'	2.29	0.47
43:B7:88:LYS:HG2	46:BA:117:G:C8	2.49	0.47
46:BA:357:U:H5''	46:BA:357:U:H6	1.79	0.47
46:BA:522:C:C5	46:BA:530:A:H5''	2.50	0.47
46:BA:714:A:H5'	48:BD:71:LYS:NZ	2.29	0.47
44:B8:108:LYS:NZ	46:BA:78:A:OP2	2.30	0.47
49:BE:104:LEU:HD23	49:BE:104:LEU:HA	1.63	0.47
50:BF:97:HIS:ND1	56:BP:27:LEU:HB3	2.29	0.47
46:BA:1201:C:O2'	56:BP:77:ARG:NH1	2.47	0.47
57:BQ:83:THR:OG1	57:BQ:123:ARG:NH1	2.48	0.47
63:BW:201:LEU:HB3	63:BW:204:ARG:HH21	1.79	0.47
63:BW:78:ILE:HG22	63:BW:80:TYR:H	1.79	0.47
1:AA:522:A:H2'	1:AA:523:C:O4'	2.13	0.47
8:AJ:83:HIS:CE1	11:AN:122:GLY:HA3	2.50	0.47
12:AO:69:PRO:HD2	12:AO:72:MET:HG3	1.95	0.47
49:BE:175:LYS:HB3	49:BE:296:LEU:HD23	1.95	0.47
51:BI:84:GLU:HG3	51:BI:85:ASP:N	2.28	0.47
57:BQ:71:ASP:OD1	57:BQ:72:ILE:HG13	2.14	0.47
1:AA:438:C:H2'	1:AA:439:A:O4'	2.14	0.47
1:AA:899:C:O3'	1:AA:900:A:H4'	2.15	0.47
7:AI:198:SER:HA	7:AI:247:ARG:O	2.14	0.47
15:AR:86:SER:HA	15:AR:93:TYR:OH	2.15	0.47
17:AY:28:Y5P:H6	17:AY:28:Y5P:O5'	2.14	0.47
37:B1:197:PRO:HG2	37:B1:200:GLU:HG3	1.97	0.47
44:B8:132:LYS:O	44:B8:136:LYS:HG3	2.15	0.47
46:BA:521:U:O2'	46:BA:522:C:O5'	2.29	0.47
49:BE:123:GLN:HG2	49:BE:124:VAL:O	2.15	0.47
54:BN:128:PHE:HA	54:BN:129:PRO:HD3	1.71	0.47
38:B2:190:TRP:HB3	65:BY:216:TYR:CE1	2.49	0.47
1:AA:256:G:O6	18:AX:21:Y5P:HC	2.13	0.47
1:AA:31:U:OP1	10:AL:134:HIS:HE1	1.97	0.47
2:AB:161:CYS:O	2:AB:260:LYS:NZ	2.37	0.47
4:AE:256:PHE:CZ	4:AE:347:ARG:HG2	2.49	0.47
7:AI:202:ILE:HG13	7:AI:205:GLU:HG3	1.95	0.47
1:AA:815:U:OP1	7:AI:278:LYS:HG2	2.14	0.47
11:AN:33:LYS:HB3	11:AN:90:ARG:NH2	2.30	0.47
17:AV:24:Y5P:C4	17:AV:25:Y5P:H4	2.43	0.47
92:AA:8113:HOH:O	17:AV:30:Y5P:C4	2.52	0.47
38:B2:115:LEU:HB3	64:BX:27:GLN:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:1551:A:H3'	46:BA:1552:G:H8	1.79	0.47
46:BA:890:G:H2'	46:BA:891:U:H6	1.80	0.47
46:BA:809:A:N3	49:BE:230:THR:HG21	2.30	0.47
49:BE:275:ARG:HD2	49:BE:333:TYR:CE1	2.49	0.47
59:BS:176:ARG:HG2	59:BS:177:ARG:H	1.78	0.47
1:AA:168:A:O2'	1:AA:170:A:N1	2.47	0.47
6:AG:194:LYS:NZ	6:AG:218:PRO:HB2	2.30	0.47
7:AI:316:PHE:HB3	7:AI:317:PRO:HD3	1.97	0.47
9:AK:154:LYS:HA	9:AK:180:ASN:O	2.14	0.47
44:B8:101:LYS:HE3	46:BA:75:A:C2	2.48	0.47
46:BA:1494:C:H5'	49:BE:220:ARG:NH1	2.29	0.47
46:BA:777:G:C2	46:BA:778:G:H1'	2.50	0.47
48:BD:165:LEU:HB3	48:BD:181:ASP:OD1	2.14	0.47
49:BE:187:ILE:HG22	49:BE:188:LYS:N	2.29	0.47
55:BO:40:VAL:HA	55:BO:105:VAL:HG23	1.97	0.47
56:BP:157:GLN:HA	56:BP:177:ALA:O	2.14	0.47
62:BV:112:VAL:HG13	62:BV:199:ILE:HG21	1.97	0.47
65:BY:172:ASP:HB3	65:BY:176:ASP:HB2	1.97	0.47
41:B5:84:ARG:HB2	46:BA:1010:U:O2	2.15	0.47
46:BA:120:C:H2'	46:BA:121:C:H6	1.79	0.47
46:BA:197:U:H2'	46:BA:198:A:H8	1.80	0.47
53:BK:66:LEU:HB3	53:BK:85:PRO:HG3	1.96	0.47
57:BQ:124:VAL:HA	57:BQ:158:ARG:NH2	2.28	0.47
65:BY:59:GLY:H	65:BY:76:VAL:HB	1.80	0.47
2:AB:140:ILE:HG23	2:AB:164:TYR:CD2	2.50	0.47
5:AF:3:ARG:HG2	5:AF:4:TYR:CE1	2.50	0.47
8:AJ:81:LYS:HE2	8:AJ:140:TYR:HE1	1.80	0.47
10:AL:69:LYS:HZ3	10:AL:77:ASN:HB3	1.79	0.47
39:B3:142:ASN:OD1	39:B3:144:GLU:HB3	2.15	0.47
46:BA:1328:U:H2'	46:BA:1329:G:O4'	2.15	0.47
46:BA:76:G:N2	46:BA:88:G:H2'	2.30	0.47
46:BA:85:A:C5	46:BA:86:U:H1'	2.49	0.47
53:BK:43:GLY:HA3	53:BK:76:ARG:NH1	2.24	0.47
46:BA:799:G:H4'	55:BO:36:THR:HG22	1.97	0.47
55:BO:57:CYS:SG	55:BO:58:ILE:N	2.88	0.47
55:BO:96:MET:HG2	60:BT:164:PHE:CD1	2.49	0.47
46:BA:440:A:H5'	57:BQ:66:ARG:HB2	1.96	0.47
64:BX:2:ALA:HB2	64:BX:19:VAL:HG11	1.96	0.47
1:AA:234:A:N6	1:AA:250:A:N1	2.62	0.47
3:AC:144:SER:HA	3:AC:149:CYS:O	2.15	0.47
39:B3:72:ILE:CD1	39:B3:118:ARG:HD3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:B5:157:VAL:HA	58:BR:130:CYS:SG	2.55	0.47
46:BA:1044:A:C2	46:BA:1435:A:C2	3.03	0.47
46:BA:438:A:OP1	57:BQ:73:ARG:NH2	2.48	0.47
46:BA:521:U:HO2'	46:BA:522:C:C5'	2.28	0.47
46:BA:895:A:H2'	46:BA:896:C:C6	2.50	0.47
46:BA:960:U:H2'	46:BA:961:G:C8	2.50	0.47
46:BA:733:A:OP2	48:BD:103:ARG:NH2	2.48	0.47
49:BE:205:ASP:CG	49:BE:302:SER:HA	2.35	0.47
46:BA:787:A:O2'	49:BE:215:PHE:O	2.24	0.47
50:BF:69:LEU:HD22	50:BF:193:LEU:HD12	1.97	0.47
46:BA:224:C:OP1	56:BP:132:SER:OG	2.33	0.47
56:BP:39:ARG:O	56:BP:41:ARG:N	2.45	0.47
58:BR:108:LEU:HD11	58:BR:136:LEU:HD22	1.97	0.47
1:AA:317:A:C2	1:AA:318:C:C5	3.03	0.46
1:AA:535:U:H2'	1:AA:536:C:O4'	2.15	0.46
1:AA:959:U:H4'	1:AA:960:A:O5'	2.15	0.46
2:AB:146:ARG:HG2	2:AB:205:HIS:CD2	2.49	0.46
8:AJ:109:HIS:CE1	8:AJ:142:CYS:HB3	2.50	0.46
1:AA:606:A:O2'	11:AN:28:TYR:OH	2.16	0.46
9:AK:160:ARG:HH12	16:AU:27:ASN:HD21	1.62	0.46
17:AV:48:Y5P:OP2	17:AV:48:Y5P:H6	2.15	0.46
17:AY:54:Y5P:H4A	17:AY:55:Y5P:C5	2.45	0.46
47:BB:9:P5P:H1'	47:BB:46:P5P:C2	2.45	0.46
49:BE:90:TRP:HA	49:BE:316:PHE:CE2	2.47	0.46
61:BU:69:ILE:O	61:BU:73:THR:OG1	2.27	0.46
63:BW:152:LYS:HD3	63:BW:164:ILE:HD11	1.97	0.46
63:BW:85:MET:HG3	63:BW:145:SER:OG	2.15	0.46
1:AA:348:A:OP2	9:AK:122:ALA:HB2	2.15	0.46
1:AA:456:A:OP2	1:AA:952:C:O2'	2.30	0.46
6:AG:113:GLN:OE1	6:AG:202:PRO:HG2	2.15	0.46
37:B1:202:GLU:HG3	37:B1:203:TRP:CD1	2.50	0.46
46:BA:163:A:H2'	46:BA:163:A:N3	2.30	0.46
46:BA:220:A:N7	50:BF:281:THR:OG1	2.41	0.46
59:BS:72:TRP:CG	59:BS:73:PRO:HA	2.50	0.46
1:AA:256:G:OP1	1:AA:257:U:H5'	2.14	0.46
12:AO:155:ARG:HE	12:AO:159:MET:HE1	1.80	0.46
37:B1:202:GLU:HG3	37:B1:203:TRP:HD1	1.81	0.46
37:B1:21:TYR:HE2	37:B1:208:LEU:HD21	1.80	0.46
37:B1:65:VAL:HG22	51:BI:71:PRO:HG2	1.98	0.46
44:B8:96:TYR:CD1	44:B8:96:TYR:N	2.84	0.46
46:BA:473:A:N6	46:BA:594:A:C6	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:BJ:95:MET:HB3	52:BJ:156:SER:HB2	1.96	0.46
56:BP:114:GLN:HB3	56:BP:115:PRO:HD2	1.97	0.46
61:BU:91:ILE:O	61:BU:94:GLN:N	2.44	0.46
1:AA:259:A:O2'	1:AA:260:U:H5''	2.15	0.46
1:AA:439:A:H5'	1:AA:440:C:OP2	2.15	0.46
1:AA:498:U:H5'	1:AA:499:C:OP2	2.16	0.46
5:AF:6:LEU:HG	5:AF:8:LEU:HG	1.96	0.46
2:AB:164:TYR:CD1	7:AI:149:PHE:HA	2.51	0.46
39:B3:76:LYS:HZ3	46:BA:472:G:H8	1.56	0.46
40:B4:55:VAL:HG21	40:B4:69:TYR:HB3	1.97	0.46
43:B7:93:LEU:HD22	43:B7:93:LEU:HA	1.85	0.46
46:BA:1072:U:H3'	46:BA:1073:U:H5''	1.98	0.46
46:BA:1202:A:C2	46:BA:1203:G:H1'	2.50	0.46
46:BA:1557:A:H4'	49:BE:263:ASN:ND2	2.29	0.46
60:BT:224:MET:HB2	60:BT:248:CYS:SG	2.55	0.46
61:BU:65:ARG:HA	61:BU:68:TRP:CE3	2.50	0.46
1:AA:185:A:O2'	1:AA:213:G:N2	2.48	0.46
1:AA:914:A:H2'	1:AA:915:G:O4'	2.16	0.46
6:AG:62:GLU:HG2	6:AG:66:ARG:HE	1.80	0.46
7:AI:129:GLU:HG3	7:AI:130:GLU:HG3	1.98	0.46
9:AK:181:THR:O	9:AK:183:ILE:HG13	2.14	0.46
13:AP:100:HIS:ND1	13:AP:101:PRO:HD2	2.30	0.46
37:B1:94:ASN:HD21	51:BI:81:LYS:HB2	1.80	0.46
46:BA:378:U:OP2	56:BP:62:ARG:NH1	2.48	0.46
46:BA:392:A:C2	46:BA:418:A:C2	3.03	0.46
46:BA:485:A:H61	46:BA:580:C:H42	1.63	0.46
49:BE:66:SER:O	49:BE:69:ASN:HB2	2.15	0.46
55:BO:60:VAL:HG22	55:BO:62:ASN:H	1.80	0.46
57:BQ:172:VAL:HA	57:BQ:175:PHE:CE2	2.50	0.46
59:BS:133:ALA:HB1	59:BS:168:GLY:HA3	1.98	0.46
1:AA:485:G:H2'	1:AA:486:C:O4'	2.16	0.46
2:AB:87:ARG:HG3	2:AB:243:PRO:HG2	1.96	0.46
7:AI:276:LYS:HE3	7:AI:281:LYS:HE2	1.98	0.46
10:AL:32:THR:OG1	10:AL:35:GLN:HG3	2.16	0.46
15:AR:104:LYS:HD3	15:AR:104:LYS:HA	1.59	0.46
17:AV:58:Y5P:H6	17:AV:58:Y5P:H2'	1.74	0.46
41:B5:119:LYS:NZ	49:BE:46:VAL:O	2.47	0.46
46:BA:493:A:OP1	46:BA:557:A:N6	2.49	0.46
46:BA:913:C:H6	46:BA:913:C:O5'	1.99	0.46
49:BE:90:TRP:CH2	49:BE:312:LYS:HE2	2.51	0.46
49:BE:74:ALA:O	49:BE:77:LEU:HB3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:BO:107:LEU:HA	55:BO:107:LEU:HD23	1.61	0.46
46:BA:1232:U:H5'	56:BP:79:PRO:HB3	1.98	0.46
1:AA:615:A:C6	1:AA:691:G:C5	3.03	0.46
4:AE:200:GLY:O	4:AE:221:ARG:HD2	2.16	0.46
4:AE:215:TYR:HB3	4:AE:218:PHE:HD2	1.81	0.46
7:AI:341:GLN:O	7:AI:345:VAL:HG23	2.15	0.46
11:AN:93:MET:H	11:AN:93:MET:HG2	1.40	0.46
5:AF:9:ILE:HD11	15:AR:118:LEU:O	2.16	0.46
39:B3:41:ILE:HA	39:B3:42:PRO:HD2	1.68	0.46
46:BA:1139:A:H2'	46:BA:1140:U:H6	1.78	0.46
46:BA:1491:A:C5	58:BR:14:VAL:HG21	2.50	0.46
46:BA:396:C:C4	46:BA:397:A:C2	3.04	0.46
46:BA:767:A:H8	46:BA:767:A:H5''	1.80	0.46
46:BA:841:C:H4'	48:BD:258:ILE:HG22	1.97	0.46
46:BA:975:G:N7	92:BA:1882:HOH:O	2.36	0.46
37:B1:91:TYR:CD2	51:BI:79:VAL:HG11	2.51	0.46
55:BO:69:VAL:HG12	55:BO:127:LEU:HD21	1.97	0.46
55:BO:91:MET:HG2	55:BO:92:PRO:HD2	1.97	0.46
60:BT:260:TRP:O	60:BT:262:GLN:HG3	2.15	0.46
65:BY:149:ARG:HD3	65:BY:150:SER:OG	2.16	0.46
2:AB:180:LEU:HD12	2:AB:180:LEU:HA	1.77	0.46
4:AE:180:ASP:O	4:AE:184:LYS:HG2	2.16	0.46
5:AF:105:CYS:HB3	15:AR:69:CYS:SG	2.55	0.46
10:AL:32:THR:O	10:AL:36:MET:HG3	2.16	0.46
17:AY:38:Y5P:H4A	17:AY:39:Y5P:C4	2.45	0.46
43:B7:77:THR:HA	43:B7:80:GLN:HG3	1.98	0.46
46:BA:1301:C:H2'	46:BA:1302:G:H5'	1.98	0.46
46:BA:1409:G:H2'	46:BA:1410:A:O4'	2.16	0.46
46:BA:69:C:HO2'	46:BA:70:A:P	2.34	0.46
46:BA:72:U:C4	46:BA:73:A:N7	2.84	0.46
57:BQ:127:PRO:HA	57:BQ:152:THR:OG1	2.15	0.46
57:BQ:39:PHE:HB3	57:BQ:42:VAL:HG23	1.98	0.46
64:BX:26:ILE:HD12	64:BX:56:TYR:CE1	2.51	0.46
1:AA:704:U:H2'	1:AA:705:G:C8	2.50	0.46
36:B0:40:LYS:HE3	36:B0:40:LYS:HB2	1.57	0.46
46:BA:1030:G:H2'	46:BA:1031:G:C8	2.51	0.46
46:BA:1339:A:N3	46:BA:1339:A:H2'	2.30	0.46
46:BA:1382:A:H2'	46:BA:1383:U:O4'	2.16	0.46
46:BA:289:A:C2	46:BA:301:A:C2	3.03	0.46
46:BA:446:A:N7	46:BA:448:C:C2	2.83	0.46
50:BF:103:GLN:HE22	50:BF:250:VAL:H	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BF:283:LEU:HD23	50:BF:284:TYR:CE2	2.51	0.46
49:BE:212:GLY:O	58:BR:11:HIS:CE1	2.69	0.46
59:BS:125:CYS:SG	59:BS:157:SER:HB2	2.56	0.46
1:AA:752:A:H3'	1:AA:753:A:H5'	1.98	0.46
1:AA:768:A:H2'	1:AA:769:A:H8	1.81	0.46
4:AE:305:MET:HE2	4:AE:332:LEU:HD21	1.97	0.46
2:AB:164:TYR:HD1	7:AI:149:PHE:HA	1.81	0.46
11:AN:125:ARG:NH1	11:AN:125:ARG:HG2	2.31	0.46
5:AF:105:CYS:HA	15:AR:103:LYS:NZ	2.31	0.46
43:B7:82:ILE:HG23	43:B7:93:LEU:HD13	1.97	0.46
46:BA:220:A:H5''	46:BA:221:G:OP2	2.16	0.46
46:BA:63:A:OP2	92:BA:1924:HOH:O	2.21	0.46
46:BA:924:U:O2'	46:BA:925:A:C8	2.67	0.46
55:BO:118:ARG:HA	55:BO:140:ILE:HB	1.98	0.46
62:BV:114:ALA:O	62:BV:115:GLU:HB2	2.16	0.46
1:AA:287:C:OP1	14:AQ:38:TYR:OH	2.31	0.45
1:AA:757:U:H2'	1:AA:758:U:O4'	2.15	0.45
6:AG:200:LEU:HA	6:AG:200:LEU:HD22	1.79	0.45
7:AI:376:ARG:HH11	7:AI:376:ARG:HG3	1.81	0.45
15:AR:65:LYS:HB3	15:AR:69:CYS:CB	2.47	0.45
46:BA:1159:G:H2'	46:BA:1160:G:H8	1.81	0.45
46:BA:1312:U:O2'	46:BA:1313:U:O4'	2.34	0.45
46:BA:960:U:H2'	46:BA:961:G:H8	1.80	0.45
50:BF:103:GLN:HE22	50:BF:250:VAL:N	2.14	0.45
57:BQ:89:ILE:HG13	57:BQ:161:VAL:HB	1.97	0.45
58:BR:93:LEU:HA	58:BR:93:LEU:HD12	1.68	0.45
62:BV:113:THR:O	62:BV:199:ILE:HG12	2.16	0.45
1:AA:950:U:H2'	1:AA:951:G:C8	2.51	0.45
17:AV:70:Y5P:H4A	17:AV:71:Y5P:H4	1.98	0.45
39:B3:125:PRO:HG2	39:B3:144:GLU:HG3	1.97	0.45
42:B6:38:ARG:NH2	42:B6:39:GLU:OE1	2.49	0.45
44:B8:98:SER:HG	44:B8:102:GLY:N	2.14	0.45
46:BA:1264:U:C2	46:BA:1265:A:C8	3.04	0.45
46:BA:566:C:N4	46:BA:567:C:N3	2.64	0.45
46:BA:718:C:H6	46:BA:718:C:OP1	2.00	0.45
49:BE:202:GLN:O	49:BE:272:LYS:HA	2.16	0.45
50:BF:284:TYR:HB2	50:BF:285:PRO:HD2	1.97	0.45
57:BQ:183:LEU:HA	57:BQ:183:LEU:HD23	1.75	0.45
62:BV:91:ILE:HG22	62:BV:206:PRO:HA	1.98	0.45
63:BW:57:TYR:HD2	63:BW:67:ARG:NH1	2.14	0.45
1:AA:629:C:H2'	1:AA:630:A:H8	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AJ:109:HIS:NE2	8:AJ:142:CYS:HB3	2.32	0.45
18:AX:20:Y5P:H4A	18:AX:21:Y5P:H4	1.99	0.45
37:B1:27:HIS:CD2	37:B1:28:TYR:N	2.85	0.45
46:BA:1258:U:H2'	46:BA:1259:U:H6	1.81	0.45
46:BA:1348:G:H1	46:BA:1357:C:H42	1.62	0.45
46:BA:187:C:C4	46:BA:1023:A:N1	2.84	0.45
47:BB:37:P5P:OP2	47:BB:37:P5P:H8	2.15	0.45
53:BK:29:ALA:HB3	53:BK:54:ASN:ND2	2.31	0.45
56:BP:142:GLU:OE1	56:BP:142:GLU:N	2.49	0.45
63:BW:57:TYR:CD2	63:BW:67:ARG:NH1	2.84	0.45
65:BY:153:ILE:HG13	65:BY:153:ILE:O	2.15	0.45
3:AC:100:PHE:CE2	3:AC:155:LEU:HD21	2.51	0.45
3:AC:43:ARG:HA	3:AC:43:ARG:HD3	1.74	0.45
4:AE:324:CYS:HB3	4:AE:329:ILE:HB	1.99	0.45
9:AK:195:ARG:HD3	9:AK:195:ARG:HA	1.53	0.45
11:AN:80:ARG:O	11:AN:86:ARG:HD2	2.16	0.45
12:AO:172:ARG:NH1	14:AQ:88:VAL:HG21	2.31	0.45
5:AF:105:CYS:HB2	15:AR:70:GLU:H	1.81	0.45
43:B7:57:GLN:O	46:BA:253:G:H8	1.99	0.45
46:BA:1045:A:O4'	49:BE:244:SER:HB3	2.16	0.45
46:BA:1535:A:H2'	46:BA:1536:A:O4'	2.17	0.45
46:BA:216:A:O2'	46:BA:218:A:H4'	2.17	0.45
46:BA:481:G:H2'	46:BA:482:U:O4'	2.17	0.45
46:BA:48:U:H1'	51:BI:78:ARG:HH12	1.80	0.45
46:BA:54:A:H5''	46:BA:55:A:OP2	2.16	0.45
52:BJ:34:THR:OG1	52:BJ:35:ARG:N	2.49	0.45
46:BA:93:U:H5'	56:BP:196:ARG:HD3	1.98	0.45
57:BQ:53:VAL:HG21	57:BQ:102:PHE:HB3	1.99	0.45
60:BT:118:ARG:HA	60:BT:133:PHE:O	2.16	0.45
64:BX:15:PRO:HA	65:BY:208:ARG:NH1	2.32	0.45
1:AA:348:A:P	9:AK:122:ALA:HB2	2.56	0.45
1:AA:526:G:N2	1:AA:840:A:C4	2.84	0.45
1:AA:861:A:C6	1:AA:908:A:C6	3.04	0.45
3:AC:76:LEU:HD22	8:AJ:138:THR:HG23	1.97	0.45
16:AU:46:GLU:OE2	16:AU:54:ARG:NH1	2.49	0.45
37:B1:25:PRO:HB2	37:B1:27:HIS:CE1	2.51	0.45
42:B6:43:LEU:O	42:B6:55:LEU:HA	2.17	0.45
46:BA:1052:A:C5	46:BA:1324:A:C2	3.05	0.45
49:BE:199:ARG:CG	49:BE:199:ARG:HH11	2.29	0.45
57:BQ:42:VAL:HG21	57:BQ:166:ARG:HA	1.97	0.45
59:BS:127:SER:O	59:BS:131:VAL:HG23	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:BT:168:ASN:ND2	60:BT:170:ARG:HB2	2.31	0.45
62:BV:180:LYS:O	62:BV:181:ARG:HG2	2.17	0.45
64:BX:141:ARG:HD2	64:BX:141:ARG:HA	1.64	0.45
65:BY:59:GLY:N	65:BY:76:VAL:O	2.49	0.45
1:AA:180:U:H2'	1:AA:181:A:H8	1.80	0.45
1:AA:232:G:O6	1:AA:250:A:N6	2.50	0.45
1:AA:665:A:H62	8:AJ:85:LYS:HE3	1.82	0.45
1:AA:826:C:H2'	1:AA:827:A:C8	2.46	0.45
4:AE:289:THR:HG21	4:AE:308:GLN:N	2.31	0.45
5:AF:75:VAL:HA	5:AF:78:MET:SD	2.56	0.45
14:AQ:55:LEU:HG	14:AQ:55:LEU:H	1.53	0.45
37:B1:91:TYR:HE2	51:BI:79:VAL:HG11	1.79	0.45
38:B2:123:ARG:NH1	64:BX:30:ARG:HB3	2.32	0.45
46:BA:104:C:H5''	46:BA:105:G:OP1	2.17	0.45
46:BA:444:A:OP1	52:BJ:35:ARG:NH2	2.36	0.45
46:BA:532:A:H5''	57:BQ:134:LYS:NZ	56.93	0.45
44:B8:103:LYS:NZ	46:BA:76:G:OP2	2.43	0.45
51:BI:130:VAL:HB	51:BI:136:ASN:HD21	1.80	0.45
56:BP:205:LEU:HA	56:BP:205:LEU:HD23	1.74	0.45
58:BR:16:ARG:HG2	58:BR:51:GLU:OE1	2.16	0.45
59:BS:133:ALA:O	59:BS:136:CYS:HB2	2.16	0.45
61:BU:137:GLU:HB2	61:BU:138:PRO:HD3	1.98	0.45
62:BV:60:LEU:HD23	62:BV:60:LEU:HA	1.78	0.45
1:AA:792:U:H2'	1:AA:793:A:H8	1.80	0.45
2:AB:158:ALA:HB2	2:AB:165:ALA:HB2	1.99	0.45
8:AJ:132:VAL:HG21	11:AN:112:ARG:NH1	2.31	0.45
46:BA:1349:U:OP2	46:BA:1349:U:H6	1.99	0.45
46:BA:15:A:H2'	46:BA:16:A:C8	2.49	0.45
57:BQ:101:HIS:O	57:BQ:105:MET:HG3	2.16	0.45
59:BS:177:ARG:HD3	59:BS:180:GLU:HG3	1.97	0.45
4:AE:303:ILE:HD12	4:AE:303:ILE:HA	1.76	0.45
1:AA:368:A:O5'	9:AK:186:ASN:ND2	2.50	0.45
10:AL:64:ARG:HG3	10:AL:66:PHE:HD2	1.82	0.45
12:AO:99:ALA:HB1	12:AO:103:GLU:HG3	1.98	0.45
13:AP:54:TYR:CD1	13:AP:66:VAL:HG22	2.47	0.45
36:B0:126:LEU:HA	36:B0:126:LEU:HD13	1.82	0.45
46:BA:160:A:N6	46:BA:1034:A:N6	2.64	0.45
46:BA:110:A:C5	46:BA:111:G:C8	3.05	0.45
46:BA:1388:G:H2'	46:BA:1389:U:C6	2.52	0.45
46:BA:1476:U:H2'	46:BA:1477:G:C8	2.49	0.45
46:BA:521:U:H4'	46:BA:522:C:H5'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:BD:74:VAL:HG13	48:BD:151:TRP:NE1	2.31	0.45
54:BN:160:GLN:HA	54:BN:163:ILE:HD12	1.97	0.45
58:BR:46:TRP:CD1	58:BR:122:ALA:HB2	2.50	0.45
46:BA:177:C:H1'	61:BU:55:ARG:NH2	2.31	0.45
11:AN:115:ALA:HA	11:AN:120:LEU:HB2	1.98	0.45
16:AU:77:ARG:O	16:AU:80:ARG:NH1	2.50	0.45
46:BA:128:A:C6	46:BA:129:A:C6	3.05	0.45
46:BA:1341:C:HO2'	46:BA:1386:A:HO2'	1.64	0.45
46:BA:742:A:OP1	46:BA:742:A:H4'	2.16	0.45
46:BA:790:G:H2'	46:BA:791:A:C8	2.50	0.45
47:BB:38:P5P:H2'	47:BB:39:P5P:H8	1.98	0.45
56:BP:142:GLU:HB2	56:BP:162:LEU:HD23	1.98	0.45
60:BT:244:ARG:HG2	60:BT:246:ASP:OD1	2.17	0.45
1:AA:503:A:HO2'	1:AA:504:C:P	2.37	0.45
1:AA:532:G:H2'	1:AA:533:C:O4'	2.16	0.45
7:AI:145:ARG:HA	7:AI:146:PRO:HD3	1.75	0.45
1:AA:647:A:C6	16:AU:82:ASP:HB3	2.52	0.45
46:BA:1268:G:C5	46:BA:1322:C:N3	2.84	0.45
46:BA:160:A:H5'	46:BA:161:G:C2	2.52	0.45
46:BA:288:U:H2'	46:BA:289:A:C8	2.52	0.45
46:BA:828:U:C4	46:BA:834:A:C4	3.05	0.45
47:BB:23:P5P:H8	47:BB:48:Y5P:H4	1.99	0.45
49:BE:222:TRP:CE2	49:BE:256:LYS:HB3	2.52	0.45
50:BF:166:PRO:HG2	50:BF:169:VAL:CG2	2.47	0.45
54:BN:112:LEU:HB3	54:BN:113:PRO:HD2	1.98	0.45
56:BP:61:THR:HG22	56:BP:61:THR:O	2.16	0.45
57:BQ:107:LEU:O	57:BQ:111:ARG:HG2	2.17	0.45
57:BQ:133:ARG:HA	57:BQ:133:ARG:HD3	1.72	0.45
57:BQ:51:ARG:O	57:BQ:106:ARG:HD2	2.17	0.45
62:BV:91:ILE:HD11	62:BV:145:PHE:CZ	2.51	0.45
63:BW:147:ARG:NH1	63:BW:150:TYR:CE1	2.85	0.45
63:BW:99:GLN:O	63:BW:102:ALA:HB3	2.17	0.45
64:BX:138:ASP:HB3	64:BX:141:ARG:HG2	1.99	0.45
65:BY:62:VAL:HG12	65:BY:122:LEU:HA	1.99	0.45
1:AA:155:A:H2'	1:AA:156:C:C6	2.52	0.44
1:AA:296:G:H4'	1:AA:297:A:H5''	1.98	0.44
1:AA:630:A:H2'	1:AA:631:A:C8	2.51	0.44
1:AA:937:A:H2'	1:AA:938:U:O4'	2.17	0.44
4:AE:203:LEU:HD11	4:AE:268:PHE:HB3	1.98	0.44
8:AJ:76:LEU:HD23	8:AJ:145:LEU:HD12	1.99	0.44
37:B1:77:LEU:HA	37:B1:77:LEU:HD12	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:1164:A:C2	46:BA:1170:A:N7	2.85	0.44
46:BA:508:C:H42	46:BA:512:A:H3'	1.83	0.44
48:BD:127:VAL:HG12	48:BD:160:ALA:HA	1.98	0.44
48:BD:74:VAL:HG22	48:BD:151:TRP:CD1	2.52	0.44
50:BF:87:PHE:O	50:BF:179:THR:HG23	2.17	0.44
62:BV:88:ASN:ND2	62:BV:208:LEU:H	2.15	0.44
64:BX:66:ALA:N	64:BX:98:GLN:O	2.44	0.44
1:AA:180:U:O4	1:AA:181:A:N6	2.51	0.44
4:AE:193:TRP:HZ2	4:AE:319:ALA:HA	1.82	0.44
6:AG:236:LEU:O	6:AG:239:TYR:HB2	2.17	0.44
8:AJ:75:ARG:H	8:AJ:175:THR:HG23	1.82	0.44
10:AL:69:LYS:HA	10:AL:70:PRO:HD3	1.67	0.44
36:B0:45:LYS:HB2	36:B0:45:LYS:HE3	1.77	0.44
36:B0:62:HIS:H	36:B0:65:ASN:ND2	2.15	0.44
38:B2:155:LEU:HD23	65:BY:193:THR:HG23	1.98	0.44
44:B8:116:ARG:NH1	44:B8:167:LYS:HG2	2.32	0.44
46:BA:1343:A:C2	46:BA:1364:A:N6	2.83	0.44
46:BA:397:A:H2'	46:BA:398:A:H5'	1.98	0.44
46:BA:774:C:O2'	46:BA:775:A:H2'	2.17	0.44
46:BA:882:U:H2'	46:BA:883:G:O4'	2.17	0.44
48:BD:148:ARG:HE	48:BD:150:ARG:HG2	1.82	0.44
52:BJ:176:LEU:HB3	52:BJ:188:ARG:NH1	2.32	0.44
56:BP:130:GLN:NE2	92:BP:402:HOH:O	2.23	0.44
56:BP:223:LEU:HA	56:BP:223:LEU:HD23	1.84	0.44
64:BX:2:ALA:HA	64:BX:23:ASN:H	1.81	0.44
64:BX:75:GLY:N	64:BX:91:ASP:OD1	2.46	0.44
1:AA:318:C:O2'	1:AA:319:A:OP2	2.34	0.44
1:AA:836:G:H2'	1:AA:837:C:H6	1.80	0.44
1:AA:931:G:H4'	1:AA:932:U:H5''	1.99	0.44
2:AB:168:ARG:HA	2:AB:168:ARG:HD3	1.58	0.44
4:AE:215:TYR:HB3	4:AE:218:PHE:CD2	2.53	0.44
9:AK:175:ILE:HA	16:AU:14:VAL:HG22	1.99	0.44
12:AO:158:LEU:HA	12:AO:158:LEU:HD12	1.81	0.44
38:B2:98:GLU:O	38:B2:101:HIS:HB3	2.17	0.44
39:B3:136:ASN:O	39:B3:149:TRP:HB2	2.17	0.44
42:B6:36:ARG:NH1	46:BA:1184:U:OP1	2.50	0.44
41:B5:82:LYS:O	46:BA:1010:U:H4'	2.17	0.44
46:BA:114:A:O2'	46:BA:115:U:H5''	2.17	0.44
46:BA:1157:U:H1'	46:BA:1249:C:H2'	1.99	0.44
46:BA:691:U:H1'	46:BA:692:A:H5'	1.99	0.44
50:BF:227:PRO:HG2	50:BF:230:VAL:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:BW:147:ARG:CZ	63:BW:150:TYR:CE1	3.00	0.44
46:BA:673:U:C5	64:BX:74:TYR:CD2	3.05	0.44
1:AA:142:G:C2	1:AA:143:C:C2	3.05	0.44
1:AA:344:G:O2'	1:AA:437:C:H4'	2.18	0.44
1:AA:433:U:O2	1:AA:942:G:H4'	2.17	0.44
1:AA:672:A:H2'	1:AA:673:A:O4'	2.18	0.44
1:AA:822:A:N3	1:AA:822:A:H3'	2.32	0.44
1:AA:825:C:HO2'	1:AA:826:C:P	2.40	0.44
4:AE:161:SER:OG	4:AE:164:ASP:HB2	2.16	0.44
8:AJ:164:LEU:HD21	8:AJ:170:MET:HB2	1.99	0.44
11:AN:64:PRO:HG2	11:AN:67:LEU:HB2	1.99	0.44
17:AY:25:Y5P:O5'	17:AY:25:Y5P:H6	2.17	0.44
36:B0:90:TYR:CE1	36:B0:92:LEU:HD21	2.52	0.44
40:B4:44:LEU:HD23	40:B4:46:ARG:H	1.83	0.44
46:BA:1232:U:H3'	46:BA:1233:C:H6	1.82	0.44
50:BF:190:VAL:HG13	50:BF:191:ASP:O	2.18	0.44
51:BI:105:LEU:HD22	51:BI:112:VAL:HG21	2.00	0.44
56:BP:237:ALA:O	56:BP:241:GLY:N	2.50	0.44
60:BT:99:MET:HB3	60:BT:145:LEU:HD12	2.00	0.44
1:AA:232:G:H5''	4:AE:196:ASN:HD22	1.83	0.44
2:AB:142:LEU:HA	2:AB:164:TYR:O	2.17	0.44
3:AC:89:ASP:CG	3:AC:110:LEU:HD12	2.37	0.44
6:AG:190:GLU:O	6:AG:194:LYS:HG2	2.18	0.44
6:AG:204:LYS:O	6:AG:208:GLU:HG2	2.17	0.44
1:AA:687:A:C4	11:AN:109:ILE:HG21	2.53	0.44
37:B1:155:SER:HB2	37:B1:158:GLY:H	1.82	0.44
37:B1:173:ASP:HA	37:B1:174:PRO:HD3	1.80	0.44
44:B8:95:THR:HB	44:B8:105:LYS:HB2	1.99	0.44
44:B8:142:ARG:HB2	44:B8:142:ARG:CZ	2.46	0.44
46:BA:1178:G:C2	46:BA:1179:A:C8	3.06	0.44
46:BA:777:G:H5'	46:BA:778:G:OP2	2.18	0.44
53:BK:60:ILE:HG21	53:BK:64:ILE:HG13	1.99	0.44
44:B8:172:TYR:CE1	56:BP:90:ARG:NH1	2.86	0.44
60:BT:229:TRP:HH2	60:BT:249:LEU:HD21	1.83	0.44
62:BV:137:VAL:HG12	62:BV:153:LEU:HD23	1.99	0.44
63:BW:76:ARG:CA	63:BW:171:HIS:HD2	2.28	0.44
63:BW:49:TRP:HD1	63:BW:74:CYS:HG	1.66	0.44
1:AA:85:G:H2'	1:AA:86:A:C8	2.53	0.44
13:AP:110:LEU:O	13:AP:114:ARG:HG2	2.16	0.44
5:AF:92:ASN:OD1	15:AR:118:LEU:HD22	2.16	0.44
36:B0:51:PHE:HA	36:B0:69:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B3:81:TRP:CD1	39:B3:82:GLU:N	2.86	0.44
46:BA:108:A:C2	46:BA:131:G:C8	3.05	0.44
46:BA:163:A:P	61:BU:52:LYS:NZ	2.90	0.44
46:BA:346:U:O4'	46:BA:348:A:H5'	2.17	0.44
46:BA:838:C:H2'	46:BA:839:A:O4'	2.18	0.44
47:BB:32:P5P:C5	47:BB:33:Y5P:H4	2.48	0.44
50:BF:105:ASN:O	50:BF:107:LYS:N	2.50	0.44
50:BF:192:SER:O	50:BF:193:LEU:HB2	2.18	0.44
53:BK:111:LEU:HD11	53:BK:154:ARG:HE	1.82	0.44
56:BP:244:LEU:HD12	56:BP:245:PRO:HD2	1.99	0.44
56:BP:51:ARG:HH11	56:BP:51:ARG:HB3	1.82	0.44
58:BR:15:PHE:HB3	58:BR:25:ARG:HH12	1.82	0.44
47:BB:24:P5P:H4'	59:BS:108:ARG:HD2	2.00	0.44
36:B0:76:HIS:CD2	59:BS:70:THR:HG21	2.52	0.44
46:BA:163:A:P	61:BU:52:LYS:HZ3	2.39	0.44
1:AA:333:A:N7	1:AA:361:A:H2	2.16	0.44
1:AA:557:G:C2	1:AA:558:U:C2	3.06	0.44
3:AC:91:PHE:HD2	3:AC:147:TYR:HH	1.65	0.44
4:AE:128:ARG:HD3	4:AE:179:TRP:CZ2	2.53	0.44
7:AI:331:CYS:SG	7:AI:332:ALA:N	2.91	0.44
1:AA:794:A:OP1	7:AI:390:ARG:NH1	2.50	0.44
1:AA:202:A:H5'	13:AP:102:MET:CE	2.48	0.44
39:B3:67:HIS:NE2	39:B3:102:ASN:OD1	2.49	0.44
45:B9:63:PHE:N	46:BA:1347:G:N3	2.66	0.44
46:BA:163:A:C2'	61:BU:35:LYS:HZ1	2.29	0.44
46:BA:230:C:OP2	46:BA:230:C:H6	1.99	0.44
46:BA:774:C:O2'	46:BA:775:A:O5'	2.30	0.44
53:BK:23:ILE:HA	53:BK:67:PRO:HA	2.00	0.44
56:BP:142:GLU:HB3	56:BP:162:LEU:HB3	2.00	0.44
57:BQ:213:TRP:CZ3	57:BQ:217:ARG:NH1	2.85	0.44
60:BT:54:UNK:O	60:BT:54:UNK:HG2	2.18	0.44
65:BY:159:PHE:CD1	65:BY:160:PRO:HD2	2.53	0.44
1:AA:25:U:H2'	1:AA:26:A:C8	2.52	0.44
2:AB:241:SER:HA	2:AB:242:PRO:HD3	1.85	0.44
7:AI:294:ILE:HG23	7:AI:301:TYR:CD1	2.53	0.44
9:AK:141:ALA:O	9:AK:146:VAL:HG22	2.17	0.44
13:AP:77:ILE:HD11	13:AP:83:LEU:HD11	2.00	0.44
38:B2:144:LEU:O	38:B2:148:VAL:HG23	2.17	0.44
39:B3:73:LYS:HB3	39:B3:73:LYS:HE2	1.66	0.44
40:B4:42:THR:O	40:B4:68:ARG:NH1	2.48	0.44
46:BA:13:U:C2	46:BA:105:G:C2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:214:A:H2'	46:BA:215:C:O4'	2.17	0.44
46:BA:724:A:H4'	46:BA:725:A:OP1	2.18	0.44
46:BA:801:A:H61	46:BA:809:A:H61	1.64	0.44
49:BE:235:LYS:O	49:BE:239:ARG:HD2	2.18	0.44
46:BA:1557:A:H4'	49:BE:263:ASN:HD21	1.83	0.44
50:BF:262:THR:O	50:BF:265:THR:HB	2.18	0.44
56:BP:54:LYS:HB3	56:BP:55:GLY:H	1.45	0.44
59:BS:81:LEU:HD12	59:BS:93:LEU:O	2.17	0.44
60:BT:234:GLU:HG2	60:BT:234:GLU:H	1.42	0.44
4:AE:321:MET:HE2	4:AE:325:ARG:HH22	1.83	0.44
5:AF:50:LYS:HD2	5:AF:57:ARG:NH2	2.33	0.44
2:AB:168:ARG:HG2	7:AI:159:TYR:CZ	2.53	0.44
7:AI:158:TYR:OH	7:AI:218:ASP:O	2.34	0.44
9:AK:194:ARG:O	9:AK:195:ARG:NH1	2.51	0.44
1:AA:318:C:H3'	15:AR:106:LYS:NZ	2.32	0.44
41:B5:95:ARG:HH11	46:BA:156:A:H5'	1.83	0.44
46:BA:1037:A:H2'	46:BA:1038:A:O4'	2.17	0.44
46:BA:1192:U:H2'	46:BA:1193:A:H5''	2.00	0.44
46:BA:222:A:O2'	46:BA:223:A:C8	2.71	0.44
46:BA:356:U:H5'	46:BA:357:U:P	2.58	0.44
46:BA:911:G:HO2'	46:BA:913:C:N4	2.16	0.44
52:BJ:161:VAL:HB	52:BJ:195:SER:HA	1.99	0.44
53:BK:137:LEU:HD12	53:BK:137:LEU:HA	1.82	0.44
56:BP:100:ARG:HH11	56:BP:100:ARG:HG3	1.82	0.44
92:BA:1912:HOH:O	56:BP:130:GLN:NE2	2.51	0.44
57:BQ:211:ASN:HA	57:BQ:212:PRO:HD3	1.67	0.44
60:BT:100:LEU:HA	60:BT:100:LEU:HD23	1.78	0.44
3:AC:92:LEU:HA	3:AC:92:LEU:HD23	1.74	0.43
37:B1:216:ARG:HD3	37:B1:217:LEU:HD23	2.00	0.43
46:BA:1340:C:C5	46:BA:1362:A:C6	3.06	0.43
46:BA:160:A:H62	46:BA:1034:A:H62	1.66	0.43
46:BA:197:U:H2'	46:BA:198:A:C8	2.53	0.43
46:BA:30:U:H5'	46:BA:31:A:OP1	2.18	0.43
46:BA:378:U:H1'	56:BP:68:GLU:OE1	2.18	0.43
46:BA:462:A:H3'	46:BA:463:U:C5'	2.47	0.43
46:BA:64:C:N3	46:BA:65:C:C4	2.86	0.43
46:BA:812:C:O2	46:BA:812:C:H2'	2.17	0.43
49:BE:165:TYR:CD2	49:BE:172:PRO:HA	2.53	0.43
50:BF:63:GLN:HE21	50:BF:81:GLU:HG3	1.83	0.43
50:BF:95:ILE:H	50:BF:95:ILE:HG13	1.51	0.43
1:AA:225:A:N1	1:AA:272:A:O2'	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:386:U:H2'	1:AA:387:C:C6	2.54	0.43
7:AI:376:ARG:HG3	7:AI:376:ARG:NH1	2.33	0.43
42:B6:47:ASP:HA	42:B6:48:PRO:HD3	1.68	0.43
38:B2:175:PHE:CZ	43:B7:82:ILE:HG21	2.53	0.43
46:BA:1030:G:H2'	46:BA:1031:G:H8	1.83	0.43
46:BA:980:U:H2'	46:BA:980:U:O2	2.17	0.43
52:BJ:117:ARG:HD3	52:BJ:117:ARG:HA	1.75	0.43
55:BO:69:VAL:CG1	55:BO:127:LEU:HD21	2.48	0.43
56:BP:83:PHE:HD1	56:BP:83:PHE:HA	1.66	0.43
60:BT:74:ARG:HB3	60:BT:283:TRP:CH2	2.53	0.43
1:AA:127:A:C2	1:AA:128:C:C4	3.06	0.43
1:AA:612:U:H5'	1:AA:613:A:OP1	2.18	0.43
1:AA:761:U:H2'	1:AA:762:G:O4'	2.17	0.43
7:AI:309:GLN:HG2	7:AI:313:GLN:HE21	1.82	0.43
38:B2:115:LEU:O	38:B2:118:GLU:HB3	2.18	0.43
46:BA:196:U:H2'	46:BA:197:U:C6	2.53	0.43
46:BA:217:A:H4'	46:BA:218:A:H5'	2.00	0.43
46:BA:697:G:H2'	46:BA:698:A:C8	2.53	0.43
46:BA:699:U:H2'	46:BA:700:A:O4'	2.18	0.43
49:BE:208:ALA:HB3	49:BE:290:PRO:O	2.18	0.43
50:BF:205:GLU:CG	50:BF:208:ARG:HH12	2.24	0.43
50:BF:63:GLN:HA	50:BF:80:THR:O	2.18	0.43
58:BR:13:ARG:HG3	58:BR:13:ARG:HH11	1.84	0.43
59:BS:178:ILE:HG22	59:BS:179:TYR:HD1	1.84	0.43
63:BW:150:TYR:HE2	63:BW:168:VAL:HG13	1.83	0.43
65:BY:196:GLU:O	65:BY:200:GLU:HB3	2.17	0.43
1:AA:48:C:N4	1:AA:172:A:OP2	2.46	0.43
1:AA:835:C:H2'	1:AA:836:G:H8	1.77	0.43
1:AA:938:U:H2'	1:AA:939:A:C8	2.53	0.43
6:AG:68:PHE:HB3	7:AI:367:GLN:NE2	2.33	0.43
46:BA:1230:G:C8	46:BA:1230:G:H5''	2.51	0.43
36:B0:74:ARG:HG3	46:BA:401:A:O4'	2.18	0.43
44:B8:163:THR:HG21	46:BA:76:G:H5''	1.99	0.43
46:BA:82:G:H5'	46:BA:83:A:H5'	2.00	0.43
46:BA:857:A:H5''	48:BD:67:LYS:HE2	1.99	0.43
46:BA:899:C:C5	46:BA:923:G:C6	3.05	0.43
47:BB:61:Y5P:H2'	47:BB:62:Y5P:H6	1.99	0.43
48:BD:198:GLU:HA	48:BD:205:ALA:HA	2.01	0.43
49:BE:296:LEU:HD12	49:BE:296:LEU:HA	1.61	0.43
52:BJ:163:GLU:N	52:BJ:163:GLU:OE1	2.52	0.43
59:BS:52:ASN:OD1	59:BS:55:ASN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:BV:180:LYS:O	62:BV:182:LYS:HG2	2.18	0.43
4:AE:260:LYS:HB3	4:AE:260:LYS:HE2	1.70	0.43
6:AG:45:GLN:HB3	6:AG:51:TYR:OH	2.18	0.43
16:AU:50:ARG:HH11	16:AU:50:ARG:CG	2.32	0.43
38:B2:192:LEU:HD23	38:B2:192:LEU:HA	1.81	0.43
46:BA:1228:U:H5'	46:BA:1229:U:O5'	2.18	0.43
46:BA:162:C:H2'	46:BA:162:C:O2	2.18	0.43
46:BA:397:A:C5	46:BA:398:A:C8	3.06	0.43
46:BA:537:U:O4	46:BA:538:A:N6	2.51	0.43
49:BE:297:VAL:HG12	49:BE:298:LYS:N	2.33	0.43
57:BQ:88:ALA:HA	57:BQ:161:VAL:O	2.17	0.43
1:AA:670:A:H2'	1:AA:671:U:C6	2.53	0.43
1:AA:792:U:H4'	7:AI:389:ARG:HG3	2.00	0.43
8:AJ:179:GLN:HG2	8:AJ:179:GLN:H	1.59	0.43
12:AO:68:PRO:HG2	12:AO:108:LYS:HE3	1.99	0.43
13:AP:86:PRO:HA	13:AP:89:LYS:HG2	2.01	0.43
17:AV:51:Y5P:H2'	17:AV:52:Y5P:H6	1.98	0.43
37:B1:118:ILE:O	37:B1:168:ARG:HD3	2.18	0.43
40:B4:73:ARG:NH2	40:B4:76:LEU:HD13	2.32	0.43
43:B7:85:ARG:NH1	43:B7:90:ARG:HD2	2.33	0.43
46:BA:112:A:C2	46:BA:114:A:C6	3.06	0.43
46:BA:242:A:C6	46:BA:243:A:C6	3.06	0.43
46:BA:355:G:N2	46:BA:356:U:H1'	2.34	0.43
46:BA:654:C:O2	46:BA:655:U:N3	2.42	0.43
50:BF:92:ARG:HG2	50:BF:95:ILE:HG13	2.01	0.43
56:BP:247:ILE:H	56:BP:247:ILE:HD12	1.83	0.43
56:BP:56:GLU:OE2	56:BP:61:THR:HB	2.17	0.43
59:BS:88:HIS:HB3	59:BS:89:HIS:CD2	2.43	0.43
65:BY:25:ARG:HA	65:BY:26:PRO:HD2	1.74	0.43
1:AA:750:G:N2	1:AA:776:A:N7	2.67	0.43
1:AA:825:C:O2'	1:AA:826:C:O5'	2.33	0.43
1:AA:861:A:C2	1:AA:910:G:C6	3.07	0.43
3:AC:89:ASP:O	3:AC:93:ARG:HG2	2.19	0.43
4:AE:238:LYS:HB2	4:AE:238:LYS:HE3	1.67	0.43
38:B2:158:LEU:HD12	38:B2:158:LEU:HA	1.75	0.43
38:B2:236:LEU:HD13	65:BY:48:PRO:HG3	2.01	0.43
38:B2:66:LEU:HA	38:B2:66:LEU:HD12	1.87	0.43
38:B2:75:ASN:HA	38:B2:75:ASN:HD22	1.62	0.43
42:B6:44:LEU:HA	42:B6:54:VAL:O	2.19	0.43
45:B9:92:ASN:HB3	45:B9:94:LYS:HG2	2.01	0.43
46:BA:1048:C:H5'	46:BA:1049:G:OP1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:209:A:H2'	46:BA:210:U:C6	2.54	0.43
39:B3:76:LYS:NZ	46:BA:472:G:C8	2.81	0.43
46:BA:774:C:HO2'	46:BA:775:A:P	2.41	0.43
46:BA:794:U:H4'	60:BT:260:TRP:HZ3	1.83	0.43
46:BA:956:U:H6	46:BA:956:U:H2'	1.57	0.43
52:BJ:140:TYR:HB3	52:BJ:143:LEU:HD12	2.01	0.43
53:BK:104:THR:HG21	53:BK:150:SER:C	2.39	0.43
56:BP:180:ASP:HB3	56:BP:204:MET:HB2	2.00	0.43
57:BQ:121:LEU:N	57:BQ:162:GLU:O	2.52	0.43
59:BS:145:VAL:HG22	59:BS:174:GLU:HB2	1.99	0.43
61:BU:29:ARG:HA	61:BU:29:ARG:HD3	1.72	0.43
65:BY:107:THR:HG22	65:BY:109:ILE:HG13	2.00	0.43
1:AA:561:U:H1'	1:AA:711:A:H62	1.83	0.43
1:AA:871:U:H3	1:AA:896:A:H61	1.66	0.43
2:AB:262:LYS:O	2:AB:266:VAL:HG23	2.19	0.43
6:AG:81:LYS:HB2	6:AG:81:LYS:HE3	1.75	0.43
9:AK:88:ALA:HB3	9:AK:151:VAL:HG23	2.00	0.43
37:B1:143:PHE:O	37:B1:147:LYS:N	2.47	0.43
39:B3:66:LEU:HA	39:B3:66:LEU:HD23	1.74	0.43
42:B6:37:LEU:HD21	42:B6:40:LYS:HE3	2.01	0.43
46:BA:1314:U:H2'	46:BA:1315:A:O4'	2.19	0.43
46:BA:1330:G:C2	46:BA:1401:U:O2	2.72	0.43
46:BA:431:A:H4'	46:BA:432:G:OP2	2.18	0.43
46:BA:656:U:H2'	46:BA:657:U:O4'	2.18	0.43
46:BA:737:U:H2'	46:BA:738:U:C6	2.54	0.43
46:BA:904:G:C2	46:BA:914:C:C2	3.06	0.43
49:BE:219:MET:O	49:BE:223:GLY:N	2.51	0.43
52:BJ:41:HIS:CD2	52:BJ:43:GLU:H	2.36	0.43
53:BK:111:LEU:HD12	53:BK:154:ARG:HB3	2.01	0.43
56:BP:210:LEU:HD23	56:BP:210:LEU:HA	1.81	0.43
57:BQ:118:MET:HE2	57:BQ:172:VAL:HG22	1.99	0.43
1:AA:898:A:H3'	1:AA:898:A:N3	2.33	0.43
6:AG:168:TYR:HB3	6:AG:236:LEU:HD13	2.00	0.43
7:AI:266:UNK:HG1	7:AI:268:MET:HE2	2.00	0.43
1:AA:102:G:H5'	14:AQ:75:LYS:HZ2	1.83	0.43
38:B2:95:LYS:NZ	65:BY:181:ASP:O	2.51	0.43
49:BE:56:GLU:O	49:BE:59:PRO:HD2	2.18	0.43
55:BO:42:ASP:HB3	55:BO:119:ILE:HG12	2.01	0.43
55:BO:58:ILE:HD12	55:BO:74:LEU:HG	2.01	0.43
60:BT:82:PRO:HA	60:BT:83:PRO:HD3	1.88	0.43
46:BA:642:G:O6	63:BW:81:SER:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:BY:188:VAL:HA	65:BY:189:PRO:HD3	1.85	0.43
2:AB:66:LEU:HD23	2:AB:133:HIS:HE1	1.84	0.43
7:AI:321:LEU:HB3	7:AI:323:ARG:HD2	1.99	0.43
5:AF:65:LEU:HD21	15:AR:76:LYS:HD3	2.01	0.43
16:AU:50:ARG:HD2	16:AU:50:ARG:HA	1.53	0.43
16:AU:50:ARG:HH11	16:AU:50:ARG:HG2	1.83	0.43
17:AV:43:Y5P:H2'	17:AV:44:Y5P:H6	2.01	0.43
17:AY:29:Y5P:H2'	17:AY:30:Y5P:O4'	2.19	0.43
37:B1:202:GLU:OE1	37:B1:214:LYS:NZ	2.34	0.43
37:B1:92:VAL:CG2	37:B1:98:SER:HB3	2.48	0.43
49:BE:203:TYR:CE1	49:BE:272:LYS:HB2	2.54	0.43
49:BE:58:VAL:HB	49:BE:59:PRO:HD3	2.00	0.43
51:BI:118:VAL:O	51:BI:122:ARG:HB2	2.19	0.43
52:BJ:65:LEU:HD22	52:BJ:66:PRO:HD2	2.01	0.43
54:BN:67:PHE:HB2	54:BN:72:TRP:NE1	2.34	0.43
58:BR:131:LEU:HA	58:BR:131:LEU:HD23	1.83	0.43
59:BS:39:VAL:HB	59:BS:42:GLU:HB2	2.01	0.43
59:BS:56:LEU:O	59:BS:60:ALA:N	2.51	0.43
59:BS:56:LEU:CB	59:BS:62:ALA:HB2	2.48	0.43
1:AA:203:G:H2'	1:AA:204:U:C6	2.53	0.42
2:AB:83:LEU:HB2	2:AB:117:LEU:HD13	2.00	0.42
4:AE:374:ARG:HB3	4:AE:377:CYS:HB2	2.00	0.42
6:AG:68:PHE:HB3	7:AI:367:GLN:HE21	1.84	0.42
37:B1:146:LEU:HA	37:B1:162:LYS:HE3	2.01	0.42
46:BA:1049:G:C2	46:BA:1050:A:C8	3.08	0.42
46:BA:366:A:O2'	46:BA:367:A:OP2	2.29	0.42
50:BF:217:LEU:HB2	50:BF:256:HIS:ND1	2.34	0.42
52:BJ:162:LYS:O	52:BJ:166:ARG:HB2	2.19	0.42
53:BK:124:LYS:NZ	53:BK:124:LYS:HB3	2.31	0.42
54:BN:173:PRO:HG2	54:BN:176:TYR:HB2	2.01	0.42
60:BT:145:LEU:HA	60:BT:145:LEU:HD12	1.85	0.42
61:BU:41:LEU:H	61:BU:41:LEU:HG	1.25	0.42
62:BV:91:ILE:CG2	62:BV:206:PRO:HA	2.49	0.42
1:AA:302:U:O5'	1:AA:302:U:H6	2.03	0.42
1:AA:30:A:C6	1:AA:31:U:C4	3.07	0.42
4:AE:289:THR:HG21	4:AE:308:GLN:H	1.84	0.42
5:AF:42:LEU:HB2	5:AF:63:TYR:HB3	2.01	0.42
8:AJ:157:LEU:HA	8:AJ:157:LEU:HD23	1.83	0.42
13:AP:110:LEU:O	13:AP:113:LYS:HG2	2.20	0.42
13:AP:114:ARG:HA	13:AP:114:ARG:HD2	1.79	0.42
13:AP:19:ILE:HG23	13:AP:51:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AV:43:Y5P:C4	17:AV:44:Y5P:H4	2.47	0.42
37:B1:72:PRO:O	37:B1:75:SER:HB3	2.19	0.42
38:B2:197:ASN:HA	38:B2:197:ASN:HD22	1.53	0.42
44:B8:113:ARG:HD2	56:BP:75:TYR:O	2.19	0.42
46:BA:1154:A:H2'	46:BA:1155:C:O4'	2.19	0.42
46:BA:194:G:H21	61:BU:44:ARG:NH2	2.17	0.42
46:BA:57:A:H8	46:BA:57:A:H5'	1.84	0.42
49:BE:128:HIS:CD2	49:BE:173:LYS:HZ2	2.37	0.42
51:BI:55:ILE:O	51:BI:83:VAL:HG22	2.20	0.42
58:BR:16:ARG:HH11	58:BR:47:ALA:HB1	1.84	0.42
59:BS:89:HIS:HA	59:BS:119:THR:CG2	2.49	0.42
61:BU:11:ARG:CZ	61:BU:13:ARG:HD2	2.49	0.42
64:BX:64:PRO:HG2	64:BX:103:GLN:NE2	2.32	0.42
1:AA:317:A:H2	1:AA:318:C:C5	2.37	0.42
1:AA:670:A:N7	92:AA:8087:HOH:O	2.37	0.42
2:AB:221:ILE:HA	2:AB:235:VAL:HG13	2.01	0.42
4:AE:243:VAL:HG11	4:AE:268:PHE:CE1	2.54	0.42
1:AA:811:U:C5'	8:AJ:131:ARG:NH1	2.82	0.42
10:AL:45:PRO:HA	10:AL:46:PRO:HD3	1.93	0.42
15:AR:87:PRO:HA	15:AR:126:LYS:HB2	2.01	0.42
38:B2:134:LEU:HD12	38:B2:134:LEU:HA	1.72	0.42
39:B3:81:TRP:CD1	39:B3:82:GLU:HG2	2.54	0.42
46:BA:1494:C:OP1	49:BE:213:LYS:HE2	2.19	0.42
46:BA:27:A:H2'	46:BA:28:A:C8	2.53	0.42
48:BD:86:ASN:ND2	48:BD:90:GLN:HB2	2.28	0.42
50:BF:66:ILE:HD13	50:BF:263:LEU:HD11	2.00	0.42
54:BN:24:LYS:HE2	54:BN:24:LYS:HB3	1.76	0.42
56:BP:156:VAL:O	56:BP:176:THR:HA	2.19	0.42
56:BP:184:LEU:O	56:BP:187:LEU:HB3	2.18	0.42
56:BP:118:LEU:HB3	56:BP:187:LEU:HD21	2.02	0.42
60:BT:209:GLN:HE21	60:BT:211:PHE:HA	1.84	0.42
1:AA:527:G:N2	1:AA:839:C:C2	2.88	0.42
1:AA:581:A:N7	1:AA:802:A:H2	2.17	0.42
1:AA:685:C:C3'	1:AA:686:A:H5'	2.48	0.42
4:AE:130:GLN:HE21	4:AE:176:ARG:HH22	1.68	0.42
4:AE:320:ILE:HG12	4:AE:349:LEU:HD22	2.01	0.42
8:AJ:122:LYS:HG3	8:AJ:132:VAL:HG22	2.02	0.42
37:B1:96:LYS:HG2	37:B1:96:LYS:O	2.20	0.42
38:B2:122:LYS:HB3	38:B2:122:LYS:NZ	2.35	0.42
45:B9:81:ARG:NH1	46:BA:1523:C:C5	2.88	0.42
45:B9:84:ARG:NH1	45:B9:99:GLN:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:129:A:H2'	46:BA:130:A:C8	2.54	0.42
46:BA:1519:U:H3'	46:BA:1520:A:H5'	2.01	0.42
46:BA:83:A:H4'	46:BA:84:G:O5'	2.18	0.42
50:BF:67:GLU:O	50:BF:190:VAL:HA	2.19	0.42
50:BF:243:VAL:HG22	50:BF:244:PRO:O	2.19	0.42
50:BF:67:GLU:HA	50:BF:75:GLU:O	2.19	0.42
54:BN:7:ALA:N	54:BN:8:PRO:HD2	2.34	0.42
58:BR:109:GLN:NE2	58:BR:120:LYS:HG3	2.35	0.42
61:BU:67:LEU:HD21	61:BU:71:ARG:NH1	2.34	0.42
1:AA:658:C:H2'	1:AA:659:A:O4'	2.19	0.42
1:AA:708:A:H5'	1:AA:709:A:OP1	2.19	0.42
2:AB:168:ARG:HH22	16:AU:87:CYS:C	2.23	0.42
4:AE:255:GLY:HA3	4:AE:278:TYR:O	2.19	0.42
6:AG:59:THR:HG22	6:AG:63:LYS:HE3	2.00	0.42
11:AN:102:ARG:HG3	11:AN:102:ARG:HH11	1.84	0.42
5:AF:92:ASN:CG	15:AR:118:LEU:HD22	2.40	0.42
42:B6:38:ARG:HG3	42:B6:39:GLU:N	2.34	0.42
46:BA:521:U:O2	46:BA:530:A:H5'	2.18	0.42
46:BA:570:A:C6	46:BA:571:A:C6	3.08	0.42
17:AY:54:Y5P:HB2	57:BQ:106:ARG:NH2	2.34	0.42
57:BQ:96:TYR:HE1	57:BQ:153:PRO:HG3	1.84	0.42
59:BS:137:LEU:HD11	59:BS:168:GLY:O	2.19	0.42
61:BU:16:ASP:OD1	61:BU:16:ASP:N	2.30	0.42
54:BN:46:VAL:HB	63:BW:206:ILE:HG23	2.02	0.42
1:AA:102:G:H5'	14:AQ:75:LYS:NZ	2.35	0.42
1:AA:937:A:H2'	1:AA:938:U:C6	2.54	0.42
2:AB:117:LEU:HA	2:AB:120:THR:HB	2.01	0.42
4:AE:193:TRP:CE3	4:AE:199:GLY:HA3	2.55	0.42
14:AQ:98:LYS:HD2	14:AQ:107:GLU:O	2.20	0.42
14:AQ:18:ILE:HA	14:AQ:18:ILE:HD13	1.93	0.42
17:AY:74:Y5P:H6	17:AY:74:Y5P:HB2	2.00	0.42
42:B6:19:LYS:HG3	42:B6:30:PHE:CE2	2.54	0.42
44:B8:119:SER:OG	44:B8:183:ARG:HD3	2.20	0.42
46:BA:1280:A:C6	46:BA:1315:A:C2	3.08	0.42
46:BA:1436:U:H2'	46:BA:1437:C:H6	1.84	0.42
46:BA:1455:A:O4'	46:BA:1457:U:H1'	2.20	0.42
46:BA:1482:C:C2	46:BA:1494:C:N4	2.87	0.42
46:BA:1556:U:H4'	58:BR:11:HIS:CG	2.55	0.42
46:BA:207:A:H2'	46:BA:208:A:O4'	2.20	0.42
46:BA:538:A:H2	53:BK:38:ILE:HG12	1.83	0.42
46:BA:58:C:O5'	46:BA:58:C:H6	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:686:A:C3'	46:BA:687:A:H4'	2.49	0.42
46:BA:998:A:H2'	46:BA:999:A:C8	2.53	0.42
47:BB:9:P5P:H5'2	47:BB:47:P5P:H1'	2.01	0.42
48:BD:83:GLY:O	48:BD:85:ARG:HG2	2.18	0.42
52:BJ:53:TYR:HB2	57:BQ:251:VAL:CG2	2.50	0.42
53:BK:33:PRO:HA	53:BK:37:PRO:HD2	2.02	0.42
54:BN:119:ARG:HD3	54:BN:119:ARG:HA	1.86	0.42
54:BN:40:GLN:OE1	54:BN:113:PRO:HD3	2.19	0.42
64:BX:63:VAL:HA	64:BX:64:PRO:HD3	1.70	0.42
1:AA:419:A:N6	1:AA:420:A:N1	2.68	0.42
4:AE:323:ILE:O	4:AE:327:ILE:HG13	2.20	0.42
13:AP:41:CYS:HB2	13:AP:42:PRO:HD2	2.02	0.42
7:AI:224:ARG:HG3	16:AU:85:GLN:HE22	1.83	0.42
17:AV:36:P5P:N1	18:AX:16:Y5P:N3	2.67	0.42
37:B1:81:GLY:O	37:B1:130:ARG:NH1	2.52	0.42
42:B6:42:THR:CG2	42:B6:55:LEU:HD13	2.48	0.42
43:B7:50:LYS:HB3	43:B7:50:LYS:HE2	1.89	0.42
44:B8:169:ARG:HD2	44:B8:170:ASN:H	1.84	0.42
45:B9:78:LEU:HD13	45:B9:87:ILE:CD1	2.48	0.42
46:BA:1506:A:H2	46:BA:1536:A:N7	2.16	0.42
46:BA:215:C:O2	46:BA:219:G:H5''	2.19	0.42
46:BA:826:G:C2	46:BA:839:A:C2	3.07	0.42
49:BE:221:ARG:NH1	49:BE:259:GLY:CA	2.82	0.42
50:BF:108:ARG:HG2	50:BF:161:TYR:CD1	2.54	0.42
50:BF:126:LYS:HG3	50:BF:127:PRO:HD2	2.01	0.42
61:BU:94:GLN:HE22	61:BU:146:VAL:N	2.18	0.42
61:BU:129:ALA:HB2	62:BV:68:ILE:HD12	2.01	0.42
64:BX:3:ARG:O	64:BX:4:ASN:HB2	2.19	0.42
1:AA:104:A:OP2	14:AQ:49:TYR:OH	2.30	0.42
1:AA:87:U:H2'	1:AA:88:C:C6	2.54	0.42
4:AE:287:ASP:O	4:AE:330:LYS:HE3	2.20	0.42
8:AJ:166:GLU:OE1	8:AJ:166:GLU:N	2.40	0.42
46:BA:1043:U:H1'	49:BE:257:MET:CE	2.50	0.42
46:BA:1236:A:H5'	46:BA:1237:A:OP2	2.20	0.42
46:BA:1069:U:H5	46:BA:1417:C:C2	2.37	0.42
46:BA:149:A:H2'	46:BA:150:A:C8	2.55	0.42
46:BA:324:G:C6	46:BA:325:U:N3	2.87	0.42
46:BA:330:A:H8	46:BA:330:A:H5''	1.85	0.42
46:BA:353:U:H2'	46:BA:354:G:C8	2.54	0.42
46:BA:570:A:H4'	46:BA:570:A:OP1	2.19	0.42
44:B8:98:SER:HB2	46:BA:76:G:O6	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:809:A:H1'	49:BE:230:THR:HG23	2.02	0.42
46:BA:96:U:C1'	46:BA:97:A:H5''	2.50	0.42
49:BE:122:LEU:HD13	49:BE:299:ILE:HD11	2.01	0.42
50:BF:199:ASP:HA	50:BF:200:PRO:HD2	1.94	0.42
51:BI:94:LEU:HB2	51:BI:116:LYS:HG2	2.01	0.42
53:BK:104:THR:HG21	53:BK:150:SER:HA	2.02	0.42
56:BP:11:ARG:CG	56:BP:11:ARG:NH1	2.76	0.42
57:BQ:214:THR:O	57:BQ:218:ILE:HG13	2.20	0.42
1:AA:636:U:P	2:AB:213:LYS:NZ	2.92	0.42
4:AE:254:ALA:O	4:AE:280:HIS:N	2.33	0.42
7:AI:127:HIS:CD2	7:AI:128:PRO:HD2	2.55	0.42
36:B0:76:HIS:HB2	36:B0:130:PHE:CD1	2.55	0.42
43:B7:74:ARG:HD3	43:B7:74:ARG:HA	1.71	0.42
46:BA:210:U:H2'	46:BA:211:C:C6	2.54	0.42
46:BA:265:C:H5''	46:BA:266:A:H5'	2.00	0.42
46:BA:68:A:N3	46:BA:69:C:H5'	2.35	0.42
46:BA:991:U:H2'	46:BA:992:A:C8	2.54	0.42
49:BE:80:LEU:O	49:BE:84:PRO:HG3	2.19	0.42
50:BF:108:ARG:HG2	50:BF:161:TYR:CE1	2.55	0.42
52:BJ:143:LEU:HD11	52:BJ:180:CYS:HB2	2.01	0.42
53:BK:87:VAL:HG12	53:BK:91:LEU:HD12	2.01	0.42
54:BN:28:PRO:HB3	54:BN:65:ILE:HD13	2.01	0.42
58:BR:134:LEU:HA	58:BR:134:LEU:HD12	1.83	0.42
46:BA:1555:C:H4'	60:BT:86:ARG:HH12	1.85	0.42
61:BU:39:TYR:O	61:BU:43:VAL:HG23	2.20	0.42
63:BW:101:LEU:HD23	63:BW:101:LEU:HA	1.82	0.42
1:AA:190:G:H21	1:AA:192:C:H41	1.67	0.42
1:AA:254:C:H4'	1:AA:261:A:C6	2.55	0.42
1:AA:454:A:H2'	1:AA:456:A:OP1	2.20	0.42
1:AA:460:A:H4'	1:AA:461:A:OP2	2.20	0.42
1:AA:650:A:N6	2:AB:176:THR:OG1	2.53	0.42
5:AF:22:LEU:O	5:AF:26:LEU:HG	2.19	0.42
7:AI:176:HIS:ND1	7:AI:233:PRO:HG2	2.34	0.42
17:AV:66:Y5P:H4A	17:AV:67:Y5P:N3	2.35	0.42
36:B0:64:GLY:N	36:B0:91:ALA:O	2.44	0.42
46:BA:1060:A:C2	46:BA:1062:G:C8	3.08	0.42
46:BA:1129:U:H2'	46:BA:1130:G:H8	1.85	0.42
46:BA:328:A:OP1	48:BD:274:GLY:N	2.53	0.42
46:BA:365:A:H2'	46:BA:365:A:N3	2.35	0.42
46:BA:528:A:O2'	46:BA:545:A:N6	2.53	0.42
47:BB:25:P5P:H5'1	47:BB:25:P5P:H8	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:BE:293:LYS:HB3	49:BE:293:LYS:HE2	1.78	0.42
49:BE:96:ARG:HH12	49:BE:301:ASP:CG	2.20	0.42
52:BJ:53:TYR:HB2	57:BQ:251:VAL:HG22	2.02	0.42
56:BP:184:LEU:HD12	56:BP:184:LEU:HA	1.80	0.42
58:BR:38:ARG:HG2	58:BR:39:HIS:CD2	2.55	0.42
65:BY:194:LEU:HD23	65:BY:195:GLU:OE2	2.20	0.42
65:BY:62:VAL:HB	65:BY:120:VAL:HG13	2.02	0.42
1:AA:305:A:H2'	1:AA:306:G:O4'	2.19	0.41
1:AA:462:A:C6	1:AA:463:U:C4	3.08	0.41
1:AA:4:C:C4	4:AE:427:ARG:HD3	2.55	0.41
6:AG:131:ALA:HA	6:AG:134:GLN:HB2	2.02	0.41
7:AI:127:HIS:CD2	7:AI:129:GLU:HG2	2.54	0.41
10:AL:115:THR:HG22	10:AL:117:ASP:H	1.84	0.41
15:AR:79:GLN:HG3	15:AR:133:ASP:OD2	2.18	0.41
17:AY:8:Y5P:N3	17:AY:14:Y5P:H4	2.35	0.41
41:B5:138:ARG:HA	41:B5:141:MET:HG2	2.01	0.41
43:B7:73:LEU:HD12	46:BA:31:A:H1'	2.02	0.41
44:B8:106:THR:OG1	44:B8:162:THR:HA	2.20	0.41
46:BA:389:A:H2'	46:BA:390:A:C8	2.56	0.41
55:BO:45:ALA:O	55:BO:49:THR:HG22	2.20	0.41
65:BY:81:ARG:HG2	65:BY:81:ARG:NH1	2.35	0.41
3:AC:58:ALA:HB3	3:AC:60:HIS:CE1	2.55	0.41
4:AE:244:LEU:HD12	4:AE:257:ALA:O	2.20	0.41
6:AG:163:LYS:HE3	18:AX:12:Y5P:HA1	2.02	0.41
7:AI:116:LEU:O	7:AI:122:ARG:NH1	2.53	0.41
15:AR:56:GLU:CD	15:AR:56:GLU:H	2.22	0.41
37:B1:128:THR:HG22	37:B1:129:MET:H	1.85	0.41
41:B5:177:ARG:CG	41:B5:177:ARG:HH11	2.32	0.41
44:B8:94:VAL:HB	44:B8:96:TYR:CE1	2.56	0.41
46:BA:1149:G:C2	46:BA:1150:G:C4	3.08	0.41
46:BA:1355:C:H3'	46:BA:1356:G:H5''	2.02	0.41
46:BA:715:A:H2'	46:BA:716:A:C8	2.55	0.41
47:BB:29:P5P:H2'	47:BB:30:P5P:C8	2.43	0.41
53:BK:103:HIS:HB3	53:BK:106:LYS:HD2	2.02	0.41
56:BP:176:THR:OG1	56:BP:219:ASN:O	2.38	0.41
57:BQ:194:THR:O	57:BQ:197:LYS:HB3	2.20	0.41
57:BQ:97:LEU:HD11	57:BQ:160:ILE:HD12	2.02	0.41
64:BX:16:GLN:NE2	64:BX:17:LEU:O	2.49	0.41
6:AG:155:VAL:H	6:AG:227:HIS:HE1	1.67	0.41
8:AJ:135:GLU:HB2	11:AN:126:ALA:HB2	2.03	0.41
10:AL:64:ARG:HG3	10:AL:66:PHE:CD2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AO:133:LEU:HD23	12:AO:133:LEU:HA	1.83	0.41
14:AQ:16:LYS:N	14:AQ:29:ARG:O	2.51	0.41
46:BA:1144:G:H1'	46:BA:1248:A:C2	2.55	0.41
46:BA:163:A:H4'	46:BA:164:A:O4'	2.20	0.41
46:BA:518:C:O2'	53:BK:103:HIS:HE1	2.03	0.41
50:BF:279:ARG:NH1	50:BF:282:PRO:HD3	2.34	0.41
58:BR:65:LEU:HD23	58:BR:65:LEU:HA	1.73	0.41
58:BR:91:GLN:O	58:BR:95:PRO:HG2	2.20	0.41
60:BT:288:ALA:HA	60:BT:291:ASN:HD22	1.85	0.41
62:BV:98:ARG:HD3	62:BV:113:THR:HG21	2.03	0.41
63:BW:104:LEU:HD11	63:BW:115:ILE:HG22	2.01	0.41
1:AA:162:C:H5''	1:AA:163:A:N7	2.36	0.41
5:AF:114:GLU:HG2	5:AF:117:LEU:HD21	2.01	0.41
17:AV:43:Y5P:H2'	17:AV:44:Y5P:C6	2.50	0.41
46:BA:1180:G:H4'	46:BA:1228:U:O2'	2.19	0.41
46:BA:442:G:N2	46:BA:445:C:H3'	2.35	0.41
46:BA:473:A:O2'	46:BA:474:C:P	2.78	0.41
46:BA:856:U:O2'	48:BD:67:LYS:NZ	2.53	0.41
52:BJ:89:VAL:O	52:BJ:93:ASN:ND2	2.53	0.41
53:BK:124:LYS:HZ2	53:BK:124:LYS:HB3	1.86	0.41
55:BO:138:LEU:HA	55:BO:138:LEU:HD12	1.78	0.41
56:BP:202:LYS:HZ1	56:BP:263:ARG:HH12	1.67	0.41
60:BT:68:UNK:O	60:BT:68:UNK:CG	2.68	0.41
61:BU:116:LEU:O	61:BU:119:LEU:HB3	2.20	0.41
62:BV:139:LEU:HD13	62:BV:148:LEU:CD2	2.49	0.41
62:BV:119:LEU:HD11	62:BV:194:GLN:HB3	2.01	0.41
1:AA:128:C:H2'	1:AA:129:G:O4'	2.20	0.41
1:AA:228:G:H2'	1:AA:229:U:O4'	2.21	0.41
1:AA:630:A:H2	1:AA:654:A:N6	2.19	0.41
1:AA:746:A:H2'	1:AA:747:C:O4'	2.20	0.41
1:AA:916:A:H2'	1:AA:917:C:C1'	2.51	0.41
7:AI:88:LEU:HD11	7:AI:107:ALA:HB1	2.02	0.41
10:AL:39:LEU:HD22	10:AL:39:LEU:HA	1.73	0.41
13:AP:20:ARG:HA	13:AP:87:VAL:HG21	2.02	0.41
15:AR:57:ASN:HA	15:AR:58:PRO:HD3	1.74	0.41
16:AU:59:THR:O	16:AU:63:ILE:HG13	2.20	0.41
17:AY:55:Y5P:C6	17:AY:57:Y5P:H5	2.44	0.41
37:B1:190:ARG:HG2	37:B1:190:ARG:H	1.69	0.41
37:B1:201:ALA:O	37:B1:204:VAL:HG12	2.21	0.41
38:B2:126:LEU:HA	38:B2:126:LEU:HD12	1.74	0.41
38:B2:221:ILE:HG13	38:B2:221:ILE:H	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:1081:C:H2'	46:BA:1082:C:C6	2.55	0.41
46:BA:1129:U:H2'	46:BA:1130:G:C8	2.56	0.41
46:BA:1312:U:HO2'	46:BA:1313:U:H6	1.65	0.41
46:BA:214:A:P	50:BF:92:ARG:HH22	2.43	0.41
46:BA:219:G:N3	46:BA:230:C:O2'	2.53	0.41
46:BA:870:A:H5''	46:BA:871:U:OP2	2.20	0.41
47:BB:33:Y5P:H2'	47:BB:34:Y5P:HA1	2.03	0.41
47:BB:65:Y5P:H2'	47:BB:66:P5P:C8	2.33	0.41
54:BN:112:LEU:HA	54:BN:112:LEU:HD23	1.76	0.41
55:BO:52:HIS:HD2	55:BO:53:ARG:HG3	1.86	0.41
56:BP:100:ARG:O	56:BP:103:TYR:HB3	2.21	0.41
56:BP:178:PHE:HB2	56:BP:214:TYR:CE2	2.55	0.41
58:BR:64:LYS:HE2	58:BR:97:PHE:O	2.21	0.41
59:BS:68:TRP:C	59:BS:70:THR:H	2.23	0.41
59:BS:74:SER:HB3	59:BS:147:HIS:HE1	1.85	0.41
60:BT:117:LEU:HD22	60:BT:176:VAL:HG22	2.02	0.41
61:BU:64:LEU:HD22	61:BU:64:LEU:HA	1.58	0.41
65:BY:159:PHE:CG	65:BY:160:PRO:HD2	2.56	0.41
1:AA:246:A:H2'	1:AA:247:G:O4'	2.21	0.41
1:AA:677:C:H2'	1:AA:678:G:O4'	2.21	0.41
1:AA:823:G:H5'	1:AA:824:G:OP2	2.21	0.41
7:AI:389:ARG:HD3	7:AI:389:ARG:HA	1.89	0.41
12:AO:68:PRO:HA	12:AO:69:PRO:HD3	1.80	0.41
16:AU:68:MET:O	16:AU:72:ILE:HG12	2.20	0.41
17:AV:53:Y5P:O5'	17:AV:53:Y5P:H6	2.19	0.41
17:AY:32:Y5P:H4A	17:AY:33:Y5P:C4	2.40	0.41
17:AY:62:Y5P:N3	17:AY:63:Y5P:H4	2.35	0.41
38:B2:72:ASP:HA	38:B2:73:PRO:HD3	1.95	0.41
46:BA:1452:C:H2'	46:BA:1453:C:O4'	2.21	0.41
46:BA:48:U:O2'	46:BA:49:A:H4'	2.20	0.41
46:BA:529:G:H1	46:BA:544:C:N4	2.13	0.41
46:BA:672:U:H6	46:BA:672:U:O5'	2.04	0.41
46:BA:680:G:H1	46:BA:695:C:H42	1.69	0.41
48:BD:82:SER:O	48:BD:82:SER:OG	2.34	0.41
56:BP:160:SER:O	56:BP:164:ILE:HG13	2.21	0.41
56:BP:56:GLU:HG2	56:BP:62:ARG:CA	2.49	0.41
1:AA:559:U:H3	1:AA:712:A:H61	1.68	0.41
1:AA:925:A:O2'	1:AA:946:A:H5'	2.21	0.41
6:AG:154:PRO:HG3	6:AG:186:TRP:CH2	2.56	0.41
7:AI:201:LEU:HB3	7:AI:205:GLU:HB2	2.03	0.41
8:AJ:179:GLN:HG3	8:AJ:180:LEU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AK:176:SER:HB2	16:AU:13:MET:HG2	2.02	0.41
12:AO:223:LYS:HB2	12:AO:223:LYS:HE3	1.81	0.41
12:AO:69:PRO:HA	12:AO:70:PRO:HD3	1.84	0.41
13:AP:59:ASN:OD1	13:AP:63:GLU:N	2.47	0.41
17:AY:61:Y5P:H4A	17:AY:62:Y5P:H4	2.02	0.41
37:B1:173:ASP:HB3	37:B1:175:GLN:HG2	2.01	0.41
37:B1:42:HIS:HE1	37:B1:84:GLY:H	1.68	0.41
37:B1:226:LEU:HB2	38:B2:158:LEU:HD12	2.02	0.41
46:BA:1021:U:H2'	46:BA:1022:G:C8	2.54	0.41
46:BA:288:U:O2'	46:BA:289:A:H5'	2.21	0.41
44:B8:103:LYS:NZ	46:BA:76:G:P	2.93	0.41
48:BD:128:ILE:HD11	48:BD:144:ALA:CB	2.50	0.41
54:BN:81:THR:HB	54:BN:83:TYR:CD2	2.52	0.41
46:BA:441:G:OP1	57:BQ:144:LYS:HE3	2.20	0.41
57:BQ:185:PHE:CD1	57:BQ:185:PHE:N	2.87	0.41
65:BY:133:VAL:CG1	65:BY:145:ARG:HB3	2.46	0.41
65:BY:212:LYS:NZ	65:BY:214:TYR:CE1	2.85	0.41
1:AA:124:A:H1'	1:AA:125:U:H5	1.84	0.41
1:AA:57:A:P	1:AA:203:G:H21	2.43	0.41
6:AG:153:GLU:HG3	6:AG:179:ARG:HB3	2.03	0.41
8:AJ:165:PRO:HB2	8:AJ:168:VAL:HG22	2.02	0.41
11:AN:71:ALA:O	11:AN:75:ILE:HG12	2.21	0.41
17:AV:53:Y5P:H2'	17:AV:54:Y5P:H6	2.01	0.41
17:AY:54:Y5P:H4A	17:AY:55:Y5P:C4	2.47	0.41
37:B1:37:THR:HA	37:B1:38:PRO:HD2	1.91	0.41
39:B3:148:ARG:NH2	39:B3:151:LEU:HD22	2.35	0.41
39:B3:89:LEU:HA	39:B3:89:LEU:HD23	1.79	0.41
46:BA:1159:G:H4'	46:BA:1227:A:H5'	2.02	0.41
46:BA:192:U:H2'	46:BA:193:G:H8	1.86	0.41
49:BE:104:LEU:HB2	49:BE:121:LEU:O	2.21	0.41
49:BE:243:ILE:H	49:BE:243:ILE:HG12	1.70	0.41
60:BT:103:ARG:NE	60:BT:108:ILE:HD12	2.36	0.41
60:BT:194:LEU:HA	60:BT:195:PRO:HD3	1.91	0.41
64:BX:144:VAL:HA	64:BX:145:PRO:HD3	1.79	0.41
64:BX:77:ASN:HD22	64:BX:77:ASN:HA	1.61	0.41
65:BY:73:GLN:NE2	65:BY:128:ARG:O	2.54	0.41
1:AA:805:G:H2'	1:AA:806:A:O4'	2.21	0.41
1:AA:942:G:N1	1:AA:945:A:OP2	2.54	0.41
2:AB:174:LEU:HA	2:AB:174:LEU:HD12	1.64	0.41
4:AE:198:TRP:O	4:AE:222:ILE:HB	2.21	0.41
4:AE:289:THR:HG22	4:AE:290:ILE:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AF:2:PRO:HB2	5:AF:96:HIS:CG	2.56	0.41
1:AA:687:A:O2'	11:AN:96:ARG:HB2	2.21	0.41
16:AU:25:THR:O	16:AU:29:ILE:HG12	2.21	0.41
17:AV:25:Y5P:H4A	17:AV:26:Y5P:H4	2.01	0.41
36:B0:120:LEU:HA	36:B0:121:PRO:HD2	1.87	0.41
38:B2:123:ARG:HH12	64:BX:30:ARG:CB	2.32	0.41
44:B8:116:ARG:HG3	44:B8:122:TRP:CE2	2.56	0.41
46:BA:1198:A:H2'	46:BA:1200:C:OP2	2.21	0.41
46:BA:251:G:C6	46:BA:320:A:C4	3.09	0.41
46:BA:356:U:C6	46:BA:356:U:H5''	2.55	0.41
46:BA:532:A:H2'	46:BA:533:G:O4'	2.21	0.41
46:BA:632:G:N3	46:BA:632:G:H2'	2.36	0.41
46:BA:658:C:O3'	58:BR:81:THR:HG21	2.21	0.41
46:BA:812:C:O2	46:BA:812:C:H5'	2.21	0.41
50:BF:220:ASP:OD1	50:BF:221:LEU:N	2.54	0.41
50:BF:263:LEU:N	50:BF:264:PRO:HD2	2.35	0.41
54:BN:116:LEU:HA	54:BN:116:LEU:HD23	1.66	0.41
58:BR:84:ASP:O	58:BR:87:PRO:HD2	2.21	0.41
60:BT:185:ASN:N	60:BT:185:ASN:OD1	2.54	0.41
60:BT:76:LEU:HB2	60:BT:283:TRP:HZ3	1.85	0.41
1:AA:102:G:P	14:AQ:75:LYS:HZ2	2.44	0.41
1:AA:190:G:H21	1:AA:192:C:N4	2.19	0.41
1:AA:345:U:O4	9:AK:122:ALA:HA	2.21	0.41
1:AA:387:C:H5''	5:AF:95:LYS:HG3	2.03	0.41
1:AA:873:A:O2'	1:AA:874:U:H5'	2.20	0.41
4:AE:255:GLY:N	4:AE:279:LEU:HD23	2.36	0.41
7:AI:397:ARG:HE	17:AV:33:Y5P:H5	1.86	0.41
36:B0:76:HIS:O	36:B0:130:PHE:HA	2.21	0.41
37:B1:16:LEU:O	37:B1:21:TYR:HB2	2.20	0.41
37:B1:43:TYR:HB3	37:B1:67:ILE:HD12	2.02	0.41
41:B5:131:ARG:HA	41:B5:131:ARG:HD2	1.85	0.41
46:BA:1293:G:O2'	46:BA:1299:A:N6	2.52	0.41
46:BA:1307:U:H2'	46:BA:1308:A:H8	1.86	0.41
46:BA:1015:U:O2'	46:BA:1438:U:H5'	2.20	0.41
46:BA:242:A:C4	46:BA:350:A:C2	3.08	0.41
46:BA:513:A:C8	46:BA:539:A:H4'	2.56	0.41
46:BA:750:U:C2'	46:BA:751:G:H5'	2.51	0.41
46:BA:774:C:O2'	46:BA:775:A:H8	2.04	0.41
46:BA:885:C:H5'	46:BA:886:A:OP2	2.21	0.41
47:BB:25:P5P:O5'	59:BS:86:THR:HG21	2.21	0.41
48:BD:288:ARG:HA	48:BD:289:PRO:HD2	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:BE:116:LYS:C	49:BE:117:HIS:HD1	2.24	0.41
49:BE:80:LEU:HA	49:BE:80:LEU:HD12	1.87	0.41
49:BE:98:GLY:HA3	49:BE:179:PHE:CE1	2.55	0.41
50:BF:205:GLU:HA	50:BF:208:ARG:HB2	2.03	0.41
53:BK:94:ALA:HB1	53:BK:116:HIS:CD2	2.56	0.41
55:BO:95:ARG:HA	55:BO:95:ARG:HH11	1.85	0.41
46:BA:658:C:C4'	58:BR:81:THR:HG21	2.47	0.41
61:BU:68:TRP:CZ2	61:BU:100:LYS:HB2	2.56	0.41
1:AA:308:A:OP2	1:AA:308:A:H8	2.03	0.41
1:AA:540:U:H1'	1:AA:541:C:H5	1.86	0.41
1:AA:679:U:H2'	1:AA:680:U:C6	2.56	0.41
4:AE:206:PRO:HA	4:AE:272:LYS:HD2	2.03	0.41
4:AE:270:LYS:O	4:AE:274:ARG:HB2	2.21	0.41
1:AA:475:A:P	5:AF:123:ARG:HH22	2.42	0.41
5:AF:58:HIS:CD2	5:AF:89:ILE:HD11	2.56	0.41
6:AG:223:LYS:O	6:AG:226:MET:HB3	2.20	0.41
1:AA:816:U:H5''	7:AI:339:SER:HB2	2.03	0.41
7:AI:71:VAL:HG12	7:AI:75:LYS:HE3	2.03	0.41
12:AO:96:LEU:HD13	12:AO:104:LYS:HG2	2.03	0.41
12:AO:67:ASP:O	12:AO:69:PRO:HD3	2.21	0.41
14:AQ:98:LYS:HE3	14:AQ:109:PRO:HG3	2.03	0.41
17:AV:21:Y5P:HC	17:AV:48:Y5P:H4	2.03	0.41
17:AY:8:Y5P:C4	17:AY:14:Y5P:H5	2.51	0.41
41:B5:178:GLU:N	41:B5:178:GLU:OE1	2.54	0.41
46:BA:1052:A:H5'	46:BA:1053:A:OP2	2.21	0.41
46:BA:1413:G:H2'	46:BA:1414:G:O4'	2.20	0.41
46:BA:1439:A:H2'	46:BA:1440:U:O4'	2.20	0.41
46:BA:438:A:H2'	46:BA:439:A:H5''	2.02	0.41
46:BA:470:U:C4	46:BA:471:U:C4	3.09	0.41
46:BA:750:U:O2'	46:BA:751:G:H5'	2.21	0.41
48:BD:73:THR:HG22	48:BD:75:MET:N	2.33	0.41
49:BE:95:SER:OG	49:BE:181:VAL:HA	2.20	0.41
49:BE:82:ASP:O	49:BE:83:GLU:HG3	2.20	0.41
53:BK:124:LYS:HE3	53:BK:124:LYS:HB3	1.81	0.41
53:BK:104:THR:HG23	53:BK:152:GLY:HA2	2.03	0.41
56:BP:247:ILE:H	56:BP:247:ILE:CD1	2.34	0.41
62:BV:63:PRO:HA	62:BV:64:PRO:HD3	1.76	0.41
64:BX:105:PHE:CG	64:BX:106:THR:N	2.89	0.41
1:AA:365:A:H1'	1:AA:417:C:N3	2.36	0.40
1:AA:434:A:H2'	1:AA:435:C:H6	1.86	0.40
2:AB:115:ILE:H	2:AB:115:ILE:HG12	1.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:71:PHE:HE2	2:AB:262:LYS:HG2	1.85	0.40
4:AE:140:LEU:HB3	4:AE:146:ILE:HD13	2.03	0.40
5:AF:42:LEU:HD12	5:AF:63:TYR:HB3	2.03	0.40
7:AI:276:LYS:CE	7:AI:281:LYS:HE2	2.51	0.40
7:AI:358:THR:HG23	7:AI:360:ASP:H	1.86	0.40
8:AJ:181:PRO:O	8:AJ:184:ILE:HG22	2.22	0.40
1:AA:358:U:OP1	9:AK:154:LYS:HD3	2.21	0.40
17:AY:31:Y5P:H4A	17:AY:32:Y5P:C4	2.48	0.40
45:B9:88:TYR:CE1	45:B9:96:LYS:HE2	2.56	0.40
46:BA:1130:G:C6	46:BA:1131:G:C5	3.08	0.40
46:BA:1393:A:H8	46:BA:1393:A:OP2	2.04	0.40
46:BA:1423:A:H4'	46:BA:1424:G:H5'	2.04	0.40
46:BA:270:U:H5'	46:BA:271:A:OP2	2.21	0.40
46:BA:568:A:H2'	46:BA:569:A:C8	2.57	0.40
46:BA:570:A:N6	46:BA:571:A:C6	2.89	0.40
46:BA:598:C:O2'	46:BA:599:C:H5'	2.21	0.40
46:BA:801:A:N6	46:BA:809:A:H61	2.20	0.40
46:BA:805:C:N4	46:BA:806:G:C6	2.89	0.40
47:BB:43:Y5P:C2'	47:BB:44:Y5P:HA1	2.50	0.40
48:BD:188:LEU:HA	48:BD:188:LEU:HD23	1.79	0.40
41:B5:185:PHE:CE2	58:BR:132:PRO:HA	2.56	0.40
58:BR:150:LEU:HD23	58:BR:150:LEU:HA	1.70	0.40
58:BR:153:LEU:HD23	58:BR:153:LEU:HA	1.86	0.40
59:BS:78:TRP:N	59:BS:174:GLU:OE1	2.43	0.40
60:BT:74:ARG:HD3	60:BT:283:TRP:CE2	2.56	0.40
62:BV:147:LEU:HA	62:BV:147:LEU:HD23	1.76	0.40
46:BA:297:A:O4'	63:BW:159:ARG:HA	2.21	0.40
1:AA:586:U:H4'	11:AN:88:ARG:HG2	2.03	0.40
4:AE:261:ALA:HB2	4:AE:270:LYS:HZ2	1.86	0.40
6:AG:170:VAL:HA	6:AG:171:PRO:HD3	1.93	0.40
7:AI:100:THR:O	7:AI:104:ILE:HG13	2.22	0.40
8:AJ:122:LYS:HA	8:AJ:132:VAL:HG23	2.03	0.40
11:AN:67:LEU:HD23	11:AN:67:LEU:HA	1.91	0.40
12:AO:126:LEU:HB2	12:AO:171:LEU:HD21	2.02	0.40
9:AK:177:ILE:HD11	16:AU:19:VAL:HG13	2.03	0.40
36:B0:102:GLU:HB2	36:B0:130:PHE:CD2	2.56	0.40
36:B0:56:MET:N	36:B0:59:HIS:HD2	2.18	0.40
37:B1:139:CYS:SG	51:BI:133:SER:HB2	2.61	0.40
41:B5:87:ILE:HD13	41:B5:91:ARG:HG3	2.03	0.40
42:B6:36:ARG:NH1	46:BA:1184:U:P	2.94	0.40
44:B8:175:ASP:HB3	44:B8:178:GLN:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:1157:U:C6	46:BA:1249:C:C5	3.08	0.40
46:BA:1308:A:H2'	46:BA:1309:G:O4'	2.21	0.40
39:B3:35:LYS:N	46:BA:437:A:HO2'	2.19	0.40
46:BA:494:C:C4	46:BA:554:A:C2	3.09	0.40
51:BI:118:VAL:HG13	51:BI:122:ARG:HD3	2.02	0.40
56:BP:233:ARG:HG2	56:BP:234:LEU:N	2.35	0.40
62:BV:139:LEU:HD13	62:BV:148:LEU:HG	2.02	0.40
63:BW:58:PRO:HA	63:BW:59:PRO:HD3	1.93	0.40
64:BX:15:PRO:HA	65:BY:208:ARG:HH11	1.86	0.40
3:AC:72:HIS:CD2	3:AC:74:GLY:H	2.35	0.40
4:AE:261:ALA:HB2	4:AE:270:LYS:HZ1	1.87	0.40
8:AJ:104:ILE:O	8:AJ:105:SER:OG	2.39	0.40
9:AK:85:ILE:O	9:AK:150:ARG:NE	2.54	0.40
17:AY:11:Y5P:H6	17:AY:11:Y5P:O5'	2.21	0.40
46:BA:367:A:N3	46:BA:367:A:H2'	2.36	0.40
47:BB:13:Y5P:H4	47:BB:24:P5P:C2	2.51	0.40
48:BD:76:PRO:HB2	48:BD:103:ARG:HD2	2.02	0.40
49:BE:131:LYS:H	49:BE:146:THR:HB	1.87	0.40
49:BE:314:LEU:HA	49:BE:314:LEU:HD23	1.77	0.40
50:BF:65:TRP:CE3	50:BF:76:ARG:HB2	2.57	0.40
54:BN:102:ALA:O	54:BN:106:LEU:HG	2.20	0.40
55:BO:128:ARG:HH22	60:BT:126:ALA:HB2	1.86	0.40
59:BS:64:LYS:HD3	59:BS:76:GLU:HG3	2.02	0.40
59:BS:85:ARG:HB3	59:BS:120:ARG:HH12	1.86	0.40
61:BU:11:ARG:HH12	61:BU:13:ARG:HH11	1.70	0.40
46:BA:139:A:OP2	65:BY:94:HIS:NE2	2.55	0.40
1:AA:210:U:O4	1:AA:211:A:N6	2.54	0.40
1:AA:432:A:O2'	1:AA:434:A:N7	2.47	0.40
1:AA:527:G:C6	1:AA:528:C:C4	3.09	0.40
7:AI:395:LYS:HE3	7:AI:395:LYS:HB3	1.95	0.40
9:AK:91:LYS:O	9:AK:97:THR:HA	2.21	0.40
10:AL:96:PRO:HD3	10:AL:124:THR:HG23	2.04	0.40
17:AV:27:Y5P:C4	17:AV:28:Y5P:H4	2.52	0.40
17:AV:63:Y5P:H2'	17:AV:64:Y5P:C6	2.51	0.40
37:B1:16:LEU:HD12	37:B1:21:TYR:CD2	2.56	0.40
38:B2:204:MET:CE	38:B2:205:PRO:HD2	2.52	0.40
41:B5:101:ILE:HD11	63:BW:87:TYR:HB3	2.02	0.40
45:B9:71:LYS:HE2	45:B9:77:TYR:HA	2.03	0.40
46:BA:242:A:C5	46:BA:350:A:C2	3.08	0.40
46:BA:993:C:H2'	46:BA:994:U:C6	2.56	0.40
49:BE:177:LYS:HB3	49:BE:298:LYS:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:BJ:90:PHE:CD1	52:BJ:96:ILE:HD13	2.57	0.40
56:BP:28:LYS:HE3	56:BP:29:PRO:O	2.21	0.40
46:BA:428:G:C5'	56:BP:57:ARG:HD2	2.52	0.40
58:BR:134:LEU:O	58:BR:136:LEU:N	2.55	0.40
63:BW:150:TYR:HB3	63:BW:166:GLU:HG2	2.03	0.40
63:BW:194:ALA:O	63:BW:198:ILE:HG12	2.21	0.40
1:AA:39:A:N6	1:AA:40:A:C6	2.90	0.40
1:AA:938:U:H2'	1:AA:939:A:H8	1.86	0.40
1:AA:95:A:H2'	1:AA:96:U:C6	2.57	0.40
4:AE:282:ILE:HG21	4:AE:353:LEU:HD13	2.03	0.40
6:AG:121:LYS:NZ	6:AG:210:LEU:HD12	2.37	0.40
8:AJ:81:LYS:HG2	8:AJ:140:TYR:CE1	2.57	0.40
9:AK:113:SER:HB3	9:AK:116:THR:OG1	2.21	0.40
1:AA:763:A:H4'	11:AN:75:ILE:HD12	2.03	0.40
15:AR:75:TYR:CE1	15:AR:114:ARG:HD3	2.56	0.40
17:AV:13:Y5P:OP2	17:AV:13:Y5P:H6	2.22	0.40
17:AV:2:Y5P:H4A	17:AV:3:Y5P:H4	2.04	0.40
17:AY:8:Y5P:H4	17:AY:14:Y5P:H5	2.03	0.40
37:B1:148:THR:HG23	37:B1:152:ASP:HB3	2.03	0.40
38:B2:112:ASN:ND2	64:BX:26:ILE:HB	2.36	0.40
44:B8:113:ARG:HG3	44:B8:114:PHE:CE1	2.57	0.40
46:BA:376:G:N1	46:BA:377:U:C2	2.90	0.40
46:BA:876:G:C6	46:BA:877:C:C4	3.10	0.40
48:BD:185:LEU:HD22	48:BD:217:LEU:HD22	2.04	0.40
46:BA:857:A:OP2	48:BD:66:TRP:HZ2	2.05	0.40
49:BE:201:GLY:O	49:BE:202:GLN:HB2	2.20	0.40
46:BA:1400:C:H4'	49:BE:236:THR:OG1	2.20	0.40
52:BJ:67:PRO:HA	52:BJ:68:PRO:HD3	1.89	0.40
54:BN:145:LEU:HA	54:BN:146:PRO:HD3	1.91	0.40
55:BO:95:ARG:O	55:BO:96:MET:HB2	2.21	0.40
60:BT:268:ASP:O	60:BT:270:MET:N	2.54	0.40
63:BW:51:LYS:HB3	63:BW:51:LYS:HE2	1.83	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	
2	AB	218/220 (99%)	212 (97%)	6 (3%)	0	100	100
3	AC	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
4	AE	324/328 (99%)	305 (94%)	18 (6%)	1 (0%)	46	83
5	AF	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
6	AG	206/208 (99%)	203 (98%)	3 (2%)	0	100	100
7	AI	291/311 (94%)	283 (97%)	8 (3%)	0	100	100
8	AJ	127/201 (63%)	119 (94%)	6 (5%)	2 (2%)	12	58
9	AK	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
10	AL	107/109 (98%)	101 (94%)	6 (6%)	0	100	100
11	AN	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
12	AO	173/239 (72%)	166 (96%)	7 (4%)	0	100	100
13	AP	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
14	AQ	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
15	AR	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
16	AU	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
19	Aa	243/356 (68%)	238 (98%)	4 (2%)	1 (0%)	39	80
20	Ab	133/190 (70%)	127 (96%)	6 (4%)	0	100	100
21	Ac	167/169 (99%)	157 (94%)	9 (5%)	1 (1%)	30	74
22	Ad	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
24	Af	97/188 (52%)	90 (93%)	7 (7%)	0	100	100
25	Ag	327/397 (82%)	317 (97%)	10 (3%)	0	100	100
26	Ah	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
27	Ai	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
28	Aj	204/218 (94%)	194 (95%)	10 (5%)	0	100	100
29	Ak	273/275 (99%)	265 (97%)	7 (3%)	1 (0%)	39	80
30	Am	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
31	An	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
32	Ao	87/530 (16%)	83 (95%)	4 (5%)	0	100	100
33	Ap	186/188 (99%)	175 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	B0	112/148 (76%)	109 (97%)	3 (3%)	0	100	100
37	B1	242/256 (94%)	237 (98%)	5 (2%)	0	100	100
38	B2	176/252 (70%)	167 (95%)	9 (5%)	0	100	100
39	B3	116/161 (72%)	112 (97%)	4 (3%)	0	100	100
40	B4	43/126 (34%)	40 (93%)	3 (7%)	0	100	100
41	B5	108/188 (57%)	107 (99%)	1 (1%)	0	100	100
42	B6	46/65 (71%)	45 (98%)	1 (2%)	0	100	100
43	B7	44/95 (46%)	44 (100%)	0	0	100	100
44	B8	93/188 (50%)	90 (97%)	3 (3%)	0	100	100
45	B9	36/100 (36%)	36 (100%)	0	0	100	100
48	BD	238/306 (78%)	228 (96%)	10 (4%)	0	100	100
49	BE	305/348 (88%)	278 (91%)	24 (8%)	3 (1%)	19	66
50	BF	248/294 (84%)	232 (94%)	16 (6%)	0	100	100
51	BI	96/268 (36%)	91 (95%)	5 (5%)	0	100	100
52	BJ	166/262 (63%)	158 (95%)	8 (5%)	0	100	100
53	BK	140/192 (73%)	134 (96%)	6 (4%)	0	100	100
54	BN	175/178 (98%)	170 (97%)	5 (3%)	0	100	100
55	BO	113/145 (78%)	108 (96%)	5 (4%)	0	100	100
56	BP	286/296 (97%)	273 (96%)	13 (4%)	0	100	100
57	BQ	219/251 (87%)	218 (100%)	1 (0%)	0	100	100
58	BR	151/169 (89%)	145 (96%)	6 (4%)	0	100	100
59	BS	141/180 (78%)	128 (91%)	12 (8%)	1 (1%)	26	72
60	BT	223/292 (76%)	216 (97%)	7 (3%)	0	100	100
61	BU	138/149 (93%)	132 (96%)	6 (4%)	0	100	100
62	BV	153/209 (73%)	146 (95%)	7 (5%)	0	100	100
63	BW	164/210 (78%)	159 (97%)	5 (3%)	0	100	100
64	BX	130/150 (87%)	126 (97%)	4 (3%)	0	100	100
65	BY	202/216 (94%)	190 (94%)	12 (6%)	0	100	100
66	Ba	391/423 (92%)	374 (96%)	17 (4%)	0	100	100
67	Bb	352/380 (93%)	330 (94%)	21 (6%)	1 (0%)	46	83
68	Bc	293/334 (88%)	281 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	Bd	97/206 (47%)	92 (95%)	5 (5%)	0	100	100
70	Be	119/135 (88%)	115 (97%)	4 (3%)	0	100	100
71	Bf	82/142 (58%)	81 (99%)	1 (1%)	0	100	100
72	Bg	146/159 (92%)	138 (94%)	8 (6%)	0	100	100
73	Bh	287/332 (86%)	269 (94%)	18 (6%)	0	100	100
74	Bi	240/312 (77%)	227 (95%)	12 (5%)	1 (0%)	39	80
75	Bj	211/279 (76%)	198 (94%)	12 (6%)	1 (0%)	34	77
76	Bk	132/212 (62%)	125 (95%)	7 (5%)	0	100	100
77	Bl	131/166 (79%)	130 (99%)	1 (1%)	0	100	100
78	Bm	107/159 (67%)	102 (95%)	5 (5%)	0	100	100
79	Bn	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
80	Bo	92/124 (74%)	88 (96%)	4 (4%)	0	100	100
81	Bp	95/112 (85%)	90 (95%)	5 (5%)	0	100	100
82	Bq	35/138 (25%)	34 (97%)	1 (3%)	0	100	100
83	Bt	92/102 (90%)	89 (97%)	3 (3%)	0	100	100
84	Bu	137/205 (67%)	129 (94%)	8 (6%)	0	100	100
85	Bv	118/222 (53%)	116 (98%)	2 (2%)	0	100	100
86	Bw	385/433 (89%)	359 (93%)	25 (6%)	1 (0%)	46	83
87	Bx	160/196 (82%)	154 (96%)	5 (3%)	1 (1%)	30	74
All	All	12706/16216 (78%)	12149 (96%)	542 (4%)	15 (0%)	59	90

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
49	BE	264	ILE
86	Bw	159	VAL
87	Bx	93	ILE
8	AJ	179	GLN
8	AJ	185	ARG
49	BE	202	GLN
19	Aa	281	ASP
49	BE	317	PRO
74	Bi	174	TRP
29	Ak	213	ARG
75	Bj	84	TYR

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Mol	Chain	Res	Type
67	Bb	330	VAL
4	AE	154	VAL
21	Ac	105	ILE
59	BS	45	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	187/187 (100%)	168 (90%)	19 (10%)	9	43
3	AC	115/115 (100%)	101 (88%)	14 (12%)	6	34
4	AE	273/273 (100%)	245 (90%)	28 (10%)	9	42
5	AF	108/109 (99%)	99 (92%)	9 (8%)	14	52
6	AG	181/181 (100%)	169 (93%)	12 (7%)	21	62
7	AI	250/250 (100%)	236 (94%)	14 (6%)	26	67
8	AJ	119/181 (66%)	107 (90%)	12 (10%)	9	43
9	AK	102/102 (100%)	89 (87%)	13 (13%)	5	32
10	AL	92/92 (100%)	82 (89%)	10 (11%)	8	40
11	AN	92/114 (81%)	79 (86%)	13 (14%)	4	29
12	AO	159/205 (78%)	155 (98%)	4 (2%)	55	83
13	AP	97/97 (100%)	93 (96%)	4 (4%)	37	74
14	AQ	94/94 (100%)	87 (93%)	7 (7%)	17	57
15	AR	89/89 (100%)	83 (93%)	6 (7%)	20	62
16	AU	77/77 (100%)	65 (84%)	12 (16%)	3	24
19	Aa	222/272 (82%)	207 (93%)	15 (7%)	20	61
20	Ab	113/162 (70%)	106 (94%)	7 (6%)	23	64
21	Ac	152/152 (100%)	138 (91%)	14 (9%)	11	48
22	Ad	149/149 (100%)	142 (95%)	7 (5%)	32	72
24	Af	86/160 (54%)	80 (93%)	6 (7%)	19	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	Ag	290/334 (87%)	268 (92%)	22 (8%)	16	56
26	Ah	95/95 (100%)	93 (98%)	2 (2%)	61	86
27	Ai	86/86 (100%)	80 (93%)	6 (7%)	19	60
28	Aj	182/184 (99%)	171 (94%)	11 (6%)	24	65
29	Ak	249/249 (100%)	227 (91%)	22 (9%)	12	50
30	Am	100/100 (100%)	90 (90%)	10 (10%)	9	43
31	An	66/66 (100%)	57 (86%)	9 (14%)	5	30
32	Ao	79/118 (67%)	74 (94%)	5 (6%)	22	63
33	Ap	168/168 (100%)	152 (90%)	16 (10%)	11	46
36	B0	92/115 (80%)	83 (90%)	9 (10%)	10	44
37	B1	219/229 (96%)	195 (89%)	24 (11%)	8	39
38	B2	164/228 (72%)	143 (87%)	21 (13%)	5	32
39	B3	110/147 (75%)	101 (92%)	9 (8%)	14	53
40	B4	42/114 (37%)	39 (93%)	3 (7%)	18	59
41	B5	99/163 (61%)	89 (90%)	10 (10%)	9	43
42	B6	45/60 (75%)	37 (82%)	8 (18%)	2	17
43	B7	41/78 (53%)	36 (88%)	5 (12%)	6	34
44	B8	87/162 (54%)	77 (88%)	10 (12%)	7	37
45	B9	36/77 (47%)	32 (89%)	4 (11%)	8	39
48	BD	193/248 (78%)	161 (83%)	32 (17%)	3	20
49	BE	263/290 (91%)	239 (91%)	24 (9%)	12	48
50	BF	217/251 (86%)	191 (88%)	26 (12%)	6	34
51	BI	88/228 (39%)	85 (97%)	3 (3%)	44	79
52	BJ	154/230 (67%)	142 (92%)	12 (8%)	16	55
53	BK	115/151 (76%)	109 (95%)	6 (5%)	29	69
54	BN	156/157 (99%)	138 (88%)	18 (12%)	7	37
55	BO	99/123 (80%)	88 (89%)	11 (11%)	8	39
56	BP	245/249 (98%)	208 (85%)	37 (15%)	3	25
57	BQ	189/210 (90%)	170 (90%)	19 (10%)	9	43
58	BR	132/143 (92%)	114 (86%)	18 (14%)	5	30
59	BS	123/153 (80%)	114 (93%)	9 (7%)	17	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
60	BT	206/243 (85%)	187 (91%)	19 (9%)	11	48
61	BU	118/127 (93%)	109 (92%)	9 (8%)	16	56
62	BV	136/178 (76%)	121 (89%)	15 (11%)	8	39
63	BW	144/180 (80%)	125 (87%)	19 (13%)	5	31
64	BX	119/134 (89%)	102 (86%)	17 (14%)	4	28
65	BY	183/192 (95%)	159 (87%)	24 (13%)	5	31
66	Ba	348/365 (95%)	310 (89%)	38 (11%)	8	40
67	Bb	310/328 (94%)	283 (91%)	27 (9%)	13	50
68	Bc	271/299 (91%)	253 (93%)	18 (7%)	21	62
69	Bd	92/181 (51%)	86 (94%)	6 (6%)	21	62
70	Be	100/108 (93%)	89 (89%)	11 (11%)	8	39
71	Bf	80/110 (73%)	70 (88%)	10 (12%)	6	33
72	Bg	128/136 (94%)	111 (87%)	17 (13%)	5	31
73	Bh	251/284 (88%)	226 (90%)	25 (10%)	9	43
74	Bi	218/281 (78%)	204 (94%)	14 (6%)	22	63
75	Bj	190/242 (78%)	176 (93%)	14 (7%)	17	57
76	Bk	119/181 (66%)	111 (93%)	8 (7%)	20	62
77	Bl	122/147 (83%)	104 (85%)	18 (15%)	4	26
78	Bm	103/145 (71%)	97 (94%)	6 (6%)	25	66
79	Bn	88/113 (78%)	77 (88%)	11 (12%)	6	33
80	Bo	74/97 (76%)	65 (88%)	9 (12%)	6	34
81	Bp	79/88 (90%)	74 (94%)	5 (6%)	22	63
82	Bq	36/114 (32%)	34 (94%)	2 (6%)	26	67
83	Bt	75/82 (92%)	62 (83%)	13 (17%)	2	18
84	Bu	126/169 (75%)	119 (94%)	7 (6%)	26	67
85	Bv	102/173 (59%)	96 (94%)	6 (6%)	24	66
86	Bw	340/373 (91%)	296 (87%)	44 (13%)	5	32
87	Bx	149/173 (86%)	135 (91%)	14 (9%)	11	47
All	All	11288/13510 (84%)	10215 (90%)	1073 (10%)	15	46

All (1073) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	57	LEU
2	AB	79	SER
2	AB	133	HIS
2	AB	144	VAL
2	AB	147	HIS
2	AB	149	GLN
2	AB	153	LEU
2	AB	159	ARG
2	AB	168	ARG
2	AB	176	THR
2	AB	177	ASN
2	AB	180	LEU
2	AB	181	LEU
2	AB	195	LEU
2	AB	197	THR
2	AB	206	VAL
2	AB	235	VAL
2	AB	247	LEU
2	AB	250	ARG
3	AC	38	ARG
3	AC	41	ARG
3	AC	44	VAL
3	AC	71	LEU
3	AC	77	ASP
3	AC	89	ASP
3	AC	112	ARG
3	AC	115	ASN
3	AC	116	GLN
3	AC	117	LEU
3	AC	125	ARG
3	AC	127	LEU
3	AC	132	PHE
3	AC	152	HIS
4	AE	91	THR
4	AE	96	ASP
4	AE	105	GLU
4	AE	131	ILE
4	AE	132	ILE
4	AE	156	THR
4	AE	165	GLN
4	AE	215	TYR
4	AE	220	THR
4	AE	228	VAL

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Mol	Chain	Res	Type
4	AE	234	LYS
4	AE	239	ARG
4	AE	242	ARG
4	AE	243	VAL
4	AE	245	VAL
4	AE	266	ASP
4	AE	274	ARG
4	AE	276	VAL
4	AE	288	HIS
4	AE	289	THR
4	AE	293	ASP
4	AE	305	MET
4	AE	314	LEU
4	AE	340	VAL
4	AE	341	ASN
4	AE	370	VAL
4	AE	419	ARG
4	AE	420	SER
5	AF	17	GLU
5	AF	39	LEU
5	AF	45	ARG
5	AF	65	LEU
5	AF	86	ILE
5	AF	89	ILE
5	AF	105	CYS
5	AF	120	THR
5	AF	123	ARG
6	AG	46	ILE
6	AG	57	GLU
6	AG	67	ASP
6	AG	85	VAL
6	AG	98	MET
6	AG	109	SER
6	AG	139	ARG
6	AG	197	ARG
6	AG	200	LEU
6	AG	205	LEU
6	AG	219	VAL
6	AG	224	HIS
7	AI	99	PHE
7	AI	100	THR
7	AI	202	ILE

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Mol	Chain	Res	Type
7	AI	206	LEU
7	AI	212	GLU
7	AI	217	GLN
7	AI	229	LEU
7	AI	234	CYS
7	AI	237	THR
7	AI	294	ILE
7	AI	308	THR
7	AI	310	ASP
7	AI	338	ARG
7	AI	357	VAL
8	AJ	72	LEU
8	AJ	80	VAL
8	AJ	92	GLU
8	AJ	121	LEU
8	AJ	123	SER
8	AJ	126	ILE
8	AJ	136	MET
8	AJ	143	LEU
8	AJ	145	LEU
8	AJ	148	LEU
8	AJ	149	THR
8	AJ	166	GLU
9	AK	65	TYR
9	AK	87	ILE
9	AK	128	ILE
9	AK	149	VAL
9	AK	151	VAL
9	AK	152	VAL
9	AK	153	VAL
9	AK	160	ARG
9	AK	161	LEU
9	AK	164	ILE
9	AK	175	ILE
9	AK	178	THR
9	AK	194	ARG
10	AL	32	THR
10	AL	39	LEU
10	AL	52	THR
10	AL	55	ARG
10	AL	61	VAL
10	AL	64	ARG

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Mol	Chain	Res	Type
10	AL	81	CYS
10	AL	103	GLN
10	AL	110	VAL
10	AL	114	ARG
11	AN	28	TYR
11	AN	35	LEU
11	AN	57	LEU
11	AN	58	ARG
11	AN	75	ILE
11	AN	81	ASP
11	AN	93	MET
11	AN	101	LYS
11	AN	102	ARG
11	AN	108	ARG
11	AN	109	ILE
11	AN	123	VAL
11	AN	125	ARG
12	AO	80	VAL
12	AO	181	LYS
12	AO	198	ARG
12	AO	210	LEU
13	AP	10	ARG
13	AP	44	ASP
13	AP	97	TYR
13	AP	110	LEU
14	AQ	13	VAL
14	AQ	55	LEU
14	AQ	57	GLN
14	AQ	59	THR
14	AQ	74	THR
14	AQ	90	GLN
14	AQ	96	THR
15	AR	55	MET
15	AR	56	GLU
15	AR	69	CYS
15	AR	91	CYS
15	AR	117	ILE
15	AR	142	ARG
16	AU	27	ASN
16	AU	32	MET
16	AU	33	ASP
16	AU	47	LYS

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Mol	Chain	Res	Type
16	AU	49	CYS
16	AU	50	ARG
16	AU	52	ARG
16	AU	61	ARG
16	AU	68	MET
16	AU	77	ARG
16	AU	80	ARG
16	AU	82	ASP
19	Aa	103	LYS
19	Aa	124	ARG
19	Aa	160	ILE
19	Aa	174	ARG
19	Aa	175	GLU
19	Aa	181	ARG
19	Aa	204	LEU
19	Aa	205	THR
19	Aa	221	ASP
19	Aa	226	VAL
19	Aa	259	ASP
19	Aa	262	ARG
19	Aa	272	TRP
19	Aa	286	ASP
19	Aa	306	LEU
20	Ab	6	LEU
20	Ab	30	LEU
20	Ab	62	ASP
20	Ab	67	GLU
20	Ab	95	THR
20	Ab	109	LEU
20	Ab	112	THR
21	Ac	3	MET
21	Ac	9	ILE
21	Ac	13	LEU
21	Ac	23	PHE
21	Ac	25	ASP
21	Ac	31	THR
21	Ac	52	ILE
21	Ac	63	GLN
21	Ac	84	GLU
21	Ac	106	LEU
21	Ac	137	ARG
21	Ac	141	CYS

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Mol	Chain	Res	Type
21	Ac	142	GLU
21	Ac	152	LEU
22	Ad	41	ARG
22	Ad	54	PHE
22	Ad	115	ARG
22	Ad	166	THR
22	Ad	191	ILE
22	Ad	197	VAL
22	Ad	198	VAL
24	Af	85	LEU
24	Af	113	LEU
24	Af	145	LEU
24	Af	155	LEU
24	Af	160	ASP
24	Af	162	THR
25	Ag	111	LEU
25	Ag	134	THR
25	Ag	135	LEU
25	Ag	138	CYS
25	Ag	139	HIS
25	Ag	150	LEU
25	Ag	171	ASN
25	Ag	178	ASP
25	Ag	181	LEU
25	Ag	209	TRP
25	Ag	215	THR
25	Ag	231	ARG
25	Ag	246	LEU
25	Ag	265	ASN
25	Ag	296	VAL
25	Ag	300	TRP
25	Ag	305	ILE
25	Ag	311	GLN
25	Ag	336	LEU
25	Ag	337	ASP
25	Ag	382	LEU
25	Ag	397	LEU
26	Ah	302	LEU
26	Ah	372	PHE
27	Ai	11	MET
27	Ai	17	ARG
27	Ai	26	THR

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Mol	Chain	Res	Type
27	Ai	31	MET
27	Ai	67	PHE
27	Ai	79	ARG
28	Aj	21	LEU
28	Aj	29	ARG
28	Aj	52	MET
28	Aj	57	ASP
28	Aj	65	LEU
28	Aj	133	GLN
28	Aj	136	TYR
28	Aj	164	VAL
28	Aj	170	LEU
28	Aj	184	THR
28	Aj	186	THR
29	Ak	60	GLU
29	Ak	72	TYR
29	Ak	74	VAL
29	Ak	79	LYS
29	Ak	85	LEU
29	Ak	93	VAL
29	Ak	125	CYS
29	Ak	134	GLU
29	Ak	145	CYS
29	Ak	152	GLU
29	Ak	157	ASP
29	Ak	160	SER
29	Ak	165	ILE
29	Ak	199	ARG
29	Ak	213	ARG
29	Ak	216	LEU
29	Ak	234	GLU
29	Ak	288	THR
29	Ak	298	VAL
29	Ak	306	ASP
29	Ak	309	ASN
29	Ak	317	SER
30	Am	6	LEU
30	Am	13	LEU
30	Am	18	ARG
30	Am	29	LEU
30	Am	33	VAL
30	Am	37	ARG

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Mol	Chain	Res	Type
30	Am	39	GLU
30	Am	44	THR
30	Am	48	GLU
30	Am	63	ASP
31	An	132	LYS
31	An	133	ILE
31	An	136	ARG
31	An	144	ARG
31	An	147	VAL
31	An	155	ARG
31	An	168	LYS
31	An	175	ARG
31	An	191	THR
32	Ao	68	VAL
32	Ao	107	LEU
32	Ao	126	LYS
32	Ao	132	ILE
32	Ao	141	MET
33	Ap	53	ASP
33	Ap	80	ASN
33	Ap	95	ILE
33	Ap	103	ASN
33	Ap	108	CYS
33	Ap	113	LEU
33	Ap	128	CYS
33	Ap	134	ILE
33	Ap	167	ILE
33	Ap	173	ARG
33	Ap	177	PHE
33	Ap	193	LEU
33	Ap	199	TRP
33	Ap	202	TRP
33	Ap	214	SER
33	Ap	215	ARG
36	B0	50	ARG
36	B0	65	ASN
36	B0	66	ILE
36	B0	85	LYS
36	B0	94	GLU
36	B0	122	GLN
36	B0	126	LEU
36	B0	132	HIS

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Mol	Chain	Res	Type
36	B0	133	VAL
37	B1	6	VAL
37	B1	32	LEU
37	B1	46	HIS
37	B1	59	ARG
37	B1	61	ARG
37	B1	74	GLU
37	B1	93	ASN
37	B1	100	ARG
37	B1	104	VAL
37	B1	116	SER
37	B1	126	THR
37	B1	128	THR
37	B1	143	PHE
37	B1	152	ASP
37	B1	155	SER
37	B1	172	GLN
37	B1	177	HIS
37	B1	179	ASP
37	B1	190	ARG
37	B1	196	ILE
37	B1	206	LEU
37	B1	216	ARG
37	B1	222	ASP
37	B1	224	ILE
38	B2	67	GLU
38	B2	75	ASN
38	B2	79	GLU
38	B2	89	CYS
38	B2	96	SER
38	B2	132	GLU
38	B2	140	SER
38	B2	141	MET
38	B2	149	GLN
38	B2	150	GLU
38	B2	153	ASP
38	B2	158	LEU
38	B2	160	THR
38	B2	171	ARG
38	B2	174	ILE
38	B2	197	ASN
38	B2	204	MET

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Mol	Chain	Res	Type
38	B2	209	ARG
38	B2	228	LEU
38	B2	230	ARG
38	B2	238	GLU
39	B3	41	ILE
39	B3	72	ILE
39	B3	75	THR
39	B3	78	ARG
39	B3	86	ILE
39	B3	99	VAL
39	B3	118	ARG
39	B3	142	ASN
39	B3	147	VAL
40	B4	42	THR
40	B4	49	TYR
40	B4	57	LEU
41	B5	87	ILE
41	B5	103	VAL
41	B5	109	VAL
41	B5	115	HIS
41	B5	136	GLU
41	B5	153	THR
41	B5	168	GLN
41	B5	170	GLN
41	B5	177	ARG
41	B5	186	THR
42	B6	18	VAL
42	B6	20	MET
42	B6	26	THR
42	B6	38	ARG
42	B6	42	THR
42	B6	54	VAL
42	B6	55	LEU
42	B6	57	VAL
43	B7	52	ARG
43	B7	63	ARG
43	B7	65	HIS
43	B7	71	ARG
43	B7	93	LEU
44	B8	100	ARG
44	B8	106	THR
44	B8	116	ARG

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Mol	Chain	Res	Type
44	B8	142	ARG
44	B8	148	VAL
44	B8	163	THR
44	B8	168	ARG
44	B8	182	ASP
44	B8	183	ARG
44	B8	186	LEU
45	B9	63	PHE
45	B9	65	THR
45	B9	70	LYS
45	B9	75	ASP
48	BD	62	THR
48	BD	69	ARG
48	BD	70	THR
48	BD	82	SER
48	BD	92	GLN
48	BD	101	LYS
48	BD	111	ARG
48	BD	117	GLU
48	BD	136	ARG
48	BD	148	ARG
48	BD	150	ARG
48	BD	152	ILE
48	BD	155	THR
48	BD	167	SER
48	BD	175	VAL
48	BD	178	ARG
48	BD	181	ASP
48	BD	190	VAL
48	BD	213	THR
48	BD	224	THR
48	BD	227	ILE
48	BD	236	GLN
48	BD	239	GLU
48	BD	240	THR
48	BD	245	VAL
48	BD	256	ARG
48	BD	263	ARG
48	BD	273	SER
48	BD	277	GLN
48	BD	288	ARG
48	BD	290	LEU

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Mol	Chain	Res	Type
48	BD	295	SER
49	BE	46	VAL
49	BE	80	LEU
49	BE	96	ARG
49	BE	109	LEU
49	BE	113	ASP
49	BE	130	LEU
49	BE	146	THR
49	BE	168	LEU
49	BE	181	VAL
49	BE	211	ILE
49	BE	218	VAL
49	BE	227	GLN
49	BE	236	THR
49	BE	237	HIS
49	BE	239	ARG
49	BE	250	ARG
49	BE	251	VAL
49	BE	273	VAL
49	BE	296	LEU
49	BE	304	LEU
49	BE	310	PHE
49	BE	311	CYS
49	BE	318	THR
49	BE	335	GLU
50	BF	47	VAL
50	BF	59	ARG
50	BF	76	ARG
50	BF	77	VAL
50	BF	79	LEU
50	BF	92	ARG
50	BF	95	ILE
50	BF	101	ILE
50	BF	106	PHE
50	BF	110	SER
50	BF	111	TYR
50	BF	129	VAL
50	BF	147	ARG
50	BF	167	MET
50	BF	172	GLN
50	BF	190	VAL
50	BF	203	LEU

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Mol	Chain	Res	Type
50	BF	214	ASP
50	BF	215	SER
50	BF	234	THR
50	BF	239	THR
50	BF	246	VAL
50	BF	269	LEU
50	BF	277	ASN
50	BF	281	THR
50	BF	292	ASP
51	BI	76	ARG
51	BI	82	LEU
51	BI	108	ARG
52	BJ	34	THR
52	BJ	38	ARG
52	BJ	43	GLU
52	BJ	60	ILE
52	BJ	63	ARG
52	BJ	65	LEU
52	BJ	73	GLN
52	BJ	76	THR
52	BJ	93	ASN
52	BJ	116	LEU
52	BJ	150	HIS
52	BJ	152	LEU
53	BK	57	THR
53	BK	64	ILE
53	BK	113	THR
53	BK	127	ASP
53	BK	135	VAL
53	BK	137	LEU
54	BN	10	GLN
54	BN	60	MET
54	BN	67	PHE
54	BN	74	GLN
54	BN	78	SER
54	BN	81	THR
54	BN	104	VAL
54	BN	111	MET
54	BN	118	ARG
54	BN	122	MET
54	BN	123	GLN
54	BN	130	ASP

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Mol	Chain	Res	Type
54	BN	140	ASN
54	BN	143	GLU
54	BN	153	ARG
54	BN	154	ARG
54	BN	156	ASP
54	BN	177	ARG
55	BO	32	ILE
55	BO	48	THR
55	BO	60	VAL
55	BO	73	ILE
55	BO	75	LEU
55	BO	77	ILE
55	BO	91	MET
55	BO	95	ARG
55	BO	102	SER
55	BO	110	ASP
55	BO	138	LEU
56	BP	11	ARG
56	BP	37	GLU
56	BP	38	ARG
56	BP	44	ARG
56	BP	49	CYS
56	BP	51	ARG
56	BP	57	ARG
56	BP	58	GLN
56	BP	64	ARG
56	BP	65	LEU
56	BP	71	GLN
56	BP	77	ARG
56	BP	83	PHE
56	BP	88	SER
56	BP	94	GLN
56	BP	97	SER
56	BP	110	VAL
56	BP	127	VAL
56	BP	130	GLN
56	BP	135	ASP
56	BP	139	GLN
56	BP	141	VAL
56	BP	146	ASP
56	BP	157	GLN
56	BP	174	VAL

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Mol	Chain	Res	Type
56	BP	175	THR
56	BP	176	THR
56	BP	203	ARG
56	BP	233	ARG
56	BP	234	LEU
56	BP	247	ILE
56	BP	250	ASP
56	BP	251	GLU
56	BP	257	SER
56	BP	259	ARG
56	BP	277	MET
56	BP	286	THR
57	BQ	62	VAL
57	BQ	73	ARG
57	BQ	77	THR
57	BQ	84	GLU
57	BQ	89	ILE
57	BQ	96	TYR
57	BQ	106	ARG
57	BQ	111	ARG
57	BQ	114	ASP
57	BQ	131	ILE
57	BQ	147	ILE
57	BQ	166	ARG
57	BQ	171	GLU
57	BQ	209	ASN
57	BQ	214	THR
57	BQ	217	ARG
57	BQ	220	THR
57	BQ	226	ILE
57	BQ	231	SER
58	BR	17	ARG
58	BR	24	SER
58	BR	25	ARG
58	BR	26	ILE
58	BR	28	LEU
58	BR	82	GLU
58	BR	83	LYS
58	BR	84	ASP
58	BR	96	ARG
58	BR	98	GLN
58	BR	110	ILE

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Mol	Chain	Res	Type
58	BR	118	ARG
58	BR	121	MET
58	BR	134	LEU
58	BR	139	ARG
58	BR	142	ASN
58	BR	143	LEU
58	BR	154	ARG
59	BS	44	VAL
59	BS	52	ASN
59	BS	71	VAL
59	BS	80	ARG
59	BS	82	ARG
59	BS	103	VAL
59	BS	107	THR
59	BS	112	ILE
59	BS	141	ILE
60	BT	77	SER
60	BT	79	GLU
60	BT	87	THR
60	BT	105	ILE
60	BT	130	THR
60	BT	136	ILE
60	BT	162	ILE
60	BT	165	GLU
60	BT	185	ASN
60	BT	187	LEU
60	BT	203	ASN
60	BT	208	THR
60	BT	219	GLN
60	BT	246	ASP
60	BT	254	MET
60	BT	260	TRP
60	BT	270	MET
60	BT	272	GLU
60	BT	275	THR
61	BU	10	LEU
61	BU	12	SER
61	BU	25	LEU
61	BU	37	ARG
61	BU	46	VAL
61	BU	53	CYS
61	BU	59	LEU

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Mol	Chain	Res	Type
61	BU	64	LEU
61	BU	102	LEU
62	BV	120	ILE
62	BV	126	VAL
62	BV	128	CYS
62	BV	133	ARG
62	BV	140	VAL
62	BV	153	LEU
62	BV	158	VAL
62	BV	159	ARG
62	BV	176	MET
62	BV	186	ARG
62	BV	190	THR
62	BV	195	THR
62	BV	198	ARG
62	BV	199	ILE
62	BV	200	ASN
63	BW	60	GLN
63	BW	67	ARG
63	BW	75	ARG
63	BW	80	TYR
63	BW	81	SER
63	BW	105	GLU
63	BW	108	ASP
63	BW	131	ASN
63	BW	135	ARG
63	BW	136	SER
63	BW	145	SER
63	BW	149	GLN
63	BW	161	ARG
63	BW	164	ILE
63	BW	170	CYS
63	BW	191	VAL
63	BW	199	GLN
63	BW	206	ILE
63	BW	207	THR
64	BX	14	ASN
64	BX	18	ARG
64	BX	35	GLN
64	BX	39	THR
64	BX	40	VAL
64	BX	49	THR

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Mol	Chain	Res	Type
64	BX	57	LEU
64	BX	71	ARG
64	BX	77	ASN
64	BX	78	ARG
64	BX	81	ASP
64	BX	85	ILE
64	BX	104	THR
64	BX	109	ASP
64	BX	141	ARG
64	BX	148	PHE
64	BX	150	LEU
65	BY	29	LEU
65	BY	40	ARG
65	BY	44	VAL
65	BY	66	GLU
65	BY	69	ASP
65	BY	78	GLN
65	BY	79	VAL
65	BY	86	VAL
65	BY	96	ARG
65	BY	105	ARG
65	BY	131	THR
65	BY	137	PHE
65	BY	138	THR
65	BY	144	VAL
65	BY	145	ARG
65	BY	149	ARG
65	BY	153	ILE
65	BY	166	VAL
65	BY	181	ASP
65	BY	186	THR
65	BY	193	THR
65	BY	202	MET
65	BY	208	ARG
65	BY	216	TYR
66	Ba	42	GLU
66	Ba	64	MET
66	Ba	67	MET
66	Ba	72	ARG
66	Ba	96	HIS
66	Ba	111	CYS
66	Ba	124	THR

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Mol	Chain	Res	Type
66	Ba	128	LEU
66	Ba	149	ASN
66	Ba	151	ASP
66	Ba	163	LEU
66	Ba	167	THR
66	Ba	169	ASP
66	Ba	175	THR
66	Ba	180	ILE
66	Ba	202	ILE
66	Ba	207	ASN
66	Ba	210	SER
66	Ba	222	VAL
66	Ba	256	PHE
66	Ba	259	ILE
66	Ba	268	CYS
66	Ba	277	THR
66	Ba	307	ASP
66	Ba	316	PHE
66	Ba	334	LYS
66	Ba	335	VAL
66	Ba	336	LEU
66	Ba	337	GLU
66	Ba	342	VAL
66	Ba	347	THR
66	Ba	367	ASP
66	Ba	372	ASN
66	Ba	388	CYS
66	Ba	391	VAL
66	Ba	396	VAL
66	Ba	398	VAL
66	Ba	415	LEU
67	Bb	40	ILE
67	Bb	51	TYR
67	Bb	52	ARG
67	Bb	53	SER
67	Bb	90	ILE
67	Bb	101	GLN
67	Bb	118	GLU
67	Bb	209	ASP
67	Bb	210	GLU
67	Bb	222	ASP
67	Bb	240	ILE

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Mol	Chain	Res	Type
67	Bb	258	PHE
67	Bb	261	ARG
67	Bb	279	ILE
67	Bb	281	PHE
67	Bb	284	ASP
67	Bb	288	SER
67	Bb	303	PHE
67	Bb	312	THR
67	Bb	322	ARG
67	Bb	324	ASP
67	Bb	334	LEU
67	Bb	337	MET
67	Bb	356	ARG
67	Bb	360	ARG
67	Bb	364	ARG
67	Bb	376	THR
68	Bc	56	THR
68	Bc	67	VAL
68	Bc	87	SER
68	Bc	98	ARG
68	Bc	106	ASP
68	Bc	111	ASP
68	Bc	129	ASP
68	Bc	131	ASP
68	Bc	140	TRP
68	Bc	142	SER
68	Bc	143	CYS
68	Bc	157	ASP
68	Bc	177	CYS
68	Bc	222	VAL
68	Bc	236	PHE
68	Bc	256	ASP
68	Bc	280	VAL
68	Bc	291	ARG
69	Bd	89	ILE
69	Bd	99	ARG
69	Bd	123	LEU
69	Bd	136	ILE
69	Bd	150	LEU
69	Bd	163	LYS
70	Be	23	SER
70	Be	28	ARG

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Mol	Chain	Res	Type
70	Be	60	VAL
70	Be	63	LEU
70	Be	66	PHE
70	Be	68	LEU
70	Be	72	VAL
70	Be	78	GLU
70	Be	106	THR
70	Be	111	HIS
70	Be	127	GLN
71	Bf	39	LEU
71	Bf	44	ASN
71	Bf	56	ARG
71	Bf	59	VAL
71	Bf	102	HIS
71	Bf	109	ILE
71	Bf	122	ARG
71	Bf	126	ARG
71	Bf	131	ARG
71	Bf	134	ARG
72	Bg	6	THR
72	Bg	12	THR
72	Bg	14	VAL
72	Bg	21	ARG
72	Bg	33	LEU
72	Bg	34	SER
72	Bg	41	ARG
72	Bg	68	ARG
72	Bg	70	CYS
72	Bg	90	HIS
72	Bg	93	SER
72	Bg	108	SER
72	Bg	112	VAL
72	Bg	117	LYS
72	Bg	119	PHE
72	Bg	125	SER
72	Bg	126	ILE
73	Bh	33	LYS
73	Bh	51	LEU
73	Bh	53	CYS
73	Bh	78	ARG
73	Bh	82	THR
73	Bh	84	SER

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Mol	Chain	Res	Type
73	Bh	96	CYS
73	Bh	98	ILE
73	Bh	121	ASP
73	Bh	145	PHE
73	Bh	153	VAL
73	Bh	191	LEU
73	Bh	213	LEU
73	Bh	216	ARG
73	Bh	231	MET
73	Bh	251	SER
73	Bh	259	ARG
73	Bh	263	SER
73	Bh	267	LEU
73	Bh	288	THR
73	Bh	289	VAL
73	Bh	293	GLU
73	Bh	294	GLU
73	Bh	301	LEU
73	Bh	307	PHE
74	Bi	74	ARG
74	Bi	144	ILE
74	Bi	145	PHE
74	Bi	165	THR
74	Bi	175	ASP
74	Bi	181	VAL
74	Bi	196	GLN
74	Bi	221	THR
74	Bi	230	ARG
74	Bi	237	ASP
74	Bi	242	VAL
74	Bi	244	GLU
74	Bi	258	SER
74	Bi	276	ILE
75	Bj	51	LEU
75	Bj	52	CYS
75	Bj	55	ARG
75	Bj	60	THR
75	Bj	142	LYS
75	Bj	145	ASP
75	Bj	169	ASP
75	Bj	179	GLN
75	Bj	198	ASN

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Mol	Chain	Res	Type
75	Bj	243	PHE
75	Bj	264	LEU
75	Bj	265	LYS
75	Bj	274	ARG
75	Bj	276	LEU
76	Bk	49	ARG
76	Bk	50	SER
76	Bk	81	ASN
76	Bk	92	ASN
76	Bk	100	MET
76	Bk	147	ASP
76	Bk	150	LEU
76	Bk	165	THR
77	Bl	42	VAL
77	Bl	57	ILE
77	Bl	73	GLN
77	Bl	77	ASP
77	Bl	89	SER
77	Bl	90	ARG
77	Bl	94	ILE
77	Bl	100	ILE
77	Bl	101	THR
77	Bl	108	THR
77	Bl	111	ARG
77	Bl	113	VAL
77	Bl	125	GLU
77	Bl	128	LEU
77	Bl	131	LEU
77	Bl	138	THR
77	Bl	141	ASN
77	Bl	155	GLN
78	Bm	56	ILE
78	Bm	67	LEU
78	Bm	71	LEU
78	Bm	121	MET
78	Bm	126	ASP
78	Bm	144	LEU
79	Bn	32	PHE
79	Bn	44	VAL
79	Bn	46	ARG
79	Bn	48	ASN
79	Bn	53	MET

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Mol	Chain	Res	Type
79	Bn	60	ILE
79	Bn	66	PHE
79	Bn	92	ILE
79	Bn	98	VAL
79	Bn	104	ILE
79	Bn	105	ASP
80	Bo	25	SER
80	Bo	31	GLN
80	Bo	40	TYR
80	Bo	64	LEU
80	Bo	65	ARG
80	Bo	72	LYS
80	Bo	75	ARG
80	Bo	84	MET
80	Bo	110	LEU
81	Bp	15	GLN
81	Bp	28	GLU
81	Bp	55	VAL
81	Bp	82	THR
81	Bp	84	GLN
82	Bq	121	LEU
82	Bq	128	ARG
83	Bt	9	ARG
83	Bt	10	ASN
83	Bt	25	ARG
83	Bt	27	VAL
83	Bt	35	MET
83	Bt	40	GLU
83	Bt	45	ASN
83	Bt	55	THR
83	Bt	57	GLU
83	Bt	81	ARG
83	Bt	82	PHE
83	Bt	88	LEU
83	Bt	99	ARG
84	Bu	56	ASP
84	Bu	97	LYS
84	Bu	123	LYS
84	Bu	138	CYS
84	Bu	140	ARG
84	Bu	159	GLU
84	Bu	184	ARG

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Mol	Chain	Res	Type
85	Bv	38	ARG
85	Bv	44	ASP
85	Bv	47	THR
85	Bv	52	LEU
85	Bv	59	LYS
85	Bv	74	SER
86	Bw	43	ARG
86	Bw	51	LEU
86	Bw	55	SER
86	Bw	77	ASP
86	Bw	81	ARG
86	Bw	92	VAL
86	Bw	96	GLN
86	Bw	98	PHE
86	Bw	100	LEU
86	Bw	153	ARG
86	Bw	162	ASP
86	Bw	196	CYS
86	Bw	216	ARG
86	Bw	236	ARG
86	Bw	237	ILE
86	Bw	241	LEU
86	Bw	245	VAL
86	Bw	248	ASP
86	Bw	258	MET
86	Bw	263	ASP
86	Bw	267	LEU
86	Bw	270	ARG
86	Bw	271	GLN
86	Bw	274	ASN
86	Bw	278	ILE
86	Bw	282	THR
86	Bw	284	ASP
86	Bw	291	THR
86	Bw	315	GLU
86	Bw	326	LEU
86	Bw	330	THR
86	Bw	335	MET
86	Bw	336	TYR
86	Bw	347	ARG
86	Bw	378	ASP
86	Bw	383	ARG

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Mol	Chain	Res	Type
86	Bw	395	LEU
86	Bw	399	ILE
86	Bw	402	ASN
86	Bw	404	VAL
86	Bw	405	LYS
86	Bw	410	ASP
86	Bw	420	LEU
86	Bw	421	ASN
87	Bx	54	THR
87	Bx	92	PHE
87	Bx	100	LEU
87	Bx	111	GLU
87	Bx	121	MET
87	Bx	128	LEU
87	Bx	148	ASN
87	Bx	149	ARG
87	Bx	152	THR
87	Bx	155	SER
87	Bx	157	ARG
87	Bx	162	ILE
87	Bx	190	ARG
87	Bx	193	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (246) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	133	HIS
3	AC	57	HIS
3	AC	72	HIS
3	AC	75	ASN
3	AC	115	ASN
3	AC	126	GLN
3	AC	154	HIS
3	AC	156	GLN
4	AE	130	GLN
4	AE	145	ASN
4	AE	196	ASN
4	AE	277	HIS
4	AE	288	HIS
4	AE	292	HIS
4	AE	317	HIS
4	AE	360	GLN

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Mol	Chain	Res	Type
4	AE	369	HIS
5	AF	41	ASN
5	AF	54	HIS
5	AF	58	HIS
6	AG	146	HIS
6	AG	227	HIS
6	AG	233	ASN
7	AI	87	HIS
7	AI	90	ASN
7	AI	127	HIS
7	AI	148	HIS
7	AI	156	GLN
7	AI	163	HIS
7	AI	313	GLN
7	AI	327	HIS
8	AJ	83	HIS
8	AJ	183	HIS
9	AK	95	ASN
10	AL	34	ASN
10	AL	35	GLN
10	AL	44	HIS
10	AL	57	GLN
10	AL	100	HIS
10	AL	134	HIS
11	AN	60	ASN
11	AN	117	HIS
12	AO	153	HIS
13	AP	28	ASN
14	AQ	9	HIS
14	AQ	23	GLN
14	AQ	56	GLN
14	AQ	57	GLN
15	AR	72	HIS
16	AU	3	ASN
16	AU	27	ASN
16	AU	85	GLN
19	Aa	75	GLN
19	Aa	107	GLN
19	Aa	222	GLN
19	Aa	247	HIS
19	Aa	266	HIS
19	Aa	276	ASN

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Mol	Chain	Res	Type
19	Aa	287	GLN
21	Ac	51	ASN
21	Ac	56	GLN
21	Ac	59	ASN
21	Ac	63	GLN
21	Ac	69	ASN
21	Ac	95	ASN
21	Ac	101	HIS
21	Ac	125	HIS
21	Ac	146	GLN
22	Ad	31	HIS
22	Ad	65	GLN
22	Ad	109	ASN
24	Af	98	ASN
25	Ag	80	HIS
25	Ag	153	HIS
25	Ag	210	ASN
25	Ag	386	ASN
25	Ag	389	GLN
26	Ah	309	ASN
26	Ah	323	HIS
27	Ai	75	HIS
28	Aj	111	HIS
29	Ak	104	ASN
29	Ak	124	HIS
29	Ak	187	HIS
29	Ak	263	ASN
29	Ak	303	ASN
30	Am	31	ASN
30	Am	109	HIS
30	Am	113	ASN
30	Am	116	HIS
31	An	129	ASN
31	An	178	GLN
32	Ao	129	GLN
33	Ap	130	HIS
33	Ap	136	HIS
33	Ap	147	HIS
36	B0	59	HIS
36	B0	76	HIS
37	B1	27	HIS
37	B1	42	HIS

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Mol	Chain	Res	Type
37	B1	94	ASN
37	B1	172	GLN
38	B2	75	ASN
38	B2	90	GLN
38	B2	119	GLN
38	B2	197	ASN
40	B4	37	ASN
41	B5	83	ASN
41	B5	144	GLN
41	B5	168	GLN
41	B5	170	GLN
42	B6	45	HIS
48	BD	196	ASN
49	BE	128	HIS
49	BE	156	HIS
49	BE	197	HIS
49	BE	281	ASN
49	BE	292	HIS
50	BF	63	GLN
50	BF	74	GLN
50	BF	83	HIS
50	BF	103	GLN
50	BF	105	ASN
50	BF	153	HIS
50	BF	201	GLN
50	BF	241	ASN
50	BF	249	ASN
50	BF	251	HIS
51	BI	88	HIS
51	BI	136	ASN
52	BJ	41	HIS
52	BJ	93	ASN
52	BJ	119	HIS
53	BK	84	GLN
53	BK	103	HIS
54	BN	10	GLN
54	BN	56	HIS
54	BN	74	GLN
54	BN	80	HIS
56	BP	53	HIS
56	BP	71	GLN
56	BP	157	GLN

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Mol	Chain	Res	Type
56	BP	170	ASN
57	BQ	98	HIS
57	BQ	110	ASN
57	BQ	209	ASN
57	BQ	211	ASN
58	BR	11	HIS
58	BR	39	HIS
58	BR	112	ASN
59	BS	52	ASN
59	BS	115	HIS
59	BS	147	HIS
60	BT	212	ASN
60	BT	291	ASN
61	BU	79	HIS
61	BU	94	GLN
62	BV	88	ASN
62	BV	104	HIS
62	BV	109	GLN
62	BV	122	ASN
62	BV	192	ASN
63	BW	123	GLN
63	BW	171	HIS
63	BW	203	ASN
64	BX	14	ASN
64	BX	77	ASN
65	BY	35	ASN
65	BY	78	GLN
65	BY	117	HIS
66	Ba	108	HIS
66	Ba	150	GLN
66	Ba	156	ASN
66	Ba	195	HIS
66	Ba	221	GLN
66	Ba	223	HIS
66	Ba	269	ASN
66	Ba	289	HIS
66	Ba	358	GLN
67	Bb	224	HIS
67	Bb	266	HIS
67	Bb	308	GLN
67	Bb	354	GLN
68	Bc	229	HIS

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Mol	Chain	Res	Type
68	Bc	230	ASN
68	Bc	243	GLN
68	Bc	282	ASN
68	Bc	294	GLN
68	Bc	305	HIS
68	Bc	310	ASN
69	Bd	143	GLN
70	Be	42	HIS
70	Be	50	GLN
71	Bf	44	ASN
71	Bf	62	HIS
71	Bf	121	HIS
72	Bg	17	ASN
72	Bg	127	GLN
72	Bg	131	HIS
72	Bg	135	ASN
73	Bh	73	GLN
73	Bh	118	ASN
73	Bh	177	GLN
73	Bh	222	GLN
73	Bh	260	GLN
74	Bi	193	GLN
74	Bi	196	GLN
75	Bj	87	HIS
75	Bj	150	HIS
75	Bj	251	HIS
75	Bj	252	HIS
76	Bk	92	ASN
76	Bk	158	GLN
76	Bk	175	HIS
76	Bk	177	ASN
77	Bl	141	ASN
78	Bm	96	HIS
79	Bn	69	HIS
79	Bn	122	ASN
80	Bo	63	GLN
81	Bp	15	GLN
81	Bp	72	HIS
82	Bq	125	ASN
82	Bq	129	HIS
83	Bt	34	ASN
83	Bt	45	ASN

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Mol	Chain	Res	Type
83	Bt	85	HIS
84	Bu	103	HIS
84	Bu	124	ASN
84	Bu	145	ASN
86	Bw	60	GLN
86	Bw	96	GLN
86	Bw	101	ASN
86	Bw	146	GLN
86	Bw	173	GLN
86	Bw	185	HIS
86	Bw	226	GLN
86	Bw	233	ASN
86	Bw	271	GLN
86	Bw	313	GLN
86	Bw	385	ASN
86	Bw	421	ASN
87	Bx	112	HIS
87	Bx	164	ASN
87	Bx	170	ASN
87	Bx	184	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	959/962 (99%)	308 (32%)	7 (0%)
17	AV	0/69	-	-
17	AY	0/69	-	-
18	AX	0/13	-	-
46	BA	1508/1570 (96%)	620 (41%)	30 (1%)
47	BB	0/51	-	-
All	All	2467/2734 (90%)	928 (37%)	37 (1%)

All (928) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	A
1	AA	10	U
1	AA	11	G
1	AA	14	C
1	AA	18	G
1	AA	34	U

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Mol	Chain	Res	Type
1	AA	36	A
1	AA	39	A
1	AA	42	A
1	AA	45	A
1	AA	49	A
1	AA	51	G
1	AA	54	A
1	AA	55	G
1	AA	58	U
1	AA	61	G
1	AA	63	G
1	AA	65	C
1	AA	77	G
1	AA	78	C
1	AA	83	C
1	AA	92	A
1	AA	98	A
1	AA	102	G
1	AA	104	A
1	AA	111	A
1	AA	115	A
1	AA	118	A
1	AA	120	A
1	AA	124	A
1	AA	125	U
1	AA	126	A
1	AA	127	A
1	AA	128	C
1	AA	129	G
1	AA	139	A
1	AA	142	G
1	AA	147	G
1	AA	151	A
1	AA	152	A
1	AA	160	C
1	AA	161	C
1	AA	162	C
1	AA	163	A
1	AA	165	G
1	AA	168	A
1	AA	170	A
1	AA	171	C

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Mol	Chain	Res	Type
1	AA	173	G
1	AA	175	A
1	AA	184	A
1	AA	186	U
1	AA	191	C
1	AA	192	C
1	AA	194	U
1	AA	198	C
1	AA	199	G
1	AA	202	A
1	AA	203	G
1	AA	216	A
1	AA	217	U
1	AA	222	A
1	AA	223	U
1	AA	224	U
1	AA	225	A
1	AA	227	A
1	AA	231	G
1	AA	237	U
1	AA	238	C
1	AA	244	C
1	AA	245	C
1	AA	246	A
1	AA	247	G
1	AA	253	G
1	AA	257	U
1	AA	258	C
1	AA	259	A
1	AA	265	U
1	AA	273	A
1	AA	281	G
1	AA	285	C
1	AA	286	A
1	AA	288	G
1	AA	293	A
1	AA	294	A
1	AA	297	A
1	AA	298	G
1	AA	309	A
1	AA	310	A
1	AA	311	A

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Mol	Chain	Res	Type
1	AA	313	A
1	AA	316	C
1	AA	317	A
1	AA	318	C
1	AA	319	A
1	AA	320	A
1	AA	330	A
1	AA	340	A
1	AA	345	U
1	AA	354	C
1	AA	360	A
1	AA	361	A
1	AA	362	A
1	AA	367	A
1	AA	368	A
1	AA	369	U
1	AA	372	C
1	AA	381	G
1	AA	392	A
1	AA	393	A
1	AA	394	U
1	AA	395	C
1	AA	396	C
1	AA	399	A
1	AA	400	C
1	AA	417	C
1	AA	421	A
1	AA	425	G
1	AA	433	U
1	AA	434	A
1	AA	439	A
1	AA	444	G
1	AA	445	C
1	AA	448	A
1	AA	454	A
1	AA	455	A
1	AA	456	A
1	AA	457	C
1	AA	458	C
1	AA	459	C
1	AA	461	A
1	AA	465	G

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Mol	Chain	Res	Type
1	AA	471	U
1	AA	472	A
1	AA	477	A
1	AA	479	C
1	AA	481	A
1	AA	487	C
1	AA	488	A
1	AA	489	G
1	AA	493	A
1	AA	498	U
1	AA	501	C
1	AA	502	A
1	AA	504	C
1	AA	505	U
1	AA	506	G
1	AA	513	A
1	AA	515	U
1	AA	517	A
1	AA	518	A
1	AA	526	G
1	AA	530	G
1	AA	536	C
1	AA	538	C
1	AA	540	U
1	AA	547	A
1	AA	559	U
1	AA	561	U
1	AA	562	A
1	AA	564	A
1	AA	566	U
1	AA	571	A
1	AA	574	C
1	AA	576	C
1	AA	577	C
1	AA	579	A
1	AA	581	A
1	AA	582	G
1	AA	588	A
1	AA	589	C
1	AA	592	A
1	AA	593	C
1	AA	594	C

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Mol	Chain	Res	Type
1	AA	597	U
1	AA	604	U
1	AA	606	A
1	AA	607	G
1	AA	609	C
1	AA	610	U
1	AA	612	U
1	AA	613	A
1	AA	619	C
1	AA	620	C
1	AA	625	U
1	AA	626	C
1	AA	627	A
1	AA	628	G
1	AA	630	A
1	AA	633	C
1	AA	635	C
1	AA	637	A
1	AA	638	A
1	AA	639	A
1	AA	640	A
1	AA	644	A
1	AA	645	A
1	AA	646	C
1	AA	647	A
1	AA	648	A
1	AA	649	U
1	AA	650	A
1	AA	654	A
1	AA	655	G
1	AA	656	C
1	AA	661	U
1	AA	662	C
1	AA	665	A
1	AA	666	G
1	AA	667	C
1	AA	669	C
1	AA	681	A
1	AA	682	G
1	AA	686	A
1	AA	693	A
1	AA	694	G

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Mol	Chain	Res	Type
1	AA	695	C
1	AA	698	A
1	AA	707	A
1	AA	708	A
1	AA	711	A
1	AA	720	A
1	AA	722	A
1	AA	723	U
1	AA	732	U
1	AA	733	A
1	AA	734	A
1	AA	739	A
1	AA	740	U
1	AA	742	C
1	AA	744	C
1	AA	745	C
1	AA	746	A
1	AA	747	C
1	AA	748	A
1	AA	752	A
1	AA	753	A
1	AA	761	U
1	AA	765	A
1	AA	766	C
1	AA	775	A
1	AA	790	A
1	AA	791	G
1	AA	802	A
1	AA	803	U
1	AA	804	A
1	AA	807	G
1	AA	808	U
1	AA	821	A
1	AA	822	A
1	AA	823	G
1	AA	824	G
1	AA	825	C
1	AA	826	C
1	AA	835	C
1	AA	838	A
1	AA	841	C
1	AA	842	A

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Mol	Chain	Res	Type
1	AA	861	A
1	AA	862	A
1	AA	863	G
1	AA	867	G
1	AA	868	U
1	AA	869	A
1	AA	870	G
1	AA	874	U
1	AA	875	A
1	AA	876	A
1	AA	877	A
1	AA	878	A
1	AA	880	U
1	AA	881	A
1	AA	884	C
1	AA	885	U
1	AA	886	A
1	AA	890	U
1	AA	891	C
1	AA	894	U
1	AA	895	U
1	AA	896	A
1	AA	897	C
1	AA	898	A
1	AA	899	C
1	AA	900	A
1	AA	901	A
1	AA	902	C
1	AA	910	G
1	AA	912	A
1	AA	915	G
1	AA	917	C
1	AA	918	A
1	AA	919	A
1	AA	920	G
1	AA	923	G
1	AA	925	A
1	AA	928	A
1	AA	930	G
1	AA	932	U
1	AA	933	A
1	AA	934	A

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Mol	Chain	Res	Type
1	AA	943	G
1	AA	945	A
1	AA	946	A
1	AA	955	G
1	AA	956	G
1	AA	958	U
1	AA	959	U
1	AA	962	C
46	BA	4	A
46	BA	5	A
46	BA	7	G
46	BA	11	G
46	BA	16	A
46	BA	27	A
46	BA	30	U
46	BA	31	A
46	BA	32	C
46	BA	36	A
46	BA	37	A
46	BA	39	A
46	BA	40	C
46	BA	41	A
46	BA	42	C
46	BA	43	C
46	BA	44	A
46	BA	45	A
46	BA	46	A
46	BA	48	U
46	BA	49	A
46	BA	54	A
46	BA	56	A
46	BA	57	A
46	BA	58	C
46	BA	59	A
46	BA	60	U
46	BA	61	U
46	BA	63	A
46	BA	66	U
46	BA	67	A
46	BA	68	A
46	BA	69	C
46	BA	70	A

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Mol	Chain	Res	Type
46	BA	71	U
46	BA	72	U
46	BA	82	G
46	BA	83	A
46	BA	84	G
46	BA	96	U
46	BA	97	A
46	BA	98	U
46	BA	99	C
46	BA	100	C
46	BA	101	U
46	BA	102	G
46	BA	104	C
46	BA	105	G
46	BA	108	A
46	BA	109	U
46	BA	110	A
46	BA	112	A
46	BA	113	G
46	BA	115	U
46	BA	116	A
46	BA	117	G
46	BA	119	A
46	BA	128	A
46	BA	129	A
46	BA	131	G
46	BA	133	U
46	BA	136	A
46	BA	138	G
46	BA	139	A
46	BA	140	A
46	BA	148	A
46	BA	152	U
46	BA	156	A
46	BA	157	A
46	BA	158	A
46	BA	159	A
46	BA	160	A
46	BA	161	G
46	BA	162	C
46	BA	163	A
46	BA	164	A

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Mol	Chain	Res	Type
46	BA	167	A
46	BA	168	U
46	BA	169	U
46	BA	171	C
46	BA	178	U
46	BA	179	A
46	BA	187	C
46	BA	189	U
46	BA	191	A
46	BA	203	G
46	BA	204	A
46	BA	206	A
46	BA	207	A
46	BA	209	A
46	BA	217	A
46	BA	218	A
46	BA	219	G
46	BA	220	A
46	BA	222	A
46	BA	223	A
46	BA	224	C
46	BA	225	U
46	BA	227	U
46	BA	228	A
46	BA	229	G
46	BA	230	C
46	BA	236	A
46	BA	237	C
46	BA	238	C
46	BA	242	A
46	BA	253	G
46	BA	258	C
46	BA	262	G
46	BA	270	U
46	BA	271	A
46	BA	272	A
46	BA	274	A
46	BA	275	G
46	BA	276	A
46	BA	277	A
46	BA	293	G
46	BA	294	G

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Mol	Chain	Res	Type
46	BA	302	G
46	BA	305	A
46	BA	308	A
46	BA	310	A
46	BA	311	C
46	BA	321	G
46	BA	322	A
46	BA	323	G
46	BA	328	A
46	BA	329	A
46	BA	330	A
46	BA	331	G
46	BA	335	A
46	BA	336	A
46	BA	337	C
46	BA	338	G
46	BA	339	A
46	BA	344	G
46	BA	347	G
46	BA	348	A
46	BA	351	G
46	BA	356	U
46	BA	357	U
46	BA	358	G
46	BA	361	C
46	BA	363	A
46	BA	365	A
46	BA	367	A
46	BA	368	G
46	BA	370	A
46	BA	372	U
46	BA	374	U
46	BA	375	A
46	BA	380	A
46	BA	382	C
46	BA	389	A
46	BA	390	A
46	BA	391	U
46	BA	392	A
46	BA	393	C
46	BA	396	C
46	BA	397	A

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Mol	Chain	Res	Type
46	BA	398	A
46	BA	401	A
46	BA	403	C
46	BA	404	C
46	BA	405	U
46	BA	406	A
46	BA	408	A
46	BA	413	A
46	BA	416	G
46	BA	417	U
46	BA	419	U
46	BA	426	G
46	BA	427	A
46	BA	428	G
46	BA	432	G
46	BA	433	U
46	BA	439	A
46	BA	444	A
46	BA	445	C
46	BA	447	G
46	BA	448	C
46	BA	458	A
46	BA	459	C
46	BA	460	G
46	BA	462	A
46	BA	463	U
46	BA	464	A
46	BA	466	A
46	BA	467	A
46	BA	471	U
46	BA	472	G
46	BA	473	A
46	BA	474	C
46	BA	475	U
46	BA	476	A
46	BA	477	G
46	BA	478	A
46	BA	479	G
46	BA	480	A
46	BA	486	U
46	BA	487	C
46	BA	488	U

*Continued on next page...*

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Mol	Chain	Res	Type
46	BA	490	A
46	BA	491	A
46	BA	492	U
46	BA	493	A
46	BA	495	U
46	BA	496	A
46	BA	497	C
46	BA	498	C
46	BA	499	A
46	BA	501	A
46	BA	503	U
46	BA	504	A
46	BA	505	G
46	BA	508	C
46	BA	509	U
46	BA	510	A
46	BA	512	A
46	BA	513	A
46	BA	514	G
46	BA	515	C
46	BA	516	A
46	BA	519	C
46	BA	521	U
46	BA	522	C
46	BA	524	A
46	BA	525	U
46	BA	526	U
46	BA	527	G
46	BA	528	A
46	BA	529	G
46	BA	530	A
46	BA	533	G
46	BA	539	A
46	BA	542	C
46	BA	543	U
46	BA	545	A
46	BA	546	A
46	BA	548	A
46	BA	549	A
46	BA	550	A
46	BA	552	U
46	BA	553	C

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Mol	Chain	Res	Type
46	BA	554	A
46	BA	556	C
46	BA	557	A
46	BA	558	A
46	BA	559	C
46	BA	560	A
46	BA	561	U
46	BA	564	U
46	BA	567	C
46	BA	568	A
46	BA	570	A
46	BA	571	A
46	BA	572	A
46	BA	573	C
46	BA	574	U
46	BA	576	A
46	BA	577	U
46	BA	578	A
46	BA	579	A
46	BA	581	A
46	BA	582	A
46	BA	583	A
46	BA	584	C
46	BA	587	C
46	BA	588	U
46	BA	590	G
46	BA	591	C
46	BA	593	C
46	BA	594	A
46	BA	598	C
46	BA	600	G
46	BA	611	U
46	BA	614	A
46	BA	615	A
46	BA	616	A
46	BA	617	C
46	BA	618	A
46	BA	619	U
46	BA	620	A
46	BA	623	A
46	BA	624	G
46	BA	626	A

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Mol	Chain	Res	Type
46	BA	629	A
46	BA	630	A
46	BA	632	G
46	BA	638	A
46	BA	641	A
46	BA	646	C
46	BA	647	A
46	BA	648	A
46	BA	653	C
46	BA	654	C
46	BA	655	U
46	BA	658	C
46	BA	659	U
46	BA	672	U
46	BA	673	U
46	BA	682	A
46	BA	687	A
46	BA	688	U
46	BA	689	A
46	BA	692	A
46	BA	693	U
46	BA	695	C
46	BA	702	U
46	BA	703	U
46	BA	705	A
46	BA	706	C
46	BA	707	A
46	BA	710	C
46	BA	711	A
46	BA	716	A
46	BA	717	C
46	BA	718	C
46	BA	719	A
46	BA	720	A
46	BA	722	A
46	BA	723	C
46	BA	724	A
46	BA	725	A
46	BA	726	C
46	BA	734	C
46	BA	735	G
46	BA	741	U

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Mol	Chain	Res	Type
46	BA	742	A
46	BA	743	A
46	BA	744	U
46	BA	745	U
46	BA	746	A
46	BA	747	C
46	BA	748	A
46	BA	751	G
46	BA	761	C
46	BA	762	A
46	BA	763	C
46	BA	764	A
46	BA	768	G
46	BA	772	A
46	BA	773	C
46	BA	774	C
46	BA	775	A
46	BA	776	A
46	BA	777	G
46	BA	778	G
46	BA	779	A
46	BA	780	A
46	BA	781	A
46	BA	787	A
46	BA	802	A
46	BA	807	G
46	BA	812	C
46	BA	813	A
46	BA	816	A
46	BA	817	A
46	BA	822	G
46	BA	823	C
46	BA	826	G
46	BA	831	C
46	BA	832	C
46	BA	833	A
46	BA	838	C
46	BA	844	C
46	BA	845	U
46	BA	846	C
46	BA	847	U
46	BA	848	A

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Mol	Chain	Res	Type
46	BA	849	G
46	BA	850	C
46	BA	851	A
46	BA	852	U
46	BA	853	U
46	BA	857	A
46	BA	858	G
46	BA	862	U
46	BA	866	G
46	BA	870	A
46	BA	880	A
46	BA	881	G
46	BA	885	C
46	BA	886	A
46	BA	890	G
46	BA	892	U
46	BA	893	U
46	BA	895	A
46	BA	897	G
46	BA	898	G
46	BA	899	C
46	BA	900	C
46	BA	904	G
46	BA	905	U
46	BA	906	A
46	BA	920	A
46	BA	921	A
46	BA	922	G
46	BA	923	G
46	BA	924	U
46	BA	925	A
46	BA	926	G
46	BA	929	U
46	BA	931	A
46	BA	932	U
46	BA	933	C
46	BA	937	U
46	BA	946	A
46	BA	948	U
46	BA	956	U
46	BA	957	G
46	BA	958	U

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Mol	Chain	Res	Type
46	BA	959	A
46	BA	962	A
46	BA	963	A
46	BA	965	G
46	BA	968	C
46	BA	975	G
46	BA	977	G
46	BA	979	U
46	BA	980	U
46	BA	981	U
46	BA	984	U
46	BA	989	C
46	BA	990	U
46	BA	997	C
46	BA	1013	C
46	BA	1014	C
46	BA	1016	U
46	BA	1023	A
46	BA	1025	G
46	BA	1026	A
46	BA	1032	G
46	BA	1036	A
46	BA	1039	A
46	BA	1043	U
46	BA	1048	C
46	BA	1049	G
46	BA	1051	G
46	BA	1052	A
46	BA	1053	A
46	BA	1054	G
46	BA	1055	A
46	BA	1060	A
46	BA	1061	U
46	BA	1062	G
46	BA	1063	G
46	BA	1071	A
46	BA	1073	U
46	BA	1078	A
46	BA	1087	G
46	BA	1088	U
46	BA	1089	U
46	BA	1125	A

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Mol	Chain	Res	Type
46	BA	1127	C
46	BA	1135	A
46	BA	1136	G
46	BA	1138	A
46	BA	1140	U
46	BA	1144	G
46	BA	1147	U
46	BA	1149	G
46	BA	1157	U
46	BA	1161	A
46	BA	1162	G
46	BA	1164	A
46	BA	1165	C
46	BA	1166	A
46	BA	1167	A
46	BA	1176	C
46	BA	1181	U
46	BA	1182	G
46	BA	1184	U
46	BA	1185	U
46	BA	1186	U
46	BA	1187	U
46	BA	1193	A
46	BA	1199	A
46	BA	1204	U
46	BA	1205	C
46	BA	1211	A
46	BA	1224	C
46	BA	1226	U
46	BA	1230	G
46	BA	1232	U
46	BA	1236	A
46	BA	1237	A
46	BA	1238	A
46	BA	1239	U
46	BA	1240	U
46	BA	1241	U
46	BA	1243	G
46	BA	1244	A
46	BA	1245	U
46	BA	1246	C
46	BA	1247	A

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Mol	Chain	Res	Type
46	BA	1249	C
46	BA	1251	G
46	BA	1252	A
46	BA	1262	C
46	BA	1266	G
46	BA	1268	G
46	BA	1269	A
46	BA	1284	U
46	BA	1285	G
46	BA	1286	U
46	BA	1289	U
46	BA	1290	A
46	BA	1292	A
46	BA	1294	U
46	BA	1295	U
46	BA	1297	C
46	BA	1301	C
46	BA	1305	A
46	BA	1306	A
46	BA	1309	G
46	BA	1312	U
46	BA	1313	U
46	BA	1315	A
46	BA	1322	C
46	BA	1323	G
46	BA	1324	A
46	BA	1326	G
46	BA	1327	U
46	BA	1330	G
46	BA	1339	A
46	BA	1340	C
46	BA	1344	A
46	BA	1346	U
46	BA	1347	G
46	BA	1349	U
46	BA	1350	G
46	BA	1351	C
46	BA	1355	C
46	BA	1356	G
46	BA	1375	U
46	BA	1377	C
46	BA	1383	U

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Mol	Chain	Res	Type
46	BA	1385	A
46	BA	1387	A
46	BA	1388	G
46	BA	1394	C
46	BA	1397	G
46	BA	1399	U
46	BA	1402	G
46	BA	1406	U
46	BA	1407	C
46	BA	1411	C
46	BA	1412	C
46	BA	1420	U
46	BA	1423	A
46	BA	1424	G
46	BA	1426	U
46	BA	1427	C
46	BA	1428	G
46	BA	1429	G
46	BA	1430	U
46	BA	1431	U
46	BA	1432	U
46	BA	1433	C
46	BA	1434	U
46	BA	1436	U
46	BA	1443	U
46	BA	1446	A
46	BA	1450	C
46	BA	1451	U
46	BA	1453	C
46	BA	1455	A
46	BA	1456	G
46	BA	1457	U
46	BA	1465	G
46	BA	1466	A
46	BA	1471	A
46	BA	1472	G
46	BA	1474	A
46	BA	1480	A
46	BA	1488	C
46	BA	1489	A
46	BA	1490	C
46	BA	1491	A

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Mol	Chain	Res	Type
46	BA	1492	A
46	BA	1493	A
46	BA	1496	C
46	BA	1501	C
46	BA	1502	A
46	BA	1503	G
46	BA	1506	A
46	BA	1507	U
46	BA	1508	A
46	BA	1510	U
46	BA	1511	U
46	BA	1512	A
46	BA	1516	A
46	BA	1518	U
46	BA	1519	U
46	BA	1520	A
46	BA	1522	U
46	BA	1523	C
46	BA	1524	U
46	BA	1525	U
46	BA	1526	A
46	BA	1529	C
46	BA	1530	U
46	BA	1531	A
46	BA	1532	A
46	BA	1534	U
46	BA	1541	U
46	BA	1542	A
46	BA	1543	A
46	BA	1546	A
46	BA	1547	A
46	BA	1548	U
46	BA	1549	C
46	BA	1550	C
46	BA	1551	A
46	BA	1552	G
46	BA	1556	U
46	BA	1557	A
46	BA	1568	C
46	BA	1569	A

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	124	A
1	AA	127	A
1	AA	317	A
1	AA	395	C
1	AA	825	C
1	AA	900	A
1	AA	901	A
46	BA	39	A
46	BA	48	U
46	BA	69	C
46	BA	96	U
46	BA	100	C
46	BA	112	A
46	BA	160	A
46	BA	275	G
46	BA	292	U
46	BA	294	G
46	BA	347	G
46	BA	350	A
46	BA	431	A
46	BA	446	A
46	BA	463	U
46	BA	467	A
46	BA	512	A
46	BA	521	U
46	BA	555	C
46	BA	572	A
46	BA	573	C
46	BA	583	A
46	BA	653	C
46	BA	774	C
46	BA	812	C
46	BA	936	U
46	BA	1139	A
46	BA	1423	A
46	BA	1431	U
46	BA	1518	U

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

202 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
17	Y5P	AV	1	-	15,16,20	3.46	3 (20%)	18,22,29	2.87	3 (16%)
17	Y5P	AV	10	-	14,19,20	3.59	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AV	11	-	14,19,20	4.79	3 (21%)	18,26,29	1.84	1 (5%)
17	Y5P	AV	12	-	14,19,20	3.10	2 (14%)	18,26,29	2.99	2 (11%)
17	Y5P	AV	13	-	14,19,20	4.65	3 (21%)	18,26,29	1.80	1 (5%)
17	Y5P	AV	14	-	14,19,20	3.65	3 (21%)	18,26,29	2.86	2 (11%)
17	Y5P	AV	15	-	14,19,20	3.60	3 (21%)	18,26,29	2.82	2 (11%)
17	Y5P	AV	2	-	14,19,20	5.10	3 (21%)	18,26,29	1.56	1 (5%)
17	Y5P	AV	21	-	14,19,20	3.69	3 (21%)	18,26,29	2.87	2 (11%)
17	Y5P	AV	22	-	14,19,20	3.61	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AV	23	-	14,19,20	3.59	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AV	24	-	14,19,20	3.62	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AV	25	-	14,19,20	4.96	3 (21%)	18,26,29	1.57	1 (5%)
17	Y5P	AV	26	-	14,19,20	3.62	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AV	27	-	14,19,20	3.66	3 (21%)	18,26,29	2.87	2 (11%)
17	Y5P	AV	28	-	14,19,20	3.61	3 (21%)	18,26,29	2.82	2 (11%)
17	Y5P	AV	29	-	14,19,20	3.55	3 (21%)	18,26,29	2.88	2 (11%)
17	Y5P	AV	3	-	14,19,20	5.02	3 (21%)	18,26,29	1.59	1 (5%)
17	Y5P	AV	30	-	14,19,20	3.62	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AV	31	-	14,19,20	3.62	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AV	32	-	14,19,20	3.28	2 (14%)	18,26,29	2.88	2 (11%)
17	Y5P	AV	33	-	14,19,20	3.73	2 (14%)	18,26,29	2.39	2 (11%)
17	P5P	AV	34	-	16,23,24	1.48	2 (12%)	15,33,36	2.00	2 (13%)
17	P5P	AV	35	-	16,23,24	0.77	1 (6%)	15,33,36	0.76	0
17	P5P	AV	36	-	16,23,24	0.74	0	15,33,36	0.77	0
17	Y5P	AV	37	-	14,19,20	3.64	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AV	38	-	14,19,20	3.59	3 (21%)	18,26,29	2.82	2 (11%)
17	Y5P	AV	39	-	14,19,20	3.35	2 (14%)	18,26,29	2.90	2 (11%)
17	Y5P	AV	4	-	14,19,20	5.00	3 (21%)	18,26,29	1.66	1 (5%)
17	Y5P	AV	40	-	14,19,20	5.04	3 (21%)	18,26,29	1.66	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	Y5P	AV	41	-	14,19,20	5.23	3 (21%)	18,26,29	1.61	1 (5%)
17	Y5P	AV	42	-	14,19,20	5.13	3 (21%)	18,26,29	1.60	1 (5%)
17	Y5P	AV	43	-	14,19,20	4.99	3 (21%)	18,26,29	1.61	1 (5%)
17	Y5P	AV	44	-	14,19,20	3.65	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AV	45	-	14,19,20	3.28	2 (14%)	18,26,29	2.62	2 (11%)
17	Y5P	AV	48	-	14,19,20	5.03	3 (21%)	18,26,29	1.73	1 (5%)
17	Y5P	AV	49	-	14,19,20	4.77	3 (21%)	18,26,29	1.72	1 (5%)
17	Y5P	AV	5	-	14,19,20	3.64	3 (21%)	18,26,29	2.83	2 (11%)
17	Y5P	AV	50	-	14,19,20	3.25	3 (21%)	18,26,29	2.79	2 (11%)
17	Y5P	AV	51	-	14,19,20	3.25	2 (14%)	18,26,29	2.73	2 (11%)
17	Y5P	AV	52	-	14,19,20	3.62	3 (21%)	18,26,29	2.87	2 (11%)
17	Y5P	AV	53	-	14,19,20	3.60	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AV	54	-	14,19,20	3.20	2 (14%)	18,26,29	2.95	2 (11%)
17	Y5P	AV	55	-	14,19,20	3.28	2 (14%)	18,26,29	2.73	2 (11%)
17	Y5P	AV	56	-	14,19,20	4.85	3 (21%)	18,26,29	1.67	1 (5%)
17	Y5P	AV	57	-	14,19,20	3.67	3 (21%)	18,26,29	2.86	2 (11%)
17	Y5P	AV	58	-	14,19,20	3.63	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AV	59	-	14,19,20	3.33	3 (21%)	18,26,29	2.89	2 (11%)
17	Y5P	AV	6	-	14,19,20	3.60	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AV	60	-	14,19,20	3.32	2 (14%)	18,26,29	2.84	2 (11%)
17	Y5P	AV	61	-	14,19,20	4.92	3 (21%)	18,26,29	1.67	1 (5%)
17	Y5P	AV	62	-	14,19,20	4.87	3 (21%)	18,26,29	1.82	1 (5%)
17	Y5P	AV	63	-	14,19,20	3.61	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AV	64	-	14,19,20	3.66	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AV	65	-	14,19,20	3.62	3 (21%)	18,26,29	2.83	2 (11%)
17	Y5P	AV	66	-	14,19,20	3.24	2 (14%)	18,26,29	2.72	2 (11%)
17	Y5P	AV	67	-	14,19,20	4.91	3 (21%)	18,26,29	1.66	1 (5%)
17	Y5P	AV	68	-	14,19,20	4.91	3 (21%)	18,26,29	1.65	1 (5%)
17	Y5P	AV	69	-	14,19,20	3.62	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AV	7	-	14,19,20	3.57	3 (21%)	18,26,29	2.83	2 (11%)
17	Y5P	AV	70	-	14,19,20	3.63	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AV	71	-	14,19,20	3.60	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AV	72	-	14,19,20	4.96	3 (21%)	18,26,29	1.56	1 (5%)
17	Y5P	AV	73	-	14,19,20	3.66	3 (21%)	18,26,29	2.96	4 (22%)
17	Y5P	AV	74	-	14,19,20	4.86	3 (21%)	18,26,29	1.64	1 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	Y5P	AV	75	-	14,19,20	4.94	2 (14%)	18,26,29	1.68	1 (5%)
17	P5P	AV	76	-	16,23,24	0.67	0	15,33,36	0.75	1 (6%)
17	Y5P	AV	8	-	14,19,20	3.26	2 (14%)	18,26,29	3.08	2 (11%)
17	Y5P	AV	9	-	14,19,20	3.59	3 (21%)	18,26,29	2.86	2 (11%)
18	Y5P	AX	12	-	15,16,20	3.04	2 (13%)	18,22,29	2.94	2 (11%)
18	Y5P	AX	13	-	14,19,20	3.26	3 (21%)	18,26,29	2.91	2 (11%)
18	Y5P	AX	14	-	14,19,20	3.23	3 (21%)	18,26,29	2.70	2 (11%)
18	Y5P	AX	15	-	14,19,20	3.07	3 (21%)	18,26,29	2.95	2 (11%)
18	Y5P	AX	16	-	14,19,20	3.29	3 (21%)	18,26,29	2.93	2 (11%)
18	Y5P	AX	17	-	14,19,20	3.43	2 (14%)	18,26,29	2.88	2 (11%)
18	Y5P	AX	18	-	14,19,20	4.96	3 (21%)	18,26,29	1.62	1 (5%)
18	Y5P	AX	19	-	14,19,20	3.38	3 (21%)	18,26,29	2.80	2 (11%)
18	Y5P	AX	20	-	14,19,20	3.32	2 (14%)	18,26,29	2.87	2 (11%)
18	Y5P	AX	21	-	14,19,20	5.12	3 (21%)	18,26,29	1.61	1 (5%)
18	Y5P	AX	22	-	14,19,20	3.18	3 (21%)	18,26,29	2.92	2 (11%)
18	Y5P	AX	23	-	14,19,20	3.11	3 (21%)	18,26,29	2.97	2 (11%)
18	Y5P	AX	24	-	14,19,20	3.26	3 (21%)	18,26,29	2.72	2 (11%)
17	Y5P	AY	1	-	15,16,20	3.49	3 (20%)	18,22,29	2.84	2 (11%)
17	Y5P	AY	10	-	14,19,20	3.58	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AY	11	-	14,19,20	4.89	3 (21%)	18,26,29	1.65	1 (5%)
17	Y5P	AY	12	-	14,19,20	3.25	2 (14%)	18,26,29	2.89	2 (11%)
17	Y5P	AY	13	-	14,19,20	4.83	3 (21%)	18,26,29	1.80	1 (5%)
17	Y5P	AY	14	-	14,19,20	3.59	3 (21%)	18,26,29	2.81	2 (11%)
17	Y5P	AY	15	-	14,19,20	3.60	3 (21%)	18,26,29	2.88	3 (16%)
17	Y5P	AY	2	-	14,19,20	4.77	3 (21%)	18,26,29	1.76	1 (5%)
17	Y5P	AY	21	-	14,19,20	3.60	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AY	22	-	14,19,20	3.61	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AY	23	-	14,19,20	3.60	3 (21%)	18,26,29	2.83	2 (11%)
17	Y5P	AY	24	-	14,19,20	3.60	3 (21%)	18,26,29	2.82	2 (11%)
17	Y5P	AY	25	-	14,19,20	4.95	3 (21%)	18,26,29	1.77	1 (5%)
17	Y5P	AY	26	-	14,19,20	3.67	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AY	27	-	14,19,20	3.63	3 (21%)	18,26,29	2.88	3 (16%)
17	Y5P	AY	28	-	14,19,20	3.61	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AY	29	-	14,19,20	3.60	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AY	3	-	14,19,20	4.75	2 (14%)	18,26,29	1.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	Y5P	AY	30	-	14,19,20	3.60	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AY	31	-	14,19,20	3.62	3 (21%)	18,26,29	2.83	2 (11%)
17	Y5P	AY	32	-	14,19,20	3.38	2 (14%)	18,26,29	2.78	2 (11%)
17	Y5P	AY	33	-	14,19,20	3.53	2 (14%)	18,26,29	2.63	2 (11%)
17	P5P	AY	34	-	16,23,24	1.36	2 (12%)	15,33,36	1.97	3 (20%)
17	P5P	AY	35	-	16,23,24	0.73	0	15,33,36	0.77	0
17	P5P	AY	36	-	16,23,24	0.74	0	15,33,36	1.02	0
17	Y5P	AY	37	-	14,19,20	3.63	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AY	38	-	14,19,20	3.61	3 (21%)	18,26,29	2.83	2 (11%)
17	Y5P	AY	39	-	14,19,20	3.24	2 (14%)	18,26,29	2.97	2 (11%)
17	Y5P	AY	4	-	14,19,20	4.89	3 (21%)	18,26,29	1.82	1 (5%)
17	Y5P	AY	40	-	14,19,20	4.99	2 (14%)	18,26,29	1.82	1 (5%)
17	Y5P	AY	41	-	14,19,20	4.97	3 (21%)	18,26,29	1.80	1 (5%)
17	Y5P	AY	42	-	14,19,20	4.86	3 (21%)	18,26,29	1.87	1 (5%)
17	Y5P	AY	43	-	14,19,20	4.90	3 (21%)	18,26,29	1.82	1 (5%)
17	Y5P	AY	44	-	14,19,20	3.64	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AY	45	-	14,19,20	3.38	2 (14%)	18,26,29	2.95	2 (11%)
17	Y5P	AY	48	-	14,19,20	4.96	3 (21%)	18,26,29	1.69	1 (5%)
17	Y5P	AY	49	-	14,19,20	4.84	3 (21%)	18,26,29	1.77	1 (5%)
17	Y5P	AY	5	-	14,19,20	3.59	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AY	50	-	14,19,20	3.33	2 (14%)	18,26,29	2.93	2 (11%)
17	Y5P	AY	51	-	14,19,20	3.16	2 (14%)	18,26,29	3.05	2 (11%)
17	Y5P	AY	52	-	14,19,20	3.58	3 (21%)	18,26,29	2.86	2 (11%)
17	Y5P	AY	53	-	14,19,20	3.60	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AY	54	-	14,19,20	3.16	2 (14%)	18,26,29	3.04	2 (11%)
17	Y5P	AY	55	-	14,19,20	3.53	3 (21%)	18,26,29	2.83	3 (16%)
17	Y5P	AY	56	-	14,19,20	4.86	3 (21%)	18,26,29	1.71	1 (5%)
17	Y5P	AY	57	-	14,19,20	3.62	3 (21%)	18,26,29	2.83	2 (11%)
17	Y5P	AY	58	-	14,19,20	3.61	3 (21%)	18,26,29	2.86	2 (11%)
17	Y5P	AY	59	-	14,19,20	3.26	2 (14%)	18,26,29	2.87	2 (11%)
17	Y5P	AY	6	-	14,19,20	3.60	3 (21%)	18,26,29	2.85	2 (11%)
17	Y5P	AY	60	-	14,19,20	3.21	2 (14%)	18,26,29	2.85	2 (11%)
17	Y5P	AY	61	-	14,19,20	4.94	3 (21%)	18,26,29	1.78	1 (5%)
17	Y5P	AY	62	-	14,19,20	4.94	3 (21%)	18,26,29	1.86	1 (5%)
17	Y5P	AY	63	-	14,19,20	3.61	3 (21%)	18,26,29	2.84	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	Y5P	AY	64	-	14,19,20	3.64	3 (21%)	18,26,29	2.87	2 (11%)
17	Y5P	AY	65	-	14,19,20	3.63	3 (21%)	18,26,29	2.86	2 (11%)
17	Y5P	AY	66	-	14,19,20	3.23	2 (14%)	18,26,29	2.88	2 (11%)
17	Y5P	AY	67	-	14,19,20	4.98	3 (21%)	18,26,29	1.65	1 (5%)
17	Y5P	AY	68	-	14,19,20	4.82	3 (21%)	18,26,29	1.75	1 (5%)
17	Y5P	AY	69	-	14,19,20	3.63	3 (21%)	18,26,29	2.90	3 (16%)
17	Y5P	AY	7	-	14,19,20	3.59	3 (21%)	18,26,29	2.83	2 (11%)
17	Y5P	AY	70	-	14,19,20	3.66	3 (21%)	18,26,29	2.84	2 (11%)
17	Y5P	AY	71	-	14,19,20	3.64	3 (21%)	18,26,29	2.87	2 (11%)
17	Y5P	AY	72	-	14,19,20	4.91	3 (21%)	18,26,29	1.51	1 (5%)
17	Y5P	AY	73	-	14,19,20	3.70	3 (21%)	18,26,29	3.00	4 (22%)
17	Y5P	AY	74	-	14,19,20	4.80	3 (21%)	18,26,29	1.62	1 (5%)
17	Y5P	AY	75	-	14,19,20	4.82	3 (21%)	18,26,29	1.70	1 (5%)
17	P5P	AY	76	-	16,23,24	0.69	0	15,33,36	0.75	0
17	Y5P	AY	8	-	14,19,20	3.20	2 (14%)	18,26,29	2.94	2 (11%)
17	Y5P	AY	9	-	14,19,20	3.60	3 (21%)	18,26,29	2.83	2 (11%)
47	P5P	BB	10	47	16,23,24	1.28	3 (18%)	15,33,36	1.90	3 (20%)
47	Y5P	BB	11	47	14,19,20	5.08	3 (21%)	18,26,29	1.56	1 (5%)
47	Y5P	BB	12	47	14,19,20	3.15	2 (14%)	18,26,29	2.78	2 (11%)
47	Y5P	BB	13	47	14,19,20	3.14	2 (14%)	18,26,29	3.06	2 (11%)
47	P5P	BB	14	47	16,23,24	0.69	0	15,33,36	0.94	0
47	P5P	BB	15	47	16,23,24	0.69	0	15,33,36	0.70	0
47	P5P	BB	23	47	16,23,24	0.74	1 (6%)	15,33,36	2.05	3 (20%)
47	P5P	BB	24	47	16,23,24	0.86	1 (6%)	15,33,36	0.90	0
47	P5P	BB	25	47	16,23,24	1.43	3 (18%)	15,33,36	2.09	3 (20%)
47	Y5P	BB	26	47	14,19,20	4.91	3 (21%)	18,26,29	1.88	1 (5%)
47	P5P	BB	27	47	16,23,24	0.71	0	15,33,36	1.04	1 (6%)
47	P5P	BB	28	47	16,23,24	0.70	0	15,33,36	0.69	0
47	P5P	BB	29	47	16,23,24	1.34	2 (12%)	15,33,36	2.07	3 (20%)
47	P5P	BB	30	47	16,23,24	1.31	2 (12%)	15,33,36	1.75	2 (13%)
47	Y5P	BB	31	47	14,19,20	5.08	3 (21%)	18,26,29	1.73	1 (5%)
47	P5P	BB	32	47	16,23,24	0.74	0	15,33,36	0.81	0
47	Y5P	BB	33	47	14,19,20	5.04	3 (21%)	18,26,29	1.77	1 (5%)
47	Y5P	BB	34	47	14,19,20	3.26	3 (21%)	18,26,29	2.71	2 (11%)
47	P5P	BB	35	47	16,23,24	1.40	2 (12%)	15,33,36	1.96	2 (13%)
47	P5P	BB	36	47	16,23,24	0.73	0	15,33,36	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
47	P5P	BB	37	47	16,23,24	0.75	0	15,33,36	1.08	1 (6%)
47	P5P	BB	38	47	16,23,24	0.76	0	15,33,36	0.84	0
47	P5P	BB	39	47	16,23,24	0.74	0	15,33,36	0.76	0
47	Y5P	BB	40	47	14,19,20	3.34	2 (14%)	18,26,29	2.73	2 (11%)
47	P5P	BB	41	47	16,23,24	1.36	3 (18%)	15,33,36	2.02	2 (13%)
47	Y5P	BB	42	47	14,19,20	4.92	3 (21%)	18,26,29	1.71	1 (5%)
47	Y5P	BB	43	47	14,19,20	4.84	3 (21%)	18,26,29	1.77	1 (5%)
47	Y5P	BB	44	47	14,19,20	3.38	2 (14%)	18,26,29	2.65	2 (11%)
47	P5P	BB	45	47	16,23,24	0.73	0	15,33,36	0.77	0
47	P5P	BB	46	47	16,23,24	1.26	3 (18%)	15,33,36	1.74	2 (13%)
47	P5P	BB	47	47	16,23,24	0.67	0	15,33,36	0.92	1 (6%)
47	Y5P	BB	48	47	14,19,20	3.18	2 (14%)	18,26,29	2.92	2 (11%)
47	P5P	BB	49	47	16,23,24	1.38	2 (12%)	15,33,36	1.96	2 (13%)
47	P5P	BB	5	47	16,23,24	0.71	0	15,33,36	0.75	0
47	P5P	BB	50	47	16,23,24	0.76	0	15,33,36	0.87	0
47	P5P	BB	51	47	16,23,24	1.35	2 (12%)	15,33,36	1.91	2 (13%)
47	Y5P	BB	52	47	14,19,20	4.95	3 (21%)	18,26,29	1.75	1 (5%)
47	Y5P	BB	53	47	14,19,20	4.95	3 (21%)	18,26,29	1.75	1 (5%)
47	P5P	BB	58	47	16,23,24	0.70	0	15,33,36	0.73	0
47	P5P	BB	59	47	16,23,24	1.35	2 (12%)	15,33,36	1.87	2 (13%)
47	Y5P	BB	6	47	14,19,20	3.31	2 (14%)	18,26,29	2.77	2 (11%)
47	Y5P	BB	60	47	14,19,20	4.75	3 (21%)	18,26,29	1.85	1 (5%)
47	Y5P	BB	61	47	14,19,20	3.15	2 (14%)	18,26,29	2.75	2 (11%)
47	Y5P	BB	62	47	14,19,20	3.20	2 (14%)	18,26,29	2.93	2 (11%)
47	Y5P	BB	63	47	14,19,20	4.98	3 (21%)	18,26,29	1.72	1 (5%)
47	P5P	BB	64	47	16,23,24	0.70	0	15,33,36	0.81	0
47	Y5P	BB	65	47	14,19,20	3.30	2 (14%)	18,26,29	2.93	2 (11%)
47	P5P	BB	66	47	16,23,24	0.73	0	15,33,36	0.77	0
47	P5P	BB	7	47	16,23,24	1.32	2 (12%)	15,33,36	1.92	2 (13%)
47	Y5P	BB	8	47	14,19,20	3.19	2 (14%)	18,26,29	3.04	2 (11%)
47	P5P	BB	9	47	16,23,24	0.70	0	15,33,36	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Y5P	AV	1	-	-	0/6/30/34	0/2/2/2
17	Y5P	AV	10	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	11	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	12	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	13	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	14	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	15	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	2	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	21	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	22	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	23	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	24	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	25	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	26	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	27	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	28	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	29	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	3	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	30	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	31	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	32	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	33	-	-	0/7/33/34	0/2/2/2
17	P5P	AV	34	-	-	0/3/25/26	0/3/3/3
17	P5P	AV	35	-	-	0/3/25/26	0/3/3/3
17	P5P	AV	36	-	-	0/3/25/26	0/3/3/3
17	Y5P	AV	37	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	38	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	39	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	4	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	40	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	41	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	42	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	43	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	44	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	45	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	48	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	49	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	5	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	50	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	51	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	52	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	53	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	54	-	-	0/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Y5P	AV	55	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	56	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	57	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	58	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	59	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	6	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	60	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	61	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	62	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	63	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	64	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	65	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	66	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	67	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	68	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	69	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	7	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	70	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	71	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	72	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	73	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	74	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	75	-	-	0/7/33/34	0/2/2/2
17	P5P	AV	76	-	-	0/3/25/26	0/3/3/3
17	Y5P	AV	8	-	-	0/7/33/34	0/2/2/2
17	Y5P	AV	9	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	12	-	-	0/6/30/34	0/2/2/2
18	Y5P	AX	13	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	14	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	15	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	16	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	17	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	18	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	19	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	20	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	21	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	22	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	23	-	-	0/7/33/34	0/2/2/2
18	Y5P	AX	24	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	1	-	-	0/6/30/34	0/2/2/2
17	Y5P	AY	10	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	11	-	-	0/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Y5P	AY	12	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	13	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	14	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	15	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	2	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	21	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	22	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	23	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	24	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	25	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	26	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	27	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	28	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	29	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	3	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	30	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	31	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	32	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	33	-	-	0/7/33/34	0/2/2/2
17	P5P	AY	34	-	-	0/3/25/26	0/3/3/3
17	P5P	AY	35	-	-	0/3/25/26	0/3/3/3
17	P5P	AY	36	-	-	0/3/25/26	0/3/3/3
17	Y5P	AY	37	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	38	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	39	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	4	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	40	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	41	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	42	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	43	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	44	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	45	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	48	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	49	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	5	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	50	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	51	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	52	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	53	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	54	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	55	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	56	-	-	0/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Y5P	AY	57	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	58	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	59	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	6	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	60	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	61	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	62	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	63	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	64	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	65	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	66	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	67	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	68	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	69	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	7	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	70	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	71	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	72	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	73	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	74	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	75	-	-	0/7/33/34	0/2/2/2
17	P5P	AY	76	-	-	0/3/25/26	0/3/3/3
17	Y5P	AY	8	-	-	0/7/33/34	0/2/2/2
17	Y5P	AY	9	-	-	0/7/33/34	0/2/2/2
47	P5P	BB	10	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	11	47	-	0/7/33/34	0/2/2/2
47	Y5P	BB	12	47	-	0/7/33/34	0/2/2/2
47	Y5P	BB	13	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	14	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	15	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	23	47	-	1/3/25/26	0/3/3/3
47	P5P	BB	24	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	25	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	26	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	27	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	28	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	29	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	30	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	31	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	32	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	33	47	-	0/7/33/34	0/2/2/2
47	Y5P	BB	34	47	-	0/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	P5P	BB	35	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	36	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	37	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	38	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	39	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	40	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	41	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	42	47	-	0/7/33/34	0/2/2/2
47	Y5P	BB	43	47	-	0/7/33/34	0/2/2/2
47	Y5P	BB	44	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	45	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	46	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	47	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	48	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	49	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	5	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	50	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	51	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	52	47	-	0/7/33/34	0/2/2/2
47	Y5P	BB	53	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	58	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	59	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	6	47	-	0/7/33/34	0/2/2/2
47	Y5P	BB	60	47	-	0/7/33/34	0/2/2/2
47	Y5P	BB	61	47	-	0/7/33/34	0/2/2/2
47	Y5P	BB	62	47	-	0/7/33/34	0/2/2/2
47	Y5P	BB	63	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	64	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	65	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	66	47	-	0/3/25/26	0/3/3/3
47	P5P	BB	7	47	-	0/3/25/26	0/3/3/3
47	Y5P	BB	8	47	-	0/7/33/34	0/2/2/2
47	P5P	BB	9	47	-	0/3/25/26	0/3/3/3

All (486) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AV	41	Y5P	C4-N3	-19.22	1.33	1.46
18	AX	21	Y5P	C4-N3	-18.84	1.33	1.46
17	AV	42	Y5P	C4-N3	-18.82	1.33	1.46
17	AV	2	Y5P	C4-N3	-18.61	1.33	1.46
47	BB	31	Y5P	C4-N3	-18.55	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	BB	33	Y5P	C4-N3	-18.49	1.33	1.46
47	BB	11	Y5P	C4-N3	-18.48	1.33	1.46
17	AV	40	Y5P	C4-N3	-18.42	1.33	1.46
17	AV	48	Y5P	C4-N3	-18.39	1.33	1.46
17	AY	40	Y5P	C4-N3	-18.33	1.33	1.46
17	AV	3	Y5P	C4-N3	-18.28	1.33	1.46
17	AV	4	Y5P	C4-N3	-18.22	1.33	1.46
17	AV	75	Y5P	C4-N3	-18.21	1.33	1.46
47	BB	63	Y5P	C4-N3	-18.15	1.33	1.46
17	AY	48	Y5P	C4-N3	-18.13	1.33	1.46
17	AY	25	Y5P	C4-N3	-18.13	1.33	1.46
17	AY	67	Y5P	C4-N3	-18.13	1.33	1.46
17	AY	41	Y5P	C4-N3	-18.13	1.33	1.46
17	AY	61	Y5P	C4-N3	-18.11	1.33	1.46
18	AX	18	Y5P	C4-N3	-18.08	1.33	1.46
47	BB	53	Y5P	C4-N3	-18.05	1.33	1.46
47	BB	52	Y5P	C4-N3	-18.02	1.33	1.46
17	AV	43	Y5P	C4-N3	-18.01	1.33	1.46
17	AV	72	Y5P	C4-N3	-18.01	1.33	1.46
47	BB	42	Y5P	C4-N3	-17.97	1.33	1.46
17	AV	61	Y5P	C4-N3	-17.96	1.33	1.46
17	AY	62	Y5P	C4-N3	-17.93	1.33	1.46
17	AV	68	Y5P	C4-N3	-17.91	1.33	1.46
17	AV	25	Y5P	C4-N3	-17.91	1.33	1.46
17	AY	43	Y5P	C4-N3	-17.88	1.34	1.46
17	AY	11	Y5P	C4-N3	-17.86	1.34	1.46
47	BB	26	Y5P	C4-N3	-17.86	1.34	1.46
17	AV	67	Y5P	C4-N3	-17.83	1.34	1.46
17	AV	62	Y5P	C4-N3	-17.81	1.34	1.46
17	AY	4	Y5P	C4-N3	-17.75	1.34	1.46
17	AY	72	Y5P	C4-N3	-17.73	1.34	1.46
17	AY	42	Y5P	C4-N3	-17.70	1.34	1.46
17	AY	56	Y5P	C4-N3	-17.67	1.34	1.46
17	AY	49	Y5P	C4-N3	-17.65	1.34	1.46
17	AY	13	Y5P	C4-N3	-17.62	1.34	1.46
47	BB	43	Y5P	C4-N3	-17.61	1.34	1.46
17	AV	74	Y5P	C4-N3	-17.61	1.34	1.46
17	AV	56	Y5P	C4-N3	-17.60	1.34	1.46
17	AY	68	Y5P	C4-N3	-17.52	1.34	1.46
17	AY	75	Y5P	C4-N3	-17.51	1.34	1.46
17	AV	11	Y5P	C4-N3	-17.47	1.34	1.46
17	AY	3	Y5P	C4-N3	-17.36	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AY	74	Y5P	C4-N3	-17.34	1.34	1.46
17	AV	49	Y5P	C4-N3	-17.31	1.34	1.46
47	BB	60	Y5P	C4-N3	-17.30	1.34	1.46
17	AY	2	Y5P	C4-N3	-17.20	1.34	1.46
17	AV	13	Y5P	C4-N3	-16.86	1.34	1.46
17	AV	33	Y5P	C4-N3	-13.21	1.37	1.46
17	AY	33	Y5P	C4-N3	-12.49	1.37	1.46
18	AX	17	Y5P	C4-N3	-12.21	1.37	1.46
17	AY	73	Y5P	C4-N3	-12.20	1.37	1.46
17	AV	24	Y5P	C4-N3	-12.19	1.37	1.46
17	AY	55	Y5P	C4-N3	-12.19	1.37	1.46
17	AY	26	Y5P	C4-N3	-12.17	1.37	1.46
17	AV	52	Y5P	C4-N3	-12.16	1.37	1.46
17	AV	21	Y5P	C4-N3	-12.16	1.37	1.46
17	AY	22	Y5P	C4-N3	-12.16	1.37	1.46
17	AV	64	Y5P	C4-N3	-12.16	1.37	1.46
17	AY	69	Y5P	C4-N3	-12.16	1.37	1.46
17	AY	70	Y5P	C4-N3	-12.15	1.37	1.46
17	AV	73	Y5P	C4-N3	-12.15	1.37	1.46
17	AV	37	Y5P	C4-N3	-12.14	1.38	1.46
17	AV	29	Y5P	C4-N3	-12.13	1.38	1.46
17	AV	28	Y5P	C4-N3	-12.13	1.38	1.46
17	AY	9	Y5P	C4-N3	-12.13	1.38	1.46
17	AY	29	Y5P	C4-N3	-12.12	1.38	1.46
17	AY	44	Y5P	C4-N3	-12.12	1.38	1.46
17	AY	57	Y5P	C4-N3	-12.11	1.38	1.46
17	AY	27	Y5P	C4-N3	-12.11	1.38	1.46
17	AV	5	Y5P	C4-N3	-12.11	1.38	1.46
17	AV	57	Y5P	C4-N3	-12.10	1.38	1.46
17	AY	37	Y5P	C4-N3	-12.10	1.38	1.46
17	AY	31	Y5P	C4-N3	-12.10	1.38	1.46
17	AV	44	Y5P	C4-N3	-12.10	1.38	1.46
17	AY	63	Y5P	C4-N3	-12.10	1.38	1.46
17	AV	63	Y5P	C4-N3	-12.09	1.38	1.46
17	AY	58	Y5P	C4-N3	-12.09	1.38	1.46
17	AV	14	Y5P	C4-N3	-12.09	1.38	1.46
17	AY	65	Y5P	C4-N3	-12.09	1.38	1.46
17	AY	71	Y5P	C4-N3	-12.09	1.38	1.46
17	AV	27	Y5P	C4-N3	-12.08	1.38	1.46
17	AV	65	Y5P	C4-N3	-12.08	1.38	1.46
17	AV	58	Y5P	C4-N3	-12.08	1.38	1.46
17	AY	38	Y5P	C4-N3	-12.07	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AV	69	Y5P	C4-N3	-12.07	1.38	1.46
17	AV	31	Y5P	C4-N3	-12.07	1.38	1.46
17	AV	30	Y5P	C4-N3	-12.07	1.38	1.46
17	AV	23	Y5P	C4-N3	-12.07	1.38	1.46
17	AV	15	Y5P	C4-N3	-12.06	1.38	1.46
17	AV	71	Y5P	C4-N3	-12.06	1.38	1.46
17	AY	52	Y5P	C4-N3	-12.06	1.38	1.46
17	AV	1	Y5P	C4-N3	-12.06	1.38	1.46
17	AY	28	Y5P	C4-N3	-12.05	1.38	1.46
17	AV	26	Y5P	C4-N3	-12.05	1.38	1.46
17	AY	53	Y5P	C4-N3	-12.05	1.38	1.46
17	AY	24	Y5P	C4-N3	-12.05	1.38	1.46
17	AV	22	Y5P	C4-N3	-12.05	1.38	1.46
17	AV	9	Y5P	C4-N3	-12.04	1.38	1.46
17	AY	6	Y5P	C4-N3	-12.04	1.38	1.46
17	AV	7	Y5P	C4-N3	-12.04	1.38	1.46
17	AY	64	Y5P	C4-N3	-12.03	1.38	1.46
17	AY	1	Y5P	C4-N3	-12.03	1.38	1.46
17	AV	38	Y5P	C4-N3	-12.03	1.38	1.46
17	AV	53	Y5P	C4-N3	-12.03	1.38	1.46
17	AY	7	Y5P	C4-N3	-12.02	1.38	1.46
17	AV	10	Y5P	C4-N3	-12.02	1.38	1.46
17	AV	70	Y5P	C4-N3	-12.02	1.38	1.46
17	AV	6	Y5P	C4-N3	-12.01	1.38	1.46
17	AY	30	Y5P	C4-N3	-12.01	1.38	1.46
17	AY	14	Y5P	C4-N3	-12.01	1.38	1.46
17	AY	5	Y5P	C4-N3	-12.00	1.38	1.46
17	AY	15	Y5P	C4-N3	-11.98	1.38	1.46
17	AY	10	Y5P	C4-N3	-11.97	1.38	1.46
17	AY	23	Y5P	C4-N3	-11.94	1.38	1.46
17	AY	21	Y5P	C4-N3	-11.93	1.38	1.46
17	AY	45	Y5P	C4-N3	-11.93	1.38	1.46
17	AY	32	Y5P	C4-N3	-11.90	1.38	1.46
47	BB	40	Y5P	C4-N3	-11.81	1.38	1.46
47	BB	44	Y5P	C4-N3	-11.81	1.38	1.46
18	AX	19	Y5P	C4-N3	-11.75	1.38	1.46
17	AV	39	Y5P	C4-N3	-11.70	1.38	1.46
17	AY	50	Y5P	C4-N3	-11.68	1.38	1.46
18	AX	20	Y5P	C4-N3	-11.66	1.38	1.46
47	BB	65	Y5P	C4-N3	-11.58	1.38	1.46
47	BB	6	Y5P	C4-N3	-11.53	1.38	1.46
17	AV	60	Y5P	C4-N3	-11.49	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AV	59	Y5P	C4-N3	-11.49	1.38	1.46
17	AV	32	Y5P	C4-N3	-11.46	1.38	1.46
17	AV	8	Y5P	C4-N3	-11.46	1.38	1.46
18	AX	16	Y5P	C4-N3	-11.45	1.38	1.46
17	AV	55	Y5P	C4-N3	-11.36	1.38	1.46
17	AY	39	Y5P	C4-N3	-11.32	1.38	1.46
17	AY	12	Y5P	C4-N3	-11.28	1.38	1.46
17	AY	59	Y5P	C4-N3	-11.26	1.38	1.46
17	AY	66	Y5P	C4-N3	-11.23	1.38	1.46
17	AV	51	Y5P	C4-N3	-11.19	1.38	1.46
18	AX	13	Y5P	C4-N3	-11.17	1.38	1.46
17	AV	45	Y5P	C4-N3	-11.16	1.38	1.46
17	AY	8	Y5P	C4-N3	-11.12	1.38	1.46
47	BB	8	Y5P	C4-N3	-11.10	1.38	1.46
17	AV	66	Y5P	C4-N3	-11.10	1.38	1.46
17	AV	50	Y5P	C4-N3	-11.09	1.38	1.46
17	AY	60	Y5P	C4-N3	-11.09	1.38	1.46
47	BB	34	Y5P	C4-N3	-11.07	1.38	1.46
47	BB	48	Y5P	C4-N3	-11.04	1.38	1.46
47	BB	62	Y5P	C4-N3	-11.00	1.38	1.46
18	AX	14	Y5P	C4-N3	-10.95	1.38	1.46
17	AV	54	Y5P	C4-N3	-10.93	1.38	1.46
17	AY	54	Y5P	C4-N3	-10.91	1.38	1.46
17	AY	51	Y5P	C4-N3	-10.88	1.38	1.46
18	AX	24	Y5P	C4-N3	-10.87	1.38	1.46
47	BB	13	Y5P	C4-N3	-10.87	1.38	1.46
47	BB	61	Y5P	C4-N3	-10.85	1.38	1.46
47	BB	12	Y5P	C4-N3	-10.81	1.38	1.46
18	AX	22	Y5P	C4-N3	-10.79	1.38	1.46
18	AX	12	Y5P	C4-N3	-10.77	1.38	1.46
17	AV	12	Y5P	C4-N3	-10.55	1.39	1.46
18	AX	23	Y5P	C4-N3	-10.54	1.39	1.46
18	AX	15	Y5P	C4-N3	-10.25	1.39	1.46
47	BB	25	P5P	C8-N7	-2.28	1.30	1.34
47	BB	10	P5P	C8-N7	-2.12	1.30	1.34
47	BB	46	P5P	C8-N7	-2.05	1.30	1.34
47	BB	41	P5P	C8-N7	-2.01	1.30	1.34
47	BB	24	P5P	C8-N7	-2.01	1.30	1.34
18	AX	21	Y5P	C2-N1	2.00	1.39	1.36
18	AX	14	Y5P	C2-N1	2.01	1.39	1.36
17	AV	35	P5P	C6-N1	2.02	1.36	1.32
47	BB	30	P5P	C2-N1	2.03	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	AX	19	Y5P	C2-N1	2.06	1.39	1.36
47	BB	34	Y5P	C2-N1	2.07	1.39	1.36
17	AY	25	Y5P	C2-N1	2.08	1.39	1.36
18	AX	22	Y5P	C2-N1	2.08	1.39	1.36
18	AX	23	Y5P	C2-N1	2.09	1.39	1.36
17	AV	50	Y5P	C2-N1	2.09	1.39	1.36
17	AV	42	Y5P	C2-N1	2.10	1.39	1.36
18	AX	16	Y5P	C2-N1	2.10	1.39	1.36
18	AX	13	Y5P	C2-N1	2.11	1.39	1.36
17	AV	59	Y5P	C2-N1	2.11	1.39	1.36
47	BB	23	P5P	C6-N1	2.13	1.36	1.32
47	BB	46	P5P	C2-N1	2.14	1.37	1.33
18	AX	15	Y5P	C2-N1	2.15	1.39	1.36
17	AV	41	Y5P	C2-N1	2.18	1.39	1.36
17	AY	11	Y5P	C2-N1	2.18	1.39	1.36
17	AY	13	Y5P	C2-N1	2.21	1.40	1.36
17	AV	40	Y5P	C2-N1	2.21	1.40	1.36
17	AY	61	Y5P	C2-N1	2.22	1.40	1.36
47	BB	33	Y5P	C2-N1	2.25	1.40	1.36
47	BB	29	P5P	C2-N1	2.28	1.37	1.33
17	AV	62	Y5P	C2-N1	2.28	1.40	1.36
47	BB	10	P5P	C2-N1	2.28	1.37	1.33
47	BB	41	P5P	C2-N1	2.29	1.37	1.33
17	AV	61	Y5P	C2-N1	2.30	1.40	1.36
47	BB	7	P5P	C2-N1	2.30	1.37	1.33
17	AY	48	Y5P	C2-N1	2.34	1.40	1.36
47	BB	35	P5P	C2-N1	2.35	1.37	1.33
47	BB	59	P5P	C2-N1	2.36	1.37	1.33
47	BB	51	P5P	C2-N1	2.36	1.37	1.33
47	BB	60	Y5P	C2-N1	2.40	1.40	1.36
17	AV	2	Y5P	C2-N1	2.41	1.40	1.36
17	AV	13	Y5P	C2-N1	2.41	1.40	1.36
47	BB	25	P5P	C2-N1	2.41	1.38	1.33
17	AV	68	Y5P	C2-N1	2.43	1.40	1.36
47	BB	63	Y5P	C2-N1	2.43	1.40	1.36
47	BB	49	P5P	C2-N1	2.47	1.38	1.33
47	BB	42	Y5P	C2-N1	2.47	1.40	1.36
17	AY	43	Y5P	C2-N1	2.47	1.40	1.36
17	AV	11	Y5P	C2-N1	2.49	1.40	1.36
17	AY	49	Y5P	C2-N1	2.49	1.40	1.36
17	AV	3	Y5P	C2-N1	2.51	1.40	1.36
17	AY	68	Y5P	C2-N1	2.51	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	AX	24	Y5P	C2-N1	2.53	1.40	1.36
17	AY	42	Y5P	C2-N1	2.54	1.40	1.36
17	AV	75	Y5P	C2-N3	2.54	1.34	1.29
17	AV	49	Y5P	C2-N1	2.55	1.40	1.36
17	AY	56	Y5P	C2-N1	2.55	1.40	1.36
17	AV	48	Y5P	C2-N1	2.56	1.40	1.36
17	AY	75	Y5P	C2-N1	2.56	1.40	1.36
17	AY	67	Y5P	C2-N1	2.57	1.40	1.36
47	BB	43	Y5P	C2-N1	2.57	1.40	1.36
47	BB	53	Y5P	C2-N1	2.58	1.40	1.36
47	BB	52	Y5P	C2-N1	2.58	1.40	1.36
17	AV	4	Y5P	C2-N1	2.59	1.40	1.36
17	AY	34	P5P	C2-N1	2.59	1.38	1.33
17	AV	34	P5P	C2-N1	2.60	1.38	1.33
18	AX	18	Y5P	C2-N1	2.60	1.40	1.36
17	AY	41	Y5P	C2-N1	2.66	1.40	1.36
17	AV	74	Y5P	C2-N1	2.66	1.40	1.36
17	AY	55	Y5P	C2-N1	2.68	1.40	1.36
17	AV	56	Y5P	C2-N1	2.68	1.40	1.36
47	BB	31	Y5P	C2-N1	2.69	1.40	1.36
17	AV	67	Y5P	C2-N1	2.71	1.40	1.36
17	AV	29	Y5P	C1'-N1	2.72	1.54	1.46
17	AY	40	Y5P	C2-N3	2.75	1.35	1.29
17	AY	74	Y5P	C2-N1	2.76	1.40	1.36
17	AV	41	Y5P	C2-N3	2.77	1.35	1.29
18	AX	21	Y5P	C2-N3	2.78	1.35	1.29
17	AY	4	Y5P	C2-N1	2.83	1.41	1.36
47	BB	26	Y5P	C2-N1	2.84	1.41	1.36
47	BB	33	Y5P	C2-N3	2.87	1.35	1.29
17	AY	62	Y5P	C2-N1	2.88	1.41	1.36
47	BB	11	Y5P	C2-N1	2.89	1.41	1.36
17	AV	42	Y5P	C2-N3	2.90	1.35	1.29
17	AV	48	Y5P	C2-N3	2.90	1.35	1.29
17	AY	61	Y5P	C2-N3	2.90	1.35	1.29
17	AV	72	Y5P	C2-N1	2.90	1.41	1.36
17	AY	48	Y5P	C2-N3	2.93	1.35	1.29
17	AY	2	Y5P	C2-N1	2.94	1.41	1.36
17	AY	25	Y5P	C2-N3	2.96	1.35	1.29
18	AX	18	Y5P	C2-N3	2.97	1.35	1.29
17	AV	25	Y5P	C2-N1	2.99	1.41	1.36
17	AY	49	Y5P	C2-N3	3.00	1.35	1.29
17	AY	41	Y5P	C2-N3	3.01	1.35	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	BB	42	Y5P	C2-N3	3.01	1.35	1.29
47	BB	31	Y5P	C2-N3	3.01	1.35	1.29
17	AV	62	Y5P	C2-N3	3.01	1.35	1.29
17	AV	40	Y5P	C2-N3	3.04	1.35	1.29
17	AV	4	Y5P	C2-N3	3.05	1.35	1.29
17	AY	72	Y5P	C2-N1	3.07	1.41	1.36
17	AY	43	Y5P	C2-N3	3.07	1.35	1.29
47	BB	26	Y5P	C2-N3	3.07	1.35	1.29
17	AV	11	Y5P	C2-N3	3.08	1.35	1.29
47	BB	53	Y5P	C2-N3	3.08	1.35	1.29
17	AY	62	Y5P	C2-N3	3.09	1.35	1.29
17	AV	61	Y5P	C2-N3	3.10	1.35	1.29
17	AY	3	Y5P	C2-N3	3.11	1.36	1.29
17	AY	11	Y5P	C2-N3	3.12	1.36	1.29
47	BB	52	Y5P	C2-N3	3.13	1.36	1.29
17	AY	67	Y5P	C2-N3	3.14	1.36	1.29
47	BB	43	Y5P	C2-N3	3.14	1.36	1.29
47	BB	60	Y5P	C2-N3	3.14	1.36	1.29
47	BB	11	Y5P	C2-N3	3.15	1.36	1.29
17	AV	2	Y5P	C2-N3	3.16	1.36	1.29
17	AV	68	Y5P	C2-N3	3.17	1.36	1.29
17	AY	13	Y5P	C2-N3	3.17	1.36	1.29
17	AY	42	Y5P	C2-N3	3.17	1.36	1.29
17	AY	56	Y5P	C2-N3	3.18	1.36	1.29
17	AV	43	Y5P	C2-N1	3.20	1.41	1.36
47	BB	63	Y5P	C2-N3	3.22	1.36	1.29
17	AV	67	Y5P	C2-N3	3.23	1.36	1.29
17	AV	3	Y5P	C2-N3	3.23	1.36	1.29
17	AV	7	Y5P	C1'-N1	3.23	1.56	1.46
17	AY	68	Y5P	C2-N3	3.24	1.36	1.29
17	AY	75	Y5P	C2-N3	3.26	1.36	1.29
17	AV	56	Y5P	C2-N3	3.26	1.36	1.29
17	AV	72	Y5P	C2-N3	3.26	1.36	1.29
17	AY	4	Y5P	C2-N3	3.32	1.36	1.29
17	AV	25	Y5P	C2-N3	3.36	1.36	1.29
17	AV	43	Y5P	C2-N3	3.36	1.36	1.29
17	AV	49	Y5P	C2-N3	3.36	1.36	1.29
17	AV	13	Y5P	C2-N3	3.36	1.36	1.29
17	AY	72	Y5P	C2-N3	3.39	1.36	1.29
17	AV	74	Y5P	C2-N3	3.44	1.36	1.29
17	AY	2	Y5P	C2-N3	3.46	1.36	1.29
17	AY	74	Y5P	C2-N3	3.46	1.36	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AV	1	Y5P	C1'-N1	3.47	1.56	1.46
17	AY	52	Y5P	C1'-N1	3.49	1.56	1.46
17	AY	22	Y5P	C1'-N1	3.52	1.57	1.46
17	AY	29	Y5P	C1'-N1	3.52	1.57	1.46
17	AY	9	Y5P	C1'-N1	3.53	1.57	1.46
17	AV	52	Y5P	C1'-N1	3.59	1.57	1.46
17	AV	23	Y5P	C1'-N1	3.61	1.57	1.46
17	AV	9	Y5P	C1'-N1	3.63	1.57	1.46
17	AV	63	Y5P	C1'-N1	3.64	1.57	1.46
17	AV	38	Y5P	C1'-N1	3.65	1.57	1.46
17	AV	24	Y5P	C1'-N1	3.68	1.57	1.46
17	AV	28	Y5P	C1'-N1	3.68	1.57	1.46
17	AV	10	Y5P	C1'-N1	3.68	1.57	1.46
17	AV	71	Y5P	C1'-N1	3.70	1.57	1.46
17	AV	15	Y5P	C1'-N1	3.70	1.57	1.46
17	AY	10	Y5P	C1'-N1	3.71	1.57	1.46
17	AY	58	Y5P	C1'-N1	3.72	1.57	1.46
17	AY	5	Y5P	C1'-N1	3.72	1.57	1.46
17	AY	63	Y5P	C1'-N1	3.73	1.57	1.46
17	AY	53	Y5P	C1'-N1	3.73	1.57	1.46
17	AY	7	Y5P	C1'-N1	3.75	1.57	1.46
18	AX	17	Y5P	C2-N3	3.75	1.37	1.29
17	AY	6	Y5P	C1'-N1	3.76	1.57	1.46
17	AV	53	Y5P	C1'-N1	3.77	1.57	1.46
17	AY	69	Y5P	C1'-N1	3.77	1.57	1.46
17	AV	33	Y5P	C2-N3	3.79	1.37	1.29
17	AV	6	Y5P	C1'-N1	3.80	1.57	1.46
17	AY	14	Y5P	C1'-N1	3.81	1.57	1.46
17	AV	8	Y5P	C2-N3	3.81	1.37	1.29
17	AY	24	Y5P	C1'-N1	3.81	1.57	1.46
17	AY	33	Y5P	C2-N3	3.82	1.37	1.29
17	AY	30	Y5P	C1'-N1	3.83	1.58	1.46
17	AY	57	Y5P	C1'-N1	3.83	1.58	1.46
17	AY	45	Y5P	C2-N3	3.85	1.37	1.29
17	AY	38	Y5P	C1'-N1	3.85	1.58	1.46
18	AX	16	Y5P	C2-N3	3.87	1.37	1.29
17	AV	65	Y5P	C1'-N1	3.88	1.58	1.46
47	BB	65	Y5P	C2-N3	3.89	1.37	1.29
17	AY	32	Y5P	C2-N3	3.89	1.37	1.29
47	BB	46	P5P	C6-N1	3.90	1.39	1.32
17	AY	28	Y5P	C1'-N1	3.90	1.58	1.46
47	BB	40	Y5P	C2-N3	3.90	1.37	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	AX	20	Y5P	C2-N3	3.91	1.37	1.29
17	AV	39	Y5P	C2-N3	3.92	1.37	1.29
17	AV	37	Y5P	C1'-N1	3.94	1.58	1.46
47	BB	10	P5P	C6-N1	3.94	1.39	1.32
17	AV	22	Y5P	C1'-N1	3.94	1.58	1.46
17	AV	69	Y5P	C1'-N1	3.95	1.58	1.46
17	AY	27	Y5P	C1'-N1	3.96	1.58	1.46
47	BB	44	Y5P	C2-N3	3.96	1.37	1.29
17	AV	31	Y5P	C1'-N1	3.96	1.58	1.46
17	AY	15	Y5P	C1'-N1	3.96	1.58	1.46
17	AY	31	Y5P	C1'-N1	3.97	1.58	1.46
47	BB	6	Y5P	C2-N3	3.97	1.37	1.29
17	AY	50	Y5P	C2-N3	3.97	1.37	1.29
17	AY	39	Y5P	C2-N3	3.97	1.37	1.29
17	AY	37	Y5P	C1'-N1	3.98	1.58	1.46
17	AV	30	Y5P	C1'-N1	3.98	1.58	1.46
17	AV	58	Y5P	C1'-N1	3.99	1.58	1.46
18	AX	19	Y5P	C2-N3	4.00	1.37	1.29
17	AY	12	Y5P	C2-N3	4.02	1.37	1.29
47	BB	13	Y5P	C2-N3	4.03	1.37	1.29
17	AY	8	Y5P	C2-N3	4.03	1.37	1.29
17	AV	26	Y5P	C1'-N1	4.04	1.58	1.46
17	AY	1	Y5P	C1'-N1	4.05	1.58	1.46
17	AY	23	Y5P	C1'-N1	4.06	1.58	1.46
17	AY	66	Y5P	C2-N3	4.07	1.38	1.29
47	BB	30	P5P	C6-N1	4.09	1.39	1.32
17	AV	55	Y5P	C2-N3	4.09	1.38	1.29
17	AY	60	Y5P	C2-N3	4.09	1.38	1.29
17	AY	54	Y5P	C2-N3	4.10	1.38	1.29
47	BB	8	Y5P	C2-N3	4.10	1.38	1.29
17	AY	44	Y5P	C1'-N1	4.10	1.58	1.46
17	AY	71	Y5P	C1'-N1	4.10	1.58	1.46
17	AV	59	Y5P	C2-N3	4.11	1.38	1.29
47	BB	7	P5P	C6-N1	4.11	1.39	1.32
17	AV	5	Y5P	C1'-N1	4.12	1.58	1.46
47	BB	48	Y5P	C2-N3	4.13	1.38	1.29
17	AY	59	Y5P	C2-N3	4.13	1.38	1.29
17	AY	65	Y5P	C1'-N1	4.14	1.58	1.46
17	AV	60	Y5P	C2-N3	4.14	1.38	1.29
47	BB	61	Y5P	C2-N3	4.14	1.38	1.29
17	AV	32	Y5P	C2-N3	4.15	1.38	1.29
17	AY	55	Y5P	C2-N3	4.15	1.38	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AY	21	Y5P	C1'-N1	4.17	1.59	1.46
17	AY	51	Y5P	C2-N3	4.18	1.38	1.29
18	AX	13	Y5P	C2-N3	4.19	1.38	1.29
47	BB	29	P5P	C6-N1	4.19	1.39	1.32
17	AY	70	Y5P	C1'-N1	4.19	1.59	1.46
18	AX	12	Y5P	C2-N3	4.20	1.38	1.29
47	BB	59	P5P	C6-N1	4.20	1.39	1.32
47	BB	62	Y5P	C2-N3	4.20	1.38	1.29
47	BB	12	Y5P	C2-N3	4.21	1.38	1.29
17	AV	44	Y5P	C1'-N1	4.21	1.59	1.46
47	BB	51	P5P	C6-N1	4.22	1.39	1.32
17	AV	12	Y5P	C2-N3	4.23	1.38	1.29
17	AV	64	Y5P	C1'-N1	4.24	1.59	1.46
17	AV	73	Y5P	C1'-N1	4.25	1.59	1.46
17	AV	51	Y5P	C2-N3	4.25	1.38	1.29
18	AX	23	Y5P	C2-N3	4.27	1.38	1.29
17	AV	54	Y5P	C2-N3	4.27	1.38	1.29
18	AX	22	Y5P	C2-N3	4.27	1.38	1.29
17	AY	64	Y5P	C1'-N1	4.27	1.59	1.46
17	AY	26	Y5P	C1'-N1	4.28	1.59	1.46
17	AV	70	Y5P	C1'-N1	4.29	1.59	1.46
17	AV	66	Y5P	C2-N3	4.29	1.38	1.29
17	AV	50	Y5P	C2-N3	4.29	1.38	1.29
17	AY	63	Y5P	C2-N3	4.29	1.38	1.29
17	AV	14	Y5P	C2-N3	4.30	1.38	1.29
17	AY	34	P5P	C6-N1	4.30	1.39	1.32
17	AY	1	Y5P	C2-N3	4.30	1.38	1.29
17	AV	5	Y5P	C2-N3	4.31	1.38	1.29
47	BB	41	P5P	C6-N1	4.31	1.39	1.32
17	AY	38	Y5P	C2-N3	4.31	1.38	1.29
17	AV	28	Y5P	C2-N3	4.31	1.38	1.29
17	AY	31	Y5P	C2-N3	4.31	1.38	1.29
17	AY	21	Y5P	C2-N3	4.31	1.38	1.29
17	AY	24	Y5P	C2-N3	4.31	1.38	1.29
17	AV	26	Y5P	C2-N3	4.31	1.38	1.29
17	AY	65	Y5P	C2-N3	4.31	1.38	1.29
17	AY	27	Y5P	C2-N3	4.31	1.38	1.29
17	AV	15	Y5P	C2-N3	4.32	1.38	1.29
17	AV	70	Y5P	C2-N3	4.32	1.38	1.29
17	AY	58	Y5P	C2-N3	4.32	1.38	1.29
47	BB	34	Y5P	C2-N3	4.32	1.38	1.29
17	AY	70	Y5P	C2-N3	4.32	1.38	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AY	52	Y5P	C2-N3	4.32	1.38	1.29
17	AV	64	Y5P	C2-N3	4.32	1.38	1.29
17	AY	37	Y5P	C2-N3	4.33	1.38	1.29
17	AV	21	Y5P	C2-N3	4.33	1.38	1.29
17	AY	71	Y5P	C2-N3	4.33	1.38	1.29
17	AV	45	Y5P	C2-N3	4.33	1.38	1.29
17	AY	9	Y5P	C2-N3	4.33	1.38	1.29
17	AY	30	Y5P	C2-N3	4.33	1.38	1.29
17	AV	31	Y5P	C2-N3	4.33	1.38	1.29
17	AV	58	Y5P	C2-N3	4.33	1.38	1.29
18	AX	14	Y5P	C2-N3	4.33	1.38	1.29
17	AY	64	Y5P	C2-N3	4.33	1.38	1.29
17	AV	38	Y5P	C2-N3	4.33	1.38	1.29
17	AV	7	Y5P	C2-N3	4.33	1.38	1.29
17	AV	10	Y5P	C2-N3	4.34	1.38	1.29
17	AV	53	Y5P	C2-N3	4.34	1.38	1.29
17	AV	37	Y5P	C2-N3	4.34	1.38	1.29
17	AY	6	Y5P	C2-N3	4.34	1.38	1.29
17	AY	7	Y5P	C2-N3	4.34	1.38	1.29
17	AY	53	Y5P	C2-N3	4.34	1.38	1.29
17	AV	24	Y5P	C2-N3	4.34	1.38	1.29
17	AV	6	Y5P	C2-N3	4.34	1.38	1.29
17	AV	65	Y5P	C2-N3	4.34	1.38	1.29
17	AY	26	Y5P	C2-N3	4.34	1.38	1.29
17	AV	14	Y5P	C1'-N1	4.34	1.59	1.46
17	AY	14	Y5P	C2-N3	4.34	1.38	1.29
17	AY	22	Y5P	C2-N3	4.34	1.38	1.29
17	AV	71	Y5P	C2-N3	4.34	1.38	1.29
17	AY	15	Y5P	C2-N3	4.34	1.38	1.29
17	AV	22	Y5P	C2-N3	4.34	1.38	1.29
17	AV	1	Y5P	C2-N3	4.34	1.38	1.29
17	AV	29	Y5P	C2-N3	4.35	1.38	1.29
17	AY	28	Y5P	C2-N3	4.35	1.38	1.29
17	AY	10	Y5P	C2-N3	4.35	1.38	1.29
17	AY	44	Y5P	C2-N3	4.35	1.38	1.29
17	AV	44	Y5P	C2-N3	4.35	1.38	1.29
17	AV	27	Y5P	C2-N3	4.35	1.38	1.29
17	AV	30	Y5P	C2-N3	4.35	1.38	1.29
17	AY	57	Y5P	C2-N3	4.35	1.38	1.29
17	AY	23	Y5P	C2-N3	4.35	1.38	1.29
17	AY	73	Y5P	C2-N3	4.35	1.38	1.29
17	AY	29	Y5P	C2-N3	4.35	1.38	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AY	5	Y5P	C2-N3	4.35	1.38	1.29
17	AY	69	Y5P	C2-N3	4.35	1.38	1.29
47	BB	25	P5P	C6-N1	4.36	1.40	1.32
17	AV	23	Y5P	C2-N3	4.36	1.38	1.29
17	AV	52	Y5P	C2-N3	4.36	1.38	1.29
17	AV	9	Y5P	C2-N3	4.36	1.38	1.29
17	AV	73	Y5P	C2-N3	4.36	1.38	1.29
17	AV	57	Y5P	C2-N3	4.36	1.38	1.29
17	AV	63	Y5P	C2-N3	4.37	1.38	1.29
17	AV	69	Y5P	C2-N3	4.37	1.38	1.29
17	AV	27	Y5P	C1'-N1	4.42	1.59	1.46
47	BB	49	P5P	C6-N1	4.43	1.40	1.32
47	BB	35	P5P	C6-N1	4.45	1.40	1.32
18	AX	15	Y5P	C2-N3	4.46	1.38	1.29
18	AX	24	Y5P	C2-N3	4.47	1.38	1.29
17	AV	57	Y5P	C1'-N1	4.48	1.59	1.46
17	AV	21	Y5P	C1'-N1	4.52	1.60	1.46
17	AY	73	Y5P	C1'-N1	4.54	1.60	1.46
17	AV	34	P5P	C6-N1	4.78	1.40	1.32

All (322) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AV	8	Y5P	N1-C2-N3	-12.27	114.18	125.85
47	BB	13	Y5P	N1-C2-N3	-12.16	114.28	125.85
17	AY	51	Y5P	N1-C2-N3	-12.09	114.35	125.85
17	AY	54	Y5P	N1-C2-N3	-12.08	114.36	125.85
47	BB	8	Y5P	N1-C2-N3	-12.06	114.38	125.85
17	AV	12	Y5P	N1-C2-N3	-11.86	114.57	125.85
17	AY	39	Y5P	N1-C2-N3	-11.78	114.65	125.85
18	AX	23	Y5P	N1-C2-N3	-11.76	114.66	125.85
18	AX	12	Y5P	N1-C2-N3	-11.67	114.75	125.85
17	AY	8	Y5P	N1-C2-N3	-11.66	114.76	125.85
18	AX	15	Y5P	N1-C2-N3	-11.63	114.79	125.85
17	AV	54	Y5P	N1-C2-N3	-11.58	114.84	125.85
18	AX	16	Y5P	N1-C2-N3	-11.56	114.85	125.85
47	BB	62	Y5P	N1-C2-N3	-11.56	114.86	125.85
47	BB	48	Y5P	N1-C2-N3	-11.55	114.86	125.85
18	AX	13	Y5P	N1-C2-N3	-11.55	114.87	125.85
17	AY	50	Y5P	N1-C2-N3	-11.53	114.88	125.85
17	AV	39	Y5P	N1-C2-N3	-11.52	114.90	125.85
17	AY	45	Y5P	N1-C2-N3	-11.51	114.91	125.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	BB	65	Y5P	N1-C2-N3	-11.46	114.95	125.85
17	AY	12	Y5P	N1-C2-N3	-11.43	114.97	125.85
17	AV	32	Y5P	N1-C2-N3	-11.40	115.01	125.85
17	AV	59	Y5P	N1-C2-N3	-11.37	115.04	125.85
18	AX	17	Y5P	N1-C2-N3	-11.36	115.04	125.85
18	AX	22	Y5P	N1-C2-N3	-11.31	115.09	125.85
17	AY	66	Y5P	N1-C2-N3	-11.29	115.11	125.85
17	AY	59	Y5P	N1-C2-N3	-11.29	115.11	125.85
18	AX	20	Y5P	N1-C2-N3	-11.26	115.14	125.85
17	AV	52	Y5P	N1-C2-N3	-11.23	115.17	125.85
17	AY	60	Y5P	N1-C2-N3	-11.23	115.17	125.85
17	AY	6	Y5P	N1-C2-N3	-11.22	115.18	125.85
17	AV	73	Y5P	N1-C2-N3	-11.22	115.18	125.85
17	AV	70	Y5P	N1-C2-N3	-11.22	115.18	125.85
17	AY	15	Y5P	N1-C2-N3	-11.21	115.18	125.85
17	AY	22	Y5P	N1-C2-N3	-11.21	115.19	125.85
17	AV	9	Y5P	N1-C2-N3	-11.21	115.19	125.85
17	AY	64	Y5P	N1-C2-N3	-11.21	115.19	125.85
17	AV	27	Y5P	N1-C2-N3	-11.21	115.19	125.85
17	AV	53	Y5P	N1-C2-N3	-11.21	115.19	125.85
17	AV	14	Y5P	N1-C2-N3	-11.21	115.19	125.85
17	AV	69	Y5P	N1-C2-N3	-11.20	115.19	125.85
17	AV	71	Y5P	N1-C2-N3	-11.20	115.19	125.85
17	AY	44	Y5P	N1-C2-N3	-11.20	115.19	125.85
17	AV	64	Y5P	N1-C2-N3	-11.20	115.19	125.85
17	AV	6	Y5P	N1-C2-N3	-11.20	115.20	125.85
17	AV	23	Y5P	N1-C2-N3	-11.20	115.20	125.85
17	AY	65	Y5P	N1-C2-N3	-11.19	115.21	125.85
17	AY	30	Y5P	N1-C2-N3	-11.19	115.21	125.85
17	AV	57	Y5P	N1-C2-N3	-11.19	115.21	125.85
17	AY	31	Y5P	N1-C2-N3	-11.19	115.21	125.85
17	AY	37	Y5P	N1-C2-N3	-11.18	115.21	125.85
17	AY	71	Y5P	N1-C2-N3	-11.18	115.21	125.85
17	AV	26	Y5P	N1-C2-N3	-11.18	115.21	125.85
17	AV	24	Y5P	N1-C2-N3	-11.18	115.21	125.85
17	AY	53	Y5P	N1-C2-N3	-11.18	115.22	125.85
17	AY	57	Y5P	N1-C2-N3	-11.18	115.22	125.85
17	AV	44	Y5P	N1-C2-N3	-11.18	115.22	125.85
17	AY	29	Y5P	N1-C2-N3	-11.18	115.22	125.85
17	AY	28	Y5P	N1-C2-N3	-11.18	115.22	125.85
17	AY	70	Y5P	N1-C2-N3	-11.18	115.22	125.85
17	AV	37	Y5P	N1-C2-N3	-11.17	115.22	125.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AY	7	Y5P	N1-C2-N3	-11.17	115.22	125.85
17	AY	1	Y5P	N1-C2-N3	-11.17	115.22	125.85
17	AV	63	Y5P	N1-C2-N3	-11.17	115.22	125.85
17	AY	73	Y5P	N1-C2-N3	-11.17	115.22	125.85
17	AV	30	Y5P	N1-C2-N3	-11.17	115.22	125.85
17	AV	1	Y5P	N1-C2-N3	-11.17	115.22	125.85
17	AY	23	Y5P	N1-C2-N3	-11.17	115.23	125.85
17	AV	29	Y5P	N1-C2-N3	-11.17	115.23	125.85
17	AY	26	Y5P	N1-C2-N3	-11.17	115.23	125.85
17	AV	7	Y5P	N1-C2-N3	-11.17	115.23	125.85
17	AV	31	Y5P	N1-C2-N3	-11.16	115.23	125.85
17	AV	22	Y5P	N1-C2-N3	-11.16	115.24	125.85
17	AY	63	Y5P	N1-C2-N3	-11.16	115.24	125.85
17	AV	5	Y5P	N1-C2-N3	-11.16	115.24	125.85
17	AY	58	Y5P	N1-C2-N3	-11.16	115.24	125.85
17	AY	69	Y5P	N1-C2-N3	-11.16	115.24	125.85
17	AY	5	Y5P	N1-C2-N3	-11.15	115.25	125.85
17	AY	38	Y5P	N1-C2-N3	-11.15	115.25	125.85
17	AV	65	Y5P	N1-C2-N3	-11.14	115.25	125.85
17	AY	21	Y5P	N1-C2-N3	-11.14	115.25	125.85
17	AY	27	Y5P	N1-C2-N3	-11.14	115.25	125.85
17	AY	52	Y5P	N1-C2-N3	-11.14	115.25	125.85
17	AV	28	Y5P	N1-C2-N3	-11.14	115.25	125.85
17	AV	10	Y5P	N1-C2-N3	-11.14	115.26	125.85
17	AV	21	Y5P	N1-C2-N3	-11.13	115.26	125.85
17	AY	10	Y5P	N1-C2-N3	-11.13	115.26	125.85
17	AV	38	Y5P	N1-C2-N3	-11.13	115.27	125.85
17	AV	15	Y5P	N1-C2-N3	-11.13	115.27	125.85
17	AV	58	Y5P	N1-C2-N3	-11.13	115.27	125.85
17	AY	14	Y5P	N1-C2-N3	-11.13	115.27	125.85
17	AY	24	Y5P	N1-C2-N3	-11.12	115.27	125.85
17	AY	9	Y5P	N1-C2-N3	-11.12	115.27	125.85
47	BB	12	Y5P	N1-C2-N3	-11.01	115.38	125.85
17	AY	32	Y5P	N1-C2-N3	-10.96	115.42	125.85
17	AV	60	Y5P	N1-C2-N3	-10.96	115.43	125.85
18	AX	19	Y5P	N1-C2-N3	-10.95	115.43	125.85
17	AV	50	Y5P	N1-C2-N3	-10.91	115.47	125.85
47	BB	6	Y5P	N1-C2-N3	-10.86	115.52	125.85
47	BB	61	Y5P	N1-C2-N3	-10.85	115.53	125.85
47	BB	40	Y5P	N1-C2-N3	-10.77	115.60	125.85
17	AY	55	Y5P	N1-C2-N3	-10.76	115.61	125.85
17	AV	66	Y5P	N1-C2-N3	-10.63	115.73	125.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	AX	24	Y5P	N1-C2-N3	-10.57	115.80	125.85
17	AV	51	Y5P	N1-C2-N3	-10.51	115.85	125.85
18	AX	14	Y5P	N1-C2-N3	-10.47	115.89	125.85
47	BB	34	Y5P	N1-C2-N3	-10.46	115.90	125.85
17	AV	55	Y5P	N1-C2-N3	-10.46	115.91	125.85
47	BB	44	Y5P	N1-C2-N3	-10.31	116.05	125.85
17	AY	33	Y5P	N1-C2-N3	-10.09	116.25	125.85
17	AV	45	Y5P	N1-C2-N3	-10.09	116.26	125.85
17	AV	33	Y5P	N1-C2-N3	-9.10	117.19	125.85
17	AY	62	Y5P	N1-C2-N3	-7.51	118.70	125.85
47	BB	26	Y5P	N1-C2-N3	-7.51	118.70	125.85
17	AY	3	Y5P	N1-C2-N3	-7.51	118.71	125.85
17	AY	42	Y5P	N1-C2-N3	-7.49	118.72	125.85
17	AV	11	Y5P	N1-C2-N3	-7.47	118.75	125.85
17	AV	62	Y5P	N1-C2-N3	-7.43	118.78	125.85
17	AY	40	Y5P	N1-C2-N3	-7.42	118.80	125.85
17	AY	43	Y5P	N1-C2-N3	-7.39	118.82	125.85
17	AY	13	Y5P	N1-C2-N3	-7.38	118.83	125.85
47	BB	60	Y5P	N1-C2-N3	-7.35	118.86	125.85
17	AY	4	Y5P	N1-C2-N3	-7.34	118.87	125.85
17	AY	41	Y5P	N1-C2-N3	-7.28	118.92	125.85
17	AV	13	Y5P	N1-C2-N3	-7.26	118.94	125.85
17	AY	61	Y5P	N1-C2-N3	-7.23	118.97	125.85
17	AY	25	Y5P	N1-C2-N3	-7.23	118.97	125.85
47	BB	33	Y5P	N1-C2-N3	-7.20	119.00	125.85
17	AY	49	Y5P	N1-C2-N3	-7.18	119.02	125.85
17	AY	68	Y5P	N1-C2-N3	-7.13	119.07	125.85
17	AY	2	Y5P	N1-C2-N3	-7.12	119.08	125.85
47	BB	52	Y5P	N1-C2-N3	-7.09	119.11	125.85
47	BB	31	Y5P	N1-C2-N3	-7.08	119.12	125.85
47	BB	53	Y5P	N1-C2-N3	-7.02	119.17	125.85
47	BB	43	Y5P	N1-C2-N3	-7.00	119.19	125.85
17	AY	56	Y5P	N1-C2-N3	-6.96	119.22	125.85
17	AV	49	Y5P	N1-C2-N3	-6.93	119.25	125.85
47	BB	63	Y5P	N1-C2-N3	-6.89	119.30	125.85
17	AY	75	Y5P	N1-C2-N3	-6.87	119.32	125.85
47	BB	42	Y5P	N1-C2-N3	-6.85	119.33	125.85
17	AV	75	Y5P	N1-C2-N3	-6.85	119.34	125.85
17	AY	48	Y5P	N1-C2-N3	-6.80	119.38	125.85
17	AV	48	Y5P	N1-C2-N3	-6.76	119.42	125.85
17	AV	56	Y5P	N1-C2-N3	-6.74	119.43	125.85
17	AV	4	Y5P	N1-C2-N3	-6.74	119.44	125.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AY	11	Y5P	N1-C2-N3	-6.66	119.51	125.85
17	AV	61	Y5P	N1-C2-N3	-6.66	119.51	125.85
17	AV	68	Y5P	N1-C2-N3	-6.60	119.57	125.85
17	AV	40	Y5P	N1-C2-N3	-6.58	119.59	125.85
17	AV	41	Y5P	N1-C2-N3	-6.58	119.59	125.85
17	AV	42	Y5P	N1-C2-N3	-6.52	119.64	125.85
17	AY	74	Y5P	N1-C2-N3	-6.50	119.67	125.85
18	AX	18	Y5P	N1-C2-N3	-6.49	119.67	125.85
17	AV	43	Y5P	N1-C2-N3	-6.46	119.71	125.85
17	AV	67	Y5P	N1-C2-N3	-6.45	119.71	125.85
17	AV	74	Y5P	N1-C2-N3	-6.42	119.74	125.85
17	AV	3	Y5P	N1-C2-N3	-6.33	119.83	125.85
18	AX	21	Y5P	N1-C2-N3	-6.32	119.84	125.85
17	AY	67	Y5P	N1-C2-N3	-6.30	119.85	125.85
47	BB	23	P5P	C1'-N9-C4	-6.28	119.80	126.81
47	BB	11	Y5P	N1-C2-N3	-6.28	119.88	125.85
17	AV	2	Y5P	N1-C2-N3	-6.27	119.89	125.85
17	AV	25	Y5P	N1-C2-N3	-6.23	119.92	125.85
17	AV	72	Y5P	N1-C2-N3	-6.15	120.00	125.85
17	AY	72	Y5P	N1-C2-N3	-5.85	120.28	125.85
47	BB	41	P5P	N1-C2-N3	-3.44	123.14	127.66
47	BB	29	P5P	N1-C2-N3	-3.37	123.23	127.66
17	AY	73	Y5P	C1'-N1-C6	-3.33	113.35	120.80
47	BB	35	P5P	N1-C2-N3	-3.29	123.34	127.66
17	AV	34	P5P	N1-C2-N3	-3.24	123.40	127.66
47	BB	29	P5P	C1'-N9-C4	-3.21	123.23	126.81
47	BB	51	P5P	N1-C2-N3	-3.01	123.71	127.66
47	BB	30	P5P	N1-C2-N3	-3.00	123.71	127.66
47	BB	59	P5P	N1-C2-N3	-2.98	123.74	127.66
47	BB	49	P5P	N1-C2-N3	-2.98	123.75	127.66
47	BB	25	P5P	N1-C2-N3	-2.94	123.79	127.66
47	BB	7	P5P	N1-C2-N3	-2.83	123.94	127.66
17	AY	34	P5P	N1-C2-N3	-2.81	123.96	127.66
17	AY	69	Y5P	C1'-N1-C6	-2.67	114.83	120.80
17	AY	27	Y5P	C1'-N1-C6	-2.65	114.86	120.80
47	BB	10	P5P	N1-C2-N3	-2.47	124.42	127.66
47	BB	46	P5P	N1-C2-N3	-2.46	124.42	127.66
17	AV	73	Y5P	C1'-N1-C6	-2.41	115.40	120.80
17	AV	1	Y5P	C1'-N1-C6	-2.20	115.86	120.80
17	AY	55	Y5P	C1'-N1-C6	-2.06	116.19	120.80
17	AY	15	Y5P	C1'-N1-C6	-2.04	116.23	120.80
17	AV	76	P5P	C6-N1-C2	2.00	118.88	115.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AY	34	P5P	C1'-N9-C4	2.04	129.08	126.81
17	AV	73	Y5P	O4'-C1'-N1	2.07	112.03	108.09
47	BB	47	P5P	C6-N1-C2	2.15	119.09	115.99
47	BB	23	P5P	C6-N1-C2	2.46	119.54	115.99
17	AY	73	Y5P	O4'-C1'-N1	2.51	112.87	108.09
47	BB	23	P5P	O4'-C1'-N9	2.60	113.01	108.11
47	BB	10	P5P	C1'-N9-C4	2.63	129.74	126.81
47	BB	37	P5P	C1'-N9-C4	2.77	129.89	126.81
47	BB	27	P5P	C1'-N9-C4	2.94	130.09	126.81
47	BB	13	Y5P	C4-N3-C2	3.42	125.88	117.71
17	AV	33	Y5P	C4-N3-C2	3.61	126.34	117.71
17	AV	66	Y5P	C4-N3-C2	3.69	126.53	117.71
47	BB	40	Y5P	C4-N3-C2	3.69	126.53	117.71
17	AV	39	Y5P	C4-N3-C2	3.69	126.53	117.71
47	BB	12	Y5P	C4-N3-C2	3.70	126.56	117.71
47	BB	61	Y5P	C4-N3-C2	3.72	126.59	117.71
17	AY	7	Y5P	C4-N3-C2	3.73	126.62	117.71
17	AY	23	Y5P	C4-N3-C2	3.73	126.62	117.71
17	AV	15	Y5P	C4-N3-C2	3.73	126.63	117.71
17	AY	10	Y5P	C4-N3-C2	3.73	126.63	117.71
17	AY	9	Y5P	C4-N3-C2	3.74	126.64	117.71
17	AY	28	Y5P	C4-N3-C2	3.74	126.64	117.71
17	AV	1	Y5P	C4-N3-C2	3.74	126.64	117.71
17	AV	22	Y5P	C4-N3-C2	3.74	126.64	117.71
17	AV	10	Y5P	C4-N3-C2	3.74	126.64	117.71
17	AY	5	Y5P	C4-N3-C2	3.74	126.64	117.71
17	AY	52	Y5P	C4-N3-C2	3.74	126.64	117.71
17	AV	58	Y5P	C4-N3-C2	3.74	126.64	117.71
17	AV	23	Y5P	C4-N3-C2	3.74	126.64	117.71
17	AY	14	Y5P	C4-N3-C2	3.74	126.64	117.71
17	AV	57	Y5P	C4-N3-C2	3.74	126.65	117.71
17	AV	26	Y5P	C4-N3-C2	3.74	126.65	117.71
17	AV	63	Y5P	C4-N3-C2	3.74	126.65	117.71
17	AV	30	Y5P	C4-N3-C2	3.74	126.65	117.71
17	AV	65	Y5P	C4-N3-C2	3.74	126.65	117.71
17	AY	24	Y5P	C4-N3-C2	3.74	126.65	117.71
17	AV	7	Y5P	C4-N3-C2	3.74	126.65	117.71
17	AY	30	Y5P	C4-N3-C2	3.74	126.65	117.71
17	AV	28	Y5P	C4-N3-C2	3.74	126.65	117.71
17	AV	38	Y5P	C4-N3-C2	3.74	126.66	117.71
17	AV	9	Y5P	C4-N3-C2	3.74	126.66	117.71
17	AY	73	Y5P	C4-N3-C2	3.75	126.66	117.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AV	29	Y5P	C4-N3-C2	3.75	126.66	117.71
17	AY	21	Y5P	C4-N3-C2	3.75	126.66	117.71
17	AY	64	Y5P	C4-N3-C2	3.75	126.66	117.71
17	AV	44	Y5P	C4-N3-C2	3.75	126.67	117.71
17	AV	71	Y5P	C4-N3-C2	3.75	126.67	117.71
17	AY	27	Y5P	C4-N3-C2	3.75	126.67	117.71
17	AV	37	Y5P	C4-N3-C2	3.75	126.67	117.71
17	AV	64	Y5P	C4-N3-C2	3.75	126.67	117.71
17	AV	31	Y5P	C4-N3-C2	3.75	126.67	117.71
17	AY	29	Y5P	C4-N3-C2	3.75	126.68	117.71
17	AV	21	Y5P	C4-N3-C2	3.75	126.68	117.71
17	AY	38	Y5P	C4-N3-C2	3.75	126.68	117.71
17	AY	53	Y5P	C4-N3-C2	3.75	126.68	117.71
17	AY	37	Y5P	C4-N3-C2	3.75	126.68	117.71
17	AY	26	Y5P	C4-N3-C2	3.75	126.68	117.71
17	AY	69	Y5P	C4-N3-C2	3.75	126.68	117.71
17	AY	71	Y5P	C4-N3-C2	3.76	126.68	117.71
17	AY	44	Y5P	C4-N3-C2	3.76	126.68	117.71
17	AV	27	Y5P	C4-N3-C2	3.76	126.68	117.71
17	AY	15	Y5P	C4-N3-C2	3.76	126.69	117.71
17	AY	57	Y5P	C4-N3-C2	3.76	126.69	117.71
17	AV	5	Y5P	C4-N3-C2	3.76	126.69	117.71
17	AY	31	Y5P	C4-N3-C2	3.76	126.69	117.71
17	AY	63	Y5P	C4-N3-C2	3.76	126.69	117.71
17	AY	58	Y5P	C4-N3-C2	3.76	126.69	117.71
17	AV	53	Y5P	C4-N3-C2	3.76	126.69	117.71
17	AY	6	Y5P	C4-N3-C2	3.76	126.70	117.71
17	AV	69	Y5P	C4-N3-C2	3.76	126.70	117.71
17	AV	24	Y5P	C4-N3-C2	3.76	126.70	117.71
17	AV	6	Y5P	C4-N3-C2	3.77	126.71	117.71
17	AV	73	Y5P	C4-N3-C2	3.77	126.71	117.71
17	AV	14	Y5P	C4-N3-C2	3.77	126.71	117.71
17	AY	70	Y5P	C4-N3-C2	3.77	126.71	117.71
17	AY	22	Y5P	C4-N3-C2	3.77	126.72	117.71
17	AV	70	Y5P	C4-N3-C2	3.77	126.72	117.71
17	AV	52	Y5P	C4-N3-C2	3.77	126.72	117.71
17	AY	1	Y5P	C4-N3-C2	3.77	126.72	117.71
17	AY	65	Y5P	C4-N3-C2	3.78	126.73	117.71
47	BB	25	P5P	C1'-N9-C4	3.78	131.02	126.81
17	AY	33	Y5P	C4-N3-C2	3.82	126.83	117.71
17	AY	32	Y5P	C4-N3-C2	3.82	126.85	117.71
18	AX	16	Y5P	C4-N3-C2	3.90	127.04	117.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	BB	44	Y5P	C4-N3-C2	3.94	127.12	117.71
47	BB	34	Y5P	C4-N3-C2	3.94	127.13	117.71
18	AX	20	Y5P	C4-N3-C2	3.96	127.18	117.71
17	AY	8	Y5P	C4-N3-C2	4.00	127.26	117.71
18	AX	12	Y5P	C4-N3-C2	4.00	127.27	117.71
17	AV	55	Y5P	C4-N3-C2	4.00	127.28	117.71
47	BB	6	Y5P	C4-N3-C2	4.01	127.29	117.71
17	AV	8	Y5P	C4-N3-C2	4.02	127.31	117.71
17	AV	50	Y5P	C4-N3-C2	4.02	127.31	117.71
17	AY	66	Y5P	C4-N3-C2	4.02	127.32	117.71
17	AY	50	Y5P	C4-N3-C2	4.03	127.34	117.71
18	AX	13	Y5P	C4-N3-C2	4.04	127.35	117.71
17	AY	12	Y5P	C4-N3-C2	4.04	127.36	117.71
47	BB	65	Y5P	C4-N3-C2	4.04	127.36	117.71
18	AX	14	Y5P	C4-N3-C2	4.06	127.40	117.71
47	BB	48	Y5P	C4-N3-C2	4.06	127.42	117.71
17	AV	60	Y5P	C4-N3-C2	4.06	127.42	117.71
47	BB	8	Y5P	C4-N3-C2	4.07	127.43	117.71
17	AY	60	Y5P	C4-N3-C2	4.07	127.43	117.71
17	AY	39	Y5P	C4-N3-C2	4.07	127.44	117.71
17	AV	45	Y5P	C4-N3-C2	4.08	127.46	117.71
18	AX	22	Y5P	C4-N3-C2	4.10	127.50	117.71
17	AV	12	Y5P	C4-N3-C2	4.10	127.50	117.71
17	AV	32	Y5P	C4-N3-C2	4.11	127.52	117.71
18	AX	17	Y5P	C4-N3-C2	4.12	127.54	117.71
18	AX	15	Y5P	C4-N3-C2	4.12	127.55	117.71
17	AY	54	Y5P	C4-N3-C2	4.12	127.55	117.71
17	AV	51	Y5P	C4-N3-C2	4.12	127.56	117.71
18	AX	23	Y5P	C4-N3-C2	4.13	127.57	117.71
17	AY	59	Y5P	C4-N3-C2	4.17	127.67	117.71
18	AX	19	Y5P	C4-N3-C2	4.17	127.67	117.71
47	BB	62	Y5P	C4-N3-C2	4.20	127.75	117.71
17	AV	59	Y5P	C4-N3-C2	4.21	127.77	117.71
18	AX	24	Y5P	C4-N3-C2	4.23	127.82	117.71
17	AY	51	Y5P	C4-N3-C2	4.25	127.87	117.71
17	AY	55	Y5P	C4-N3-C2	4.28	127.94	117.71
17	AV	54	Y5P	C4-N3-C2	4.36	128.12	117.71
17	AY	45	Y5P	C4-N3-C2	4.40	128.21	117.71
47	BB	30	P5P	C6-N1-C2	5.81	124.36	115.99
47	BB	25	P5P	C6-N1-C2	5.95	124.57	115.99
47	BB	46	P5P	C6-N1-C2	6.08	124.75	115.99
47	BB	10	P5P	C6-N1-C2	6.13	124.83	115.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	BB	59	P5P	C6-N1-C2	6.22	124.96	115.99
47	BB	35	P5P	C6-N1-C2	6.31	125.08	115.99
47	BB	29	P5P	C6-N1-C2	6.31	125.09	115.99
47	BB	51	P5P	C6-N1-C2	6.34	125.13	115.99
47	BB	49	P5P	C6-N1-C2	6.39	125.20	115.99
17	AY	34	P5P	C6-N1-C2	6.53	125.41	115.99
47	BB	41	P5P	C6-N1-C2	6.55	125.43	115.99
47	BB	7	P5P	C6-N1-C2	6.61	125.52	115.99
17	AV	34	P5P	C6-N1-C2	6.82	125.83	115.99

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	BB	23	P5P	P-O5'-C5'-C4'

There are no ring outliers.

141 monomers are involved in 183 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AV	10	Y5P	2	0
17	AV	11	Y5P	2	0
17	AV	12	Y5P	1	0
17	AV	13	Y5P	1	0
17	AV	14	Y5P	1	0
17	AV	2	Y5P	2	0
17	AV	21	Y5P	1	0
17	AV	24	Y5P	2	0
17	AV	25	Y5P	3	0
17	AV	26	Y5P	2	0
17	AV	27	Y5P	4	0
17	AV	28	Y5P	6	0
17	AV	29	Y5P	4	0
17	AV	3	Y5P	1	0
17	AV	30	Y5P	3	0
17	AV	31	Y5P	2	0
17	AV	32	Y5P	1	0
17	AV	33	Y5P	1	0
17	AV	34	P5P	1	0
17	AV	35	P5P	1	0
17	AV	36	P5P	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AV	37	Y5P	5	0
17	AV	38	Y5P	4	0
17	AV	4	Y5P	1	0
17	AV	41	Y5P	1	0
17	AV	42	Y5P	3	0
17	AV	43	Y5P	6	0
17	AV	44	Y5P	4	0
17	AV	48	Y5P	2	0
17	AV	49	Y5P	1	0
17	AV	5	Y5P	1	0
17	AV	50	Y5P	1	0
17	AV	51	Y5P	2	0
17	AV	52	Y5P	2	0
17	AV	53	Y5P	2	0
17	AV	54	Y5P	6	0
17	AV	55	Y5P	7	0
17	AV	57	Y5P	5	0
17	AV	58	Y5P	4	0
17	AV	59	Y5P	2	0
17	AV	60	Y5P	2	0
17	AV	62	Y5P	2	0
17	AV	63	Y5P	4	0
17	AV	64	Y5P	3	0
17	AV	65	Y5P	1	0
17	AV	66	Y5P	3	0
17	AV	67	Y5P	4	0
17	AV	68	Y5P	1	0
17	AV	70	Y5P	1	0
17	AV	71	Y5P	1	0
17	AV	8	Y5P	1	0
17	AV	9	Y5P	2	0
18	AX	12	Y5P	1	0
18	AX	16	Y5P	1	0
18	AX	17	Y5P	1	0
18	AX	18	Y5P	2	0
18	AX	20	Y5P	1	0
18	AX	21	Y5P	3	0
18	AX	22	Y5P	1	0
17	AY	11	Y5P	2	0
17	AY	12	Y5P	1	0
17	AY	14	Y5P	6	0
17	AY	15	Y5P	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AY	2	Y5P	1	0
17	AY	22	Y5P	6	0
17	AY	23	Y5P	1	0
17	AY	24	Y5P	3	0
17	AY	25	Y5P	6	0
17	AY	26	Y5P	3	0
17	AY	27	Y5P	1	0
17	AY	28	Y5P	2	0
17	AY	29	Y5P	2	0
17	AY	3	Y5P	3	0
17	AY	30	Y5P	2	0
17	AY	31	Y5P	3	0
17	AY	32	Y5P	4	0
17	AY	33	Y5P	2	0
17	AY	34	P5P	2	0
17	AY	36	P5P	2	0
17	AY	37	Y5P	3	0
17	AY	38	Y5P	3	0
17	AY	39	Y5P	2	0
17	AY	4	Y5P	1	0
17	AY	42	Y5P	1	0
17	AY	43	Y5P	2	0
17	AY	44	Y5P	1	0
17	AY	45	Y5P	1	0
17	AY	50	Y5P	1	0
17	AY	51	Y5P	1	0
17	AY	52	Y5P	1	0
17	AY	53	Y5P	1	0
17	AY	54	Y5P	6	0
17	AY	55	Y5P	14	0
17	AY	56	Y5P	1	0
17	AY	57	Y5P	3	0
17	AY	58	Y5P	11	0
17	AY	6	Y5P	3	0
17	AY	61	Y5P	1	0
17	AY	62	Y5P	2	0
17	AY	63	Y5P	1	0
17	AY	66	Y5P	1	0
17	AY	67	Y5P	3	0
17	AY	68	Y5P	4	0
17	AY	69	Y5P	2	0
17	AY	7	Y5P	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AY	70	Y5P	2	0
17	AY	71	Y5P	2	0
17	AY	74	Y5P	2	0
17	AY	76	P5P	1	0
17	AY	8	Y5P	5	0
17	AY	9	Y5P	6	0
47	BB	11	Y5P	1	0
47	BB	12	Y5P	1	0
47	BB	13	Y5P	2	0
47	BB	23	P5P	1	0
47	BB	24	P5P	4	0
47	BB	25	P5P	3	0
47	BB	26	Y5P	1	0
47	BB	28	P5P	1	0
47	BB	29	P5P	3	0
47	BB	30	P5P	3	0
47	BB	31	Y5P	1	0
47	BB	32	P5P	1	0
47	BB	33	Y5P	2	0
47	BB	34	Y5P	1	0
47	BB	36	P5P	1	0
47	BB	37	P5P	2	0
47	BB	38	P5P	2	0
47	BB	39	P5P	2	0
47	BB	43	Y5P	2	0
47	BB	44	Y5P	3	0
47	BB	45	P5P	1	0
47	BB	46	P5P	1	0
47	BB	47	P5P	1	0
47	BB	48	Y5P	1	0
47	BB	61	Y5P	2	0
47	BB	62	Y5P	3	0
47	BB	63	Y5P	1	0
47	BB	65	Y5P	2	0
47	BB	66	P5P	2	0
47	BB	9	P5P	2	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.



## 5.6 Ligand geometry ⓘ

Of 358 ligands modelled in this entry, 357 are monoatomic - leaving 1 for Mogul analysis.

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$
91	GDP	Ag	500	-	24,30,30	1.41	3 (12%)	26,47,47	1.94	6 (23%)

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
91	GDP	Ag	500	-	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	Ag	500	GDP	O4'-C1'	2.28	1.44	1.41
91	Ag	500	GDP	C5-C4	3.69	1.48	1.40
91	Ag	500	GDP	C6-C5	4.46	1.50	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	Ag	500	GDP	C5-C6-N1	-4.35	117.84	123.52
91	Ag	500	GDP	N3-C2-N1	-3.65	122.59	127.56
91	Ag	500	GDP	C6-C5-C4	-3.11	117.30	120.86
91	Ag	500	GDP	C2'-C1'-N9	-2.02	108.05	113.47
91	Ag	500	GDP	O4'-C1'-N9	2.01	111.90	108.11
91	Ag	500	GDP	C6-N1-C2	5.70	122.56	115.88

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
32	Ao	26
88	Bz	4
23	Ae	4
17	AY	3
47	BB	2
17	AV	2
4	AE	1
7	AI	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Bz	36:UNK	C	99:UNK	N	56.86
1	Bz	425:UNK	C	601:UNK	N	55.59
1	Ae	262:UNK	C	263:UNK	N	42.03
1	Ae	309:UNK	C	354:UNK	N	28.87
1	Bz	106:UNK	C	300:UNK	N	28.46
1	AI	177:ASN	C	195:PRO	N	26.78
1	Ao	143:GLU	C	153:UNK	N	24.92
1	Bz	315:UNK	C	399:UNK	N	22.81
1	Ao	405:UNK	C	410:UNK	N	21.39
1	BB	53:Y5P	O3'	58:P5P	P	17.94
1	Ao	368:UNK	C	371:UNK	N	16.08
1	AE	106:SER	C	122:ARG	N	16.04
1	AV	15:Y5P	O3'	21:Y5P	P	14.94
1	AY	15:Y5P	O3'	21:Y5P	P	14.74
1	Ao	292:UNK	C	295:UNK	N	14.07
1	Ao	250:UNK	C	260:UNK	N	13.92
1	Ao	181:UNK	C	185:UNK	N	13.52
1	Ao	349:UNK	C	355:UNK	N	13.13
1	Ae	292:UNK	C	293:UNK	N	12.58
1	Ao	607:UNK	C	651:UNK	N	12.48

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ao	585:UNK	C	593:UNK	N	12.31
1	Ao	310:UNK	C	315:UNK	N	11.71
1	Ao	215:UNK	C	220:UNK	N	11.36
1	Ao	330:UNK	C	335:UNK	N	11.30
1	Ao	560:UNK	C	575:UNK	N	11.29
1	Ao	447:UNK	C	456:UNK	N	11.26
1	AY	45:Y5P	O3'	48:Y5P	P	10.79
1	Ao	198:UNK	C	200:UNK	N	10.76
1	Ao	661:UNK	C	666:UNK	N	10.72
1	BB	15:P5P	O3'	23:P5P	P	9.76
1	Ao	275:UNK	C	277:UNK	N	9.70
1	Ae	211:UNK	C	212:UNK	N	9.63
1	Ao	490:UNK	C	492:UNK	N	9.62
1	AV	45:Y5P	O3'	48:Y5P	P	9.50
1	Ao	525:UNK	C	531:UNK	N	9.11
1	Ao	470:UNK	C	475:UNK	N	8.37
1	Ao	235:UNK	C	237:UNK	N	7.59
1	Ao	385:UNK	C	390:UNK	N	7.45
1	Ao	165:UNK	C	167:UNK	N	6.98
1	Ao	507:UNK	C	510:UNK	N	6.97
1	Ao	430:UNK	C	433:UNK	N	6.37
1	Ao	542:UNK	C	546:UNK	N	5.15
1	AY	7:Y5P	O3'	8:Y5P	P	3.72