



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:34 pm BST

PDB ID : 5TBW
Title : Crystal structure of chlorolissoclimide bound to the yeast 80S ribosome
Authors : Konst, Z.A.; Szklarski, A.R.; Pellegrino, S.; Michalak, S.E.; Meyer, M.; Zquette, C.; Cencic, R.; Nam, S.; Horne, D.A.; Pelletier, J.; Mobley, D.L.; Yusupova, G.; Yusupov, M.; Vanderwal, C.D.
Deposited on : 2016-09-13
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

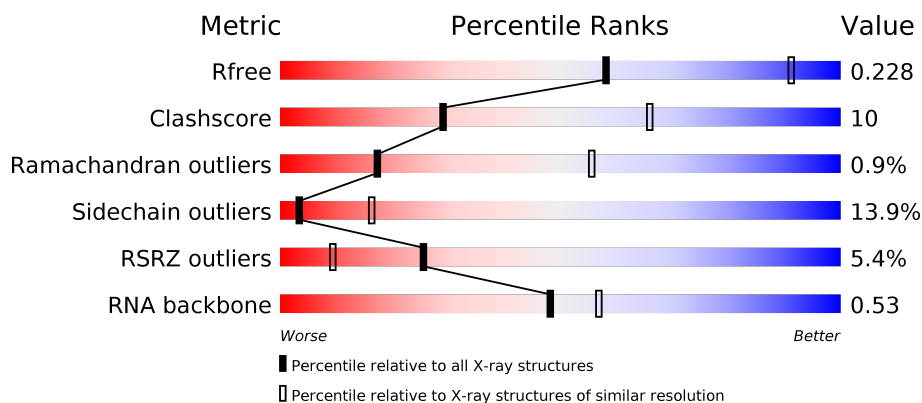
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.





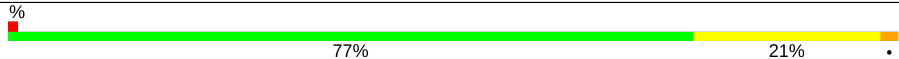
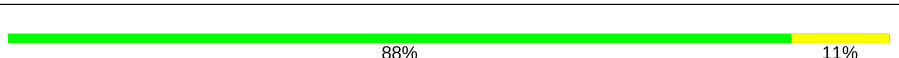
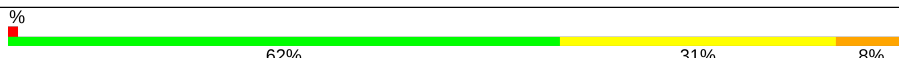
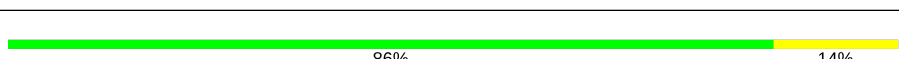
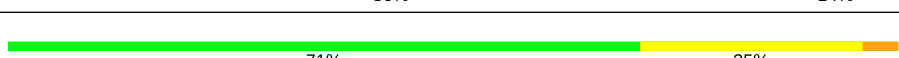
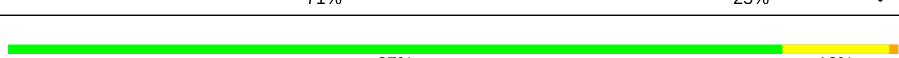
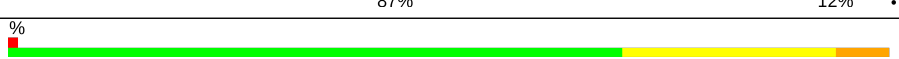

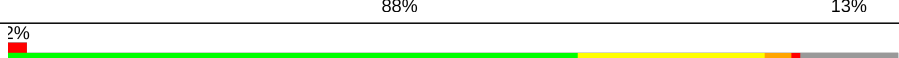



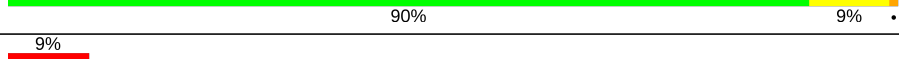



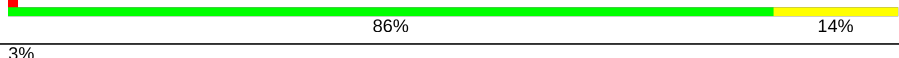
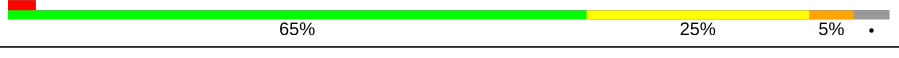

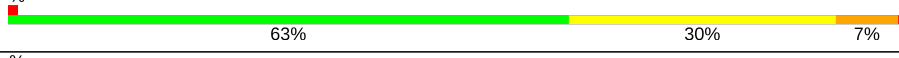



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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

Mol	Chain	Length	Quality of chain
1	1	3149	<div> <div>2%</div> <div>62%</div> <div>30%</div> <div>7%</div> </div>
1	AR	3149	<div> <div>3%</div> <div>60%</div> <div>32%</div> <div>8%</div> </div>
2	3	121	<div> <div>70%</div> <div>27%</div> </div>
2	AS	121	<div> <div>66%</div> <div>31%</div> </div>











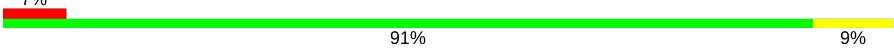


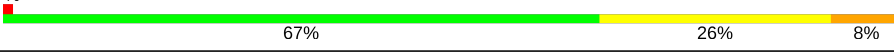
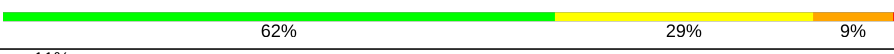
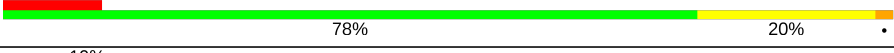

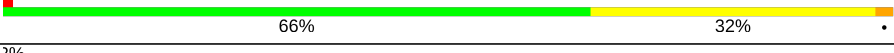







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Mol	Chain	Length	Quality of chain
3	4	158	
3	AT	158	
4	CD	252	
4	j	252	
5	CE	386	
5	k	386	
6	CF	361	
6	l	361	
7	CG	296	
7	m	296	
8	CH	175	
8	n	175	
9	CI	222	
9	o	222	
10	CJ	233	
10	p	233	
11	CK	191	
11	q	191	
12	CL	220	
12	r	220	
13	CM	169	
13	s	169	
14	CN	193	
14	t	193	
15	CO	136	

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Mol	Chain	Length	Quality of chain
15	u	136	
16	CP	203	
16	v	203	
17	CQ	197	
17	w	197	
18	CR	183	
18	x	183	
19	CS	185	
19	y	185	
20	CT	188	
20	z	188	
21	0	172	
21	CU	172	
22	2	159	
22	CV	159	
23	5	100	
23	CW	100	
24	6	136	
24	CX	136	
25	7	98	
25	CY	98	
26	8	121	
26	CZ	121	
27	9	126	
27	DA	126	

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Mol	Chain	Length	Quality of chain
28	AA	135	
28	DB	135	
29	AB	148	
29	DC	148	
30	AC	58	
30	DD	58	
31	AD	97	
31	DE	97	
32	AE	109	
32	DF	109	
33	AF	127	
33	DG	127	
34	AG	106	
34	DH	106	
35	AH	112	
35	DI	112	
36	AI	119	
36	DJ	119	
37	AJ	99	
37	DK	99	
38	AK	87	
38	DL	87	
39	AL	77	
39	DM	77	
40	AM	50	

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Mol	Chain	Length	Quality of chain
40	DN	50	
41	AN	52	
41	DO	52	
42	AO	25	
42	DP	25	
43	AP	105	
43	DQ	105	
44	AQ	91	
44	DR	91	
45	i	168	
46	p0	219	
47	sM	104	
48	A	1800	
48	sR	1800	
49	B	206	
49	s0	206	
50	C	216	
50	s1	216	
51	D	217	
51	s2	217	
52	E	223	
52	s3	223	
53	F	260	
53	s4	260	
54	G	206	

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Mol	Chain	Length	Quality of chain
54	s5	206	
55	H	226	
55	s6	226	
56	I	186	
56	s7	186	
57	J	199	
57	s8	199	
58	K	185	
58	s9	185	
59	L	105	
59	c0	105	
60	M	155	
60	c1	155	
61	N	143	
61	c2	143	
62	O	150	
62	c3	150	
63	P	128	
63	c4	128	
64	Q	135	
64	c5	135	
65	R	142	
65	c6	142	
66	S	125	
67	T	145	


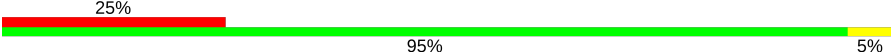
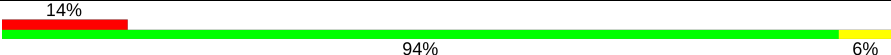
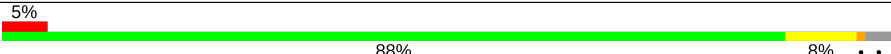
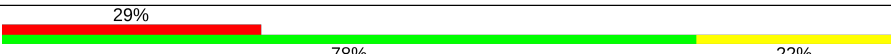
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Mol	Chain	Length	Quality of chain
67	c8	145	<div> <div>9%</div> <div>86%</div> <div>14%</div> </div>
68	U	143	<div> <div>7%</div> <div>69%</div> <div>26%</div> <div>5%</div> </div>
68	c9	143	<div> <div>8%</div> <div>92%</div> <div>6%</div> </div>
69	V	110	<div> <div>22%</div> <div>55%</div> <div>33%</div> <div>10%</div> </div>
69	d0	110	<div> <div>25%</div> <div>87%</div> <div>12%</div> </div>
70	W	87	<div> <div>8%</div> <div>60%</div> <div>34%</div> <div>6%</div> </div>
70	d1	87	<div> <div>6%</div> <div>86%</div> <div>14%</div> </div>
71	X	129	<div> <div>%</div> <div>57%</div> <div>33%</div> <div>8%</div> </div>
71	d2	129	<div> <div>91%</div> <div>8%</div> </div>
72	Y	144	<div> <div>67%</div> <div>28%</div> <div>6%</div> </div>
72	d3	144	<div> <div>%</div> <div>91%</div> <div>9%</div> </div>
73	Z	134	<div> <div>5%</div> <div>63%</div> <div>32%</div> </div>
73	d4	134	<div> <div>4%</div> <div>91%</div> <div>8%</div> </div>
74	a	70	<div> <div>33%</div> <div>71%</div> <div>27%</div> </div>
74	d5	70	<div> <div>31%</div> <div>91%</div> <div>7%</div> </div>
75	b	97	<div> <div>15%</div> <div>86%</div> <div>14%</div> </div>
75	d6	97	<div> <div>2%</div> <div>92%</div> <div>8%</div> </div>
76	c	81	<div> <div>12%</div> <div>90%</div> <div>10%</div> </div>
76	d7	81	<div> <div>15%</div> <div>89%</div> <div>11%</div> </div>
77	d	63	<div> <div>17%</div> <div>89%</div> <div>11%</div> </div>
77	d8	63	<div> <div>32%</div> <div>90%</div> <div>10%</div> </div>
78	d9	53	<div> <div>4%</div> <div>81%</div> <div>17%</div> </div>
78	e	53	<div> <div>2%</div> <div>85%</div> <div>15%</div> </div>
79	e0	62	<div> <div>10%</div> <div>84%</div> <div>16%</div> </div>
79	f	62	<div> <div>13%</div> <div>82%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
80	g	71	
81	Rb	318	
81	h	318	
82	c7	121	
83	e1	51	

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
84	OHX	1	3406	-	-	X	-
84	OHX	1	3437	-	-	X	-
84	OHX	1	3474	-	-	X	-
84	OHX	1	3540	-	-	X	-
84	OHX	1	3580	-	-	X	-
84	OHX	1	3592	-	-	X	-
84	OHX	1	3673	-	-	-	X
84	OHX	1	3697	-	-	X	-
84	OHX	1	3705	-	-	X	-
84	OHX	1	3713	-	-	X	-
84	OHX	1	3718	-	-	-	X
84	OHX	1	3730	-	-	X	-
84	OHX	A	1909	-	-	X	-
84	OHX	A	2009	-	-	X	-
84	OHX	A	2024	-	-	X	-
84	OHX	A	2039	-	-	-	X
84	OHX	AP	502	-	-	X	-
84	OHX	AR	3445	-	-	X	-
84	OHX	AR	3465	-	-	X	-
84	OHX	AR	3507	-	-	X	-
84	OHX	AR	3516	-	-	X	-
84	OHX	AR	3526	-	-	X	-
84	OHX	AR	3599	-	-	X	-
84	OHX	AR	3677	-	-	X	-
84	OHX	AR	3703	-	-	X	-
84	OHX	AR	3705	-	-	X	-
84	OHX	AR	3721	-	-	X	-
84	OHX	AR	3738	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	AR	3740	-	-	-	X
84	OHX	AT	212	-	-	X	-
84	OHX	CL	301	-	-	X	-
84	OHX	sR	2040	-	-	-	X
85	MG	1	3772	-	-	-	X
85	MG	1	3787	-	-	-	X
85	MG	1	3790	-	-	-	X
85	MG	1	3802	-	-	-	X
85	MG	1	3822	-	-	-	X
85	MG	1	3834	-	-	-	X
85	MG	1	3866	-	-	-	X
85	MG	1	3878	-	-	-	X
85	MG	1	3913	-	-	-	X
85	MG	1	3985	-	-	-	X
85	MG	1	3988	-	-	-	X
85	MG	1	3994	-	-	-	X
85	MG	1	4001	-	-	-	X
85	MG	1	4003	-	-	-	X
85	MG	1	4032	-	-	-	X
85	MG	1	4104	-	-	-	X
85	MG	1	4108	-	-	-	X
85	MG	1	4116	-	-	-	X
85	MG	1	4155	-	-	-	X
85	MG	1	4162	-	-	-	X
85	MG	1	4194	-	-	-	X
85	MG	3	210	-	-	-	X
85	MG	3	216	-	-	-	X
85	MG	A	2068	-	-	-	X
85	MG	A	2102	-	-	-	X
85	MG	A	2104	-	-	-	X
85	MG	A	2113	-	-	-	X
85	MG	A	2119	-	-	-	X
85	MG	A	2134	-	-	-	X
85	MG	AR	3803	-	-	-	X
85	MG	AR	3834	-	-	-	X
85	MG	AR	3966	-	-	-	X
85	MG	AR	3972	-	-	-	X
85	MG	AR	3974	-	-	-	X
85	MG	AR	3989	-	-	-	X
85	MG	AR	4038	-	-	-	X
85	MG	AR	4055	-	-	-	X
85	MG	AR	4085	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	AR	4091	-	-	-	X
85	MG	AR	4102	-	-	-	X
85	MG	AR	4113	-	-	-	X
85	MG	AR	4126	-	-	-	X
85	MG	AR	4138	-	-	-	X
85	MG	AR	4156	-	-	-	X
85	MG	AR	4157	-	-	-	X
85	MG	AR	4169	-	-	-	X
85	MG	AR	4171	-	-	-	X
85	MG	AR	4186	-	-	-	X
85	MG	AR	4227	-	-	-	X
85	MG	AR	4233	-	-	-	X
85	MG	AR	4236	-	-	-	X
85	MG	AT	221	-	-	-	X
85	MG	AT	225	-	-	-	X
85	MG	l	403	-	-	-	X
85	MG	l	404	-	-	-	X
85	MG	l	406	-	-	-	X
85	MG	sR	2066	-	-	-	X
85	MG	sR	2082	-	-	-	X
85	MG	sR	2157	-	-	-	X
85	MG	sR	2159	-	-	-	X
85	MG	sR	2185	-	-	-	X
85	MG	sR	2187	-	-	-	X
85	MG	sR	2188	-	-	-	X
85	MG	x	206	-	-	-	X

2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 409612 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			
1	AR	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
2	AS	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			
3	AT	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	j	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
4	CD	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	k	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
5	CE	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	l	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
6	CF	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	m	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
7	CG	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	n	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
8	CH	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	o	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
9	CI	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	p	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	q	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
11	CK	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	r	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			
12	CL	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			

- Molecule 13 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	s	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			
13	CM	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	t	193	Total	C	N	O	0	0	0
			1543	962	315	266			
14	CN	193	Total	C	N	O	0	0	0
			1543	962	315	266			

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	u	136	Total	C	N	O	0	0	0
			1053	675	199	177			
15	CO	136	Total	C	N	O	0	0	0
			1053	675	199	177			

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	v	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			
16	CP	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	w	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			
17	CQ	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	x	183	Total	C	N	O	S	0	0	0
			1420	882	281	257				
18	CR	183	Total	C	N	O	S	0	0	0
			1420	882	281	257				

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	y	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			
19	CS	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	z	188	Total	C	N	O	S	0	0	0
			1521	935	326	260				
20	CT	188	Total	C	N	O	S	0	0	0
			1521	935	326	260				

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
21	CU	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	2	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			
22	CV	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	5	100	Total	C	N	O		0	0	0
			796	516	131	149				
23	CW	100	Total	C	N	O		0	0	0
			796	516	131	149				

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	6	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
24	CX	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	7	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			
25	CY	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	8	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	CZ	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			

- Molecule 27 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	9	126	Total	C	N	O		0	0	0
			993	625	192	176				
27	DA	126	Total	C	N	O		0	0	0
			993	625	192	176				

- Molecule 28 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	AA	135	Total	C	N	O		0	0	0
			1092	710	202	180				
28	DB	135	Total	C	N	O		0	0	0
			1092	710	202	180				

- Molecule 29 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	AB	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			
29	DC	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	AC	58	Total	C	N	O		0	0	0
			462	289	100	73				
30	DD	58	Total	C	N	O		0	0	0
			462	289	100	73				

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	AD	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			
31	DE	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AE	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			
32	DF	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	AF	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			
33	DG	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	AG	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			
34	DH	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			

- Molecule 35 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	AH	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			
35	DI	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			

- Molecule 36 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	AI	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			
36	DJ	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			

- Molecule 37 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	AJ	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			
37	DK	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			

- Molecule 38 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	AK	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			
38	DL	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			

- Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	AL	77	Total	C	N	O		0	0	0
			612	391	115	106				
39	DM	77	Total	C	N	O		0	0	0
			612	391	115	106				

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	AM	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			
40	DN	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	AN	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			
41	DO	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			

- Molecule 42 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	AO	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	DP	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

- Molecule 43 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	AP	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			
43	DQ	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	AQ	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			
44	DR	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			

- Molecule 45 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	i	159	Total	C	N	O	0	0	0
			1104	654	221	229			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	134	LEU	ASP	conflict	UNP P39015

- Molecule 46 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	p0	143	Total	C	N	O	S	0	0	0
			1077	687	192	195	3			

- Molecule 47 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	sM	104	Total	C	N	O	0	0	0
			681	404	140	137			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
sM	59	ALA	GLY	conflict	UNP P39015

- Molecule 48 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	A	1781	Total	C	N	O	P	0	0	0
			37948	16965	6715	12487	1781			
48	sR	1783	Total	C	N	O	P	0	0	0
			37990	16984	6723	12500	1783			

- Molecule 49 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B	206	Total	C	N	O	S	0	0	0
			1577	1014	278	283	2			
49	s0	206	Total	C	N	O	S	0	0	0
			1583	1017	281	283	2			

- Molecule 50 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	C	214	Total	C	N	O	S	0	0	0
			1709	1084	310	311	4			
50	s1	216	Total	C	N	O	S	0	0	0
			1722	1091	312	315	4			

- Molecule 51 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	D	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			
51	s2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			

- Molecule 52 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	E	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			
52	s3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			

- Molecule 53 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	F	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			
53	s4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			

- Molecule 54 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	G	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			
54	s5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			

- Molecule 55 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	H	226	Total	C	N	O	S	0	0	0
			1799	1129	346	321	3			
55	s6	218	Total	C	N	O	S	0	0	0
			1755	1102	337	313	3			

- Molecule 56 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	I	184	Total	C	N	O	0	0	0
			1481	951	265	265			
56	s7	186	Total	C	N	O	0	0	0
			1491	957	267	267			

- Molecule 57 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	J	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			
57	s8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

- Molecule 58 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	K	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			
58	s9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

- Molecule 59 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	L	96	Total	C	N	O	S	0	0	0
			772	499	126	145	2			
59	c0	96	Total	C	N	O	S	0	0	0
			760	489	125	144	2			

- Molecule 60 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	M	155	Total	C	N	O	S	0	0	0
			1213	774	230	206	3			
60	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

- Molecule 61 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	N	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			
61	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

- Molecule 62 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
62	O	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			
62	c3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			

- Molecule 63 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
63	P	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
63	c4	128	Total	C	N	O	S	0	0	0
			949	582	188	176	3			

- Molecule 64 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	Q	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			
64	c5	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	7			

- Molecule 65 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
65	R	141	Total	C	N	O	S	0	0	0
			1105	708	203	194				
65	c6	142	Total	C	N	O	S	0	0	0
			1111	711	204	196				

- Molecule 66 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	S	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			

- Molecule 67 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	T	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			
67	c8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			

- Molecule 68 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	U	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			
68	c9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			

- Molecule 69 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	V	107	Total	C	N	O	S	0	0	0
			855	539	156	159	1			
69	d0	110	Total	C	N	O	S	0	0	0
			882	554	161	166	1			

- Molecule 70 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
70	W	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			
70	d1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			

- Molecule 71 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
71	X	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			
71	d2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			

- Molecule 72 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	Y	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			
72	d3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			

- Molecule 73 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
73	Z	134	Total	C	N	O	0	0	0
			1073	676	208	189			
73	d4	134	Total	C	N	O	0	0	0
			1073	676	208	189			

- Molecule 74 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
74	a	70	Total	C	N	O	0	0	0
			563	360	104	99			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
74	d5	69	Total	C	N	O	0	0	0
			558	357	103	98			

- Molecule 75 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	b	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			
75	d6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

- Molecule 76 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	c	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			
76	d7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			

- Molecule 77 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	d	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			
77	d8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			

- Molecule 78 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	e	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			
78	d9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			

- Molecule 79 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	f	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			
79	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

- Molecule 80 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	g	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			

- Molecule 81 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	h	318	Total	C	N	O	S	0	0	0
			2437	1541	418	470	8			
81	Rb	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

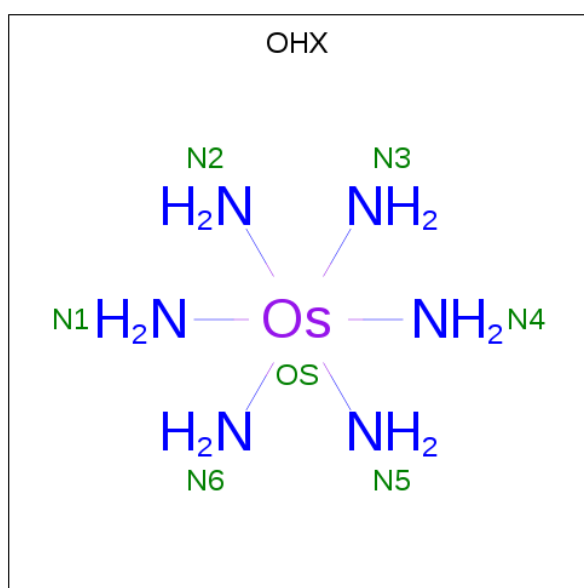
- Molecule 82 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

- Molecule 83 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
83	e1	51	Total	C	N	O	S	0	0	0
			397	249	73	71	4			

- Molecule 84 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
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			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	3	1	Total	N	Os	0	0
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84	3	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	r	1	Total	N	Os	0	0
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84	v	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	x	1	Total 7	N 6	Os 1	0	0
84	y	1	Total 7	N 6	Os 1	0	0
84	z	1	Total 7	N 6	Os 1	0	0
84	AC	1	Total 7	N 6	Os 1	0	0
84	AG	1	Total 7	N 6	Os 1	0	0
84	AK	1	Total 7	N 6	Os 1	0	0
84	AK	1	Total 7	N 6	Os 1	0	0
84	AP	1	Total 7	N 6	Os 1	0	0
84	AR	1	Total 7	N 6	Os 1	0	0
84	AR	1	Total 7	N 6	Os 1	0	0
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84	AR	1	Total 7	N 6	Os 1	0	0
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84	AR	1	Total 7	N 6	Os 1	0	0
84	AR	1	Total 7	N 6	Os 1	0	0
84	AR	1	Total 7	N 6	Os 1	0	0
84	AR	1	Total 7	N 6	Os 1	0	0
84	AR	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	AR	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AS	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AS	1	Total	N	Os	0	0
			7	6	1		
84	AS	1	Total	N	Os	0	0
			7	6	1		
84	AS	1	Total	N	Os	0	0
			7	6	1		
84	AS	1	Total	N	Os	0	0
			7	6	1		
84	AS	1	Total	N	Os	0	0
			7	6	1		
84	AS	1	Total	N	Os	0	0
			7	6	1		
84	AS	1	Total	N	Os	0	0
			7	6	1		
84	AS	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
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84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
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84	CE	1	Total	N	Os	0	0
			7	6	1		
84	CE	1	Total	N	Os	0	0
			7	6	1		
84	CF	1	Total	N	Os	0	0
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84	CF	1	Total	N	Os	0	0
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84	CG	1	Total	N	Os	0	0
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84	CG	1	Total	N	Os	0	0
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84	CG	1	Total	N	Os	0	0
			7	6	1		
84	CK	1	Total	N	Os	0	0
			7	6	1		
84	CL	1	Total	N	Os	0	0
			7	6	1		
84	CL	1	Total	N	Os	0	0
			7	6	1		
84	CM	1	Total	N	Os	0	0
			7	6	1		
84	CO	1	Total	N	Os	0	0
			7	6	1		
84	CP	1	Total	N	Os	0	0
			7	6	1		
84	CS	1	Total	Os		0	0
			1	1			
84	CV	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	CX	1	Total	N	Os	0	0
			7	6	1		
84	CX	1	Total	N	Os	0	0
			7	6	1		
84	DD	1	Total	N	Os	0	0
			7	6	1		
84	DH	1	Total	N	Os	0	0
			7	6	1		
84	DL	1	Total	N	Os	0	0
			7	6	1		
84	DQ	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	A	1	Total	N	Os	0	0
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84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	A	1	Total 7	N 6	Os 1	0	0
84	H	1	Total 7	N 6	Os 1	0	0
84	J	1	Total 7	N 6	Os 1	0	0
84	M	1	Total 7	N 6	Os 1	0	0
84	O	1	Total 7	N 6	Os 1	0	0
84	Q	1	Total 7	N 6	Os 1	0	0
84	T	1	Total 7	N 6	Os 1	0	0
84	e	1	Total 7	N 6	Os 1	0	0
84	h	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0
84	sR	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		
84	Rb	1	Total	N	Os	0	0
			7	6	1		
84	s1	1	Total	N	Os	0	0
			7	6	1		
84	s4	1	Total	N	Os	0	0
			7	6	1		
84	s8	1	Total	N	Os	0	0
			7	6	1		
84	c3	1	Total	N	Os	0	0
			7	6	1		
84	c5	1	Total	N	Os	0	0
			7	6	1		
84	c8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	d4	1	Total	N	Os	0	0
			7	6	1		
84	d9	1	Total	N	Os	0	0
			7	6	1		

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	AP	1	Total	Mg	0	0
			1	1		
85	AK	1	Total	Mg	0	0
			1	1		
85	AB	4	Total	Mg	0	0
			4	4		
85	c6	1	Total	Mg	0	0
			1	1		
85	6	2	Total	Mg	0	0
			2	2		
85	DO	1	Total	Mg	0	0
			1	1		
85	sM	1	Total	Mg	0	0
			1	1		
85	d5	1	Total	Mg	0	0
			1	1		
85	t	3	Total	Mg	0	0
			3	3		
85	CD	2	Total	Mg	0	0
			2	2		
85	CR	6	Total	Mg	0	0
			6	6		
85	o	1	Total	Mg	0	0
			1	1		
85	DC	6	Total	Mg	0	0
			6	6		
85	AS	17	Total	Mg	0	0
			17	17		
85	DH	2	Total	Mg	0	0
			2	2		
85	J	1	Total	Mg	0	0
			1	1		
85	k	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	CU	1	Total 1	Mg 1	0	0
85	b	1	Total 1	Mg 1	0	0
85	DR	2	Total 2	Mg 2	0	0
85	w	1	Total 1	Mg 1	0	0
85	c8	1	Total 1	Mg 1	0	0
85	A	109	Total 109	Mg 109	0	0
85	CQ	3	Total 3	Mg 3	0	0
85	n	1	Total 1	Mg 1	0	0
85	x	5	Total 5	Mg 5	0	0
85	AR	504	Total 504	Mg 504	0	0
85	d6	2	Total 2	Mg 2	0	0
85	s	1	Total 1	Mg 1	0	0
85	CG	1	Total 1	Mg 1	0	0
85	j	1	Total 1	Mg 1	0	0
85	1	485	Total 485	Mg 485	0	0
85	CN	1	Total 1	Mg 1	0	0
85	DD	1	Total 1	Mg 1	0	0
85	e	1	Total 1	Mg 1	0	0
85	d3	2	Total 2	Mg 2	0	0
85	c1	1	Total 1	Mg 1	0	0
85	v	2	Total 2	Mg 2	0	0

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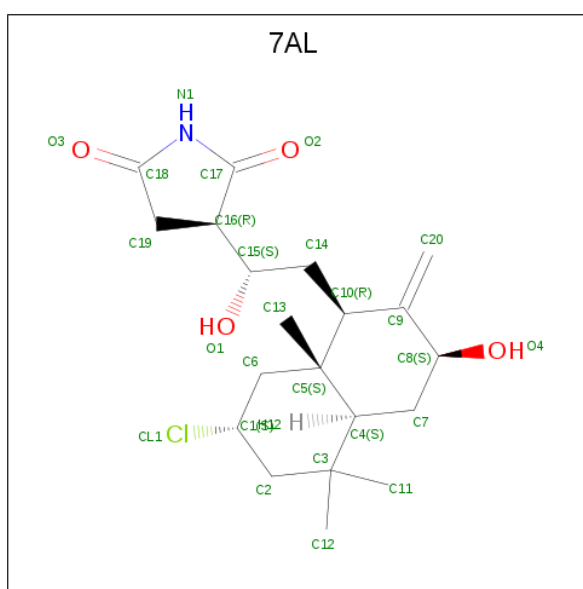
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	CJ	1	Total 1	Mg 1	0	0
85	CP	4	Total 4	Mg 4	0	0
85	4	19	Total 19	Mg 19	0	0
85	DA	1	Total 1	Mg 1	0	0
85	O	1	Total 1	Mg 1	0	0
85	r	2	Total 2	Mg 2	0	0
85	CF	1	Total 1	Mg 1	0	0
85	CX	3	Total 3	Mg 3	0	0
85	CM	2	Total 2	Mg 2	0	0
85	s1	1	Total 1	Mg 1	0	0
85	AH	1	Total 1	Mg 1	0	0
85	DP	1	Total 1	Mg 1	0	0
85	s8	1	Total 1	Mg 1	0	0
85	D	1	Total 1	Mg 1	0	0
85	d9	1	Total 1	Mg 1	0	0
85	c7	1	Total 1	Mg 1	0	0
85	sR	139	Total 139	Mg 139	0	0
85	z	1	Total 1	Mg 1	0	0
85	AT	13	Total 13	Mg 13	0	0
85	d4	1	Total 1	Mg 1	0	0
85	u	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	CE	2	Total	Mg	0	0
			2	2		
85	Y	1	Total	Mg	0	0
			1	1		
85	l	5	Total	Mg	0	0
			5	5		
85	3	12	Total	Mg	0	0
			12	12		

- Molecule 86 is Chlorolissoclimide (three-letter code: 7AL) (formula: $C_{20}H_{30}ClNO_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
86	1	1	Total	C	Cl	N	O	0	0
			26	20	1	1	4		
86	AR	1	Total	C	Cl	N	O	0	0
			26	20	1	1	4		

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	AP	1	Total	Zn	0	0
			1	1		
87	g	1	Total	Zn	0	0
			1	1		
87	AQ	1	Total	Zn	0	0
			1	1		

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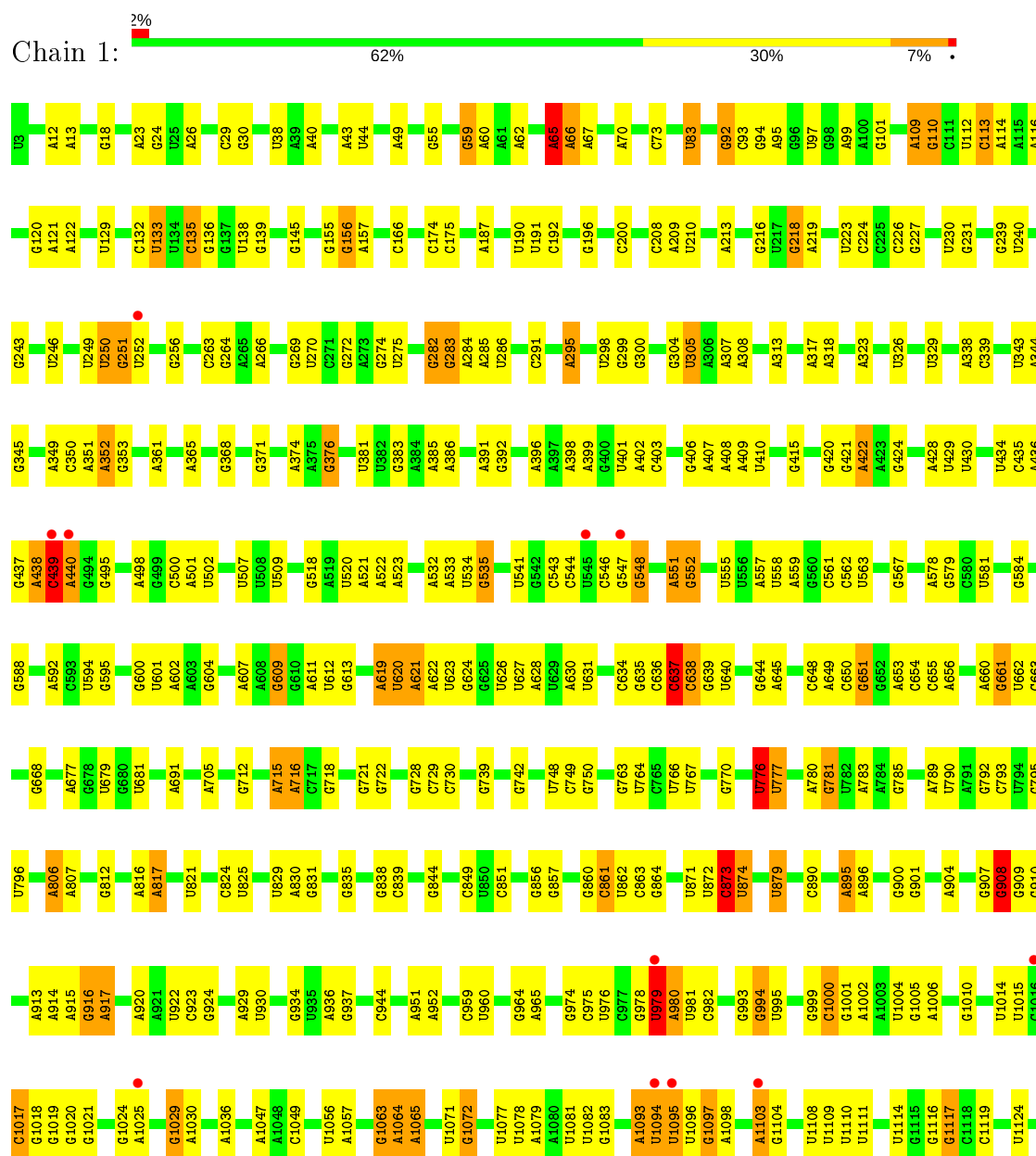
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	AK	1	Total 1	Zn 1	0	0
87	DQ	1	Total 1	Zn 1	0	0
87	e	1	Total 1	Zn 1	0	0
87	b	1	Total 1	Zn 1	0	0
87	e1	1	Total 1	Zn 1	0	0
87	c	1	Total 1	Zn 1	0	0
87	DL	1	Total 1	Zn 1	0	0
87	d9	1	Total 1	Zn 1	0	0
87	DR	1	Total 1	Zn 1	0	0
87	DO	1	Total 1	Zn 1	0	0
87	AN	1	Total 1	Zn 1	0	0
87	d7	1	Total 1	Zn 1	0	0
87	d6	1	Total 1	Zn 1	0	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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

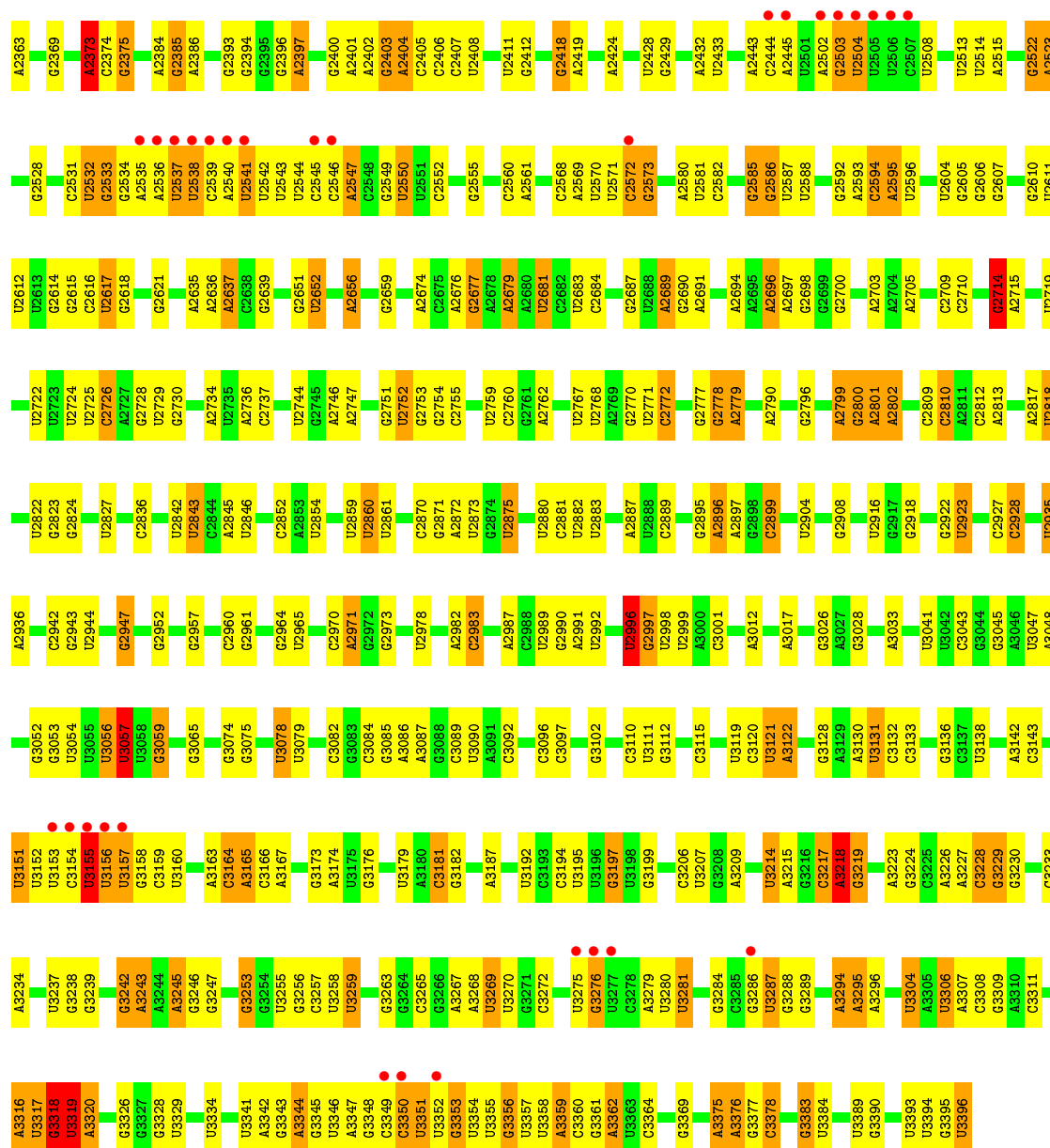
• Molecule 1: 25S ribosomal RNA



U2683	C2566	A2296	U2209	C2098	U1853	G1761	G1634	U1554	G1434	G1321	U1241	G1131
C2684	C2567	A2299	G2210	A2099	C1854	C1762	G1635	U1555	A1435	U1329	G1242	A1135
C2420	A2219	G2302	C2211	C2100	U1855	U1763	U1636	U1556	U1436	A1330	G1243	A1136
U2427	G2307	G2302	A2213	U2102	C1857	U1765	C1639	G1560	G1440	U1331	A1245	G1145
U2428	C2308	G2435	G2218	A2107	G1861	G1769	A1643	C1561	G1441	A1332	U1247	C1146
G2429	A2309	U2439	A2219	C2108	U1862	G1770	C1644	C1562	U1445	G1340	C1248	A1183
G2435	U2310	U2438	A2220	G2111	C1866	G1780	G1646	U1564	U1446	U1341	C1249	C1156
G2690	G2311	A2438	G2221	U2112	C1866	G1786	G1650	U1565	G1450	U1251	A1251	A1159
A2691	A2312	A2439	A2222	A2113	U1871	A1787	C1657	U1567	A1450	A1252	A1252	C1160
A2694	G2313	A2443	A2224	C2114	G1786	A1787	C1657	U1568	A1450	C1255	C1255	G1166
A2695	U2315	C2444	A2225	A2120	G1790	G1790	G1658	U1569	A1461	G1257	G1257	G1167
A2696	G2316	U2226	U2226	G2121	G1878	G1790	G1659	U1570	A1462	A1352	U1258	A1170
A2697	A2317	G2327	G2227	G2122	A1879	A1797	C1660	A1571	G1464	G1353	U1259	G1171
G2698	U2318	A2228	A2228	C2128	A1886	A1798	A1676	U1572	C1478	A1355	A1260	C1176
A2705	G2334	A2229	A2232	G2131	A1887	A1799	A1667	C1574	U1479	U1356	G1261	G1177
A2712	U2336	A2232	A2233	A2134	G1892	A1804	G1668	A1575	U1481	G1357	G1262	G1177
A2713	G2353	G2234	G2234	G2134	A1895	C1805	C1669	G1576	A1482	G1362	A1263	A1180
A2714	C2354	A2242	A2242	U2137	A1896	A1806	G1674	C1577	G1483	A1363	G1264	U1181
A2715	G2355	A2243	A2243	A2138	G1898	A1807	G1675	C1578	U1484	C1364	U1265	U1182
A2716	A2356	A2244	A2244	A2139	A1809	A1809	A1676	A1580	G1485	G1365	U1267	C1185
A2717	G2357	A2245	A2245	U2140	A1810	A1810	A1683	C1581	G1486	A1366	U1268	C1185
A2718	A2358	A2246	G2247	U2141	G1811	G1811	U1688	A1582	U1487	U1367	U1269	A1190
A2719	G2359	A2247	G2248	G2145	A1812	A1812	U1689	A1583	A1489	A1369	A1270	A1191
A2720	A2360	A2248	G2249	G2146	A1813	A1813	A1699	A1584	A1490	G1380	C1272	C1192
A2721	G2361	A2249	G2250	A2147	U1814	U1814	A1699	A1585	A1491	A1273	A1273	C1201
A2722	A2362	A2250	A2251	A2148	U1815	U1815	A1706	A1586	A1492	A1386	A1274	C1201
A2723	G2363	A2252	A2252	G2149	A1816	A1816	A1707	A1587	U1495	G1389	A1278	G1209
A2724	C2364	A2253	A2253	G2150	U1817	U1817	A1707	A1588	A1498	A1389	C1279	U1210
A2725	G2365	A2254	A2254	G2151	U1818	U1818	U1716	A1589	C1499	A1399	C1280	U1211
A2726	A2366	A2255	A2255	A2152	U1819	U1819	U1717	C1596	C1502	G1400	G1285	A1212
A2727	G2367	A2256	A2256	G2153	U1820	U1820	U1718	C1597	A1503	A1407	A1286	G1213
A2728	A2368	A2257	A2257	A2154	U1821	U1821	G1718	G1598	C1502	A1287	A1287	C1216
A2729	G2369	A2258	A2258	G2155	G1825	G1825	U1724	G1599	A1503	G1408	A1217	A1217
A2730	A2370	A2259	A2259	A2156	G1833	G1833	C1725	A1603	G1507	C1292	C1292	G1222
A2731	G2371	A2260	A2260	G2157	U1834	U1834	G1726	G1604	G1409	U1293	U1293	G1222
A2732	A2372	A2261	A2261	A2158	U1835	U1835	G1727	A1605	C1508	A1294	A1294	A1225
A2733	G2373	A2262	A2262	G2159	G1838	G1838	G1734	U1606	U1522	G1412	C1296	G1225
A2734	A2374	A2263	A2263	G2160	U1839	U1839	G1735	C1608	A1524	G1413	C1297	C1227
A2735	G2375	A2264	A2264	G2161	U1840	U1840	G1736	C1609	C1527	A1301	A1301	G1230
A2736	A2376	A2265	A2265	A2162	A1841	A1841	U1740	C1615	A1418	A1302	A1302	A1231
A2737	G2377	A2266	A2266	G2163	U1842	U1842	A1741	U1616	A1419	G1307	G1307	G1232
A2738	A2378	A2267	A2267	G2164	G1843	G1843	U1742	U1617	A1534	A1308	A1308	G1233
A2739	G2379	A2268	A2268	A2165	U1844	U1844	G1743	G1618	U1425	G1234	G1234	G1234
A2740	A2380	A2269	A2269	G2166	G1845	G1845	G1744	G1619	A1426	U1309	U1309	G1235
A2741	G2381	A2270	A2270	G2167	U1846	U1846	U1750	U1620	A1427	U1236	G1236	U1236
A2742	A2382	A2271	A2271	A2168	C1849	C1849	G1751	A1621	G1429	G1313	G1313	G1237
A2743	G2383	A2272	A2272	G2169	U1850	U1850	A1751	U1622	U1430	A1317	A1317	G1238
A2744	A2384	A2273	A2273	A2170	G1851	G1851	A1760	U1629	G1542	C1320	C1320	C1239
A2745	G2385	A2274	A2274	G2171	G1852	G1852	A1760	U1629	G1543	A1433	A1433	A1240
A2746	A2386	A2275	A2275	G2172	U1853	U1853	A1760	U1629	G1543	A1433	A1433	A1240
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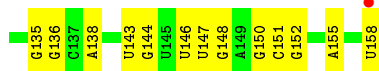
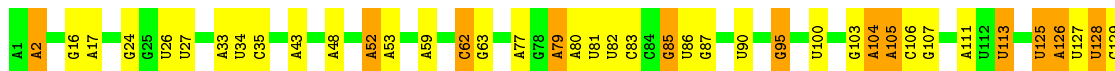








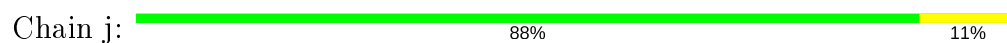
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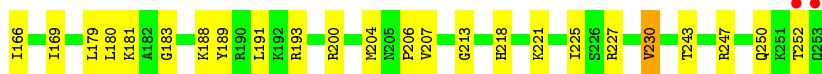
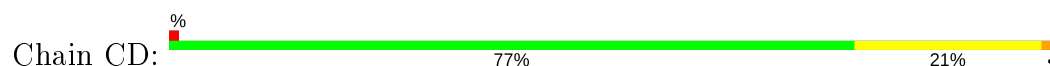
- Molecule 3: 5.8S ribosomal RNA



- Molecule 4: 60S ribosomal protein L2-A

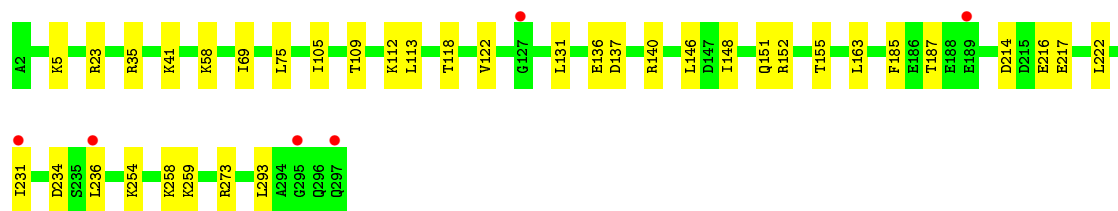


- Molecule 4: 60S ribosomal protein L2-A

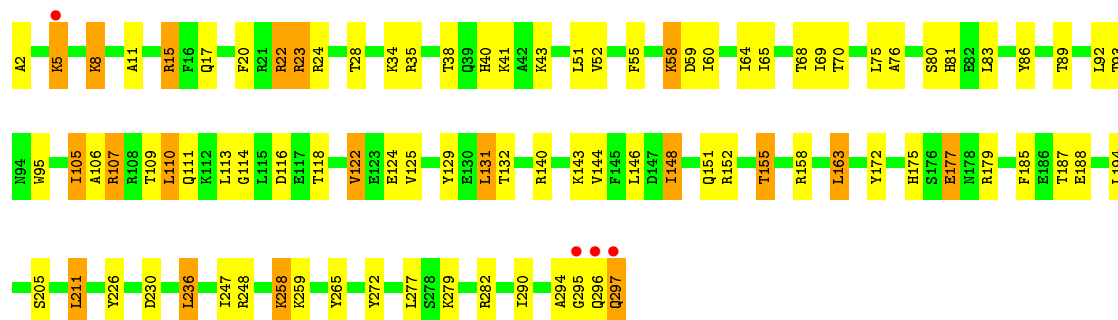
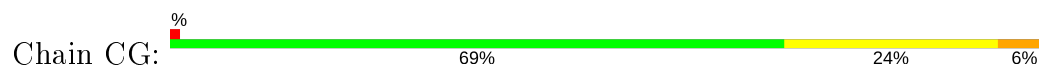


- Molecule 5: 60S ribosomal protein L3

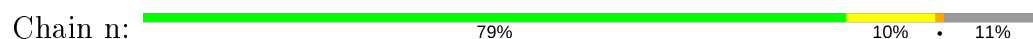




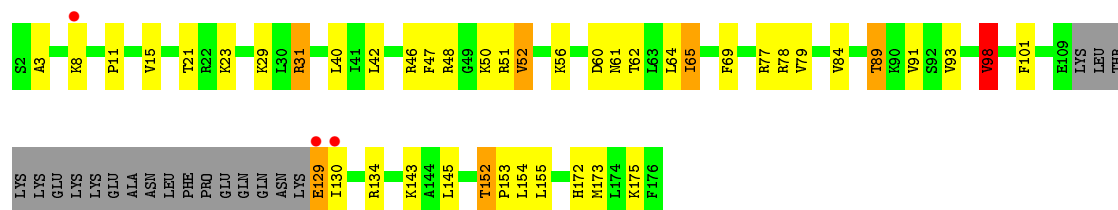
• Molecule 7: 60S ribosomal protein L5



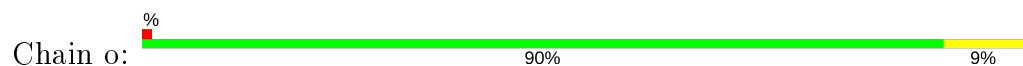
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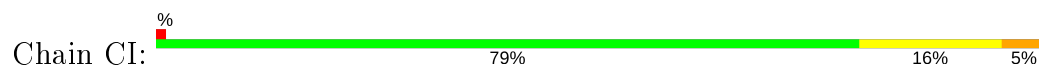
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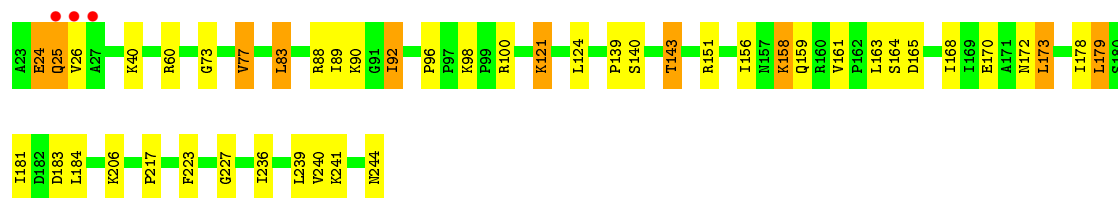


• Molecule 9: 60S ribosomal protein L7-A

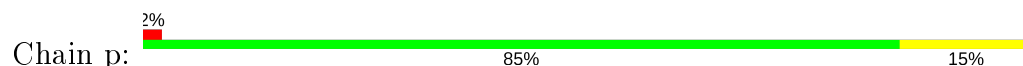


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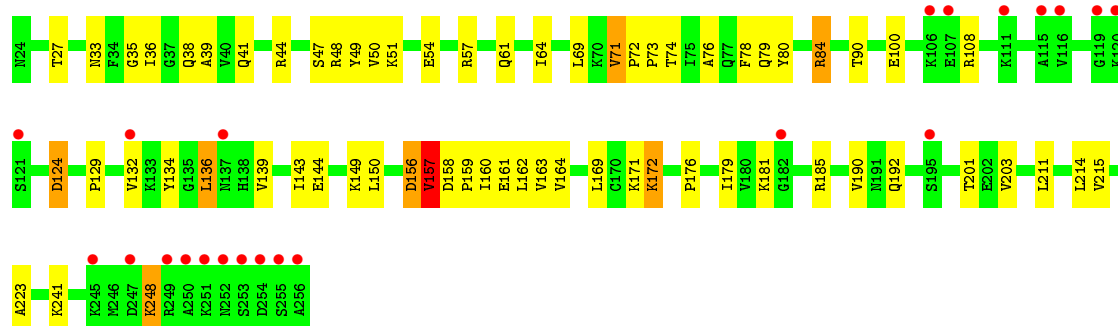
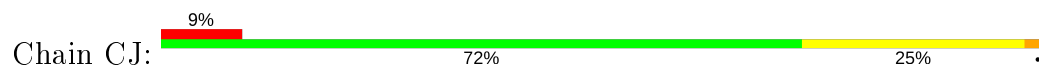




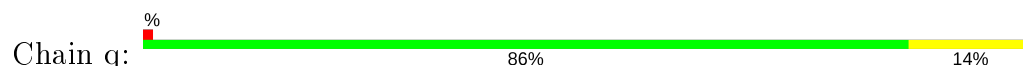
- Molecule 10: 60S ribosomal protein L8-A



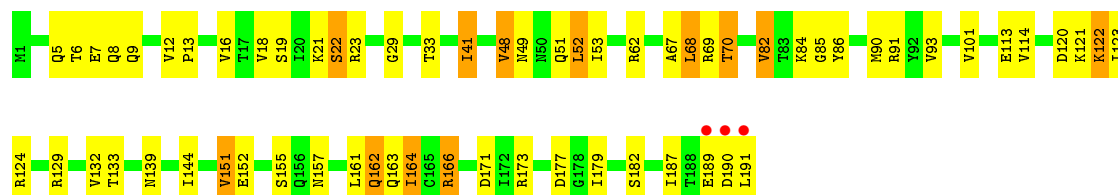
- Molecule 10: 60S ribosomal protein L8-A



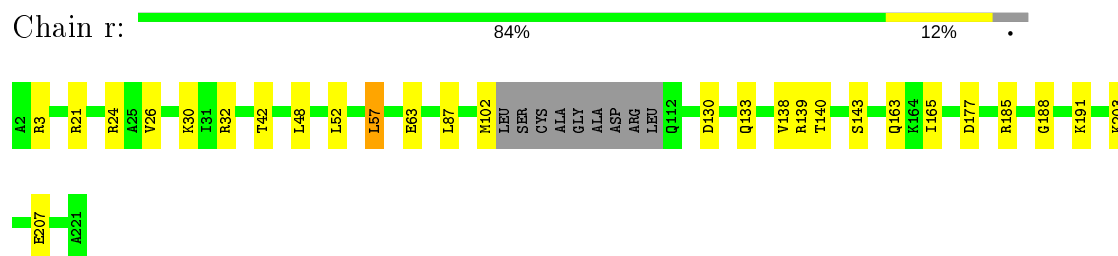
- Molecule 11: 60S ribosomal protein L9-A



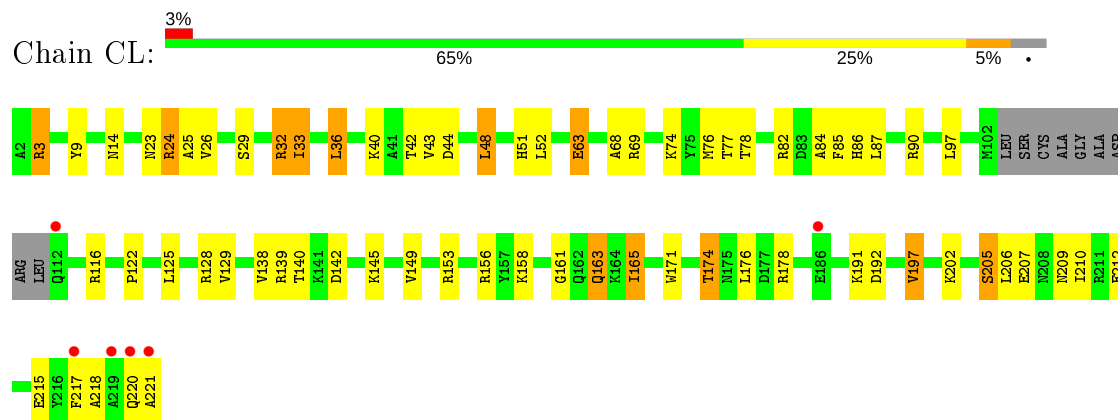
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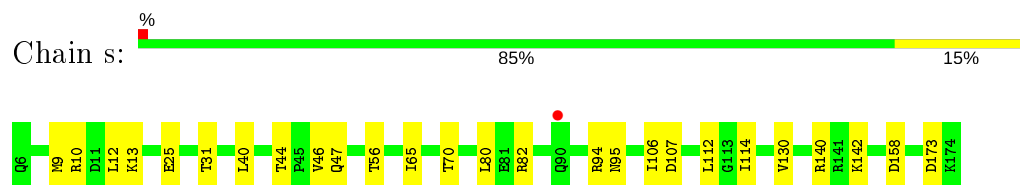
- Molecule 12: 60S ribosomal protein L10



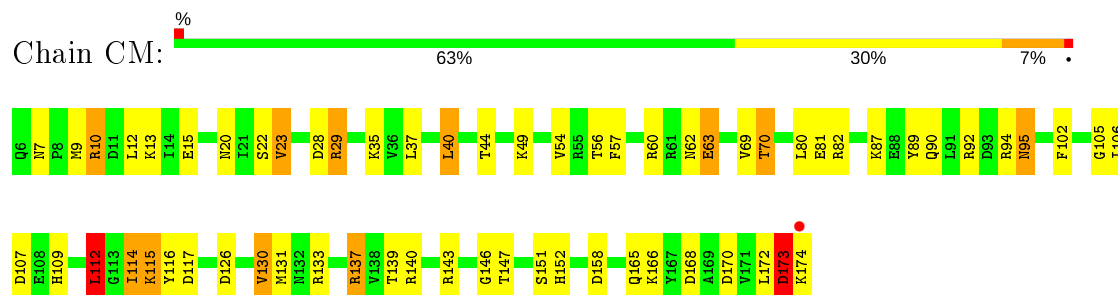
- Molecule 12: 60S ribosomal protein L10



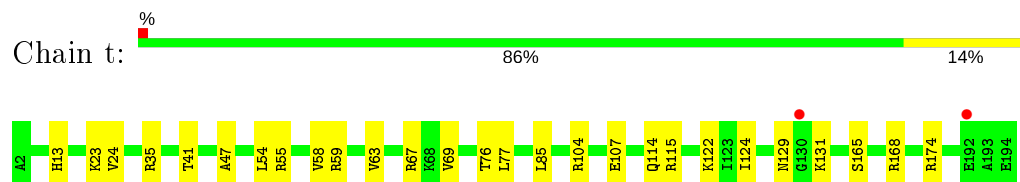
- Molecule 13: 60S ribosomal protein L11-B



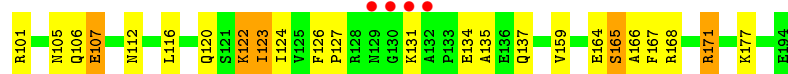
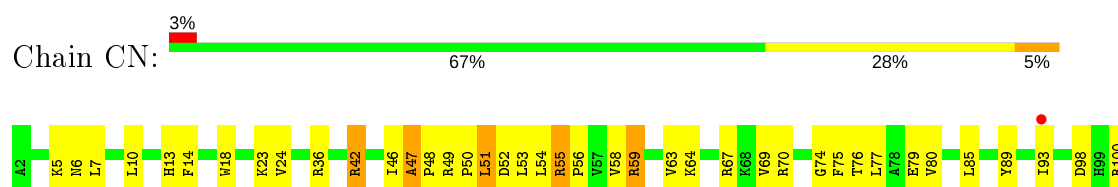
- Molecule 13: 60S ribosomal protein L11-B



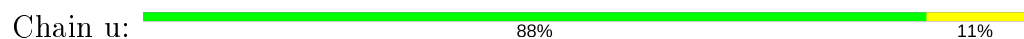
- Molecule 14: 60S ribosomal protein L13-A



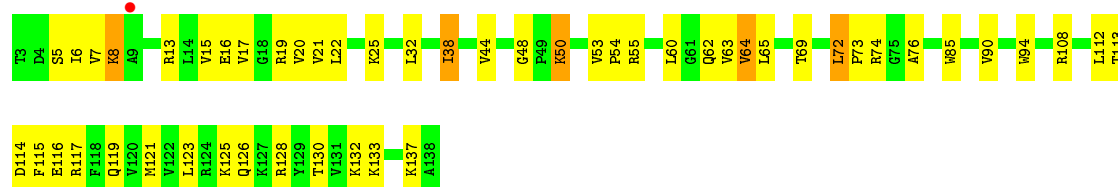
- Molecule 14: 60S ribosomal protein L13-A



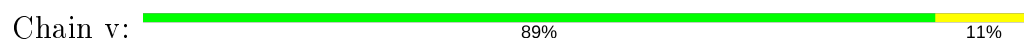
- Molecule 15: 60S ribosomal protein L14-A



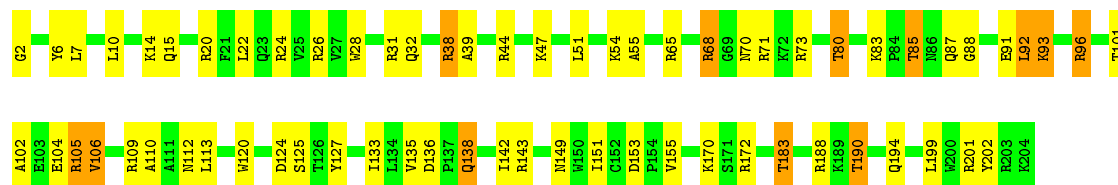
- Molecule 15: 60S ribosomal protein L14-A



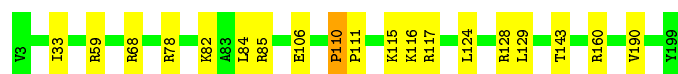
- Molecule 16: 60S ribosomal protein L15-A



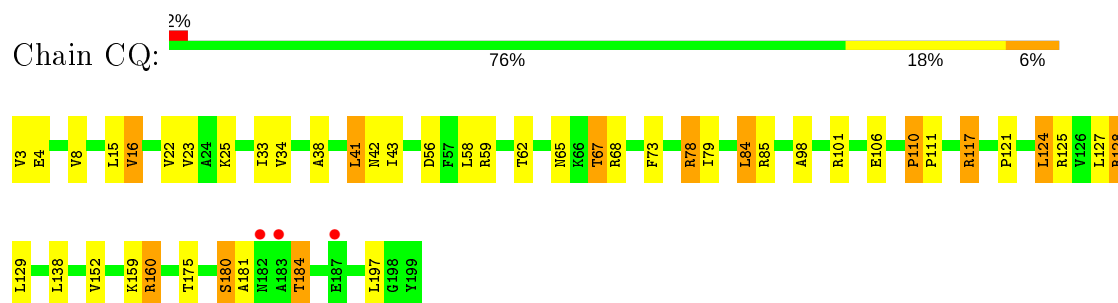
- Molecule 16: 60S ribosomal protein L15-A



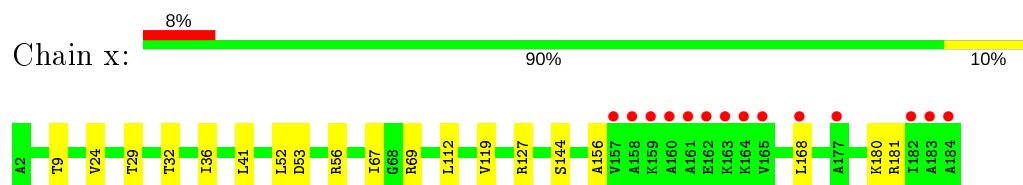
- Molecule 17: 60S ribosomal protein L16-A



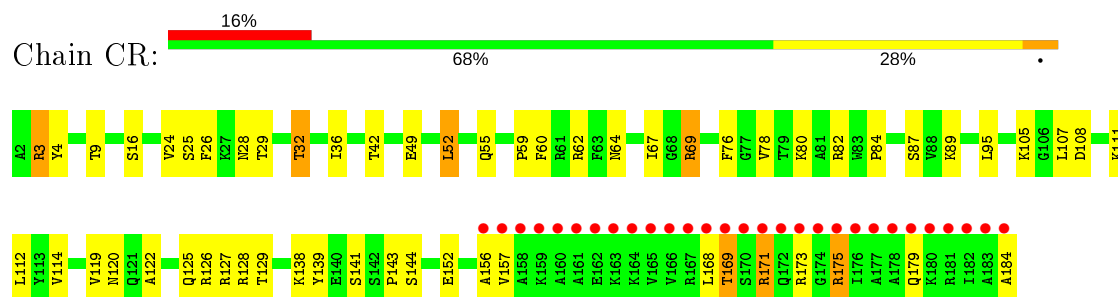
- Molecule 17: 60S ribosomal protein L16-A



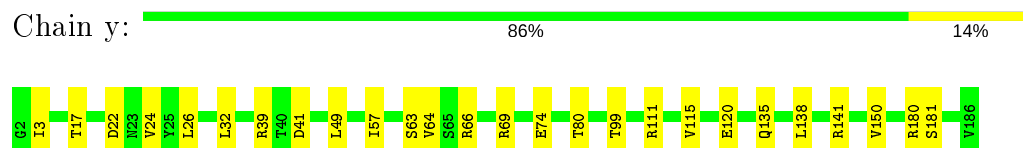
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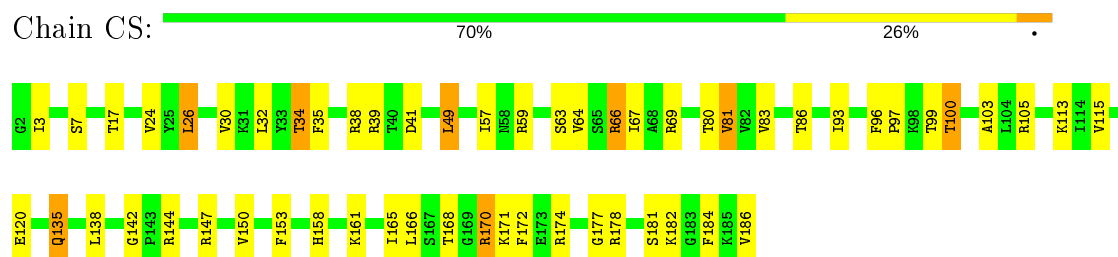
- Molecule 18: 60S ribosomal protein L17-A



- Molecule 19: 60S ribosomal protein L18-A

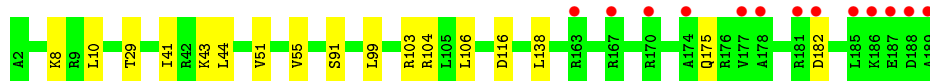


- Molecule 19: 60S ribosomal protein L18-A

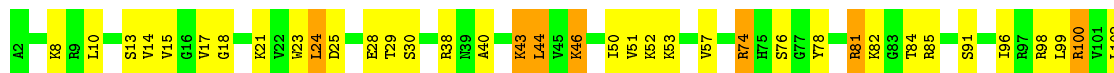


- Molecule 20: 60S ribosomal protein L19-A

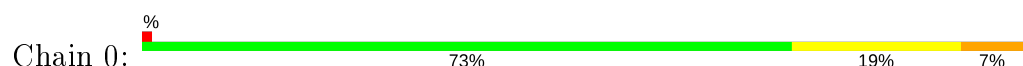




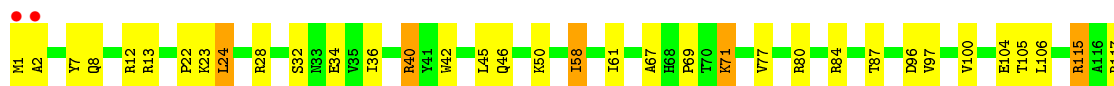
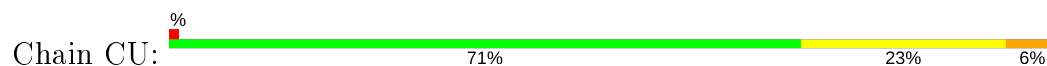
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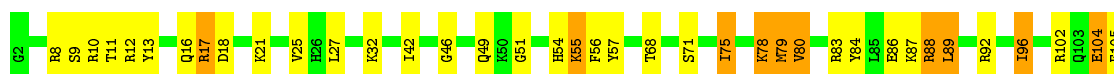
- Molecule 21: 60S ribosomal protein L20-A



- Molecule 21: 60S ribosomal protein L20-A

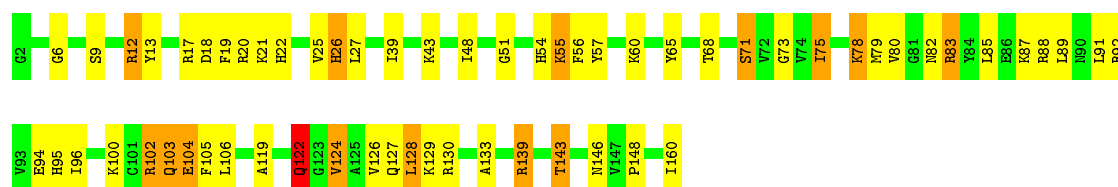


- Molecule 22: 60S ribosomal protein L21-A

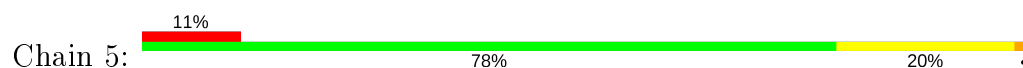


- Molecule 22: 60S ribosomal protein L21-A

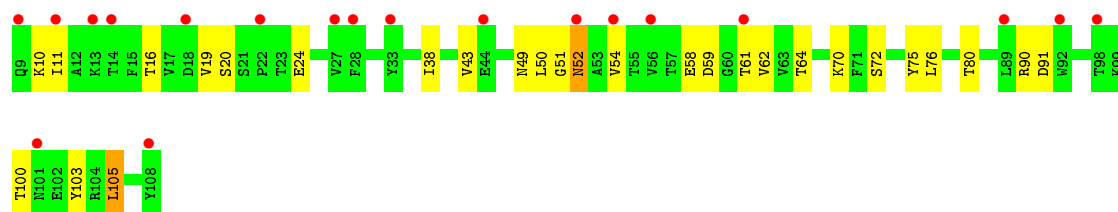
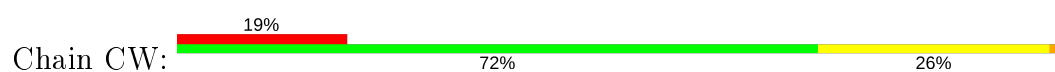




- Molecule 23: 60S ribosomal protein L22-A



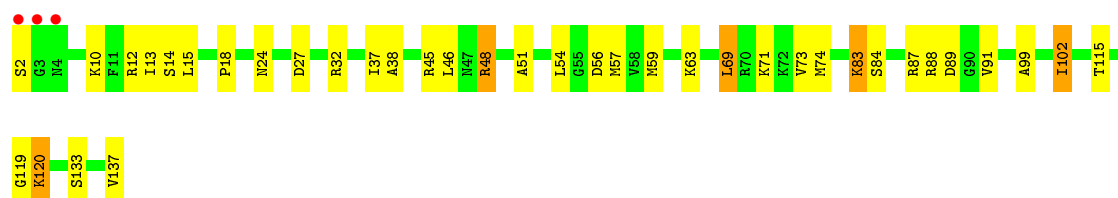
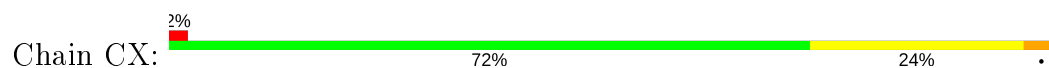
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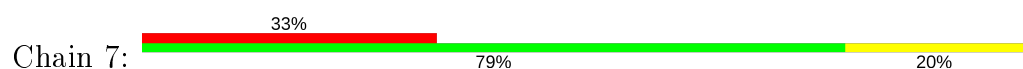
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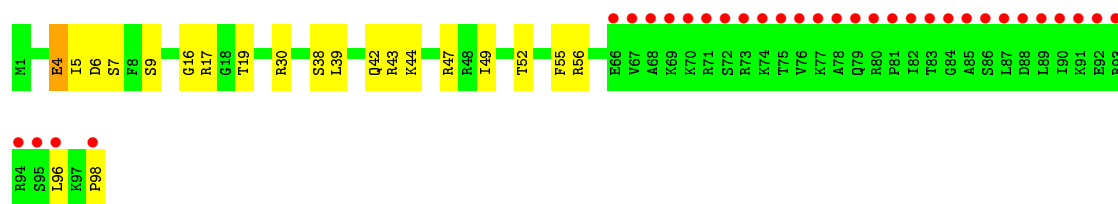


- Molecule 24: 60S ribosomal protein L23-A

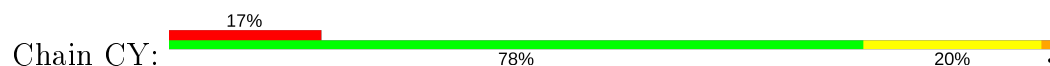


- Molecule 25: 60S ribosomal protein L24-A

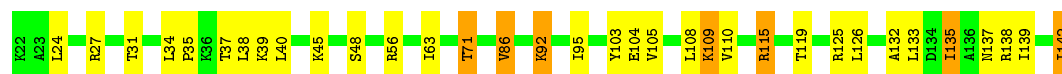




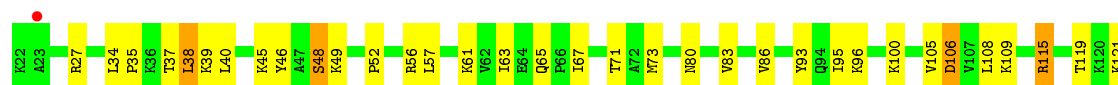
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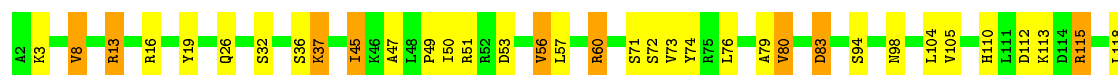
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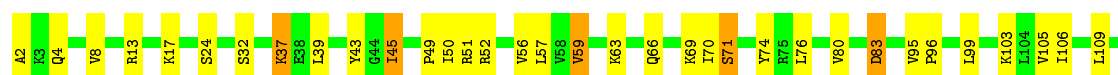
- Molecule 26: 60S ribosomal protein L25



- Molecule 27: 60S ribosomal protein L26-A

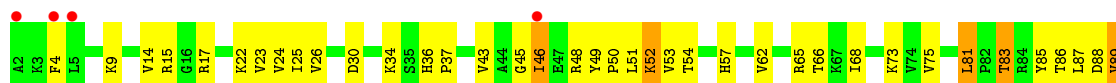


- Molecule 27: 60S ribosomal protein L26-A





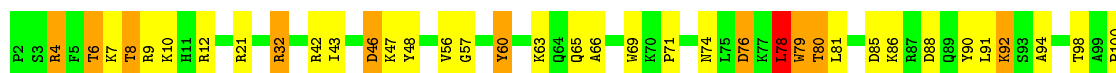
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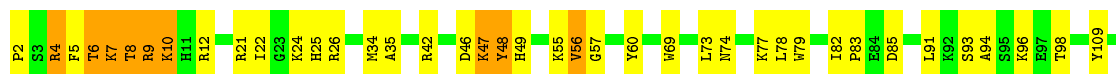
- Molecule 28: 60S ribosomal protein L27-A



- Molecule 29: 60S ribosomal protein L28



- Molecule 29: 60S ribosomal protein L28

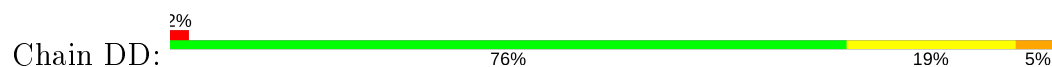


- Molecule 30: 60S ribosomal protein L29





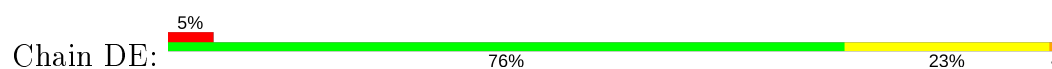
- Molecule 30: 60S ribosomal protein L29



- Molecule 31: 60S ribosomal protein L30



- Molecule 31: 60S ribosomal protein L30



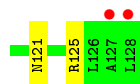
- Molecule 32: 60S ribosomal protein L31-A



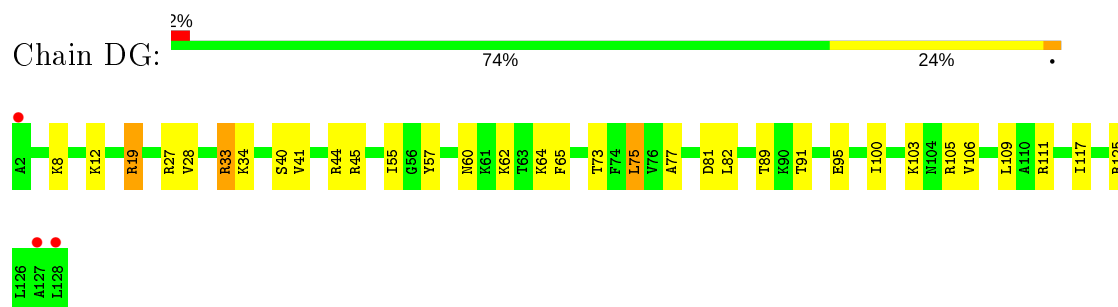
- Molecule 32: 60S ribosomal protein L31-A



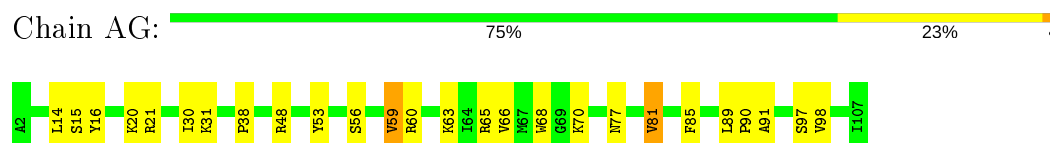
- Molecule 33: 60S ribosomal protein L32



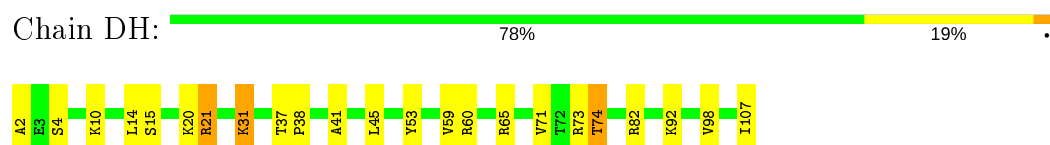
- Molecule 33: 60S ribosomal protein L32



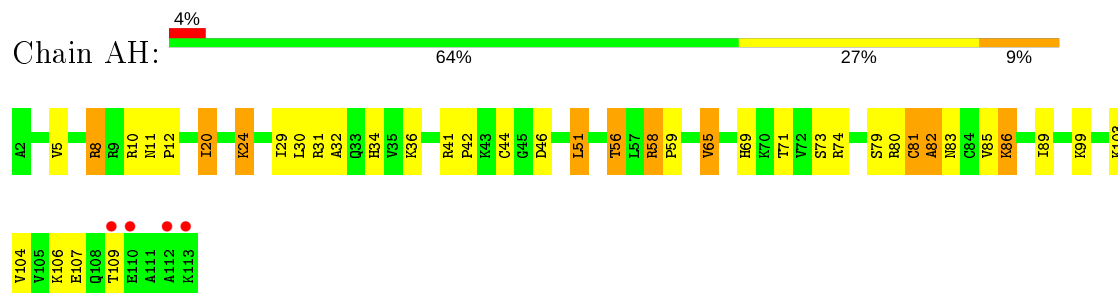
- Molecule 34: 60S ribosomal protein L33-A



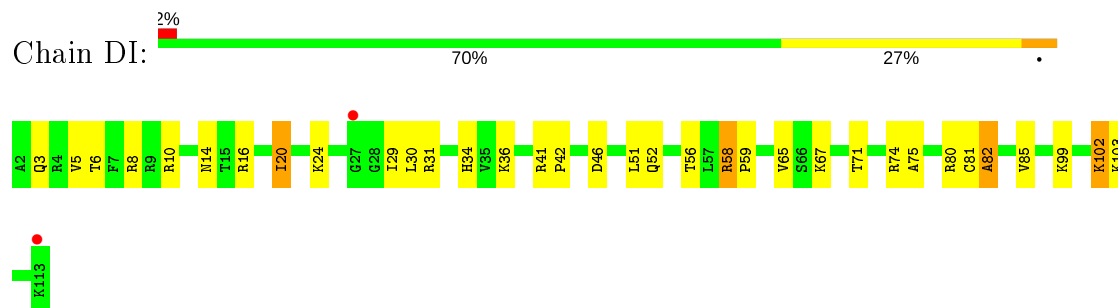
- Molecule 34: 60S ribosomal protein L33-A



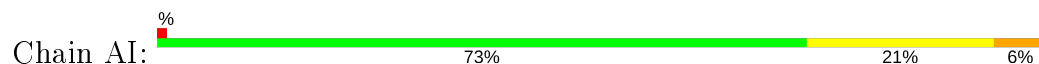
- Molecule 35: 60S ribosomal protein L34-A

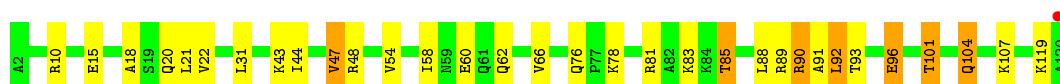


- Molecule 35: 60S ribosomal protein L34-A

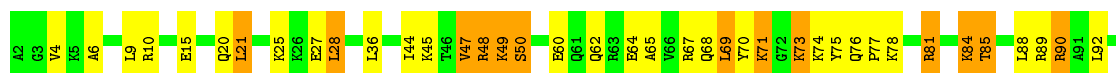


- Molecule 36: 60S ribosomal protein L35-A

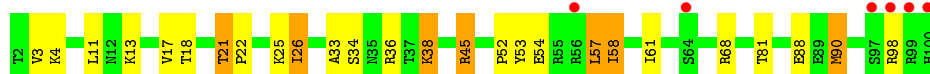




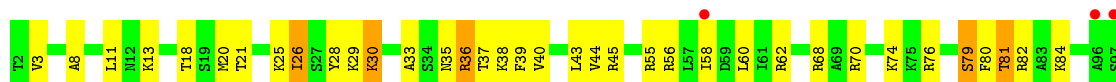
- Molecule 36: 60S ribosomal protein L35-A



- Molecule 37: 60S ribosomal protein L36-A



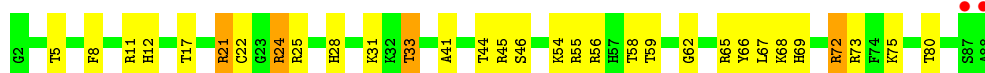
- Molecule 37: 60S ribosomal protein L36-A



- Molecule 38: 60S ribosomal protein L37-A



- Molecule 38: 60S ribosomal protein L37-A

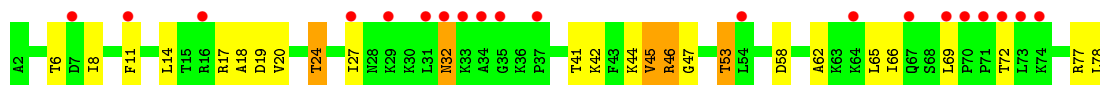


- Molecule 39: 60S ribosomal protein L38





- Molecule 39: 60S ribosomal protein L38



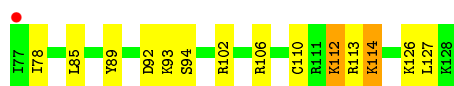
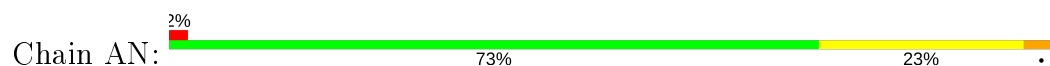
- Molecule 40: 60S ribosomal protein L39



- Molecule 40: 60S ribosomal protein L39



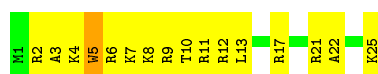
- Molecule 41: Ubiquitin-60S ribosomal protein L40



- Molecule 41: Ubiquitin-60S ribosomal protein L40



- Molecule 42: 60S ribosomal protein L41-A

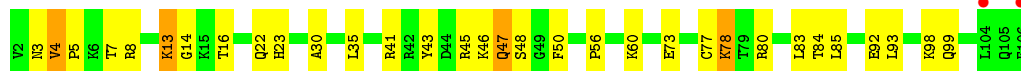


- Molecule 42: 60S ribosomal protein L41-A

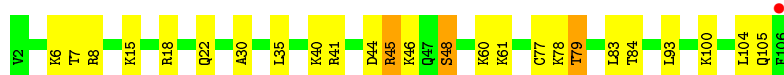
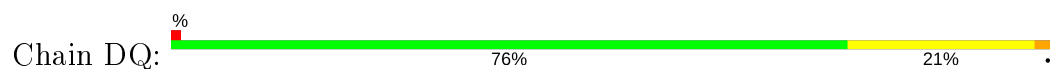




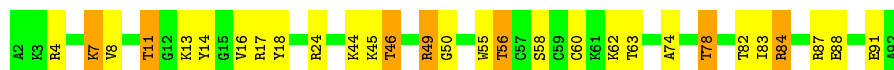
- Molecule 43: 60S ribosomal protein L42-A



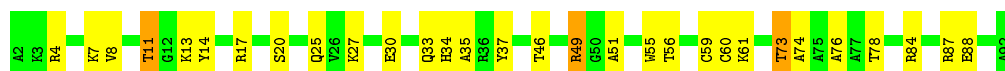
- Molecule 43: 60S ribosomal protein L42-A



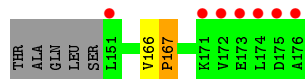
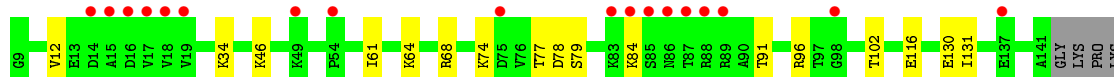
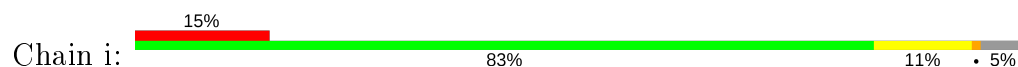
- Molecule 44: 60S ribosomal protein L43-A



- Molecule 44: 60S ribosomal protein L43-A

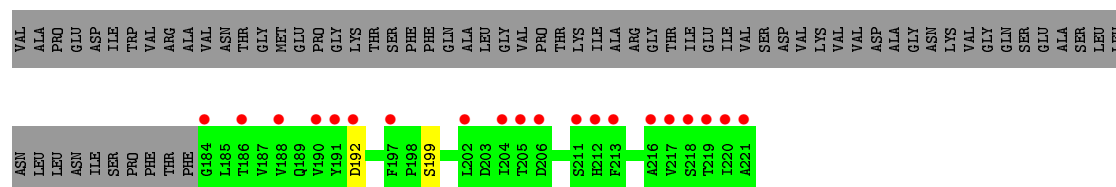


- Molecule 45: Suppressor protein STM1



- Molecule 46: 60S acidic ribosomal protein P0

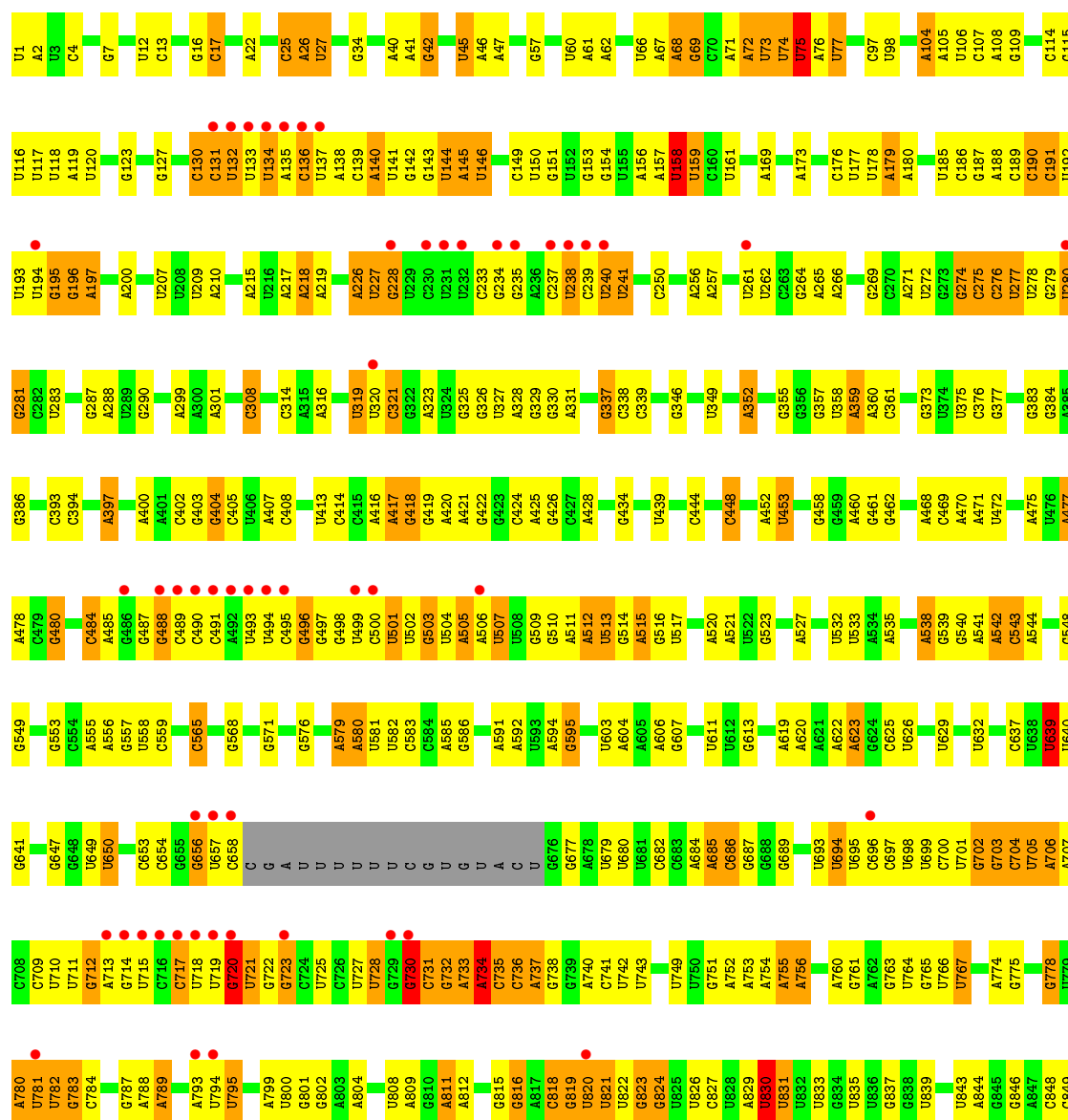


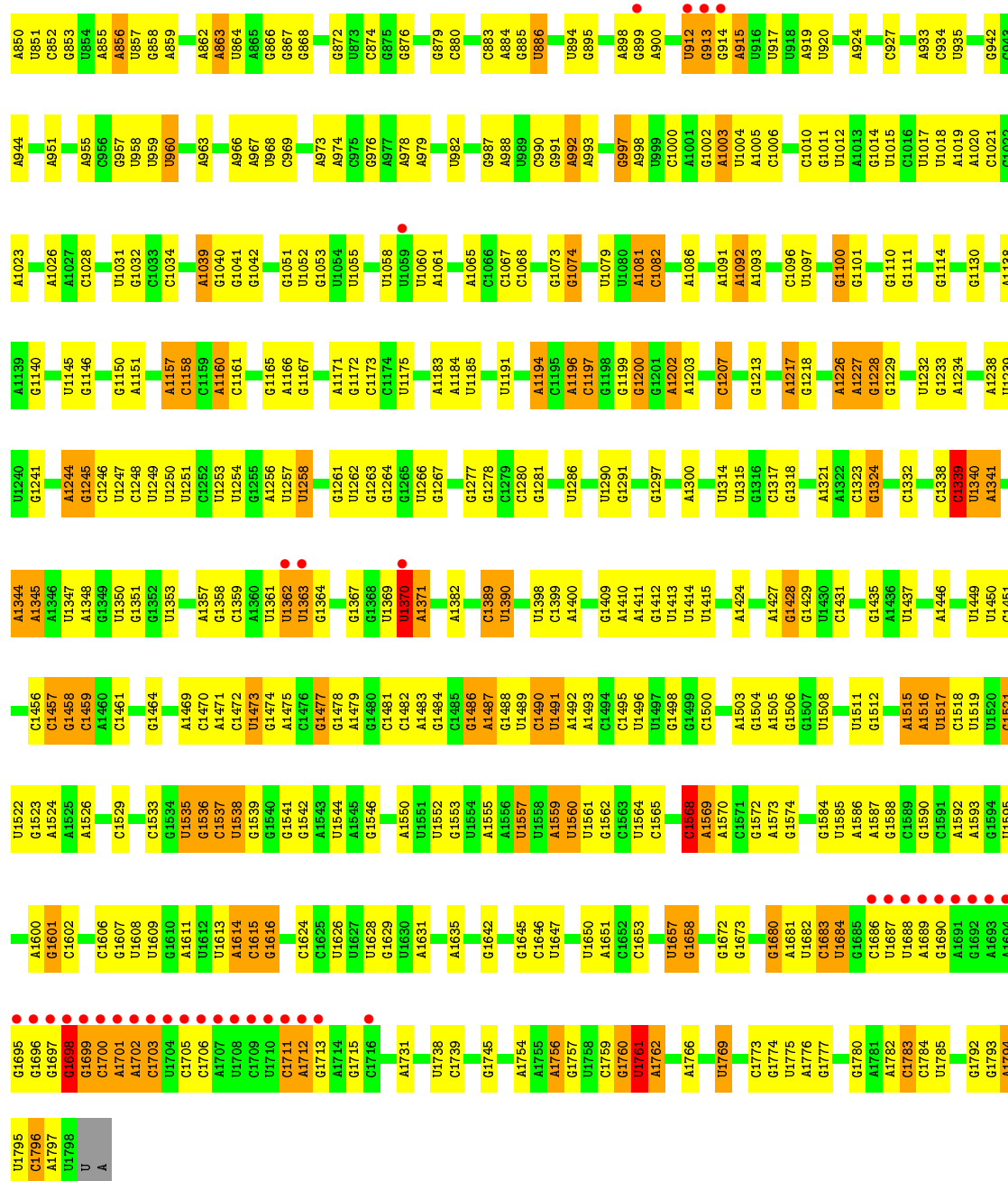


• Molecule 47: Suppressor protein STM1

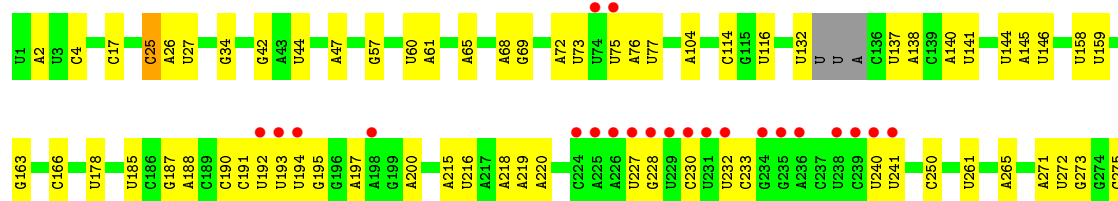
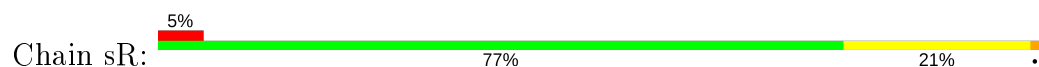


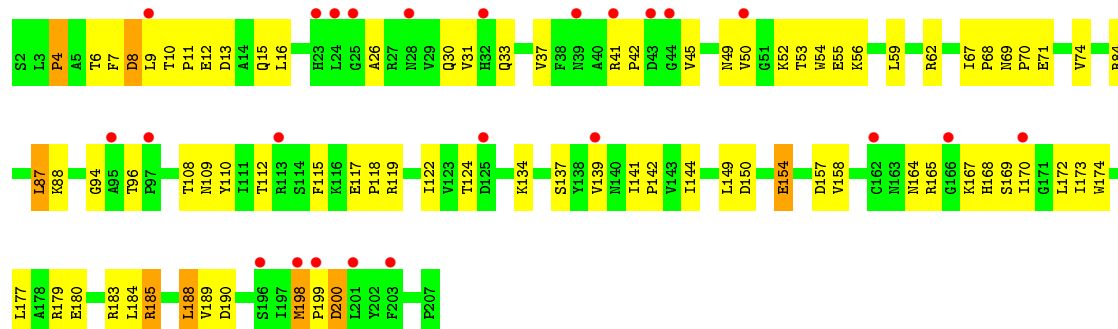
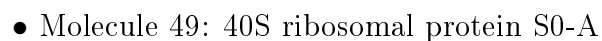
• Molecule 48: 18S ribosomal RNA



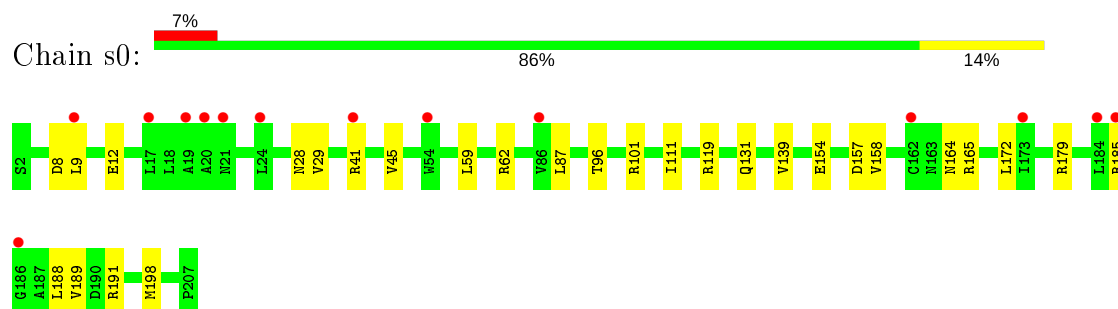


• Molecule 48: 18S ribosomal RNA

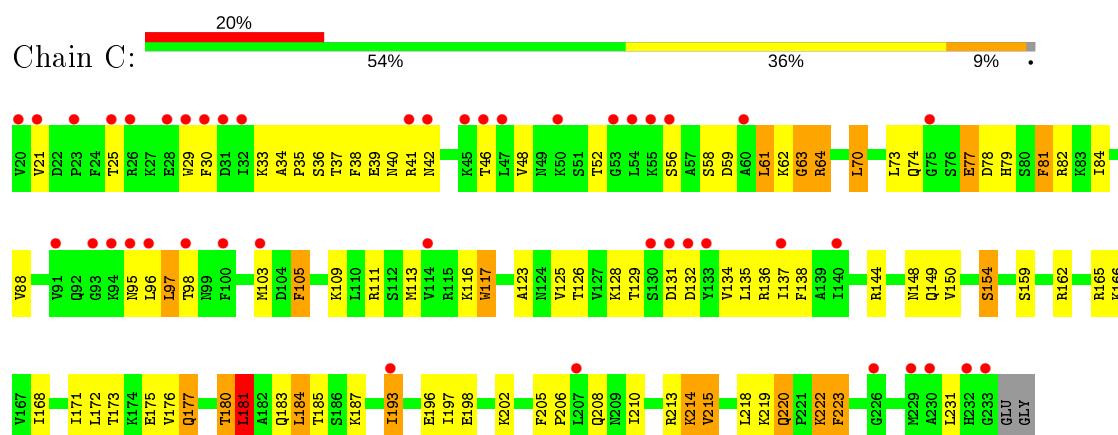




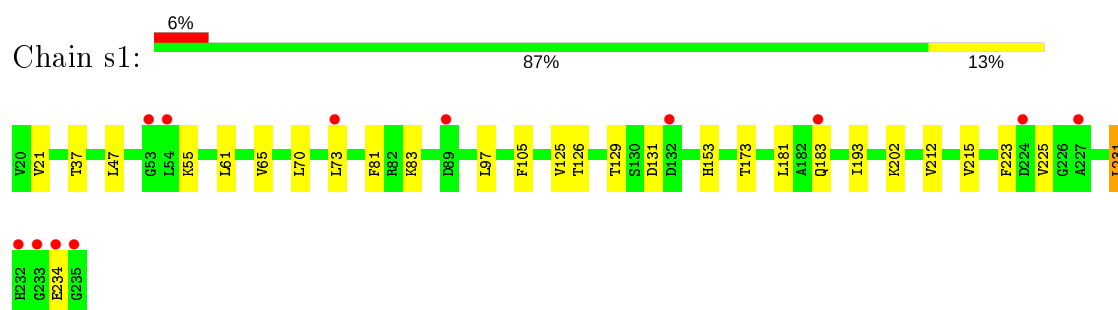
- Molecule 49: 40S ribosomal protein S0-A



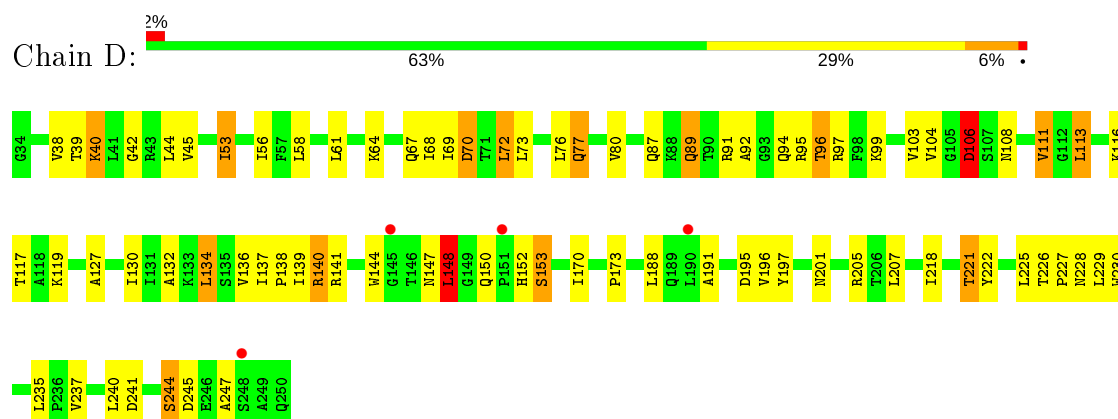
- Molecule 50: 40S ribosomal protein S1-A



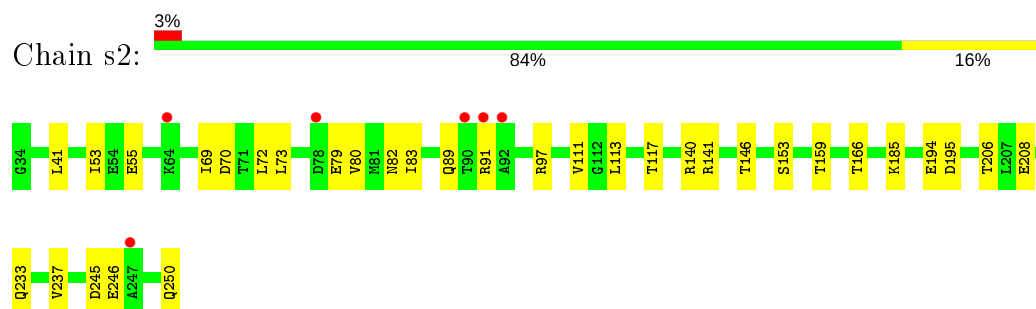
- Molecule 50: 40S ribosomal protein S1-A



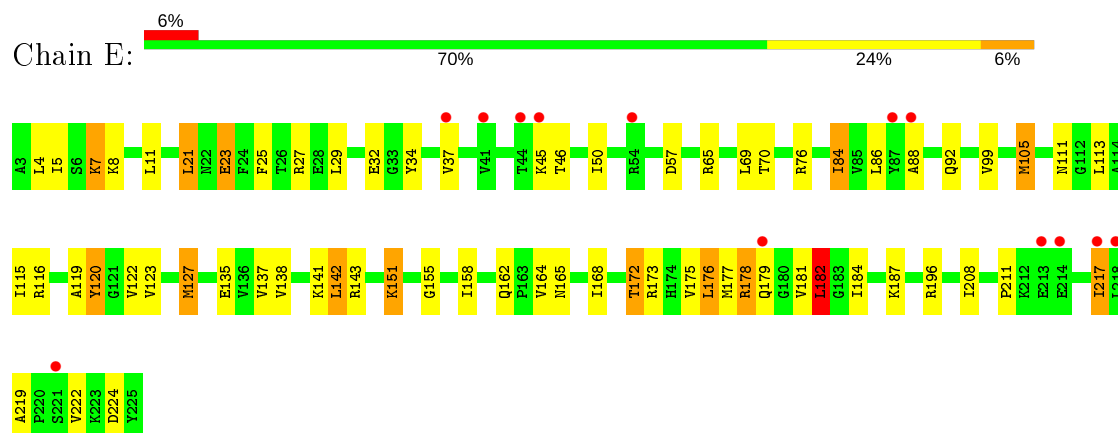
- Molecule 51: 40S ribosomal protein S2



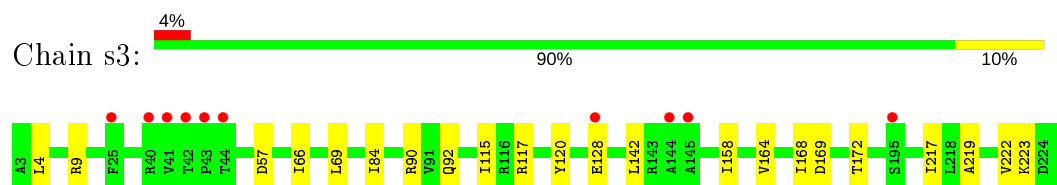
- Molecule 51: 40S ribosomal protein S2



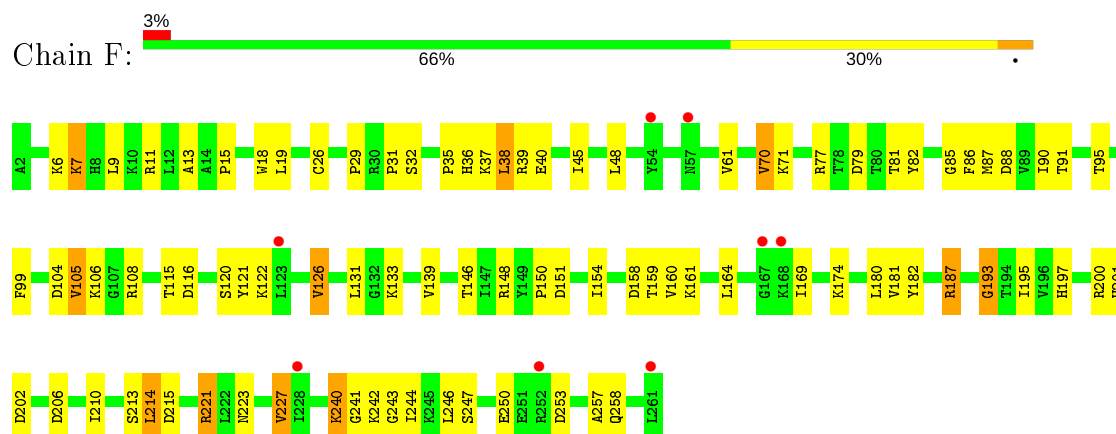
- Molecule 52: 40S ribosomal protein S3



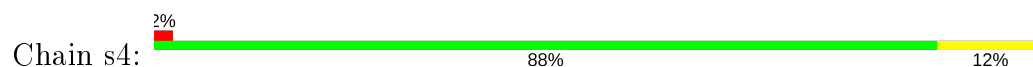
- Molecule 52: 40S ribosomal protein S3

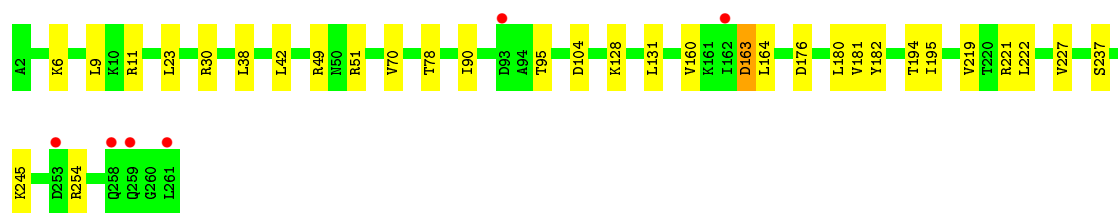


- Molecule 53: 40S ribosomal protein S4-A

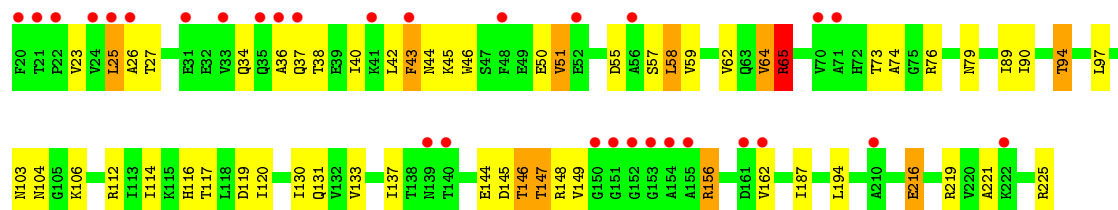
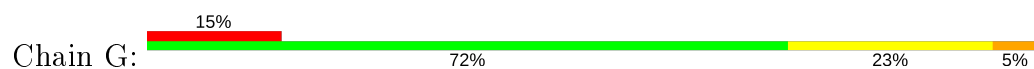


- Molecule 53: 40S ribosomal protein S4-A

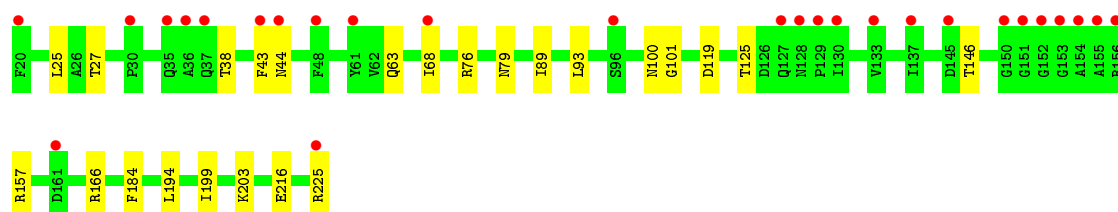
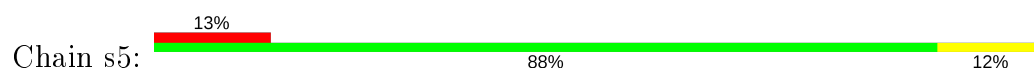




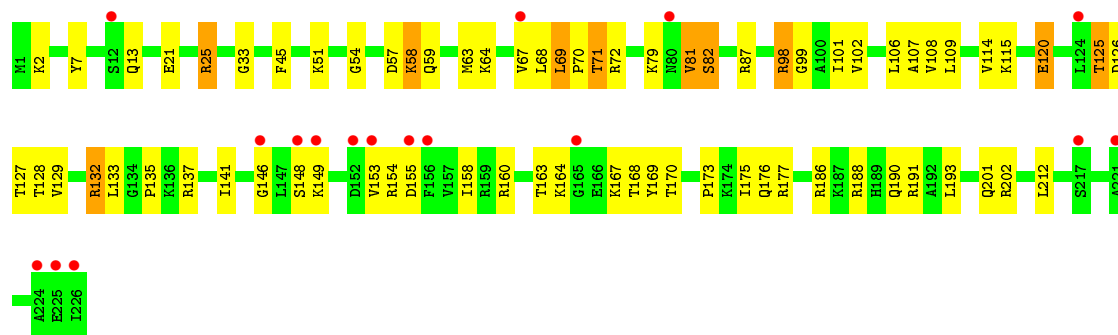
- Molecule 54: 40S ribosomal protein S5



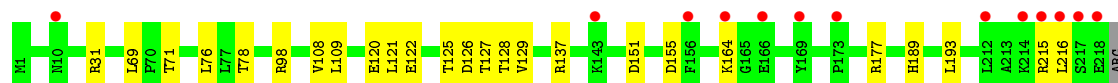
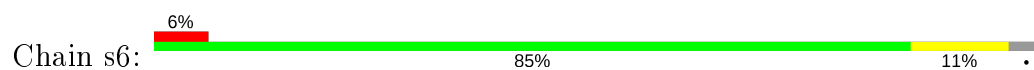
- Molecule 54: 40S ribosomal protein S5



- Molecule 55: 40S ribosomal protein S6-A

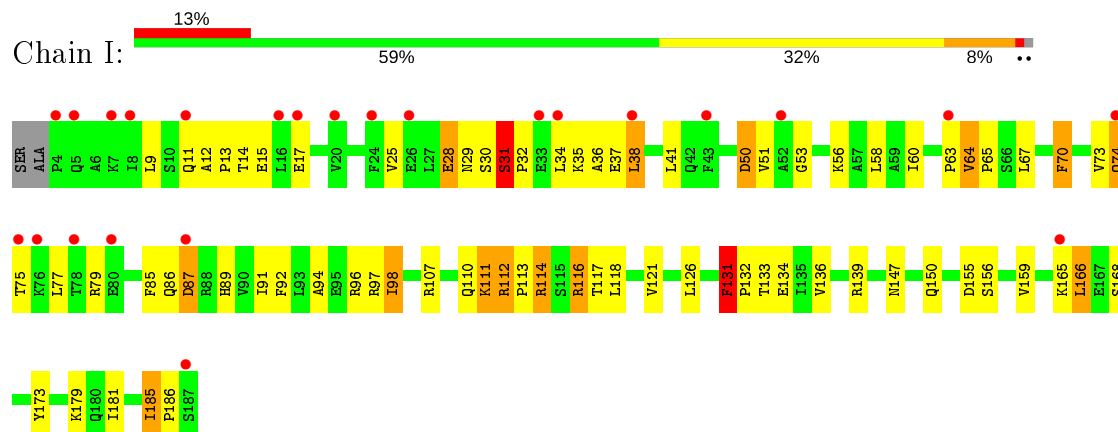


- Molecule 55: 40S ribosomal protein S6-A

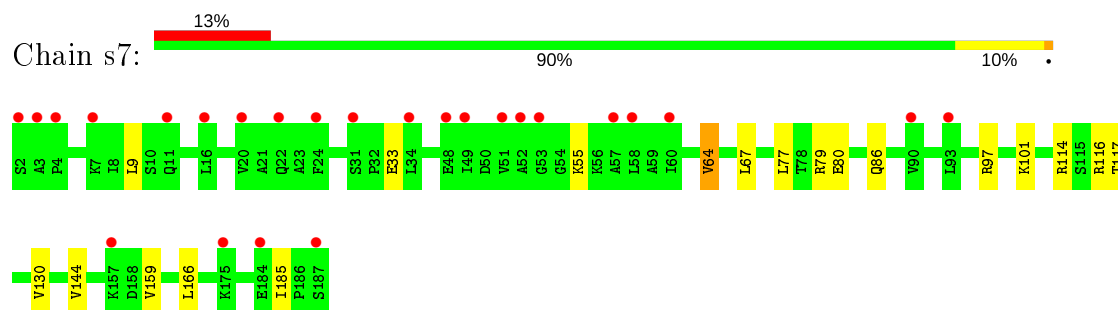


LYS
ALA
GLU
LYS
ALA
GLU
ILE

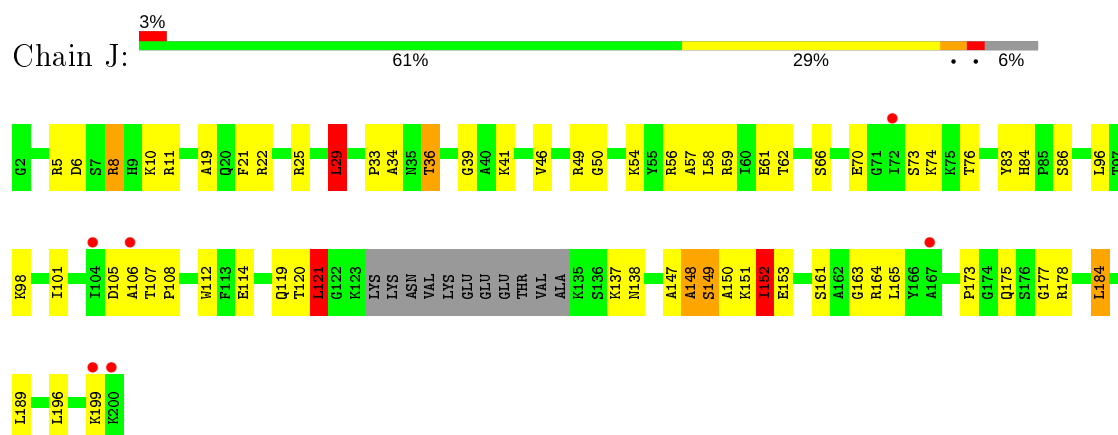
• Molecule 56: 40S ribosomal protein S7-A



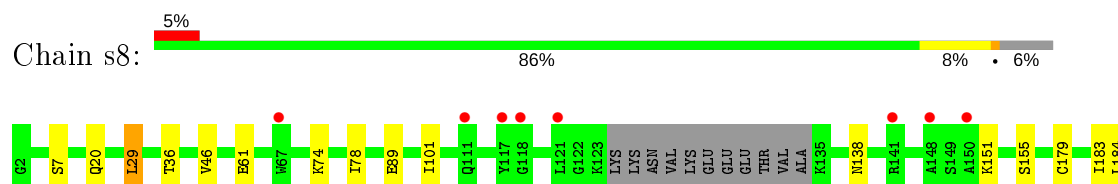
• Molecule 56: 40S ribosomal protein S7-A



• Molecule 57: 40S ribosomal protein S8-A

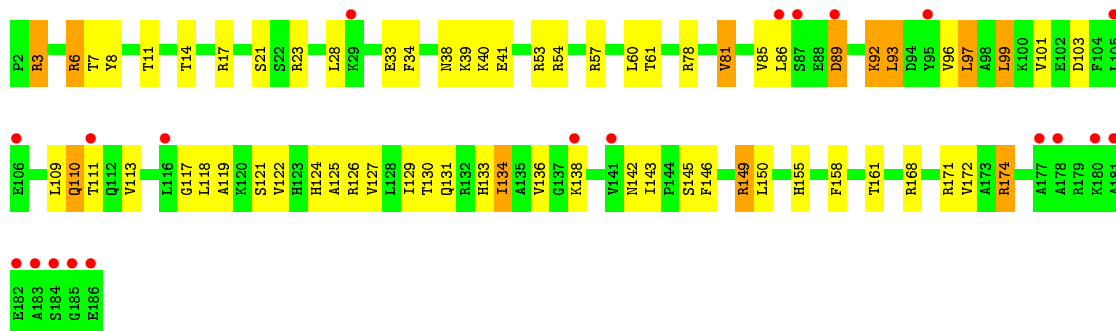


• Molecule 57: 40S ribosomal protein S8-A

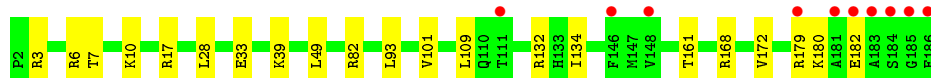
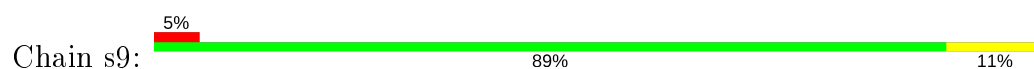




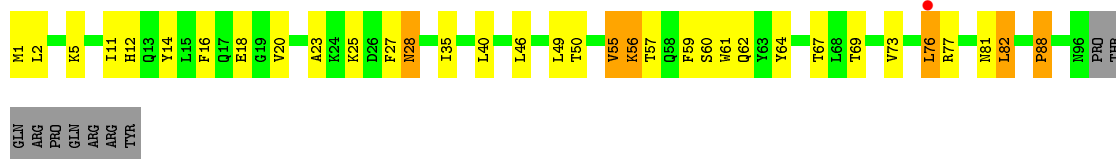
- Molecule 58: 40S ribosomal protein S9-A



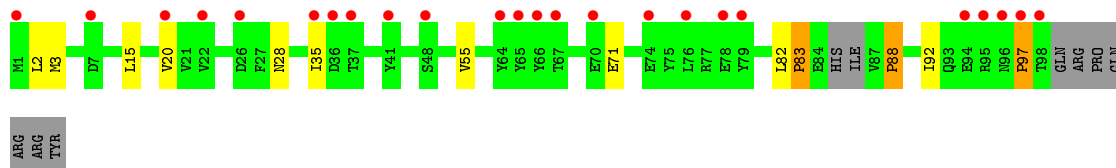
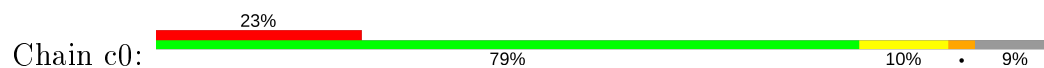
- Molecule 58: 40S ribosomal protein S9-A



- Molecule 59: 40S ribosomal protein S10-A

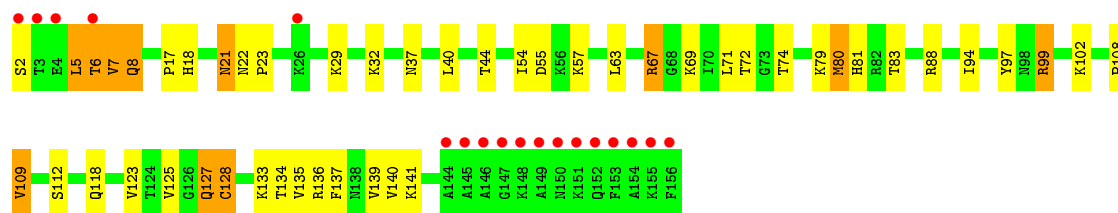


- Molecule 59: 40S ribosomal protein S10-A

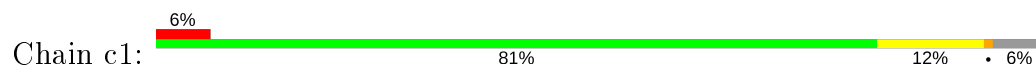


- Molecule 60: 40S ribosomal protein S11-A

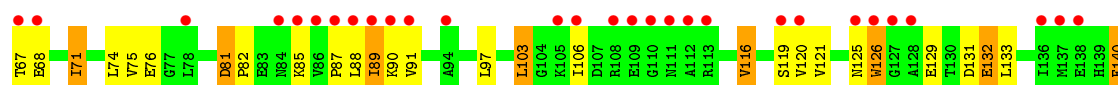
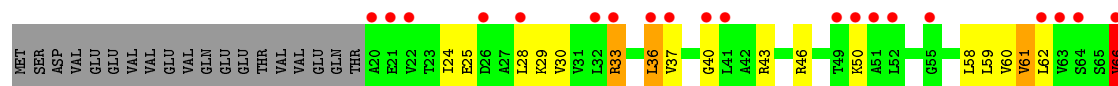




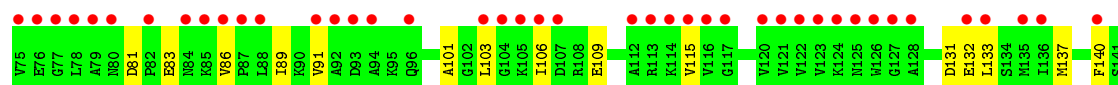
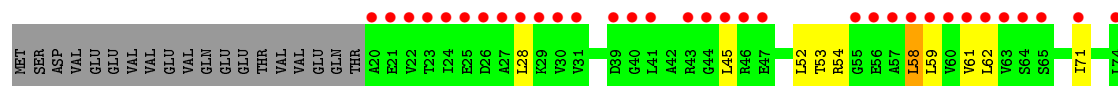
• Molecule 60: 40S ribosomal protein S11-A



• Molecule 61: 40S ribosomal protein S12



• Molecule 61: 40S ribosomal protein S12



• Molecule 62: 40S ribosomal protein S13

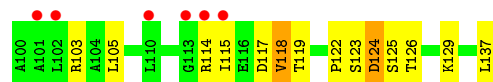
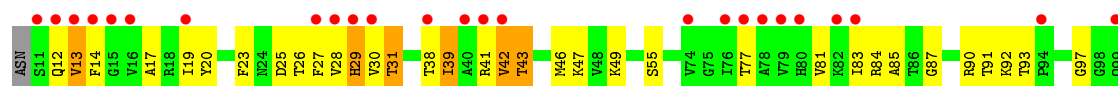




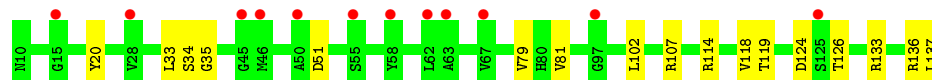
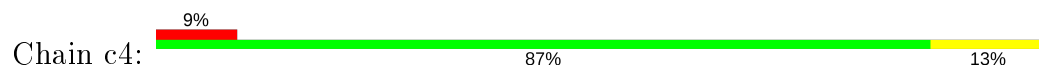
- Molecule 62: 40S ribosomal protein S13



- Molecule 63: 40S ribosomal protein S14-B



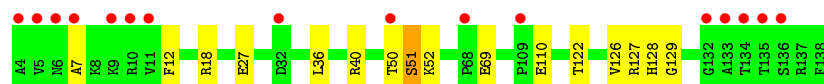
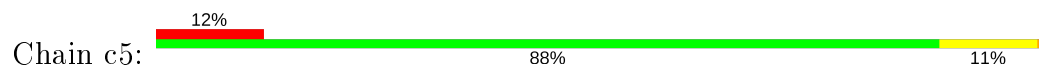
- Molecule 63: 40S ribosomal protein S14-B



- Molecule 64: 40S ribosomal protein S15

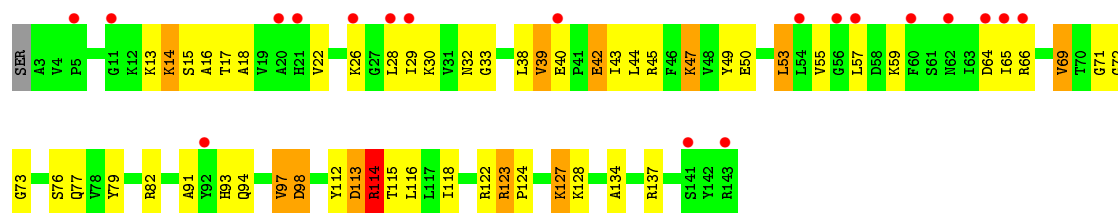


- Molecule 64: 40S ribosomal protein S15

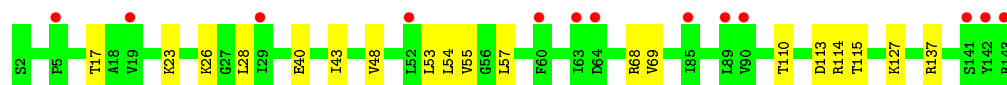
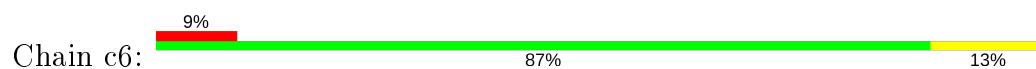


- Molecule 65: 40S ribosomal protein S16-A





- Molecule 65: 40S ribosomal protein S16-A



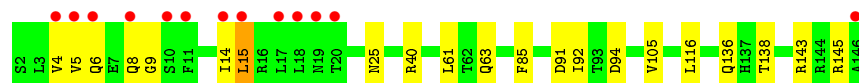
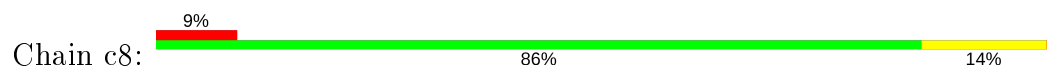
- Molecule 66: 40S ribosomal protein S17-A



- Molecule 67: 40S ribosomal protein S18-A

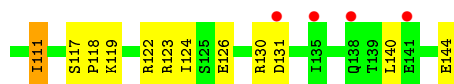


- Molecule 67: 40S ribosomal protein S18-A

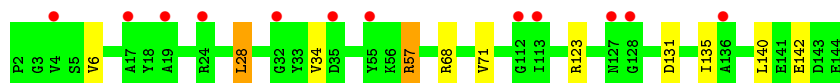


- Molecule 68: 40S ribosomal protein S19-A

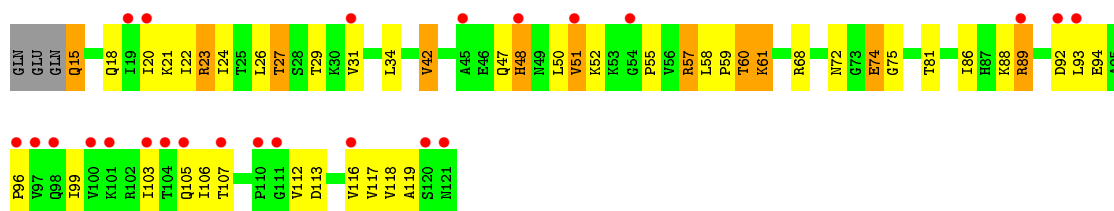




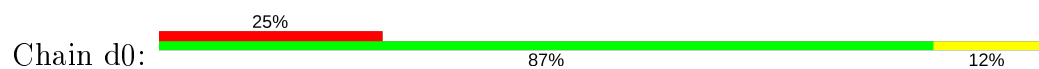
- Molecule 68: 40S ribosomal protein S19-A



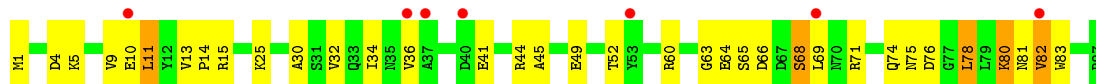
- Molecule 69: 40S ribosomal protein S20



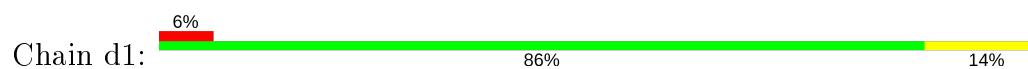
- Molecule 69: 40S ribosomal protein S20



- Molecule 70: 40S ribosomal protein S21-A

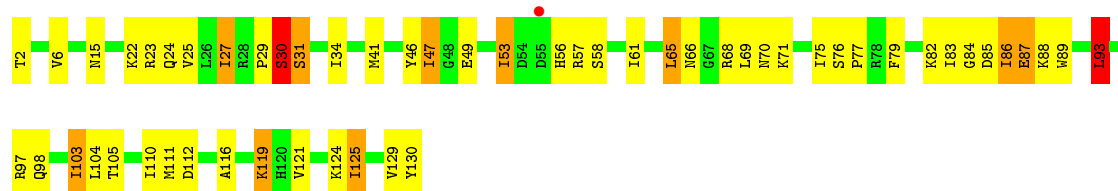


- Molecule 70: 40S ribosomal protein S21-A



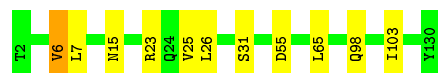
- Molecule 71: 40S ribosomal protein S22-A





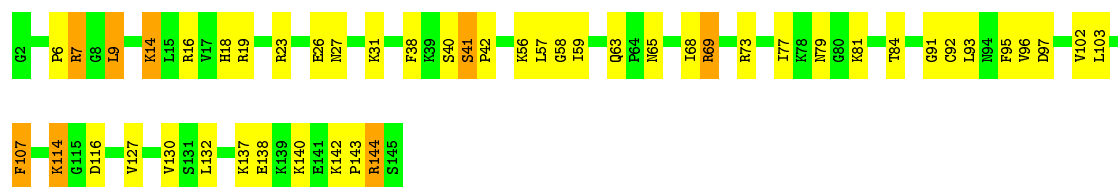
- Molecule 71: 40S ribosomal protein S22-A

Chain d2: 91% 8%



- Molecule 72: 40S ribosomal protein S23-A

Chain Y: 67% 28% 6%



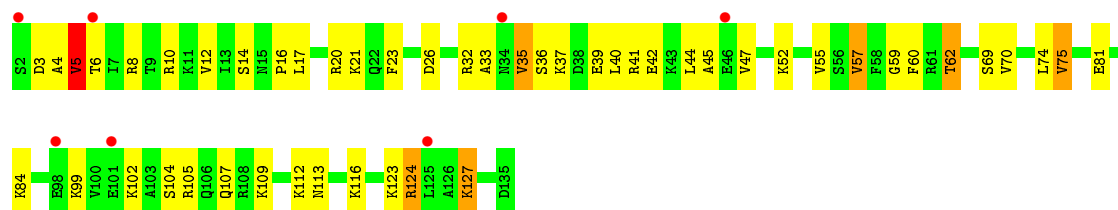
- Molecule 72: 40S ribosomal protein S23-A

Chain d3: 91% 9%



- Molecule 73: 40S ribosomal protein S24-A

Chain Z: 5% 63% 32%

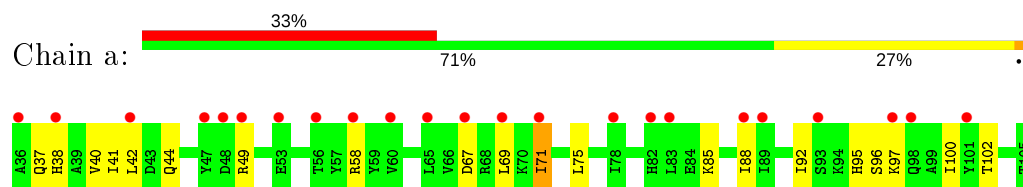


- Molecule 73: 40S ribosomal protein S24-A

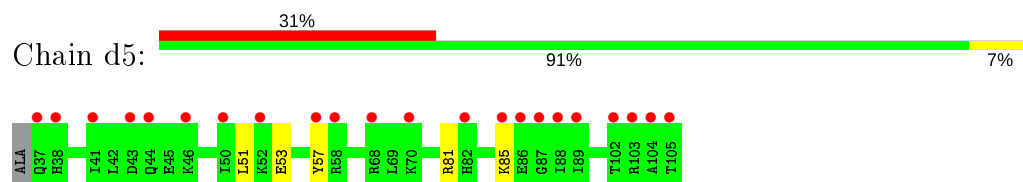
Chain d4: 4% 91% 8%



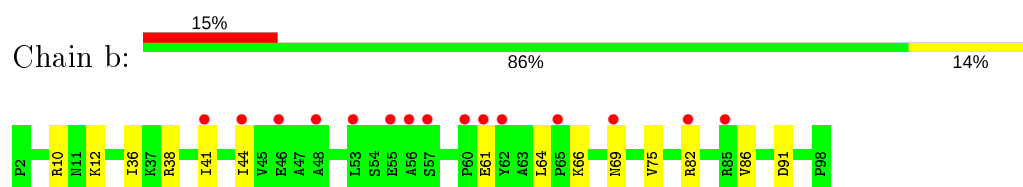
• Molecule 74: 40S ribosomal protein S25-A



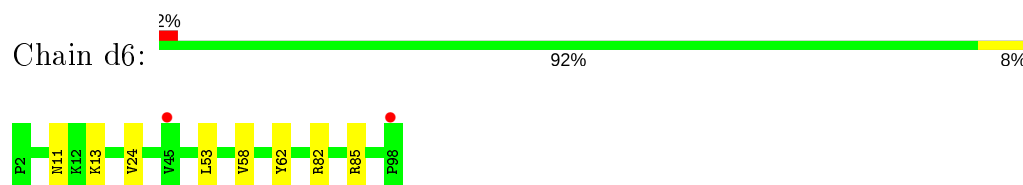
• Molecule 74: 40S ribosomal protein S25-A



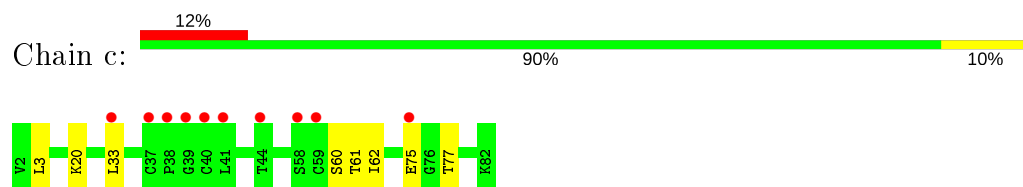
• Molecule 75: 40S ribosomal protein S26-B



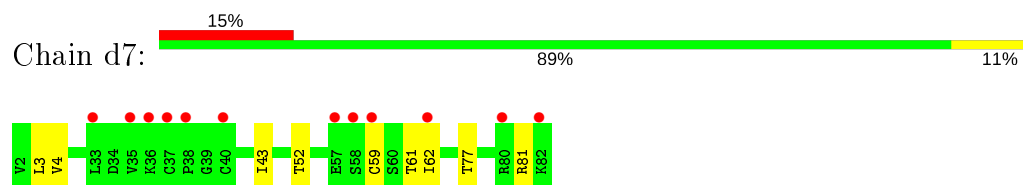
• Molecule 75: 40S ribosomal protein S26-B



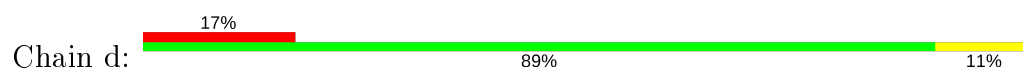
• Molecule 76: 40S ribosomal protein S27-A

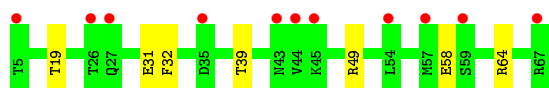


• Molecule 76: 40S ribosomal protein S27-A

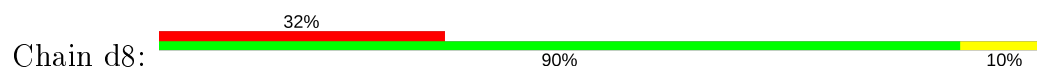


• Molecule 77: 40S ribosomal protein S28-A

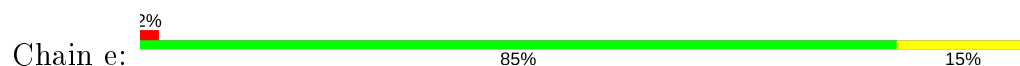




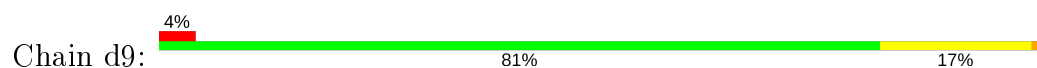
- Molecule 77: 40S ribosomal protein S28-A



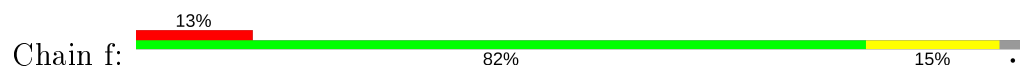
- Molecule 78: 40S ribosomal protein S29-A



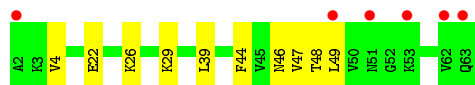
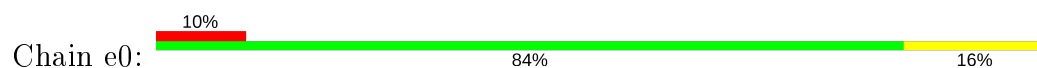
- Molecule 78: 40S ribosomal protein S29-A



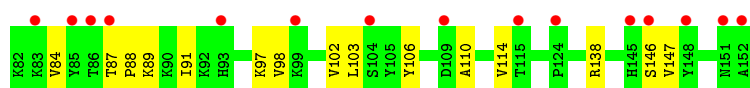
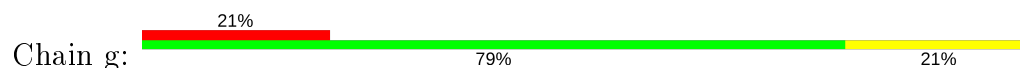
- Molecule 79: 40S ribosomal protein S30-A



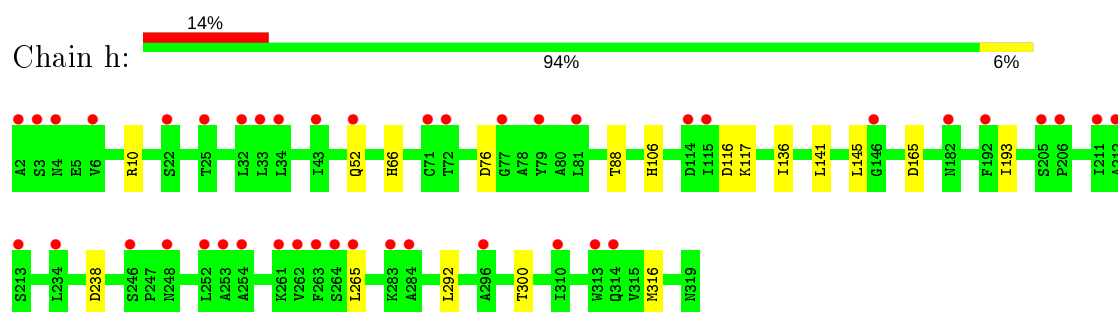
- Molecule 79: 40S ribosomal protein S30-A



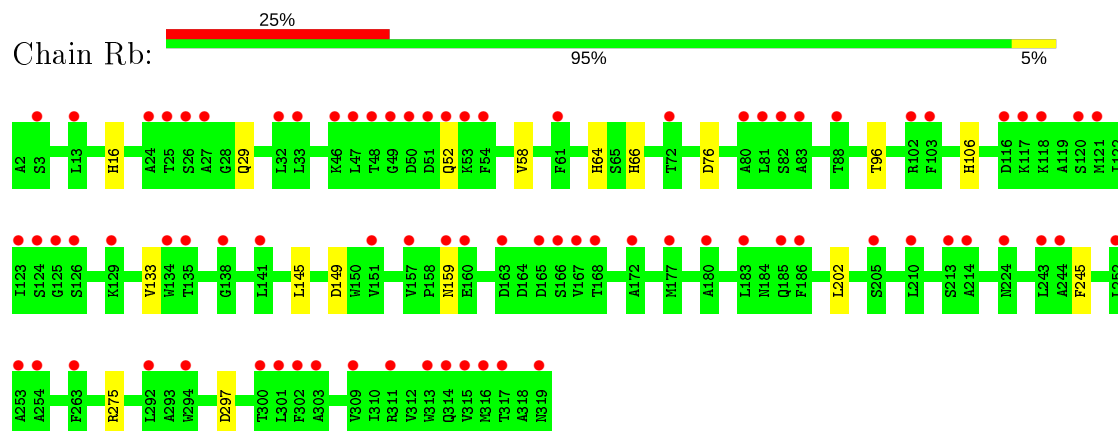
- Molecule 80: Ubiquitin-40S ribosomal protein S31



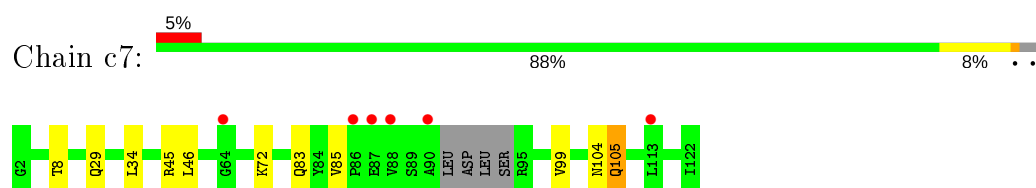
- Molecule 81: Guanine nucleotide-binding protein subunit beta-like protein



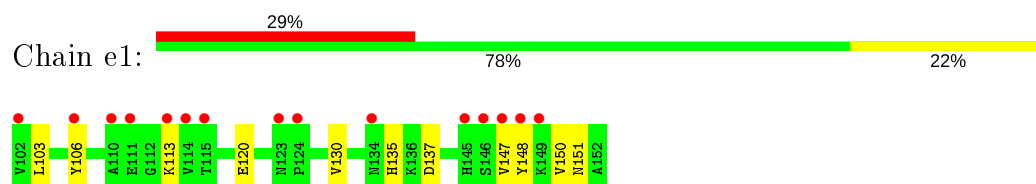
- Molecule 81: Guanine nucleotide-binding protein subunit beta-like protein



- Molecule 82: 40S ribosomal protein S17-A



- Molecule 83: Ubiquitin-40S ribosomal protein S31



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	304.80Å 288.20Å 437.68Å 90.00° 98.71° 90.00°	Depositor
Resolution (Å)	99.86 – 3.00 99.86 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (99.86-3.00) 100.0 (99.86-3.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.194 , 0.227 0.196 , 0.228	Depositor DCC
R_{free} test set	29480 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	409612	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 7AL, OHX, 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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.54	0/75394	1.00	128/117545 (0.1%)
1	AR	0.54	0/75394	0.98	102/117545 (0.1%)
2	3	0.47	0/2883	0.88	0/4491
2	AS	0.52	0/2883	0.94	1/4491 (0.0%)
3	4	0.52	0/3746	0.96	1/5832 (0.0%)
3	AT	0.46	0/3746	0.91	4/5832 (0.1%)
4	CD	0.37	0/1948	0.60	0/2617
4	j	0.41	0/1948	0.65	1/2617 (0.0%)
5	CE	0.45	0/3146	0.66	1/4228 (0.0%)
5	k	0.41	0/3146	0.63	0/4228
6	CF	0.40	0/2800	0.67	2/3790 (0.1%)
6	l	0.44	0/2800	0.70	3/3790 (0.1%)
7	CG	0.39	0/2425	0.60	0/3271
7	m	0.34	0/2425	0.54	0/3271
8	CH	0.40	0/1260	0.58	0/1694
8	n	0.40	0/1260	0.58	0/1694
9	CI	0.43	0/1821	0.61	0/2451
9	o	0.43	0/1821	0.63	1/2451 (0.0%)
10	CJ	0.32	0/1836	0.54	1/2481 (0.0%)
10	p	0.34	0/1836	0.58	0/2481
11	CK	0.39	0/1539	0.58	0/2073
11	q	0.38	0/1539	0.58	0/2073
12	CL	0.40	0/1741	0.60	0/2335
12	r	0.42	0/1741	0.64	1/2335 (0.0%)
13	CM	0.39	0/1374	0.62	1/1842 (0.1%)
13	s	0.33	0/1374	0.57	0/1842
14	CN	0.39	0/1568	0.61	0/2106
14	t	0.41	0/1568	0.64	0/2106
15	CO	0.41	0/1068	0.60	0/1438
15	u	0.39	0/1068	0.59	0/1438
16	CP	0.39	0/1757	0.62	1/2354 (0.0%)
16	v	0.44	0/1757	0.66	1/2354 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	CQ	0.53	0/1585	0.63	1/2128 (0.0%)
17	w	0.47	0/1585	0.61	0/2128
18	CR	0.45	0/1443	0.66	0/1944
18	x	0.43	0/1443	0.63	0/1944
19	CS	0.41	0/1465	0.66	1/1965 (0.1%)
19	y	0.44	0/1465	0.67	0/1965
20	CT	0.34	0/1538	0.55	0/2050
20	z	0.33	0/1538	0.52	0/2050
21	0	0.40	0/1481	0.61	0/1990
21	CU	0.42	0/1481	0.60	0/1990
22	2	0.40	0/1300	0.60	0/1743
22	CV	0.43	0/1300	0.61	0/1743
23	5	0.29	0/812	0.49	0/1099
23	CW	0.32	0/812	0.54	0/1099
24	6	0.42	0/1018	0.60	0/1369
24	CX	0.44	0/1018	0.60	0/1369
25	7	0.35	0/712	0.51	0/958
25	CY	0.37	0/712	0.60	0/958
26	8	0.34	0/979	0.59	0/1321
26	CZ	0.36	0/979	0.60	1/1321 (0.1%)
27	9	0.39	0/1004	0.67	1/1341 (0.1%)
27	DA	0.39	0/1004	0.62	0/1341
28	AA	0.33	0/1118	0.52	0/1497
28	DB	0.31	0/1118	0.54	0/1497
29	AB	0.45	0/1204	0.70	1/1612 (0.1%)
29	DC	0.44	0/1204	0.65	0/1612
30	AC	0.38	0/473	0.65	1/629 (0.2%)
30	DD	0.38	0/473	0.60	0/629
31	AD	0.31	0/751	0.52	0/1008
31	DE	0.30	0/751	0.52	1/1008 (0.1%)
32	AE	0.35	0/890	0.57	0/1196
32	DF	0.39	0/890	0.57	0/1196
33	AF	0.43	0/1041	0.60	0/1394
33	DG	0.42	0/1041	0.62	0/1394
34	AG	0.48	0/868	0.62	0/1168
34	DH	0.46	0/868	0.63	0/1168
35	AH	0.37	0/890	0.60	0/1189
35	DI	0.35	0/890	0.57	0/1189
36	AI	0.39	0/978	0.57	0/1301
36	DJ	0.34	0/978	0.50	1/1301 (0.1%)
37	AJ	0.37	0/778	0.59	0/1034
37	DK	0.32	0/778	0.57	0/1034
38	AK	0.49	0/696	0.71	0/923

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DL	0.41	0/696	0.65	0/923
39	AL	0.33	0/618	0.51	0/826
39	DM	0.30	0/618	0.52	0/826
40	AM	0.42	0/443	0.67	0/588
40	DN	0.35	0/443	0.63	0/588
41	AN	0.44	0/423	0.65	0/562
41	DO	0.44	0/423	0.66	0/562
42	AO	0.36	0/234	0.57	0/300
42	DP	0.37	0/234	0.56	0/300
43	AP	0.42	0/860	0.64	0/1136
43	DQ	0.43	0/860	0.65	0/1136
44	AQ	0.40	0/701	0.64	1/934 (0.1%)
44	DR	0.37	0/701	0.63	0/934
45	i	0.33	0/1113	0.56	1/1502 (0.1%)
46	p0	0.31	0/1092	0.54	0/1474
47	sM	0.34	0/481	0.61	0/644
48	A	0.36	0/42443	0.87	45/66134 (0.1%)
48	sR	0.40	0/42490	0.88	45/66207 (0.1%)
49	B	0.29	0/1617	0.57	0/2215
49	s0	0.31	0/1623	0.55	0/2222
50	C	0.29	0/1735	0.58	1/2335 (0.0%)
50	s1	0.31	0/1748	0.59	1/2352 (0.0%)
51	D	0.30	0/1665	0.54	0/2263
51	s2	0.33	0/1665	0.60	0/2263
52	E	0.29	0/1759	0.50	1/2368 (0.0%)
52	s3	0.27	0/1759	0.47	0/2368
53	F	0.32	0/2109	0.60	1/2839 (0.0%)
53	s4	0.32	0/2109	0.60	0/2839
54	G	0.27	0/1629	0.51	0/2202
54	s5	0.28	0/1629	0.52	0/2202
55	H	0.29	0/1823	0.50	0/2439
55	s6	0.32	0/1779	0.52	0/2379
56	I	0.31	0/1506	0.54	0/2028
56	s7	0.31	0/1516	0.53	0/2043
57	J	0.33	0/1514	0.62	2/2021 (0.1%)
57	s8	0.34	0/1514	0.56	1/2021 (0.0%)
58	K	0.30	0/1519	0.56	0/2035
58	s9	0.31	0/1519	0.51	0/2035
59	L	0.32	0/789	0.64	1/1067 (0.1%)
59	c0	0.31	0/775	0.63	3/1045 (0.3%)
60	M	0.37	0/1239	0.61	0/1673
60	c1	0.35	0/1194	0.60	0/1610
61	N	0.33	0/898	0.59	0/1220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
61	c2	0.26	0/898	0.57	1/1220 (0.1%)
62	O	0.32	0/1215	0.52	0/1638
62	c3	0.33	0/1215	0.55	0/1638
63	P	0.29	0/901	0.59	0/1217
63	c4	0.33	0/960	0.61	0/1290
64	Q	0.31	0/998	0.56	0/1341
64	c5	0.32	0/1060	0.58	0/1426
65	R	0.29	0/1125	0.58	0/1510
65	c6	0.30	0/1131	0.54	0/1518
66	S	0.32	0/935	0.66	2/1254 (0.2%)
67	T	0.31	0/1211	0.55	0/1628
67	c8	0.30	0/1211	0.53	1/1628 (0.1%)
68	U	0.29	0/1130	0.49	0/1517
68	c9	0.29	0/1130	0.55	1/1517 (0.1%)
69	V	0.29	0/865	0.54	0/1169
69	d0	0.30	0/892	0.56	0/1205
70	W	0.29	0/693	0.51	0/935
70	d1	0.29	0/693	0.56	0/935
71	X	0.31	0/1038	0.61	1/1395 (0.1%)
71	d2	0.34	0/1038	0.57	0/1395
72	Y	0.35	0/1139	0.60	0/1518
72	d3	0.39	0/1139	0.58	0/1518
73	Z	0.30	0/1087	0.49	0/1449
73	d4	0.33	0/1087	0.58	0/1449
74	a	0.29	0/571	0.64	0/768
74	d5	0.27	0/566	0.47	0/761
75	b	0.30	0/782	0.58	0/1047
75	d6	0.33	0/782	0.55	0/1047
76	c	0.27	0/620	0.52	0/838
76	d7	0.30	0/620	0.57	0/838
77	d	0.25	0/499	0.49	0/670
77	d8	0.26	0/499	0.53	0/670
78	d9	0.32	0/452	0.52	0/600
78	e	0.37	0/452	0.61	0/600
79	e0	0.32	0/499	0.60	0/665
79	f	0.31	0/483	0.56	0/643
80	g	0.39	0/577	0.76	0/770
81	Rb	0.26	0/2495	0.47	0/3395
81	h	0.26	0/2490	0.49	0/3389
82	c7	0.29	0/914	0.50	0/1224
83	e1	0.30	0/404	0.63	0/542
All	All	0.44	0/429965	0.83	366/631328 (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
6	l	0	1
7	CG	0	2
10	p	0	1
12	r	0	1
17	CQ	0	1
17	w	0	1
21	0	0	1
22	2	0	1
22	CV	0	1
25	CY	0	1
27	9	0	1
27	DA	0	1
28	AA	0	1
28	DB	0	1
30	AC	0	1
30	DD	0	1
32	DF	0	1
36	DJ	0	1
39	AL	0	1
44	DR	0	1
51	D	0	1
52	E	0	1
52	s3	0	1
53	F	0	1
53	s4	0	1
54	G	0	2
54	s5	0	2
55	s6	0	1
56	I	0	3
56	s7	0	2
57	J	0	1
61	c2	0	1
63	P	0	1
63	c4	0	1
64	Q	0	1
64	c5	0	2
65	R	0	4
65	c6	0	2
66	S	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
67	T	0	1
70	d1	0	1
72	Y	0	1
73	d4	0	1
75	b	0	1
80	g	0	2
83	e1	0	1
All	All	0	60

There are no bond length outliers.

All (366) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1308	A	O5'-P-OP1	-10.26	96.47	105.70
1	1	1307	G	P-O3'-C3'	10.16	131.89	119.70
1	AR	3217	C	N1-C2-O2	9.74	124.75	118.90
1	1	406	G	O4'-C1'-N9	9.62	115.89	108.20
1	1	3278	C	N1-C2-O2	9.04	124.32	118.90
1	1	1495	U	C5-C6-N1	-9.04	118.18	122.70
48	sR	453	U	C2-N1-C1'	9.02	128.52	117.70
48	A	553	G	N1-C6-O6	8.84	125.20	119.90
1	AR	2846	U	N3-C2-O2	-8.72	116.10	122.20
1	AR	2714	G	N3-C4-C5	8.71	132.96	128.60
1	AR	3306	U	N3-C2-O2	-8.61	116.17	122.20
48	sR	163	G	N3-C4-N9	-8.61	120.83	126.00
1	1	3217	C	N1-C2-O2	8.46	123.98	118.90
1	1	2714	G	N3-C4-C5	8.42	132.81	128.60
1	AR	3217	C	C2-N1-C1'	8.41	128.05	118.80
1	AR	3344	A	C8-N9-C4	-8.38	102.45	105.80
66	S	85	VAL	C-N-CD	-8.36	102.20	120.60
1	AR	3344	A	N7-C8-N9	8.31	117.95	113.80
1	AR	2714	G	N3-C4-N9	-8.24	121.06	126.00
1	1	3217	C	N3-C2-O2	-8.17	116.18	121.90
3	AT	125	U	C2-N1-C1'	8.15	127.48	117.70
1	AR	3217	C	N3-C2-O2	-8.14	116.20	121.90
1	1	1495	U	C4-C5-C6	8.10	124.56	119.70
1	AR	2846	U	C5-C4-O4	7.94	130.66	125.90
1	AR	2726	C	N3-C2-O2	-7.86	116.40	121.90
1	1	3217	C	C2-N1-C1'	7.78	127.35	118.80
1	1	3278	C	N3-C2-O2	-7.68	116.52	121.90
53	F	193	GLY	N-CA-C	7.54	131.95	113.10
48	sR	453	U	N3-C2-O2	-7.47	116.97	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2726	C	N3-C2-O2	-7.39	116.72	121.90
1	AR	1495	U	C5-C6-N1	-7.39	119.00	122.70
1	1	2572	C	N1-C2-O2	7.36	123.31	118.90
1	AR	406	G	O4'-C1'-N9	7.32	114.06	108.20
6	l	327	LEU	CA-CB-CG	7.30	132.10	115.30
48	sR	1473	U	C2-N1-C1'	7.25	126.40	117.70
1	1	3278	C	C2-N1-C1'	7.22	126.74	118.80
3	AT	125	U	N1-C2-O2	7.16	127.81	122.80
1	AR	2362	C	N3-C2-O2	-7.09	116.94	121.90
48	A	1200	G	N1-C6-O6	7.05	124.13	119.90
1	AR	2362	C	C6-N1-C2	-7.04	117.49	120.30
1	AR	2385	G	O5'-P-OP1	-7.03	99.37	105.70
1	1	2846	U	N3-C2-O2	-7.01	117.29	122.20
1	1	835	G	O4'-C1'-N9	7.01	113.81	108.20
1	1	2978	U	O4'-C1'-N1	7.00	113.80	108.20
1	AR	2272	G	O4'-C1'-N9	7.00	113.80	108.20
6	l	313	LEU	CA-CB-CG	6.98	131.36	115.30
1	1	3217	C	C6-N1-C2	-6.97	117.51	120.30
6	l	182	LEU	CA-CB-CG	6.97	131.34	115.30
1	AR	2617	U	C5-C6-N1	-6.96	119.22	122.70
1	1	2572	C	N3-C2-O2	-6.96	117.03	121.90
48	A	639	U	N3-C2-O2	-6.95	117.34	122.20
48	A	553	G	C5-C6-O6	-6.92	124.45	128.60
1	AR	2726	C	C6-N1-C2	-6.92	117.53	120.30
12	r	57	LEU	CA-CB-CG	6.90	131.18	115.30
1	1	3306	U	N3-C2-O2	-6.90	117.37	122.20
48	A	728	U	C2-N1-C1'	6.87	125.94	117.70
48	sR	453	U	N1-C2-O2	6.84	127.59	122.80
1	AR	2996	U	N1-C2-O2	6.84	127.58	122.80
50	s1	231	LEU	CA-CB-CG	6.83	131.02	115.30
48	sR	1473	U	N3-C2-O2	-6.80	117.44	122.20
1	1	2870	C	C2-N1-C1'	-6.80	111.32	118.80
48	A	507	U	C2-N1-C1'	6.77	125.83	117.70
48	A	1339	C	P-O3'-C3'	6.75	127.80	119.70
1	1	2726	C	C6-N1-C2	-6.74	117.60	120.30
1	1	2714	G	N3-C4-N9	-6.71	121.97	126.00
1	1	2870	C	C6-N1-C1'	6.70	128.84	120.80
1	AR	1495	U	C4-C5-C6	6.70	123.72	119.70
48	sR	163	G	N3-C4-C5	6.68	131.94	128.60
1	1	2714	G	C2-N3-C4	-6.68	108.56	111.90
48	A	507	U	N3-C2-O2	-6.67	117.53	122.20
48	A	453	U	C2-N1-C1'	6.65	125.68	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A	507	U	N1-C2-O2	6.65	127.45	122.80
3	AT	125	U	N3-C2-O2	-6.64	117.56	122.20
1	1	2550	U	N3-C2-O2	-6.63	117.56	122.20
1	AR	640	U	O5'-P-OP1	-6.61	99.75	105.70
61	c2	58	LEU	CA-CB-CG	6.60	130.47	115.30
1	1	637	C	C2-N1-C1'	-6.57	111.58	118.80
1	1	2617	U	C5-C6-N1	-6.56	119.42	122.70
1	1	2572	C	C2-N1-C1'	6.55	126.01	118.80
59	L	88	PRO	N-CA-CB	6.55	111.16	103.30
1	1	1365	G	N3-C4-C5	-6.55	125.33	128.60
48	sR	1773	C	N3-C4-C5	-6.53	119.29	121.90
1	AR	3155	U	C2-N1-C1'	6.52	125.53	117.70
1	1	1556	C	C2-N1-C1'	6.50	125.96	118.80
1	AR	3057	U	C5-C4-O4	6.48	129.79	125.90
1	1	1849	C	O5'-P-OP1	-6.48	99.87	105.70
6	CF	182	LEU	CA-CB-CG	6.48	130.21	115.30
1	1	65	A	P-O3'-C3'	6.48	127.47	119.70
1	AR	439	C	C2-N1-C1'	6.46	125.91	118.80
1	AR	3155	U	N1-C2-O2	6.46	127.32	122.80
48	sR	453	U	C6-N1-C1'	-6.41	112.22	121.20
1	AR	979	U	P-O3'-C3'	6.41	127.39	119.70
1	AR	2550	U	N3-C2-O2	-6.41	117.72	122.20
1	AR	2846	U	N3-C4-O4	-6.37	114.94	119.40
48	sR	813	U	N1-C2-O2	6.37	127.26	122.80
48	A	934	C	C2-N1-C1'	6.36	125.79	118.80
1	1	776	U	C4-C5-C6	6.34	123.51	119.70
1	AR	776	U	C5-C6-N1	-6.32	119.54	122.70
1	1	3181	C	N3-C2-O2	-6.30	117.49	121.90
1	1	2373	A	O5'-P-OP1	-6.29	100.04	105.70
1	1	3214	U	N3-C2-O2	-6.28	117.81	122.20
1	1	2572	C	C6-N1-C2	-6.27	117.79	120.30
1	AR	2418	G	OP1-P-O3'	6.26	118.98	105.20
1	AR	3344	A	C5-N7-C8	-6.26	100.77	103.90
1	1	2726	C	C5-C4-N4	6.25	124.58	120.20
1	AR	2714	G	C2-N3-C4	-6.25	108.77	111.90
1	AR	2726	C	C5-C4-N4	6.24	124.57	120.20
48	A	1039	A	O4'-C1'-N9	6.23	113.19	108.20
45	i	167	PRO	N-CA-CB	6.21	110.75	103.30
1	1	1556	C	N1-C2-O2	6.21	122.63	118.90
1	AR	3344	A	O4'-C1'-N9	6.20	113.16	108.20
48	A	75	U	N1-C2-O2	6.19	127.14	122.80
1	AR	3181	C	N3-C2-O2	-6.19	117.57	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	895	A	C5-N7-C8	-6.16	100.82	103.90
1	AR	3306	U	N1-C2-O2	6.15	127.11	122.80
1	1	2899	C	N3-C2-O2	-6.13	117.61	121.90
1	AR	1495	U	C5-C4-O4	6.12	129.57	125.90
57	J	29	LEU	CA-CB-CG	6.12	129.38	115.30
1	1	645	A	C6-N1-C2	-6.12	114.93	118.60
48	sR	1473	U	N1-C2-O2	6.11	127.08	122.80
5	CE	102	LEU	CA-CB-CG	6.10	129.33	115.30
48	sR	813	U	C2-N1-C1'	6.10	125.02	117.70
1	AR	2263	C	C4-C5-C6	-6.10	114.35	117.40
1	1	1495	U	N1-C2-N3	6.08	118.55	114.90
1	1	3344	A	N7-C8-N9	6.05	116.83	113.80
1	1	3362	A	O4'-C1'-N9	6.05	113.04	108.20
48	A	158	U	P-O3'-C3'	6.04	126.95	119.70
57	J	121	LEU	CA-CB-CG	6.04	129.18	115.30
1	1	2302	G	N1-C6-O6	-6.01	116.29	119.90
1	1	2617	U	C5-C4-O4	5.98	129.49	125.90
1	AR	2550	U	C5-C4-O4	5.97	129.48	125.90
1	AR	1495	U	N1-C2-N3	5.97	118.48	114.90
48	A	1761	U	P-O3'-C3'	5.96	126.86	119.70
1	1	3057	U	N3-C2-O2	-5.96	118.03	122.20
1	1	922	U	N1-C2-O2	5.96	126.97	122.80
1	1	2617	U	N1-C2-N3	5.96	118.47	114.90
48	sR	1274	C	N1-C2-O2	5.95	122.47	118.90
48	sR	65	A	C2-N3-C4	-5.94	107.63	110.60
48	A	728	U	N1-C2-O2	5.93	126.95	122.80
1	AR	439	C	N1-C2-O2	5.92	122.45	118.90
1	AR	3217	C	C6-N1-C1'	-5.90	113.72	120.80
1	AR	3309	G	N3-C4-N9	5.90	129.54	126.00
48	sR	158	U	P-O3'-C3'	5.90	126.78	119.70
1	1	979	U	P-O3'-C3'	5.89	126.77	119.70
1	AR	2846	U	N1-C2-O2	5.89	126.92	122.80
1	1	1556	C	N3-C2-O2	-5.88	117.78	121.90
48	sR	858	G	O4'-C1'-N9	5.88	112.90	108.20
1	1	282	G	P-O3'-C3'	5.88	126.75	119.70
1	AR	65	A	P-O3'-C3'	5.87	126.74	119.70
13	CM	112	LEU	CA-CB-CG	5.87	128.80	115.30
1	1	2550	U	N1-C2-O2	5.87	126.91	122.80
1	1	1820	U	P-O3'-C3'	5.86	126.74	119.70
48	A	720	G	OP1-P-O3'	5.85	118.07	105.20
1	1	1365	G	N3-C4-N9	5.85	129.51	126.00
1	1	3140	G	C5-C6-O6	-5.84	125.09	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2302	G	C5-C6-O6	5.84	132.10	128.60
1	1	2176	U	N3-C2-O2	-5.84	118.11	122.20
1	AR	895	A	C5-N7-C8	-5.82	100.99	103.90
48	A	1200	G	C5-C6-O6	-5.82	125.11	128.60
1	AR	2362	C	N1-C2-O2	5.81	122.39	118.90
1	1	1279	C	C6-N1-C2	-5.80	117.98	120.30
1	AR	835	G	O4'-C1'-N9	5.79	112.84	108.20
48	sR	1000	C	C2-N1-C1'	5.79	125.17	118.80
1	1	1269	U	C2-N1-C1'	5.79	124.65	117.70
1	1	776	U	C5-C6-N1	-5.78	119.81	122.70
1	1	2719	U	N1-C2-O2	-5.78	118.75	122.80
1	1	3278	C	C6-N1-C2	-5.78	117.99	120.30
1	1	2996	U	N1-C2-O2	5.77	126.84	122.80
1	1	908	G	O4'-C1'-N9	-5.76	103.59	108.20
1	AR	3155	U	N3-C2-O2	-5.75	118.17	122.20
6	CF	313	LEU	CA-CB-CG	5.75	128.53	115.30
1	AR	895	A	N7-C8-N9	5.75	116.67	113.80
1	AR	2679	A	O4'-C1'-N9	5.75	112.80	108.20
48	A	453	U	N1-C2-O2	5.75	126.82	122.80
1	AR	2978	U	O4'-C1'-N1	5.74	112.79	108.20
1	AR	2827	U	C5-C6-N1	-5.74	119.83	122.70
1	1	439	C	C2-N1-C1'	5.73	125.10	118.80
48	A	1698	G	P-O3'-C3'	5.73	126.57	119.70
48	sR	1097	U	P-O3'-C3'	5.71	126.56	119.70
1	1	116	A	O4'-C1'-N9	5.71	112.77	108.20
1	1	1495	U	N1-C2-O2	-5.70	118.81	122.80
48	A	75	U	N3-C2-O2	-5.70	118.21	122.20
48	A	75	U	C2-N1-C1'	5.69	124.53	117.70
1	1	895	A	C6-C5-N7	-5.68	128.32	132.30
1	AR	2257	C	C2-N1-C1'	5.66	125.03	118.80
1	AR	3214	U	N3-C2-O2	-5.66	118.24	122.20
1	1	2816	G	O4'-C1'-N9	5.66	112.72	108.20
48	A	501	U	OP1-P-O3'	5.65	117.64	105.20
44	AQ	50	GLY	N-CA-C	-5.65	98.98	113.10
1	AR	1483	G	O4'-C1'-N9	5.65	112.72	108.20
68	c9	57	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	AR	2714	G	C5-N7-C8	-5.64	101.48	104.30
1	1	635	G	C5-C6-O6	-5.61	125.23	128.60
9	o	83	LEU	CA-CB-CG	5.61	128.19	115.30
48	sR	965	U	N1-C2-O2	5.60	126.72	122.80
48	sR	1773	C	C6-N1-C2	-5.60	118.06	120.30
48	sR	557	G	P-O3'-C3'	5.59	126.41	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	c0	83	PRO	N-CA-CB	5.59	110.01	103.30
48	A	73	U	OP1-P-O3'	5.58	117.49	105.20
48	A	1458	G	C4-N9-C1'	5.58	133.75	126.50
48	sR	337	G	C4-N9-C1'	5.57	133.74	126.50
1	1	282	G	C2'-C3'-O3'	5.57	122.61	113.70
27	9	126	LEU	CA-CB-CG	5.56	128.09	115.30
59	c0	97	PRO	N-CA-CB	5.55	109.96	103.30
1	AR	1604	G	C4-N9-C1'	5.54	133.70	126.50
66	S	85	VAL	C-N-CA	5.54	145.26	122.00
59	c0	88	PRO	N-CA-CB	5.54	109.94	103.30
1	1	218	G	O5'-P-OP2	-5.53	100.72	105.70
1	1	1858	A	C4-N9-C1'	5.52	136.24	126.30
4	j	191	LEU	CA-CB-CG	-5.52	102.60	115.30
1	AR	1556	C	N1-C2-O2	5.52	122.21	118.90
48	A	639	U	N1-C2-O2	5.51	126.66	122.80
1	AR	3354	U	C2-N1-C1'	5.51	124.31	117.70
1	1	639	G	N1-C6-O6	5.50	123.20	119.90
1	1	1556	C	C6-N1-C2	-5.50	118.10	120.30
1	1	3344	A	O4'-C1'-N9	5.49	112.59	108.20
1	1	344	A	N1-C6-N6	-5.48	115.31	118.60
1	1	2818	U	C5-C6-N1	5.48	125.44	122.70
1	AR	2375	G	N1-C6-O6	-5.48	116.61	119.90
48	sR	813	U	N3-C2-O2	-5.48	118.37	122.20
1	1	895	A	C4-C5-N7	5.47	113.44	110.70
1	AR	1844	C	C6-N1-C2	-5.47	118.11	120.30
71	X	93	LEU	CA-CB-CG	5.47	127.88	115.30
29	AB	42	ARG	NE-CZ-NH2	-5.46	117.57	120.30
48	sR	1058	U	OP1-P-O3'	5.46	117.21	105.20
1	AR	2263	C	C6-N1-C1'	-5.46	114.25	120.80
48	sR	542	A	P-O3'-C3'	5.45	126.24	119.70
1	1	2836	C	N3-C2-O2	-5.45	118.09	121.90
1	1	3362	A	C2-N3-C4	-5.45	107.88	110.60
48	A	767	U	N3-C2-O2	-5.45	118.39	122.20
1	1	2772	C	O4'-C1'-N1	5.44	112.56	108.20
1	1	648	C	C2-N1-C1'	5.44	124.78	118.80
1	1	922	U	C2-N1-C1'	5.44	124.23	117.70
30	AC	20	GLY	N-CA-C	5.43	126.66	113.10
1	1	97	U	C5-C6-N1	-5.42	119.99	122.70
1	1	1156	C	N1-C2-O2	5.42	122.15	118.90
1	1	1484	U	P-O3'-C3'	5.42	126.20	119.70
1	AR	2996	U	C2-N1-C1'	5.42	124.20	117.70
1	AR	934	G	C8-N9-C1'	-5.40	119.98	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AR	2870	C	C6-N1-C1'	5.40	127.28	120.80
48	sR	1560	U	N3-C2-O2	-5.39	118.43	122.20
1	1	651	G	N3-C4-C5	-5.39	125.91	128.60
17	CQ	84	LEU	CB-CG-CD1	-5.39	101.84	111.00
1	AR	1419	A	O5'-P-OP2	-5.38	100.86	105.70
1	1	3140	G	N1-C6-O6	5.38	123.13	119.90
1	1	1117	G	O5'-P-OP1	-5.37	100.87	105.70
50	C	181	LEU	CA-CB-CG	5.37	127.65	115.30
1	1	439	C	N1-C2-O2	5.37	122.12	118.90
48	A	728	U	N3-C2-O2	-5.37	118.44	122.20
1	1	3275	U	OP1-P-O3'	5.36	116.99	105.20
48	sR	163	G	C2-N3-C4	-5.36	109.22	111.90
48	A	501	U	P-O3'-C3'	5.35	126.12	119.70
1	1	637	C	O4'-C1'-N1	5.35	112.48	108.20
1	AR	718	G	C5-N7-C8	-5.35	101.62	104.30
48	sR	1389	C	C2-N1-C1'	5.35	124.68	118.80
1	AR	908	G	O4'-C1'-N9	-5.34	103.93	108.20
1	1	2227	C	P-O3'-C3'	5.34	126.10	119.70
1	AR	2281	A	O4'-C1'-N9	5.33	112.47	108.20
1	AR	3362	A	O4'-C1'-N9	5.33	112.47	108.20
26	CZ	38	LEU	CA-CB-CG	5.33	127.56	115.30
1	AR	2824	G	O5'-P-OP2	-5.33	100.90	105.70
48	A	934	C	C6-N1-C1'	-5.33	114.41	120.80
1	1	2983	C	N3-C2-O2	-5.32	118.17	121.90
1	AR	1556	C	C2-N1-C1'	5.32	124.66	118.80
1	AR	1858	A	C4-N9-C1'	5.31	135.87	126.30
1	1	2827	U	C2-N3-C4	-5.30	123.82	127.00
16	CP	93	LYS	N-CA-C	5.30	125.31	111.00
1	AR	3217	C	C6-N1-C2	-5.30	118.18	120.30
1	AR	3269	U	N3-C2-O2	-5.30	118.49	122.20
48	A	1370	U	P-O3'-C3'	5.29	126.05	119.70
48	sR	1246	C	C2-N1-C1'	5.29	124.62	118.80
48	sR	1274	C	C2-N1-C1'	5.29	124.62	118.80
1	1	2679	A	C2-N3-C4	-5.29	107.96	110.60
1	1	895	A	N1-C6-N6	5.28	121.77	118.60
48	sR	187	G	P-O3'-C3'	5.28	126.04	119.70
1	1	2983	C	C5-C4-N4	5.28	123.89	120.20
1	AR	3319	U	P-O3'-C3'	5.27	126.03	119.70
48	sR	25	C	P-O3'-C3'	5.27	126.02	119.70
48	A	720	G	P-O3'-C3'	5.26	126.02	119.70
1	1	895	A	N7-C8-N9	5.26	116.43	113.80
2	AS	98	C	C6-N1-C2	5.26	122.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3362	A	N1-C2-N3	5.26	131.93	129.30
1	1	2719	U	N1-C2-N3	5.25	118.05	114.90
48	A	730	G	C4-N9-C1'	5.25	133.33	126.50
48	A	1258	U	N3-C2-O2	-5.25	118.53	122.20
1	1	2772	C	C2-N1-C1'	5.24	124.57	118.80
57	s8	29	LEU	CA-CB-CG	5.24	127.34	115.30
1	1	2797	C	O5'-P-OP1	-5.23	100.99	105.70
52	E	182	LEU	CA-CB-CG	5.23	127.32	115.30
1	AR	3318	G	C4-N9-C1'	5.22	133.29	126.50
48	sR	795	U	N3-C2-O2	-5.21	118.55	122.20
67	c8	15	LEU	CA-CB-CG	5.21	127.28	115.30
10	CJ	35	GLY	N-CA-C	5.21	126.12	113.10
48	sR	1389	C	N1-C2-O2	5.21	122.02	118.90
1	1	637	C	C6-N1-C1'	5.20	127.04	120.80
1	AR	2373	A	O5'-P-OP1	-5.20	101.02	105.70
48	sR	1458	G	C4-N9-C1'	5.20	133.25	126.50
1	1	2418	G	OP1-P-O3'	5.19	116.61	105.20
1	AR	1097	G	P-O3'-C3'	5.19	125.92	119.70
48	A	553	G	C6-C5-N7	-5.18	127.29	130.40
3	AT	125	U	C6-N1-C1'	-5.18	113.95	121.20
1	1	979	U	C6-N1-C2	-5.17	117.89	121.00
1	1	873	C	P-O3'-C3'	5.17	125.91	119.70
1	1	2257	C	C2-N1-C1'	5.17	124.49	118.80
1	AR	644	G	C8-N9-C4	-5.17	104.33	106.40
1	1	101	G	O4'-C1'-N9	5.17	112.33	108.20
1	AR	1495	U	C2-N1-C1'	-5.17	111.50	117.70
48	A	1389	C	C2-N1-C1'	5.16	124.48	118.80
1	AR	439	C	C6-N1-C2	-5.16	118.23	120.30
1	AR	101	G	O4'-C1'-N9	5.16	112.33	108.20
1	1	770	G	O4'-C1'-N9	5.15	112.32	108.20
1	AR	2541	U	P-O3'-C3'	5.15	125.88	119.70
1	1	326	U	C5-C6-N1	5.15	125.28	122.70
1	AR	2281	A	C8-N9-C4	5.15	107.86	105.80
1	1	1716	U	P-O3'-C3'	5.15	125.88	119.70
1	AR	3057	U	N3-C2-O2	-5.14	118.60	122.20
48	sR	558	U	C2-N1-C1'	5.14	123.87	117.70
1	AR	1377	G	N1-C6-O6	-5.14	116.82	119.90
19	CS	161	LYS	N-CA-C	5.14	124.87	111.00
48	A	73	U	P-O3'-C3'	5.14	125.86	119.70
48	A	734	A	OP1-P-O3'	5.13	116.50	105.20
1	1	1858	A	N3-C4-N9	5.13	131.50	127.40
1	1	2101	C	P-O3'-C3'	5.13	125.86	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A	734	A	P-O3'-C3'	5.12	125.85	119.70
1	AR	1556	C	N3-C2-O2	-5.12	118.31	121.90
31	DE	41	LEU	CA-CB-CG	5.12	127.08	115.30
1	1	1604	G	C4-N9-C1'	5.11	133.15	126.50
48	A	287	G	O4'-C1'-N9	5.11	112.29	108.20
48	sR	610	G	C8-N9-C1'	-5.11	120.36	127.00
1	AR	718	G	C4-C5-N7	5.11	112.84	110.80
1	AR	3354	U	O4'-C1'-N1	5.11	112.29	108.20
48	sR	687	G	N3-C2-N2	-5.11	116.33	119.90
1	AR	1556	C	C6-N1-C2	-5.10	118.26	120.30
3	4	100	U	C2-N1-C1'	5.10	123.81	117.70
36	DJ	28	LEU	CA-CB-CG	5.10	127.02	115.30
48	A	1761	U	C5-C4-O4	5.09	128.96	125.90
48	sR	1058	U	P-O3'-C3'	5.09	125.81	119.70
48	sR	1503	A	O4'-C1'-N9	5.08	112.26	108.20
1	1	1116	G	OP2-P-O3'	5.07	116.35	105.20
1	1	2634	U	C5-C6-N1	-5.07	120.17	122.70
48	sR	280	U	C2-N1-C1'	5.07	123.78	117.70
1	1	2679	A	O4'-C1'-N9	5.06	112.25	108.20
48	sR	337	G	C8-N9-C1'	-5.05	120.43	127.00
1	1	2541	U	P-O3'-C3'	5.05	125.76	119.70
1	AR	3078	U	N3-C2-O2	-5.05	118.67	122.20
1	1	639	G	C5-C6-O6	-5.05	125.57	128.60
1	AR	1858	A	N3-C4-C5	-5.04	123.27	126.80
48	A	1560	U	N3-C2-O2	-5.04	118.67	122.20
1	1	1308	A	O5'-P-OP2	5.04	116.75	110.70
1	AR	1047	A	C5-C6-N6	-5.04	119.67	123.70
1	AR	2772	C	C2-N1-C1'	5.04	124.35	118.80
48	A	1568	C	P-O3'-C3'	5.04	125.75	119.70
48	sR	1039	A	O4'-C1'-N9	5.04	112.23	108.20
1	1	2314	U	C2-N1-C1'	5.03	123.73	117.70
1	AR	1047	A	N1-C6-N6	5.03	121.62	118.60
48	A	1241	G	O4'-C1'-N9	5.03	112.22	108.20
48	sR	187	G	OP1-P-O3'	5.03	116.26	105.20
1	AR	1815	U	P-O3'-C3'	5.03	125.73	119.70
48	A	830	U	N1-C2-O2	5.03	126.32	122.80
1	1	1858	A	C8-N9-C1'	-5.02	118.66	127.70
16	v	93	LYS	N-CA-C	5.02	124.54	111.00
1	AR	2412	G	C8-N9-C4	-5.01	104.39	106.40
1	AR	3218	A	P-O3'-C3'	5.01	125.72	119.70
48	sR	1573	A	P-O3'-C3'	5.01	125.71	119.70
1	AR	1103	A	C2-N3-C4	5.00	113.10	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	1	635	G	N3-C4-N9	5.00	129.00	126.00

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	0	133	ALA	Peptide
22	2	122	GLN	Peptide
27	9	83	ASP	Peptide
28	AA	101	PHE	Peptide
30	AC	19	ASN	Peptide
39	AL	17	ARG	Peptide
7	CG	294	ALA	Peptide
7	CG	58	LYS	Peptide
17	CQ	110	PRO	Peptide
22	CV	122	GLN	Peptide
25	CY	80	ARG	Peptide
51	D	106	ASP	Peptide
27	DA	83	ASP	Peptide
28	DB	3	LYS	Peptide
30	DD	19	ASN	Peptide
32	DF	82	GLU	Peptide
36	DJ	118	ILE	Peptide
44	DR	49	ARG	Peptide
52	E	219	ALA	Peptide
53	F	213	SER	Peptide
54	G	44	ASN	Peptide
54	G	65	ARG	Peptide
56	I	131	PHE	Peptide
56	I	31	SER	Peptide
56	I	64	VAL	Peptide
57	J	148	ALA	Peptide
63	P	123	SER	Peptide
64	Q	124	THR	Peptide
65	R	114	ARG	Peptide
65	R	33	GLY	Peptide
65	R	39	VAL	Peptide
65	R	40	GLU	Peptide
66	S	22	PRO	Peptide
66	S	85	VAL	Peptide
66	S	86	PRO	Peptide
67	T	83	ALA	Peptide

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Mol	Chain	Res	Type	Group
72	Y	137	LYS	Peptide
75	b	10	ARG	Peptide
61	c2	101	ALA	Peptide
63	c4	34	SER	Peptide
64	c5	50	THR	Peptide
64	c5	52	LYS	Peptide
65	c6	114	ARG	Peptide
65	c6	40	GLU	Peptide
70	d1	43	GLY	Peptide
73	d4	29	HIS	Peptide
83	e1	106	TYR	Peptide
80	g	110	ALA	Peptide
80	g	146	SER	Peptide
6	l	338	LYS	Peptide
10	p	30	THR	Peptide
12	r	188	GLY	Peptide
52	s3	219	ALA	Peptide
53	s4	163	ASP	Peptide
54	s5	100	ASN	Peptide
54	s5	44	ASN	Peptide
55	s6	164	LYS	Peptide
56	s7	130	VAL	Peptide
56	s7	64	VAL	Peptide
17	w	110	PRO	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	1	67355	0	33847	742	0
1	AR	67355	0	33847	869	0
2	3	2579	0	1304	21	0
2	AS	2579	0	1304	32	0
3	4	3353	0	1695	29	0
3	AT	3353	0	1695	46	0
4	CD	1914	0	1981	33	0
4	j	1914	0	1981	0	0
5	CE	3075	0	3142	107	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	k	3075	0	3142	0	0
6	CF	2748	0	2859	62	0
6	l	2748	0	2859	0	0
7	CG	2375	0	2325	61	0
7	m	2375	0	2325	0	0
8	CH	1239	0	1326	30	0
8	n	1239	0	1326	0	0
9	CI	1784	0	1862	26	0
9	o	1784	0	1862	0	0
10	CJ	1804	0	1877	44	0
10	p	1804	0	1877	0	0
11	CK	1518	0	1587	40	0
11	q	1518	0	1587	0	0
12	CL	1705	0	1736	52	0
12	r	1705	0	1736	0	0
13	CM	1353	0	1383	37	0
13	s	1353	0	1383	0	0
14	CN	1543	0	1608	44	0
14	t	1543	0	1608	0	0
15	CO	1053	0	1149	32	0
15	u	1053	0	1149	0	0
16	CP	1720	0	1779	47	0
16	v	1720	0	1779	0	0
17	CQ	1555	0	1659	26	0
17	w	1555	0	1659	0	0
18	CR	1420	0	1437	36	0
18	x	1420	0	1437	0	0
19	CS	1441	0	1543	32	0
19	y	1441	0	1543	0	0
20	CT	1521	0	1617	43	0
20	z	1521	0	1617	0	0
21	0	1445	0	1487	24	0
21	CU	1445	0	1487	31	0
22	2	1276	0	1323	32	0
22	CV	1276	0	1323	43	0
23	5	796	0	812	7	0
23	CW	796	0	812	11	0
24	6	1003	0	1048	23	0
24	CX	1003	0	1048	24	0
25	7	699	0	640	12	0
25	CY	699	0	640	9	0
26	8	964	0	1025	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	CZ	964	0	1025	24	0
27	9	993	0	1081	22	0
27	DA	993	0	1081	22	0
28	AA	1092	0	1155	36	0
28	DB	1092	0	1155	27	0
29	AB	1173	0	1215	37	0
29	DC	1173	0	1215	43	0
30	AC	462	0	491	14	0
30	DD	462	0	491	13	0
31	AD	743	0	797	18	0
31	DE	743	0	797	11	0
32	AE	876	0	912	20	0
32	DF	876	0	912	16	0
33	AF	1020	0	1090	20	0
33	DG	1020	0	1090	20	0
34	AG	850	0	880	16	0
34	DH	850	0	880	11	0
35	AH	880	0	945	27	0
35	DI	880	0	945	23	0
36	AI	969	0	1078	17	0
36	DJ	969	0	1078	32	0
37	AJ	771	0	849	12	0
37	DK	771	0	849	21	0
38	AK	681	0	683	22	0
38	DL	681	0	683	20	0
39	AL	612	0	682	11	0
39	DM	612	0	682	15	0
40	AM	436	0	475	16	0
40	DN	436	0	475	16	0
41	AN	417	0	455	6	0
41	DO	417	0	455	6	0
42	AO	233	0	284	11	0
42	DP	233	0	284	4	0
43	AP	847	0	914	19	0
43	DQ	847	0	914	9	0
44	AQ	694	0	734	17	0
44	DR	694	0	734	17	0
45	i	1104	0	1003	0	0
46	p0	1077	0	1041	0	0
47	sM	681	0	541	0	0
48	A	37948	0	19094	565	0
48	sR	37990	0	19116	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	B	1577	0	1567	54	0
49	s0	1583	0	1578	0	0
50	C	1709	0	1784	68	0
50	s1	1722	0	1793	0	0
51	D	1635	0	1723	42	0
51	s2	1635	0	1723	0	0
52	E	1734	0	1817	42	0
52	s3	1734	0	1817	0	0
53	F	2068	0	2154	52	0
53	s4	2068	0	2154	0	0
54	G	1609	0	1675	46	0
54	s5	1609	0	1675	0	0
55	H	1799	0	1878	42	0
55	s6	1755	0	1846	0	0
56	I	1481	0	1572	55	0
56	s7	1491	0	1578	0	0
57	J	1489	0	1525	46	0
57	s8	1489	0	1525	0	0
58	K	1494	0	1573	41	0
58	s9	1494	0	1573	0	0
59	L	772	0	727	26	0
59	c0	760	0	696	0	0
60	M	1213	0	1257	31	0
60	c1	1168	0	1233	0	0
61	N	890	0	887	25	0
61	c2	890	0	887	0	0
62	O	1192	0	1255	31	0
62	c3	1192	0	1255	0	0
63	P	891	0	883	33	0
63	c4	949	0	985	0	0
64	Q	977	0	1002	25	0
64	c5	1039	0	1050	0	0
65	R	1105	0	1166	41	0
65	c6	1111	0	1171	0	0
66	S	926	0	930	33	0
67	T	1192	0	1222	37	0
67	c8	1192	0	1222	0	0
68	U	1112	0	1124	22	0
68	c9	1112	0	1124	0	0
69	V	855	0	917	35	0
69	d0	882	0	939	0	0
70	W	684	0	672	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	d1	684	0	672	0	0
71	X	1021	0	1060	40	0
71	d2	1021	0	1060	0	0
72	Y	1121	0	1196	28	0
72	d3	1121	0	1196	0	0
73	Z	1073	0	1132	38	0
73	d4	1073	0	1132	0	0
74	a	563	0	603	0	0
74	d5	558	0	598	0	0
75	b	769	0	814	0	0
75	d6	769	0	814	0	0
76	c	610	0	633	0	0
76	d7	610	0	633	0	0
77	d	497	0	535	0	0
77	d8	497	0	535	0	0
78	d9	442	0	428	0	0
78	e	442	0	428	0	0
79	e0	491	0	542	0	0
79	f	475	0	525	0	0
80	g	566	0	601	0	0
81	Rb	2442	0	2392	0	0
81	h	2437	0	2386	0	0
82	c7	906	0	909	0	0
83	e1	397	0	397	0	0
84	1	2317	0	0	252	0
84	3	56	0	0	5	0
84	4	105	0	0	8	0
84	A	994	0	0	109	0
84	AC	7	0	0	2	0
84	AG	7	0	0	1	0
84	AK	14	0	0	3	0
84	AP	7	0	0	5	0
84	AR	2422	0	0	306	0
84	AS	77	0	0	7	0
84	AT	119	0	0	20	0
84	CE	14	0	0	4	0
84	CF	14	0	0	4	0
84	CG	21	0	0	4	0
84	CK	7	0	0	0	0
84	CL	14	0	0	5	0
84	CM	7	0	0	1	0
84	CO	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	CP	7	0	0	1	0
84	CS	1	0	0	0	0
84	CV	7	0	0	1	0
84	CX	14	0	0	2	0
84	DD	7	0	0	1	0
84	DH	7	0	0	0	0
84	DL	7	0	0	2	0
84	DQ	7	0	0	3	0
84	H	7	0	0	0	0
84	J	7	0	0	1	0
84	M	7	0	0	1	0
84	O	7	0	0	1	0
84	Q	7	0	0	2	0
84	Rb	7	0	0	0	0
84	T	7	0	0	1	0
84	c3	7	0	0	0	0
84	c5	7	0	0	0	0
84	c8	7	0	0	0	0
84	d4	7	0	0	0	0
84	d9	7	0	0	0	0
84	e	7	0	0	0	0
84	h	7	0	0	0	0
84	k	7	0	0	0	0
84	l	7	0	0	0	0
84	r	7	0	0	0	0
84	s1	7	0	0	0	0
84	s4	7	0	0	0	0
84	s8	7	0	0	0	0
84	sR	1064	0	0	0	0
84	v	14	0	0	0	0
84	x	14	0	0	0	0
84	y	7	0	0	0	0
84	z	7	0	0	0	0
85	1	485	0	0	0	0
85	3	12	0	0	0	0
85	4	19	0	0	0	0
85	6	2	0	0	0	0
85	A	109	0	0	0	0
85	AB	4	0	0	0	0
85	AH	1	0	0	0	0
85	AK	1	0	0	0	0
85	AP	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	AR	504	0	0	0	0
85	AS	17	0	0	0	0
85	AT	13	0	0	0	0
85	CD	2	0	0	0	0
85	CE	2	0	0	0	0
85	CF	1	0	0	0	0
85	CG	1	0	0	0	0
85	CJ	1	0	0	0	0
85	CM	2	0	0	0	0
85	CN	1	0	0	0	0
85	CP	4	0	0	0	0
85	CQ	3	0	0	0	0
85	CR	6	0	0	0	0
85	CU	1	0	0	0	0
85	CX	3	0	0	0	0
85	D	1	0	0	0	0
85	DA	1	0	0	0	0
85	DC	6	0	0	0	0
85	DD	1	0	0	0	0
85	DH	2	0	0	0	0
85	DO	1	0	0	0	0
85	DP	1	0	0	0	0
85	DR	2	0	0	0	0
85	J	1	0	0	0	0
85	O	1	0	0	0	0
85	Y	1	0	0	0	0
85	b	1	0	0	0	0
85	c1	1	0	0	0	0
85	c6	1	0	0	0	0
85	c7	1	0	0	0	0
85	c8	1	0	0	0	0
85	d3	2	0	0	0	0
85	d4	1	0	0	0	0
85	d5	1	0	0	0	0
85	d6	2	0	0	0	0
85	d9	1	0	0	0	0
85	e	1	0	0	0	0
85	j	1	0	0	0	0
85	k	2	0	0	0	0
85	l	5	0	0	0	0
85	n	1	0	0	0	0
85	o	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	r	2	0	0	0	0
85	s	1	0	0	0	0
85	s1	1	0	0	0	0
85	s8	1	0	0	0	0
85	sM	1	0	0	0	0
85	sR	139	0	0	0	0
85	t	3	0	0	0	0
85	u	1	0	0	0	0
85	v	2	0	0	0	0
85	w	1	0	0	0	0
85	x	5	0	0	0	0
85	z	1	0	0	0	0
86	1	26	0	0	0	0
86	AR	26	0	0	1	0
87	AK	1	0	0	0	0
87	AN	1	0	0	0	0
87	AP	1	0	0	0	0
87	AQ	1	0	0	0	0
87	DL	1	0	0	0	0
87	DO	1	0	0	0	0
87	DQ	1	0	0	0	0
87	DR	1	0	0	0	0
87	b	1	0	0	0	0
87	c	1	0	0	0	0
87	d6	1	0	0	0	0
87	d7	1	0	0	0	0
87	d9	1	0	0	0	0
87	e	1	0	0	0	0
87	e1	1	0	0	0	0
87	g	1	0	0	0	0
All	All	409612	0	296692	4353	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 10.

All (4353) 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)
5:CE:41:VAL:HA	5:CE:185:GLY:HA3	1.34	1.05
12:CL:174:THR:HG23	12:CL:176:LEU:H	1.29	0.95
56:I:11:GLN:HG3	56:I:13:PRO:HD2	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2736:A:OP1	22:2:92:ARG:NH1	2.00	0.93
48:A:1339:C:O2'	48:A:1341:A:N7	2.01	0.93
63:P:85:ALA:H	63:P:119:THR:HG22	1.30	0.93
1:AR:3182:G:OP1	17:CQ:160:ARG:NH2	2.04	0.91
1:1:1222:G:HO2'	1:1:1285:G:H1	1.16	0.89
2:AS:49:G:N7	7:CG:58:LYS:HG3	1.85	0.89
38:AK:88:ALA:O	84:AK:102:OHX:N1	2.05	0.89
1:1:1171:G:N7	84:1:3494:OHX:N2	2.20	0.89
48:A:991:G:OP2	84:A:2009:OHX:N1	2.06	0.89
1:1:3118:C:H4'	41:AN:106:ARG:HH22	1.35	0.89
1:1:640:U:OP1	29:AB:21:ARG:NH2	2.06	0.88
1:AR:2198:A:OP2	84:AR:3697:OHX:N6	2.07	0.88
1:AR:2854:U:OP2	12:CL:3:ARG:NH2	2.07	0.88
11:CK:22:SER:OG	11:CK:23:ARG:N	2.05	0.88
1:1:679:U:O4	84:1:3508:OHX:N1	2.07	0.88
84:AR:3407:OHX:N1	3:AT:2:A:OP2	2.07	0.87
1:1:3344:A:H2	1:1:3361:G:H21	1.21	0.87
1:1:1486:G:N7	84:1:3688:OHX:N2	2.24	0.86
15:CO:55:ARG:NH2	15:CO:76:ALA:O	2.08	0.86
1:AR:3194:C:O2	1:AR:3197:G:N2	2.09	0.86
1:AR:1565:G:N2	1:AR:1574:C:N3	2.24	0.85
1:1:3120:C:OP2	84:1:3427:OHX:N3	2.10	0.85
36:DJ:64:GLU:HA	36:DJ:67:ARG:HB2	1.59	0.84
56:I:51:VAL:HG23	56:I:53:GLY:H	1.43	0.84
1:AR:1639:C:OP2	35:DI:74:ARG:NH2	2.10	0.84
1:AR:283:G:OP2	43:DQ:45:ARG:NH2	2.11	0.84
53:F:79:ASP:HB3	53:F:82:TYR:HB2	1.60	0.84
1:AR:2836:C:H5	1:AR:2852:C:H42	1.23	0.84
53:F:193:GLY:HA3	53:F:210:ILE:HG22	1.60	0.84
6:CF:16:THR:HG22	6:CF:18:ASN:H	1.40	0.83
1:1:1481:A:O2'	1:1:1858:A:N3	2.10	0.83
1:1:1541:G:OP2	84:1:3556:OHX:N2	2.11	0.83
1:AR:778:U:O4	84:AR:3593:OHX:N1	2.12	0.83
1:1:1414:G:N7	84:1:3656:OHX:N2	2.27	0.83
6:CF:204:GLY:O	6:CF:246:ARG:NH1	2.11	0.82
72:Y:102:VAL:HG12	72:Y:127:VAL:HG12	1.60	0.82
48:A:40:A:OP1	58:K:3:ARG:NH1	2.12	0.82
24:6:48:ARG:HG3	24:6:48:ARG:HH11	1.43	0.82
1:1:509:U:O4	84:1:3705:OHX:N2	2.13	0.82
1:AR:3128:G:OP2	84:AR:3664:OHX:N3	2.12	0.82
1:1:371:G:O6	84:1:3712:OHX:N4	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:2:A:OP2	84:4:202:OHX:N5	2.13	0.81
1:AR:1481:A:O2'	1:AR:1858:A:N3	2.11	0.81
1:AR:2273:G:O6	84:AR:3703:OHX:N5	2.13	0.81
1:AR:31:C:OP2	16:CP:188:ARG:NH2	2.14	0.81
57:J:76:THR:HG22	57:J:108:PRO:HG2	1.62	0.81
1:AR:1486:G:N7	84:AR:3539:OHX:N4	2.28	0.81
5:CE:171:LEU:O	84:CE:401:OHX:N3	2.14	0.81
1:1:3346:U:H3	1:1:3359:A:H61	1.25	0.81
1:1:1230:G:H1	1:1:1279:C:H42	1.29	0.81
48:A:1585:U:H3	48:A:1611:A:H2	1.27	0.81
48:A:237:C:H5''	48:A:238:U:H5'	1.62	0.80
1:1:3343:G:H21	1:1:3362:A:H2	1.25	0.80
22:CV:39:ILE:HD12	22:CV:102:ARG:HD3	1.62	0.80
48:A:169:A:H5''	55:H:176:GLN:HG2	1.62	0.80
50:C:129:THR:HA	50:C:177:GLN:HA	1.62	0.80
71:X:15:ASN:HD21	71:X:71:LYS:HA	1.46	0.80
1:AR:2703:A:OP2	7:CG:23:ARG:NH1	2.15	0.80
16:CP:31:ARG:NH1	16:CP:124:ASP:OD2	2.14	0.80
11:CK:41:ILE:HD11	11:CK:67:ALA:HB1	1.62	0.80
1:AR:430:U:OP1	84:AR:3613:OHX:N5	2.14	0.80
51:D:38:VAL:HG13	51:D:39:THR:HG23	1.64	0.80
48:A:1318:G:N7	84:A:1963:OHX:N6	2.29	0.79
36:DJ:85:THR:HG22	36:DJ:88:LEU:H	1.47	0.79
56:I:50:ASP:HB3	56:I:56:LYS:HG2	1.62	0.79
48:A:1429:G:H1'	69:V:74:GLU:HG2	1.63	0.79
1:1:2836:C:H5	1:1:2852:C:H42	1.29	0.79
84:AT:203:OHX:N3	38:DL:62:GLY:O	2.15	0.79
1:1:2233:A:OP2	84:1:3580:OHX:N5	2.15	0.79
1:1:581:U:O4	84:1:3544:OHX:N4	2.15	0.79
2:3:85:G:N7	84:3:202:OHX:N4	2.31	0.79
19:CS:34:THR:HG22	19:CS:49:LEU:HD21	1.65	0.79
48:A:1757:G:O6	84:A:1901:OHX:N2	2.15	0.79
48:A:1015:U:OP1	84:A:1923:OHX:N3	2.16	0.79
53:F:240:LYS:H	53:F:240:LYS:HE2	1.46	0.79
1:1:2818:U:H6	1:1:2818:U:H5'	1.45	0.79
36:AI:85:THR:HG22	36:AI:88:LEU:H	1.45	0.79
48:A:1110:G:N7	84:A:1947:OHX:N3	2.31	0.79
3:4:62:C:O2	84:4:208:OHX:N5	2.16	0.78
48:A:123:G:H21	53:F:146:THR:HG21	1.48	0.78
36:AI:78:LYS:HA	36:AI:81:ARG:HD2	1.63	0.78
48:A:1234:A:OP2	84:A:2030:OHX:N3	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:CL:220:GLN:O	84:CL:301:OHX:N2	2.16	0.78
1:AR:2818:U:H6	1:AR:2818:U:H5'	1.47	0.78
48:A:140:A:N6	48:A:281:G:OP1	2.16	0.78
48:A:339:C:OP2	57:J:10:LYS:NZ	2.17	0.78
1:AR:2700:G:N7	84:AR:3434:OHX:N6	2.32	0.78
1:1:2663:G:O6	84:1:3405:OHX:N6	2.16	0.78
1:1:1740:U:H1'	1:1:1741:A:H2	1.49	0.78
69:V:68:ARG:HG2	69:V:68:ARG:HH11	4.47	0.78
1:AR:2108:C:H1'	1:AR:3344:A:C8	2.19	0.77
1:AR:640:U:OP1	29:DC:21:ARG:NH2	2.18	0.77
1:1:3375:A:O2'	1:1:3378:C:OP2	2.03	0.77
84:AR:3408:OHX:N3	3:AT:15:G:OP2	2.17	0.77
6:CF:20:LEU:HD11	6:CF:252:GLU:HG3	1.66	0.77
11:CK:22:SER:HG	11:CK:23:ARG:H	1.31	0.77
48:A:1140:G:OP2	84:A:1943:OHX:N2	2.18	0.77
1:1:1951:C:H42	1:1:2095:G:H1	1.30	0.77
1:1:621:A:O2'	84:1:3697:OHX:N5	2.17	0.77
48:A:1382:A:H5''	69:V:60:THR:HG22	1.67	0.77
48:A:22:A:OP2	84:A:1997:OHX:N4	2.18	0.77
3:AT:62:C:O2	84:AT:207:OHX:N4	2.17	0.77
58:K:110:GLN:HE22	58:K:126:ARG:HG2	1.49	0.77
1:AR:2317:A:OP2	84:AR:3692:OHX:N6	2.18	0.77
1:1:283:G:OP1	43:AP:45:ARG:NH2	2.17	0.76
66:S:82:ASP:O	66:S:83:GLN:NE2	2.16	0.76
69:V:27:THR:HG23	69:V:113:ASP:HB3	1.67	0.76
26:CZ:57:LEU:HD12	26:CZ:61:LYS:HG2	1.66	0.76
48:A:820:U:H2'	48:A:821:U:H4'	1.66	0.76
48:A:355:G:OP2	84:A:1914:OHX:N4	2.18	0.76
3:4:95:G:OP2	38:AK:72:ARG:NH1	2.17	0.76
1:AR:2582:C:OP1	84:AR:3635:OHX:N3	2.19	0.76
21:CU:2:ALA:HB3	21:CU:32:SER:HB3	1.68	0.76
1:1:964:G:OP1	84:1:3500:OHX:N2	2.18	0.76
1:1:1015:U:O2'	1:1:1017:C:OP2	2.04	0.76
1:1:1427:U:OP2	29:AB:4:ARG:NH2	2.19	0.76
1:1:1639:C:OP2	35:AH:74:ARG:NH2	2.19	0.76
1:1:2128:C:OP1	84:1:3493:OHX:N6	2.18	0.75
28:AA:15:ARG:NH2	35:AH:83:ASN:OD1	2.18	0.75
33:DG:100:ILE:O	33:DG:105:ARG:NH1	2.18	0.75
3:4:135:G:OP2	26:8:56:ARG:NH2	2.20	0.75
70:W:74:GLN:NE2	70:W:81:ASN:O	2.19	0.75
48:A:373:G:N7	84:A:2037:OHX:N6	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AC:18:ARG:O	84:AC:101:OHX:N2	2.19	0.75
48:A:1353:U:O4	84:A:1973:OHX:N5	2.20	0.75
1:AR:373:A:OP1	84:AR:3655:OHX:N6	2.20	0.75
5:CE:296:THR:HG22	5:CE:298:PHE:H	1.51	0.75
1:AR:3045:G:OP1	5:CE:19:ARG:NH2	2.19	0.75
13:CM:82:ARG:HG2	13:CM:112:LEU:HB2	1.68	0.75
1:1:978:G:O2'	1:1:979:U:O2	2.03	0.75
1:AR:2964:G:N7	84:AR:3486:OHX:N2	2.34	0.75
29:DC:47:LYS:O	29:DC:49:HIS:N	2.18	0.75
1:1:3224:G:O6	84:1:3429:OHX:N4	2.20	0.74
48:A:1202:A:OP1	84:A:1988:OHX:N1	2.20	0.74
48:A:702:G:O6	48:A:736:C:N4	2.19	0.74
1:AR:1440:G:N7	84:AR:3467:OHX:N6	2.35	0.74
7:CG:111:GLN:HA	7:CG:116:ASP:HB2	1.69	0.74
1:1:392:G:O6	84:1:3679:OHX:N5	2.21	0.74
7:CG:76:ALA:HB3	7:CG:109:THR:HG22	1.69	0.74
19:CS:86:THR:HG22	19:CS:105:ARG:HB2	1.69	0.74
1:1:624:G:OP2	84:1:3665:OHX:N3	2.20	0.74
51:D:45:VAL:HG21	51:D:68:ILE:HG23	1.70	0.74
1:AR:3377:G:O6	84:AR:3594:OHX:N1	2.20	0.74
1:1:1464:G:O2'	84:1:3414:OHX:N1	2.20	0.74
48:A:1595:U:H3	48:A:1600:A:H2	1.34	0.74
24:CX:133:SER:O	84:CX:202:OHX:N3	2.20	0.74
1:1:1538:G:OP2	84:1:3668:OHX:N1	2.21	0.74
1:1:637:C:H2'	1:1:638:C:C6	2.21	0.74
1:AR:658:G:OP1	84:AT:209:OHX:N5	2.21	0.74
18:CR:125:GLN:HB2	18:CR:141:SER:HB2	1.69	0.74
60:M:18:HIS:O	84:M:201:OHX:N6	2.20	0.74
1:1:3019:U:O4	84:1:3524:OHX:N1	2.21	0.74
60:M:7:VAL:HG13	60:M:8:GLN:H	1.52	0.74
1:1:1170:A:OP2	84:1:3494:OHX:N3	2.20	0.74
1:AR:3272:C:OP2	8:CH:78:ARG:NH1	2.21	0.74
48:A:874:C:OP1	84:A:1911:OHX:N2	2.20	0.74
48:A:895:G:H1	48:A:917:U:H3	1.34	0.73
1:AR:510:G:O6	84:AR:3529:OHX:N2	2.21	0.73
50:C:61:LEU:HG	50:C:64:ARG:HH21	1.52	0.73
17:CQ:3:VAL:HG22	17:CQ:4:GLU:HG3	1.70	0.73
3:AT:67:U:O4	84:AT:214:OHX:N3	2.22	0.73
48:A:142:G:H22	48:A:173:A:H2	1.34	0.73
1:1:626:U:O4	84:1:3535:OHX:N3	2.21	0.73
33:AF:100:ILE:O	33:AF:105:ARG:NH1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:471:A:OP2	84:A:1954:OHX:N4	2.22	0.73
49:B:150:ASP:OD2	49:B:165:ARG:NH2	2.22	0.73
14:CN:47:ALA:HB1	14:CN:48:PRO:HD2	1.69	0.73
1:AR:1493:G:O6	40:DN:2:ALA:N	2.22	0.73
1:1:3200:G:O6	84:1:3661:OHX:N4	2.21	0.73
1:AR:1734:G:O6	84:AR:3472:OHX:N5	2.22	0.73
1:AR:72:C:H5'	14:CN:63:VAL:HG22	1.70	0.73
6:CF:283:THR:HG22	6:CF:285:ASP:H	1.52	0.73
48:A:68:A:OP1	55:H:160:ARG:NH2	2.22	0.73
38:AK:21:ARG:NH2	38:AK:41:ALA:O	2.21	0.73
1:1:3289:G:N7	84:1:3664:OHX:N4	2.37	0.72
1:1:3111:U:OP2	84:1:3427:OHX:N2	2.22	0.72
56:I:64:VAL:HG22	56:I:94:ALA:HB1	1.69	0.72
57:J:39:GLY:HA2	57:J:61:GLU:HB3	1.70	0.72
1:AR:733:G:N7	84:AR:3570:OHX:N5	2.38	0.72
1:AR:744:A:OP1	19:CS:66:ARG:NH2	2.22	0.72
5:CE:169:THR:HG23	5:CE:171:LEU:H	1.54	0.72
55:H:135:PRO:HB2	55:H:141:ILE:HG12	1.70	0.72
48:A:818:C:N4	48:A:819:G:O6	2.22	0.72
1:AR:3214:U:OP2	15:CO:128:ARG:NH2	2.21	0.72
1:AR:1752:A:OP2	84:AR:3586:OHX:N6	2.23	0.72
48:A:1672:G:N7	84:A:1922:OHX:N5	2.37	0.72
48:A:422:G:OP1	84:A:1920:OHX:N6	2.22	0.72
1:AR:3319:U:O2'	1:AR:3320:A:OP1	2.06	0.72
55:H:2:LYS:HB3	55:H:108:VAL:HG22	1.72	0.72
21:0:91:TYR:O	21:0:137:ARG:NH1	2.23	0.72
21:0:2:ALA:HB3	21:0:32:SER:HB3	1.70	0.72
48:A:1508:U:O4	84:A:1909:OHX:N2	2.23	0.72
1:AR:1851:G:OP2	84:AR:3545:OHX:N2	2.22	0.72
1:AR:1471:U:OP2	84:AR:3460:OHX:N6	2.23	0.72
48:A:475:A:OP2	58:K:126:ARG:NH1	2.23	0.72
3:4:16:G:O6	84:4:201:OHX:N4	2.23	0.72
48:A:131:C:OP1	84:A:1951:OHX:N1	2.23	0.72
1:AR:1015:U:O2'	1:AR:1017:C:OP2	2.06	0.72
1:AR:2261:G:O2'	1:AR:2263:C:N4	2.22	0.72
48:A:732:G:O2'	48:A:733:A:O4'	2.08	0.71
1:AR:621:A:O2'	84:AR:3627:OHX:N6	2.23	0.71
48:A:523:G:OP2	73:Z:37:LYS:NZ	2.21	0.71
1:1:3134:A:OP1	84:1:3437:OHX:N4	2.23	0.71
48:A:377:G:O6	84:A:1956:OHX:N5	2.23	0.71
1:AR:1381:A:OP1	6:CF:197:ARG:NH1	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1861:G:O6	84:1:3532:OHX:N1	2.23	0.71
1:AR:1028:U:O2	13:CM:94:ARG:NH1	2.23	0.71
1:AR:2234:G:N7	84:AR:3465:OHX:N1	2.39	0.71
50:C:34:ALA:HB3	50:C:41:ARG:HA	1.69	0.71
56:I:31:SER:HB3	56:I:32:PRO:HD3	1.70	0.71
1:1:129:U:O4	84:1:3426:OHX:N5	2.23	0.71
48:A:1459:C:OP2	67:T:138:THR:OG1	2.07	0.71
48:A:190:C:N4	48:A:196:G:O6	2.22	0.71
1:AR:1591:G:OP1	35:DI:16:ARG:NH1	2.23	0.71
1:AR:440:A:OP1	1:AR:494:G:O2'	2.06	0.71
2:AS:81:U:O4	84:AS:210:OHX:N6	2.23	0.71
14:CN:165:SER:O	14:CN:167:PHE:N	2.24	0.71
71:X:82:LYS:O	71:X:84:GLY:N	2.20	0.71
48:A:1754:A:O2'	84:A:1936:OHX:N5	2.23	0.71
1:1:1320:C:O2	21:0:115:ARG:NH2	2.24	0.71
48:A:1521:G:O6	68:U:68:ARG:NH1	2.24	0.71
1:1:2895:G:H2'	1:1:2896:A:H5''	1.73	0.71
1:1:2386:A:OP1	84:1:3561:OHX:N1	2.24	0.71
1:1:742:G:O6	84:1:3510:OHX:N1	2.24	0.71
1:1:979:U:H1'	1:1:980:A:C8	2.26	0.71
4:CD:27:ALA:O	4:CD:128:ARG:NH2	2.24	0.71
48:A:542:A:H8	48:A:543:C:H5'	1.55	0.71
1:AR:2108:C:H1'	1:AR:3344:A:H8	1.56	0.70
57:J:106:ALA:HB2	57:J:165:LEU:HG	1.72	0.70
1:1:420:G:O6	84:1:3436:OHX:N6	2.24	0.70
1:AR:2768:U:OP2	84:AR:3674:OHX:N5	2.24	0.70
1:AR:419:G:N7	84:AR:3407:OHX:N3	2.38	0.70
22:CV:51:GLY:HA3	22:CV:92:ARG:HG3	1.71	0.70
54:G:117:THR:HG21	54:G:194:LEU:HD12	1.72	0.70
1:1:2960:C:OP1	84:1:3538:OHX:N4	2.25	0.70
48:A:992:A:OP1	84:A:1913:OHX:N2	2.25	0.70
1:AR:2310:U:OP1	84:AR:3703:OHX:N2	2.23	0.70
61:N:75:VAL:HG21	61:N:120:VAL:HG21	1.72	0.70
48:A:1542:G:N2	48:A:1569:A:OP2	2.24	0.70
1:AR:2580:A:O2'	84:AR:3635:OHX:N1	2.25	0.70
1:AR:3328:G:OP2	84:AR:3541:OHX:N1	2.25	0.70
84:AT:212:OHX:N2	27:DA:114:ASP:OD1	2.25	0.70
56:I:35:LYS:HG2	56:I:36:ALA:H	1.56	0.70
48:A:623:A:OP1	84:A:2035:OHX:N1	2.24	0.70
26:CZ:115:ARG:HH11	26:CZ:115:ARG:HG3	1.56	0.70
48:A:1291:G:N2	48:A:1324:G:H22	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:AR:3694:OHX:N2	37:DK:28:TYR:O	2.24	0.70
1:AR:1543:G:O6	84:AR:3706:OHX:N1	2.23	0.70
1:AR:3115:C:OP1	11:CK:62:ARG:NH2	2.24	0.70
31:DE:100:ILE:HG13	31:DE:101:LEU:HD22	1.74	0.70
1:1:1114:U:OP2	84:1:3500:OHX:N4	2.24	0.70
48:A:1238:A:OP2	84:A:1925:OHX:N2	2.25	0.70
1:1:3346:U:H3	1:1:3359:A:N6	1.89	0.70
1:AR:1507:G:N7	18:CR:129:THR:HG22	2.06	0.70
1:AR:3230:G:O6	84:AR:3569:OHX:N3	2.25	0.70
49:B:189:VAL:HG22	49:B:190:ASP:H	1.56	0.70
10:CJ:156:ASP:OD1	10:CJ:156:ASP:N	2.24	0.70
31:DE:22:LYS:HB2	31:DE:94:GLU:HB2	1.73	0.70
1:1:1634:G:N7	28:AA:17:ARG:NH2	2.37	0.69
28:AA:52:LYS:O	28:AA:65:ARG:NH1	2.25	0.69
1:AR:2560:C:O2	84:AR:3537:OHX:N2	2.25	0.69
1:AR:1630:U:OP1	28:DB:67:LYS:NZ	2.23	0.69
1:AR:3054:U:O4	84:AR:3677:OHX:N4	2.25	0.69
13:CM:60:ARG:O	13:CM:63:GLU:HB2	1.93	0.69
57:J:76:THR:HB	57:J:105:ASP:HB2	1.72	0.69
1:1:2274:U:OP2	84:1:3501:OHX:N4	2.25	0.69
48:A:1535:U:O2'	48:A:1536:G:N3	2.24	0.69
48:A:280:U:O2'	48:A:281:G:OP2	2.11	0.69
1:AR:187:A:OP2	84:AR:3413:OHX:N2	2.25	0.69
65:R:50:GLU:OE1	65:R:114:ARG:NH1	2.25	0.69
1:1:838:G:O6	44:AQ:4:ARG:NH2	2.25	0.69
1:AR:318:A:OP1	84:AR:3458:OHX:N5	2.25	0.69
22:CV:18:ASP:OD1	84:CV:201:OHX:N3	2.25	0.69
48:A:7:G:O6	51:D:205:ARG:NH2	2.25	0.69
23:5:51:GLY:O	23:5:52:ASN:ND2	2.19	0.69
1:AR:1538:G:OP2	84:AR:3511:OHX:N4	2.24	0.69
1:AR:79:U:OP2	84:AR:3464:OHX:N4	2.25	0.69
7:CG:68:THR:HG22	7:CG:70:THR:H	1.57	0.69
65:R:82:ARG:HH22	65:R:114:ARG:HB2	1.58	0.69
1:1:1056:U:O2	84:1:3520:OHX:N4	2.25	0.69
48:A:149:C:O2'	55:H:132:ARG:NH1	2.25	0.69
26:CZ:86:VAL:HG11	26:CZ:95:ILE:HG12	1.75	0.69
48:A:1522:U:OP2	84:A:1937:OHX:N3	2.25	0.69
48:A:1140:G:OP2	84:A:1943:OHX:N6	2.25	0.69
1:AR:1887:A:OP1	84:AR:3619:OHX:N3	2.26	0.69
70:W:60:ARG:HA	70:W:65:SER:HB2	1.75	0.69
1:1:781:G:O6	84:1:3476:OHX:N3	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:2880:U:H1'	5:CE:250:ALA:HB3	1.75	0.69
1:AR:3230:G:H4'	15:CO:132:LYS:HD3	1.75	0.69
1:AR:2278:C:OP1	84:AR:3597:OHX:N6	2.26	0.69
28:DB:3:LYS:O	28:DB:5:LEU:N	2.25	0.69
1:1:1817:G:OP1	84:1:3626:OHX:N1	2.25	0.68
48:A:1034:C:HO2'	71:X:2:THR:N	1.89	0.68
42:AO:2:ARG:NH1	48:A:1773:C:OP2	2.26	0.68
5:CE:218:ILE:HG13	5:CE:276:THR:HG23	1.75	0.68
48:A:383:G:N7	84:A:2008:OHX:N4	2.41	0.68
1:AR:1599:G:OP1	84:AR:3642:OHX:N4	2.26	0.68
5:CE:53:MET:HG2	5:CE:77:THR:HG22	1.76	0.68
48:A:1794:A:OP1	84:A:1970:OHX:N4	2.27	0.68
1:AR:2895:G:H2'	1:AR:2896:A:H5''	1.75	0.68
1:AR:368:G:OP1	84:AR:3427:OHX:N1	2.25	0.68
1:AR:838:G:O6	44:DR:4:ARG:NH2	2.26	0.68
1:1:1192:C:OP2	84:1:3586:OHX:N4	2.27	0.68
1:1:904:A:OP2	38:AK:30:GLN:NE2	2.26	0.68
1:AR:3349:C:H42	1:AR:3356:G:H1	1.40	0.68
15:CO:16:GLU:HB3	21:CU:149:LYS:HB3	1.76	0.68
67:T:94:ASP:OD2	67:T:98:TYR:OH	2.11	0.68
24:6:10:LYS:NZ	24:6:56:ASP:OD1	2.22	0.68
50:C:123:ALA:HB2	50:C:165:ARG:HG2	1.75	0.68
36:DJ:10:ARG:NH1	36:DJ:60:GLU:OE1	2.25	0.68
44:DR:84:ARG:NH1	44:DR:88:GLU:OE2	2.27	0.68
2:3:112:G:OP2	84:3:206:OHX:N3	2.27	0.68
1:AR:2400:G:OP1	84:AR:3615:OHX:N1	2.27	0.68
48:A:283:U:H5''	55:H:188:ARG:HD3	1.75	0.68
27:9:45:ILE:HD12	27:9:119:ILE:HG23	1.75	0.68
48:A:1203:A:OP2	84:A:1988:OHX:N5	2.26	0.68
1:AR:617:G:H4'	18:CR:171:ARG:HH21	1.58	0.68
54:G:40:ILE:HG23	54:G:42:LEU:HD22	1.74	0.68
1:1:249:U:O2	1:1:250:U:N3	2.23	0.68
1:1:256:G:N7	84:1:3692:OHX:N4	2.42	0.68
48:A:45:U:O2'	48:A:46:A:H2'	1.94	0.68
14:CN:46:ILE:HG22	14:CN:49:ARG:HB2	1.74	0.68
24:CX:133:SER:O	84:CX:202:OHX:N5	2.26	0.68
1:AR:354:U:OP1	84:DL:101:OHX:N2	2.27	0.68
1:1:2946:A:H5''	1:1:2947:G:H5'	1.75	0.68
1:1:2925:C:O2	84:1:3554:OHX:N1	2.26	0.68
48:A:384:G:O6	84:A:2008:OHX:N6	2.27	0.68
1:AR:2687:G:N7	84:AR:3421:OHX:N1	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CE:152:LYS:HG2	5:CE:192:VAL:HG11	1.74	0.68
84:1:3404:OHX:N4	61:N:29:LYS:O	188.12	0.68
1:1:3143:C:O2'	84:1:3436:OHX:N2	2.27	0.68
1:1:3376:A:OP2	84:1:3442:OHX:N2	2.27	0.68
48:A:62:A:OP1	84:A:1944:OHX:N4	2.26	0.68
43:AP:7:THR:HB	43:AP:22:GLN:HE21	1.57	0.68
1:AR:891:G:OP1	84:AR:3419:OHX:N2	2.26	0.68
6:CF:203:ARG:NH1	6:CF:226:GLU:OE2	2.27	0.68
58:K:109:LEU:HB2	58:K:146:PHE:HB3	1.76	0.68
65:R:38:LEU:O	65:R:45:ARG:NE	2.27	0.68
70:W:71:ARG:O	70:W:75:ASN:ND2	2.27	0.68
1:1:2356:A:H61	1:1:2983:C:H5	1.42	0.67
36:AI:101:THR:HG22	36:AI:104:GLN:H	1.59	0.67
1:AR:2744:U:OP1	84:AR:3600:OHX:N1	2.26	0.67
7:CG:34:LYS:O	7:CG:38:THR:HG23	1.95	0.67
1:1:1898:G:OP2	84:1:3466:OHX:N4	2.27	0.67
31:AD:40:LYS:HB3	31:AD:101:LEU:HD11	1.77	0.67
1:AR:1466:G:O6	84:AR:3415:OHX:N5	2.27	0.67
1:AR:739:G:O6	84:AR:3469:OHX:N6	2.28	0.67
1:AR:912:G:OP2	4:CD:9:ARG:NH1	2.28	0.67
58:K:93:LEU:HA	58:K:96:VAL:HG13	1.76	0.67
1:1:3050:U:OP2	84:1:3713:OHX:N1	2.26	0.67
1:AR:393:U:OP2	84:AR:3455:OHX:N1	2.28	0.67
9:CI:143:THR:HG22	9:CI:241:LYS:HE3	1.75	0.67
1:AR:2604:U:O4	84:AR:3406:OHX:N5	2.27	0.67
1:AR:409:A:OP2	84:AR:3608:OHX:N5	2.27	0.67
5:CE:92:TYR:HB2	5:CE:157:VAL:HG22	1.76	0.67
13:CM:168:ASP:OD1	84:CM:201:OHX:N3	2.27	0.67
67:T:100:THR:HG21	67:T:108:LYS:HG3	1.77	0.67
1:1:1485:G:N7	84:1:3511:OHX:N1	2.41	0.67
1:1:3319:U:O2'	1:1:3320:A:OP1	2.10	0.67
2:3:79:A:OP2	84:3:203:OHX:N6	2.27	0.67
1:AR:3166:C:H42	1:AR:3284:G:H1	1.43	0.67
6:CF:361:HIS:O	21:CU:28:ARG:NH2	2.27	0.67
12:CL:77:THR:HG22	12:CL:82:ARG:HA	1.75	0.67
3:4:136:G:OP1	26:8:48:SER:OG	2.11	0.67
1:AR:1365:G:OP2	84:AR:3535:OHX:N3	2.27	0.67
1:AR:155:G:H5''	1:AR:156:G:C8	2.30	0.67
1:AR:1740:U:H1'	1:AR:1741:A:H2	1.60	0.67
1:AR:2213:A:H2'	1:AR:2214:A:C8	2.30	0.67
1:AR:2239:G:N7	84:AR:3697:OHX:N5	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:CH:40:LEU:HD13	8:CH:84:VAL:HG11	1.77	0.67
10:CJ:100:GLU:OE2	10:CJ:108:ARG:NH1	2.27	0.67
64:Q:68:PRO:HB2	64:Q:71:GLU:HB3	1.77	0.67
1:1:1313:G:O6	84:1:3627:OHX:N4	2.28	0.67
84:AR:3408:OHX:N6	3:AT:16:G:O6	2.27	0.67
11:CK:21:LYS:HG3	15:CO:8:LYS:HD2	1.77	0.67
23:CW:19:VAL:HG12	23:CW:105:LEU:HD22	1.75	0.67
52:E:164:VAL:HG13	52:E:168:ILE:HD11	1.77	0.67
48:A:1559:A:H5''	67:T:135:GLY:HA3	1.77	0.67
48:A:1542:G:H22	48:A:1568:C:H1'	1.59	0.67
48:A:1738:U:O4	84:A:1919:OHX:N4	2.28	0.67
55:H:71:THR:OG1	55:H:72:ARG:N	2.28	0.67
3:4:150:G:N7	84:4:207:OHX:N4	2.43	0.67
34:AG:14:LEU:HD11	34:AG:31:LYS:HB2	1.75	0.67
1:AR:2356:A:OP1	18:CR:138:LYS:NZ	2.27	0.67
40:DN:9:ILE:HG22	40:DN:13:MET:HE2	1.75	0.67
63:P:13:VAL:HG13	63:P:77:THR:H	1.60	0.67
48:A:144:U:HO2'	48:A:145:A:H8	1.43	0.67
48:A:452:A:OP2	84:A:1916:OHX:N5	2.28	0.67
48:A:795:U:OP1	71:X:82:LYS:NZ	2.27	0.67
1:AR:3375:A:O2'	1:AR:3378:C:OP2	2.12	0.67
1:AR:773:G:O6	84:AR:3441:OHX:N5	2.28	0.67
1:1:3113:A:OP2	84:1:3563:OHX:N5	2.28	0.66
30:AC:28:LYS:HD3	30:AC:29:TYR:H	1.60	0.66
63:P:122:PRO:HB2	63:P:124:ASP:HA	1.77	0.66
1:AR:1058:U:O4	84:AR:3689:OHX:N1	2.28	0.66
1:1:1887:A:OP2	84:1:3428:OHX:N4	2.28	0.66
1:AR:1852:G:N7	84:AR:3545:OHX:N6	2.44	0.66
1:AR:718:G:C2	1:AR:721:G:H1'	2.30	0.66
15:CO:19:ARG:HA	15:CO:69:THR:HG22	1.75	0.66
68:U:37:VAL:HG11	68:U:100:ILE:HD11	1.76	0.66
71:X:86:ILE:HD12	71:X:87:GLU:HG3	1.77	0.66
48:A:42:G:N7	84:A:1918:OHX:N4	2.44	0.66
48:A:778:G:H3'	48:A:780:A:H2	1.60	0.66
1:AR:2585:G:N7	10:CJ:47:SER:OG	2.27	0.66
1:AR:2287:C:O2'	84:AR:3449:OHX:N3	2.29	0.66
1:AR:3136:G:OP2	84:AR:3612:OHX:N3	2.28	0.66
51:D:56:ILE:HG23	51:D:61:LEU:HB2	1.76	0.66
28:DB:25:ILE:HG23	28:DB:41:ALA:HB1	1.78	0.66
1:1:2561:A:HO2'	1:1:2562:A:H8	1.42	0.66
48:A:1564:U:OP1	68:U:38:LYS:NZ	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:AE:13:THR:HG22	32:AE:72:ARG:HH11	1.61	0.66
1:AR:2610:G:O6	84:AR:3678:OHX:N3	2.28	0.66
3:AT:87:G:O6	84:AT:212:OHX:N1	2.28	0.66
12:CL:191:LYS:HE2	12:CL:212:GLU:HB3	1.76	0.66
27:DA:71:SER:HB3	27:DA:83:ASP:HB2	1.76	0.66
48:A:656:G:O2'	48:A:657:U:O4'	2.13	0.66
1:AR:1141:C:OP2	84:AR:3618:OHX:N2	2.29	0.66
1:AR:3053:G:O6	84:AR:3677:OHX:N3	2.29	0.66
1:AR:870:G:N7	84:AR:3470:OHX:N5	2.43	0.66
1:AR:979:U:H1'	1:AR:980:A:C8	2.31	0.66
56:I:98:ILE:HG12	56:I:121:VAL:HG21	1.77	0.66
58:K:38:ASN:HB2	58:K:41:GLU:HG3	1.78	0.66
1:1:541:U:O4	84:1:3725:OHX:N6	2.28	0.66
48:A:867:G:N7	84:A:1910:OHX:N2	2.44	0.66
1:AR:1940:G:H21	1:AR:3362:A:H8	1.40	0.66
6:CF:226:GLU:OE2	6:CF:246:ARG:NH2	2.29	0.66
1:1:1534:A:OP1	84:1:3411:OHX:N1	2.28	0.66
1:1:2418:G:O6	84:1:3652:OHX:N4	2.29	0.66
48:A:1367:G:O6	84:A:1986:OHX:N3	2.29	0.66
50:C:61:LEU:HD23	50:C:62:LYS:H	1.61	0.66
5:CE:4:ARG:O	5:CE:5:LYS:HB3	1.96	0.66
1:AR:1696:A:OP2	84:AR:3690:OHX:N6	2.29	0.66
48:A:868:G:H1	48:A:960:U:H3	1.42	0.65
1:AR:2734:A:OP1	84:AR:3552:OHX:N6	2.28	0.65
1:AR:1345:G:N7	84:AR:3572:OHX:N5	2.44	0.65
11:CK:49:ASN:ND2	11:CK:51:GLN:H	1.93	0.65
29:DC:6:THR:HG23	29:DC:8:THR:HG23	1.78	0.65
1:1:1854:C:OP2	84:1:3570:OHX:N5	2.29	0.65
1:1:3074:G:O6	84:1:3667:OHX:N5	2.29	0.65
1:AR:1924:U:OP1	42:DP:25:LYS:NZ	2.29	0.65
12:CL:174:THR:HG23	12:CL:176:LEU:N	2.06	0.65
61:N:103:LEU:HG	61:N:116:VAL:HG22	1.76	0.65
84:1:3406:OHX:N1	38:AK:46:SER:OG	2.30	0.65
48:A:1414:U:O2'	84:A:1903:OHX:N6	2.30	0.65
1:AR:25:U:O4	84:AR:3410:OHX:N5	2.29	0.65
30:DD:14:ARG:HH22	30:DD:18:ARG:HH11	1.43	0.65
1:1:18:G:OP1	36:AI:81:ARG:NH2	2.29	0.65
1:1:2370:G:N7	84:1:3408:OHX:N4	2.45	0.65
1:1:3010:U:O4	84:1:3437:OHX:N2	2.30	0.65
1:1:300:G:O6	84:1:3683:OHX:N1	2.29	0.65
48:A:867:G:OP2	62:O:3:ARG:NH1	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:3376:A:OP2	84:AR:3437:OHX:N4	2.29	0.65
9:CI:158:LYS:HE2	9:CI:159:GLN:H	1.60	0.65
1:1:2560:C:O2	84:1:3461:OHX:N1	2.29	0.65
84:A:2038:OHX:N1	58:K:8:TYR:O	2.30	0.65
1:AR:1549:U:O4	84:AR:3706:OHX:N2	2.29	0.65
1:AR:625:G:OP1	84:AR:3640:OHX:N6	2.30	0.65
6:CF:299:ILE:HG23	19:CS:39:ARG:HB3	1.77	0.65
6:CF:60:THR:HG21	6:CF:77:VAL:HG22	1.78	0.65
28:DB:46:ILE:HD13	28:DB:68:ILE:HG23	1.79	0.65
48:A:823:G:H2'	48:A:824:G:C8	2.31	0.65
51:D:137:ILE:HG12	51:D:138:PRO:HD2	1.79	0.65
51:D:170:ILE:HB	51:D:197:TYR:HB2	1.78	0.65
35:DI:82:ALA:O	35:DI:85:VAL:N	2.30	0.65
48:A:144:U:H5	55:H:137:ARG:HH12	1.44	0.65
48:A:800:U:O4	84:A:1932:OHX:N5	2.30	0.65
1:AR:3329:U:H5''	5:CE:308:MET:HE3	1.77	0.65
18:CR:179:GLN:O	18:CR:184:ALA:N	2.29	0.65
32:DF:23:VAL:O	32:DF:28:ARG:NH1	2.28	0.65
63:P:81:VAL:HG22	63:P:115:ILE:HB	1.77	0.65
64:Q:128:HIS:O	64:Q:130:ARG:NH1	2.30	0.65
48:A:138:A:OP2	48:A:1706:C:O2'	2.14	0.65
1:AR:2534:G:H1	1:AR:2545:C:H42	1.43	0.65
1:AR:2513:U:OP2	84:AR:3468:OHX:N3	2.30	0.65
2:AS:85:G:N7	84:AS:204:OHX:N2	2.45	0.65
7:CG:58:LYS:HA	7:CG:93:THR:HB	1.78	0.65
31:DE:24:THR:HG22	31:DE:91:SER:HB3	1.78	0.65
71:X:30:SER:OG	71:X:31:SER:N	2.26	0.65
48:A:1014:G:OP1	84:A:1902:OHX:N5	2.30	0.65
48:A:1114:G:O2'	48:A:1130:G:O6	2.14	0.65
39:DM:14:LEU:HD23	39:DM:17:ARG:HD3	1.79	0.65
48:A:1769:U:OP2	84:A:2023:OHX:N4	2.30	0.64
1:AR:2822:U:OP2	84:AR:3456:OHX:N1	2.30	0.64
38:DL:21:ARG:NH2	38:DL:41:ALA:O	2.30	0.64
1:1:1674:G:OP2	84:1:3483:OHX:N2	2.30	0.64
48:A:1339:C:O2'	48:A:1340:U:OP1	2.15	0.64
48:A:734:A:H5''	48:A:735:C:OP1	1.96	0.64
1:AR:1447:G:H3'	18:CR:67:ILE:HD11	1.79	0.64
1:AR:581:U:O4	84:AR:3529:OHX:N6	2.30	0.64
5:CE:10:ARG:NH2	5:CE:263:SER:O	2.30	0.64
1:1:2112:U:H4'	1:1:2113:A:H5'	1.78	0.64
1:1:1166:G:N7	84:1:3401:OHX:N4	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:1192:C:OP2	84:AR:3598:OHX:N2	2.30	0.64
1:AR:3075:G:O6	84:AR:3611:OHX:N6	2.30	0.64
5:CE:173:GLN:HG3	5:CE:175:LYS:H	1.62	0.64
1:1:430:U:OP1	84:1:3665:OHX:N6	2.30	0.64
1:1:1407:A:O3'	33:AF:33:ARG:NH2	2.31	0.64
1:AR:1095:U:H4'	1:AR:1096:U:H5''	1.79	0.64
1:AR:1794:G:H4'	4:CD:191:LEU:HD13	1.78	0.64
1:AR:2111:G:OP1	84:AR:3445:OHX:N5	2.30	0.64
7:CG:290:ILE:HG22	12:CL:210:ILE:HD11	1.78	0.64
1:AR:300:G:N7	84:AR:3696:OHX:N1	2.46	0.64
12:CL:84:ALA:O	12:CL:140:THR:HG22	1.97	0.64
61:N:119:SER:OG	61:N:120:VAL:N	2.31	0.64
1:1:2976:A:OP1	84:1:3653:OHX:N6	2.30	0.64
27:9:71:SER:HB3	27:9:83:ASP:HB2	1.79	0.64
29:AB:6:THR:HG23	29:AB:8:THR:HG23	1.79	0.64
1:AR:917:A:OP2	84:AR:3718:OHX:N1	2.30	0.64
1:1:2535:A:H61	1:1:2544:U:H3	1.45	0.64
48:A:458:G:OP2	73:Z:105:ARG:NH2	2.31	0.64
19:CS:100:THR:HG23	19:CS:120:GLU:HB3	1.79	0.64
1:1:2108:C:H1'	1:1:3344:A:C8	2.33	0.64
1:1:567:G:O6	84:1:3539:OHX:N1	2.31	0.64
1:1:1124:U:O4	84:1:3604:OHX:N3	2.31	0.64
1:AR:770:G:N7	84:AR:3602:OHX:N6	2.45	0.64
49:B:118:PRO:HG2	49:B:141:ILE:HD13	1.80	0.64
50:C:180:THR:HG22	50:C:181:LEU:HD13	1.80	0.64
48:A:66:U:C5	55:H:173:PRO:HG3	2.33	0.64
1:1:2572:C:O2'	1:1:2573:G:O4'	2.15	0.64
43:DQ:48:SER:O	84:DQ:201:OHX:N3	2.31	0.64
52:E:178:ARG:H	52:E:178:ARG:HE	1.46	0.64
53:F:104:ASP:HB2	53:F:108:ARG:H	1.63	0.64
1:1:777:U:O4	84:1:3542:OHX:N2	2.31	0.64
1:AR:2211:U:O4	84:AR:3465:OHX:N4	2.30	0.64
1:AR:1892:G:N7	84:AR:3620:OHX:N1	2.46	0.64
50:C:154:SER:O	50:C:154:SER:OG	2.13	0.64
13:CM:81:GLU:OE2	13:CM:89:TYR:OH	2.11	0.64
51:D:218:ILE:O	51:D:221:THR:OG1	2.15	0.64
27:DA:45:ILE:HD12	27:DA:119:ILE:HG23	1.80	0.64
53:F:48:LEU:HD21	53:F:70:VAL:HG11	1.79	0.64
1:1:1365:G:OP2	84:1:3503:OHX:N3	2.30	0.63
1:1:381:U:O4	84:1:3598:OHX:N4	2.31	0.63
1:AR:1819:U:O4	84:AR:3556:OHX:N3	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CF:300:ARG:O	19:CS:39:ARG:NH1	2.30	0.63
1:1:2278:C:OP1	84:1:3493:OHX:N5	2.32	0.63
48:A:701:U:H3	48:A:737:A:H61	1.44	0.63
1:1:662:U:OP1	29:AB:8:THR:HG21	1.98	0.63
38:AK:86:ALA:O	84:AK:102:OHX:N5	2.32	0.63
1:AR:1353:U:O2'	8:CH:8:LYS:O	2.16	0.63
29:DC:112:ILE:HB	29:DC:130:VAL:HG12	1.80	0.63
48:A:780:A:H8	73:Z:8:ARG:HB3	1.62	0.63
1:1:1841:A:N3	40:AM:45:ARG:NH2	2.45	0.63
11:CK:49:ASN:ND2	11:CK:51:GLN:OE1	2.31	0.63
39:DM:44:LYS:HG2	39:DM:53:THR:HB	1.80	0.63
48:A:1473:U:O2'	54:G:103:ASN:ND2	2.32	0.63
48:A:1173:C:OP1	67:T:132:ARG:NH1	2.31	0.63
1:AR:80:G:OP2	84:AR:3464:OHX:N1	2.31	0.63
49:B:55:GLU:OE2	70:W:80:LYS:N	2.25	0.63
10:CJ:61:GLN:HA	10:CJ:64:ILE:HD12	1.80	0.63
1:1:1543:G:O6	84:1:3593:OHX:N2	2.32	0.63
1:1:718:G:C2	1:1:721:G:H1'	2.34	0.63
84:AR:3582:OHX:N2	20:CT:14:VAL:O	2.32	0.63
18:CR:25:SER:O	18:CR:29:THR:HG23	1.99	0.63
55:H:64:LYS:HZ1	55:H:81:VAL:HG22	1.63	0.63
57:J:61:GLU:HG3	57:J:62:THR:HG23	1.79	0.63
72:Y:69:ARG:NH1	72:Y:116:ASP:OD2	2.31	0.63
48:A:649:U:O2'	48:A:650:U:O5'	2.16	0.63
1:AR:2177:G:OP2	4:CD:128:ARG:NH1	2.32	0.63
5:CE:238:LEU:HB3	5:CE:242:THR:HG21	1.79	0.63
1:1:1235:U:H4'	1:1:1236:G:H5'	1.81	0.63
1:1:863:C:OP1	84:1:3418:OHX:N6	2.31	0.63
48:A:839:U:O4	84:A:1915:OHX:N4	2.32	0.63
1:AR:1854:C:OP2	84:AR:3562:OHX:N6	2.31	0.63
1:AR:364:G:OP1	6:CF:60:THR:HG23	1.98	0.63
5:CE:37:ARG:HG3	5:CE:186:GLY:HA2	1.81	0.63
6:CF:143:GLU:O	84:CF:401:OHX:N1	2.31	0.63
18:CR:25:SER:HB3	18:CR:28:ASN:HB2	1.80	0.63
51:D:67:GLN:HA	51:D:70:ASP:HB2	1.79	0.63
53:F:158:ASP:OD2	53:F:174:LYS:NZ	2.32	0.63
28:AA:46:ILE:HD13	28:AA:68:ILE:HG23	1.79	0.63
1:AR:3026:G:N7	84:AR:3443:OHX:N3	2.46	0.63
1:AR:508:U:O4	84:AR:3526:OHX:N3	2.32	0.63
1:AR:44:U:O3'	84:DQ:201:OHX:N2	2.31	0.63
50:C:63:GLY:HA2	50:C:88:VAL:HB	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CE:37:ARG:HG2	5:CE:187:SER:H	1.63	0.63
35:DI:8:ARG:HH21	35:DI:31:ARG:HD2	1.62	0.63
1:1:2211:U:O4	84:1:3580:OHX:N4	2.31	0.63
1:AR:1938:U:O4	84:AR:3453:OHX:N4	2.32	0.63
1:AR:2120:A:OP2	84:AR:3577:OHX:N4	2.32	0.63
1:AR:3112:G:N7	84:AR:3420:OHX:N6	2.46	0.63
17:CQ:15:LEU:HD21	17:CQ:125:ARG:HG3	1.79	0.63
36:DJ:101:THR:HG22	36:DJ:104:GLN:HB2	1.81	0.63
53:F:104:ASP:HB3	53:F:106:LYS:H	1.64	0.63
1:1:1238:C:N4	1:1:1245:A:OP2	2.32	0.62
48:A:134:U:OP1	48:A:136:C:N4	2.32	0.62
1:AR:2973:G:OP1	84:AR:3656:OHX:N3	2.32	0.62
1:AR:2264:U:OP2	84:AR:3459:OHX:N4	2.32	0.62
54:G:57:SER:O	54:G:59:VAL:N	2.27	0.62
65:R:32:ASN:HD21	65:R:69:VAL:H	1.46	0.62
48:A:992:A:H2	48:A:1012:U:H3	1.48	0.62
31:AD:16:LEU:HB3	31:AD:98:SER:HB2	1.81	0.62
1:AR:2617:U:O3'	12:CL:116:ARG:NH2	2.30	0.62
1:AR:2700:G:OP1	22:CV:17:ARG:HB2	1.98	0.62
26:CZ:34:LEU:HD22	26:CZ:35:PRO:HD2	1.81	0.62
1:1:595:G:H1	1:1:609:G:H5''	1.63	0.62
1:AR:2759:U:H5''	1:AR:2760:C:H5'	1.81	0.62
1:AR:402:A:OP1	40:DN:36:ARG:NH2	2.28	0.62
48:A:1232:U:H4'	59:L:2:LEU:HD21	1.82	0.62
65:R:16:ALA:HB2	65:R:72:GLY:HA3	1.80	0.62
67:T:95:GLY:O	84:T:201:OHX:N2	2.31	0.62
1:AR:1410:U:O4	84:AR:3667:OHX:N6	2.31	0.62
2:AS:17:A:OP1	7:CG:2:ALA:N	2.33	0.62
50:C:70:LEU:HA	50:C:73:LEU:HB3	1.79	0.62
24:CX:54:LEU:HD21	24:CX:119:GLY:HA3	1.80	0.62
1:AR:2767:U:O2'	43:DQ:30:ALA:O	2.14	0.62
48:A:513:U:H2'	48:A:514:G:C8	2.34	0.62
12:CL:14:ASN:O	12:CL:128:ARG:NH2	2.32	0.62
55:H:120:GLU:HG3	55:H:125:THR:HB	1.81	0.62
1:1:1786:G:H2'	1:1:1787:A:C8	2.35	0.62
48:A:1370:U:O4	84:A:1998:OHX:N1	2.33	0.62
1:AR:172:G:N7	84:AR:3583:OHX:N4	2.47	0.62
1:AR:2736:A:OP1	22:CV:92:ARG:NH1	2.32	0.62
3:AT:81:U:O2'	3:AT:82:U:OP2	2.15	0.62
65:R:71:GLY:O	65:R:77:GLN:NE2	2.31	0.62
67:T:83:ALA:HA	67:T:86:LEU:HD22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1699:A:OP1	84:1:3711:OHX:N1	2.32	0.62
1:1:1599:G:OP1	84:1:3620:OHX:N5	2.33	0.62
48:A:1065:A:OP1	84:A:1911:OHX:N3	2.32	0.62
48:A:1010:C:OP2	84:A:2009:OHX:N6	2.33	0.62
43:AP:48:SER:O	84:AP:502:OHX:N6	2.32	0.62
1:AR:1088:U:OP2	84:AR:3695:OHX:N4	2.33	0.62
50:C:40:ASN:ND2	50:C:42:ASN:O	2.32	0.62
54:G:94:THR:HG22	54:G:114:ILE:HG13	1.81	0.62
69:V:106:ILE:HG23	69:V:107:THR:HG23	1.81	0.62
69:V:42:VAL:HG13	69:V:52:LYS:HZ1	1.65	0.62
48:A:25:C:O2	84:A:1962:OHX:N4	2.32	0.62
1:AR:1845:G:O2'	38:DL:5:THR:HG22	2.00	0.62
16:CP:110:ALA:HB1	16:CP:113:LEU:HD23	1.82	0.62
48:A:1300:A:OP1	51:D:99:LYS:NZ	2.32	0.62
1:1:2310:U:OP1	84:1:3671:OHX:N1	2.33	0.62
1:1:2896:A:OP1	41:AN:102:ARG:NE	2.25	0.62
48:A:1570:A:OP1	84:A:2032:OHX:N5	2.33	0.62
1:1:1278:A:O2'	1:1:1279:C:O5'	2.18	0.62
1:AR:2369:G:OP2	84:AR:3412:OHX:N5	2.32	0.62
10:CJ:157:VAL:HG21	10:CJ:163:VAL:HG21	1.82	0.62
11:CK:49:ASN:HD21	11:CK:51:GLN:HB2	1.65	0.62
35:DI:102:LYS:HB3	35:DI:103:LYS:HE3	1.81	0.62
39:DM:46:ARG:NH1	39:DM:47:GLY:O	2.33	0.62
65:R:22:VAL:HG22	65:R:65:ILE:HD13	1.82	0.62
1:1:1352:A:H4'	1:1:1353:U:OP1	2.00	0.61
48:A:1498:G:O6	84:A:1909:OHX:N5	2.32	0.61
48:A:625:C:H2'	48:A:626:U:C6	2.36	0.61
1:AR:20:A:OP2	36:DJ:90:ARG:NH1	2.33	0.61
1:AR:3316:A:OP1	1:AR:3318:G:N2	2.33	0.61
12:CL:221:ALA:O	84:CL:301:OHX:N2	2.33	0.61
65:R:127:LYS:HA	65:R:134:ALA:HA	1.81	0.61
72:Y:79:ASN:HB3	72:Y:81:LYS:H	1.65	0.61
1:1:3195:U:O2'	1:1:3197:G:N2	2.33	0.61
1:1:541:U:O4	84:1:3725:OHX:N2	2.33	0.61
48:A:1291:G:H22	48:A:1324:G:H22	1.46	0.61
48:A:1450:U:OP2	84:A:1940:OHX:N2	2.33	0.61
1:AR:356:C:OP2	84:AR:3713:OHX:N2	2.33	0.61
49:B:10:THR:OG1	49:B:12:GLU:OE1	2.17	0.61
1:1:2273:G:O6	84:1:3417:OHX:N5	2.33	0.61
1:1:1077:U:O4	84:1:3502:OHX:N1	2.33	0.61
24:6:87:ARG:HH12	24:6:137:VAL:HG11	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:409:A:OP2	84:AR:3608:OHX:N3	2.33	0.61
1:AR:3334:U:OP2	84:AR:3738:OHX:N2	2.33	0.61
17:CQ:65:ASN:HB3	17:CQ:68:ARG:HD3	1.81	0.61
56:I:13:PRO:HB3	56:I:14:THR:HB	1.82	0.61
71:X:103:ILE:HA	71:X:112:ASP:HA	1.82	0.61
1:1:2107:A:H2	1:1:3344:A:H8	1.46	0.61
1:1:776:U:H5	1:1:2719:U:O2	1.84	0.61
12:CL:142:ASP:OD2	12:CL:178:ARG:NH2	2.33	0.61
1:1:1790:G:O6	84:1:3701:OHX:N4	2.33	0.61
26:8:115:ARG:NH1	26:8:119:THR:OG1	2.34	0.61
27:9:126:LEU:HD12	27:9:127:GLU:H	1.65	0.61
15:CO:128:ARG:HD3	15:CO:132:LYS:HD2	1.80	0.61
54:G:57:SER:C	54:G:59:VAL:H	2.03	0.61
54:G:62:VAL:HG13	54:G:89:ILE:HG12	1.82	0.61
56:I:113:PRO:HG2	56:I:116:ARG:HB2	1.80	0.61
59:L:59:PHE:CZ	59:L:62:GLN:HA	2.36	0.61
1:1:1853:U:OP2	84:1:3570:OHX:N4	2.34	0.61
1:1:619:A:H5''	1:1:620:U:OP1	2.00	0.61
39:AL:12:LEU:HB3	39:AL:16:ARG:HH12	1.65	0.61
61:N:66:VAL:HG11	61:N:71:ILE:HD12	1.81	0.61
1:1:1412:G:OP1	33:AF:105:ARG:NH2	2.34	0.61
1:AR:3128:G:OP2	84:AR:3664:OHX:N5	2.33	0.61
58:K:110:GLN:NE2	58:K:126:ARG:HG2	2.16	0.61
64:Q:126:VAL:HG13	64:Q:127:ARG:H	1.66	0.61
48:A:326:G:OP1	60:M:57:LYS:NZ	2.29	0.61
1:AR:2875:U:H3	1:AR:2952:G:H1	1.48	0.61
1:AR:2843:U:OP1	84:AR:3643:OHX:N1	2.34	0.61
60:M:94:ILE:HG12	72:Y:16:ARG:HD2	1.83	0.61
71:X:30:SER:HB2	71:X:61:ILE:HD11	1.81	0.61
1:1:1317:A:OP1	84:1:3600:OHX:N2	2.34	0.61
3:4:107:G:OP2	84:4:213:OHX:N2	2.34	0.61
35:AH:82:ALA:O	35:AH:85:VAL:N	2.33	0.61
1:AR:2809:C:O2'	84:AR:3718:OHX:N5	2.33	0.61
48:A:1145:U:O2'	51:D:89:GLN:O	2.16	0.61
29:DC:47:LYS:C	29:DC:49:HIS:H	2.03	0.61
8:CH:31:ARG:NH1	34:DH:107:ILE:O	2.34	0.61
57:J:147:ALA:HA	57:J:150:ALA:HB2	1.83	0.61
61:N:61:VAL:HG13	61:N:121:VAL:HG23	1.83	0.61
65:R:73:GLY:H	65:R:76:SER:HB3	1.66	0.61
48:A:478:A:O2'	58:K:124:HIS:ND1	2.25	0.61
40:AM:9:ILE:HG22	40:AM:13:MET:HE2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:AO:22:ALA:HA	42:AO:25:LYS:HG3	1.81	0.61
1:AR:2268:U:H3'	1:AR:2269:U:H5''	1.81	0.61
1:AR:2970:C:HO2'	1:AR:2971:A:H2	1.48	0.61
1:AR:3074:G:OP1	84:AR:3624:OHX:N4	2.34	0.61
1:AR:3157:U:H4'	1:AR:3158:G:H5'	1.83	0.61
84:AR:3612:OHX:N4	5:CE:30:LYS:O	2.34	0.61
18:CR:108:ASP:N	18:CR:152:GLU:OE2	2.23	0.61
1:1:1596:C:H2'	1:1:1597:C:C6	2.35	0.60
1:1:3082:C:OP2	84:1:3471:OHX:N2	2.34	0.60
1:1:1877:U:OP2	84:1:3462:OHX:N2	2.34	0.60
48:A:320:U:H3'	48:A:321:C:H5''	1.81	0.60
1:AR:1733:G:OP2	84:AR:3472:OHX:N6	2.34	0.60
62:O:132:VAL:HG23	62:O:134:VAL:HG13	1.83	0.60
1:1:1798:A:H2'	1:1:1799:A:C8	2.36	0.60
1:AR:994:G:O6	84:AR:3663:OHX:N1	2.34	0.60
50:C:109:LYS:HG3	50:C:113:MET:HE3	1.82	0.60
22:CV:103:GLN:HE21	22:CV:104:GLU:N	1.98	0.60
56:I:86:GLN:HG2	56:I:87:ASP:H	1.66	0.60
68:U:57:ARG:HH21	68:U:80:TYR:HB3	1.65	0.60
48:A:761:G:OP1	58:K:54:ARG:NH1	2.34	0.60
1:AR:421:G:OP1	84:AR:3524:OHX:N2	2.34	0.60
20:CT:21:LYS:O	20:CT:53:LYS:HB2	2.02	0.60
44:AQ:84:ARG:NH1	44:AQ:88:GLU:OE1	2.35	0.60
1:AR:3122:A:N1	11:CK:70:THR:HG21	2.17	0.60
1:AR:508:U:O4	84:AR:3721:OHX:N1	2.34	0.60
28:DB:27:LYS:HB3	28:DB:42:LEU:HB2	1.84	0.60
1:1:59:G:H2'	3:4:33:A:O2'	2.01	0.60
1:AR:2299:A:OP2	84:AR:3463:OHX:N1	2.35	0.60
1:AR:2310:U:O4	84:AR:3488:OHX:N5	2.34	0.60
14:CN:123:ILE:HG22	36:DJ:118:ILE:HG12	1.84	0.60
35:DI:58:ARG:HG3	35:DI:59:PRO:HD2	1.84	0.60
1:1:1833:G:OP1	40:AM:10:LYS:NZ	2.30	0.60
1:1:2997:G:N7	84:1:3690:OHX:N5	2.50	0.60
1:1:3348:G:H1	1:1:3357:U:H3	1.48	0.60
1:1:1222:G:O6	84:1:3648:OHX:N2	2.34	0.60
1:1:2840:C:OP1	84:1:3675:OHX:N6	2.34	0.60
48:A:1564:U:H2'	48:A:1565:C:C6	2.36	0.60
48:A:480:G:H22	48:A:509:G:H1'	1.65	0.60
1:AR:1235:U:H4'	1:AR:1236:G:H5'	1.83	0.60
1:AR:2308:C:O2	84:AR:3744:OHX:N4	2.34	0.60
1:AR:1580:A:H5'	1:AR:2522:G:N7	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:2998:U:O4	84:AR:3647:OHX:N4	2.34	0.60
1:AR:3316:A:O2'	1:AR:3317:U:OP2	2.17	0.60
1:AR:2965:U:O2	4:CD:221:LYS:NZ	2.33	0.60
1:1:2513:U:OP2	84:1:3444:OHX:N3	2.34	0.60
1:1:408:A:OP1	84:1:3592:OHX:N3	2.35	0.60
1:1:1409:G:N7	84:1:3603:OHX:N3	2.50	0.60
1:AR:2656:A:O2'	84:AR:3411:OHX:N1	2.34	0.60
1:AR:830:A:OP1	84:AR:3568:OHX:N2	2.35	0.60
49:B:179:ARG:HD3	49:B:183:ARG:HH11	1.67	0.60
19:CS:30:VAL:O	19:CS:34:THR:HG23	2.01	0.60
65:R:123:ARG:HG3	65:R:124:PRO:HD2	1.82	0.60
1:1:353:G:N7	38:AK:55:ARG:HD3	2.16	0.60
84:AR:3445:OHX:N1	84:AR:3738:OHX:N4	2.50	0.60
12:CL:149:VAL:HG13	12:CL:165:ILE:HG13	1.84	0.60
1:AR:1065:A:N1	30:DD:26:THR:OG1	2.35	0.60
48:A:68:A:H5'	55:H:160:ARG:HH12	1.67	0.60
67:T:139:LYS:O	67:T:143:ARG:NH1	2.35	0.60
1:1:391:A:OP2	84:1:3679:OHX:N1	2.35	0.60
48:A:104:A:OP2	48:A:308:C:N4	2.35	0.60
48:A:1173:C:H3'	67:T:141:THR:HG21	1.84	0.60
48:A:1588:G:H1	48:A:1608:U:H3	1.49	0.60
48:A:453:U:O4	84:A:1916:OHX:N5	2.35	0.60
1:AR:2767:U:O4	84:AR:3623:OHX:N3	2.34	0.60
84:AR:3445:OHX:N2	84:AR:3738:OHX:N4	2.50	0.60
3:AT:137:C:OP2	84:AT:217:OHX:N4	2.34	0.60
3:AT:63:G:O2'	36:DJ:49:LYS:NZ	2.35	0.60
5:CE:167:ARG:O	84:CE:401:OHX:N5	2.34	0.60
15:CO:50:LYS:HD3	15:CO:85:TRP:CD1	2.37	0.60
37:DK:33:ALA:HB1	37:DK:38:LYS:HE3	1.84	0.60
52:E:105:MET:HG2	52:E:122:VAL:HG21	1.84	0.60
53:F:139:VAL:HG13	53:F:150:PRO:HG3	1.84	0.60
1:1:2762:A:OP2	84:1:3469:OHX:N4	2.35	0.60
48:A:108:A:H2'	48:A:109:G:C8	2.37	0.60
1:AR:2193:U:H5'	1:AR:2194:G:H5'	1.83	0.60
1:AR:3284:G:OP1	84:AR:3687:OHX:N3	2.35	0.60
1:AR:911:C:H42	4:CD:3:ARG:HD3	1.67	0.60
1:AR:103:G:OP1	14:CN:70:ARG:NH2	2.35	0.60
19:CS:158:HIS:H	19:CS:186:VAL:HG12	1.67	0.60
49:B:52:LYS:HD2	70:W:82:VAL:HA	1.84	0.60
48:A:1435:G:N7	59:L:25:LYS:NZ	2.48	0.59
48:A:145:A:O2'	48:A:146:U:O5'	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:AH:44:CYS:SG	35:AH:81:CYS:HB3	2.41	0.59
1:AR:3090:U:OP1	5:CE:270:ARG:NH2	2.27	0.59
19:CS:170:ARG:O	19:CS:171:LYS:HB2	2.02	0.59
55:H:33:GLY:HA2	55:H:51:LYS:HE2	1.84	0.59
1:1:3192:U:O4	84:1:3661:OHX:N1	2.36	0.59
1:AR:18:G:OP1	36:DJ:81:ARG:NH2	2.34	0.59
5:CE:296:THR:HG22	5:CE:298:PHE:N	2.16	0.59
13:CM:139:THR:HG22	13:CM:147:THR:HA	1.84	0.59
48:A:1615:C:O2'	48:A:1616:G:OP2	2.20	0.59
48:A:1653:C:OP2	84:A:1964:OHX:N4	2.35	0.59
48:A:647:G:N2	48:A:687:G:H22	2.01	0.59
44:AQ:56:THR:HG22	44:AQ:63:THR:HG23	1.83	0.59
1:AR:2818:U:C6	1:AR:2818:U:H5'	2.34	0.59
1:AR:2897:A:H2'	1:AR:2899:C:H5''	1.84	0.59
1:AR:2908:G:OP1	84:AR:3446:OHX:N1	2.35	0.59
1:AR:2705:A:OP2	84:AR:3401:OHX:N4	2.35	0.59
4:CD:79:ASN:ND2	4:CD:166:ILE:O	2.31	0.59
7:CG:143:LYS:HG3	7:CG:172:TYR:HD2	1.66	0.59
37:DK:74:LYS:HD2	37:DK:80:PHE:HD1	1.67	0.59
48:A:325:G:H4'	60:M:83:THR:HG21	1.83	0.59
63:P:19:ILE:HB	63:P:83:ILE:HD12	1.84	0.59
1:1:2255:A:H5'	1:1:2261:G:H22	1.68	0.59
84:1:3594:OHX:N3	2:3:87:G:OP2	2.35	0.59
1:AR:3056:U:OP2	84:AR:3444:OHX:N2	2.35	0.59
1:AR:361:A:O3'	38:DL:45:ARG:NH2	2.35	0.59
48:A:131:C:OP1	84:A:1951:OHX:N4	2.36	0.59
48:A:469:C:O2	84:A:1962:OHX:N5	2.36	0.59
1:AR:715:A:H8	29:DC:115:LYS:HG2	1.66	0.59
40:DN:23:LEU:HD22	40:DN:24:PRO:HD2	1.85	0.59
3:4:77:A:OP2	84:4:206:OHX:N2	2.35	0.59
48:A:1600:A:O2'	48:A:1602:C:N4	2.35	0.59
48:A:927:C:H1'	63:P:125:SER:HB2	1.85	0.59
1:AR:3239:G:N7	84:AR:3492:OHX:N5	2.49	0.59
3:AT:135:G:OP2	26:CZ:56:ARG:NH2	2.35	0.59
50:C:103:MET:HB3	50:C:215:VAL:HG13	1.85	0.59
73:Z:5:VAL:O	73:Z:6:THR:OG1	2.17	0.59
1:AR:1580:A:H4'	1:AR:1581:C:H5'	1.85	0.59
1:AR:3344:A:H2	1:AR:3361:G:H21	1.49	0.59
3:AT:77:A:OP2	84:AT:206:OHX:N1	2.36	0.59
5:CE:173:GLN:O	5:CE:174:LYS:HB2	2.01	0.59
5:CE:188:ILE:HD12	5:CE:189:SER:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:CL:43:VAL:HG21	12:CL:197:VAL:HB	1.83	0.59
20:CT:175:GLN:HA	20:CT:178:ALA:HB3	1.85	0.59
1:1:1724:U:H1'	1:1:1725:C:C6	2.37	0.59
38:AK:65:ARG:HG3	38:AK:65:ARG:HH11	1.68	0.59
1:AR:1808:G:O6	84:AR:3530:OHX:N4	2.36	0.59
1:AR:2284:C:O2	84:AR:3684:OHX:N1	2.36	0.59
6:CF:354:VAL:O	6:CF:358:THR:HG23	2.02	0.59
54:G:42:LEU:HB2	54:G:46:TRP:O	2.02	0.59
55:H:114:VAL:HG12	55:H:115:LYS:HD3	1.83	0.59
71:X:105:THR:HG23	71:X:110:ILE:HG12	1.84	0.59
48:A:1207:C:H42	48:A:1456:C:H5	1.49	0.59
48:A:301:A:OP2	84:A:1942:OHX:N2	2.35	0.59
48:A:591:A:H2'	48:A:592:A:C8	2.37	0.59
1:AR:2982:A:OP1	84:AR:3733:OHX:N3	2.36	0.59
1:AR:705:A:H62	29:DC:74:ASN:HD21	1.50	0.59
84:AR:3495:OHX:N4	3:AT:112:U:O2	2.36	0.59
7:CG:131:LEU:H	7:CG:131:LEU:HD22	1.68	0.59
9:CI:178:ILE:HA	9:CI:183:ASP:HB3	1.84	0.59
16:CP:149:ASN:OD1	84:CP:501:OHX:N1	2.36	0.59
1:1:2676:A:H4'	1:1:2677:G:O5'	2.03	0.59
48:A:1592:A:H2'	48:A:1593:A:C8	2.38	0.59
48:A:68:A:O2'	48:A:69:G:OP2	2.19	0.59
29:AB:80:THR:HG22	29:AB:81:LEU:HD23	1.84	0.59
30:AC:17:HIS:O	84:AC:101:OHX:N6	2.36	0.59
40:AM:23:LEU:HD22	40:AM:24:PRO:HD2	1.83	0.59
84:AR:3445:OHX:N1	84:AR:3738:OHX:N3	2.50	0.59
19:CS:170:ARG:HA	19:CS:174:ARG:HD2	1.85	0.59
27:DA:45:ILE:HD11	27:DA:122:LYS:HB2	1.84	0.59
34:DH:14:LEU:HD11	34:DH:31:LYS:HB2	1.84	0.59
65:R:42:GLU:HA	65:R:45:ARG:HB2	1.83	0.59
68:U:49:ASP:HB3	68:U:53:TRP:HB3	1.85	0.59
1:1:2177:G:O6	84:1:3459:OHX:N2	2.36	0.58
1:1:1170:A:OP2	84:1:3494:OHX:N5	2.36	0.58
48:A:1101:G:H5''	71:X:76:SER:HB3	1.85	0.58
31:AD:26:GLY:O	31:AD:30:THR:HG23	2.03	0.58
1:AR:2294:U:OP2	24:CX:71:LYS:NZ	2.35	0.58
1:1:155:G:H5''	1:1:156:G:C8	2.38	0.58
1:1:1688:U:H2'	1:1:1689:U:C6	2.37	0.58
1:AR:1298:C:OP2	84:AR:3519:OHX:N2	2.36	0.58
84:AR:3445:OHX:N2	84:AR:3738:OHX:N6	2.51	0.58
7:CG:279:LYS:HE3	7:CG:282:ARG:HH12	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DI:46:ASP:OD1	35:DI:80:ARG:NH1	2.34	0.58
52:E:46:THR:HB	52:E:84:ILE:HG12	1.85	0.58
65:R:79:TYR:HA	65:R:82:ARG:HD3	1.86	0.58
1:1:1942:U:HO2'	1:1:3345:G:HO2'	1.50	0.58
14:CN:24:VAL:HG12	16:CP:199:LEU:HB2	1.85	0.58
28:DB:83:THR:HG23	28:DB:85:TYR:H	1.68	0.58
48:A:1529:C:OP1	54:G:112:ARG:NH1	2.36	0.58
1:1:1636:U:H5''	28:AA:73:LYS:NZ	2.17	0.58
1:1:2107:A:H2	1:1:3344:A:C8	2.21	0.58
1:1:2751:G:N7	84:1:3642:OHX:N6	2.50	0.58
1:1:595:G:N1	1:1:609:G:H5''	2.18	0.58
48:A:1745:G:O6	84:A:1964:OHX:N2	2.36	0.58
1:AR:2999:U:O4	84:AR:3647:OHX:N4	2.36	0.58
1:AR:3268:A:OP1	8:CH:46:ARG:NH2	2.36	0.58
1:AR:495:G:H2'	1:AR:496:C:O4'	2.03	0.58
1:AR:900:G:H1'	1:AR:1589:A:N6	2.18	0.58
1:AR:412:G:OP1	18:CR:62:ARG:NH1	2.37	0.58
1:1:1245:A:H3'	1:1:1246:G:H5''	1.84	0.58
1:1:2818:U:C6	1:1:2818:U:H5'	2.34	0.58
1:1:2960:C:H2'	1:1:2961:G:H8	1.69	0.58
48:A:329:G:N7	84:A:1984:OHX:N6	2.51	0.58
1:AR:1110:U:H2'	1:AR:1111:U:C6	2.37	0.58
1:AR:541:U:O4	84:AR:3518:OHX:N4	2.36	0.58
41:DO:99:CYS:HB2	41:DO:114:LYS:HD3	1.84	0.58
56:I:73:VAL:O	56:I:75:THR:N	2.34	0.58
57:J:36:THR:HB	57:J:57:ALA:O	2.03	0.58
63:P:30:VAL:HG13	63:P:39:ILE:HG13	1.85	0.58
1:1:1145:G:OP1	33:AF:44:ARG:NH1	2.36	0.58
48:A:687:G:H5'	71:X:119:LYS:HD2	1.85	0.58
31:AD:74:ASN:OD1	31:AD:74:ASN:N	2.35	0.58
1:AR:1171:G:O6	84:AR:3507:OHX:N1	2.37	0.58
1:AR:1249:G:H2'	1:AR:1250:G:H8	1.69	0.58
1:AR:299:G:N7	84:AR:3694:OHX:N1	2.50	0.58
17:CQ:79:ILE:HG21	17:CQ:138:LEU:HD11	1.85	0.58
4:CD:96:LEU:O	44:DR:87:ARG:HD3	2.02	0.58
57:J:120:THR:O	84:J:301:OHX:N5	2.36	0.58
63:P:85:ALA:N	63:P:119:THR:HG22	2.12	0.58
69:V:20:ILE:HD13	69:V:22:ILE:HD13	1.84	0.58
1:1:1108:U:H2'	1:1:1109:U:C6	2.39	0.58
1:1:1580:A:H5'	1:1:2522:G:C5	2.38	0.58
1:1:2247:G:OP1	84:1:3601:OHX:N6	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:6:13:ILE:HG12	24:6:53:SER:HB2	1.86	0.58
48:A:513:U:OP1	58:K:133:HIS:NE2	2.34	0.58
48:A:900:A:OP1	63:P:43:THR:OG1	2.21	0.58
1:AR:3350:C:H2'	1:AR:3351:U:H2'	1.86	0.58
84:AR:3445:OHX:N5	84:AR:3738:OHX:N6	2.51	0.58
49:B:124:THR:HG22	49:B:174:TRP:HE1	1.68	0.58
1:AR:2146:C:OP1	4:CD:200:ARG:NH1	2.36	0.58
4:CD:45:VAL:HG22	4:CD:84:THR:HA	1.84	0.58
2:AS:44:C:OP2	13:CM:137:ARG:NH2	2.36	0.58
42:DP:8:LYS:HD3	42:DP:12:ARG:NH2	2.18	0.58
55:H:163:THR:HG22	55:H:168:THR:HG22	1.86	0.58
57:J:121:LEU:H	57:J:121:LEU:HD22	1.68	0.58
1:1:1108:U:H2'	1:1:1109:U:H6	1.68	0.58
1:1:1595:U:OP2	35:AH:36:LYS:NZ	2.26	0.58
1:1:2429:G:OP2	84:1:3522:OHX:N6	2.37	0.58
1:1:410:U:O4	84:1:3592:OHX:N5	2.36	0.58
1:AR:2605:G:N7	84:AR:3521:OHX:N1	2.51	0.58
1:AR:1196:C:O2	84:AR:3504:OHX:N1	2.36	0.58
1:AR:2355:G:H4'	18:CR:139:TYR:CE1	2.38	0.58
31:DE:99:ASP:OD1	31:DE:99:ASP:N	2.34	0.58
39:DM:24:THR:HG23	39:DM:44:LYS:HB2	1.85	0.58
65:R:82:ARG:HH12	65:R:114:ARG:HB3	1.68	0.58
73:Z:3:ASP:O	73:Z:5:VAL:N	2.36	0.58
1:1:900:G:H1'	1:1:1589:A:N6	2.18	0.58
33:AF:81:ASP:O	33:AF:84:THR:HG23	2.03	0.58
49:B:70:PRO:HB2	49:B:94:GLY:HA3	1.86	0.58
24:CX:87:ARG:HB2	24:CX:89:ASP:OD1	2.04	0.58
1:1:2924:U:O2'	84:1:3666:OHX:N2	2.37	0.58
48:A:1017:U:H2'	48:A:1018:U:C6	2.39	0.58
1:AR:1064:A:H4'	1:AR:1065:A:O5'	2.04	0.58
1:AR:2169:G:O6	84:AR:3457:OHX:N2	2.37	0.58
1:AR:2429:G:OP2	84:AR:3551:OHX:N5	2.37	0.58
49:B:164:ASN:OD1	49:B:165:ARG:NH1	2.37	0.58
33:DG:40:SER:O	33:DG:44:ARG:HG3	2.03	0.58
33:DG:89:THR:HG22	33:DG:117:ILE:HG12	1.85	0.58
1:1:2278:C:OP1	84:1:3493:OHX:N3	2.37	0.57
48:A:1557:U:OP2	48:A:1559:A:O2'	2.16	0.57
34:AG:59:VAL:HG23	34:AG:60:ARG:H	1.69	0.57
1:AR:1915:A:H2'	1:AR:1916:U:C6	2.38	0.57
1:AR:275:U:O4	84:AR:3571:OHX:N5	2.37	0.57
4:CD:206:PRO:HD3	4:CD:213:GLY:HA3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:1114:U:H5''	29:DC:22:ILE:HD12	1.87	0.57
48:A:579:A:H2	52:E:143:ARG:HG3	1.68	0.57
28:AA:53:VAL:HA	28:AA:57:HIS:HD2	1.69	0.57
32:AE:82:GLU:O	32:AE:84:ASP:N	2.37	0.57
44:AQ:83:ILE:HG23	57:J:96:LEU:HD22	103.35	0.57
4:CD:62:VAL:HA	4:CD:73:GLU:HA	1.87	0.57
14:CN:56:PRO:HG3	14:CN:74:GLY:O	2.04	0.57
21:CU:155:ARG:HD3	21:CU:172:TYR:CG	2.39	0.57
24:CX:10:LYS:NZ	24:CX:56:ASP:OD1	2.34	0.57
48:A:1555:A:OP2	64:Q:47:ARG:NH2	2.37	0.57
73:Z:21:LYS:HE3	73:Z:55:VAL:HA	11.86	0.57
1:1:1542:G:N7	84:1:3556:OHX:N6	2.51	0.57
1:1:2635:A:H2	22:2:10:ARG:HH21	1.51	0.57
1:1:3060:C:OP1	84:1:3575:OHX:N4	2.37	0.57
1:1:728:G:OP1	84:1:3639:OHX:N5	2.37	0.57
28:AA:50:PRO:HD3	28:AA:68:ILE:HG12	1.85	0.57
1:AR:3317:U:H4'	1:AR:3318:G:O5'	2.05	0.57
1:AR:2386:A:OP1	84:AR:3524:OHX:N1	2.37	0.57
50:C:88:VAL:HG11	50:C:96:LEU:HD12	1.87	0.57
1:AR:73:C:N3	14:CN:59:ARG:NH1	2.52	0.57
1:AR:1916:U:O3'	20:CT:85:ARG:NH2	2.37	0.57
66:S:71:PHE:HD1	66:S:73:LEU:HB3	1.69	0.57
1:1:439:C:H5'	1:1:440:A:C8	2.40	0.57
1:1:655:C:H2'	1:1:656:A:C8	2.40	0.57
48:A:1239:U:O4	84:A:1925:OHX:N4	2.37	0.57
48:A:1533:C:H4'	48:A:1539:G:N1	2.20	0.57
48:A:118:U:OP1	84:A:2012:OHX:N3	2.37	0.57
2:AS:110:G:OP2	7:CG:279:LYS:NZ	2.34	0.57
51:D:77:GLN:NE2	51:D:106:ASP:O	2.38	0.57
67:T:130:GLY:O	67:T:145:ARG:NH1	2.38	0.57
1:1:1159:A:O2'	1:1:1160:C:H5''	2.03	0.57
1:1:2314:U:O2'	1:1:2315:G:OP1	2.22	0.57
1:1:318:A:OP1	84:1:3446:OHX:N2	2.37	0.57
1:1:3259:U:H6	1:1:3259:U:H5'	1.68	0.57
27:9:45:ILE:HD11	27:9:122:LYS:HB2	1.85	0.57
48:A:1562:G:OP1	68:U:89:ARG:NH2	2.38	0.57
32:AE:77:ARG:HD2	32:AE:89:LEU:HD23	1.86	0.57
1:AR:566:G:O6	84:AR:3636:OHX:N2	2.38	0.57
5:CE:227:GLU:HG2	5:CE:270:ARG:HD3	1.86	0.57
5:CE:25:ILE:H	5:CE:25:ILE:HD13	1.70	0.57
51:D:116:LYS:HG2	51:D:127:ALA:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:CS:170:ARG:HH11	29:DC:57:GLY:H	1.52	0.57
56:I:131:PHE:O	56:I:133:THR:N	2.37	0.57
1:1:2573:G:O6	84:1:3534:OHX:N3	2.37	0.57
48:A:835:U:OP1	84:A:2019:OHX:N6	2.37	0.57
1:AR:291:C:H5''	16:CP:68:ARG:HH12	1.69	0.57
1:AR:3159:C:H2'	1:AR:3160:U:C6	2.39	0.57
51:D:144:TRP:CE2	51:D:173:PRO:HG3	2.40	0.57
52:E:127:MET:HE1	52:E:155:GLY:HA3	1.86	0.57
66:S:25:THR:HB	66:S:27:ASP:H	1.68	0.57
1:1:1369:A:OP1	29:AB:21:ARG:NH1	2.38	0.57
48:A:491:C:H42	48:A:496:G:H1	1.53	0.57
1:AR:1409:G:OP1	84:AR:3533:OHX:N5	2.38	0.57
2:AS:91:G:H2'	2:AS:92:A:C8	2.39	0.57
16:CP:96:ARG:HG2	16:CP:96:ARG:HH11	1.69	0.57
24:6:15:LEU:HD23	24:6:53:SER:HB3	1.85	0.57
25:7:9:SER:HA	25:7:52:THR:HG22	1.86	0.57
48:A:142:G:N2	48:A:173:A:H2	2.03	0.57
28:AA:53:VAL:HG21	28:AA:62:VAL:HG13	1.86	0.57
39:AL:8:ILE:H	39:AL:8:ILE:HD12	1.70	0.57
1:AR:1441:G:OP1	84:AT:216:OHX:N5	2.37	0.57
1:AR:2770:G:O6	84:AR:3661:OHX:N2	2.38	0.57
6:CF:145:ILE:O	84:CF:401:OHX:N3	2.37	0.57
24:CX:120:LYS:H	24:CX:137:VAL:HG23	1.70	0.57
64:Q:81:ARG:NH1	64:Q:97:TYR:O	2.34	0.57
1:1:1564:U:H2'	1:1:1565:G:C8	2.40	0.57
48:A:1280:C:H2'	48:A:1281:G:H8	1.69	0.57
48:A:1362:U:O2'	48:A:1363:U:O2	2.23	0.57
48:A:480:G:N2	48:A:509:G:H1'	2.20	0.57
48:A:607:G:H5'	48:A:613:G:N2	2.20	0.57
50:C:77:GLU:OE1	63:P:114:ARG:NH2	2.29	0.57
12:CL:68:ALA:HB2	12:CL:158:LYS:HB2	1.86	0.57
16:CP:73:ARG:NH1	16:CP:88:GLY:O	2.38	0.57
1:AR:670:C:OP1	19:CS:147:ARG:NH2	2.38	0.57
21:CU:137:ARG:HG2	21:CU:139:TYR:CZ	2.40	0.57
51:D:38:VAL:HG22	51:D:39:THR:H	1.69	0.57
52:E:208:ILE:HD12	66:S:16:LEU:HD21	1.85	0.57
53:F:200:ARG:NH2	53:F:202:ASP:OD2	2.38	0.57
48:A:868:G:OP1	62:O:121:ARG:NH1	2.37	0.57
67:T:30:TYR:HE2	67:T:40:ARG:HH11	1.52	0.57
48:A:1711:C:H2'	48:A:1712:A:H5''	1.87	0.57
48:A:753:A:H5'	53:F:221:ARG:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1926:C:H3'	44:AQ:7:LYS:HG3	1.87	0.57
1:AR:2356:A:H61	1:AR:2983:C:H5	1.51	0.57
7:CG:258:LYS:O	7:CG:259:LYS:HB3	2.04	0.57
28:DB:23:VAL:HG12	28:DB:45:GLY:HA3	1.86	0.57
53:F:88:ASP:OD1	53:F:122:LYS:NZ	2.38	0.57
48:A:116:U:H2'	48:A:117:U:C6	2.40	0.56
3:4:52:A:H62	40:AM:27:ILE:HD13	1.70	0.56
1:AR:392:G:O6	84:AR:3573:OHX:N3	2.38	0.56
1:AR:1485:G:O6	84:AR:3587:OHX:N1	2.38	0.56
13:CM:109:HIS:O	13:CM:112:LEU:HD23	2.05	0.56
21:0:82:ASP:OD1	21:0:87:THR:HB	2.04	0.56
1:1:994:G:N2	1:1:995:U:O4	2.35	0.56
39:AL:24:THR:HG23	39:AL:44:LYS:HB2	1.85	0.56
50:C:61:LEU:HD22	50:C:61:LEU:H	1.69	0.56
20:CT:157:GLU:O	20:CT:160:GLU:HB2	2.06	0.56
24:CX:45:ARG:HD2	24:CX:46:LEU:H	1.70	0.56
56:I:150:GLN:HB3	56:I:181:ILE:HD12	1.86	0.56
1:1:3155:U:H3'	1:1:3156:U:H4'	1.88	0.56
43:AP:50:PHE:O	84:AP:502:OHX:N2	2.38	0.56
1:AR:656:A:H2'	1:AR:657:A:C8	2.40	0.56
49:B:31:VAL:HG12	49:B:33:GLN:H	1.69	0.56
5:CE:103:THR:HG21	5:CE:147:GLU:OE2	2.05	0.56
52:E:176:LEU:HD12	52:E:176:LEU:H	1.70	0.56
1:1:2790:A:O2'	84:1:3518:OHX:N5	2.39	0.56
35:AH:99:LYS:O	35:AH:103:LYS:HG2	2.05	0.56
1:AR:860:G:O5'	4:CD:181:LYS:NZ	2.38	0.56
11:CK:8:GLN:HG2	11:CK:68:LEU:HD13	1.87	0.56
21:CU:12:ARG:HB3	21:CU:24:LEU:HD23	1.87	0.56
28:DB:97:SER:HB2	28:DB:99:GLU:HG3	1.87	0.56
36:DJ:76:GLN:O	36:DJ:81:ARG:NH1	2.38	0.56
57:J:114:GLU:HG2	57:J:120:THR:HA	1.87	0.56
64:Q:67:ALA:O	84:Q:201:OHX:N1	2.39	0.56
1:1:1064:A:H4'	1:1:1065:A:O5'	2.05	0.56
1:1:3253:G:N7	84:1:3591:OHX:N1	2.53	0.56
27:9:112:ASP:HB2	27:9:115:ARG:HB2	1.88	0.56
48:A:1542:G:N2	48:A:1568:C:H1'	2.19	0.56
48:A:523:G:O6	84:A:1931:OHX:N4	2.38	0.56
1:AR:1352:A:H4'	1:AR:1353:U:OP1	2.04	0.56
1:AR:2180:G:H2'	1:AR:2181:C:C6	2.40	0.56
1:AR:3238:G:N7	84:AR:3492:OHX:N2	2.53	0.56
18:CR:122:ALA:HB3	18:CR:143:PRO:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:1720:U:OP2	20:CT:110:ARG:NH1	2.39	0.56
22:CV:82:ASN:O	30:DD:21:ILE:HA	2.05	0.56
63:P:19:ILE:HD11	63:P:105:LEU:HD21	1.88	0.56
1:1:23:A:OP1	84:1:3406:OHX:N5	2.37	0.56
48:A:1609:U:OP 2	65:R:14:LYS:NZ	2.39	0.56
48:A:477:A:H2'	48:A:478:A:H8	1.71	0.56
48:A:855:A:C2	48:A:857:U:H1'	2.41	0.56
1:AR:3243:A:OP1	17:CQ:159:LYS:NZ	2.38	0.56
1:AR:1196:C:O2	84:AS:208:OHX:N1	2.38	0.56
5:CE:166:ILE:O	5:CE:169:THR:HG22	2.06	0.56
20:CT:23:TRP:HB3	20:CT:51:VAL:HG22	1.88	0.56
84:AR:3410:OHX:N2	38:DL:46:SER:OG	2.38	0.56
1:AR:1841:A:N3	40:DN:45:ARG:NH2	2.54	0.56
53:F:13:ALA:O	53:F:39:ARG:NH2	2.38	0.56
59:L:23:ALA:O	59:L:64:TYR:HB2	2.06	0.56
68:U:28:LEU:HD13	68:U:30:VAL:HG22	1.87	0.56
1:1:2419:A:H2'	1:1:2420:C:C6	2.41	0.56
1:1:2523:A:OP1	26:8:31:THR:OG1	2.16	0.56
1:1:3340:G:N7	84:1:3588:OHX:N2	2.53	0.56
1:1:437:G:OP 2	84:1:3719:OHX:N3	2.39	0.56
1:1:200:C:OP 1	27:9:60:ARG:NH1	2.38	0.56
48:A:422:G:N7	84:A:1985:OHX:N5	2.53	0.56
28:AA:4:PHE:CZ	31:AD:35:ARG:HA	2.41	0.56
1:AR:2535:A:H2'	1:AR:2536:A:H5'	1.88	0.56
1:AR:3348:G:H1	1:AR:3357:U:H3	1.53	0.56
10:CJ:41:GLN:HG3	10:CJ:44:ARG:HH12	1.69	0.56
57:J:36:THR:HG21	57:J:173:PRO:HB2	1.87	0.56
52:E:8:LYS:HE2	69:V:61:LYS:HD3	1.87	0.56
84:1:3425:OHX:N4	22:2:18:ASP:OD1	2.39	0.56
48:A:1290:U:H2'	48:A:1291:G:C8	2.41	0.56
48:A:1680:G:O6	84:A:1987:OHX:N5	2.39	0.56
32:AE:51:LEU:HD22	32:AE:55:LEU:HD12	1.87	0.56
32:AE:6:ASP:HB2	32:AE:77:ARG:NH2	2.21	0.56
1:AR:2659:G:H4'	1:AR:2751:G:O2'	2.06	0.56
3:AT:18:U:OP1	84:AT:209:OHX:N1	2.39	0.56
62:O:91:LEU:HB3	62:O:122:ILE:HG12	1.86	0.56
48:A:1479:A:OP 1	68:U:57:ARG:NH1	2.39	0.56
1:1:1110:U:H2'	1:1:1111:U:C6	2.41	0.56
48:A:1041:G:H2'	48:A:1042:G:C8	2.41	0.56
48:A:1672:G:O6	84:A:1922:OHX:N3	2.38	0.56
48:A:761:G:N7	84:A:1939:OHX:N1	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:880:C:OP2	84:A:1999:OHX:N1	2.38	0.56
48:A:720:G:H1'	48:A:721:U:H5''	1.88	0.56
29:AB:94:ALA:HB1	29:AB:121:VAL:HA	1.87	0.56
1:AR:742:G:N7	84:AR:3508:OHX:N4	2.54	0.56
1:1:1307:G:H1'	1:1:1308:A:C8	2.40	0.56
1:1:1940:G:H21	1:1:3362:A:H8	1.52	0.56
1:1:3085:G:OP2	84:1:3422:OHX:N2	2.38	0.56
48:A:1600:A:HO2'	48:A:1602:C:N4	2.04	0.56
48:A:782:U:H4'	48:A:783:G:OP2	2.05	0.56
32:AE:51:LEU:HD23	32:AE:93:VAL:HB	1.88	0.56
1:AR:3151:U:OP2	5:CE:132:LYS:NZ	2.34	0.56
21:CU:155:ARG:NH2	21:CU:171:PHE:O	2.37	0.56
22:CV:12:ARG:HD3	22:CV:13:TYR:CZ	2.41	0.56
61:N:30:VAL:HB	61:N:132:GLU:HG3	1.88	0.56
62:O:55:ARG:NH1	62:O:56:ASP:OD1	2.39	0.56
48:A:1041:G:OP1	84:A:2027:OHX:N5	2.38	0.56
48:A:487:G:H3'	48:A:488:G:H5''	1.88	0.56
1:AR:1331:U:OP2	84:AR:3402:OHX:N4	2.39	0.56
50:C:183:GLN:HG2	50:C:187:LYS:HE3	1.87	0.56
5:CE:188:ILE:O	5:CE:192:VAL:HG12	2.05	0.56
6:CF:145:ILE:O	84:CF:401:OHX:N4	2.38	0.56
1:AR:3206:C:O2	21:CU:155:ARG:NH1	2.39	0.56
28:DB:41:ALA:HB2	28:DB:77:TYR:HE1	1.70	0.56
62:O:34:ILE:HG13	62:O:67:THR:HG21	1.87	0.56
71:X:70:ASN:ND2	71:X:130:TYR:O	2.35	0.56
73:Z:62:THR:HA	73:Z:69:SER:HA	1.86	0.56
1:1:3121:U:H1'	1:1:3122:A:H5''	1.88	0.55
1:1:2579:G:O6	84:1:3461:OHX:N6	2.39	0.55
27:9:47:ALA:O	27:9:122:LYS:NZ	2.39	0.55
48:A:1600:A:H4'	48:A:1601:G:OP1	2.05	0.55
29:AB:46:ASP:N	29:AB:46:ASP:OD1	2.38	0.55
1:AR:1863:G:N1	1:AR:1866:C:OP2	2.38	0.55
1:AR:94:G:H2'	1:AR:95:A:C8	2.41	0.55
50:C:48:VAL:HG13	50:C:61:LEU:HD21	1.88	0.55
7:CG:205:SER:HB3	7:CG:236:LEU:HD22	1.88	0.55
48:A:1228:G:H1	61:N:67:THR:HB	1.71	0.55
48:A:337:G:H3'	60:M:133:LYS:HB2	1.86	0.55
1:AR:3047:U:O2'	1:AR:3048:A:H5'	2.07	0.55
1:AR:3102:G:N7	84:AR:3416:OHX:N6	2.54	0.55
1:AR:1443:G:N7	84:AR:3514:OHX:N2	2.54	0.55
11:CK:120:ASP:OD2	11:CK:124:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:CX:38:ALA:HB3	24:CX:59:MET:HB2	1.89	0.55
29:DC:46:ASP:O	29:DC:47:LYS:HG2	2.06	0.55
57:J:8:ARG:HD3	57:J:21:PHE:HB3	1.86	0.55
60:M:125:VAL:HG12	60:M:139:VAL:HA	1.87	0.55
61:N:76:GLU:HG3	61:N:88:LEU:HD21	1.87	0.55
67:T:14:ILE:O	67:T:14:ILE:HG13	2.07	0.55
1:1:1014:U:H2'	1:1:1015:U:H5''	1.88	0.55
1:1:1495:U:H5	1:1:1835:A:N1	2.05	0.55
1:1:2960:C:H2'	1:1:2961:G:C8	2.41	0.55
1:1:3275:U:H5'	34:AG:68:TRP:HZ2	1.71	0.55
48:A:778:G:H22	73:Z:10:ARG:CZ	2.19	0.55
35:AH:41:ARG:HG2	35:AH:56:THR:HG21	1.88	0.55
1:AR:1243:G:N2	1:AR:1270:A:O2'	2.21	0.55
1:AR:1541:G:OP2	84:AR:3599:OHX:N3	2.39	0.55
1:AR:2752:U:O2	84:AR:3736:OHX:N3	2.40	0.55
1:AR:595:G:N1	1:AR:609:G:H5''	2.22	0.55
3:AT:90:U:O2	84:AT:207:OHX:N2	2.39	0.55
1:AR:911:C:N4	4:CD:3:ARG:HD3	2.21	0.55
8:CH:11:PRO:HD2	33:DG:91:THR:HG21	1.89	0.55
43:DQ:15:LYS:HG2	43:DQ:18:ARG:HH11	1.71	0.55
1:1:518:G:O6	84:1:3644:OHX:N6	2.39	0.55
48:A:1488:G:H3'	48:A:1515:A:H61	1.70	0.55
1:AR:1114:U:OP2	84:AR:3513:OHX:N5	2.40	0.55
1:AR:687:U:OP2	14:CN:36:ARG:NH2	2.39	0.55
26:CZ:49:LYS:HD2	26:CZ:52:PRO:HA	1.87	0.55
42:DP:16:LYS:O	42:DP:20:VAL:HG23	2.05	0.55
48:A:579:A:C2	52:E:143:ARG:HG3	2.41	0.55
53:F:122:LYS:HD2	53:F:164:LEU:HD21	1.88	0.55
48:A:1011:G:OP2	84:A:1968:OHX:N5	2.39	0.55
48:A:1437:U:H5'	52:E:176:LEU:HD23	1.89	0.55
48:A:1628:U:H2'	48:A:1629:G:C8	2.42	0.55
28:AA:22:LYS:NZ	28:AA:132:SER:O	2.29	0.55
48:A:885:G:OP1	50:C:136:ARG:NH1	2.40	0.55
37:AJ:58:ILE:HG22	37:AJ:90:MET:HG3	1.87	0.55
1:AR:3155:U:O2	84:AR:3730:OHX:N6	2.39	0.55
49:B:41:ARG:HD2	49:B:42:PRO:O	2.07	0.55
1:1:3174:A:OP1	34:AG:97:SER:OG	2.19	0.55
48:A:976:G:O6	84:A:1928:OHX:N3	2.40	0.55
1:AR:1317:A:OP1	84:AR:3603:OHX:N4	2.39	0.55
1:AR:3215:A:O5'	15:CO:121:MET:HE1	2.06	0.55
1:AR:3353:G:OP2	84:AR:3734:OHX:N5	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:964:G:OP1	84:AR:3513:OHX:N1	2.40	0.55
15:CO:48:GLY:HA3	15:CO:53:VAL:HG13	1.88	0.55
1:AR:1507:G:C8	18:CR:129:THR:HG22	2.42	0.55
37:DK:25:LYS:HB2	37:DK:28:TYR:HD2	1.71	0.55
1:1:2592:G:H4'	1:1:2594:C:C2	2.41	0.55
1:1:3009:G:O6	84:1:3437:OHX:N2	2.40	0.55
48:A:1500:C:OP1	68:U:122:ARG:NH2	2.38	0.55
36:AI:10:ARG:NH1	36:AI:60:GLU:OE1	2.39	0.55
1:AR:860:G:OP1	44:DR:17:ARG:NH1	2.39	0.55
2:AS:121:U:OP2	7:CG:265:TYR:OH	2.18	0.55
7:CG:64:ILE:HG13	7:CG:105:ILE:HD12	1.88	0.55
7:CG:107:ARG:HD3	7:CG:248:ARG:HG2	1.88	0.55
11:CK:9:GLN:HB3	11:CK:52:LEU:HD21	1.89	0.55
37:DK:70:ARG:HD3	37:DK:84:LYS:HG2	1.89	0.55
58:K:129:ILE:HG12	58:K:134:ILE:HD11	1.88	0.55
1:1:1567:U:O2	1:1:1571:A:N6	2.37	0.55
1:AR:1054:A:OP1	84:AR:3592:OHX:N4	2.39	0.55
1:AR:3255:U:H2'	1:AR:3256:G:H8	1.71	0.55
1:AR:528:U:H2'	1:AR:529:A:C8	2.42	0.55
3:AT:74:U:O2	84:AT:206:OHX:N5	2.40	0.55
5:CE:41:VAL:HA	5:CE:185:GLY:CA	2.25	0.55
6:CF:141:ARG:NH1	6:CF:180:LYS:HD3	2.21	0.55
14:CN:14:PHE:HB3	14:CN:18:TRP:CD1	2.42	0.55
48:A:637:C:O2	56:I:114:ARG:NH2	2.39	0.55
67:T:91:ASP:OD1	67:T:93:THR:N	2.38	0.55
1:AR:781:G:O6	84:AR:3496:OHX:N6	2.40	0.55
1:AR:67:A:OP1	84:AR:3458:OHX:N6	2.40	0.55
1:AR:715:A:H4'	1:AR:716:A:OP1	2.07	0.55
50:C:81:PHE:HD1	50:C:82:ARG:HG3	1.71	0.55
10:CJ:134:TYR:CG	10:CJ:190:VAL:HG21	2.42	0.55
1:AR:2433:U:H1'	16:CP:125:SER:HB3	1.88	0.55
58:K:6:ARG:HH11	58:K:6:ARG:HB2	1.72	0.55
65:R:97:VAL:HG12	65:R:98:ASP:H	1.71	0.55
67:T:99:HIS:HD2	67:T:101:LEU:HD21	1.71	0.55
2:3:3:U:H2'	2:3:4:U:C6	2.42	0.54
2:3:4:U:H2'	2:3:5:G:C8	2.42	0.54
48:A:386:G:OP2	57:J:25:ARG:NH2	2.39	0.54
50:C:175:GLU:HG3	50:C:193:ILE:HD12	1.88	0.54
1:AR:824:C:H5''	4:CD:21:ARG:HD3	1.88	0.54
13:CM:20:ASN:HB3	13:CM:126:ASP:HB2	1.90	0.54
15:CO:13:ARG:NH1	15:CO:65:LEU:O	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:Z:35:VAL:HG13	73:Z:36:SER:H	1.71	0.54
73:Z:36:SER:OG	73:Z:37:LYS:N	2.39	0.54
1:1:409:A:OP2	84:1:3592:OHX:N5	2.40	0.54
1:1:551:A:O2'	1:1:552:G:O5'	2.25	0.54
1:1:94:G:H2'	1:1:95:A:C8	2.43	0.54
48:A:702:G:O2'	48:A:703:G:H8	1.90	0.54
1:AR:2181:C:H5''	4:CD:193:ARG:NH2	2.22	0.54
29:DC:34:MET:HE2	29:DC:34:MET:HA	1.88	0.54
57:J:8:ARG:NH2	57:J:19:ALA:O	2.39	0.54
58:K:34:PHE:HD2	58:K:111:THR:HG21	1.71	0.54
71:X:76:SER:OG	71:X:77:PRO:HD3	2.06	0.54
1:1:2234:G:O6	84:1:3580:OHX:N4	2.41	0.54
1:1:523:A:OP2	84:1:3539:OHX:N5	2.39	0.54
48:A:1698:G:H22	48:A:1703:C:H42	1.56	0.54
1:AR:2927:C:H2'	1:AR:2928:C:C6	2.42	0.54
1:AR:3214:U:C4	15:CO:121:MET:HG3	2.42	0.54
1:AR:3164:C:N4	1:AR:3287:U:O4	2.40	0.54
1:AR:3383:G:H2'	1:AR:3384:U:H6	1.73	0.54
1:AR:1134:G:O6	84:AR:3490:OHX:N3	2.40	0.54
1:AR:2123:G:O6	84:AR:3605:OHX:N5	2.41	0.54
84:AR:3612:OHX:N1	5:CE:30:LYS:O	2.41	0.54
10:CJ:190:VAL:HG13	10:CJ:192:GLN:HG2	1.89	0.54
1:AR:1369:A:OP1	29:DC:21:ARG:NH1	2.40	0.54
58:K:119:ALA:HA	58:K:124:HIS:HD2	1.73	0.54
1:1:1915:A:H2'	1:1:1916:U:C6	2.43	0.54
1:1:2248:C:OP2	84:1:3417:OHX:N3	2.41	0.54
24:6:81:GLN:O	24:6:95:PHE:HB2	2.08	0.54
48:A:1449:U:H2'	48:A:1450:U:C6	2.43	0.54
31:AD:34:LEU:HD23	31:AD:59:TYR:HB3	1.89	0.54
1:AR:2298:U:O4	1:AR:2923:U:H5	1.89	0.54
1:AR:3052:G:O6	84:AR:3677:OHX:N3	2.40	0.54
1:AR:3082:C:OP2	84:AR:3444:OHX:N4	2.40	0.54
1:AR:1389:G:N7	84:AR:3516:OHX:N5	2.56	0.54
48:A:1067:C:H5''	50:C:150:VAL:HG23	1.89	0.54
6:CF:181:VAL:O	6:CF:182:LEU:HB2	2.07	0.54
8:CH:3:ALA:HB1	33:DG:75:LEU:HD13	1.88	0.54
12:CL:29:SER:HB2	12:CL:125:LEU:HD12	1.90	0.54
18:CR:60:PHE:HB3	18:CR:64:ASN:HB3	1.89	0.54
70:W:36:VAL:HG11	70:W:78:LEU:HD13	1.89	0.54
1:1:2723:U:H2'	1:1:2724:U:C6	2.42	0.54
1:1:901:G:O6	84:1:3473:OHX:N2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:131:C:O2'	48:A:132:U:OP1	2.24	0.54
48:A:143:G:N7	55:H:177:ARG:NH2	2.55	0.54
1:AR:2263:C:OP1	84:AR:3459:OHX:N1	2.40	0.54
1:AR:1817:G:OP1	84:AR:3685:OHX:N1	2.40	0.54
84:AR:3445:OHX:N5	84:AR:3738:OHX:N3	2.56	0.54
49:B:134:LYS:O	49:B:137:SER:OG	2.23	0.54
10:CJ:33:ASN:O	10:CJ:39:ALA:HB3	2.07	0.54
51:D:87:GLN:HG2	51:D:96:THR:HB	1.89	0.54
43:DQ:77:CYS:SG	43:DQ:79:THR:OG1	2.66	0.54
1:1:246:U:OP1	1:AR:176:G:O2'	2.26	0.54
1:1:3233:C:H2'	1:1:3234:A:C8	2.43	0.54
48:A:1495:C:OP1	84:A:1953:OHX:N5	2.40	0.54
40:AM:21:ARG:HD3	40:AM:22:PRO:O	2.07	0.54
1:AR:3192:U:O4	84:AR:3649:OHX:N6	2.40	0.54
7:CG:297:GLN:O	84:CG:302:OHX:N5	2.40	0.54
25:CY:47:ARG:HG3	25:CY:54:LEU:HD23	1.90	0.54
44:DR:49:ARG:HB2	44:DR:55:TRP:CZ3	2.43	0.54
57:J:39:GLY:O	57:J:59:ARG:HB3	2.07	0.54
58:K:133:HIS:O	58:K:134:ILE:HG12	2.06	0.54
59:L:56:LYS:HG2	59:L:67:THR:HB	1.89	0.54
1:1:522:A:OP1	84:1:3479:OHX:N5	2.40	0.54
1:1:1807:G:H5''	28:AA:135:ARG:HH22	1.72	0.54
1:AR:917:A:OP2	84:AR:3728:OHX:N3	2.40	0.54
50:C:70:LEU:O	50:C:74:GLN:N	2.27	0.54
5:CE:293:ASN:HB2	5:CE:304:THR:HA	1.89	0.54
5:CE:53:MET:HE2	5:CE:77:THR:HG22	1.90	0.54
6:CF:295:ILE:O	6:CF:299:ILE:HG12	2.07	0.54
8:CH:42:LEU:HD23	8:CH:84:VAL:HG22	1.89	0.54
36:DJ:119:LYS:HE2	36:DJ:119:LYS:HA	1.90	0.54
36:DJ:21:LEU:HD22	36:DJ:25:LYS:HE3	1.90	0.54
60:M:17:PRO:HG3	60:M:63:LEU:HD11	1.90	0.54
69:V:48:HIS:O	69:V:48:HIS:ND1	2.41	0.54
1:1:2242:A:OP2	84:1:3492:OHX:N2	2.41	0.54
1:1:2778:G:H2'	1:1:2779:A:H5'	1.90	0.54
1:1:3316:A:OP1	1:1:3318:G:N2	2.40	0.54
1:1:2259:A:OP2	84:1:3468:OHX:N2	2.41	0.54
23:5:39:ASP:O	23:5:47:VAL:HB	2.08	0.54
48:A:1233:G:OP2	84:A:2030:OHX:N5	2.41	0.54
48:A:352:A:H8	48:A:352:A:OP2	1.91	0.54
1:AR:599:C:OP1	6:CF:332:LYS:NZ	2.39	0.54
2:AS:76:A:OP2	84:AS:201:OHX:N3	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:CP:47:LYS:HE3	16:CP:51:LEU:HD11	1.90	0.54
18:CR:59:PRO:HG3	18:CR:76:PHE:CD2	2.42	0.54
27:DA:32:SER:HA	27:DA:49:PRO:HA	1.90	0.54
31:DE:26:GLY:O	31:DE:30:THR:HG23	2.08	0.54
53:F:253:ASP:O	53:F:257:ALA:N	2.41	0.54
56:I:25:VAL:HA	56:I:28:GLU:HB2	1.90	0.54
67:T:11:PHE:HD1	67:T:59:GLY:HA3	1.71	0.54
1:1:1727:G:OP1	44:AQ:44:LYS:NZ	2.40	0.54
1:1:2850:G:O6	84:1:3611:OHX:N6	2.41	0.54
3:4:43:A:OP1	84:4:215:OHX:N2	2.40	0.54
48:A:749:U:H3	48:A:800:U:H3	1.55	0.54
29:AB:47:LYS:HE2	29:AB:48:TYR:CZ	2.43	0.54
13:CM:133:ARG:HD2	13:CM:152:HIS:O	2.08	0.54
13:CM:90:GLN:HG2	13:CM:170:ASP:HB2	1.89	0.54
51:D:147:ASN:HB3	70:W:4:ASP:HA	1.89	0.54
41:DO:99:CYS:HB3	41:DO:115:CYS:HB3	1.90	0.54
60:M:21:ASN:HD22	60:M:32:LYS:H	1.53	0.54
1:1:1029:G:H2'	1:1:1030:A:C8	2.43	0.54
1:1:434:U:O4	84:1:3697:OHX:N2	2.40	0.54
1:1:817:A:N3	38:AK:11:ARG:HB3	2.23	0.54
24:6:104:ASN:ND2	24:6:106:LYS:H	2.06	0.54
48:A:138:A:N6	48:A:266:A:H61	2.04	0.54
48:A:780:A:C8	73:Z:8:ARG:HB3	2.42	0.54
1:AR:1222:G:OP2	1:AR:1222:G:H8	1.90	0.54
1:AR:1348:U:O2	1:AR:1349:G:N2	2.41	0.54
1:AR:1639:C:H5'	35:DI:52:GLN:HG2	1.88	0.54
1:AR:1717:U:H2'	1:AR:1718:G:C8	2.43	0.54
11:CK:91:ARG:HG2	11:CK:182:SER:HB3	1.89	0.54
52:E:178:ARG:H	52:E:178:ARG:NE	2.05	0.54
61:N:61:VAL:HA	61:N:89:ILE:HG22	1.90	0.54
1:1:114:A:N1	1:1:266:A:O2'	2.35	0.53
48:A:264:G:N7	84:A:1912:OHX:N4	2.57	0.53
29:AB:90:TYR:CG	29:AB:100:PRO:HG3	2.42	0.53
39:AL:31:LEU:HA	39:AL:37:PRO:HA	1.91	0.53
43:AP:48:SER:O	84:AP:502:OHX:N2	2.41	0.53
1:AR:271:C:OP1	84:AR:3580:OHX:N6	2.41	0.53
1:AR:2725:U:O4	84:AR:3462:OHX:N1	2.40	0.53
10:CJ:90:THR:HA	10:CJ:214:LEU:HD21	1.89	0.53
2:AS:39:C:N3	13:CM:70:THR:HG23	2.23	0.53
13:CM:92:ARG:NH2	13:CM:94:ARG:HH21	2.06	0.53
18:CR:64:ASN:HB2	18:CR:80:LYS:HE3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DI:41:ARG:HG2	35:DI:56:THR:HG21	1.89	0.53
44:DR:84:ARG:O	44:DR:88:GLU:HG2	2.08	0.53
71:X:6:VAL:HG13	71:X:29:PRO:HD2	1.90	0.53
71:X:85:ASP:HA	71:X:88:LYS:HG3	1.89	0.53
21:O:137:ARG:HG2	21:O:139:TYR:CE2	2.43	0.53
1:AR:2311:G:OP2	84:AR:3481:OHX:N1	2.41	0.53
3:AT:100:U:OP2	84:AT:204:OHX:N1	2.41	0.53
50:C:137:ILE:HD11	50:C:172:LEU:HB3	1.89	0.53
25:CY:14:TYR:O	25:CY:17:ARG:HB2	2.08	0.53
57:J:11:ARG:O	60:M:133:LYS:NZ	2.40	0.53
69:V:34:LEU:HD23	69:V:112:VAL:HG13	1.89	0.53
72:Y:92:CYS:HA	72:Y:95:PHE:CD2	2.42	0.53
1:1:1815:U:O2'	1:1:1816:A:OP2	2.21	0.53
1:1:2736:A:O2'	22:2:68:THR:HG21	2.08	0.53
26:8:105:VAL:HG11	26:8:126:LEU:HD22	1.91	0.53
48:A:583:C:OP1	84:A:1904:OHX:N4	2.40	0.53
48:A:581:U:OP2	52:E:143:ARG:NH1	2.41	0.53
1:AR:1246:G:O2'	1:AR:1264:G:OP2	2.26	0.53
1:AR:83:U:OP2	84:AR:3711:OHX:N4	2.41	0.53
50:C:35:PRO:HD3	50:C:98:THR:HG23	1.89	0.53
23:CW:76:LEU:O	23:CW:80:THR:HG23	2.08	0.53
26:CZ:115:ARG:NH1	26:CZ:115:ARG:HG3	2.24	0.53
66:S:71:PHE:CD1	66:S:73:LEU:HB3	2.42	0.53
72:Y:79:ASN:HB3	72:Y:81:LYS:HG3	1.91	0.53
48:A:1317:C:H2'	48:A:1318:G:O4'	2.07	0.53
48:A:144:U:H5	55:H:137:ARG:NH1	2.06	0.53
48:A:1762:A:H1'	48:A:1783:C:H5'	1.91	0.53
48:A:732:G:O6	84:A:2007:OHX:N5	2.42	0.53
31:AD:13:LYS:HB3	31:AD:100:ILE:HG23	1.91	0.53
1:AR:1877:U:H5''	1:AR:1878:G:O4'	2.09	0.53
1:AR:2722:U:OP1	30:DD:33:LYS:NZ	2.32	0.53
1:AR:328:U:O4	84:AR:3528:OHX:N1	2.41	0.53
1:AR:849:C:H2'	1:AR:850:U:C6	2.43	0.53
61:N:40:GLY:HA3	61:N:125:ASN:HB3	1.89	0.53
1:1:2689:A:H2'	1:1:2689:A:N3	2.23	0.53
1:1:3159:C:OP1	84:1:3682:OHX:N1	2.42	0.53
1:1:3275:U:O4'	34:AG:66:VAL:HG21	2.08	0.53
1:1:637:C:O2'	1:1:638:C:O5'	2.26	0.53
1:1:792:G:H2'	1:1:793:C:C6	2.44	0.53
1:1:807:A:H61	1:1:934:G:H22	1.57	0.53
48:A:1592:A:H2'	48:A:1593:A:H8	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:915:A:OP1	84:A:1972:OHX:N3	2.41	0.53
48:A:1239:U:OP1	84:A:2022:OHX:N5	2.41	0.53
48:A:417:A:H4'	48:A:418:G:O5'	2.09	0.53
48:A:702:G:HO2'	48:A:703:G:H8	1.55	0.53
48:A:778:G:H22	73:Z:10:ARG:NH2	2.07	0.53
1:AR:1103:A:H2'	1:AR:1103:A:N3	2.24	0.53
1:AR:1340:G:H2'	1:AR:1341:U:H6	1.74	0.53
1:AR:3396:U:O2	84:AR:3688:OHX:N6	2.41	0.53
54:G:26:ALA:HB2	65:R:26:LYS:HG3	1.90	0.53
48:A:329:G:H5''	57:J:98:LYS:HB3	1.91	0.53
48:A:1544:U:OP1	67:T:136:GLN:NE2	2.41	0.53
72:Y:92:CYS:HA	72:Y:95:PHE:HD2	1.71	0.53
1:1:1895:A:O2'	1:1:3053:G:H4'	2.08	0.53
1:1:272:G:OP2	84:1:3567:OHX:N6	2.41	0.53
1:1:3092:C:O2'	1:1:3094:A:OP2	2.19	0.53
1:1:3291:G:O6	84:1:3664:OHX:N2	2.42	0.53
1:1:715:A:H4'	1:1:716:A:OP1	2.09	0.53
2:3:109:G:N7	84:3:204:OHX:N5	2.56	0.53
48:A:1595:U:N3	48:A:1600:A:H2	2.06	0.53
1:AR:1688:U:H2'	1:AR:1689:U:C6	2.44	0.53
1:AR:2754:G:OP2	84:AR:3552:OHX:N3	2.42	0.53
1:AR:30:G:P	16:CP:172:ARG:HE	2.32	0.53
1:AR:3155:U:H3'	1:AR:3156:U:H4'	1.90	0.53
1:AR:1940:G:N2	1:AR:3362:A:H8	2.06	0.53
2:AS:107:C:H2'	2:AS:108:A:C8	2.44	0.53
1:AR:291:C:H5''	16:CP:68:ARG:NH1	2.24	0.53
28:DB:5:LEU:HD11	31:DE:35:ARG:HD2	1.90	0.53
58:K:134:ILE:HA	58:K:158:PHE:HA	1.89	0.53
63:P:125:SER:OG	63:P:126:THR:N	2.40	0.53
64:Q:25:LEU:HA	64:Q:28:MET:HE2	1.91	0.53
65:R:18:ALA:HB2	65:R:69:VAL:HG13	1.89	0.53
1:1:2611:U:H2'	1:1:2612:U:C6	2.43	0.53
1:1:2309:A:H4'	84:1:3671:OHX:N1	2.23	0.53
1:1:535:G:O2'	84:1:3485:OHX:N3	2.42	0.53
3:4:151:C:C4	26:8:24:LEU:HD11	2.44	0.53
48:A:1280:C:H2'	48:A:1281:G:C8	2.44	0.53
31:AD:22:LYS:HB2	31:AD:94:GLU:HB2	1.90	0.53
35:AH:42:PRO:HB2	35:AH:51:LEU:HD21	1.91	0.53
1:AR:1586:G:OP1	84:AR:3495:OHX:N3	2.42	0.53
1:AR:2943:G:OP2	5:CE:2:SER:OG	2.27	0.53
14:CN:50:PRO:O	14:CN:52:ASP:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CT:159:ALA:O	20:CT:163:ARG:HB2	2.08	0.53
30:DD:14:ARG:HH12	30:DD:18:ARG:NH1	2.07	0.53
31:DE:13:LYS:HB3	31:DE:100:ILE:HG22	1.91	0.53
39:DM:18:ALA:O	39:DM:20:VAL:N	2.41	0.53
48:A:1515:A:OP2	52:E:7:LYS:HB2	2.09	0.53
58:K:143:ILE:HG22	58:K:145:SER:H	1.73	0.53
1:1:872:U:H2'	1:1:873:C:C6	2.43	0.53
48:A:1338:C:H1'	48:A:1410:A:C4	2.43	0.53
48:A:514:G:O2'	48:A:515:A:H5'	2.08	0.53
50:C:36:SER:HB2	50:C:231:LEU:HB3	1.91	0.53
11:CK:29:GLY:HA3	11:CK:82:VAL:HG13	1.89	0.53
12:CL:171:TRP:CE3	12:CL:178:ARG:HD2	2.43	0.53
14:CN:126:PHE:HZ	14:CN:135:ALA:HB2	1.74	0.53
37:DK:56:ARG:O	37:DK:60:LEU:HD23	2.09	0.53
48:A:858:G:OP1	56:I:116:ARG:NH2	2.42	0.53
71:X:6:VAL:HG12	71:X:34:ILE:HD11	1.91	0.53
73:Z:23:PHE:HE1	73:Z:75:VAL:HG12	1.74	0.53
1:1:1852:G:N7	84:1:3513:OHX:N3	2.57	0.53
1:1:2294:U:OP2	24:6:71:LYS:HE2	2.09	0.53
2:3:19:C:H2'	2:3:20:A:H8	1.74	0.53
27:9:118:LEU:O	27:9:122:LYS:HG3	2.09	0.53
1:AR:1659:U:H2'	1:AR:1660:C:C6	2.44	0.53
1:AR:1661:G:H2'	1:AR:1662:G:C8	2.44	0.53
1:AR:339:C:OP1	1:AR:1380:G:O2'	2.26	0.53
20:CT:43:LYS:HA	20:CT:46:LYS:HD3	1.91	0.53
63:P:17:ALA:HB3	63:P:81:VAL:HA	1.91	0.53
1:1:156:G:OP2	37:AJ:25:LYS:HB3	2.08	0.53
1:1:795:G:O6	84:1:3430:OHX:N3	2.42	0.53
48:A:1561:U:H2'	48:A:1562:G:H8	1.74	0.53
48:A:927:C:H1'	63:P:125:SER:CB	2.39	0.53
1:AR:3364:C:OP1	84:AR:3445:OHX:N1	2.41	0.53
84:AR:3526:OHX:N3	84:AR:3721:OHX:N1	2.56	0.53
6:CF:16:THR:HG22	6:CF:18:ASN:N	2.19	0.53
14:CN:42:ARG:HE	14:CN:51:LEU:HD22	1.73	0.53
14:CN:75:PHE:O	14:CN:79:GLU:HB2	2.08	0.53
22:CV:12:ARG:HD3	22:CV:13:TYR:CE1	2.44	0.53
59:L:50:THR:HA	59:L:55:VAL:HG13	1.91	0.53
64:Q:128:HIS:O	64:Q:130:ARG:HG2	2.09	0.53
66:S:85:VAL:HG12	66:S:86:PRO:HA	1.91	0.53
71:X:86:ILE:HD12	71:X:87:GLU:H	1.74	0.53
1:1:2218:G:H2'	1:1:2219:A:C8	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:130:C:O2'	48:A:131:C:OP1	2.26	0.52
1:AR:1781:C:H2'	1:AR:1782:U:C6	2.44	0.52
1:AR:229:G:H5''	27:DA:4:GLN:HB2	1.90	0.52
1:AR:2916:U:H5	1:AR:2935:U:HO2'	1.57	0.52
7:CG:106:ALA:O	7:CG:110:LEU:HB2	2.09	0.52
1:AR:1722:U:OP1	20:CT:100:ARG:HD3	2.09	0.52
48:A:778:G:H1	73:Z:10:ARG:HG2	1.75	0.52
1:1:1464:G:OP2	84:1:3730:OHX:N3	2.42	0.52
48:A:1683:C:O2'	48:A:1684:U:O5'	2.25	0.52
48:A:61:A:H8	48:A:269:G:HO2'	1.57	0.52
1:AR:2801:A:O2'	1:AR:2802:A:H2'	2.08	0.52
1:AR:3255:U:H2'	1:AR:3256:G:C8	2.45	0.52
1:AR:3343:G:H21	1:AR:3362:A:H2	1.56	0.52
1:AR:2790:A:O2'	84:AR:3574:OHX:N4	2.42	0.52
1:AR:916:G:H5'	1:AR:917:A:OP1	2.09	0.52
28:DB:50:PRO:HD3	28:DB:68:ILE:HG12	1.90	0.52
56:I:30:SER:HB2	56:I:34:LEU:HB2	1.91	0.52
58:K:96:VAL:HA	58:K:99:LEU:HD22	1.91	0.52
1:1:2261:G:O6	84:1:3468:OHX:N4	2.43	0.52
48:A:1484:G:H21	48:A:1606:C:H1'	1.73	0.52
48:A:218:A:N6	48:A:844:A:H1'	2.24	0.52
48:A:912:U:H4'	48:A:913:G:H2'	1.91	0.52
1:1:715:A:H8	29:AB:115:LYS:HG2	1.74	0.52
29:AB:90:TYR:CD1	29:AB:100:PRO:HG3	2.45	0.52
1:AR:1063:G:OP2	1:AR:1097:G:H3'	2.09	0.52
1:AR:3353:G:OP2	84:AR:3734:OHX:N1	2.42	0.52
1:AR:66:A:OP2	14:CN:100:ARG:NH2	2.33	0.52
3:AT:139:U:O4	84:AT:210:OHX:N5	2.41	0.52
50:C:48:VAL:CG1	50:C:61:LEU:HD21	2.39	0.52
11:CK:12:VAL:HG13	11:CK:16:VAL:HG22	1.90	0.52
53:F:246:LEU:HB3	53:F:250:GLU:HB2	1.92	0.52
62:O:21:ASN:N	62:O:21:ASN:OD1	2.41	0.52
1:1:1176:C:H2'	1:1:1177:G:N2	2.24	0.52
1:1:1355:A:H5''	1:1:1356:U:H5	1.75	0.52
1:1:2947:G:H4'	1:1:2947:G:OP2	2.10	0.52
1:1:2317:A:OP2	84:1:3606:OHX:N2	2.43	0.52
2:3:106:U:H2'	2:3:107:C:C6	2.44	0.52
48:A:1511:U:H2'	48:A:1512:G:C8	2.44	0.52
48:A:1559:A:C6	67:T:134:ARG:HD2	2.44	0.52
48:A:1006:C:OP1	84:A:1913:OHX:N5	2.42	0.52
1:AR:59:G:H4'	1:AR:60:A:H4'	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:CI:168:ILE:O	9:CI:172:ASN:ND2	2.39	0.52
1:1:2683:U:H2'	1:1:2684:C:C6	2.43	0.52
1:AR:1508:C:OP1	18:CR:127:ARG:NH2	2.38	0.52
15:CO:17:VAL:HG21	15:CO:74:ARG:HB2	1.91	0.52
17:CQ:121:PRO:HA	17:CQ:124:LEU:HD22	1.92	0.52
26:CZ:67:ILE:HD12	26:CZ:121:LYS:HG3	1.91	0.52
48:A:1183:A:C4	64:Q:100:LYS:HD3	2.44	0.52
1:1:621:A:O2'	84:1:3697:OHX:N1	2.43	0.52
25:7:52:THR:O	25:7:56:ARG:HG3	2.10	0.52
48:A:565:C:O2	84:A:1917:OHX:N5	2.42	0.52
1:AR:1427:U:OP2	29:DC:4:ARG:NH2	2.38	0.52
1:AR:196:G:N7	84:AR:3447:OHX:N3	2.57	0.52
5:CE:286:GLY:HA3	5:CE:321:PHE:CE2	2.44	0.52
12:CL:74:LYS:O	12:CL:78:THR:HG23	2.09	0.52
16:CP:112:ASN:ND2	16:CP:113:LEU:HD22	2.25	0.52
56:I:38:LEU:HD23	56:I:41:LEU:HD12	1.92	0.52
1:1:2165:G:OP1	84:1:3536:OHX:N6	2.43	0.52
1:1:383:G:O6	84:1:3629:OHX:N3	2.43	0.52
48:A:1031:U:H4'	48:A:1032:G:OP2	2.10	0.52
1:AR:1724:U:H1'	1:AR:1725:C:C6	2.45	0.52
1:AR:2810:C:OP1	84:AR:3585:OHX:N3	2.43	0.52
1:AR:2904:U:OP1	84:AR:3548:OHX:N3	2.42	0.52
1:AR:863:C:OP1	84:AR:3419:OHX:N3	2.43	0.52
50:C:168:ILE:HG12	50:C:197:ILE:HD12	1.90	0.52
50:C:52:THR:H	50:C:56:SER:HA	1.75	0.52
14:CN:101:ARG:HH22	14:CN:112:ASN:ND2	2.07	0.52
1:1:3354:U:H1'	57:J:163:GLY:HA3	1.91	0.52
58:K:53:ARG:NH2	58:K:97:LEU:O	2.42	0.52
61:N:89:ILE:HG12	61:N:90:LYS:H	1.75	0.52
1:1:1103:A:N3	1:1:1103:A:H2'	2.25	0.52
48:A:715:U:H3	48:A:723:G:H1	1.58	0.52
32:AE:36:ILE:HD12	32:AE:59:ILE:HD11	1.92	0.52
36:AI:101:THR:HG22	36:AI:104:GLN:HB2	1.92	0.52
1:AR:1340:G:H2'	1:AR:1341:U:C6	2.44	0.52
1:AR:1779:C:N3	84:AR:3510:OHX:N4	2.57	0.52
1:AR:1743:G:N7	84:AR:3606:OHX:N5	2.58	0.52
1:AR:792:G:N7	84:AR:3691:OHX:N2	2.58	0.52
5:CE:347:SER:HB3	5:CE:350:ALA:H	1.74	0.52
7:CG:5:LYS:O	84:CG:303:OHX:N3	2.43	0.52
8:CH:175:LYS:O	15:CO:117:ARG:NH2	2.43	0.52
7:CG:17:GLN:HE22	22:CV:22:HIS:H	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:D:58:LEU:O	70:W:15:ARG:NE	2.38	0.52
69:V:118:VAL:HG22	69:V:119:ALA:H	1.74	0.52
2:3:71:G:H2'	2:3:72:A:C8	2.45	0.52
3:4:104:A:C8	3:4:105:A:C8	2.98	0.52
1:AR:2537:U:H1'	1:AR:2538:U:O4'	2.09	0.52
1:AR:1464:G:O6	84:AR:3477:OHX:N3	2.43	0.52
15:CO:32:LEU:HD11	15:CO:94:TRP:CG	2.45	0.52
51:D:139:ILE:HD12	51:D:191:ALA:HB1	1.92	0.52
1:AR:1592:G:OP1	35:DI:58:ARG:NH1	2.43	0.52
48:A:1254:U:OP2	61:N:46:ARG:NH1	2.42	0.52
65:R:47:LYS:NZ	65:R:114:ARG:HG2	2.25	0.52
72:Y:56:LYS:HE3	72:Y:96:VAL:HG23	1.91	0.52
73:Z:124:ARG:O	73:Z:127:LYS:HG3	2.10	0.52
73:Z:36:SER:O	73:Z:40:LEU:HG	2.10	0.52
1:1:2754:G:OP2	84:1:3543:OHX:N3	2.43	0.52
1:1:3228:C:H4'	1:1:3229:G:O5'	2.10	0.52
1:1:3278:C:H2'	1:1:3278:C:O2	2.08	0.52
48:A:685:A:H2'	48:A:686:C:C6	2.45	0.52
1:1:44:U:O3'	84:AP:502:OHX:N1	2.42	0.52
1:AR:1588:A:C2	40:DN:4:GLN:HG2	2.45	0.52
1:AR:955:U:H2'	1:AR:956:U:C6	2.45	0.52
12:CL:86:HIS:HB3	12:CL:139:ARG:CG	2.40	0.52
18:CR:129:THR:HG23	18:CR:139:TYR:HB2	1.92	0.52
51:D:53:ILE:HG23	51:D:72:LEU:HD23	1.92	0.52
56:I:35:LYS:C	56:I:37:GLU:H	2.14	0.52
65:R:44:LEU:O	65:R:47:LYS:HB2	2.10	0.52
69:V:72:ASN:HD22	69:V:74:GLU:H	1.58	0.52
1:1:2299:A:OP2	84:1:3482:OHX:N4	2.44	0.51
1:1:584:G:O6	84:1:3540:OHX:N2	2.43	0.51
48:A:1202:A:N6	48:A:1457:C:H5''	2.25	0.51
48:A:1247:U:OP2	84:A:2030:OHX:N6	2.42	0.51
1:AR:1056:U:O2	84:AR:3497:OHX:N5	2.43	0.51
1:AR:3267:A:H2'	8:CH:69:PHE:CZ	2.45	0.51
11:CK:48:VAL:HG13	11:CK:52:LEU:HB3	1.91	0.51
16:CP:172:ARG:O	16:CP:183:THR:OG1	2.28	0.51
51:D:39:THR:O	51:D:42:GLY:N	2.40	0.51
53:F:45:ILE:HA	53:F:61:VAL:HG11	1.92	0.51
53:F:90:ILE:HB	53:F:99:PHE:HB2	1.93	0.51
48:A:568:G:N7	72:Y:69:ARG:NH2	2.58	0.51
53:F:95:THR:HG22	73:Z:16:PRO:HG2	1.91	0.51
73:Z:12:VAL:HG13	73:Z:23:PHE:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2218:G:H2'	1:1:2219:A:H8	1.75	0.51
48:A:1606:C:H2'	48:A:1607:G:C8	2.45	0.51
28:AA:46:ILE:HD11	28:AA:49:TYR:HA	1.91	0.51
1:AR:1764:U:H5''	20:CT:43:LYS:HE2	1.92	0.51
1:AR:3346:U:H3	1:AR:3359:A:H61	1.58	0.51
3:AT:136:G:OP1	26:CZ:48:SER:OG	2.28	0.51
50:C:180:THR:HG22	50:C:181:LEU:H	1.75	0.51
54:G:187:ILE:HD12	54:G:187:ILE:H	1.75	0.51
1:1:3088:G:OP2	84:1:3713:OHX:N5	2.43	0.51
1:1:829:U:H3	1:1:895:A:H62	1.58	0.51
22:2:12:ARG:HD3	22:2:13:TYR:CE1	2.46	0.51
25:7:49:ILE:O	25:7:52:THR:OG1	2.28	0.51
1:1:1636:U:H5''	28:AA:73:LYS:HZ2	1.75	0.51
38:AK:48:ASN:OD1	38:AK:54:LYS:NZ	2.40	0.51
1:AR:2254:U:H3	1:AR:2263:C:H42	1.58	0.51
1:AR:249:U:O2	1:AR:250:U:N3	2.43	0.51
1:AR:271:C:O2	37:DK:82:ARG:NH2	2.37	0.51
2:AS:58:C:OP2	84:AS:202:OHX:N5	2.43	0.51
1:AR:827:A:H5''	35:DI:14:ASN:O	2.09	0.51
1:1:132:C:H2'	1:1:133:U:H5''	1.91	0.51
1:1:2539:C:H5'	1:1:2541:U:O4	2.10	0.51
1:1:2927:C:H2'	1:1:2928:C:C6	2.45	0.51
1:1:3395:G:O2'	84:1:3682:OHX:N2	2.43	0.51
48:A:1100:G:O2'	71:X:76:SER:N	2.44	0.51
84:A:1909:OHX:N6	84:A:2024:OHX:N2	2.58	0.51
48:A:603:U:H2'	48:A:604:A:C8	2.45	0.51
48:A:863:A:O5'	71:X:57:ARG:HG2	2.11	0.51
1:AR:1765:U:H5''	20:CT:43:LYS:HD3	1.93	0.51
1:AR:2384:A:OP1	84:AR:3483:OHX:N3	2.43	0.51
1:AR:2854:U:P	12:CL:3:ARG:HH22	2.32	0.51
1:AR:662:U:OP1	29:DC:8:THR:HG21	2.10	0.51
2:AS:3:U:H2'	2:AS:4:U:H6	1.75	0.51
34:DH:45:LEU:HA	34:DH:71:VAL:HG12	1.92	0.51
40:DN:9:ILE:O	40:DN:13:MET:HG3	2.11	0.51
53:F:11:ARG:HB2	53:F:26:CYS:O	2.10	0.51
55:H:186:ARG:O	55:H:190:GLN:HG2	2.10	0.51
66:S:34:LEU:O	66:S:38:ILE:HG22	2.10	0.51
69:V:68:ARG:HG2	69:V:68:ARG:NH1	4.71	0.51
1:1:1078:U:O4	84:1:3502:OHX:N2	2.44	0.51
1:1:250:U:H5	1:1:251:G:C5	2.29	0.51
1:1:13:A:H4'	26:8:39:LYS:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:1701:A:H3'	48:A:1702:A:H5''	1.92	0.51
48:A:603:U:H2'	48:A:604:A:H8	1.75	0.51
29:AB:74:ASN:HB2	29:AB:76:ASP:HB2	1.93	0.51
1:AR:3259:U:H5'	1:AR:3259:U:H6	1.76	0.51
1:AR:428:A:H2'	1:AR:429:U:C6	2.45	0.51
38:DL:65:ARG:HG3	38:DL:65:ARG:HH11	1.75	0.51
52:E:141:LYS:HE3	52:E:179:GLN:HG3	1.91	0.51
56:I:133:THR:O	56:I:155:ASP:HB2	2.11	0.51
61:N:62:LEU:HA	61:N:120:VAL:HA	1.93	0.51
68:U:25:GLN:HG2	68:U:27:LYS:H	1.76	0.51
1:1:1460:A:H2'	1:1:1461:A:C8	2.46	0.51
1:1:263:C:H2'	1:1:264:G:O4'	2.11	0.51
1:1:3164:C:H1'	1:1:3165:A:H5'	1.93	0.51
22:2:56:PHE:CZ	22:2:78:LYS:HD3	2.45	0.51
28:AA:17:ARG:HG3	35:AH:73:SER:HB3	1.91	0.51
29:AB:85:ASP:OD1	29:AB:86:LYS:N	2.40	0.51
1:AR:1675:G:H2'	1:AR:1676:A:C8	2.46	0.51
1:AR:3258:U:OP2	84:AR:3502:OHX:N4	2.43	0.51
1:AR:3351:U:O2'	1:AR:3353:G:N2	2.44	0.51
2:AS:3:U:H2'	2:AS:4:U:C6	2.46	0.51
5:CE:10:ARG:NH1	5:CE:11:HIS:O	2.43	0.51
5:CE:221:THR:O	5:CE:272:TYR:HA	2.11	0.51
11:CK:93:VAL:O	11:CK:177:ASP:HA	2.11	0.51
2:AS:64:A:N1	12:CL:202:LYS:HD3	2.26	0.51
51:D:106:ASP:OD1	51:D:108:ASN:N	2.39	0.51
27:DA:59:VAL:HG12	27:DA:103:LYS:O	2.11	0.51
53:F:37:LYS:HB2	53:F:40:GLU:HG2	1.92	0.51
58:K:113:VAL:HG21	58:K:134:ILE:HD12	1.93	0.51
1:1:2193:U:H5'	1:1:2194:G:H5'	1.91	0.51
1:1:2209:U:O2'	1:1:2210:G:OP1	2.29	0.51
1:1:385:A:H2'	1:1:386:A:C8	2.45	0.51
48:A:349:U:O4	84:A:2005:OHX:N3	2.44	0.51
39:AL:42:LYS:HG2	39:AL:55:VAL:HG13	1.92	0.51
44:AQ:13:LYS:HE3	44:AQ:14:TYR:CZ	2.46	0.51
1:AR:3218:A:H4'	1:AR:3219:G:O5'	2.10	0.51
1:AR:1650:G:N7	84:AR:3686:OHX:N3	2.59	0.51
6:CF:321:LYS:HA	6:CF:324:LEU:HB3	1.92	0.51
7:CG:226:TYR:HE2	7:CG:236:LEU:HD11	1.74	0.51
53:F:159:THR:HB	53:F:227:VAL:HG23	1.93	0.51
24:6:80:ARG:NE	24:6:97:ASP:OD1	2.42	0.51
28:AA:23:VAL:HG12	28:AA:45:GLY:HA3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:AB:46:ASP:O	29:AB:47:LYS:HB3	2.10	0.51
1:AR:3295:A:H2'	1:AR:3296:A:C8	2.46	0.51
1:AR:722:G:N7	84:AR:3517:OHX:N3	2.59	0.51
49:B:74:VAL:HG22	49:B:96:THR:HG23	1.93	0.51
50:C:135:LEU:HD11	50:C:176:VAL:HG11	1.93	0.51
8:CH:65:ILE:HD12	8:CH:79:VAL:HB	1.93	0.51
11:CK:86:TYR:CE2	11:CK:151:VAL:HG22	2.46	0.51
15:CO:22:LEU:HB3	15:CO:64:VAL:HG13	1.92	0.51
52:E:23:GLU:CD	59:L:61:TRP:HE1	2.14	0.51
48:A:123:G:N2	53:F:146:THR:HG21	2.23	0.51
48:A:159:U:O2'	55:H:87:ARG:NH1	2.44	0.51
71:X:47:ILE:HG22	71:X:65:LEU:HB3	1.93	0.51
73:Z:3:ASP:C	73:Z:5:VAL:H	2.14	0.51
1:1:2656:A:H4'	43:AP:98:LYS:HD2	1.93	0.51
48:A:1490:C:H4'	48:A:1491:U:OP1	2.10	0.51
48:A:992:A:O2'	48:A:1785:U:O2	2.26	0.51
48:A:982:U:OP1	84:A:2013:OHX:N1	2.44	0.51
48:A:689:G:O6	84:A:2029:OHX:N1	2.44	0.51
1:AR:2696:A:H2'	1:AR:2697:A:C8	2.46	0.51
8:CH:62:THR:OG1	8:CH:78:ARG:HD3	2.11	0.51
12:CL:36:LEU:HD21	12:CL:69:ARG:HD3	1.93	0.51
13:CM:92:ARG:HH21	13:CM:94:ARG:HH21	1.58	0.51
16:CP:190:THR:O	16:CP:194:GLN:HG2	2.11	0.51
36:DJ:6:ALA:O	36:DJ:10:ARG:HG3	2.10	0.51
54:G:116:HIS:O	54:G:120:ILE:HG13	2.11	0.51
63:P:84:ARG:HB2	63:P:118:VAL:HG23	1.92	0.51
72:Y:42:PRO:O	72:Y:79:ASN:ND2	2.43	0.51
1:1:1839:A:OP2	84:1:3511:OHX:N3	2.44	0.51
1:1:3393:U:H2'	1:1:3394:U:C6	2.46	0.51
48:A:150:U:OP1	73:Z:123:LYS:NZ	2.34	0.51
48:A:142:G:H1	48:A:173:A:H2	1.59	0.51
48:A:595:G:OP2	84:A:1954:OHX:N3	2.43	0.51
48:A:375:U:H2'	48:A:376:C:H6	1.76	0.51
1:AR:283:G:O6	1:AR:304:G:H1'	2.11	0.51
1:AR:909:G:O2'	84:AR:3584:OHX:N2	2.44	0.51
6:CF:35:VAL:HG21	6:CF:244:LEU:HD21	1.92	0.51
17:CQ:62:THR:HG22	17:CQ:65:ASN:H	1.76	0.51
19:CS:158:HIS:H	19:CS:186:VAL:CG1	2.24	0.51
23:CW:51:GLY:O	23:CW:52:ASN:ND2	2.38	0.51
30:DD:14:ARG:NH2	30:DD:18:ARG:HH11	2.08	0.51
59:L:16:PHE:HD1	59:L:76:LEU:HD23	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:U:117:SER:HB2	68:U:123:ARG:HB2	1.92	0.51
1:1:1094:U:O2'	1:1:1095:U:O5'	2.26	0.50
1:1:1952:G:H3'	1:1:1953:G:H5''	1.93	0.50
1:1:2443:A:O2'	1:1:2444:C:OP2	2.23	0.50
1:1:655:C:H2'	1:1:656:A:H8	1.76	0.50
48:A:491:C:N3	48:A:496:G:N2	2.57	0.50
38:AK:63:ARG:O	38:AK:68:LYS:HE2	2.11	0.50
1:AR:1089:G:N7	84:AR:3695:OHX:N3	2.58	0.50
1:AR:1117:G:OP1	30:DD:4:SER:HB2	2.11	0.50
1:AR:692:A:OP1	16:CP:201:ARG:NH2	2.38	0.50
1:AR:978:G:O2'	1:AR:979:U:O2	2.29	0.50
14:CN:177:LYS:HG3	37:DK:11:LEU:HD13	1.92	0.50
65:R:50:GLU:OE1	65:R:112:TYR:OH	2.30	0.50
71:X:27:ILE:HD11	71:X:61:ILE:HD12	1.93	0.50
1:1:437:G:H2'	1:1:438:A:O4'	2.11	0.50
48:A:1350:U:H2'	48:A:1351:G:C8	2.46	0.50
30:AC:28:LYS:HD3	30:AC:29:TYR:N	2.27	0.50
1:AR:1232:C:C5	1:AR:1261:G:H2'	2.46	0.50
1:AR:3383:G:H2'	1:AR:3384:U:C6	2.46	0.50
1:AR:2751:G:O6	84:AR:3660:OHX:N3	2.43	0.50
1:AR:1062:A:OP2	84:AR:3726:OHX:N3	2.44	0.50
6:CF:317:PRO:C	6:CF:319:LYS:H	2.14	0.50
6:CF:361:HIS:CG	6:CF:362:ASP:H	2.30	0.50
12:CL:33:ILE:HD11	12:CL:36:LEU:HD23	1.93	0.50
1:AR:1874:A:H5''	20:CT:18:GLY:HA3	1.93	0.50
1:AR:3215:A:H5''	34:DH:2:ALA:HB2	1.93	0.50
63:P:26:THR:HG21	63:P:97:GLY:HA3	1.92	0.50
66:S:87:GLU:O	66:S:88:VAL:HG12	2.11	0.50
73:Z:14:SER:HB2	73:Z:21:LYS:HE3	1.93	0.50
1:1:3354:U:OP1	1:1:3356:G:H5'	2.11	0.50
48:A:207:U:O2	57:J:178:ARG:NH1	2.43	0.50
30:AC:46:ALA:O	30:AC:50:THR:HG22	2.11	0.50
36:AI:90:ARG:O	36:AI:91:ALA:HB3	2.11	0.50
38:AK:5:THR:HA	38:AK:8:PHE:CD2	2.45	0.50
6:CF:59:GLN:OE1	38:DL:55:ARG:NH2	2.45	0.50
9:CI:88:ARG:HD2	9:CI:90:LYS:O	2.12	0.50
19:CS:67:ILE:HG23	19:CS:81:VAL:HG11	1.94	0.50
1:AR:2339:C:P	24:CX:48:ARG:HG2	2.52	0.50
1:AR:39:A:H5''	29:DC:35:ALA:HB2	1.93	0.50
56:I:139:ARG:HD3	71:X:53:ILE:HA	1.93	0.50
66:S:14:LYS:HE2	66:S:68:GLY:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:789:A:H2'	1:1:790:U:C6	2.46	0.50
22:2:54:HIS:CE1	22:2:55:LYS:HD3	2.46	0.50
2:3:79:A:C2	2:3:102:A:C4	3.00	0.50
48:A:1130:G:OP2	84:A:1952:OHX:N2	2.44	0.50
48:A:1171:A:H2'	48:A:1172:G:C8	2.47	0.50
48:A:1370:U:H4'	48:A:1371:A:H5'	1.92	0.50
48:A:919:A:H2'	48:A:920:U:C6	2.47	0.50
1:AR:2209:U:O2'	1:AR:2210:G:OP1	2.23	0.50
1:AR:2997:G:O6	84:AR:3688:OHX:N4	2.44	0.50
1:AR:776:U:H5	1:AR:2719:U:O2	1.93	0.50
2:AS:23:A:H2'	2:AS:24:A:C8	2.47	0.50
1:AR:59:G:H2'	3:AT:33:A:O2'	2.11	0.50
14:CN:46:ILE:HG23	14:CN:49:ARG:CZ	2.42	0.50
1:AR:3215:A:N7	15:CO:125:LYS:NZ	2.59	0.50
16:CP:91:GLU:O	16:CP:93:LYS:HE3	2.11	0.50
18:CR:105:LYS:HB3	18:CR:107:LEU:HD13	1.92	0.50
19:CS:182:LYS:HE2	29:DC:55:LYS:O	2.12	0.50
53:F:151:ASP:HB3	53:F:154:ILE:HG13	1.93	0.50
60:M:72:THR:O	60:M:88:ARG:HD2	2.11	0.50
69:V:106:ILE:HG13	69:V:107:THR:H	1.76	0.50
48:A:647:G:H22	48:A:687:G:H1	1.59	0.50
44:AQ:46:THR:HB	44:AQ:58:SER:H	1.76	0.50
1:AR:1029:G:H2'	1:AR:1030:A:C8	2.47	0.50
1:AR:2233:A:OP2	84:AR:3465:OHX:N5	2.45	0.50
1:AR:383:G:O6	84:AR:3575:OHX:N3	2.44	0.50
1:AR:501:A:H2'	1:AR:502:U:C6	2.46	0.50
5:CE:77:THR:HG23	5:CE:326:GLY:O	2.12	0.50
84:AR:3507:OHX:N2	9:CI:217:PRO:HA	2.26	0.50
19:CS:147:ARG:HB3	19:CS:150:VAL:HG13	1.94	0.50
44:DR:33:GLN:HG3	44:DR:34:HIS:CD2	2.47	0.50
64:Q:69:GLU:OE1	84:Q:201:OHX:N4	2.44	0.50
73:Z:104:SER:HB3	73:Z:107:GLN:HG3	1.93	0.50
1:1:1480:G:H4'	1:1:1481:A:OP1	2.12	0.50
1:1:1488:G:H5''	1:1:1838:G:O6	2.12	0.50
1:1:2418:G:H4'	1:1:2419:A:OP1	2.10	0.50
1:1:2730:G:OP2	84:1:3445:OHX:N5	2.44	0.50
1:1:3030:G:N7	84:1:3609:OHX:N6	2.60	0.50
48:A:848:C:H2'	48:A:849:C:C6	2.47	0.50
28:AA:14:VAL:HG13	35:AH:86:LYS:HG2	1.93	0.50
1:AR:1408:G:P	33:DG:33:ARG:HH22	2.34	0.50
1:AR:1564:U:H2'	1:AR:1565:G:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:1941:C:OP2	20:CT:74:ARG:HG2	2.12	0.50
1:AR:2618:G:P	12:CL:116:ARG:HH21	2.35	0.50
1:AR:301:G:O6	84:AR:3696:OHX:N5	2.45	0.50
50:C:70:LEU:HD21	50:C:79:HIS:ND1	2.27	0.50
5:CE:296:THR:HG21	5:CE:357:LYS:O	2.11	0.50
3:AT:59:A:O2'	26:CZ:61:LYS:NZ	2.45	0.50
55:H:57:ASP:HA	55:H:106:LEU:HA	1.93	0.50
48:A:959:U:C6	62:O:61:THR:HB	2.47	0.50
73:Z:20:ARG:HD2	73:Z:74:LEU:HB3	1.93	0.50
1:1:1460:A:H2'	1:1:1461:A:H8	1.77	0.50
1:1:3084:C:H2'	1:1:3085:G:O4'	2.12	0.50
1:1:3393:U:H2'	1:1:3394:U:H6	1.77	0.50
1:1:562:C:H2'	1:1:563:U:C6	2.46	0.50
22:2:17:ARG:O	22:2:18:ASP:HB2	2.11	0.50
29:AB:6:THR:HG22	29:AB:9:ARG:HG2	1.93	0.50
36:AI:92:LEU:HB3	36:AI:96:GLU:HG3	1.94	0.50
1:AR:172:G:N2	1:AR:247:C:O2	2.45	0.50
1:AR:2572:C:O2'	1:AR:2573:G:O4'	2.30	0.50
1:AR:1122:U:OP2	84:AR:3633:OHX:N2	2.44	0.50
8:CH:47:PHE:O	8:CH:50:LYS:HB2	2.12	0.50
28:DB:134:LEU:HD13	28:DB:136:PHE:HD2	1.77	0.50
39:DM:32:ASN:ND2	39:DM:32:ASN:O	2.44	0.50
44:DR:74:ALA:O	44:DR:78:THR:HG23	2.11	0.50
66:S:13:SER:HA	66:S:54:THR:HG22	1.93	0.50
84:A:1909:OHX:N3	84:A:2024:OHX:N5	2.60	0.50
48:A:520:A:H2'	48:A:521:A:C8	2.47	0.50
28:AA:88:ASP:HB3	28:AA:121:ARG:HH22	1.76	0.50
37:AJ:45:ARG:NH2	37:AJ:54:GLU:OE1	2.45	0.50
43:AP:46:LYS:O	84:AP:502:OHX:N6	2.45	0.50
1:AR:1942:U:OP2	20:CT:74:ARG:NH1	2.41	0.50
1:AR:2676:A:H4'	1:AR:2677:G:O5'	2.12	0.50
1:AR:3121:U:H1'	1:AR:3122:A:H5''	1.92	0.50
1:AR:422:A:C2	1:AR:2363:A:H4'	2.46	0.50
1:AR:73:C:C2	14:CN:59:ARG:HD3	2.47	0.50
50:C:176:VAL:HG12	50:C:177:GLN:H	1.77	0.50
84:AR:3405:OHX:N2	8:CH:29:LYS:O	2.45	0.50
11:CK:163:GLN:O	11:CK:166:ARG:HD3	2.12	0.50
17:CQ:73:PHE:CD2	17:CQ:78:ARG:HG2	2.46	0.50
1:AR:2737:C:H4'	22:CV:68:THR:OG1	2.11	0.50
37:DK:62:ARG:HH12	37:DK:98:ARG:HH11	1.59	0.50
52:E:211:PRO:HG3	66:S:20:TYR:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:U:57:ARG:HB2	68:U:57:ARG:HH11	1.77	0.50
49:B:56:LYS:NZ	70:W:66:ASP:OD1	2.42	0.50
72:Y:7:ARG:HH11	72:Y:7:ARG:HB2	1.77	0.50
1:1:2438:A:H2'	1:1:2439:A:C8	2.47	0.50
1:1:2882:U:H2'	1:1:2883:U:C6	2.47	0.50
48:A:1317:C:OP2	84:A:1963:OHX:N3	2.45	0.50
48:A:978:A:H2'	48:A:979:A:O4'	2.12	0.50
1:AR:1190:A:C8	1:AR:1193:A:H1'	2.46	0.50
1:AR:1701:C:H2'	1:AR:1702:U:O4'	2.11	0.50
1:AR:2251:G:O6	84:AR:3450:OHX:N6	2.45	0.50
1:AR:2922:G:O6	84:AR:3656:OHX:N2	2.45	0.50
1:AR:595:G:H1	1:AR:609:G:H5''	1.74	0.50
49:B:13:ASP:HA	49:B:16:LEU:HD12	1.94	0.50
49:B:71:GLU:O	49:B:96:THR:HG22	2.12	0.50
50:C:61:LEU:HB2	50:C:64:ARG:HE	1.76	0.50
6:CF:36:HIS:O	6:CF:40:THR:HG23	2.12	0.50
7:CG:155:THR:HG22	7:CG:179:ARG:NH1	2.27	0.50
9:CI:159:GLN:O	9:CI:161:VAL:HG23	2.11	0.50
12:CL:86:HIS:HB3	12:CL:139:ARG:HG2	1.92	0.50
11:CK:53:ILE:HD13	15:CO:7:VAL:HG21	1.93	0.50
1:AR:655:C:OP1	33:DG:27:ARG:HB3	2.11	0.50
48:A:127:G:N7	55:H:202:ARG:NH2	2.59	0.50
56:I:111:LYS:O	56:I:112:ARG:HB2	2.11	0.50
1:1:1243:G:HO2'	1:1:1271:A:HO2'	1.55	0.49
1:1:1321:G:O3'	21:O:117:ARG:NH2	2.45	0.49
1:1:1724:U:H4'	1:1:1725:C:OP1	2.10	0.49
1:1:2593:A:H4'	1:1:2594:C:O5'	2.11	0.49
84:A:1909:OHX:N4	84:A:2024:OHX:N2	2.60	0.49
37:AJ:33:ALA:HB1	37:AJ:38:LYS:HE3	1.93	0.49
11:CK:162:GLN:HG3	11:CK:163:GLN:N	2.27	0.49
29:DC:47:LYS:HE2	29:DC:48:TYR:CE1	2.47	0.49
48:A:1546:G:OP1	67:T:123:ARG:NH1	2.45	0.49
1:1:1233:G:H22	1:1:1255:C:H42	1.61	0.49
1:1:1650:G:O6	84:1:3670:OHX:N2	2.45	0.49
1:1:2744:U:OP1	84:1:3612:OHX:N1	2.45	0.49
23:5:36:TYR:OH	23:5:82:LYS:HG2	2.12	0.49
48:A:1073:G:H2'	48:A:1074:G:H5''	1.94	0.49
48:A:1175:U:H3	48:A:1464:G:H1	1.58	0.49
48:A:735:C:O2'	48:A:736:C:H5''	2.11	0.49
1:AR:3192:U:O4	84:AR:3649:OHX:N2	2.44	0.49
2:AS:91:G:H2'	2:AS:92:A:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AT:126:A:O2'	3:AT:128:U:OP2	2.19	0.49
4:CD:20:THR:HA	4:CD:23:ARG:HD2	1.94	0.49
6:CF:148:ILE:HA	6:CF:149:PRO:C	2.33	0.49
9:CI:40:LYS:HE2	9:CI:170:GLU:OE1	2.11	0.49
12:CL:210:ILE:HG23	12:CL:217:PHE:CD2	2.47	0.49
12:CL:218:ALA:HB3	84:CL:301:OHX:N3	2.26	0.49
44:DR:13:LYS:HE3	44:DR:14:TYR:CZ	2.47	0.49
52:E:142:LEU:HD11	52:E:182:LEU:HD21	1.94	0.49
53:F:32:SER:OG	53:F:81:THR:OG1	2.23	0.49
1:1:1507:G:N3	1:1:1507:G:H5'	2.27	0.49
1:1:3117:C:N3	84:1:3562:OHX:N1	2.61	0.49
1:1:501:A:H2'	1:1:502:U:C6	2.47	0.49
1:1:839:C:H4'	1:1:1724:U:H2'	1.94	0.49
2:3:112:G:H2'	2:3:113:C:C6	2.47	0.49
3:4:126:A:O2'	3:4:128:U:OP1	2.30	0.49
48:A:1498:G:OP1	68:U:75:LYS:HD3	2.12	0.49
1:AR:266:A:H2'	37:DK:30:LYS:HE2	1.94	0.49
1:AR:297:G:N2	1:AR:297:G:OP2	2.40	0.49
1:AR:830:A:H2'	1:AR:831:G:O4'	2.13	0.49
3:AT:83:C:H1'	3:AT:85:G:N2	2.27	0.49
6:CF:299:ILE:HG22	6:CF:300:ARG:O	2.12	0.49
48:A:1424:A:H1'	51:D:92:ALA:HB1	1.94	0.49
32:DF:81:GLU:O	32:DF:82:GLU:HG2	2.12	0.49
1:AR:170:G:H5'	36:DJ:109:ILE:HG23	1.94	0.49
36:DJ:74:LYS:HE3	36:DJ:75:TYR:CE2	2.47	0.49
56:I:50:ASP:N	56:I:50:ASP:OD1	2.45	0.49
71:X:46:TYR:HB3	71:X:69:LEU:HD13	1.95	0.49
1:1:2107:A:C2	1:1:3344:A:H8	2.28	0.49
84:A:1909:OHX:N3	84:A:2024:OHX:N1	2.60	0.49
48:A:393:C:H4'	48:A:1673:G:O2'	2.13	0.49
1:AR:1481:A:H2'	1:AR:1858:A:H1'	1.94	0.49
1:AR:229:G:OP2	84:AR:3638:OHX:N5	2.45	0.49
1:AR:343:U:OP2	84:AR:3427:OHX:N3	2.46	0.49
20:CT:154:ALA:O	20:CT:158:GLU:HG3	2.12	0.49
54:G:25:LEU:H	54:G:25:LEU:HD22	1.77	0.49
56:I:58:LEU:N	56:I:89:HIS:O	2.39	0.49
3:4:113:U:H5''	40:AM:7:PHE:HB3	1.94	0.49
23:5:22:PRO:HB2	23:5:28:PHE:HB2	1.95	0.49
26:8:135:ILE:O	26:8:139:ILE:HG22	2.12	0.49
48:A:1018:U:H2'	48:A:1019:A:C8	2.48	0.49
48:A:1450:U:H2'	48:A:1451:C:C6	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:1783:C:H2'	48:A:1784:C:H6	1.78	0.49
33:AF:40:SER:O	33:AF:44:ARG:HG3	2.13	0.49
1:AR:1804:A:H2'	1:AR:1805:C:C6	2.47	0.49
1:AR:1933:A:OP2	84:AR:3418:OHX:N6	2.46	0.49
1:AR:1789:G:O6	84:AR:3702:OHX:N1	2.45	0.49
9:CI:73:GLY:O	22:CV:143:THR:HB	2.12	0.49
20:CT:78:TYR:HA	20:CT:81:ARG:HD3	1.94	0.49
27:DA:71:SER:CB	27:DA:83:ASP:HB2	2.42	0.49
57:J:21:PHE:O	57:J:22:ARG:HG2	2.12	0.49
48:A:895:G:H21	63:P:38:THR:HG21	1.78	0.49
49:B:200:ASP:OD1	66:S:88:VAL:HG23	2.13	0.49
1:1:2387:A:OP2	84:1:3561:OHX:N5	2.45	0.49
1:1:637:C:HO2'	1:1:638:C:C5'	2.24	0.49
48:A:1369:U:O4	84:A:1973:OHX:N2	2.46	0.49
84:A:1909:OHX:N4	84:A:2024:OHX:N1	2.60	0.49
48:A:407:A:H2'	48:A:408:C:C6	2.48	0.49
48:A:74:U:O2'	48:A:75:U:OP2	2.30	0.49
1:AR:1039:U:H2'	1:AR:1040:A:C8	2.48	0.49
1:AR:1078:U:O4	84:AR:3503:OHX:N5	2.46	0.49
1:AR:2424:A:N1	4:CD:230:VAL:HG21	2.27	0.49
1:AR:3294:A:H2'	1:AR:3295:A:O4'	2.13	0.49
1:AR:656:A:H2'	1:AR:657:A:H8	1.76	0.49
49:B:26:ALA:HB3	49:B:149:LEU:HB2	1.94	0.49
6:CF:47:ARG:NH1	6:CF:109:TRP:O	2.45	0.49
7:CG:297:GLN:OE1	84:CG:302:OHX:N1	2.46	0.49
8:CH:56:LYS:HE3	8:CH:98:VAL:HG13	1.94	0.49
11:CK:129:ARG:O	11:CK:132:VAL:HG13	2.12	0.49
22:CV:17:ARG:O	22:CV:18:ASP:HB2	2.13	0.49
59:L:1:MET:HG2	59:L:2:LEU:N	2.27	0.49
60:M:99:ARG:NH1	72:Y:7:ARG:O	2.46	0.49
1:1:196:G:O6	84:1:3441:OHX:N6	2.46	0.49
1:1:352:A:H61	1:1:365:A:H5''	1.76	0.49
1:1:790:U:OP1	84:1:3451:OHX:N5	2.46	0.49
26:8:132:ALA:O	26:8:135:ILE:HG22	2.13	0.49
48:A:1642:G:O6	84:A:1901:OHX:N6	2.46	0.49
48:A:460:A:H5'	48:A:461:G:OP2	2.13	0.49
28:AA:87:LEU:HB2	28:AA:127:ASN:ND2	2.28	0.49
1:AR:3045:G:O3'	5:CE:275:ARG:NH1	2.45	0.49
1:AR:1409:G:O6	84:AR:3667:OHX:N6	2.45	0.49
28:DB:81:LEU:HD22	28:DB:82:PRO:HD2	1.95	0.49
52:E:116:ARG:O	52:E:120:TYR:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:E:115:ILE:HD11	52:E:138:VAL:HG21	1.95	0.49
60:M:2:SER:HB2	60:M:81:HIS:CD2	2.47	0.49
1:1:562:C:H2'	1:1:563:U:H6	1.77	0.49
23:5:32:SER:HA	23:5:35:LYS:HB3	1.95	0.49
48:A:1650:U:H2'	48:A:1651:A:C8	2.48	0.49
36:AI:76:GLN:O	36:AI:81:ARG:NH1	2.46	0.49
1:AR:1201:C:OP1	84:AR:3741:OHX:N4	2.45	0.49
1:AR:129:U:H2'	1:AR:130:A:C8	2.47	0.49
7:CG:22:ARG:HG2	7:CG:28:THR:OG1	2.13	0.49
11:CK:189:GLU:C	11:CK:191:LEU:H	2.16	0.49
51:D:188:LEU:HD13	51:D:196:VAL:HG11	1.94	0.49
40:DN:3:ALA:O	40:DN:5:LYS:HG3	2.12	0.49
55:H:67:VAL:HG21	55:H:99:GLY:HA2	1.95	0.49
57:J:70:GLU:HG3	57:J:112:TRP:CH2	2.48	0.49
1:1:2404:A:N3	1:1:2404:A:H2'	2.28	0.49
1:1:29:C:H4'	1:1:62:A:H4'	1.93	0.49
1:1:908:G:OP1	84:1:3519:OHX:N6	2.46	0.49
84:1:3540:OHX:N6	84:1:3705:OHX:N1	2.61	0.49
48:A:1000:C:N4	48:A:1003:A:OP2	2.41	0.49
48:A:1067:C:H2'	48:A:1068:C:C6	2.47	0.49
1:AR:92:G:H5'	1:AR:93:C:H5''	1.94	0.49
1:AR:993:G:N3	1:AR:2637:A:H2'	2.28	0.49
1:AR:999:G:C6	1:AR:1000:C:N4	2.81	0.49
50:C:39:GLU:HB3	50:C:73:LEU:O	2.13	0.49
10:CJ:144:GLU:OE1	37:DK:36:ARG:NH2	2.46	0.49
11:CK:101:VAL:HG22	11:CK:114:VAL:HG22	1.95	0.49
14:CN:89:TYR:CE1	14:CN:93:ILE:HD11	2.48	0.49
9:CI:121:LYS:HB2	22:CV:133:ALA:HB3	1.95	0.49
51:D:103:VAL:HG22	51:D:113:LEU:HD22	1.93	0.49
27:DA:52:ARG:O	27:DA:70:ILE:HB	2.12	0.49
57:J:5:ARG:HD3	57:J:29:LEU:O	2.13	0.49
72:Y:63:GLN:HA	72:Y:65:ASN:H	1.78	0.49
21:0:40:ARG:O	21:0:43:TYR:HB3	2.12	0.49
1:1:2419:A:H2'	1:1:2420:C:H6	1.76	0.49
1:1:3152:U:O2'	1:1:3153:U:H5'	2.13	0.49
1:1:1441:G:O6	84:1:3460:OHX:N1	2.46	0.49
1:1:2242:A:OP2	84:1:3492:OHX:N6	2.46	0.49
48:A:471:A:N7	84:A:1954:OHX:N1	2.61	0.49
48:A:800:U:H2'	48:A:801:G:H8	1.77	0.49
1:AR:2683:U:H2'	1:AR:2684:C:C6	2.48	0.49
1:AR:2989:U:O2'	5:CE:232:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CF:237:GLN:O	6:CF:246:ARG:HG3	2.13	0.49
6:CF:20:LEU:HD13	6:CF:256:THR:HG23	1.95	0.49
10:CJ:71:VAL:HG22	10:CJ:76:ALA:HB2	1.95	0.49
25:CY:17:ARG:HG3	25:CY:17:ARG:HH11	1.78	0.49
26:CZ:115:ARG:NH1	26:CZ:119:THR:OG1	2.46	0.49
38:DL:66:TYR:OH	38:DL:73:ARG:NH2	2.46	0.49
52:E:11:LEU:HD13	69:V:29:THR:HG23	1.94	0.49
58:K:125:ALA:O	58:K:129:ILE:HG13	2.12	0.49
58:K:17:ARG:O	58:K:23:ARG:NH2	2.46	0.49
54:G:37:GLN:OE1	65:R:53:LEU:HD22	2.13	0.49
69:V:18:GLN:O	69:V:96:PRO:HA	2.12	0.49
1:1:1307:G:H1'	1:1:1308:A:N7	2.28	0.48
1:1:3119:U:OP2	84:1:3427:OHX:N4	2.46	0.48
48:A:151:G:O6	73:Z:124:ARG:NH2	2.39	0.48
84:A:1909:OHX:N6	84:A:2024:OHX:N5	2.60	0.48
48:A:359:A:C2	72:Y:38:PHE:HB3	2.48	0.48
1:AR:2232:A:OP2	84:AR:3465:OHX:N3	2.46	0.48
1:AR:3228:C:H4'	1:AR:3229:G:O5'	2.13	0.48
1:AR:503:C:O2'	8:CH:23:LYS:HE2	2.13	0.48
4:CD:148:VAL:HG22	4:CD:156:LYS:O	2.12	0.48
5:CE:187:SER:O	5:CE:190:GLU:N	2.46	0.48
17:CQ:98:ALA:HA	17:CQ:101:ARG:HH11	1.76	0.48
18:CR:4:TYR:CE2	18:CR:16:SER:HB2	2.48	0.48
21:CU:24:LEU:O	22:CV:148:PRO:HA	2.13	0.48
26:CZ:115:ARG:CG	26:CZ:115:ARG:HH11	2.25	0.48
28:DB:25:ILE:HA	28:DB:43:VAL:HG12	1.95	0.48
29:DC:77:LYS:O	29:DC:79:TRP:N	2.42	0.48
1:AR:1412:G:OP1	33:DG:105:ARG:NH2	2.46	0.48
56:I:50:ASP:HA	56:I:56:LYS:HA	1.95	0.48
59:L:46:LEU:O	59:L:50:THR:HG23	2.12	0.48
66:S:88:VAL:HG13	66:S:89:SER:H	1.78	0.48
48:A:1682:U:O2'	48:A:1683:C:H5'	2.12	0.48
48:A:1756:A:OP2	48:A:1756:A:H8	1.96	0.48
36:AI:31:LEU:HD22	36:AI:47:VAL:HG11	1.95	0.48
1:AR:2689:A:H2'	1:AR:2689:A:N3	2.28	0.48
1:AR:276:U:O2	16:CP:93:LYS:NZ	2.46	0.48
1:AR:2883:U:OP2	84:AR:3567:OHX:N4	2.46	0.48
10:CJ:248:LYS:HD2	10:CJ:248:LYS:N	2.28	0.48
1:AR:3043:C:OP2	24:CX:48:ARG:NH2	2.46	0.48
36:DJ:78:LYS:HA	36:DJ:81:ARG:CD	2.43	0.48
37:DK:55:ARG:O	37:DK:58:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:I:73:VAL:C	56:I:75:THR:H	2.15	0.48
57:J:41:LYS:HA	57:J:59:ARG:O	2.13	0.48
59:L:1:MET:HG2	59:L:2:LEU:H	1.77	0.48
71:X:29:PRO:HB2	71:X:58:SER:HB3	1.95	0.48
1:1:1621:A:H2'	1:1:1622:U:C6	2.48	0.48
1:1:2924:U:O4	84:1:3554:OHX:N1	2.47	0.48
84:1:3474:OHX:N4	84:1:3730:OHX:N1	2.61	0.48
1:1:650:C:H2'	1:1:651:G:C8	2.47	0.48
2:3:62:U:O4	2:3:63:A:N6	2.46	0.48
1:1:1408:G:P	33:AF:33:ARG:HH22	2.37	0.48
1:AR:1059:G:OP2	84:AR:3653:OHX:N4	2.47	0.48
1:AR:1258:U:O2	1:AR:1260:A:H8	1.96	0.48
1:AR:1778:G:O2'	1:AR:1780:G:OP2	2.28	0.48
1:AR:3112:G:O2'	11:CK:70:THR:HB	2.14	0.48
1:AR:847:A:H2'	1:AR:848:A:C8	2.48	0.48
4:CD:83:HIS:CE1	4:CD:86:GLN:HB2	2.48	0.48
5:CE:283:TYR:OH	5:CE:325:LYS:HD3	2.14	0.48
10:CJ:171:LYS:NZ	10:CJ:223:ALA:O	2.46	0.48
16:CP:136:ASP:OD1	16:CP:138:GLN:HG2	2.14	0.48
10:CJ:162:LEU:HA	16:CP:7:LEU:HD11	1.95	0.48
53:F:160:VAL:HG13	53:F:169:ILE:HG23	1.96	0.48
55:H:64:LYS:NZ	55:H:82:SER:OG	2.46	0.48
59:L:77:ARG:HG3	59:L:82:LEU:HD12	1.96	0.48
1:1:1495:U:C5	1:1:1835:A:N1	2.81	0.48
1:1:3035:A:OP2	84:1:3610:OHX:N4	2.46	0.48
1:1:916:G:H5'	1:1:917:A:OP1	2.13	0.48
48:A:1536:G:C6	48:A:1538:U:H1'	2.48	0.48
48:A:158:U:O2'	48:A:159:U:H3'	2.13	0.48
48:A:505:A:H2'	48:A:505:A:N3	2.28	0.48
44:AQ:74:ALA:O	44:AQ:78:THR:HG23	2.12	0.48
1:AR:2533:G:H2'	1:AR:2534:G:O4'	2.12	0.48
1:AR:3089:C:H2'	1:AR:3090:U:O4'	2.13	0.48
1:AR:671:U:OP2	19:CS:57:ILE:HD12	2.13	0.48
16:CP:96:ARG:HG2	16:CP:96:ARG:NH1	2.28	0.48
62:O:87:ASP:OD1	62:O:88:LEU:N	2.45	0.48
21:O:42:TRP:O	21:O:46:GLN:HG3	2.14	0.48
1:1:307:A:H2'	1:1:308:A:C8	2.48	0.48
1:1:2418:G:O6	84:1:3652:OHX:N1	2.47	0.48
1:1:440:A:OP2	1:1:440:A:H8	1.97	0.48
48:A:1194:A:OP2	69:V:75:GLY:N	2.41	0.48
48:A:1140:G:N7	84:A:1943:OHX:N1	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:197:A:H61	57:J:138:ASN:ND2	2.11	0.48
48:A:346:G:O6	84:A:2003:OHX:N5	2.46	0.48
48:A:484:C:N4	48:A:503:G:H22	2.11	0.48
1:1:295:A:OP1	37:AJ:53:TYR:HE2	1.97	0.48
42:AO:6:ARG:O	42:AO:10:THR:HG23	2.14	0.48
1:AR:789:A:H2'	1:AR:790:U:C6	2.47	0.48
84:AR:3528:OHX:N6	3:AT:31:G:OP2	2.47	0.48
7:CG:58:LYS:HD2	7:CG:93:THR:HG21	1.96	0.48
4:CD:64:ARG:HH22	10:CJ:38:GLN:HA	1.78	0.48
13:CM:49:LYS:HB3	13:CM:62:ASN:HA	1.95	0.48
15:CO:72:LEU:HD22	15:CO:73:PRO:HD2	1.94	0.48
18:CR:28:ASN:O	18:CR:32:THR:HG23	2.13	0.48
28:DB:52:LYS:O	28:DB:65:ARG:NH2	2.45	0.48
29:DC:73:LEU:HD13	29:DC:109:TYR:CZ	2.49	0.48
54:G:216:GLU:HA	54:G:219:ARG:HB3	1.96	0.48
65:R:55:VAL:HG22	65:R:59:LYS:HE3	1.95	0.48
67:T:134:ARG:HB2	67:T:136:GLN:OE1	2.14	0.48
1:1:1742:U:H2'	1:1:1743:G:C8	2.48	0.48
1:1:2986:U:H2'	1:1:2987:A:C8	2.49	0.48
48:A:327:U:H2'	48:A:328:A:C8	2.48	0.48
48:A:859:A:C6	62:O:73:ARG:HD3	2.48	0.48
28:AA:46:ILE:HD11	28:AA:48:ARG:C	2.33	0.48
34:AG:30:ILE:HB	34:AG:81:VAL:HG12	1.96	0.48
43:AP:43:TYR:CZ	43:AP:47:GLN:NE2	2.77	0.48
1:1:860:G:OP1	44:AQ:17:ARG:NH1	2.47	0.48
1:AR:1587:A:OP1	84:AR:3495:OHX:N5	2.47	0.48
1:AR:304:G:H5'	1:AR:304:G:N3	2.28	0.48
1:AR:385:A:H2'	1:AR:386:A:C8	2.48	0.48
1:AR:728:G:OP1	84:AR:3716:OHX:N6	2.45	0.48
10:CJ:134:TYR:CD2	10:CJ:190:VAL:HG21	2.48	0.48
12:CL:25:ALA:O	12:CL:122:PRO:HG2	2.14	0.48
14:CN:10:LEU:HD23	19:CS:166:LEU:HD11	1.95	0.48
66:S:27:ASP:OD2	66:S:30:THR:HG22	2.14	0.48
67:T:28:ILE:HG13	67:T:61:LEU:HD11	1.94	0.48
1:1:2861:U:OP1	84:1:3403:OHX:N1	2.47	0.48
1:1:304:G:N3	1:1:304:G:H5'	2.28	0.48
1:1:844:G:O6	84:1:3457:OHX:N5	2.47	0.48
22:2:46:GLY:O	22:2:49:GLN:NE2	2.46	0.48
27:9:79:ALA:HB1	27:9:98:ASN:HB3	1.96	0.48
48:A:115:G:OP1	60:M:67:ARG:NH1	2.46	0.48
48:A:1207:C:N4	48:A:1456:C:H5	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:1226:A:O2'	48:A:1227:A:OP1	2.32	0.48
48:A:452:A:H3'	48:A:453:U:C5	2.49	0.48
48:A:591:A:H2'	48:A:592:A:H8	1.78	0.48
48:A:694:U:H5	56:I:96:ARG:O	1.96	0.48
41:AN:110:CYS:SG	41:AN:112:LYS:HB2	2.53	0.48
44:AQ:87:ARG:HD3	57:J:96:LEU:O	102.83	0.48
1:AR:509:U:O4	84:AR:3721:OHX:N1	2.46	0.48
1:AR:786:A:H4'	1:AR:787:G:H5'	1.96	0.48
3:AT:154:C:H5''	10:CJ:181:LYS:HG2	1.95	0.48
4:CD:45:VAL:HG12	4:CD:88:ILE:HD13	1.95	0.48
5:CE:286:GLY:HA3	5:CE:321:PHE:CZ	2.49	0.48
1:AR:992:A:H5''	22:CV:43:LYS:HD2	1.96	0.48
26:CZ:132:ALA:O	26:CZ:136:ALA:N	2.46	0.48
1:AR:1433:A:P	33:DG:19:ARG:HH22	2.37	0.48
54:G:146:THR:HG23	54:G:221:ALA:HA	1.95	0.48
69:V:42:VAL:HG21	69:V:55:PRO:HD3	1.95	0.48
72:Y:6:PRO:HG3	72:Y:14:LYS:HG2	1.95	0.48
1:1:2534:G:H2'	1:1:2535:A:H8	1.79	0.48
1:1:2771:U:O2'	1:1:2772:C:O5'	2.32	0.48
1:1:283:G:O6	1:1:304:G:H1'	2.12	0.48
1:1:1119:C:OP2	84:1:3490:OHX:N1	2.47	0.48
1:1:679:U:OP2	84:1:3646:OHX:N6	2.47	0.48
26:8:92:LYS:HE3	26:8:110:VAL:O	2.13	0.48
48:A:1486:G:H1'	48:A:1592:A:O2'	2.14	0.48
1:AR:2586:G:C5	10:CJ:241:LYS:HB2	2.49	0.48
1:AR:3155:U:H3'	1:AR:3156:U:C4'	2.44	0.48
1:AR:595:G:C8	1:AR:609:G:C6	3.01	0.48
3:AT:141:C:OP2	84:AT:218:OHX:N2	2.47	0.48
28:DB:83:THR:HG23	28:DB:85:TYR:N	2.29	0.48
52:E:29:LEU:HD21	52:E:69:LEU:HD11	1.96	0.48
54:G:147:THR:OG1	54:G:148:ARG:N	2.46	0.48
57:J:184:LEU:HB3	57:J:189:LEU:HD13	1.96	0.48
60:M:71:LEU:HB3	60:M:88:ARG:NH1	2.29	0.48
64:Q:121:ILE:HG23	64:Q:123:TYR:H	1.78	0.48
1:1:2407:C:H1'	1:1:2818:U:O2	2.14	0.48
1:1:2895:G:C2'	1:1:2896:A:H5''	2.43	0.48
1:1:1440:G:O6	84:1:3460:OHX:N1	2.47	0.48
1:1:821:U:OP2	84:1:3515:OHX:N3	2.46	0.48
2:3:60:G:H2'	2:3:61:G:C8	2.49	0.48
48:A:1776:A:H2'	48:A:1777:G:C8	2.48	0.48
35:AH:46:ASP:OD1	35:AH:80:ARG:NH1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:AL:7:ASP:HB3	39:AL:10:GLN:HB3	1.95	0.48
1:AR:439:C:H5'	1:AR:440:A:C8	2.48	0.48
1:AR:662:U:H2'	1:AR:663:C:C6	2.48	0.48
50:C:171:ILE:HD13	50:C:196:GLU:HG2	1.96	0.48
5:CE:41:VAL:CA	5:CE:185:GLY:HA3	2.23	0.48
5:CE:256:HIS:HA	5:CE:257:PRO:C	2.33	0.48
5:CE:53:MET:HE1	5:CE:327:CYS:HB3	1.94	0.48
20:CT:158:GLU:OE1	20:CT:159:ALA:N	2.47	0.48
35:DI:42:PRO:HB2	35:DI:51:LEU:HD21	1.96	0.48
56:I:51:VAL:HG11	56:I:168:SER:HB3	1.95	0.48
57:J:54:LYS:HG2	57:J:175:GLN:O	2.14	0.48
60:M:5:LEU:HD12	60:M:6:THR:HG23	1.95	0.48
62:O:27:LYS:HD2	62:O:28:LEU:HG	1.94	0.48
65:R:50:GLU:OE2	65:R:82:ARG:NH2	2.39	0.48
69:V:42:VAL:HG13	69:V:52:LYS:NZ	2.29	0.48
73:Z:113:ASN:HA	73:Z:116:LYS:HD3	1.94	0.48
1:1:1355:A:H4'	1:1:1356:U:O5'	2.13	0.48
1:1:3006:A:H2'	1:1:3007:U:O4'	2.13	0.48
1:1:1160:C:OP1	84:1:3503:OHX:N6	2.47	0.48
1:1:543:C:H42	1:1:548:G:H1	1.61	0.48
27:9:112:ASP:H	27:9:115:ARG:HB2	1.79	0.48
48:A:1017:U:H2'	48:A:1018:U:H6	1.78	0.48
48:A:1410:A:H2'	48:A:1411:A:O4'	2.14	0.48
48:A:703:G:H2'	48:A:704:C:H5'	1.95	0.48
28:AA:25:ILE:HA	28:AA:43:VAL:HG12	1.96	0.48
36:AI:31:LEU:HB3	36:AI:44:ILE:HG13	1.95	0.48
38:AK:21:ARG:HD2	38:AK:37:CYS:SG	2.54	0.48
1:AR:1662:G:N2	1:AR:1788:C:O2	2.46	0.48
5:CE:387:LEU:O	84:CE:402:OHX:N2	2.47	0.48
14:CN:64:LYS:HG3	29:DC:69:TRP:CG	2.49	0.48
1:AR:353:G:O6	38:DL:55:ARG:NH1	2.47	0.48
67:T:102:ALA:O	67:T:105:VAL:HG12	2.13	0.48
64:Q:18:ARG:HG2	67:T:92:ILE:HA	1.95	0.48
58:K:61:THR:HA	71:X:97:ARG:HH12	1.78	0.48
1:1:1367:G:OP1	33:AF:45:ARG:NH2	2.47	0.47
1:1:1599:G:OP1	84:1:3687:OHX:N5	2.47	0.47
1:1:1734:G:N7	84:1:3450:OHX:N5	2.61	0.47
1:1:174:C:H2'	1:1:175:C:C6	2.48	0.47
1:1:3295:A:H2'	1:1:3296:A:C8	2.49	0.47
1:1:1934:G:N7	84:1:3420:OHX:N2	2.62	0.47
1:1:722:G:O6	84:1:3552:OHX:N6	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:637:C:H2'	1:1:638:C:H6	1.72	0.47
1:1:83:U:OP1	84:1:3716:OHX:N3	2.47	0.47
48:A:641:G:H1	48:A:693:U:H3	1.61	0.47
1:1:3275:U:H5'	34:AG:68:TRP:CZ2	2.49	0.47
42:AO:8:LYS:HD3	42:AO:12:ARG:HH21	1.78	0.47
44:AQ:84:ARG:HG2	44:AQ:87:ARG:NH2	2.30	0.47
1:AR:1540:U:OP1	84:AR:3599:OHX:N4	2.46	0.47
1:AR:849:C:H2'	1:AR:850:U:H6	1.79	0.47
5:CE:306:THR:OG1	5:CE:316:GLU:O	2.28	0.47
7:CG:297:GLN:OE1	84:CG:302:OHX:N5	2.47	0.47
10:CJ:139:VAL:O	10:CJ:143:ILE:HG13	2.13	0.47
12:CL:9:TYR:CG	12:CL:97:LEU:HD13	2.48	0.47
20:CT:105:LEU:HD13	20:CT:138:LEU:HD12	1.96	0.47
26:CZ:105:VAL:HG13	26:CZ:130:TYR:CD2	2.48	0.47
29:DC:74:ASN:HD22	29:DC:115:LYS:H	1.62	0.47
30:DD:23:LYS:CD	30:DD:24:PRO:HD2	2.44	0.47
62:O:93:LYS:HG3	62:O:150:VAL:HG11	1.96	0.47
63:P:29:HIS:HB3	63:P:41:ARG:HG3	1.95	0.47
64:Q:87:PRO:HA	64:Q:90:ILE:HG13	1.96	0.47
21:O:167:ARG:HG3	21:O:168:PRO:HD2	1.95	0.47
1:1:2258:U:OP2	84:1:3468:OHX:N5	2.47	0.47
1:1:274:G:O6	84:1:3526:OHX:N2	2.47	0.47
1:1:994:G:O6	84:1:3622:OHX:N2	2.48	0.47
48:A:105:A:H4'	57:J:8:ARG:HH11	1.79	0.47
48:A:1487:A:OP2	52:E:8:LYS:NZ	2.47	0.47
48:A:240:U:H4'	48:A:241:U:OP2	2.13	0.47
48:A:851:U:H2'	48:A:852:C:C6	2.49	0.47
1:AR:980:A:H2	1:AR:1104:G:HO2'	1.61	0.47
84:AR:3507:OHX:N6	9:CI:217:PRO:O	2.47	0.47
7:CG:129:TYR:CD2	7:CG:177:GLU:HG2	2.49	0.47
11:CK:171:ASP:OD1	11:CK:173:ARG:HD3	2.14	0.47
12:CL:161:GLY:O	12:CL:163:GLN:NE2	2.47	0.47
16:CP:143:ARG:NH2	36:DJ:92:LEU:HD23	2.29	0.47
20:CT:129:GLY:O	20:CT:130:ASN:HB2	2.14	0.47
9:CI:77:VAL:HG13	22:CV:139:ARG:HG2	1.96	0.47
51:D:111:VAL:O	51:D:136:VAL:HA	2.14	0.47
1:AR:1410:U:O2'	33:DG:95:GLU:OE1	2.29	0.47
53:F:187:ARG:O	53:F:187:ARG:HD3	2.15	0.47
53:F:35:PRO:HB2	53:F:36:HIS:CD2	2.49	0.47
55:H:98:ARG:NH2	55:H:101:ILE:O	2.42	0.47
56:I:41:LEU:HD13	56:I:70:PHE:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:V:24:ILE:HG12	69:V:116:VAL:HG13	1.96	0.47
84:1:3474:OHX:N5	84:1:3730:OHX:N6	2.62	0.47
1:1:2172:A:OP1	84:1:3596:OHX:N4	2.47	0.47
1:1:627:U:H2'	1:1:628:A:C8	2.50	0.47
48:A:1687:U:H1'	48:A:1715:G:N2	2.29	0.47
48:A:704:C:O2	48:A:705:U:H1'	2.14	0.47
28:AA:53:VAL:HA	28:AA:57:HIS:CD2	2.50	0.47
32:AE:19:ARG:HD3	32:AE:35:GLU:HG3	1.97	0.47
43:AP:77:CYS:O	43:AP:78:LYS:HD3	2.14	0.47
1:AR:198:A:N3	1:AR:218:G:O2'	2.44	0.47
1:AR:3275:U:H5	1:AR:3276:G:H21	1.62	0.47
1:AR:2428:U:O4	84:AR:3720:OHX:N5	2.47	0.47
3:AT:16:G:OP1	84:AT:216:OHX:N2	2.47	0.47
50:C:61:LEU:CD2	50:C:62:LYS:H	2.26	0.47
5:CE:185:GLY:O	5:CE:191:LYS:NZ	2.23	0.47
5:CE:214:MET:SD	5:CE:281:LYS:HB2	2.54	0.47
6:CF:23:PRO:O	6:CF:25:VAL:HG23	2.14	0.47
7:CG:51:LEU:HB2	7:CG:144:VAL:CG1	2.45	0.47
8:CH:52:VAL:HG11	8:CH:65:ILE:HG13	1.96	0.47
18:CR:67:ILE:HG13	18:CR:82:ARG:CZ	2.45	0.47
20:CT:13:SER:OG	20:CT:38:ARG:NH2	2.48	0.47
20:CT:140:GLU:O	20:CT:144:GLN:HB2	2.13	0.47
26:CZ:105:VAL:HG12	26:CZ:106:ASP:H	1.79	0.47
28:DB:46:ILE:HD11	28:DB:48:ARG:C	2.34	0.47
1:1:1856:C:OP2	84:1:3684:OHX:N5	2.47	0.47
1:1:299:G:N7	84:1:3616:OHX:N2	2.61	0.47
48:A:71:A:H2'	48:A:72:A:O4'	2.14	0.47
48:A:848:C:H2'	48:A:849:C:H6	1.79	0.47
28:AA:9:LYS:HD2	28:AA:83:THR:O	2.14	0.47
1:AR:1682:U:O4	23:CW:90:ARG:NH1	2.47	0.47
1:AR:2432:A:OP2	84:AR:3629:OHX:N6	2.47	0.47
1:AR:92:G:H5''	1:AR:94:G:N7	2.29	0.47
5:CE:106:TRP:HB2	5:CE:133:TYR:CE2	2.50	0.47
51:D:140:ARG:HH22	51:D:228:ASN:HD21	1.61	0.47
33:DG:60:ASN:OD1	33:DG:62:LYS:HB2	2.14	0.47
38:DL:54:LYS:O	38:DL:58:THR:HG23	2.14	0.47
43:DQ:46:LYS:O	84:DQ:201:OHX:N3	2.47	0.47
66:S:66:VAL:HB	66:S:69:ILE:HD11	1.95	0.47
1:1:2617:U:H5	1:1:2621:G:OP2	1.97	0.47
3:4:26:U:H2'	3:4:27:U:C6	2.50	0.47
48:A:1183:A:C6	48:A:1184:A:N1	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:705:U:H2'	48:A:706:A:C8	2.49	0.47
1:1:661:G:OP2	29:AB:12:ARG:NH2	2.47	0.47
30:AC:14:ARG:CZ	30:AC:18:ARG:HD2	2.45	0.47
34:AG:16:TYR:OH	34:AG:91:ALA:HB2	2.14	0.47
1:AR:2100:A:N7	1:AR:2101:C:N4	2.62	0.47
1:AR:2338:C:OP1	5:CE:236:LYS:NZ	2.47	0.47
1:AR:3263:G:N7	84:AR:3625:OHX:N2	2.62	0.47
50:C:144:ARG:HB3	50:C:208:GLN:HB3	1.95	0.47
5:CE:257:PRO:HG2	5:CE:261:MET:CE	2.45	0.47
14:CN:76:THR:OG1	14:CN:77:LEU:N	2.45	0.47
8:CH:89:THR:HG21	15:CO:115:PHE:HB2	1.95	0.47
20:CT:165:LYS:C	20:CT:167:ARG:H	2.17	0.47
35:DI:74:ARG:HG2	35:DI:75:ALA:N	2.30	0.47
37:DK:79:SER:HB2	37:DK:81:THR:HG23	1.96	0.47
61:N:67:THR:HG22	61:N:68:GLU:HG3	1.96	0.47
72:Y:27:ASN:O	72:Y:31:LYS:HG2	2.14	0.47
1:1:1093:A:N3	1:1:1096:U:N3	2.63	0.47
2:3:59:U:OP2	84:3:205:OHX:N3	2.46	0.47
24:6:125:LEU:HB3	24:6:126:TRP:CD1	2.49	0.47
26:8:103:TYR:CE1	26:8:139:ILE:HD12	2.50	0.47
30:AC:23:LYS:HA	30:AC:23:LYS:HD2	1.77	0.47
32:AE:81:GLU:O	32:AE:82:GLU:HG2	2.14	0.47
1:AR:116:A:OP1	37:DK:36:ARG:NH1	2.48	0.47
1:AR:1176:C:H2'	1:AR:1177:G:N2	2.29	0.47
1:AR:212:G:OP2	27:DA:2:ALA:N	2.46	0.47
1:AR:2746:A:H2'	1:AR:2747:A:O4'	2.14	0.47
1:AR:3393:U:H2'	1:AR:3394:U:C6	2.49	0.47
1:AR:3152:U:O2	84:AR:3730:OHX:N5	2.46	0.47
48:A:1587:A:O2'	54:G:104:ASN:OD1	2.18	0.47
56:I:30:SER:O	56:I:31:SER:HB2	2.13	0.47
60:M:5:LEU:C	60:M:7:VAL:H	2.17	0.47
1:1:2660:G:O3'	1:1:2749:G:N2	2.48	0.47
1:1:23:A:OP2	84:1:3406:OHX:N3	2.47	0.47
3:4:125:U:HO2'	3:4:126:A:P	2.38	0.47
3:4:143:U:H2'	3:4:144:G:O4'	2.14	0.47
48:A:325:G:O4'	60:M:80:MET:HE1	2.15	0.47
48:A:358:U:OP2	84:A:1966:OHX:N4	2.47	0.47
29:AB:6:THR:HG23	29:AB:8:THR:H	1.79	0.47
1:AR:2799:A:H5''	1:AR:2800:G:O5'	2.14	0.47
5:CE:159:ARG:HG2	5:CE:182:GLN:HA	1.97	0.47
7:CG:179:ARG:HD3	7:CG:179:ARG:HA	1.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:563:U:OP1	21:CU:71:LYS:NZ	2.47	0.47
1:AR:1456:A:N7	32:DF:26:LYS:HE2	2.30	0.47
36:DJ:101:THR:HG22	36:DJ:104:GLN:H	1.80	0.47
52:E:32:GLU:HG3	52:E:57:ASP:HB2	1.96	0.47
48:A:169:A:OP1	55:H:137:ARG:HG3	2.14	0.47
69:V:22:ILE:HG22	69:V:93:LEU:HB2	1.96	0.47
1:1:871:U:H2'	1:1:872:U:C6	2.49	0.47
24:6:18:PRO:HA	24:6:51:ALA:HA	1.96	0.47
48:A:1517:U:OP2	48:A:1518:C:N4	2.43	0.47
48:A:1657:U:H4'	48:A:1658:G:O5'	2.13	0.47
48:A:195:G:H2'	48:A:196:G:H5'	1.96	0.47
48:A:138:A:H62	48:A:266:A:H61	1.62	0.47
28:AA:104:PRO:O	28:AA:108:GLU:HG3	2.15	0.47
32:AE:19:ARG:HD3	32:AE:35:GLU:CG	2.45	0.47
32:AE:44:MET:HB2	32:AE:46:THR:HG22	1.95	0.47
1:AR:1636:U:H5''	28:DB:73:LYS:NZ	2.30	0.47
1:AR:3376:A:H5'	1:AR:3377:G:H5''	1.95	0.47
84:AR:3526:OHX:N2	84:AR:3721:OHX:N6	2.62	0.47
50:C:58:SER:O	50:C:62:LYS:HG3	2.15	0.47
1:AR:1348:U:OP2	19:CS:38:ARG:NH2	2.48	0.47
26:CZ:48:SER:OG	26:CZ:49:LYS:N	2.48	0.47
32:DF:79:ARG:NE	32:DF:79:ARG:H	2.12	0.47
36:DJ:78:LYS:HA	36:DJ:81:ARG:HD3	1.97	0.47
37:DK:26:ILE:HG13	37:DK:26:ILE:H	1.45	0.47
52:E:119:ALA:O	52:E:123:VAL:HG23	2.15	0.47
57:J:34:ALA:HB2	57:J:56:ARG:HG3	1.96	0.47
58:K:127:VAL:HG12	58:K:131:GLN:OE1	2.15	0.47
64:Q:22:LEU:HD21	64:Q:109:PRO:HB3	1.97	0.47
1:1:1245:A:C3'	1:1:1246:G:H5''	2.45	0.47
1:1:3066:U:H2'	1:1:3067:C:C6	2.49	0.47
48:A:1291:G:H22	48:A:1324:G:N2	2.10	0.47
48:A:1537:C:N4	48:A:1572:G:H1	2.11	0.47
29:AB:74:ASN:HB3	29:AB:115:LYS:HB2	1.97	0.47
34:AG:85:PHE:O	84:AG:201:OHX:N1	2.47	0.47
1:1:1488:G:O2'	35:AH:10:ARG:O	2.30	0.47
42:AO:13:LEU:O	42:AO:17:ARG:HG3	2.15	0.47
1:AR:3017:A:OP2	84:AR:3489:OHX:N6	2.47	0.47
1:AR:3065:G:O6	84:AR:3611:OHX:N6	2.48	0.47
1:AR:627:U:H2'	1:AR:628:A:C8	2.50	0.47
50:C:125:VAL:HG21	50:C:173:THR:HG22	1.96	0.47
50:C:62:LYS:O	50:C:64:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CE:232:ARG:NH1	5:CE:269:GLN:O	2.47	0.47
9:CI:163:LEU:O	9:CI:165:ASP:N	2.46	0.47
10:CJ:84:ARG:H	10:CJ:84:ARG:HE	1.63	0.47
14:CN:42:ARG:O	14:CN:46:ILE:HG12	2.14	0.47
16:CP:65:ARG:HG2	16:CP:127:TYR:CD1	2.50	0.47
51:D:44:LEU:HD21	51:D:247:ALA:HB2	1.96	0.47
60:M:97:TYR:O	60:M:99:ARG:HG2	2.15	0.47
71:X:27:ILE:HG12	71:X:61:ILE:HB	1.96	0.47
1:1:109:A:H4'	1:1:110:G:OP1	2.14	0.47
1:1:1845:G:O2'	38:AK:5:THR:HG22	2.14	0.47
1:1:230:U:H2'	1:1:231:G:O4'	2.15	0.47
1:1:2727:A:C2	29:AB:43:ILE:HG23	2.50	0.47
27:9:37:LYS:H	27:9:37:LYS:CD	2.28	0.47
1:1:1491:A:OP2	40:AM:2:ALA:N	2.48	0.47
1:AR:2697:A:H2'	1:AR:2698:G:C8	2.50	0.47
1:AR:629:U:H2'	1:AR:630:A:C8	2.50	0.47
5:CE:114:VAL:O	5:CE:117:ARG:HB3	2.15	0.47
5:CE:303:LYS:HD2	5:CE:361:THR:HG21	1.96	0.47
17:CQ:16:VAL:HG23	17:CQ:42:ASN:O	2.15	0.47
32:DF:78:LYS:HG2	32:DF:79:ARG:HH21	1.80	0.47
53:F:36:HIS:CG	53:F:85:GLY:HA3	2.49	0.47
57:J:83:TYR:HB3	57:J:101:ILE:HB	1.95	0.47
59:L:28:ASN:N	59:L:28:ASN:OD1	2.48	0.47
70:W:71:ARG:HB2	70:W:83:TRP:CE2	2.50	0.47
1:1:2726:C:O2'	1:1:2727:A:H2'	2.15	0.47
1:1:662:U:H2'	1:1:663:C:C6	2.49	0.47
48:A:1244:A:O2'	48:A:1245:G:OP1	2.31	0.47
1:AR:1954:G:H2'	1:AR:1955:U:C6	2.50	0.47
1:AR:2263:C:O2'	1:AR:2264:U:P	2.72	0.47
1:AR:3163:A:H2'	1:AR:3164:C:H5'	1.97	0.47
1:AR:3306:U:H2'	1:AR:3307:A:H5''	1.96	0.47
1:AR:23:A:OP1	84:AR:3410:OHX:N4	2.48	0.47
2:AS:10:C:OP2	22:CV:26:HIS:ND1	2.42	0.47
2:AS:5:G:OP1	13:CM:143:ARG:NH2	2.48	0.47
49:B:169:SER:O	49:B:173:ILE:HG12	2.15	0.47
13:CM:109:HIS:CD2	13:CM:114:ILE:HG21	2.49	0.47
6:CF:112:LYS:HG3	16:CP:202:TYR:HB3	1.96	0.47
31:DE:13:LYS:HB3	31:DE:100:ILE:CG2	2.44	0.47
57:J:119:GLN:O	57:J:120:THR:OG1	2.32	0.47
57:J:84:HIS:CE1	57:J:86:SER:HB2	2.49	0.47
1:1:2778:G:C2'	1:1:2779:A:H5'	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:9:73:VAL:HA	27:9:80:VAL:HG23	1.97	0.46
48:A:1688:U:H2'	48:A:1689:A:C8	2.51	0.46
48:A:704:C:N4	48:A:735:C:N3	2.63	0.46
1:1:750:G:P	30:AC:40:ARG:HH21	2.38	0.46
1:AR:1899:G:O6	84:AR:3448:OHX:N6	2.48	0.46
1:AR:945:C:H2'	1:AR:946:U:C6	2.50	0.46
2:AS:106:U:H2'	2:AS:107:C:C6	2.50	0.46
1:1:120:G:N1	63:P:124:ASP:OD1	126.10	0.46
54:G:27:THR:HG21	65:R:30:LYS:HE3	1.97	0.46
72:Y:91:GLY:C	72:Y:93:LEU:H	2.19	0.46
1:1:1286:A:N3	1:1:1287:A:H1'	2.30	0.46
1:1:653:A:OP1	84:1:3465:OHX:N4	2.48	0.46
1:1:1615:C:OP1	84:1:3711:OHX:N5	2.47	0.46
1:1:879:U:O2	1:1:2357:A:H1'	2.15	0.46
1:1:929:A:H2'	1:1:930:U:C6	2.50	0.46
2:3:19:C:H2'	2:3:20:A:C8	2.50	0.46
1:1:2585:G:C6	26:8:24:LEU:HD13	2.49	0.46
27:9:71:SER:HB3	27:9:83:ASP:CB	2.45	0.46
1:AR:1881:A:OP2	84:AR:3536:OHX:N6	2.47	0.46
1:AR:871:U:H2'	1:AR:872:U:C6	2.51	0.46
1:AR:956:U:H2'	1:AR:957:C:C6	2.50	0.46
50:C:193:ILE:O	50:C:197:ILE:HG12	2.16	0.46
5:CE:169:THR:O	84:CE:401:OHX:N3	2.49	0.46
8:CH:65:ILE:HD13	8:CH:77:ARG:O	2.15	0.46
12:CL:76:MET:HE1	12:CL:138:VAL:HG21	1.97	0.46
13:CM:139:THR:HG22	13:CM:146:GLY:O	2.15	0.46
19:CS:83:VAL:O	19:CS:103:ALA:HA	2.15	0.46
22:CV:6:GLY:H	22:CV:9:SER:HB2	1.80	0.46
27:DA:69:LYS:O	27:DA:83:ASP:N	2.40	0.46
1:AR:1488:G:O2'	35:DI:10:ARG:O	2.32	0.46
55:H:176:GLN:HG3	55:H:177:ARG:H	1.81	0.46
48:A:1:U:O4	58:K:54:ARG:HD3	2.15	0.46
63:P:42:VAL:HA	63:P:46:MET:SD	2.55	0.46
48:A:1347:U:O2	48:A:1516:A:H5'	2.15	0.46
48:A:1681:A:H2'	48:A:1682:U:H5'	1.97	0.46
1:AR:623:U:OP2	84:AR:3613:OHX:N6	2.48	0.46
50:C:138:PHE:CD1	50:C:214:LYS:HB3	2.51	0.46
5:CE:386:ASP:HB3	5:CE:387:LEU:H	1.45	0.46
5:CE:88:GLY:O	5:CE:161:LEU:N	2.31	0.46
6:CF:82:THR:HG23	6:CF:85:SER:H	1.80	0.46
7:CG:58:LYS:HD2	7:CG:93:THR:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:CJ:149:LYS:HG2	10:CJ:201:THR:O	2.16	0.46
11:CK:122:LYS:HD3	11:CK:123:ILE:N	2.30	0.46
19:CS:177:GLY:O	19:CS:186:VAL:N	2.39	0.46
20:CT:24:LEU:HD12	20:CT:50:ILE:HG12	1.96	0.46
39:DM:27:ILE:HB	39:DM:78:LEU:HD11	1.97	0.46
56:I:155:ASP:OD1	56:I:156:SER:N	2.33	0.46
63:P:29:HIS:O	63:P:29:HIS:ND1	2.48	0.46
71:X:104:LEU:HB2	71:X:125:ILE:HA	1.96	0.46
1:1:2295:A:OP1	24:6:63:LYS:NZ	2.46	0.46
1:1:2697:A:H2'	1:1:2698:G:C8	2.51	0.46
27:9:56:VAL:HG11	27:9:104:LEU:HD13	1.98	0.46
48:A:1358:G:H2'	48:A:1359:C:C6	2.49	0.46
48:A:760:A:OP2	84:A:1939:OHX:N4	2.49	0.46
40:AM:30:ARG:HE	40:AM:30:ARG:HB2	1.46	0.46
43:AP:8:ARG:O	43:AP:23:HIS:N	2.47	0.46
1:AR:1317:A:O2'	1:AR:1318:A:H3'	2.15	0.46
1:AR:2295:A:OP1	24:6:63:LYS:NZ	2.45	0.46
1:AR:873:C:H5''	1:AR:874:U:O5'	2.16	0.46
1:AR:408:A:N6	3:AT:15:G:H1'	2.30	0.46
50:C:128:LYS:HE3	50:C:132:ASP:HB3	1.96	0.46
5:CE:221:THR:HG22	5:CE:272:TYR:H	1.80	0.46
6:CF:138:ARG:NH2	6:CF:240:PRO:HB2	2.31	0.46
6:CF:26:PHE:HA	6:CF:127:ALA:HA	1.98	0.46
10:CJ:161:GLU:OE1	16:CP:26:ARG:NH1	2.40	0.46
11:CK:86:TYR:CD1	11:CK:151:VAL:HG13	2.51	0.46
13:CM:23:VAL:HG11	13:CM:29:ARG:HG2	1.96	0.46
20:CT:40:ALA:O	20:CT:44:LEU:HD23	2.15	0.46
27:DA:37:LYS:H	27:DA:37:LYS:CD	2.27	0.46
32:DF:80:ASN:OD1	32:DF:81:GLU:N	2.49	0.46
53:F:106:LYS:HG3	53:F:108:ARG:NH1	2.30	0.46
63:P:19:ILE:HG12	63:P:28:VAL:HG22	1.96	0.46
63:P:20:TYR:HB3	63:P:27:PHE:HB2	1.97	0.46
1:1:1240:A:H3'	1:1:1241:U:C5'	2.46	0.46
1:1:1608:C:H2'	1:1:1609:C:H6	1.81	0.46
1:1:1667:A:H2'	1:1:1668:G:C8	2.51	0.46
1:1:2187:G:OP2	84:1:3538:OHX:N2	2.49	0.46
1:1:2565:U:H2'	1:1:2566:C:C6	2.51	0.46
1:1:2606:G:H2'	1:1:2606:G:N3	2.29	0.46
1:1:3242:G:H21	1:1:3245:A:H5''	1.81	0.46
1:1:2287:C:O2'	84:1:3448:OHX:N3	2.48	0.46
3:4:146:U:H2'	3:4:147:U:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:327:U:H2'	48:A:328:A:H8	1.79	0.46
48:A:733:A:H4'	48:A:734:A:C5	2.51	0.46
29:AB:65:GLN:O	29:AB:66:ALA:HB3	2.16	0.46
33:AF:67:SER:HB3	33:AF:68:PRO:HD2	1.98	0.46
1:1:361:A:O3'	38:AK:45:ARG:NH2	2.49	0.46
1:AR:2896:A:OP1	41:DO:102:ARG:NE	2.34	0.46
1:AR:2960:C:H2'	1:AR:2961:G:C8	2.50	0.46
1:AR:873:C:H3'	1:AR:874:U:H4'	1.97	0.46
50:C:126:THR:HG22	50:C:136:ARG:HE	1.80	0.46
50:C:48:VAL:HG13	50:C:61:LEU:HD11	1.96	0.46
5:CE:265:ALA:C	5:CE:266:ARG:HG2	2.36	0.46
6:CF:129:THR:O	6:CF:148:ILE:HD11	2.15	0.46
17:CQ:180:SER:OG	17:CQ:181:ALA:N	2.49	0.46
33:DG:19:ARG:HD2	33:DG:28:VAL:CG1	2.44	0.46
36:DJ:70:TYR:CE1	36:DJ:77:PRO:HD3	2.51	0.46
61:N:62:LEU:HB2	61:N:120:VAL:HG22	1.97	0.46
70:W:71:ARG:HG3	70:W:83:TRP:CH2	2.50	0.46
1:1:1645:U:H2'	1:1:1646:G:H5'	1.96	0.46
1:1:1838:G:H4'	1:1:1839:A:N3	2.29	0.46
1:1:305:U:C5	1:1:2776:C:H1'	2.51	0.46
1:1:3094:A:H2'	1:1:3095:U:C6	2.50	0.46
1:1:3276:G:O6	34:AG:60:ARG:NH1	2.48	0.46
1:1:748:U:H2'	1:1:749:C:C6	2.50	0.46
27:9:32:SER:HA	27:9:49:PRO:HA	1.98	0.46
48:A:1002:G:N1	48:A:1761:U:OP1	2.42	0.46
48:A:209:U:H2'	48:A:210:A:C8	2.50	0.46
48:A:548:G:H2'	48:A:549:G:O4'	2.15	0.46
48:A:75:U:H2'	48:A:76:A:O4'	2.16	0.46
29:AB:78:LEU:HD23	29:AB:78:LEU:HA	1.80	0.46
5:CE:49:TYR:O	5:CE:80:ASP:N	2.43	0.46
6:CF:49:ALA:HA	6:CF:109:TRP:CZ2	2.50	0.46
10:CJ:172:LYS:HD3	37:DK:39:PHE:HE1	1.80	0.46
18:CR:84:PRO:HB2	18:CR:87:SER:HB2	1.98	0.46
19:CS:150:VAL:HA	19:CS:153:PHE:CD2	2.51	0.46
54:G:73:THR:OG1	65:R:114:ARG:NH2	2.49	0.46
54:G:90:ILE:HD11	54:G:130:ILE:HG13	1.98	0.46
56:I:75:THR:O	56:I:79:ARG:HB2	2.16	0.46
57:J:66:SER:HA	57:J:73:SER:HA	1.98	0.46
61:N:33:ARG:HA	61:N:36:LEU:HB2	1.98	0.46
62:O:40:TYR:HB3	62:O:50:ILE:HG12	1.98	0.46
62:O:4:MET:HG3	62:O:5:HIS:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1211:U:H2'	1:1:1212:A:C8	2.51	0.46
1:1:1233:G:H22	1:1:1255:C:N4	2.13	0.46
1:1:2897:A:H2'	1:1:2899:C:H5''	1.98	0.46
1:1:795:G:O2'	1:1:796:U:H5'	2.15	0.46
48:A:1165:G:C6	48:A:1166:A:C6	3.04	0.46
48:A:1248:C:H2'	48:A:1249:U:C6	2.50	0.46
48:A:538:A:H8	48:A:543:C:N4	2.14	0.46
39:AL:46:ARG:HH21	39:AL:50:SER:C	2.19	0.46
1:AR:1486:G:H21	35:DI:6:THR:HG22	1.80	0.46
1:AR:2115:G:O2'	20:CT:82:LYS:HE3	2.16	0.46
1:AR:32:U:O3'	16:CP:71:ARG:NH2	2.48	0.46
84:AR:3713:OHX:N1	40:DN:49:MET:HA	2.30	0.46
49:B:137:SER:O	70:W:30:ALA:HA	2.16	0.46
5:CE:232:ARG:HG2	5:CE:233:TRP:CD1	2.51	0.46
1:AR:2947:G:C2	5:CE:250:ALA:HB1	2.50	0.46
8:CH:60:ASP:O	8:CH:61:ASN:HB2	2.16	0.46
9:CI:83:LEU:HD13	9:CI:139:PRO:HG2	1.97	0.46
10:CJ:78:PHE:C	10:CJ:80:TYR:H	2.18	0.46
13:CM:95:ASN:O	13:CM:102:PHE:HA	2.16	0.46
19:CS:165:ILE:HD11	19:CS:172:PHE:HB3	1.98	0.46
24:CX:18:PRO:HA	24:CX:51:ALA:HA	1.96	0.46
31:DE:34:LEU:HD23	31:DE:59:TYR:HB3	1.97	0.46
38:DL:56:ARG:O	84:DL:101:OHX:N3	2.49	0.46
54:G:55:ASP:HB3	54:G:58:LEU:HD12	1.98	0.46
66:S:6:THR:OG1	66:S:7:LYS:N	2.48	0.46
69:V:51:VAL:HG13	69:V:94:GLU:HB2	1.97	0.46
73:Z:21:LYS:HB2	73:Z:75:VAL:HG13	1.98	0.46
1:1:2282:U:O2	1:1:2310:U:H4'	2.15	0.46
1:1:83:U:OP1	84:1:3716:OHX:N5	2.49	0.46
1:1:1450:G:OP1	84:1:3721:OHX:N5	2.49	0.46
48:A:1239:U:O2	48:A:1246:C:N4	2.49	0.46
48:A:1511:U:H2'	48:A:1512:G:H8	1.79	0.46
48:A:237:C:O2'	48:A:240:U:O4	2.34	0.46
1:AR:1062:A:N3	22:CV:130:ARG:NH2	2.62	0.46
1:AR:1064:A:H5''	1:AR:1066:G:O4'	2.16	0.46
1:AR:114:A:H2'	1:AR:115:A:O4'	2.15	0.46
1:AR:2209:U:HO2'	1:AR:2210:G:P	2.38	0.46
1:AR:1131:G:O2'	1:AR:2373:A:N1	2.44	0.46
1:AR:2585:G:N3	1:AR:2585:G:H2'	2.31	0.46
1:AR:2611:U:H2'	1:AR:2612:U:C6	2.51	0.46
49:B:49:ASN:HB3	49:B:52:LYS:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CE:313:HIS:O	5:CE:333:LYS:HE3	2.15	0.46
7:CG:40:HIS:HB3	7:CG:43:LYS:HG3	1.98	0.46
10:CJ:211:LEU:O	10:CJ:215:VAL:HG23	2.16	0.46
12:CL:68:ALA:HA	12:CL:158:LYS:HG3	1.97	0.46
17:CQ:65:ASN:O	17:CQ:68:ARG:HG2	2.15	0.46
20:CT:153:LYS:O	20:CT:157:GLU:N	2.48	0.46
27:DA:51:ARG:HG2	27:DA:115:ARG:NH2	2.31	0.46
52:E:178:ARG:HE	52:E:178:ARG:N	2.14	0.46
58:K:174:ARG:HA	58:K:174:ARG:HE	1.81	0.46
65:R:47:LYS:HZ1	65:R:114:ARG:HG2	1.81	0.46
1:1:1340:G:H2'	1:1:1341:U:H6	1.81	0.46
1:1:1740:U:H1'	1:1:1741:A:C2	2.40	0.46
1:1:2883:U:H2'	1:1:2884:C:H6	1.81	0.46
1:1:2916:U:H5	1:1:2935:U:HO2'	1.57	0.46
27:9:3:LYS:HG3	27:9:8:VAL:HG13	1.97	0.46
48:A:1055:U:O4	84:A:2042:OHX:N3	2.49	0.46
48:A:1291:G:O5'	48:A:1291:G:H8	1.99	0.46
48:A:1347:U:C2	48:A:1517:U:C5	3.03	0.46
28:AA:88:ASP:HB3	28:AA:121:ARG:HH12	1.81	0.46
1:AR:1480:G:H4'	1:AR:1481:A:OP1	2.16	0.46
1:AR:1615:C:H2'	1:AR:1616:U:C6	2.51	0.46
1:AR:2263:C:H1'	1:AR:2264:U:H5'	1.98	0.46
1:AR:1148:G:OP2	84:AR:3715:OHX:N2	2.49	0.46
49:B:170:ILE:HD12	49:B:170:ILE:H	1.81	0.46
10:CJ:41:GLN:HG3	10:CJ:44:ARG:NH1	2.31	0.46
1:AR:2523:A:C8	10:CJ:51:LYS:HB2	2.51	0.46
21:CU:166:LYS:O	21:CU:167:ARG:HB3	2.16	0.46
22:CV:100:LYS:O	22:CV:103:GLN:HB3	2.16	0.46
51:D:241:ASP:O	51:D:244:SER:HB3	2.16	0.46
29:DC:77:LYS:C	29:DC:79:TRP:H	2.19	0.46
48:A:472:U:H5''	58:K:11:THR:HG23	1.96	0.46
68:U:63:ARG:NH1	68:U:67:MET:SD	2.89	0.46
48:A:1081:A:H5''	48:A:1082:C:OP1	2.16	0.46
48:A:1217:A:H5''	59:L:1:MET:HG3	1.97	0.46
48:A:1244:A:HO2'	48:A:1245:G:P	2.38	0.46
48:A:1607:G:H2'	48:A:1608:U:C6	2.51	0.46
48:A:799:A:H5''	53:F:201:HIS:CE1	2.51	0.46
34:AG:38:PRO:HD3	34:AG:77:ASN:O	2.16	0.46
35:AH:106:LYS:HA	35:AH:109:THR:HB	1.99	0.46
1:AR:128:G:OP2	36:DJ:74:LYS:NZ	2.38	0.46
1:AR:1613:A:OP2	39:DM:46:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:2522:G:H2'	1:AR:2522:G:N3	2.31	0.46
1:AR:2528:G:O3'	10:CJ:248:LYS:NZ	2.49	0.46
1:AR:3112:G:O6	1:AR:3120:C:H5''	2.16	0.46
1:AR:3357:U:H2'	1:AR:3358:U:C6	2.51	0.46
49:B:41:ARG:HE	49:B:45:VAL:HB	1.80	0.46
5:CE:111:SER:O	5:CE:114:VAL:HG23	2.15	0.46
6:CF:60:THR:HG22	6:CF:62:ALA:H	1.80	0.46
11:CK:85:GLY:HA3	11:CK:187:ILE:HD12	1.97	0.46
12:CL:205:SER:O	12:CL:209:ASN:HB2	2.16	0.46
17:CQ:23:VAL:CG1	17:CQ:84:LEU:HD11	2.45	0.46
54:G:90:ILE:O	54:G:94:THR:HG23	2.16	0.46
61:N:131:ASP:OD1	61:N:132:GLU:N	2.49	0.46
63:P:84:ARG:HE	63:P:84:ARG:H	7.12	0.46
66:S:88:VAL:HG13	66:S:89:SER:N	2.31	0.46
1:1:1492:G:O2'	40:AM:48:LYS:NZ	2.46	0.45
1:1:2737:C:H4'	22:2:68:THR:OG1	2.16	0.45
1:1:3356:G:H2'	1:1:3357:U:C6	2.51	0.45
1:1:3364:C:OP1	84:1:3463:OHX:N2	2.50	0.45
1:1:1410:U:OP2	84:1:3489:OHX:N4	2.49	0.45
1:1:624:G:O6	84:1:3697:OHX:N5	2.49	0.45
23:5:43:VAL:HG21	23:5:50:LEU:HA	1.97	0.45
48:A:1196:A:H4'	48:A:1197:C:O5'	2.16	0.45
48:A:1738:U:H2'	48:A:1739:C:C6	2.51	0.45
32:AE:79:ARG:H	32:AE:79:ARG:NE	2.14	0.45
1:AR:1019:G:H2'	1:AR:1020:G:O4'	2.16	0.45
1:AR:1383:G:O6	84:AR:3439:OHX:N2	2.48	0.45
1:AR:1528:G:O2'	1:AR:1588:A:N3	2.41	0.45
1:AR:1878:G:O5'	84:AR:3460:OHX:N5	2.48	0.45
1:AR:3276:G:H1	34:DH:60:ARG:NH1	2.13	0.45
1:AR:1310:G:O6	84:AR:3532:OHX:N4	2.50	0.45
1:AR:764:U:H3'	1:AR:765:C:H5''	1.98	0.45
3:AT:77:A:H2'	3:AT:78:G:O4'	2.16	0.45
9:CI:140:SER:OG	9:CI:143:THR:HG23	2.16	0.45
11:CK:7:GLU:HA	11:CK:68:LEU:HD11	1.98	0.45
12:CL:48:LEU:HB2	12:CL:142:ASP:OD1	2.16	0.45
1:AR:1112:A:P	14:CN:5:LYS:HE3	2.56	0.45
36:DJ:92:LEU:HB3	36:DJ:96:GLU:HG3	1.98	0.45
53:F:86:PHE:O	53:F:87:MET:HB2	2.15	0.45
63:P:25:ASP:N	63:P:55:SER:HB3	2.31	0.45
67:T:30:TYR:O	67:T:33:THR:OG1	2.32	0.45
21:0:109:ASP:OD1	21:0:113:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2374:C:O5'	84:1:3408:OHX:N3	2.49	0.45
1:1:250:U:H5''	1:1:251:G:H5''	1.98	0.45
1:1:2724:U:H4'	22:2:54:HIS:CD2	2.51	0.45
1:1:2881:C:H2'	1:1:2882:U:C6	2.52	0.45
1:1:3107:U:P	41:AN:112:LYS:HE2	2.56	0.45
1:1:1659:U:O4	84:1:3701:OHX:N4	2.49	0.45
22:2:79:MET:HB3	22:2:84:TYR:CE2	2.51	0.45
24:6:86:ARG:HD2	24:6:92:PHE:CZ	2.51	0.45
48:A:1018:U:OP1	62:O:107:LYS:NZ	2.48	0.45
48:A:144:U:O2'	48:A:145:A:H8	1.98	0.45
48:A:1783:C:H2'	48:A:1784:C:C6	2.51	0.45
48:A:830:U:O2'	48:A:831:U:H6	1.99	0.45
35:AH:85:VAL:O	35:AH:89:ILE:HG13	2.17	0.45
1:AR:439:C:H5'	1:AR:440:A:H8	1.81	0.45
5:CE:221:THR:HG22	5:CE:272:TYR:N	2.32	0.45
5:CE:35:ASP:HA	5:CE:184:ASN:ND2	2.31	0.45
7:CG:52:VAL:HG21	7:CG:65:ILE:HD12	1.97	0.45
3:AT:141:C:OP1	16:CP:109:ARG:NH1	2.48	0.45
18:CR:175:ARG:O	18:CR:179:GLN:HB2	2.15	0.45
25:CY:63:ILE:HG23	25:CY:64:THR:H	1.82	0.45
27:DA:39:LEU:HD22	27:DA:43:TYR:CE2	2.51	0.45
29:DC:7:LYS:HD3	29:DC:7:LYS:HA	1.77	0.45
52:E:27:ARG:HD2	59:L:60:SER:HB2	1.98	0.45
52:E:70:THR:HG22	52:E:86:LEU:HD13	1.97	0.45
55:H:98:ARG:HD3	55:H:99:GLY:N	2.30	0.45
64:Q:85:ILE:HA	64:Q:89:MET:SD	2.57	0.45
66:S:50:ILE:O	66:S:54:THR:HG23	2.15	0.45
68:U:38:LYS:O	68:U:39:THR:OG1	2.33	0.45
1:1:1063:G:N7	1:1:1097:G:H2'	2.31	0.45
1:1:2910:A:N1	84:1:3409:OHX:N1	2.64	0.45
42:AO:4:LYS:HG3	42:AO:5:TRP:CE3	2.50	0.45
1:AR:2726:C:OP1	84:AR:3659:OHX:N6	2.49	0.45
1:AR:1525:G:N7	84:AR:3553:OHX:N3	2.64	0.45
1:AR:837:A:OP2	44:DR:4:ARG:NH1	2.39	0.45
1:AR:996:A:H2'	1:AR:997:A:O4'	2.16	0.45
3:AT:85:G:HO2'	3:AT:86:U:C5'	2.30	0.45
49:B:71:GLU:HA	49:B:94:GLY:O	2.16	0.45
5:CE:66:LYS:HZ1	24:CX:120:LYS:HD3	1.81	0.45
17:CQ:8:VAL:HG12	17:CQ:117:ARG:HB3	1.98	0.45
35:DI:20:ILE:HD13	35:DI:34:HIS:HA	1.98	0.45
35:DI:3:GLN:HE22	35:DI:30:LEU:H	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:DL:69:HIS:HB3	38:DL:72:ARG:HH21	1.81	0.45
51:D:53:ILE:HB	54:G:57:SER:HB3	87.96	0.45
61:N:59:LEU:HD23	61:N:60:VAL:N	2.32	0.45
65:R:49:TYR:HB3	65:R:53:LEU:HD11	1.99	0.45
1:1:1934:G:O6	84:1:3420:OHX:N2	2.49	0.45
1:1:2396:G:OP1	1:1:2397:A:H4'	2.17	0.45
1:1:3364:C:H2'	1:1:3365:U:C6	2.52	0.45
2:3:3:U:H2'	2:3:4:U:H6	1.80	0.45
2:3:71:G:H2'	2:3:72:A:H8	1.82	0.45
48:A:523:G:H5''	73:Z:59:GLY:O	2.16	0.45
28:AA:83:THR:HG23	28:AA:85:TYR:H	1.81	0.45
44:AQ:49:ARG:HB2	44:AQ:55:TRP:CZ3	2.52	0.45
1:AR:1262:G:H5''	1:AR:1263:A:OP2	2.16	0.45
1:AR:1913:A:N3	1:AR:2120:A:H2'	2.32	0.45
1:AR:2592:G:H4'	1:AR:2594:C:C2	2.51	0.45
1:AR:792:G:H2'	1:AR:793:C:C6	2.51	0.45
1:AR:3001:C:OP1	5:CE:120:LYS:NZ	2.50	0.45
5:CE:299:ASP:OD1	5:CE:301:THR:HG23	2.16	0.45
6:CF:44:LYS:HB3	6:CF:47:ARG:NH1	2.32	0.45
7:CG:129:TYR:CG	7:CG:177:GLU:HG2	2.52	0.45
7:CG:295:GLY:O	7:CG:296:GLN:HB3	2.17	0.45
10:CJ:124:ASP:N	10:CJ:124:ASP:OD1	2.50	0.45
14:CN:126:PHE:HA	14:CN:127:PRO:HD3	1.87	0.45
1:AR:290:G:H1'	16:CP:93:LYS:HD2	1.98	0.45
21:CU:22:PRO:O	22:CV:146:ASN:ND2	2.48	0.45
31:DE:16:LEU:HB3	31:DE:98:SER:HB2	1.98	0.45
35:DI:20:ILE:HD13	35:DI:20:ILE:HA	1.76	0.45
39:DM:20:VAL:HG11	39:DM:45:VAL:HG12	1.98	0.45
57:J:10:LYS:HG2	60:M:133:LYS:HE3	1.98	0.45
62:O:105:ASN:N	62:O:105:ASN:OD1	2.49	0.45
65:R:47:LYS:O	65:R:50:GLU:HB2	2.16	0.45
1:1:415:G:OP2	84:1:3722:OHX:N3	2.50	0.45
48:A:955:A:P	62:O:3:ARG:HD2	2.56	0.45
28:AA:83:THR:HG23	28:AA:85:TYR:N	2.31	0.45
33:AF:19:ARG:HD2	33:AF:28:VAL:CG1	2.47	0.45
1:AR:1494:U:H4'	1:AR:1495:U:O5'	2.16	0.45
1:AR:1687:U:O2	23:CW:70:LYS:HE3	2.17	0.45
1:AR:230:U:H2'	1:AR:231:G:O4'	2.17	0.45
1:AR:1362:G:OP1	84:AR:3561:OHX:N3	2.50	0.45
50:C:171:ILE:HD12	50:C:197:ILE:HD13	1.99	0.45
12:CL:220:GLN:O	84:CL:301:OHX:N6	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CV:71:SER:HB3	22:CV:92:ARG:HA	1.99	0.45
48:A:1291:G:H5'	51:D:119:LYS:HD3	1.97	0.45
52:E:177:MET:SD	52:E:182:LEU:HD11	2.56	0.45
53:F:105:VAL:HG13	53:F:243:GLY:HA2	1.97	0.45
54:G:94:THR:O	54:G:97:LEU:HB2	2.17	0.45
59:L:55:VAL:HA	59:L:69:THR:HG23	1.98	0.45
64:Q:13:LYS:HD2	64:Q:13:LYS:HA	1.77	0.45
65:R:59:LYS:HE2	65:R:59:LYS:HB2	1.55	0.45
69:V:27:THR:HB	69:V:88:LYS:HG3	1.97	0.45
71:X:111:MET:HG3	71:X:116:ALA:HB2	1.99	0.45
1:1:2155:G:OP2	84:1:3637:OHX:N4	2.50	0.45
1:1:216:G:OP1	27:9:16:ARG:NH1	2.48	0.45
48:A:357:G:OP2	84:A:1938:OHX:N3	2.49	0.45
48:A:959:U:H5'	62:O:15:ALA:O	2.17	0.45
28:AA:51:LEU:HB2	28:AA:65:ARG:HD2	1.98	0.45
35:AH:20:ILE:HD13	35:AH:34:HIS:HA	1.97	0.45
1:AR:1090:G:O6	84:AR:3695:OHX:N5	2.50	0.45
1:AR:114:A:OP1	16:CP:54:LYS:NZ	2.48	0.45
1:AR:1944:U:H2'	1:AR:1945:A:C8	2.51	0.45
1:AR:2588:U:OP1	10:CJ:48:ARG:NH2	2.36	0.45
1:AR:289:A:H2'	1:AR:290:G:H8	1.80	0.45
1:AR:314:U:H2'	1:AR:315:C:C6	2.52	0.45
84:AR:3526:OHX:N2	84:AR:3721:OHX:N2	2.64	0.45
1:AR:620:U:H2'	1:AR:621:A:H4'	1.98	0.45
6:CF:317:PRO:HG3	6:CF:323:VAL:HG22	1.99	0.45
14:CN:53:LEU:HB2	14:CN:55:ARG:NH1	2.31	0.45
84:AR:3424:OHX:N1	16:CP:91:GLU:OE1	2.49	0.45
29:DC:93:SER:O	29:DC:93:SER:OG	2.33	0.45
36:DJ:47:VAL:HA	36:DJ:50:SER:HB2	1.98	0.45
55:H:21:GLU:O	55:H:25:ARG:HB2	2.17	0.45
58:K:33:GLU:O	58:K:122:VAL:HG11	2.17	0.45
69:V:96:PRO:HG2	69:V:99:ILE:HG22	1.99	0.45
1:1:112:U:O2'	1:1:113:C:OP2	2.27	0.45
1:1:1615:C:H2'	1:1:1616:U:C6	2.52	0.45
1:1:1675:G:H2'	1:1:1676:A:H8	1.80	0.45
1:1:1922:A:H2'	1:1:1923:C:O4'	2.16	0.45
1:1:3192:U:H2'	1:1:3193:C:C6	2.52	0.45
1:1:627:U:O4	84:1:3535:OHX:N5	2.50	0.45
22:2:57:TYR:CG	22:2:89:LEU:HD21	2.52	0.45
24:6:108:GLU:HG2	24:6:128:ARG:NH1	2.31	0.45
48:A:27:U:OP2	84:A:1962:OHX:N3	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:40:A:H2'	48:A:41:A:O4'	2.17	0.45
1:1:1135:A:OP1	30:AC:6:ASN:HB2	2.16	0.45
1:AR:1845:G:O2'	38:DL:8:PHE:HD2	1.99	0.45
1:AR:2881:C:H2'	1:AR:2882:U:C6	2.52	0.45
1:AR:3159:C:H4'	1:AR:3395:G:C5	2.52	0.45
1:AR:374:A:N3	1:AR:376:G:H5''	2.32	0.45
1:AR:408:A:H61	3:AT:15:G:H1'	1.81	0.45
1:AR:879:U:O2	1:AR:2357:A:H1'	2.16	0.45
5:CE:147:GLU:OE2	5:CE:150:ARG:NH1	2.49	0.45
9:CI:96:PRO:O	9:CI:100:ARG:HB2	2.17	0.45
12:CL:210:ILE:HG12	12:CL:217:PHE:CZ	2.52	0.45
18:CR:29:THR:HG22	18:CR:87:SER:OG	2.17	0.45
51:D:227:PRO:HA	51:D:230:TRP:CE2	2.51	0.45
29:DC:6:THR:HG22	29:DC:9:ARG:HG2	1.98	0.45
59:L:59:PHE:CE2	59:L:62:GLN:HA	2.52	0.45
61:N:62:LEU:HB3	61:N:75:VAL:HG11	1.98	0.45
62:O:23:PRO:HD2	62:O:26:PHE:HB3	1.99	0.45
67:T:38:VAL:HG12	67:T:42:TYR:CD1	2.52	0.45
72:Y:107:PHE:CD2	72:Y:114:LYS:HB2	2.52	0.45
21:O:16:THR:OG1	21:O:19:VAL:N	2.49	0.45
1:1:1273:A:O2'	1:1:1274:A:OP1	2.32	0.45
1:1:1892:G:N7	84:1:3614:OHX:N1	2.65	0.45
1:1:2207:A:C2'	1:1:2208:A:H5'	2.47	0.45
1:1:2611:U:H2'	1:1:2612:U:H6	1.82	0.45
3:4:103:G:O6	84:4:204:OHX:N4	2.49	0.45
3:4:24:G:OP2	27:9:13:ARG:HD3	2.17	0.45
26:8:103:TYR:O	26:8:138:ARG:NH1	2.49	0.45
48:A:119:A:H2'	48:A:120:U:O4'	2.17	0.45
2:AS:49:G:O6	7:CG:58:LYS:NZ	2.44	0.45
50:C:38:PHE:HB3	50:C:74:GLN:OE1	2.17	0.45
50:C:64:ARG:H	50:C:64:ARG:HG3	1.45	0.45
1:AR:1888:U:OP1	5:CE:247:ARG:HD3	2.16	0.45
6:CF:98:ARG:HD2	6:CF:99:MET:O	2.17	0.45
13:CM:92:ARG:H	13:CM:95:ASN:ND2	2.15	0.45
16:CP:70:ASN:HB3	16:CP:92:LEU:O	2.16	0.45
20:CT:180:LYS:HA	20:CT:183:ALA:HB3	1.97	0.45
23:CW:90:ARG:O	23:CW:91:ASP:HB2	2.16	0.45
19:CS:170:ARG:HH11	29:DC:57:GLY:N	2.15	0.45
56:I:14:THR:HG22	56:I:17:GLU:HB2	1.97	0.45
56:I:165:LYS:O	56:I:168:SER:OG	2.34	0.45
1:1:1240:A:H61	1:1:1244:A:H5''	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2443:A:N6	1:1:2504:U:C4	2.85	0.45
1:1:2617:U:C5	1:1:2621:G:OP2	2.70	0.45
1:1:1744:G:O6	84:1:3630:OHX:N2	2.50	0.45
1:1:600:G:N7	84:1:3632:OHX:N1	2.65	0.45
1:1:612:U:H2'	1:1:613:G:H8	1.82	0.45
24:6:108:GLU:HA	24:6:128:ARG:HG3	1.99	0.45
48:A:1256:A:OP1	59:L:5:LYS:NZ	2.30	0.45
42:AO:7:LYS:NZ	48:A:1774:G:OP1	2.41	0.45
1:AR:1471:U:H2'	1:AR:1472:U:C6	2.52	0.45
1:AR:156:G:OP2	37:DK:25:LYS:HB3	2.17	0.45
1:AR:1748:G:OP2	39:DM:42:LYS:NZ	2.49	0.45
1:AR:1949:G:OP2	20:CT:135:LYS:NZ	2.29	0.45
1:AR:2943:G:H2'	1:AR:2944:U:O4'	2.16	0.45
5:CE:291:GLU:O	5:CE:292:ALA:HB3	2.17	0.45
5:CE:305:ILE:HG12	5:CE:321:PHE:CZ	2.51	0.45
7:CG:55:PHE:CZ	7:CG:158:ARG:HG3	2.51	0.45
9:CI:223:PHE:HA	9:CI:227:GLY:O	2.16	0.45
15:CO:133:LYS:HE3	15:CO:133:LYS:HB3	1.73	0.45
1:AR:1296:C:H5'	21:CU:115:ARG:NH1	2.32	0.45
24:CX:83:LYS:HE2	24:CX:84:SER:O	2.16	0.45
52:E:99:VAL:HG13	52:E:173:ARG:NH2	2.32	0.45
55:H:148:SER:OG	55:H:148:SER:O	2.32	0.45
59:L:50:THR:HG22	59:L:55:VAL:HG22	1.99	0.45
59:L:50:THR:HG21	59:L:57:THR:OG1	2.17	0.45
62:O:92:ILE:HA	62:O:92:ILE:HD12	4.55	0.45
49:B:185:ARG:H	70:W:44:ARG:HA	1.82	0.45
51:D:148:LEU:O	70:W:4:ASP:HB2	2.17	0.45
1:1:1213:G:OP1	21:0:137:ARG:HD3	2.16	0.45
1:1:2120:A:OP2	84:1:3545:OHX:N2	2.50	0.45
1:1:2512:C:N4	1:1:2513:U:O4	2.50	0.45
1:1:3242:G:N2	1:1:3245:A:H5''	2.31	0.45
27:9:53:ASP:HB2	27:9:110:HIS:CD2	2.52	0.45
48:A:1695:G:N2	48:A:1706:C:H41	2.15	0.45
48:A:237:C:H4'	48:A:238:U:C6	2.52	0.45
48:A:393:C:H2'	48:A:394:C:C6	2.52	0.45
48:A:751:G:H2'	48:A:752:A:H8	1.82	0.45
1:AR:1816:A:O2'	1:AR:1817:G:OP1	2.27	0.45
1:AR:3132:C:H2'	1:AR:3133:C:C6	2.52	0.45
1:AR:3319:U:HO2'	1:AR:3320:A:P	2.37	0.45
1:AR:408:A:OP1	84:AR:3608:OHX:N6	2.49	0.45
1:AR:701:G:H2'	1:AR:702:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:929:A:H2'	1:AR:930:U:C6	2.52	0.45
50:C:149:GLN:HE22	50:C:154:SER:HB2	1.82	0.45
26:CZ:115:ARG:HD3	26:CZ:121:LYS:HE3	1.99	0.45
26:CZ:67:ILE:HB	26:CZ:83:VAL:HG12	1.99	0.45
29:DC:74:ASN:CG	29:DC:115:LYS:HB2	2.37	0.45
32:DF:13:THR:HG22	32:DF:72:ARG:HH11	1.82	0.45
55:H:72:ARG:HG2	55:H:98:ARG:HA	1.99	0.45
64:Q:67:ALA:HA	64:Q:68:PRO:HD2	1.72	0.45
70:W:13:VAL:HA	70:W:14:PRO:HD3	1.81	0.45
71:X:86:ILE:HD12	71:X:87:GLU:N	2.32	0.45
1:1:2213:A:H2'	1:1:2214:A:C8	2.52	0.44
1:1:2674:A:OP2	84:1:3584:OHX:N3	2.50	0.44
1:1:1819:U:O4	84:1:3577:OHX:N4	2.50	0.44
24:6:48:ARG:NH1	24:6:48:ARG:HG3	2.20	0.44
28:AA:26:VAL:HG21	28:AA:96:VAL:HB	1.99	0.44
1:1:716:A:N6	29:AB:117:ARG:HG3	2.30	0.44
1:AR:1235:U:C4'	1:AR:1236:G:H5'	2.47	0.44
1:AR:1709:C:H2'	1:AR:1710:C:H6	1.82	0.44
1:AR:2714:G:H4'	1:AR:2715:A:H5''	1.99	0.44
1:AR:2881:C:H2'	1:AR:2882:U:H6	1.82	0.44
1:AR:832:G:OP1	84:AR:3510:OHX:N5	2.50	0.44
1:AR:274:G:O6	84:AR:3571:OHX:N5	2.50	0.44
1:AR:436:A:N6	1:AR:621:A:C8	2.86	0.44
5:CE:37:ARG:CG	5:CE:186:GLY:HA2	2.45	0.44
5:CE:209:PHE:HB3	5:CE:282:ILE:CD1	2.47	0.44
14:CN:74:GLY:O	14:CN:101:ARG:NH1	2.50	0.44
21:CU:7:TYR:CE2	21:CU:34:GLU:HG2	2.52	0.44
1:AR:2295:A:N3	24:CX:37:ILE:HD12	2.31	0.44
25:CY:57:LYS:HE3	25:CY:57:LYS:HB2	1.79	0.44
26:CZ:80:ASN:ND2	26:CZ:126:LEU:HB2	2.32	0.44
28:DB:34:LYS:HD2	28:DB:34:LYS:HA	1.80	0.44
1:AR:1821:U:N3	35:DI:67:LYS:HD3	2.31	0.44
55:H:64:LYS:O	55:H:67:VAL:HG22	2.18	0.44
58:K:109:LEU:CB	58:K:146:PHE:HB3	2.43	0.44
60:M:54:ILE:HG23	60:M:55:ASP:N	2.33	0.44
63:P:31:THR:HB	63:P:38:THR:HA	1.99	0.44
69:V:117:VAL:HG22	69:V:118:VAL:H	1.81	0.44
69:V:58:LEU:O	69:V:60:THR:N	2.50	0.44
71:X:89:TRP:O	71:X:93:LEU:HD22	2.17	0.44
1:1:1230:G:N2	1:1:1279:C:N3	2.50	0.44
1:1:1675:G:H2'	1:1:1676:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1947:G:H1	1:1:2101:C:H42	1.64	0.44
48:A:1699:G:H2'	48:A:1700:C:H5''	1.99	0.44
48:A:702:G:C6	48:A:737:A:N6	2.86	0.44
1:AR:1604:G:H3'	1:AR:1604:G:N3	2.32	0.44
1:AR:1807:G:C6	1:AR:1808:G:N1	2.85	0.44
1:AR:1542:G:N7	84:AR:3599:OHX:N3	2.65	0.44
1:AR:980:A:H2'	1:AR:981:U:C1'	2.48	0.44
3:AT:26:U:H2'	3:AT:27:U:C6	2.52	0.44
5:CE:257:PRO:HG2	5:CE:261:MET:HE3	2.00	0.44
5:CE:299:ASP:O	5:CE:300:ARG:HB2	2.18	0.44
6:CF:131:VAL:O	6:CF:135:VAL:HG23	2.18	0.44
7:CG:110:LEU:HD12	7:CG:110:LEU:HA	1.67	0.44
12:CL:192:ASP:HA	12:CL:197:VAL:HG23	1.99	0.44
13:CM:15:GLU:HB3	13:CM:130:VAL:HG22	1.98	0.44
1:AR:1097:G:O5'	22:CV:129:LYS:HE2	2.18	0.44
22:CV:55:LYS:HG2	22:CV:56:PHE:N	2.33	0.44
28:DB:22:LYS:HD3	28:DB:129:TRP:CZ3	2.52	0.44
34:DH:73:ARG:HG3	34:DH:82:ARG:HD2	1.99	0.44
54:G:133:VAL:O	54:G:137:ILE:HG12	2.16	0.44
48:A:879:G:O2'	62:O:105:ASN:HB3	2.17	0.44
63:P:117:ASP:OD1	63:P:119:THR:HG23	2.17	0.44
69:V:61:LYS:HG3	69:V:86:ILE:HB	2.00	0.44
21:O:77:VAL:HG11	21:O:106:LEU:HD12	2.00	0.44
1:1:1522:U:H4'	1:1:1523:U:OP2	2.18	0.44
1:1:1877:U:H5''	1:1:1878:G:O4'	2.17	0.44
48:A:488:G:OP1	48:A:488:G:H4'	2.17	0.44
48:A:711:U:H1'	48:A:712:G:C8	2.53	0.44
48:A:740:A:H2'	48:A:741:C:H5''	1.99	0.44
29:AB:60:TYR:CD2	29:AB:63:LYS:HE3	2.53	0.44
38:AK:65:ARG:HG3	38:AK:65:ARG:NH1	2.32	0.44
1:AR:1686:U:O2	1:AR:1688:U:H1'	2.18	0.44
1:AR:2407:C:H2'	1:AR:2408:U:H6	1.82	0.44
1:AR:3120:C:HO2'	1:AR:3121:U:H6	1.65	0.44
1:AR:1853:U:OP2	84:AR:3562:OHX:N2	2.50	0.44
1:AR:651:G:C6	1:AR:652:G:C6	3.05	0.44
1:AR:736:A:C5	1:AR:737:G:H1'	2.52	0.44
1:AR:702:C:O2	1:AR:788:C:H4'	2.17	0.44
3:AT:70:G:N7	84:AT:212:OHX:N5	2.65	0.44
11:CK:163:GLN:O	11:CK:166:ARG:NH1	2.37	0.44
15:CO:38:ILE:HB	15:CO:44:VAL:HG12	1.99	0.44
18:CR:26:PHE:HE1	18:CR:120:ASN:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:CQ:127:LEU:HD11	21:CU:168:PRO:HG3	2.00	0.44
22:CV:57:TYR:O	22:CV:60:LYS:HB2	2.16	0.44
1:AR:715:A:C8	29:DC:115:LYS:HG2	2.51	0.44
52:E:162:GLN:NE2	52:E:165:ASN:HB2	2.32	0.44
53:F:31:PRO:HG2	53:F:38:LEU:HD13	1.98	0.44
70:W:9:VAL:HG22	70:W:10:GLU:H	1.82	0.44
1:1:1825:G:OP2	39:AL:49:SER:OG	2.35	0.44
1:1:2180:G:C6	1:1:2181:C:N4	2.86	0.44
1:1:2221:G:N2	1:1:2224:A:OP2	2.45	0.44
1:1:2812:C:H2'	1:1:2813:A:H8	1.82	0.44
1:1:2787:G:O6	84:1:3578:OHX:N4	2.51	0.44
1:1:595:G:C8	1:1:609:G:C6	3.05	0.44
48:A:489:C:H2'	48:A:490:C:C6	2.52	0.44
48:A:781:U:HO2'	48:A:782:U:H6	1.65	0.44
31:AD:86:ARG:NH1	44:AQ:44:LYS:HG2	2.31	0.44
1:AR:1063:G:N3	1:AR:1066:G:O2'	2.43	0.44
1:AR:1481:A:H2'	1:AR:1481:A:N3	2.32	0.44
1:AR:1641:U:O2'	1:AR:1643:A:OP2	2.27	0.44
1:AR:269:G:H5''	16:CP:14:LYS:HZ1	1.83	0.44
1:AR:3084:C:H2'	1:AR:3085:G:O4'	2.16	0.44
2:AS:28:C:H5''	13:CM:137:ARG:HG2	1.98	0.44
1:AR:22:G:H1'	3:AT:104:A:N3	2.32	0.44
6:CF:10:SER:OG	6:CF:14:GLU:HB2	2.17	0.44
7:CG:279:LYS:HE3	7:CG:282:ARG:NH1	2.32	0.44
14:CN:116:LEU:O	14:CN:120:GLN:HG3	2.18	0.44
17:CQ:16:VAL:HG21	17:CQ:43:ILE:HG12	2.00	0.44
1:AR:744:A:H4'	19:CS:142:GLY:O	2.17	0.44
21:CU:77:VAL:HG11	21:CU:106:LEU:HD22	1.98	0.44
28:DB:81:LEU:HD22	28:DB:81:LEU:HA	1.78	0.44
33:DG:77:ALA:HB3	33:DG:81:ASP:OD2	2.18	0.44
38:DL:5:THR:HA	38:DL:8:PHE:CD2	2.53	0.44
60:M:22:ASN:HA	60:M:23:PRO:HD3	1.84	0.44
62:O:94:LYS:HG2	62:O:118:ILE:HD13	2.00	0.44
69:V:26:LEU:HB3	69:V:34:LEU:HD21	1.98	0.44
1:1:291:C:OP1	69:V:68:ARG:NH1	123.44	0.44
49:B:154:GLU:HA	70:W:63:GLY:HA2	1.99	0.44
71:X:77:PRO:HG2	71:X:79:PHE:CZ	2.52	0.44
1:1:138:U:H2'	1:1:139:G:C8	2.53	0.44
1:1:1844:C:O2	38:AK:9:GLY:HA2	2.17	0.44
1:1:2094:C:H2'	1:1:2095:G:H8	1.83	0.44
1:1:2296:A:OP1	84:1:3680:OHX:N2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:899:G:O2'	48:A:915:A:N1	2.49	0.44
36:AI:18:ALA:O	36:AI:22:VAL:HG23	2.18	0.44
36:AI:90:ARG:HG2	36:AI:90:ARG:H	1.49	0.44
1:AR:1221:A:H3'	1:AR:1222:G:H5'	2.00	0.44
49:B:30:GLN:NE2	49:B:149:LEU:HD13	2.33	0.44
5:CE:117:ARG:CZ	5:CE:175:LYS:HD3	2.48	0.44
11:CK:113:GLU:HA	11:CK:124:ARG:O	2.17	0.44
13:CM:23:VAL:CG1	13:CM:29:ARG:HG2	2.47	0.44
14:CN:159:VAL:HB	29:DC:96:LYS:HD2	2.00	0.44
20:CT:176:ARG:HA	20:CT:176:ARG:HD3	1.82	0.44
21:CU:167:ARG:HG3	21:CU:168:PRO:HD2	2.00	0.44
36:DJ:65:ALA:O	36:DJ:69:LEU:HD23	2.17	0.44
14:CN:106:GLN:HB3	37:DK:18:THR:OG1	2.18	0.44
54:G:43:PHE:CE2	54:G:90:ILE:HG21	2.52	0.44
58:K:85:VAL:HG12	58:K:99:LEU:HD11	1.99	0.44
48:A:1073:G:H4'	62:O:10:GLY:HA2	1.99	0.44
48:A:1550:A:P	64:Q:42:ARG:NH2	2.91	0.44
72:Y:41:SER:HA	72:Y:42:PRO:HD3	1.82	0.44
1:1:1498:A:H2'	1:1:1499:C:C6	2.53	0.44
1:1:2712:U:H2'	1:1:2713:U:C6	2.53	0.44
1:1:3107:U:OP1	41:AN:114:LYS:NZ	2.47	0.44
3:4:126:A:O2'	3:4:129:C:N4	2.51	0.44
48:A:1607:G:H2'	48:A:1608:U:H6	1.83	0.44
48:A:856:A:N6	56:I:96:ARG:HB3	2.33	0.44
1:AR:1464:G:O2'	84:AR:3415:OHX:N5	2.50	0.44
1:AR:1764:U:C5	1:AR:1765:U:H1'	2.52	0.44
1:AR:1915:A:H5'	20:CT:82:LYS:O	2.17	0.44
50:C:129:THR:HG22	50:C:177:GLN:H	1.82	0.44
4:CD:206:PRO:HD3	4:CD:213:GLY:CA	2.47	0.44
5:CE:239:PRO:O	5:CE:242:THR:HG23	2.18	0.44
6:CF:178:LEU:HA	6:CF:178:LEU:HD23	1.82	0.44
13:CM:40:LEU:HG	13:CM:114:ILE:HD11	1.98	0.44
14:CN:76:THR:HA	14:CN:98:ASP:O	2.17	0.44
54:G:145:ASP:OD1	54:G:146:THR:N	2.41	0.44
54:G:64:VAL:O	54:G:65:ARG:HB2	2.18	0.44
66:S:85:VAL:HG12	66:S:86:PRO:N	2.33	0.44
68:U:15:ILE:HD13	68:U:60:SER:HA	1.98	0.44
1:1:1301:A:H4'	1:1:1302:A:O5'	2.18	0.44
1:1:1485:G:OP2	84:1:3688:OHX:N1	2.51	0.44
1:1:2536:A:H2'	1:1:2537:U:C5	2.52	0.44
1:1:343:U:OP2	84:1:3419:OHX:N2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:5:35:LYS:HA	23:5:38:ILE:HD12	1.99	0.44
27:9:36:SER:HB2	27:9:37:LYS:HE2	1.99	0.44
48:A:319:U:H1'	48:A:323:A:C4	2.52	0.44
48:A:649:U:HO2'	48:A:650:U:P	2.40	0.44
1:AR:1234:G:N7	84:AR:3454:OHX:N5	2.65	0.44
1:AR:1447:G:H3'	18:CR:67:ILE:CD1	2.47	0.44
1:AR:2746:A:C6	7:CG:148:ILE:HD12	2.52	0.44
1:AR:3041:U:OP1	24:CX:12:ARG:NH1	2.51	0.44
1:AR:425:G:O6	84:AR:3417:OHX:N3	2.50	0.44
84:AR:3516:OHX:N6	84:AR:3705:OHX:N5	2.66	0.44
1:AR:594:U:O2'	1:AR:595:G:H5'	2.18	0.44
50:C:205:PHE:CG	50:C:206:PRO:HD2	2.53	0.44
4:CD:86:GLN:HG2	4:CD:88:ILE:HD12	1.99	0.44
5:CE:188:ILE:HD12	5:CE:189:SER:N	2.33	0.44
6:CF:362:ASP:OD1	84:CF:402:OHX:N4	2.51	0.44
15:CO:17:VAL:HG11	15:CO:74:ARG:HA	1.98	0.44
1:AR:3308:C:O2	18:CR:69:ARG:HD3	2.18	0.44
22:CV:48:ILE:HG13	22:CV:94:GLU:HG2	1.99	0.44
24:CX:27:ASP:OD2	24:CX:102:ILE:HG23	2.18	0.44
43:DQ:40:LYS:HE3	43:DQ:44:ASP:OD2	2.17	0.44
44:DR:59:CYS:C	44:DR:61:LYS:H	2.21	0.44
53:F:126:VAL:HG13	53:F:158:ASP:O	2.17	0.44
1:1:1103:A:H4'	1:1:1103:A:OP2	2.17	0.44
1:1:1495:U:H5	1:1:1835:A:C2	2.36	0.44
1:1:2228:A:H2'	1:1:2229:A:C8	2.52	0.44
1:1:2407:C:H2'	1:1:2408:U:H6	1.83	0.44
1:1:1464:G:N7	84:1:3474:OHX:N3	2.65	0.44
1:1:1019:G:O6	84:1:3595:OHX:N1	2.51	0.44
1:1:501:A:OP2	84:1:3546:OHX:N4	2.51	0.44
2:3:60:G:H2'	2:3:61:G:H8	1.82	0.44
48:A:763:G:C6	48:A:764:U:C4	3.06	0.44
1:AR:1839:A:OP1	84:AR:3539:OHX:N3	2.51	0.44
1:AR:2157:G:N2	1:AR:2177:G:O2'	2.50	0.44
1:AR:1264:G:O6	84:AR:3454:OHX:N4	2.50	0.44
1:AR:627:U:H4'	1:AR:1399:A:O2'	2.18	0.44
4:CD:188:LYS:HE2	4:CD:189:TYR:CZ	2.53	0.44
21:CU:137:ARG:HG2	21:CU:139:TYR:CE2	2.53	0.44
52:E:135:GLU:HB3	52:E:187:LYS:HB3	2.00	0.44
56:I:185:ILE:HG22	56:I:186:PRO:HD2	2.00	0.44
48:A:197:A:H61	57:J:138:ASN:HD22	1.64	0.44
57:J:36:THR:HG23	57:J:96:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:P:29:HIS:HB2	63:P:41:ARG:HA	1.99	0.44
66:S:85:VAL:HG12	66:S:86:PRO:CA	2.47	0.44
1:1:1478:C:H2'	1:1:1479:U:C6	2.53	0.44
1:1:3160:U:H2'	1:1:3161:C:C6	2.52	0.44
48:A:1477:G:H2'	48:A:1478:G:C8	2.52	0.44
48:A:154:G:H5'	55:H:108:VAL:HG21	1.99	0.44
1:1:38:U:H4'	29:AB:32:ARG:HD2	1.99	0.44
35:AH:11:ASN:HA	35:AH:12:PRO:HD3	1.47	0.44
35:AH:58:ARG:HG3	35:AH:59:PRO:HD2	2.00	0.44
37:AJ:21:THR:O	37:AJ:21:THR:OG1	2.31	0.44
1:AR:1390:A:N3	1:AR:1390:A:H5'	2.33	0.44
1:AR:1495:U:H5	1:AR:1835:A:N1	2.16	0.44
49:B:67:ILE:HA	49:B:68:PRO:HD3	1.91	0.44
12:CL:215:GLU:O	84:CL:301:OHX:N1	2.51	0.44
17:CQ:128:ARG:HA	17:CQ:128:ARG:HD3	1.53	0.44
51:D:227:PRO:HA	51:D:230:TRP:CD2	2.53	0.44
54:G:89:ILE:HG13	54:G:89:ILE:H	1.61	0.44
55:H:102:VAL:HG13	55:H:106:LEU:HD12	1.99	0.44
56:I:166:LEU:HA	56:I:166:LEU:HD12	1.85	0.44
59:L:14:TYR:CE2	59:L:18:GLU:HG3	2.53	0.44
65:R:14:LYS:HB3	65:R:15:SER:H	1.52	0.44
68:U:105:LEU:HD13	68:U:122:ARG:HD3	1.99	0.44
1:1:1489:A:OP1	35:AH:10:ARG:HD2	2.18	0.43
1:1:1886:A:O4'	1:1:3307:A:H5'	2.18	0.43
1:1:2098:C:H2'	1:1:2099:A:H8	1.83	0.43
48:A:274:G:H3'	48:A:275:C:C6	2.53	0.43
48:A:512:A:H2'	48:A:513:U:C6	2.53	0.43
48:A:585:A:H2'	48:A:586:G:C8	2.53	0.43
48:A:823:G:H2'	48:A:824:G:H8	1.78	0.43
48:A:876:G:H1'	48:A:944:A:O4'	2.17	0.43
28:AA:34:LYS:HA	28:AA:34:LYS:HD2	1.64	0.43
34:AG:56:SER:O	34:AG:63:LYS:NZ	2.49	0.43
1:AR:1429:G:OP2	6:CF:107:ARG:NH2	2.40	0.43
1:AR:1816:A:HO2'	1:AR:1817:G:P	2.40	0.43
1:AR:2537:U:H2'	1:AR:2537:U:H6	1.64	0.43
1:AR:2615:G:H2'	1:AR:2616:C:C6	2.53	0.43
1:AR:2730:G:H4'	19:CS:184:PHE:CG	2.53	0.43
1:AR:2822:U:H2'	1:AR:2823:G:O4'	2.18	0.43
1:AR:2187:G:OP2	84:AR:3475:OHX:N4	2.50	0.43
1:AR:621:A:H8	1:AR:623:U:O4	2.01	0.43
1:AR:1043:C:O3'	12:CL:90:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:CM:115:LYS:HG2	13:CM:116:TYR:H	1.83	0.43
21:CU:40:ARG:HD2	21:CU:40:ARG:HA	1.53	0.43
22:CV:91:LEU:HD12	22:CV:96:ILE:HD11	2.01	0.43
25:CY:52:THR:O	25:CY:56:ARG:HG3	2.18	0.43
36:DJ:68:GLN:O	36:DJ:71:LYS:HB2	2.18	0.43
37:DK:40:VAL:O	37:DK:44:VAL:HG23	2.18	0.43
67:T:87:ASN:OD1	67:T:88:ARG:N	2.51	0.43
68:U:118:PRO:O	68:U:119:LYS:HB2	2.18	0.43
73:Z:112:LYS:HE2	73:Z:112:LYS:HB3	1.85	0.43
1:1:1481:A:H2'	1:1:1858:A:H1'	1.99	0.43
1:1:2986:U:H2'	1:1:2987:A:H8	1.82	0.43
1:1:317:A:C2	1:1:318:A:C4	3.07	0.43
1:1:739:G:O6	84:1:3453:OHX:N4	2.51	0.43
1:1:1675:G:N7	84:1:3483:OHX:N5	2.66	0.43
1:1:630:A:H2'	1:1:631:U:C6	2.53	0.43
1:1:915:A:C5	1:1:917:A:H1'	2.52	0.43
26:8:34:LEU:HD22	26:8:35:PRO:HD2	1.99	0.43
48:A:1263:G:H2'	48:A:1264:G:O4'	2.18	0.43
48:A:730:G:H21	48:A:731:C:H5''	1.83	0.43
28:AA:54:THR:HG22	28:AA:57:HIS:CG	2.52	0.43
38:AK:28:HIS:CE1	38:AK:31:LYS:HG3	2.53	0.43
38:AK:87:SER:O	84:AK:102:OHX:N3	2.51	0.43
1:AR:1066:G:OP1	84:AR:3732:OHX:N2	2.50	0.43
1:AR:2778:G:H2'	1:AR:2779:A:H5'	1.99	0.43
1:AR:2991:A:N3	18:CR:69:ARG:NH2	2.64	0.43
1:AR:3233:C:H2'	1:AR:3234:A:C8	2.52	0.43
1:AR:435:C:N4	1:AR:621:A:N7	2.66	0.43
1:AR:634:C:H5'	34:DH:21:ARG:O	2.17	0.43
2:AS:2:G:O2'	2:AS:23:A:N1	2.48	0.43
7:CG:114:GLY:C	7:CG:116:ASP:H	2.21	0.43
17:CQ:58:LEU:HA	17:CQ:58:LEU:HD12	1.78	0.43
14:CN:122:LYS:HA	36:DJ:120:ALA:HA	2.00	0.43
53:F:241:GLY:O	53:F:244:ILE:HG12	2.18	0.43
61:N:24:ILE:O	61:N:25:GLU:HG2	2.17	0.43
1:1:2131:A:N6	44:AQ:18:TYR:HA	2.34	0.43
1:1:1131:G:O2'	1:1:2373:A:N1	2.46	0.43
22:2:8:ARG:O	22:2:11:THR:OG1	2.20	0.43
48:A:276:C:O2'	48:A:277:U:H5''	2.18	0.43
48:A:489:C:N3	48:A:490:C:N4	2.66	0.43
48:A:585:A:H2'	48:A:586:G:H8	1.84	0.43
28:AA:95:VAL:HG21	28:AA:113:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AC:7:HIS:CG	30:AC:8:THR:N	2.86	0.43
32:AE:82:GLU:HG3	32:AE:83:GLU:HB2	2.00	0.43
1:AR:1616:U:H2'	1:AR:1617:G:C8	2.53	0.43
1:AR:1823:A:OP1	84:AR:3564:OHX:N4	2.51	0.43
1:AR:2268:U:H3'	1:AR:2269:U:C5'	2.48	0.43
1:AR:2896:A:H8	1:AR:2896:A:H5'	1.83	0.43
1:AR:3253:G:N7	84:AR:3743:OHX:N1	2.65	0.43
84:AR:3561:OHX:N2	6:CF:312:VAL:O	2.51	0.43
5:CE:236:LYS:HG3	5:CE:237:LYS:N	2.33	0.43
6:CF:361:HIS:CG	6:CF:362:ASP:N	2.86	0.43
7:CG:109:THR:O	7:CG:113:LEU:HB2	2.19	0.43
7:CG:11:ALA:O	7:CG:15:ARG:HG3	2.18	0.43
7:CG:64:ILE:HD12	7:CG:109:THR:HG21	1.99	0.43
12:CL:206:LEU:O	12:CL:210:ILE:HG13	2.17	0.43
15:CO:60:LEU:HD13	21:CU:152:LEU:HD11	2.00	0.43
36:DJ:44:ILE:O	36:DJ:48:ARG:HB2	2.17	0.43
53:F:71:LYS:HG3	53:F:91:THR:HB	1.99	0.43
58:K:121:SER:HB3	58:K:124:HIS:CB	2.49	0.43
58:K:92:LYS:HA	58:K:92:LYS:HE3	2.01	0.43
59:L:11:ILE:HD13	59:L:35:ILE:HG21	2.01	0.43
69:V:57:ARG:HG3	69:V:89:ARG:CZ	2.48	0.43
70:W:11:LEU:HG	70:W:11:LEU:H	1.40	0.43
48:A:533:U:H4'	73:Z:33:ALA:HB2	2.01	0.43
1:1:1004:U:C4	1:1:1005:G:N7	2.86	0.43
1:1:1057:A:O2'	84:1:3520:OHX:N3	2.51	0.43
1:1:1278:A:HO2'	1:1:1279:C:H6	1.61	0.43
1:1:1483:G:O3'	1:1:1484:U:H3'	2.18	0.43
1:1:1564:U:H2'	1:1:1565:G:H8	1.83	0.43
1:1:1603:A:H61	26:8:71:THR:HG21	1.82	0.43
1:1:2273:G:N2	1:1:2311:G:H2'	2.34	0.43
1:1:2438:A:H2'	1:1:2439:A:H8	1.83	0.43
1:1:274:G:H2'	1:1:275:U:O4'	2.18	0.43
1:1:3217:C:C5	1:1:3220:G:H1'	2.53	0.43
1:1:1362:G:OP2	84:1:3569:OHX:N6	2.52	0.43
1:1:668:G:OP1	84:1:3654:OHX:N2	2.51	0.43
1:1:1464:G:N7	84:1:3730:OHX:N6	2.66	0.43
48:A:177:U:H1'	55:H:191:ARG:NH1	2.32	0.43
48:A:629:U:OP2	48:A:969:C:N4	2.50	0.43
1:AR:3057:U:O2'	1:AR:3059:G:OP1	2.34	0.43
1:AR:3226:A:H2'	1:AR:3227:A:O4'	2.18	0.43
84:AR:3526:OHX:N6	84:AR:3721:OHX:N6	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:551:A:HO2'	1:AR:552:G:H8	1.66	0.43
50:C:33:LYS:O	50:C:98:THR:HG22	2.18	0.43
12:CL:33:ILE:O	12:CL:33:ILE:HG12	2.18	0.43
13:CM:172:LEU:HB3	13:CM:173:ASP:H	1.52	0.43
16:CP:28:TRP:O	16:CP:32:GLN:HG2	2.18	0.43
17:CQ:62:THR:HG21	17:CQ:68:ARG:HG3	2.00	0.43
22:CV:57:TYR:CG	22:CV:89:LEU:HD21	2.52	0.43
32:DF:88:PRO:HG2	32:DF:89:LEU:HD13	2.01	0.43
40:DN:2:ALA:N	40:DN:5:LYS:HZ2	2.15	0.43
41:DO:127:LEU:O	41:DO:128:LYS:HG2	2.18	0.43
57:J:6:ASP:OD2	57:J:8:ARG:HB3	2.19	0.43
60:M:109:VAL:HA	60:M:135:VAL:HG13	2.01	0.43
67:T:35:ILE:HB	67:T:38:VAL:CG2	2.48	0.43
72:Y:142:LYS:HA	72:Y:143:PRO:HD3	1.84	0.43
1:1:12:A:H1'	26:8:37:THR:HG21	2.01	0.43
1:1:1844:C:H2'	1:1:1845:G:H5''	2.00	0.43
1:1:2353:G:C5	1:1:2354:C:C5	3.06	0.43
84:1:3507:OHX:N2	84:1:3689:OHX:N6	2.67	0.43
22:2:124:VAL:HB	22:2:125:ALA:H	1.65	0.43
2:3:90:U:H2'	2:3:91:G:O4'	2.19	0.43
48:A:1213:G:O6	84:A:1907:OHX:N5	2.52	0.43
48:A:1248:C:H2'	48:A:1249:U:H6	1.84	0.43
48:A:1564:U:H2'	48:A:1565:C:H6	1.81	0.43
1:AR:1812:G:O6	28:DB:64:LYS:HD2	2.19	0.43
1:AR:2103:U:H2'	1:AR:2104:A:C8	2.53	0.43
1:AR:284:A:OP2	43:DQ:41:ARG:NH1	2.44	0.43
1:AR:3131:U:H2'	1:AR:3132:C:C6	2.54	0.43
1:AR:3378:C:OP1	84:AR:3437:OHX:N3	2.52	0.43
1:AR:407:A:C2	3:AT:17:A:H1'	2.54	0.43
1:AR:550:A:N6	1:AR:551:A:H62	2.17	0.43
5:CE:218:ILE:CG1	5:CE:276:THR:HG23	2.47	0.43
8:CH:152:THR:HA	8:CH:153:PRO:HD3	1.78	0.43
10:CJ:144:GLU:OE1	16:CP:6:TYR:OH	2.24	0.43
14:CN:46:ILE:O	14:CN:49:ARG:HB2	2.18	0.43
14:CN:6:ASN:O	14:CN:7:LEU:HD23	2.19	0.43
1:AR:149:U:H5'	16:CP:55:ALA:HB3	1.99	0.43
21:CU:132:THR:O	21:CU:133:ALA:HB3	2.18	0.43
33:DG:12:LYS:HD3	33:DG:57:TYR:O	2.18	0.43
36:DJ:70:TYR:CD1	36:DJ:77:PRO:HD3	2.53	0.43
38:DL:68:LYS:HD2	38:DL:69:HIS:CE1	2.54	0.43
48:A:789:A:OP1	53:F:108:ARG:NH2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:G:50:GLU:O	54:G:65:ARG:NH2	2.51	0.43
56:I:64:VAL:CG2	56:I:94:ALA:HB1	2.44	0.43
48:A:767:U:H5	58:K:142:ASN:OD1	2.01	0.43
1:1:2503:G:HO2'	1:1:2504:U:H5	1.65	0.43
1:1:1502:C:OP2	84:1:3414:OHX:N6	2.52	0.43
28:AA:54:THR:HG23	28:AA:57:HIS:H	1.84	0.43
33:AF:20:HIS:O	33:AF:21:HIS:HB2	2.18	0.43
1:1:1492:G:N7	40:AM:2:ALA:HB1	2.33	0.43
43:AP:13:LYS:HG2	43:AP:13:LYS:H	1.69	0.43
1:AR:1790:G:O6	84:AR:3702:OHX:N4	2.50	0.43
3:AT:145:U:H2'	3:AT:146:U:C6	2.53	0.43
49:B:139:VAL:HG13	49:B:141:ILE:HG13	1.99	0.43
49:B:180:GLU:O	49:B:184:LEU:HG	2.19	0.43
16:CP:51:LEU:HD23	16:CP:51:LEU:HA	1.85	0.43
1:AR:716:A:C6	29:DC:117:ARG:HG3	2.54	0.43
29:DC:132:LYS:O	29:DC:136:GLU:HG3	2.17	0.43
41:DO:92:ASP:O	41:DO:105:PRO:HG3	2.18	0.43
52:E:34:TYR:HE1	52:E:37:VAL:HG13	1.84	0.43
56:I:31:SER:HB3	56:I:32:PRO:CD	2.44	0.43
58:K:89:ASP:OD1	58:K:89:ASP:N	2.34	0.43
62:O:115:LEU:HD22	62:O:119:GLU:HG3	1.99	0.43
63:P:87:GLY:O	63:P:90:ARG:HB2	2.19	0.43
21:O:24:LEU:HD13	22:2:148:PRO:HG3	1.99	0.43
1:1:2943:G:H2'	1:1:2944:U:O4'	2.19	0.43
1:1:3087:A:OP1	84:1:3713:OHX:N2	2.51	0.43
1:1:3204:C:O2'	1:1:3205:G:H5'	2.19	0.43
1:1:3206:C:O2	21:O:155:ARG:NH1	2.52	0.43
1:1:532:A:O2'	1:1:533:A:H5'	2.18	0.43
1:1:729:C:H2'	1:1:730:C:H6	1.82	0.43
24:6:45:ARG:HD2	24:6:46:LEU:H	1.84	0.43
48:A:1023:A:N7	84:A:1928:OHX:N3	2.66	0.43
48:A:1496:U:H4'	48:A:1519:U:O2'	2.19	0.43
48:A:1695:G:H21	48:A:1706:C:H41	1.67	0.43
32:AE:13:THR:CG2	32:AE:72:ARG:HH11	2.29	0.43
1:AR:2213:A:N1	1:AR:2429:G:H1'	2.33	0.43
1:AR:3163:A:N6	1:AR:3288:G:O6	2.50	0.43
1:AR:2259:A:OP2	84:AR:3451:OHX:N1	2.52	0.43
3:AT:84:C:H5''	3:AT:85:G:C4	2.53	0.43
9:CI:156:ILE:O	9:CI:159:GLN:HB2	2.17	0.43
10:CJ:57:ARG:O	10:CJ:61:GLN:HG3	2.18	0.43
13:CM:37:LEU:HD13	13:CM:69:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:CO:25:LYS:HE3	15:CO:62:GLN:HG2	2.01	0.43
20:CT:102:LEU:HD23	20:CT:102:LEU:HA	1.80	0.43
21:CU:42:TRP:CZ2	21:CU:58:ILE:HD12	2.54	0.43
24:CX:69:LEU:HD12	24:CX:69:LEU:HA	1.85	0.43
26:CZ:109:LYS:HE3	26:CZ:109:LYS:HB2	1.78	0.43
32:DF:19:ARG:HB3	32:DF:35:GLU:HG2	2.01	0.43
53:F:121:TYR:CD2	53:F:161:LYS:HE3	2.53	0.43
61:N:97:LEU:HD11	61:N:121:VAL:HG22	2.01	0.43
67:T:11:PHE:CD1	67:T:59:GLY:HA3	2.52	0.43
73:Z:10:ARG:HD2	73:Z:26:ASP:HB2	2.00	0.43
1:1:1659:U:H2'	1:1:1660:C:C6	2.53	0.43
1:1:3396:U:OP2	84:1:3682:OHX:N2	2.51	0.43
1:1:368:G:OP1	84:1:3419:OHX:N5	2.52	0.43
1:1:2229:A:OP1	84:1:3724:OHX:N3	2.52	0.43
1:1:410:U:O4	84:1:3592:OHX:N2	2.51	0.43
1:1:435:C:H2'	1:1:436:A:C8	2.54	0.43
24:6:75:PRO:HB2	24:6:103:ALA:O	2.18	0.43
48:A:1091:A:H4'	48:A:1092:A:O5'	2.19	0.43
48:A:1297:G:N2	48:A:1300:A:OP2	2.45	0.43
48:A:1689:A:H2'	48:A:1690:G:C8	2.54	0.43
84:A:1968:OHX:N3	84:A:2009:OHX:N6	2.66	0.43
1:1:817:A:C4	38:AK:13:ASN:O	2.72	0.43
1:AR:1786:G:H2'	1:AR:1787:A:C8	2.54	0.43
1:AR:2407:C:H2'	1:AR:2408:U:C6	2.54	0.43
1:AR:2617:U:C5	1:AR:2621:G:OP2	2.71	0.43
1:AR:409:A:H2	1:AR:1441:G:N3	2.16	0.43
1:AR:93:C:OP1	86:AR:4246:7AL:N1	2.52	0.43
50:C:181:LEU:O	50:C:185:THR:N	2.36	0.43
10:CJ:72:PRO:HA	10:CJ:73:PRO:HD3	1.87	0.43
12:CL:156:ARG:HD3	12:CL:163:GLN:O	2.19	0.43
12:CL:74:LYS:HE3	12:CL:74:LYS:HB2	1.75	0.43
49:B:119:ARG:HE	51:D:240:LEU:HB3	1.84	0.43
40:DN:21:ARG:HD3	40:DN:22:PRO:O	2.18	0.43
53:F:247:SER:OG	53:F:250:GLU:HG3	2.19	0.43
54:G:51:VAL:HG13	54:G:131:GLN:HA	1.99	0.43
55:H:57:ASP:HA	55:H:107:ALA:H	1.83	0.43
56:I:73:VAL:HB	56:I:74:GLN:H	1.65	0.43
66:S:106:THR:O	66:S:109:LEU:HB3	2.19	0.43
66:S:115:LEU:HD23	66:S:115:LEU:HA	1.92	0.43
69:V:23:ARG:HD3	69:V:92:ASP:OD1	2.18	0.43
1:1:1524:A:OP1	26:8:92:LYS:NZ	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2166:A:H2'	1:1:2167:A:O4'	2.19	0.43
1:1:3252:G:H2'	1:1:3253:G:C8	2.54	0.43
1:1:345:G:OP1	1:1:1429:G:N2	2.49	0.43
1:1:601:U:H2'	1:1:602:A:O4'	2.19	0.43
1:1:654:C:OP1	33:AF:27:ARG:NH2	2.51	0.43
1:1:716:A:C6	29:AB:117:ARG:HG3	2.53	0.43
1:1:908:G:H4'	1:1:909:G:O5'	2.19	0.43
48:A:1565:C:OP1	67:T:41:ARG:HG3	2.18	0.43
48:A:190:C:O2'	48:A:191:C:H5'	2.18	0.43
48:A:420:A:H2'	48:A:421:A:O4'	2.19	0.43
48:A:872:G:O6	84:A:2004:OHX:N3	2.52	0.43
29:AB:78:LEU:HB3	29:AB:79:TRP:H	1.64	0.43
32:AE:12:TYR:O	32:AE:72:ARG:HD2	2.19	0.43
33:AF:24:ARG:HD3	33:AF:25:TYR:CZ	2.53	0.43
1:AR:1614:C:H2'	1:AR:1615:C:H6	1.84	0.43
1:AR:2233:A:H2'	1:AR:2234:G:O4'	2.19	0.43
49:B:87:LEU:HD12	49:B:87:LEU:HA	1.84	0.43
16:CP:65:ARG:HG2	16:CP:127:TYR:CG	2.54	0.43
30:DD:23:LYS:HD2	30:DD:24:PRO:HD2	2.01	0.43
34:DH:53:TYR:CZ	34:DH:65:ARG:HB2	2.54	0.43
1:AR:1486:G:N2	35:DI:6:THR:HG22	2.34	0.43
54:G:74:ALA:HB1	65:R:122:ARG:NH2	2.33	0.43
48:A:698:U:O4'	56:I:107:ARG:HD3	2.19	0.43
57:J:152:ILE:HB	57:J:153:GLU:H	1.53	0.43
73:Z:60:PHE:HA	73:Z:70:VAL:O	2.19	0.43
1:1:2883:U:H2'	1:1:2884:C:C6	2.54	0.43
1:1:3084:C:O2'	1:1:3332:U:OP1	2.22	0.43
1:1:1862:U:OP2	84:1:3694:OHX:N1	2.52	0.43
1:1:623:U:OP1	84:1:3665:OHX:N4	2.51	0.43
1:1:1095:U:N3	22:2:127:GLN:HG2	2.33	0.43
48:A:1323:C:H2'	48:A:1324:G:O4'	2.19	0.43
48:A:1428:G:H8	48:A:1428:G:H5'	1.83	0.43
48:A:227:U:O2'	48:A:228:G:H5''	2.19	0.43
48:A:517:U:H3	48:A:535:A:H61	1.67	0.43
48:A:639:U:OP1	56:I:118:LEU:N	2.52	0.43
48:A:924:A:O2'	48:A:987:G:OP1	2.36	0.43
35:AH:8:ARG:HB2	35:AH:34:HIS:CD2	2.54	0.43
1:AR:1677:G:OP2	23:CW:103:TYR:OH	2.22	0.43
1:AR:2403:G:N2	1:AR:2404:A:N7	2.66	0.43
1:AR:2635:A:H4'	1:AR:2636:A:O5'	2.19	0.43
1:AR:2987:A:O2'	5:CE:259:HIS:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:3257:C:H2'	1:AR:3258:U:O4'	2.19	0.43
49:B:167:LYS:HB3	49:B:168:HIS:H	1.40	0.43
6:CF:26:PHE:CD2	6:CF:130:ALA:HB2	2.54	0.43
14:CN:89:TYR:CZ	14:CN:93:ILE:HD11	2.54	0.43
22:CV:128:LEU:H	22:CV:128:LEU:HD12	1.82	0.43
24:CX:45:ARG:HD2	24:CX:46:LEU:N	2.32	0.43
38:DL:8:PHE:O	38:DL:11:ARG:HG3	2.19	0.43
54:G:216:GLU:OE2	54:G:219:ARG:HD2	2.19	0.43
62:O:129:TYR:HB3	62:O:134:VAL:HG22	2.00	0.43
48:A:1183:A:N3	64:Q:100:LYS:HD3	2.34	0.43
66:S:99:VAL:CB	66:S:118:PRO:HB2	2.49	0.43
69:V:21:LYS:HB2	69:V:21:LYS:HE3	1.70	0.43
71:X:86:ILE:HG13	71:X:86:ILE:H	1.44	0.43
73:Z:20:ARG:C	73:Z:21:LYS:HD2	2.39	0.43
21:0:13:ARG:HG2	21:0:51:VAL:CG1	2.48	0.42
1:1:2655:U:H4'	1:1:2656:A:O4'	2.18	0.42
1:1:284:A:OP2	43:AP:41:ARG:NH1	2.46	0.42
1:1:2896:A:H5'	1:1:2896:A:H8	1.84	0.42
48:A:1157:A:H2'	48:A:1160:A:N7	2.34	0.42
48:A:717:C:H42	48:A:720:G:H22	1.65	0.42
29:AB:7:LYS:HA	29:AB:7:LYS:HD3	1.72	0.42
37:AJ:57:LEU:O	37:AJ:61:ILE:HG13	2.18	0.42
1:AR:123:A:C6	1:AR:150:A:C5	3.07	0.42
1:AR:2396:G:OP1	1:AR:2397:A:H4'	2.19	0.42
1:AR:2996:U:O2	1:AR:2996:U:H2'	2.19	0.42
1:AR:3237:U:H2'	1:AR:3238:G:O4'	2.19	0.42
84:AR:3516:OHX:N3	84:AR:3705:OHX:N1	2.67	0.42
84:AR:3516:OHX:N4	84:AR:3705:OHX:N1	2.67	0.42
1:AR:678:G:O6	84:AR:3520:OHX:N2	2.52	0.42
1:AR:72:C:C2	1:AR:74:G:H1'	2.54	0.42
1:AR:80:G:H2'	1:AR:81:C:C6	2.54	0.42
49:B:9:LEU:HD23	49:B:54:TRP:CG	2.54	0.42
5:CE:186:GLY:O	5:CE:190:GLU:HB2	2.19	0.42
6:CF:271:LYS:HB2	6:CF:274:TYR:HB3	2.00	0.42
7:CG:163:LEU:HD11	7:CG:175:HIS:CG	2.54	0.42
9:CI:92:ILE:HD12	9:CI:92:ILE:HA	1.77	0.42
11:CK:151:VAL:O	11:CK:155:SER:OG	2.28	0.42
11:CK:13:PRO:HG2	11:CK:16:VAL:CG1	2.49	0.42
8:CH:51:ARG:NH1	15:CO:114:ASP:OD2	2.51	0.42
15:CO:53:VAL:HA	15:CO:54:PRO:HD3	1.70	0.42
1:AR:116:A:OP2	16:CP:2:GLY:HA3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:DB:36:HIS:N	28:DB:37:PRO:HD3	2.34	0.42
29:DC:47:LYS:HE2	29:DC:48:TYR:CZ	2.53	0.42
39:DM:78:LEU:HD13	39:DM:78:LEU:HA	1.87	0.42
53:F:37:LYS:HB2	53:F:40:GLU:CG	2.49	0.42
56:I:12:ALA:HB3	56:I:13:PRO:HD3	2.00	0.42
60:M:67:ARG:NH2	60:M:128:CYS:O	2.52	0.42
66:S:69:ILE:H	66:S:69:ILE:HG12	1.64	0.42
1:1:1560:G:C2'	1:1:1561:G:H5'	2.48	0.42
1:1:1554:U:HO2'	1:1:1582:C:H5	1.68	0.42
1:1:2191:U:H2'	1:1:2192:C:O4'	2.19	0.42
1:1:3163:A:H2'	1:1:3164:C:H5'	2.01	0.42
1:1:3254:G:N7	84:1:3591:OHX:N5	2.67	0.42
1:1:831:G:O6	84:1:3424:OHX:N1	2.52	0.42
1:1:824:C:H2'	1:1:825:U:C6	2.54	0.42
48:A:823:G:O2'	48:A:824:G:O5'	2.38	0.42
48:A:990:C:H2'	48:A:991:G:O4'	2.19	0.42
1:AR:18:G:OP2	26:CZ:46:TYR:OH	2.27	0.42
1:AR:2304:C:C5	1:AR:2305:G:C6	3.07	0.42
1:AR:537:A:H2'	1:AR:538:G:O4'	2.19	0.42
50:C:222:LYS:HD3	50:C:223:PHE:H	1.83	0.42
5:CE:53:MET:HE2	5:CE:77:THR:CG2	2.49	0.42
1:AR:1003:A:H1'	7:CG:15:ARG:CZ	2.48	0.42
7:CG:83:LEU:HD23	7:CG:83:LEU:HA	1.75	0.42
8:CH:129:GLU:OE2	8:CH:130:ILE:N	2.52	0.42
18:CR:169:THR:HG23	34:DH:60:ARG:HE	1.84	0.42
21:CU:23:LYS:HE3	21:CU:23:LYS:HB2	1.84	0.42
22:CV:83:ARG:HD2	22:CV:85:LEU:HD21	2.01	0.42
29:DC:47:LYS:C	29:DC:49:HIS:N	2.67	0.42
29:DC:74:ASN:ND2	29:DC:115:LYS:HB2	2.34	0.42
57:J:107:THR:OG1	57:J:108:PRO:HD3	2.19	0.42
57:J:199:LYS:HE3	57:J:199:LYS:HB2	1.76	0.42
58:K:149:ARG:H	58:K:149:ARG:HG2	1.59	0.42
62:O:92:ILE:O	62:O:96:VAL:HG23	2.20	0.42
65:R:91:ALA:O	65:R:94:GLN:HB3	2.19	0.42
71:X:30:SER:O	71:X:31:SER:HB3	2.20	0.42
1:1:2367:A:H2'	1:1:2368:A:C8	2.55	0.42
1:1:2534:G:H2'	1:1:2535:A:C8	2.54	0.42
1:1:776:U:C5	1:1:2719:U:O2	2.68	0.42
1:1:1940:G:N2	1:1:3362:A:H8	2.16	0.42
1:1:428:A:H2'	1:1:429:U:C6	2.55	0.42
22:2:42:ILE:HG12	22:2:96:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:1409:G:N2	48:A:1411:A:H3'	2.34	0.42
48:A:1533:C:H4'	48:A:1539:G:C6	2.53	0.42
48:A:1759:C:H2'	48:A:1760:G:O4'	2.19	0.42
48:A:240:U:H1'	48:A:241:U:OP1	2.19	0.42
1:1:1430:U:H2'	29:AB:9:ARG:HH22	1.84	0.42
37:AJ:4:LYS:HD2	37:AJ:13:LYS:O	2.20	0.42
1:AR:1542:G:O6	84:AR:3599:OHX:N5	2.52	0.42
1:AR:1798:A:H2'	1:AR:1799:A:C8	2.54	0.42
1:AR:2532:U:H5'	1:AR:2533:G:OP2	2.19	0.42
1:AR:549:U:H2'	1:AR:550:A:C8	2.53	0.42
1:AR:59:G:C4'	1:AR:60:A:H4'	2.49	0.42
2:AS:22:A:H1'	7:CG:272:TYR:CZ	2.55	0.42
3:AT:73:U:OP1	27:DA:24:SER:OG	2.28	0.42
50:C:159:SER:HA	50:C:162:ARG:NH1	2.34	0.42
50:C:131:ASP:HB3	50:C:180:THR:HG23	2.01	0.42
5:CE:306:THR:HA	5:CE:307:PRO:HD3	1.88	0.42
6:CF:295:ILE:HG23	6:CF:299:ILE:HD11	2.02	0.42
10:CJ:190:VAL:HG22	10:CJ:190:VAL:O	2.19	0.42
14:CN:165:SER:C	14:CN:167:PHE:H	2.18	0.42
17:CQ:65:ASN:OD1	17:CQ:67:THR:HB	2.18	0.42
19:CS:96:PHE:CG	19:CS:97:PRO:HD2	2.54	0.42
20:CT:43:LYS:HG2	20:CT:43:LYS:H	1.53	0.42
22:CV:56:PHE:CZ	22:CV:78:LYS:HD3	2.54	0.42
14:CN:64:LYS:HG3	29:DC:69:TRP:CD2	2.55	0.42
31:DE:43:ILE:HG22	31:DE:70:PHE:HB2	2.00	0.42
1:AR:1160:C:N3	33:DG:45:ARG:NH1	2.67	0.42
35:DI:74:ARG:HG2	35:DI:75:ALA:H	1.82	0.42
40:DN:28:ARG:HA	40:DN:33:ASN:ND2	2.34	0.42
56:I:91:ILE:HA	56:I:91:ILE:HD12	1.87	0.42
48:A:331:A:H5'	57:J:33:PRO:HA	2.01	0.42
70:W:74:GLN:HB2	70:W:74:GLN:HE21	1.72	0.42
1:1:1561:G:N1	1:1:1579:C:N3	2.67	0.42
1:1:1818:U:H2'	1:1:1819:U:O4'	2.19	0.42
1:1:1913:A:N3	1:1:2120:A:H2'	2.34	0.42
1:1:2093:A:H2'	1:1:2094:C:O4'	2.19	0.42
1:1:2435:G:N7	1:1:2593:A:H2'	2.34	0.42
1:1:2771:U:O2'	1:1:2772:C:O4'	2.34	0.42
1:1:270:U:O2'	1:1:318:A:H1'	2.20	0.42
1:1:783:A:OP2	84:1:3640:OHX:N3	2.51	0.42
1:1:999:G:C6	1:1:1000:C:N4	2.88	0.42
22:2:104:GLU:HG3	22:2:105:PHE:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:7:17:ARG:HA	25:7:17:ARG:HD3	1.57	0.42
48:A:1261:G:H2'	48:A:1262:U:C6	2.54	0.42
48:A:1266:U:H2'	48:A:1267:G:C8	2.54	0.42
48:A:1553:G:N2	48:A:1555:A:H3'	2.34	0.42
48:A:256:A:H2'	48:A:257:A:O4'	2.18	0.42
48:A:811:A:H5'	48:A:816:G:O2'	2.19	0.42
29:AB:66:ALA:HA	29:AB:69:TRP:HB2	2.00	0.42
22:2:88:ARG:NH2	30:AC:33:LYS:O	2.38	0.42
34:AG:89:LEU:HA	34:AG:90:PRO:HD3	1.68	0.42
35:AH:30:LEU:HD23	35:AH:30:LEU:HA	1.79	0.42
1:AR:1016:C:H1'	1:AR:1028:U:C2	2.54	0.42
1:AR:1355:A:H4'	1:AR:1356:U:O5'	2.18	0.42
1:AR:2230:C:H2'	1:AR:2231:C:O4'	2.20	0.42
3:AT:12:A:OP1	18:CR:3:ARG:NH2	2.49	0.42
8:CH:154:LEU:HD23	8:CH:154:LEU:HA	1.70	0.42
8:CH:172:HIS:CD2	8:CH:173:MET:HG2	2.53	0.42
15:CO:113:THR:HG22	15:CO:116:GLU:HB2	2.01	0.42
16:CP:101:THR:O	16:CP:105:ARG:HG3	2.18	0.42
16:CP:80:THR:HG21	16:CP:87:GLN:HA	2.01	0.42
17:CQ:38:ALA:O	17:CQ:41:LEU:HB2	2.18	0.42
21:CU:1:MET:SD	21:CU:36:ILE:HD13	2.59	0.42
84:AR:3513:OHX:N2	29:DC:24:LYS:O	2.51	0.42
29:DC:94:ALA:HB1	29:DC:122:PRO:HD3	2.01	0.42
38:DL:75:LYS:HE3	38:DL:75:LYS:HB3	1.79	0.42
44:DR:7:LYS:O	44:DR:27:LYS:NZ	2.36	0.42
66:S:105:GLN:CD	66:S:105:GLN:H	2.21	0.42
66:S:20:TYR:CE2	66:S:38:ILE:HD11	2.54	0.42
71:X:66:ASN:OD1	71:X:68:ARG:HG3	2.19	0.42
73:Z:42:GLU:HG3	73:Z:52:LYS:HD3	2.00	0.42
1:1:1260:A:H1'	1:1:1280:C:H1'	2.01	0.42
1:1:1294:A:O2'	1:1:1295:G:H5''	2.19	0.42
1:1:1742:U:H2'	1:1:1743:G:H8	1.83	0.42
1:1:24:G:OP2	84:1:3406:OHX:N4	2.52	0.42
1:1:2655:U:H2'	43:AP:3:ASN:O	2.20	0.42
1:1:70:A:N1	1:1:313:A:O2'	2.43	0.42
24:6:13:ILE:CD1	24:6:54:LEU:HB3	2.49	0.42
48:A:1586:A:H1'	48:A:1611:A:N6	2.34	0.42
48:A:1646:C:H2'	48:A:1647:U:C6	2.55	0.42
48:A:698:U:H2'	48:A:699:U:O4'	2.19	0.42
48:A:734:A:H4'	48:A:735:C:H5'	2.01	0.42
48:A:885:G:H2'	48:A:886:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:912:U:H4'	48:A:913:G:O5'	2.20	0.42
48:A:97:C:H2'	48:A:98:U:C6	2.55	0.42
35:AH:46:ASP:OD1	35:AH:80:ARG:HD2	2.19	0.42
1:AR:1385:C:OP1	6:CF:141:ARG:NH1	2.46	0.42
1:AR:1746:U:H2'	1:AR:1747:G:H8	1.85	0.42
1:AR:2964:G:N7	84:AR:3486:OHX:N6	2.68	0.42
49:B:110:TYR:HA	49:B:115:PHE:CE1	2.54	0.42
50:C:220:GLN:HG3	50:C:220:GLN:H	1.49	0.42
7:CG:68:THR:HG22	7:CG:70:THR:N	2.31	0.42
11:CK:51:GLN:OE1	11:CK:51:GLN:N	2.51	0.42
13:CM:12:LEU:HD12	13:CM:131:MET:HE3	2.01	0.42
14:CN:105:ASN:OD1	14:CN:107:GLU:HG2	2.19	0.42
19:CS:26:LEU:O	19:CS:30:VAL:HG23	2.19	0.42
21:CU:13:ARG:HE	21:CU:13:ARG:HB3	1.61	0.42
25:CY:8:PHE:CD2	25:CY:46:PRO:HG3	2.54	0.42
51:D:130:ILE:O	51:D:134:LEU:HD22	2.20	0.42
29:DC:56:VAL:HG23	29:DC:57:GLY:H	1.85	0.42
30:DD:14:ARG:HH22	30:DD:18:ARG:NH1	2.13	0.42
36:DJ:84:LYS:HB3	36:DJ:85:THR:H	1.63	0.42
53:F:148:ARG:NH1	55:H:201:GLN:OE1	2.49	0.42
56:I:98:ILE:HD11	56:I:121:VAL:HG11	2.01	0.42
58:K:93:LEU:O	58:K:96:VAL:HG22	2.19	0.42
59:L:12:HIS:CE1	59:L:49:LEU:HD21	2.55	0.42
64:Q:90:ILE:HD11	64:Q:112:LEU:HD21	2.01	0.42
1:1:1618:G:H2'	1:1:1619:A:O4'	2.19	0.42
1:1:2261:G:H21	1:1:2262:A:N6	2.18	0.42
1:1:2535:A:N6	1:1:2544:U:H3	2.16	0.42
1:1:2714:G:H4'	1:1:2715:A:H5''	2.01	0.42
1:1:3347:A:OP2	1:1:3347:A:H8	2.02	0.42
1:1:65:A:C4	1:1:110:G:N7	2.87	0.42
1:1:861:C:H2'	1:1:862:U:H6	1.84	0.42
1:1:92:G:OP2	1:1:93:C:H5''	2.20	0.42
22:2:119:ALA:HB1	22:2:124:VAL:O	2.19	0.42
1:1:216:G:H4'	27:9:19:TYR:CZ	2.55	0.42
48:A:1157:A:HO2'	48:A:1158:C:P	2.41	0.42
48:A:1760:G:H2'	48:A:1761:U:H5'	2.02	0.42
48:A:788:A:C4	53:F:19:LEU:HD13	2.54	0.42
28:AA:26:VAL:HA	28:AA:89:VAL:HG21	1.99	0.42
35:AH:8:ARG:HH21	35:AH:31:ARG:HD3	1.85	0.42
35:AH:42:PRO:HB2	35:AH:51:LEU:CD2	2.49	0.42
37:AJ:21:THR:HA	37:AJ:22:PRO:HD2	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:112:U:O2'	1:AR:113:C:OP2	2.29	0.42
1:AR:2358:A:H2'	1:AR:2359:C:O4'	2.20	0.42
1:AR:2532:U:H3	1:AR:2547:A:H61	1.67	0.42
1:AR:278:U:H2'	1:AR:279:U:C6	2.54	0.42
1:AR:3110:C:C4	1:AR:3111:U:C4	3.07	0.42
1:AR:1231:A:OP2	84:AR:3512:OHX:N3	2.53	0.42
1:AR:528:U:H2'	1:AR:529:A:H8	1.85	0.42
1:AR:90:C:H2'	1:AR:91:G:H5'	2.01	0.42
1:AR:976:U:OP1	19:CS:144:ARG:NH2	2.49	0.42
1:AR:976:U:H2'	1:AR:977:C:O4'	2.19	0.42
2:AS:58:C:OP1	84:AS:202:OHX:N3	2.52	0.42
50:C:129:THR:HB	50:C:180:THR:HA	2.01	0.42
5:CE:17:LEU:HD11	5:CE:233:TRP:HH2	1.84	0.42
6:CF:6:VAL:HG21	6:CF:255:PHE:CZ	2.55	0.42
2:AS:13:A:N3	7:CG:24:ARG:NH2	2.68	0.42
1:AR:1334:U:OP1	9:CI:206:LYS:HB3	2.20	0.42
12:CL:32:ARG:HA	12:CL:32:ARG:HD2	1.84	0.42
13:CM:35:LYS:HB2	13:CM:35:LYS:HE3	1.74	0.42
22:CV:19:PHE:CE2	22:CV:20:ARG:HG3	2.54	0.42
23:CW:50:LEU:HB3	23:CW:54:VAL:HG23	2.01	0.42
25:CY:35:LYS:HE2	25:CY:51:TRP:CZ2	2.55	0.42
28:DB:110:ALA:O	28:DB:114:VAL:HG23	2.20	0.42
32:DF:82:GLU:HG3	32:DF:83:GLU:CB	2.49	0.42
40:DN:21:ARG:NH1	40:DN:24:PRO:HG3	2.35	0.42
53:F:104:ASP:N	53:F:108:ARG:O	2.47	0.42
56:I:9:LEU:HD21	56:I:17:GLU:HB3	2.00	0.42
65:R:93:HIS:HA	65:R:97:VAL:HG23	2.01	0.42
67:T:15:LEU:H	67:T:15:LEU:HD23	1.85	0.42
67:T:40:ARG:HB3	68:U:45:MET:SD	2.60	0.42
73:Z:57:VAL:HG13	73:Z:60:PHE:HE2	1.85	0.42
21:O:155:ARG:HD3	21:O:172:TYR:CG	2.55	0.42
1:1:112:U:O2'	1:1:113:C:H5''	2.19	0.42
1:1:2137:U:C6	1:1:2141:U:C4	3.08	0.42
1:1:2407:C:H2'	1:1:2408:U:C6	2.55	0.42
22:2:17:ARG:NH1	22:2:21:LYS:O	2.53	0.42
26:8:142:ILE:HD13	26:8:142:ILE:HA	1.76	0.42
48:A:106:U:H2'	48:A:107:C:O4'	2.20	0.42
48:A:1332:C:O2'	52:E:162:GLN:HB3	2.20	0.42
48:A:1504:G:C6	48:A:1505:A:C6	3.07	0.42
48:A:16:G:H2'	48:A:17:C:C6	2.55	0.42
48:A:704:C:N4	48:A:735:C:C2	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:883:C:H2'	48:A:884:A:H8	1.84	0.42
1:1:952:A:OP1	30:AC:14:ARG:NH2	2.52	0.42
31:AD:32:LYS:HE2	31:AD:32:LYS:HB2	1.83	0.42
31:AD:43:ILE:HG22	31:AD:70:PHE:HB2	2.02	0.42
32:AE:54:GLU:OE2	32:AE:54:GLU:N	2.49	0.42
33:AF:9:ILE:HG12	33:AF:63:THR:HB	2.01	0.42
35:AH:65:VAL:HG22	35:AH:69:HIS:ND1	2.35	0.42
1:AR:129:U:O4	84:AR:3435:OHX:N4	2.53	0.42
1:AR:1349:G:H2'	1:AR:1350:A:C4	2.55	0.42
1:AR:2610:G:H2'	1:AR:2611:U:O4'	2.20	0.42
1:AR:2617:U:H5	1:AR:2621:G:OP2	2.03	0.42
1:AR:3279:A:N6	1:AR:3280:U:C4	2.88	0.42
1:AR:1540:U:OP1	84:AR:3599:OHX:N1	2.53	0.42
1:AR:371:G:O6	84:AR:3709:OHX:N2	2.52	0.42
1:AR:542:G:N2	1:AR:543:C:N3	2.67	0.42
2:AS:16:U:P	7:CG:8:LYS:HZ1	2.43	0.42
10:CJ:161:GLU:HA	10:CJ:164:VAL:HG22	2.02	0.42
13:CM:54:VAL:HG12	13:CM:57:PHE:H	1.84	0.42
14:CN:48:PRO:HA	14:CN:137:GLN:CB	2.50	0.42
20:CT:96:ILE:O	20:CT:100:ARG:HG3	2.19	0.42
22:CV:56:PHE:CE2	22:CV:78:LYS:HD3	2.54	0.42
22:CV:95:HIS:O	22:CV:96:ILE:HD12	2.20	0.42
23:CW:20:SER:O	23:CW:24:GLU:HG2	2.20	0.42
39:DM:14:LEU:O	39:DM:17:ARG:HB2	2.19	0.42
55:H:164:LYS:N	55:H:167:LYS:O	2.45	0.42
59:L:27:PHE:CD1	59:L:40:LEU:HD23	2.53	0.42
1:1:2631:U:OP1	1:1:2757:U:O2'	2.30	0.42
1:1:2897:A:H2'	1:1:2899:C:C5'	2.50	0.42
1:1:3008:A:N7	84:1:3437:OHX:N5	2.67	0.42
1:1:3358:U:H2'	1:1:3359:A:O4'	2.18	0.42
1:1:422:A:C2	1:1:2363:A:H4'	2.54	0.42
25:7:38:SER:O	25:7:42:GLN:HG3	2.20	0.42
48:A:156:A:H2'	48:A:157:A:O4'	2.20	0.42
36:AI:62:GLN:O	36:AI:66:VAL:HG23	2.20	0.42
1:AR:2403:G:N2	1:AR:2404:A:H62	2.18	0.42
84:AR:3516:OHX:N3	84:AR:3705:OHX:N5	2.67	0.42
1:AR:1839:A:OP2	84:AR:3587:OHX:N6	2.53	0.42
1:AR:374:A:H4'	1:AR:375:A:OP1	2.20	0.42
1:AR:661:G:P	29:DC:12:ARG:HH22	2.43	0.42
1:AR:731:U:H2'	1:AR:732:C:H6	1.84	0.42
50:C:37:THR:OG1	50:C:37:THR:O	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CF:3:ARG:HA	6:CF:4:PRO:HD3	1.83	0.42
10:CJ:136:LEU:HD11	10:CJ:162:LEU:O	2.19	0.42
10:CJ:78:PHE:CD2	10:CJ:179:ILE:HD13	2.55	0.42
11:CK:90:MET:HB2	11:CK:144:ILE:HG22	2.01	0.42
20:CT:15:VAL:HG12	20:CT:17:VAL:HG23	2.02	0.42
49:B:108:THR:HA	51:D:64:LYS:HZ1	1.84	0.42
33:DG:55:ILE:HD12	33:DG:55:ILE:HA	1.74	0.42
36:DJ:73:LYS:HB3	36:DJ:73:LYS:HE2	1.70	0.42
39:DM:8:ILE:H	39:DM:8:ILE:HD12	1.84	0.42
53:F:7:LYS:N	53:F:7:LYS:HD2	2.34	0.42
54:G:94:THR:CG2	54:G:114:ILE:HG13	2.49	0.42
64:Q:34:VAL:O	64:Q:42:ARG:HG2	2.20	0.42
60:M:99:ARG:HB3	72:Y:9:LEU:O	2.20	0.42
21:O:40:ARG:HD2	21:O:40:ARG:HA	1.66	0.42
1:1:1445:U:H5''	1:1:1446:A:OP2	2.20	0.42
1:1:249:U:H1'	1:1:250:U:C2	2.54	0.42
1:1:2768:U:H2'	1:1:2769:A:H8	1.85	0.42
1:1:2877:G:H2'	1:1:2878:G:O4'	2.19	0.42
1:1:3121:U:H4'	1:1:3122:A:OP1	2.18	0.42
1:1:3166:C:H42	1:1:3284:G:H1	1.68	0.42
1:1:3289:G:O6	84:1:3664:OHX:N6	2.53	0.42
1:1:812:G:N7	84:1:3519:OHX:N1	2.68	0.42
1:1:975:C:H2'	1:1:976:U:C6	2.54	0.42
22:2:51:GLY:HA3	22:2:92:ARG:HG3	2.02	0.42
1:1:2585:G:C2	3:4:151:C:H5	2.38	0.42
25:7:47:ARG:O	25:7:55:PHE:HD2	2.03	0.42
48:A:1344:A:H2'	48:A:1345:A:C8	2.55	0.42
48:A:1370:U:H4'	48:A:1371:A:C5'	2.49	0.42
48:A:1537:C:N4	48:A:1572:G:N1	2.68	0.42
48:A:1613:U:H2'	48:A:1614:A:H5''	2.02	0.42
48:A:755:A:O2'	48:A:756:A:OP1	2.36	0.42
42:AO:13:LEU:HD11	42:AO:17:ARG:CZ	2.49	0.42
1:AR:1833:G:H5''	40:DN:10:LYS:HD3	2.02	0.42
1:AR:2406:C:H2'	1:AR:2407:C:C6	2.55	0.42
1:AR:2550:U:H5	4:CD:40:TYR:O	2.03	0.42
1:AR:787:G:H2'	1:AR:788:C:C6	2.55	0.42
4:CD:247:ARG:HA	4:CD:247:ARG:HD2	1.84	0.42
8:CH:98:VAL:HA	8:CH:101:PHE:CE2	2.54	0.42
8:CH:175:LYS:HB3	8:CH:175:LYS:HE2	1.72	0.42
11:CK:162:GLN:HB2	11:CK:179:ILE:O	2.20	0.42
11:CK:48:VAL:CG1	11:CK:52:LEU:HB3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:CP:38:ARG:HD2	16:CP:39:ALA:N	2.35	0.42
1:AR:269:G:P	16:CP:44:ARG:HH22	2.42	0.42
19:CS:135:GLN:H	19:CS:135:GLN:CD	2.23	0.42
27:DA:80:VAL:HG12	27:DA:99:LEU:O	2.20	0.42
38:DL:31:LYS:O	38:DL:33:THR:HG22	2.20	0.42
44:DR:8:VAL:O	44:DR:11:THR:HB	2.20	0.42
52:E:137:VAL:HG22	52:E:151:LYS:HG3	2.02	0.42
53:F:214:LEU:HD12	53:F:214:LEU:HA	1.77	0.42
60:M:21:ASN:OD1	60:M:21:ASN:N	2.52	0.42
66:S:88:VAL:HG22	66:S:89:SER:H	1.84	0.42
1:1:1146:C:H4'	1:1:1331:U:C4	2.55	0.42
1:1:1340:G:H2'	1:1:1341:U:C6	2.55	0.42
1:1:1804:A:H2'	1:1:1805:C:C6	2.55	0.42
1:1:3165:A:H2'	1:1:3166:C:C6	2.55	0.42
1:1:2315:G:OP2	84:1:3538:OHX:N3	2.53	0.42
48:A:1253:U:H2'	48:A:1254:U:C6	2.55	0.42
48:A:1389:C:O2'	66:S:52:GLY:HA3	2.20	0.42
48:A:1450:U:H2'	48:A:1451:C:H6	1.84	0.42
48:A:1483:A:C2	48:A:1607:G:H1'	2.55	0.42
48:A:189:C:H2'	48:A:190:C:H5'	2.01	0.42
84:A:1968:OHX:N1	84:A:2009:OHX:N1	2.67	0.42
48:A:704:C:OP2	48:A:704:C:H3'	2.19	0.42
31:AD:13:LYS:NZ	31:AD:99:ASP:OD1	2.45	0.42
32:AE:80:ASN:OD1	32:AE:81:GLU:N	2.53	0.42
42:AO:8:LYS:O	42:AO:12:ARG:HG3	2.20	0.42
44:AQ:8:VAL:HB	44:AQ:11:THR:HG22	2.02	0.42
1:AR:2244:A:H5'	4:CD:243:THR:OG1	2.19	0.42
1:AR:2709:C:H2'	1:AR:2710:C:C6	2.55	0.42
1:AR:1895:A:O2'	1:AR:3053:G:H4'	2.19	0.42
1:AR:609:G:OP2	6:CF:315:LYS:NZ	2.40	0.42
1:AR:990:U:O4	84:AR:3689:OHX:N6	2.53	0.42
8:CH:145:LEU:HD23	8:CH:145:LEU:HA	1.85	0.42
12:CL:3:ARG:CZ	12:CL:63:GLU:HG3	2.50	0.42
24:CX:87:ARG:HH12	24:CX:137:VAL:HG21	1.85	0.42
24:CX:2:SER:N	24:CX:57:MET:H	2.18	0.42
29:DC:10:LYS:HA	29:DC:10:LYS:HD2	1.67	0.42
29:DC:2:PRO:HG2	29:DC:5:PHE:CD2	2.55	0.42
30:DD:17:HIS:O	84:DD:102:OHX:N1	2.53	0.42
3:AT:52:A:H62	40:DN:27:ILE:HD13	1.84	0.42
48:A:448:C:OP1	53:F:29:PRO:HD3	2.20	0.42
54:G:23:VAL:O	54:G:34:GLN:NE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:G:36:ALA:HB1	54:G:42:LEU:HD21	2.02	0.42
48:A:161:U:OP2	55:H:87:ARG:NH2	2.52	0.42
56:I:155:ASP:O	56:I:159:VAL:HG11	2.20	0.42
48:A:632:U:OP1	60:M:102:LYS:HG3	2.19	0.42
63:P:129:LYS:HB2	63:P:129:LYS:HE3	1.91	0.42
65:R:82:ARG:HH12	65:R:114:ARG:CB	2.32	0.42
72:Y:144:ARG:HG3	72:Y:144:ARG:H	1.47	0.42
1:1:1278:A:O2'	1:1:1279:C:H6	2.03	0.41
1:1:1565:G:N2	1:1:1574:C:N3	2.68	0.41
1:1:2108:C:H1'	1:1:3344:A:H8	1.81	0.41
1:1:2232:A:OP2	84:1:3580:OHX:N3	2.53	0.41
1:1:226:C:H2'	1:1:227:G:O4'	2.20	0.41
1:1:283:G:OP2	1:1:285:A:H4'	2.20	0.41
84:1:3540:OHX:N3	84:1:3705:OHX:N1	2.68	0.41
1:1:792:G:O6	84:1:3686:OHX:N4	2.53	0.41
1:1:1615:C:OP1	84:1:3711:OHX:N3	2.53	0.41
1:1:612:U:H2'	1:1:613:G:C8	2.55	0.41
3:4:79:A:H5''	36:AI:43:LYS:NZ	2.35	0.41
24:6:87:ARG:HB2	24:6:89:ASP:OD1	2.20	0.41
48:A:397:A:O3'	57:J:50:GLY:HA2	2.20	0.41
48:A:404:G:H2'	48:A:405:C:C6	2.55	0.41
48:A:462:G:N7	84:A:2021:OHX:N1	2.68	0.41
48:A:694:U:H3'	48:A:695:U:C6	2.55	0.41
1:1:715:A:C8	29:AB:115:LYS:HG2	2.53	0.41
30:AC:36:ASP:HA	30:AC:37:PRO:HD3	1.87	0.41
31:AD:78:GLY:HA2	31:AD:87:VAL:HG13	2.01	0.41
1:AR:1170:A:OP2	84:AR:3507:OHX:N6	2.53	0.41
1:AR:1766:G:N7	20:CT:46:LYS:NZ	2.66	0.41
1:AR:1838:G:H4'	1:AR:1839:A:N3	2.34	0.41
1:AR:2546:C:C4	1:AR:2547:A:C8	3.08	0.41
49:B:200:ASP:N	49:B:200:ASP:OD1	2.53	0.41
49:B:41:ARG:HH11	49:B:45:VAL:HG21	1.85	0.41
1:AR:2245:C:H4'	4:CD:221:LYS:O	2.20	0.41
5:CE:123:TYR:CE1	5:CE:124:LYS:HG3	2.55	0.41
10:CJ:69:LEU:HD21	16:CP:24:ARG:HG2	2.01	0.41
1:AR:1295:G:OP1	21:CU:84:ARG:HG3	2.20	0.41
24:CX:24:ASN:O	24:CX:99:ALA:HA	2.20	0.41
27:DA:63:LYS:O	27:DA:66:GLN:HG3	2.20	0.41
28:DB:46:ILE:HD11	28:DB:48:ARG:O	2.20	0.41
34:DH:41:ALA:HB3	34:DH:74:THR:HG22	2.02	0.41
36:DJ:36:LEU:HG	36:DJ:36:LEU:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:DR:73:THR:HG22	44:DR:76:ALA:CB	2.50	0.41
56:I:98:ILE:HD13	56:I:118:LEU:HD23	2.03	0.41
61:N:87:PRO:HA	61:N:140:PHE:CE2	2.55	0.41
62:O:91:LEU:HD12	62:O:125:LEU:HD12	2.02	0.41
69:V:22:ILE:HD12	69:V:118:VAL:HG23	2.02	0.41
1:1:951:A:C4	1:1:1369:A:C2	3.07	0.41
1:1:2308:C:O2	84:1:3695:OHX:N2	2.53	0.41
3:4:85:G:C8	3:4:85:G:H3'	2.55	0.41
48:A:1390:U:OP1	66:S:5:ARG:HD2	2.19	0.41
48:A:1552:U:OP2	64:Q:43:ARG:NH2	2.48	0.41
48:A:837:G:N7	84:A:1915:OHX:N6	2.67	0.41
31:AD:42:ILE:HG13	31:AD:42:ILE:O	2.19	0.41
35:AH:20:ILE:HD12	35:AH:32:ALA:HB1	2.03	0.41
1:AR:1473:G:OP2	20:CT:8:LYS:NZ	2.53	0.41
1:AR:1495:U:H5	1:AR:1835:A:C2	2.37	0.41
1:AR:1584:U:H2'	1:AR:1585:C:H6	1.85	0.41
1:AR:1770:G:H5'	1:AR:1771:C:OP2	2.20	0.41
1:AR:2282:U:O2	1:AR:2310:U:H4'	2.20	0.41
1:AR:1304:A:N6	1:AR:2860:U:OP1	2.51	0.41
1:AR:3326:G:O6	84:AR:3461:OHX:N5	2.53	0.41
84:AR:3506:OHX:N4	84:AR:3597:OHX:N1	2.68	0.41
84:AR:3506:OHX:N6	84:AR:3597:OHX:N5	2.68	0.41
1:AR:738:A:H2'	1:AR:739:G:C8	2.55	0.41
5:CE:148:LEU:HD12	5:CE:148:LEU:HA	1.78	0.41
11:CK:84:LYS:HE2	11:CK:191:LEU:HD13	2.02	0.41
1:AR:2681:U:H1'	13:CM:22:SER:OG	2.20	0.41
18:CR:141:SER:O	18:CR:143:PRO:HD3	2.19	0.41
27:DA:37:LYS:HE2	27:DA:37:LYS:H	1.85	0.41
28:DB:26:VAL:HG21	28:DB:96:VAL:HB	2.01	0.41
32:DF:84:ASP:N	32:DF:84:ASP:OD1	2.54	0.41
38:DL:22:CYS:SG	38:DL:24:ARG:HB2	2.60	0.41
39:DM:62:ALA:O	39:DM:66:ILE:HG13	2.21	0.41
54:G:43:PHE:HD1	54:G:43:PHE:HA	1.65	0.41
54:G:73:THR:HG23	65:R:114:ARG:HD2	2.02	0.41
54:G:43:PHE:CZ	54:G:90:ILE:HG21	2.55	0.41
55:H:58:LYS:O	55:H:59:GLN:HB2	2.19	0.41
63:P:12:GLN:HB3	63:P:77:THR:OG1	2.20	0.41
63:P:23:PHE:HE1	63:P:91:THR:HG21	1.84	0.41
65:R:13:LYS:HB3	65:R:13:LYS:HE2	4.05	0.41
66:S:71:PHE:HE1	66:S:73:LEU:HD22	1.85	0.41
21:0:96:ASP:OD1	21:0:97:VAL:N	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1014:U:C2'	1:1:1015:U:H5''	2.49	0.41
1:1:1820:U:H1'	1:1:1821:U:OP2	2.20	0.41
1:1:3050:U:O2'	25:7:16:GLY:O	2.38	0.41
48:A:1244:A:H3'	48:A:1244:A:N3	2.35	0.41
48:A:226:A:H2'	48:A:227:U:H5'	2.02	0.41
48:A:413:U:H2'	48:A:414:C:C6	2.55	0.41
48:A:826:U:H2'	48:A:827:C:C6	2.56	0.41
41:AN:89:TYR:O	41:AN:93:LYS:HE2	2.21	0.41
1:1:2767:U:O2'	43:AP:30:ALA:O	2.34	0.41
1:AR:2314:U:O2'	1:AR:2315:G:OP1	2.36	0.41
1:AR:2595:A:H5'	1:AR:2596:U:OP2	2.21	0.41
1:AR:3096:C:H2'	1:AR:3097:C:C6	2.55	0.41
1:AR:3155:U:H2'	1:AR:3155:U:O2	2.19	0.41
1:AR:585:A:H2'	1:AR:586:C:C6	2.56	0.41
1:AR:436:A:H61	1:AR:623:U:H3	1.67	0.41
49:B:141:ILE:HA	49:B:142:PRO:HD3	1.90	0.41
50:C:166:LYS:HB2	50:C:166:LYS:HE3	1.87	0.41
7:CG:258:LYS:HD3	7:CG:258:LYS:HA	1.37	0.41
7:CG:60:ILE:HB	7:CG:80:SER:HB3	2.02	0.41
1:AR:1334:U:OP1	9:CI:206:LYS:HE3	2.21	0.41
12:CL:149:VAL:O	12:CL:153:ARG:HB2	2.20	0.41
1:AR:269:G:H5'	16:CP:120:TRP:CE3	2.54	0.41
3:AT:131:A:H5''	26:CZ:93:TYR:CE2	2.55	0.41
32:DF:55:LEU:O	32:DF:59:ILE:HG13	2.21	0.41
54:G:156:ARG:HB2	54:G:156:ARG:HH11	1.86	0.41
54:G:97:LEU:HD23	54:G:97:LEU:HA	1.93	0.41
59:L:69:THR:O	59:L:73:VAL:HG23	2.21	0.41
65:R:115:THR:HB	65:R:118:ILE:O	2.20	0.41
65:R:28:LEU:HG	65:R:64:ASP:OD1	2.20	0.41
66:S:96:SER:HA	66:S:97:ASN:HA	1.55	0.41
67:T:54:LEU:H	67:T:54:LEU:HD22	1.84	0.41
67:T:49:LYS:NZ	67:T:80:LYS:O	2.35	0.41
71:X:41:MET:HG2	71:X:129:VAL:HG21	2.01	0.41
72:Y:23:ARG:HD2	72:Y:26:GLU:OE1	2.20	0.41
1:1:1296:C:H5'	21:0:115:ARG:NH1	2.35	0.41
1:1:138:U:H2'	1:1:139:G:H8	1.85	0.41
1:1:2266:U:H2'	1:1:2267:C:C6	2.55	0.41
1:1:2443:A:N6	1:1:2504:U:O4	2.54	0.41
1:1:2554:A:N7	44:AQ:62:LYS:NZ	2.63	0.41
1:1:3294:A:H2'	1:1:3295:A:O4'	2.21	0.41
1:1:2603:G:O6	84:1:3402:OHX:N2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:1:3540:OHX:N6	84:1:3705:OHX:N5	2.67	0.41
1:1:913:A:H2	1:1:2134:G:N3	2.18	0.41
22:2:86:GLU:OE1	22:2:88:ARG:NH1	2.53	0.41
48:A:1696:G:H21	48:A:1705:C:H5	1.68	0.41
48:A:226:A:C2'	48:A:227:U:H5'	2.50	0.41
48:A:275:C:H2'	48:A:276:C:C5	2.54	0.41
48:A:800:U:H2'	48:A:801:G:C8	2.54	0.41
48:A:802:G:O6	84:A:1932:OHX:N3	2.53	0.41
31:AD:17:VAL:O	31:AD:21:GLY:N	2.47	0.41
43:AP:14:GLY:C	43:AP:16:THR:H	2.23	0.41
1:AR:1263:A:H2'	1:AR:1263:A:N3	2.35	0.41
1:AR:379:C:H2'	1:AR:380:U:H6	1.85	0.41
1:AR:65:A:C4	1:AR:110:G:N7	2.88	0.41
49:B:122:ILE:HA	49:B:144:ILE:O	2.20	0.41
50:C:105:PHE:CD1	50:C:213:ARG:HA	2.54	0.41
7:CG:105:ILE:O	7:CG:109:THR:HG23	2.20	0.41
7:CG:86:TYR:CE2	7:CG:247:ILE:HA	2.55	0.41
17:CQ:129:LEU:HA	17:CQ:129:LEU:HD12	1.85	0.41
17:CQ:181:ALA:O	17:CQ:184:THR:HG22	2.21	0.41
18:CR:64:ASN:O	18:CR:67:ILE:HB	2.21	0.41
21:CU:167:ARG:HA	21:CU:168:PRO:HD3	1.92	0.41
22:CV:75:ILE:HA	22:CV:87:LYS:O	2.21	0.41
26:CZ:57:LEU:CD1	26:CZ:61:LYS:HG2	2.44	0.41
51:D:148:LEU:HD22	51:D:148:LEU:HA	1.83	0.41
30:DD:14:ARG:NH1	30:DD:18:ARG:HD3	2.35	0.41
34:DH:37:THR:HB	34:DH:38:PRO:HD2	2.01	0.41
35:DI:99:LYS:O	35:DI:103:LYS:HG2	2.19	0.41
43:DQ:15:LYS:HA	43:DQ:18:ARG:HG3	2.02	0.41
48:A:955:A:H5''	62:O:10:GLY:HA3	2.03	0.41
67:T:52:VAL:HG22	67:T:65:GLU:HG2	2.02	0.41
1:1:208:C:C2'	1:1:209:A:H5'	2.51	0.41
1:1:2139:A:H62	38:AK:4:GLY:HA3	1.85	0.41
1:1:2756:C:O4'	22:2:49:GLN:HG2	2.20	0.41
1:1:2765:C:H2'	1:1:2766:U:C6	2.56	0.41
1:1:3088:G:OP2	84:1:3713:OHX:N3	2.53	0.41
1:1:3239:G:O6	84:1:3504:OHX:N6	2.53	0.41
84:1:3569:OHX:N1	84:1:3581:OHX:N4	2.68	0.41
1:1:534:U:O2	21:O:146:LYS:HA	2.20	0.41
48:A:1160:A:H2'	48:A:1161:C:C6	2.55	0.41
48:A:1796:C:H4'	48:A:1797:A:OP2	2.21	0.41
48:A:77:U:O5'	48:A:77:U:H6	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:979:A:N3	48:A:1775:U:O2'	2.48	0.41
1:AR:1814:A:H4'	1:AR:1815:U:H5'	2.01	0.41
1:AR:1820:U:H1'	1:AR:1821:U:OP2	2.20	0.41
1:AR:2190:U:C4	1:AR:2191:U:C4	3.08	0.41
1:AR:3242:G:C2	1:AR:3245:A:C8	3.08	0.41
1:AR:3085:G:OP2	84:AR:3409:OHX:N1	2.54	0.41
84:AR:3481:OHX:N6	84:AR:3703:OHX:N3	2.69	0.41
1:AR:1840:U:OP2	84:AR:3545:OHX:N1	2.54	0.41
1:AR:1213:G:N7	84:AR:3554:OHX:N6	2.68	0.41
1:AR:543:C:N4	1:AR:548:G:H1	2.19	0.41
1:AR:896:A:H5'	4:CD:183:GLY:HA2	2.02	0.41
2:AS:110:G:OP2	7:CG:279:LYS:HG3	2.20	0.41
2:AS:28:C:OP1	13:CM:137:ARG:HD3	2.20	0.41
49:B:50:VAL:HA	49:B:53:THR:HB	2.02	0.41
50:C:59:ASP:N	50:C:59:ASP:OD1	2.49	0.41
50:C:33:LYS:HB3	50:C:97:LEU:HD22	2.03	0.41
5:CE:56:ILE:HD11	5:CE:359:ILE:HG12	2.01	0.41
7:CG:211:LEU:HD23	7:CG:211:LEU:HA	1.91	0.41
9:CI:236:ILE:O	9:CI:240:VAL:HG23	2.21	0.41
12:CL:23:ASN:O	12:CL:24:ARG:HB2	2.20	0.41
19:CS:178:ARG:HA	19:CS:178:ARG:HD3	1.78	0.41
24:CX:15:LEU:HD13	24:CX:51:ALA:HB3	2.01	0.41
38:DL:28:HIS:CE1	38:DL:31:LYS:HG3	2.56	0.41
53:F:193:GLY:HA3	53:F:210:ILE:CG2	2.39	0.41
54:G:103:ASN:HA	54:G:106:LYS:HD2	2.03	0.41
55:H:141:ILE:HG21	55:H:153:VAL:HG13	2.03	0.41
56:I:63:PRO:HB2	56:I:65:PRO:HD2	2.03	0.41
60:M:127:GLN:HG3	60:M:137:PHE:CE2	2.56	0.41
66:S:113:LEU:HG	66:S:114:GLY:N	2.36	0.41
67:T:28:ILE:O	67:T:32:LEU:HG	2.21	0.41
48:A:804:A:N3	71:X:105:THR:HG22	2.34	0.41
1:1:3136:G:OP2	84:1:3635:OHX:N6	2.53	0.41
1:1:655:C:OP1	33:AF:27:ARG:HB3	2.20	0.41
1:1:718:G:N1	1:1:721:G:H1'	2.35	0.41
3:4:127:U:C2'	3:4:128:U:H5'	2.50	0.41
24:6:90:GLY:O	25:7:16:GLY:HA2	2.21	0.41
25:7:6:ASP:HA	25:7:30:ARG:O	2.20	0.41
48:A:12:U:H2'	48:A:13:C:C6	2.55	0.41
48:A:1645:G:H22	48:A:1756:A:H2	1.67	0.41
42:AO:3:ALA:HB3	48:A:1773:C:OP1	2.20	0.41
48:A:788:A:H2'	53:F:19:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:AA:81:LEU:HA	28:AA:81:LEU:HD23	1.85	0.41
29:AB:92:LYS:HG2	29:AB:92:LYS:H	1.46	0.41
33:AF:121:ASN:N	33:AF:121:ASN:OD1	2.54	0.41
36:AI:54:VAL:O	36:AI:58:ILE:HG13	2.21	0.41
40:AM:21:ARG:CZ	40:AM:24:PRO:HG3	2.50	0.41
1:AR:1108:U:H2'	1:AR:1109:U:C6	2.56	0.41
1:AR:186:U:OP1	27:DA:122:LYS:HE3	2.20	0.41
1:AR:2724:U:H4'	22:CV:54:HIS:CD2	2.55	0.41
1:AR:2751:G:N7	84:AR:3660:OHX:N5	2.69	0.41
84:AR:3526:OHX:N5	84:AR:3721:OHX:N1	2.68	0.41
1:AR:506:U:H2'	1:AR:507:U:O4'	2.21	0.41
1:AR:578:A:H5''	1:AR:579:G:O5'	2.20	0.41
1:AR:589:A:H1'	1:AR:1337:A:H5''	2.02	0.41
1:AR:29:C:H4'	1:AR:62:A:H4'	2.02	0.41
1:AR:789:A:H2'	1:AR:790:U:H6	1.84	0.41
3:AT:82:U:O2'	3:AT:83:C:OP1	2.35	0.41
5:CE:339:ARG:HG2	5:CE:340:LYS:O	2.20	0.41
12:CL:51:HIS:O	12:CL:165:ILE:HA	2.20	0.41
21:CU:23:LYS:HA	22:CV:146:ASN:HD21	1.86	0.41
56:I:173:TYR:HE2	56:I:179:LYS:HB2	1.85	0.41
57:J:148:ALA:O	57:J:149:SER:HB3	2.20	0.41
21:O:138:GLN:HA	21:O:141:LYS:HB2	2.03	0.41
1:1:651:G:O2'	1:1:1435:A:OP1	2.31	0.41
1:1:1481:A:H2'	1:1:1481:A:N3	2.36	0.41
1:1:155:G:H1'	37:AJ:26:ILE:HD13	2.02	0.41
1:1:1615:C:H2'	1:1:1616:U:H6	1.85	0.41
1:1:1846:C:OP1	1:1:1849:C:N4	2.42	0.41
1:1:2375:G:O2'	1:1:2377:G:OP2	2.26	0.41
1:1:2898:G:H5''	1:1:2899:C:H5'	2.01	0.41
48:A:1490:C:O2'	48:A:1491:U:O2	2.35	0.41
48:A:1689:A:H2'	48:A:1690:G:H8	1.85	0.41
48:A:25:C:H4'	48:A:26:A:O5'	2.20	0.41
48:A:866:G:OP1	62:O:2:GLY:HA3	2.20	0.41
1:1:2787:G:O3'	29:AB:57:GLY:HA2	2.21	0.41
30:AC:23:LYS:HG3	30:AC:24:PRO:HD2	2.02	0.41
1:1:424:G:O2'	33:AF:23:ASP:OD2	2.31	0.41
37:AJ:33:ALA:O	37:AJ:34:SER:HB3	2.20	0.41
1:AR:1131:G:C4	1:AR:2373:A:C2	3.09	0.41
1:AR:2314:U:H2'	1:AR:2314:U:H6	1.63	0.41
1:AR:2714:G:H4'	1:AR:2715:A:C5'	2.51	0.41
1:AR:2897:A:H2'	1:AR:2899:C:C5'	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:3280:U:O2'	1:AR:3281:U:H5''	2.21	0.41
1:AR:508:U:H2'	1:AR:509:U:C6	2.56	0.41
1:AR:817:A:H2'	1:AR:920:A:C2	2.56	0.41
1:AR:831:G:N7	84:AR:3426:OHX:N2	2.68	0.41
1:AR:850:U:H2'	1:AR:851:C:C6	2.55	0.41
3:AT:123:G:OP2	84:AT:211:OHX:N6	2.54	0.41
49:B:69:ASN:OD1	51:D:244:SER:OG	2.33	0.41
49:B:8:ASP:N	49:B:8:ASP:OD1	2.52	0.41
5:CE:81:THR:HG21	5:CE:205:VAL:HG11	2.03	0.41
10:CJ:54:GLU:HG2	10:CJ:57:ARG:HH21	1.85	0.41
2:AS:64:A:C8	12:CL:206:LEU:HD13	2.55	0.41
13:CM:10:ARG:NH2	13:CM:151:SER:O	2.50	0.41
17:CQ:56:ASP:O	17:CQ:59:ARG:HG2	2.21	0.41
20:CT:182:ASP:OD1	20:CT:182:ASP:N	2.54	0.41
52:E:172:THR:HA	52:E:184:ILE:O	2.21	0.41
53:F:15:PRO:HG2	53:F:18:TRP:CE2	2.55	0.41
56:I:131:PHE:HA	56:I:131:PHE:HD1	1.70	0.41
62:O:135:LEU:HD22	62:O:139:TRP:CD1	2.56	0.41
64:Q:68:PRO:HG2	64:Q:71:GLU:HB3	2.03	0.41
67:T:48:LYS:HD3	68:U:35:ASP:OD1	2.21	0.41
69:V:105:GLN:HG3	69:V:106:ILE:N	2.35	0.41
1:1:1706:C:H2'	1:1:1707:A:O4'	2.21	0.41
1:1:2427:U:H2'	1:1:2428:U:C6	2.55	0.41
1:1:873:C:H5''	1:1:874:U:O5'	2.21	0.41
22:2:57:TYR:CD1	22:2:89:LEU:HD21	2.56	0.41
22:2:75:ILE:HA	22:2:87:LYS:O	2.21	0.41
25:7:4:GLU:HG2	25:7:30:ARG:CD	2.50	0.41
48:A:458:G:OP1	73:Z:109:LYS:NZ	2.54	0.41
33:AF:78:ASN:HA	33:AF:108:ILE:HD11	2.02	0.41
37:AJ:52:PRO:HD2	69:V:15:GLN:HB3	192.11	0.41
39:AL:31:LEU:H	39:AL:31:LEU:HD23	1.85	0.41
39:AL:77:ARG:O	39:AL:78:LEU:HB2	2.20	0.41
43:AP:4:VAL:HA	43:AP:5:PRO:HD3	1.90	0.41
43:AP:73:GLU:OE1	43:AP:80:ARG:NH2	2.54	0.41
1:AR:1753:G:O6	84:AR:3586:OHX:N5	2.54	0.41
1:AR:2595:A:H3'	1:AR:2596:U:H6	1.86	0.41
1:AR:2859:U:O2'	84:AR:3403:OHX:N6	2.54	0.41
1:AR:3052:G:C6	84:AR:3677:OHX:N3	2.89	0.41
84:AR:3481:OHX:N2	84:AR:3703:OHX:N5	2.68	0.41
49:B:198:MET:SD	49:B:199:PRO:HD2	2.60	0.41
50:C:219:LYS:HE2	50:C:219:LYS:HB3	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CD:46:LYS:HD2	4:CD:46:LYS:HA	1.88	0.41
5:CE:361:THR:HG23	5:CE:371:GLN:O	2.21	0.41
13:CM:87:LYS:NZ	13:CM:105:GLY:O	2.31	0.41
13:CM:166:LYS:C	13:CM:168:ASP:H	2.24	0.41
1:AR:770:G:OP1	14:CN:171:ARG:HD3	2.21	0.41
21:CU:67:ALA:O	21:CU:69:PRO:HD3	2.21	0.41
51:D:188:LEU:HD23	51:D:188:LEU:HA	1.83	0.41
28:DB:5:LEU:HD13	28:DB:77:TYR:CZ	2.56	0.41
29:DC:82:ILE:HA	29:DC:83:PRO:HD3	1.94	0.41
52:E:34:TYR:CE1	52:E:37:VAL:HG13	2.56	0.41
48:A:1217:A:C5'	59:L:1:MET:HG3	2.51	0.41
65:R:113:ASP:CG	65:R:115:THR:H	2.24	0.41
65:R:73:GLY:N	65:R:76:SER:HB3	2.35	0.41
73:Z:44:LEU:HA	73:Z:44:LEU:HD13	4.40	0.41
1:1:2207:A:H2'	1:1:2208:A:H8	1.85	0.41
1:1:2561:A:O2'	1:1:2562:A:H8	2.03	0.41
1:1:2801:A:O2'	1:1:2802:A:H2'	2.20	0.41
1:1:634:C:O3'	33:AF:47:ARG:NH1	2.54	0.41
48:A:179:A:H2'	48:A:180:A:O4'	2.21	0.41
48:A:25:C:OP2	48:A:26:A:H2'	2.21	0.41
48:A:702:G:N7	84:A:2007:OHX:N2	2.68	0.41
48:A:705:U:H2'	48:A:706:A:N7	2.36	0.41
48:A:862:A:C2	48:A:963:A:C4	3.08	0.41
48:A:967:A:H2'	48:A:968:U:O4'	2.20	0.41
31:AD:16:LEU:HD11	31:AD:97:ASP:HB3	2.03	0.41
34:AG:53:TYR:CZ	34:AG:65:ARG:HB2	2.56	0.41
35:AH:81:CYS:O	35:AH:82:ALA:HB3	2.20	0.41
43:AP:3:ASN:HA	43:AP:92:GLU:O	2.21	0.41
1:AR:1481:A:O2'	1:AR:1858:A:C2	2.69	0.41
1:AR:3165:A:H2'	1:AR:3166:C:C6	2.55	0.41
1:AR:325:A:H5''	1:AR:326:U:OP2	2.20	0.41
1:AR:2248:C:OP2	84:AR:3703:OHX:N3	2.54	0.41
1:AR:379:C:H2'	1:AR:380:U:C6	2.56	0.41
1:AR:981:U:HO2'	1:AR:982:C:P	2.44	0.41
9:CI:24:GLU:O	9:CI:26:VAL:N	2.54	0.41
11:CK:164:ILE:HA	11:CK:164:ILE:HD13	1.83	0.41
20:CT:25:ASP:HB3	20:CT:28:GLU:HB2	2.03	0.41
22:CV:104:GLU:HG3	22:CV:105:PHE:N	2.36	0.41
27:DA:125:LYS:HG2	27:DA:125:LYS:H	1.58	0.41
30:DD:23:LYS:HD2	30:DD:23:LYS:HA	1.75	0.41
37:DK:8:ALA:O	37:DK:13:LYS:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:DR:73:THR:HG23	44:DR:76:ALA:H	1.86	0.41
56:I:173:TYR:CE2	56:I:181:ILE:HD13	2.56	0.41
60:M:54:ILE:HG23	60:M:55:ASP:H	1.85	0.41
63:P:47:LYS:HD3	63:P:47:LYS:HA	1.90	0.41
71:X:65:LEU:HD13	71:X:65:LEU:H	1.86	0.41
1:1:1071:U:O2'	1:1:1072:G:OP2	2.36	0.41
1:1:656:A:C2	1:1:1440:G:C2	3.09	0.41
1:1:1492:G:O3'	40:AM:48:LYS:NZ	2.52	0.41
1:1:2219:A:H2'	1:1:2220:A:C8	2.56	0.41
1:1:2997:G:H1'	1:1:3396:U:H5'	2.01	0.41
1:1:3227:A:H2'	1:1:3228:C:H5'	2.02	0.41
1:1:3375:A:H5''	1:1:3378:C:H5	1.86	0.41
1:1:30:G:C6	1:1:55:G:C6	3.09	0.41
1:1:65:A:H4'	1:1:66:A:O5'	2.20	0.41
22:2:104:GLU:O	22:2:108:ARG:HB2	2.21	0.41
25:7:98:PRO:HD2	55:H:146:GLY:O	2.21	0.41
26:8:109:LYS:HE2	26:8:109:LYS:HB2	1.80	0.41
48:A:1469:A:H2'	48:A:1470:C:C6	2.56	0.41
48:A:196:G:O2'	48:A:197:A:H8	2.03	0.41
48:A:808:U:H2'	48:A:809:A:C8	2.56	0.41
48:A:973:A:H2'	48:A:974:A:H8	1.86	0.41
32:AE:29:ALA:HB3	32:AE:30:PRO:HD3	2.02	0.41
1:AR:1018:G:C5	1:AR:1035:G:C2	3.09	0.41
1:AR:1044:U:OP1	12:CL:90:ARG:NH1	2.54	0.41
1:AR:1382:G:OP2	6:CF:188:ARG:NH1	2.53	0.41
1:AR:1674:G:N7	84:AR:3473:OHX:N1	2.69	0.41
1:AR:230:U:O4	84:AR:3638:OHX:N6	2.54	0.41
1:AR:1410:U:OP2	84:AR:3533:OHX:N2	2.54	0.41
1:AR:535:G:O6	84:AR:3590:OHX:N2	2.54	0.41
1:AR:501:A:H2'	1:AR:502:U:H6	1.86	0.41
1:AR:908:G:H4'	1:AR:909:G:O5'	2.21	0.41
3:AT:68:G:O6	84:AT:214:OHX:N6	2.54	0.41
5:CE:151:ILE:O	5:CE:155:ALA:HB3	2.21	0.41
7:CG:122:VAL:CG2	7:CG:125:VAL:H	2.34	0.41
10:CJ:158:ASP:HB3	10:CJ:159:PRO:HD3	2.02	0.41
29:DC:73:LEU:HB2	29:DC:109:TYR:CD1	2.56	0.41
32:DF:77:ARG:HD2	32:DF:89:LEU:HD23	2.03	0.41
35:DI:81:CYS:O	35:DI:82:ALA:HB3	2.21	0.41
42:DP:4:LYS:HD2	42:DP:5:TRP:CZ3	2.55	0.41
58:K:136:VAL:O	58:K:155:HIS:HB3	2.21	0.41
60:M:108:PRO:HG3	60:M:134:THR:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:W:64:GLU:O	70:W:68:SER:HB2	2.21	0.41
72:Y:130:VAL:HG11	72:Y:143:PRO:HD3	2.02	0.41
72:Y:57:LEU:HD13	72:Y:59:ILE:HD11	2.03	0.41
1:1:1571:A:H2'	1:1:1572:U:O4'	2.20	0.41
1:1:1577:G:H2'	1:1:1578:C:O4'	2.21	0.41
1:1:1815:U:O2'	1:1:1816:A:P	2.79	0.41
1:1:1941:C:O2'	1:1:3344:A:N6	2.52	0.41
1:1:3131:U:H2'	1:1:3132:C:H6	1.86	0.41
2:3:22:A:C6	2:3:23:A:C6	3.09	0.41
1:1:407:A:C2	3:4:17:A:H1'	2.55	0.41
48:A:1067:C:H2'	48:A:1068:C:H6	1.84	0.41
48:A:1472:C:H41	48:A:1536:G:H1	1.67	0.41
48:A:1541:G:C5	48:A:1542:G:C6	3.09	0.41
48:A:330:G:H2'	48:A:331:A:O4'	2.21	0.41
48:A:632:U:OP2	60:M:102:LYS:NZ	2.49	0.41
48:A:843:U:H2'	48:A:844:A:C8	2.56	0.41
29:AB:71:PRO:HB2	29:AB:109:TYR:HA	2.03	0.41
29:AB:112:ILE:HB	29:AB:130:VAL:HG12	2.02	0.41
31:AD:25:LEU:HD23	31:AD:90:VAL:HG13	2.03	0.41
1:AR:1366:A:C2	1:AR:1367:G:C4	3.09	0.41
1:AR:1662:G:H2'	1:AR:1663:C:C6	2.56	0.41
1:AR:1656:A:O3'	84:AR:3682:OHX:N2	2.54	0.41
1:AR:620:U:C2'	1:AR:621:A:H4'	2.51	0.41
2:AS:110:G:C6	2:AS:111:U:C4	3.09	0.41
3:AT:125:U:H2'	3:AT:125:U:O2	2.20	0.41
49:B:109:ASN:O	49:B:112:THR:HG22	2.20	0.41
49:B:117:GLU:OE1	51:D:40:LYS:HG3	2.20	0.41
49:B:177:LEU:HA	49:B:177:LEU:HD23	1.87	0.41
50:C:128:LYS:HG3	50:C:134:VAL:HG22	2.03	0.41
5:CE:308:MET:HB3	5:CE:308:MET:HE3	1.89	0.41
5:CE:311:PHE:CE2	5:CE:317:ILE:HG13	2.56	0.41
8:CH:3:ALA:HB2	33:DG:77:ALA:HB2	2.01	0.41
1:AR:121:A:C6	10:CJ:129:PRO:HG3	2.55	0.41
15:CO:32:LEU:HD11	15:CO:94:TRP:CD1	2.56	0.41
1:AR:45:A:P	16:CP:85:THR:HG21	2.60	0.41
18:CR:169:THR:O	18:CR:173:ARG:N	2.54	0.41
21:CU:42:TRP:O	21:CU:46:GLN:HG3	2.20	0.41
23:CW:16:THR:HG22	23:CW:64:THR:OG1	2.21	0.41
25:CY:6:ASP:HB3	25:CY:11:ALA:H	1.85	0.41
32:DF:13:THR:HG22	32:DF:72:ARG:HD3	2.03	0.41
44:DR:30:GLU:HA	44:DR:33:GLN:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:789:A:O2'	53:F:106:LYS:NZ	2.54	0.41
55:H:54:GLY:C	55:H:63:MET:HE3	2.40	0.41
61:N:81:ASP:HA	61:N:82:PRO:HD3	1.91	0.41
64:Q:85:ILE:HD11	64:Q:116:LEU:HD23	2.03	0.41
21:0:1:MET:HB3	21:0:1:MET:HE2	1.83	0.40
1:1:3164:C:O2'	1:1:3165:A:H8	2.05	0.40
1:1:145:G:O6	84:1:3509:OHX:N4	2.54	0.40
1:1:500:C:H2'	1:1:501:A:H8	1.84	0.40
48:A:280:U:HO2'	48:A:281:G:P	2.38	0.40
48:A:819:G:O6	48:A:853:G:C6	2.74	0.40
48:A:997:G:H2'	48:A:998:A:O4'	2.21	0.40
1:1:1669:C:OP1	35:AH:24:LYS:HE2	2.21	0.40
1:AR:1940:G:H2'	1:AR:1941:C:O4'	2.21	0.40
1:AR:2260:U:H2'	1:AR:2261:G:O4'	2.22	0.40
1:AR:2523:A:H2'	10:CJ:49:TYR:O	2.22	0.40
1:AR:724:U:OP2	84:AR:3508:OHX:N5	2.54	0.40
84:AT:202:OHX:N6	84:AT:212:OHX:N4	2.68	0.40
49:B:188:LEU:HD12	49:B:189:VAL:H	1.85	0.40
1:AR:3307:A:OP1	5:CE:226:PHE:HB2	2.21	0.40
1:AR:3304:U:O3'	5:CE:334:ARG:NH2	2.53	0.40
5:CE:345:ASN:ND2	5:CE:347:SER:HB2	2.36	0.40
7:CG:55:PHE:CE2	7:CG:158:ARG:HG3	2.56	0.40
9:CI:173:LEU:HD12	9:CI:173:LEU:HA	1.81	0.40
9:CI:179:LEU:H	9:CI:179:LEU:HD22	1.87	0.40
13:CM:173:ASP:HB3	13:CM:174:LYS:H	1.49	0.40
16:CP:102:ALA:O	16:CP:106:VAL:HG13	2.21	0.40
16:CP:135:VAL:CG1	16:CP:142:ILE:HG12	2.52	0.40
17:CQ:68:ARG:H	17:CQ:68:ARG:HG2	1.78	0.40
6:CF:290:ILE:HG23	19:CS:35:PHE:CE2	2.56	0.40
22:CV:68:THR:HG22	22:CV:71:SER:O	2.21	0.40
41:DO:94:SER:OG	41:DO:104:PRO:O	2.39	0.40
54:G:144:GLU:OE1	54:G:225:ARG:NH2	2.52	0.40
56:I:67:LEU:HA	56:I:67:LEU:HD23	1.79	0.40
58:K:81:VAL:HG23	58:K:86:LEU:HD23	2.03	0.40
61:N:125:ASN:O	61:N:126:TRP:CD1	2.74	0.40
68:U:27:LYS:HB3	68:U:111:ILE:HD11	2.02	0.40
21:0:13:ARG:O	21:0:22:PRO:HG2	2.22	0.40
1:1:3131:U:H2'	1:1:3132:C:C6	2.56	0.40
1:1:3317:U:H4'	1:1:3318:G:O5'	2.21	0.40
84:1:3474:OHX:N5	84:1:3730:OHX:N2	2.69	0.40
84:1:3540:OHX:N2	84:1:3705:OHX:N5	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:561:C:H2'	1:1:562:C:H6	1.86	0.40
26:8:86:VAL:HG11	26:8:95:ILE:HD11	2.02	0.40
27:9:60:ARG:HA	27:9:60:ARG:HD3	1.83	0.40
48:A:1238:A:H2'	48:A:1239:U:O4'	2.22	0.40
48:A:1348:A:OP1	84:A:1998:OHX:N1	2.54	0.40
48:A:781:U:O2'	48:A:782:U:H6	2.04	0.40
1:1:135:C:H1'	36:AI:93:THR:HB	2.04	0.40
40:AM:9:ILE:HG22	40:AM:13:MET:CE	2.51	0.40
1:1:2802:A:C8	43:AP:56:PRO:HA	2.56	0.40
1:AR:1595:U:C2	1:AR:1596:C:C5	3.08	0.40
1:AR:2254:U:H6	1:AR:2254:U:H5''	1.86	0.40
1:AR:2812:C:H2'	1:AR:2813:A:C8	2.57	0.40
1:AR:2960:C:OP1	84:AR:3475:OHX:N3	2.54	0.40
1:AR:3138:U:OP2	5:CE:30:LYS:HD3	2.22	0.40
1:AR:1310:G:N7	84:AR:3532:OHX:N4	2.69	0.40
1:AR:796:U:H2'	1:AR:797:U:C6	2.56	0.40
49:B:185:ARG:HG3	70:W:45:ALA:O	2.21	0.40
5:CE:53:MET:HE1	5:CE:327:CYS:CB	2.51	0.40
8:CH:143:LYS:HE3	8:CH:143:LYS:HB2	1.91	0.40
9:CI:151:ARG:HD2	9:CI:244:ASN:OD1	2.21	0.40
20:CT:106:LEU:HD12	20:CT:106:LEU:HA	1.93	0.40
20:CT:158:GLU:O	20:CT:159:ALA:HB3	2.22	0.40
22:CV:65:TYR:HB3	22:CV:75:ILE:HG22	2.03	0.40
23:CW:59:ASP:HB3	23:CW:62:VAL:HB	2.03	0.40
36:DJ:74:LYS:HE3	36:DJ:75:TYR:CZ	2.56	0.40
52:E:45:LYS:HE2	52:E:45:LYS:HB2	1.84	0.40
57:J:57:ALA:HB2	57:J:177:GLY:HA2	2.03	0.40
65:R:32:ASN:ND2	65:R:69:VAL:H	2.16	0.40
71:X:77:PRO:HG3	72:Y:7:ARG:O	2.21	0.40
73:Z:36:SER:HB3	73:Z:39:GLU:HB3	2.03	0.40
1:1:1248:C:OP1	1:1:1249:G:H8	2.03	0.40
1:1:2556:C:O2'	28:AA:135:ARG:NE	2.48	0.40
1:1:2746:A:H2'	1:1:2747:A:O4'	2.22	0.40
1:1:374:A:N3	1:1:376:G:H5''	2.36	0.40
1:1:856:G:C6	1:1:857:G:N1	2.89	0.40
1:1:806:A:C4	1:1:936:A:C2	3.09	0.40
22:2:12:ARG:HD3	22:2:13:TYR:CZ	2.57	0.40
22:2:68:THR:HG22	22:2:71:SER:O	2.21	0.40
1:1:2728:G:C2	22:2:80:VAL:HG21	2.56	0.40
24:6:40:LYS:HD3	24:6:59:MET:CE	2.52	0.40
1:1:3043:C:OP2	24:6:48:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2111:G:H1'	25:7:44:LYS:HD2	2.02	0.40
48:A:1277:G:H2'	48:A:1278:G:O4'	2.20	0.40
48:A:751:G:H2'	48:A:752:A:C8	2.56	0.40
48:A:778:G:H5'	48:A:780:A:N1	2.36	0.40
48:A:811:A:C2	48:A:858:G:H1'	2.56	0.40
48:A:957:G:H2'	48:A:958:U:O4'	2.21	0.40
31:AD:56:LEU:HA	31:AD:56:LEU:HD23	1.93	0.40
39:AL:61:LYS:O	39:AL:65:LEU:HB2	2.21	0.40
1:AR:1157:G:H2'	1:AR:1158:A:O4'	2.21	0.40
1:AR:2191:U:H2'	1:AR:2192:C:O4'	2.22	0.40
1:AR:2268:U:C3'	1:AR:2269:U:H5''	2.51	0.40
1:AR:2537:U:O2'	1:AR:2538:U:O5'	2.33	0.40
1:AR:776:U:C5	1:AR:2719:U:O2	2.74	0.40
1:AR:996:A:C2	1:AR:1054:A:C4	3.09	0.40
49:B:69:ASN:HB3	49:B:71:GLU:CD	2.41	0.40
49:B:4:PRO:HG2	49:B:7:PHE:HD2	1.86	0.40
50:C:116:LYS:HE2	50:C:117:TRP:HZ3	1.86	0.40
50:C:184:LEU:HA	50:C:184:LEU:HD22	1.95	0.40
50:C:84:ILE:HD13	50:C:103:MET:HB2	2.03	0.40
5:CE:296:THR:CG2	5:CE:298:PHE:H	2.26	0.40
7:CG:59:ASP:OD2	7:CG:81:HIS:HD2	2.04	0.40
12:CL:156:ARG:HG2	12:CL:163:GLN:HG2	2.03	0.40
15:CO:108:ARG:NH1	15:CO:112:LEU:HD23	2.36	0.40
15:CO:119:GLN:O	15:CO:123:LEU:HD12	2.22	0.40
18:CR:95:LEU:HD23	18:CR:95:LEU:HA	1.87	0.40
20:CT:115:ILE:HG12	20:CT:119:LEU:HD23	2.02	0.40
51:D:152:HIS:CG	51:D:153:SER:H	2.39	0.40
32:DF:27:LYS:O	32:DF:31:ARG:HB2	2.20	0.40
33:DG:103:LYS:O	33:DG:106:VAL:HG13	2.21	0.40
37:DK:80:PHE:O	37:DK:84:LYS:HG3	2.21	0.40
39:DM:11:PHE:O	39:DM:14:LEU:HB2	2.21	0.40
40:DN:42:ARG:HG2	40:DN:43:ASN:N	2.35	0.40
52:E:21:LEU:HD22	52:E:25:PHE:CE2	2.57	0.40
52:E:50:ILE:HB	52:E:88:ALA:HA	2.03	0.40
56:I:173:TYR:CE2	56:I:179:LYS:HB2	2.55	0.40
64:Q:52:LYS:HB2	64:Q:53:PRO:HD3	2.02	0.40
67:T:60:GLU:HB2	67:T:61:LEU:H	1.65	0.40
71:X:104:LEU:HB2	71:X:124:LYS:O	2.21	0.40
48:A:571:G:H5''	72:Y:114:LYS:HD3	2.03	0.40
72:Y:58:GLY:O	72:Y:68:ILE:HG23	2.21	0.40
1:1:1717:U:H2'	1:1:1718:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1912:U:C4	1:1:1913:A:C6	3.09	0.40
1:1:2401:A:OP2	84:1:3624:OHX:N2	2.54	0.40
1:1:2622:C:H2'	1:1:2623:G:H5'	2.03	0.40
1:1:634:C:H5'	34:AG:21:ARG:O	2.21	0.40
1:1:965:A:H2	29:AB:43:ILE:HD12	1.86	0.40
22:2:18:ASP:O	22:2:21:LYS:HB2	2.20	0.40
48:A:328:A:H2'	48:A:329:G:O4'	2.21	0.40
48:A:453:U:O2	48:A:453:U:H2'	2.22	0.40
48:A:850:A:C2	48:A:851:U:C2	3.09	0.40
32:AE:46:THR:HG21	32:AE:91:SER:OG	2.21	0.40
34:AG:48:ARG:HG2	34:AG:48:ARG:HH11	1.86	0.40
3:4:52:A:N6	40:AM:27:ILE:HD13	2.35	0.40
42:AO:5:TRP:CE3	42:AO:5:TRP:HA	2.57	0.40
1:AR:1034:U:H2'	1:AR:1035:G:H8	1.86	0.40
1:AR:1764:U:H3'	1:AR:1765:U:C4'	2.52	0.40
1:AR:1915:A:H5''	20:CT:84:THR:HG22	2.03	0.40
1:AR:2263:C:HO2'	1:AR:2264:U:P	2.45	0.40
1:AR:271:C:H2'	1:AR:272:G:O4'	2.21	0.40
1:AR:289:A:H2'	1:AR:290:G:C8	2.56	0.40
1:AR:3311:C:OP1	84:AR:3735:OHX:N4	2.55	0.40
1:AR:860:G:O4'	4:CD:181:LYS:NZ	2.55	0.40
2:AS:112:G:OP2	84:AS:205:OHX:N6	2.54	0.40
3:AT:149:A:H2'	3:AT:150:G:C8	2.56	0.40
49:B:11:PRO:O	49:B:15:GLN:HG3	2.21	0.40
4:CD:65:ASP:HA	4:CD:66:PRO:HD3	1.91	0.40
6:CF:23:PRO:HD2	6:CF:26:PHE:CD1	2.57	0.40
6:CF:263:GLY:HA3	6:CF:268:ALA:O	2.22	0.40
6:CF:6:VAL:N	6:CF:20:LEU:O	2.55	0.40
18:CR:52:LEU:HA	18:CR:52:LEU:HD12	1.90	0.40
21:CU:155:ARG:HD3	21:CU:172:TYR:CD1	2.57	0.40
22:CV:119:ALA:HA	22:CV:122:GLN:HB2	2.02	0.40
51:D:104:VAL:HG22	51:D:132:ALA:HB1	2.03	0.40
32:DF:71:LEU:HA	32:DF:71:LEU:HD23	1.90	0.40
33:DG:64:LYS:HD3	33:DG:65:PHE:CE2	2.56	0.40
54:G:156:ARG:H	54:G:156:ARG:HG3	1.60	0.40
54:G:57:SER:C	54:G:59:VAL:N	2.71	0.40
56:I:60:ILE:HD12	56:I:92:PHE:CZ	2.56	0.40
58:K:117:GLY:O	58:K:119:ALA:N	2.54	0.40
68:U:66:TYR:HA	68:U:124:ILE:HB	2.03	0.40
73:Z:41:ARG:O	73:Z:45:ALA:HB2	2.22	0.40
1:1:1246:G:H8	1:1:1246:G:OP1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1362:G:H2'	1:1:1363:A:C8	2.57	0.40
1:1:1569:U:H5''	1:1:1570:U:H6	1.87	0.40
1:1:1834:U:H3'	1:1:1835:A:H5'	2.03	0.40
1:1:864:G:OP2	84:1:3418:OHX:N2	2.55	0.40
1:1:1808:G:O6	84:1:3517:OHX:N3	2.55	0.40
1:1:371:G:H4'	1:1:396:A:N1	2.36	0.40
1:1:909:G:N2	1:1:910:G:H1'	2.36	0.40
1:1:816:A:H5''	1:1:920:A:H62	1.85	0.40
48:A:1503:A:H2'	48:A:1504:G:O4'	2.22	0.40
48:A:320:U:H3'	48:A:321:C:C5'	2.49	0.40
48:A:576:G:H4'	48:A:580:A:C4	2.57	0.40
48:A:894:U:H2'	48:A:895:G:C8	2.57	0.40
28:AA:36:HIS:N	28:AA:37:PRO:HD3	2.36	0.40
29:AB:74:ASN:CB	29:AB:115:LYS:HB2	2.51	0.40
32:AE:16:LEU:HA	32:AE:16:LEU:HD13	1.73	0.40
1:1:1389:G:H5''	33:AF:101:SER:HB3	2.03	0.40
38:AK:17:THR:O	38:AK:25:ARG:HA	2.21	0.40
40:AM:5:LYS:HE3	40:AM:13:MET:HE3	2.03	0.40
1:AR:2503:G:H1'	1:AR:2504:U:H5	1.85	0.40
1:AR:255:A:H2'	1:AR:256:G:C8	2.56	0.40
1:AR:2651:G:H4'	1:AR:2652:U:OP2	2.22	0.40
1:AR:2677:G:H2'	1:AR:2679:A:H2	1.87	0.40
1:AR:1901:A:O3'	1:AR:2918:G:H5'	2.21	0.40
1:AR:915:A:N3	1:AR:915:A:H2'	2.36	0.40
10:CJ:149:LYS:O	10:CJ:176:PRO:HG2	2.21	0.40
12:CL:77:THR:HG23	12:CL:85:PHE:HZ	1.86	0.40
14:CN:116:LEU:HD23	14:CN:116:LEU:HA	1.85	0.40
14:CN:80:VAL:HG12	14:CN:85:LEU:O	2.22	0.40
15:CO:21:VAL:HB	15:CO:63:VAL:HG13	2.02	0.40
22:CV:73:GLY:HA2	22:CV:89:LEU:O	2.22	0.40
26:CZ:96:LYS:O	26:CZ:100:LYS:HB2	2.22	0.40
27:DA:106:ILE:HG21	27:DA:109:LEU:HD23	2.02	0.40
27:DA:95:VAL:HG12	27:DA:96:PRO:O	2.22	0.40
1:AR:1407:A:O3'	33:DG:33:ARG:NH2	2.54	0.40
36:DJ:4:VAL:HG21	36:DJ:9:LEU:HD11	2.04	0.40
44:DR:35:ALA:HB3	44:DR:37:TYR:CE1	2.56	0.40
52:E:113:LEU:HA	52:E:113:LEU:HD23	1.81	0.40
52:E:11:LEU:HD23	52:E:11:LEU:HA	1.80	0.40
53:F:19:LEU:HD11	53:F:108:ARG:HD2	2.04	0.40
58:K:103:ASP:OD1	58:K:103:ASP:N	2.54	0.40
62:O:150:VAL:O	84:O:201:OHX:N3	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:S:19:ARG:H	66:S:19:ARG:HG2	1.69	0.40
67:T:12:GLN:H	67:T:12:GLN:HG3	1.80	0.40
49:B:142:PRO:HB3	70:W:34:ILE:CD1	2.51	0.40
71:X:75:ILE:HG13	71:X:125:ILE:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CD	250/252 (99%)	237 (95%)	13 (5%)	0	100	100
4	j	250/252 (99%)	235 (94%)	15 (6%)	0	100	100
5	CE	384/386 (100%)	357 (93%)	27 (7%)	0	100	100
5	k	384/386 (100%)	361 (94%)	22 (6%)	1 (0%)	41	76
6	CF	359/361 (99%)	333 (93%)	25 (7%)	1 (0%)	41	76
6	l	359/361 (99%)	334 (93%)	23 (6%)	2 (1%)	25	64
7	CG	294/296 (99%)	274 (93%)	19 (6%)	1 (0%)	41	76
7	m	294/296 (99%)	268 (91%)	26 (9%)	0	100	100
8	CH	152/175 (87%)	145 (95%)	6 (4%)	1 (1%)	22	60
8	n	152/175 (87%)	146 (96%)	5 (3%)	1 (1%)	22	60
9	CI	220/222 (99%)	207 (94%)	11 (5%)	2 (1%)	17	55
9	o	220/222 (99%)	208 (94%)	9 (4%)	3 (1%)	11	43
10	CJ	231/233 (99%)	208 (90%)	21 (9%)	2 (1%)	17	55
10	p	231/233 (99%)	210 (91%)	18 (8%)	3 (1%)	12	45
11	CK	189/191 (99%)	176 (93%)	13 (7%)	0	100	100
11	q	189/191 (99%)	176 (93%)	12 (6%)	1 (0%)	29	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	CL	207/220 (94%)	194 (94%)	12 (6%)	1 (0%)	29	68
12	r	207/220 (94%)	202 (98%)	5 (2%)	0	100	100
13	CM	167/169 (99%)	148 (89%)	16 (10%)	3 (2%)	8	37
13	s	167/169 (99%)	149 (89%)	17 (10%)	1 (1%)	25	64
14	CN	191/193 (99%)	175 (92%)	13 (7%)	3 (2%)	9	40
14	t	191/193 (99%)	174 (91%)	14 (7%)	3 (2%)	9	40
15	CO	134/136 (98%)	127 (95%)	5 (4%)	2 (2%)	10	42
15	u	134/136 (98%)	126 (94%)	6 (4%)	2 (2%)	10	42
16	CP	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
16	v	201/203 (99%)	188 (94%)	11 (6%)	2 (1%)	15	53
17	CQ	195/197 (99%)	189 (97%)	3 (2%)	3 (2%)	10	42
17	w	195/197 (99%)	190 (97%)	3 (2%)	2 (1%)	15	53
18	CR	181/183 (99%)	167 (92%)	13 (7%)	1 (1%)	25	64
18	x	181/183 (99%)	172 (95%)	8 (4%)	1 (1%)	25	64
19	CS	183/185 (99%)	172 (94%)	10 (6%)	1 (0%)	29	68
19	y	183/185 (99%)	174 (95%)	8 (4%)	1 (0%)	29	68
20	CT	186/188 (99%)	172 (92%)	13 (7%)	1 (0%)	29	68
20	z	186/188 (99%)	181 (97%)	5 (3%)	0	100	100
21	0	170/172 (99%)	159 (94%)	10 (6%)	1 (1%)	25	64
21	CU	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	25	64
22	2	157/159 (99%)	147 (94%)	9 (6%)	1 (1%)	25	64
22	CV	157/159 (99%)	148 (94%)	8 (5%)	1 (1%)	25	64
23	5	98/100 (98%)	90 (92%)	7 (7%)	1 (1%)	15	53
23	CW	98/100 (98%)	90 (92%)	7 (7%)	1 (1%)	15	53
24	6	134/136 (98%)	133 (99%)	1 (1%)	0	100	100
24	CX	134/136 (98%)	133 (99%)	1 (1%)	0	100	100
25	7	96/98 (98%)	88 (92%)	7 (7%)	1 (1%)	15	53
25	CY	96/98 (98%)	89 (93%)	5 (5%)	2 (2%)	7	33
26	8	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
26	CZ	119/121 (98%)	112 (94%)	7 (6%)	0	100	100
27	9	124/126 (98%)	118 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	DA	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
28	AA	133/135 (98%)	127 (96%)	6 (4%)	0	100	100
28	DB	133/135 (98%)	121 (91%)	10 (8%)	2 (2%)	10	42
29	AB	146/148 (99%)	127 (87%)	17 (12%)	2 (1%)	11	43
29	DC	146/148 (99%)	133 (91%)	10 (7%)	3 (2%)	7	33
30	AC	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
30	DD	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
31	AD	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
31	DE	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
32	AE	107/109 (98%)	101 (94%)	3 (3%)	3 (3%)	5	25
32	DF	107/109 (98%)	103 (96%)	1 (1%)	3 (3%)	5	25
33	AF	125/127 (98%)	122 (98%)	3 (2%)	0	100	100
33	DG	125/127 (98%)	123 (98%)	2 (2%)	0	100	100
34	AG	104/106 (98%)	101 (97%)	3 (3%)	0	100	100
34	DH	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
35	AH	110/112 (98%)	105 (96%)	4 (4%)	1 (1%)	17	55
35	DI	110/112 (98%)	103 (94%)	6 (6%)	1 (1%)	17	55
36	AI	117/119 (98%)	110 (94%)	7 (6%)	0	100	100
36	DJ	117/119 (98%)	112 (96%)	5 (4%)	0	100	100
37	AJ	97/99 (98%)	88 (91%)	8 (8%)	1 (1%)	15	53
37	DK	97/99 (98%)	86 (89%)	10 (10%)	1 (1%)	15	53
38	AK	85/87 (98%)	79 (93%)	6 (7%)	0	100	100
38	DL	85/87 (98%)	79 (93%)	6 (7%)	0	100	100
39	AL	75/77 (97%)	68 (91%)	7 (9%)	0	100	100
39	DM	75/77 (97%)	69 (92%)	5 (7%)	1 (1%)	12	45
40	AM	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
40	DN	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
41	AN	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
41	DO	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
42	AO	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
42	DP	23/25 (92%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	AP	103/105 (98%)	90 (87%)	12 (12%)	1 (1%)	15	53
43	DQ	103/105 (98%)	90 (87%)	13 (13%)	0	100	100
44	AQ	89/91 (98%)	80 (90%)	9 (10%)	0	100	100
44	DR	89/91 (98%)	81 (91%)	7 (8%)	1 (1%)	14	50
45	i	155/168 (92%)	131 (84%)	21 (14%)	3 (2%)	8	36
46	p0	139/219 (64%)	123 (88%)	14 (10%)	2 (1%)	11	43
47	sM	61/104 (59%)	50 (82%)	10 (16%)	1 (2%)	9	40
49	B	204/206 (99%)	177 (87%)	25 (12%)	2 (1%)	15	53
49	s0	204/206 (99%)	179 (88%)	23 (11%)	2 (1%)	15	53
50	C	212/216 (98%)	170 (80%)	40 (19%)	2 (1%)	17	55
50	s1	214/216 (99%)	193 (90%)	21 (10%)	0	100	100
51	D	215/217 (99%)	200 (93%)	13 (6%)	2 (1%)	17	55
51	s2	215/217 (99%)	200 (93%)	15 (7%)	0	100	100
52	E	221/223 (99%)	203 (92%)	16 (7%)	2 (1%)	17	55
52	s3	221/223 (99%)	199 (90%)	20 (9%)	2 (1%)	17	55
53	F	258/260 (99%)	236 (92%)	21 (8%)	1 (0%)	34	72
53	s4	258/260 (99%)	235 (91%)	21 (8%)	2 (1%)	19	57
54	G	204/206 (99%)	180 (88%)	21 (10%)	3 (2%)	10	42
54	s5	204/206 (99%)	181 (89%)	21 (10%)	2 (1%)	15	53
55	H	224/226 (99%)	207 (92%)	14 (6%)	3 (1%)	12	45
55	s6	216/226 (96%)	198 (92%)	16 (7%)	2 (1%)	17	55
56	I	182/186 (98%)	158 (87%)	18 (10%)	6 (3%)	4	21
56	s7	184/186 (99%)	162 (88%)	21 (11%)	1 (0%)	29	68
57	J	184/199 (92%)	162 (88%)	20 (11%)	2 (1%)	14	50
57	s8	184/199 (92%)	168 (91%)	14 (8%)	2 (1%)	14	50
58	K	183/185 (99%)	165 (90%)	17 (9%)	1 (0%)	29	68
58	s9	183/185 (99%)	168 (92%)	15 (8%)	0	100	100
59	L	94/105 (90%)	77 (82%)	16 (17%)	1 (1%)	14	50
59	c0	92/105 (88%)	64 (70%)	21 (23%)	7 (8%)	1	5
60	M	153/155 (99%)	135 (88%)	15 (10%)	3 (2%)	7	34
60	c1	144/155 (93%)	133 (92%)	9 (6%)	2 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	N	122/143 (85%)	88 (72%)	30 (25%)	4 (3%)	4	21
61	c2	122/143 (85%)	94 (77%)	24 (20%)	4 (3%)	4	21
62	O	148/150 (99%)	138 (93%)	9 (6%)	1 (1%)	22	60
62	c3	148/150 (99%)	134 (90%)	11 (7%)	3 (2%)	7	34
63	P	125/128 (98%)	112 (90%)	11 (9%)	2 (2%)	9	40
63	c4	126/128 (98%)	113 (90%)	11 (9%)	2 (2%)	9	40
64	Q	122/135 (90%)	107 (88%)	12 (10%)	3 (2%)	5	28
64	c5	133/135 (98%)	105 (79%)	22 (16%)	6 (4%)	2	14
65	R	139/142 (98%)	121 (87%)	15 (11%)	3 (2%)	6	31
65	c6	140/142 (99%)	132 (94%)	7 (5%)	1 (1%)	22	60
66	S	116/125 (93%)	97 (84%)	15 (13%)	4 (3%)	3	20
67	T	143/145 (99%)	124 (87%)	15 (10%)	4 (3%)	5	25
67	c8	143/145 (99%)	123 (86%)	16 (11%)	4 (3%)	5	25
68	U	141/143 (99%)	125 (89%)	16 (11%)	0	100	100
68	c9	141/143 (99%)	131 (93%)	8 (6%)	2 (1%)	11	43
69	V	105/110 (96%)	93 (89%)	11 (10%)	1 (1%)	15	53
69	d0	108/110 (98%)	92 (85%)	15 (14%)	1 (1%)	17	55
70	W	85/87 (98%)	73 (86%)	11 (13%)	1 (1%)	13	48
70	d1	85/87 (98%)	77 (91%)	8 (9%)	0	100	100
71	X	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	6	29
71	d2	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	19	57
72	Y	142/144 (99%)	121 (85%)	20 (14%)	1 (1%)	22	60
72	d3	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
73	Z	132/134 (98%)	121 (92%)	8 (6%)	3 (2%)	6	30
73	d4	132/134 (98%)	120 (91%)	11 (8%)	1 (1%)	19	57
74	a	68/70 (97%)	55 (81%)	9 (13%)	4 (6%)	1	9
74	d5	67/70 (96%)	62 (92%)	4 (6%)	1 (2%)	10	42
75	b	95/97 (98%)	71 (75%)	21 (22%)	3 (3%)	4	22
75	d6	95/97 (98%)	78 (82%)	15 (16%)	2 (2%)	7	33
76	c	79/81 (98%)	70 (89%)	8 (10%)	1 (1%)	12	45
76	d7	79/81 (98%)	69 (87%)	8 (10%)	2 (2%)	5	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
77	d	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
77	d8	61/63 (97%)	50 (82%)	11 (18%)	0	100	100
78	d9	51/53 (96%)	44 (86%)	6 (12%)	1 (2%)	7	34
78	e	51/53 (96%)	46 (90%)	5 (10%)	0	100	100
79	e0	60/62 (97%)	52 (87%)	7 (12%)	1 (2%)	9	39
79	f	58/62 (94%)	49 (84%)	7 (12%)	2 (3%)	3	20
80	g	69/71 (97%)	44 (64%)	19 (28%)	6 (9%)	1	3
81	Rb	316/318 (99%)	294 (93%)	22 (7%)	0	100	100
81	h	316/318 (99%)	295 (93%)	21 (7%)	0	100	100
82	c7	113/121 (93%)	101 (89%)	10 (9%)	2 (2%)	8	37
83	e1	49/51 (96%)	37 (76%)	12 (24%)	0	100	100
All	All	22260/22893 (97%)	20326 (91%)	1724 (8%)	210 (1%)	17	55

All (210) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	l	339	LEU
8	n	98	VAL
11	q	50	ASN
16	v	75	VAL
17	w	111	PRO
32	AE	83	GLU
45	i	167	PRO
6	CF	292	SER
7	CG	20	PHE
8	CH	98	VAL
15	CO	8	LYS
17	CQ	111	PRO
28	DB	4	PHE
29	DC	48	TYR
56	I	111	LYS
59	L	88	PRO
60	M	8	GLN
65	R	39	VAL
66	S	85	VAL
67	T	92	ILE
70	W	82	VAL
71	X	83	ILE

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Mol	Chain	Res	Type
74	a	88	ILE
75	b	75	VAL
59	c0	88	PRO
59	c0	97	PRO
62	c3	66	ILE
68	c9	34	VAL
71	d2	6	VAL
76	d7	59	CYS
15	u	8	LYS
19	y	99	THR
20	CT	130	ASN
22	CV	124	VAL
25	CY	82	ILE
29	DC	47	LYS
32	DF	83	GLU
39	DM	19	ASP
54	G	58	LEU
56	I	74	GLN
57	J	149	SER
58	K	134	ILE
60	M	7	VAL
64	Q	126	VAL
65	R	113	ASP
66	S	86	PRO
66	S	88	VAL
73	Z	5	VAL
76	c	62	ILE
79	f	47	VAL
80	g	98	VAL
80	g	102	VAL
80	g	103	LEU
49	s0	189	VAL
59	c0	82	LEU
61	c2	91	VAL
65	c6	115	THR
82	c7	99	VAL
73	d4	52	LYS
76	d7	62	ILE
9	o	25	GLN
17	w	110	PRO
22	2	124	VAL
29	AB	79	TRP

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Mol	Chain	Res	Type
32	AE	82	GLU
14	CN	51	LEU
17	CQ	110	PRO
19	CS	99	THR
32	DF	82	GLU
46	p0	199	SER
52	E	217	ILE
54	G	64	VAL
63	P	124	ASP
67	T	91	ASP
73	Z	4	ALA
56	s7	67	LEU
60	c1	7	VAL
61	c2	109	GLU
63	c4	126	THR
64	c5	18	ARG
82	c7	105	GLN
14	t	47	ALA
14	t	76	THR
14	t	77	LEU
35	AH	82	ALA
43	AP	60	LYS
14	CN	166	ALA
18	CR	156	ALA
25	CY	25	ASP
29	DC	78	LEU
35	DI	82	ALA
49	B	4	PRO
50	C	63	GLY
57	J	152	ILE
60	M	6	THR
61	N	106	ILE
71	X	30	SER
71	X	31	SER
73	Z	35	VAL
52	s3	217	ILE
53	s4	163	ASP
54	s5	101	GLY
54	s5	184	PHE
59	c0	2	LEU
64	c5	51	SER
64	c5	128	HIS

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Mol	Chain	Res	Type
68	c9	28	LEU
13	s	114	ILE
16	v	74	PRO
18	x	156	ALA
29	AB	78	LEU
9	CI	25	GLN
9	CI	164	SER
12	CL	207	GLU
13	CM	117	ASP
14	CN	47	ALA
21	CU	167	ARG
28	DB	103	GLN
51	D	148	LEU
55	H	70	PRO
55	H	149	LYS
56	I	112	ARG
61	N	89	ILE
64	Q	125	PRO
67	T	144	ARG
80	g	88	PRO
55	s6	122	GLU
61	c2	106	ILE
64	c5	7	ALA
67	c8	8	GLN
75	d6	13	LYS
6	l	24	ALA
9	o	26	VAL
10	p	36	ILE
21	0	167	ARG
25	7	96	LEU
10	CJ	36	ILE
10	CJ	157	VAL
13	CM	114	ILE
13	CM	173	ASP
44	DR	51	ALA
49	B	158	VAL
52	E	222	VAL
56	I	132	PRO
74	a	38	HIS
80	g	84	VAL
52	s3	222	VAL
59	c0	83	PRO

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Mol	Chain	Res	Type
67	c8	9	GLY
67	c8	91	ASP
69	d0	51	VAL
74	d5	85	LYS
10	p	25	PRO
10	p	157	VAL
45	i	166	VAL
51	D	150	GLN
63	P	42	VAL
69	V	59	PRO
74	a	71	ILE
49	s0	158	VAL
62	c3	60	VAL
63	c4	35	GLY
64	c5	129	GLY
78	d9	6	VAL
15	u	6	ILE
17	CQ	16	VAL
46	p0	33	VAL
50	C	210	ILE
53	F	195	ILE
55	H	69	LEU
61	N	66	VAL
61	N	91	VAL
72	Y	41	SER
75	b	86	VAL
80	g	87	THR
55	s6	69	LEU
59	c0	35	ILE
59	c0	92	ILE
60	c1	129	ARG
67	c8	14	ILE
79	e0	47	VAL
32	AE	7	VAL
37	AJ	3	VAL
15	CO	6	ILE
23	CW	11	ILE
32	DF	7	VAL
65	R	97	VAL
67	T	14	ILE
57	s8	78	ILE
57	s8	101	ILE

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Mol	Chain	Res	Type
61	c2	115	VAL
5	k	317	ILE
9	o	178	ILE
23	5	11	ILE
45	i	12	VAL
37	DK	3	VAL
47	sM	43	ASP
54	G	51	VAL
56	I	31	SER
56	I	98	ILE
62	O	22	ALA
66	S	124	VAL
75	b	36	ILE
79	f	45	VAL
53	s4	90	ILE
62	c3	22	ALA
64	c5	126	VAL
64	Q	53	PRO
74	a	41	ILE
75	d6	58	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CD	193/194 (100%)	165 (86%)	28 (14%)	3	15
4	j	193/194 (100%)	164 (85%)	29 (15%)	3	14
5	CE	320/322 (99%)	269 (84%)	51 (16%)	2	12
5	k	320/322 (99%)	266 (83%)	54 (17%)	2	11
6	CF	288/288 (100%)	249 (86%)	39 (14%)	4	17
6	l	288/288 (100%)	243 (84%)	45 (16%)	2	13
7	CG	244/244 (100%)	206 (84%)	38 (16%)	2	13
7	m	244/244 (100%)	207 (85%)	37 (15%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CH	134/152 (88%)	119 (89%)	15 (11%)	6	24
8	n	134/152 (88%)	116 (87%)	18 (13%)	4	17
9	CI	186/186 (100%)	169 (91%)	17 (9%)	9	34
9	o	186/186 (100%)	164 (88%)	22 (12%)	5	22
10	CJ	187/191 (98%)	169 (90%)	18 (10%)	8	32
10	p	187/191 (98%)	157 (84%)	30 (16%)	2	12
11	CK	171/171 (100%)	146 (85%)	25 (15%)	3	15
11	q	171/171 (100%)	145 (85%)	26 (15%)	3	14
12	CL	177/186 (95%)	157 (89%)	20 (11%)	6	24
12	r	177/186 (95%)	151 (85%)	26 (15%)	3	15
13	CM	147/147 (100%)	123 (84%)	24 (16%)	2	11
13	s	147/147 (100%)	122 (83%)	25 (17%)	2	10
14	CN	154/154 (100%)	135 (88%)	19 (12%)	4	21
14	t	154/154 (100%)	130 (84%)	24 (16%)	2	13
15	CO	107/107 (100%)	96 (90%)	11 (10%)	7	28
15	u	107/107 (100%)	92 (86%)	15 (14%)	3	16
16	CP	175/175 (100%)	153 (87%)	22 (13%)	4	20
16	v	175/175 (100%)	156 (89%)	19 (11%)	6	25
17	CQ	160/160 (100%)	142 (89%)	18 (11%)	6	24
17	w	160/160 (100%)	143 (89%)	17 (11%)	6	26
18	CR	140/145 (97%)	116 (83%)	24 (17%)	2	10
18	x	140/145 (97%)	122 (87%)	18 (13%)	4	19
19	CS	150/150 (100%)	125 (83%)	25 (17%)	2	11
19	y	150/150 (100%)	125 (83%)	25 (17%)	2	11
20	CT	153/153 (100%)	125 (82%)	28 (18%)	1	9
20	z	153/153 (100%)	136 (89%)	17 (11%)	6	25
21	0	156/156 (100%)	131 (84%)	25 (16%)	2	12
21	CU	156/156 (100%)	132 (85%)	24 (15%)	2	13
22	2	136/136 (100%)	110 (81%)	26 (19%)	1	8
22	CV	136/136 (100%)	111 (82%)	25 (18%)	1	9
23	5	87/87 (100%)	77 (88%)	10 (12%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	CW	87/87 (100%)	76 (87%)	11 (13%)	4	20
24	6	104/104 (100%)	88 (85%)	16 (15%)	2	13
24	CX	104/104 (100%)	91 (88%)	13 (12%)	4	20
25	7	57/86 (66%)	51 (90%)	6 (10%)	7	27
25	CY	57/86 (66%)	51 (90%)	6 (10%)	7	27
26	8	104/105 (99%)	87 (84%)	17 (16%)	2	11
26	CZ	104/105 (99%)	86 (83%)	18 (17%)	2	10
27	9	109/109 (100%)	90 (83%)	19 (17%)	2	10
27	DA	109/109 (100%)	94 (86%)	15 (14%)	3	17
28	AA	115/115 (100%)	98 (85%)	17 (15%)	3	14
28	DB	115/115 (100%)	105 (91%)	10 (9%)	10	37
29	AB	118/118 (100%)	98 (83%)	20 (17%)	2	11
29	DC	118/118 (100%)	102 (86%)	16 (14%)	3	17
30	AC	46/46 (100%)	40 (87%)	6 (13%)	4	19
30	DD	46/46 (100%)	39 (85%)	7 (15%)	3	14
31	AD	81/81 (100%)	69 (85%)	12 (15%)	3	14
31	DE	81/81 (100%)	75 (93%)	6 (7%)	13	44
32	AE	92/96 (96%)	79 (86%)	13 (14%)	3	16
32	DF	92/96 (96%)	74 (80%)	18 (20%)	1	7
33	AF	109/109 (100%)	94 (86%)	15 (14%)	3	17
33	DG	109/109 (100%)	98 (90%)	11 (10%)	7	29
34	AG	90/90 (100%)	84 (93%)	6 (7%)	16	49
34	DH	90/90 (100%)	80 (89%)	10 (11%)	6	25
35	AH	95/95 (100%)	80 (84%)	15 (16%)	2	12
35	DI	95/95 (100%)	86 (90%)	9 (10%)	8	32
36	AI	104/104 (100%)	89 (86%)	15 (14%)	3	15
36	DJ	104/104 (100%)	81 (78%)	23 (22%)	1	4
37	AJ	81/81 (100%)	66 (82%)	15 (18%)	1	8
37	DK	81/81 (100%)	65 (80%)	16 (20%)	1	7
38	AK	70/70 (100%)	61 (87%)	9 (13%)	4	19
38	DL	70/70 (100%)	59 (84%)	11 (16%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	AL	68/68 (100%)	57 (84%)	11 (16%)	2	12
39	DM	68/68 (100%)	56 (82%)	12 (18%)	2	10
40	AM	45/45 (100%)	38 (84%)	7 (16%)	2	13
40	DN	45/45 (100%)	40 (89%)	5 (11%)	6	25
41	AN	47/47 (100%)	38 (81%)	9 (19%)	1	8
41	DO	47/47 (100%)	40 (85%)	7 (15%)	3	14
42	AO	23/23 (100%)	19 (83%)	4 (17%)	2	10
42	DP	23/23 (100%)	19 (83%)	4 (17%)	2	10
43	AP	90/90 (100%)	80 (89%)	10 (11%)	6	25
43	DQ	90/90 (100%)	73 (81%)	17 (19%)	1	8
44	AQ	71/71 (100%)	58 (82%)	13 (18%)	1	9
44	DR	71/71 (100%)	64 (90%)	7 (10%)	8	30
45	i	97/137 (71%)	81 (84%)	16 (16%)	2	11
46	p0	105/186 (56%)	88 (84%)	17 (16%)	2	12
47	sM	54/54 (100%)	47 (87%)	7 (13%)	4	19
49	B	164/173 (95%)	149 (91%)	15 (9%)	9	34
49	s0	165/173 (95%)	139 (84%)	26 (16%)	2	12
50	C	191/192 (100%)	160 (84%)	31 (16%)	2	12
50	s1	192/192 (100%)	164 (85%)	28 (15%)	3	15
51	D	176/176 (100%)	140 (80%)	36 (20%)	1	6
51	s2	176/176 (100%)	141 (80%)	35 (20%)	1	7
52	E	182/182 (100%)	157 (86%)	25 (14%)	3	17
52	s3	182/182 (100%)	163 (90%)	19 (10%)	7	27
53	F	221/221 (100%)	194 (88%)	27 (12%)	5	21
53	s4	221/221 (100%)	191 (86%)	30 (14%)	3	17
54	G	173/173 (100%)	158 (91%)	15 (9%)	10	37
54	s5	173/173 (100%)	153 (88%)	20 (12%)	5	23
55	H	188/193 (97%)	159 (85%)	29 (15%)	2	13
55	s6	187/193 (97%)	165 (88%)	22 (12%)	5	22
56	I	165/166 (99%)	144 (87%)	21 (13%)	4	19
56	s7	165/166 (99%)	148 (90%)	17 (10%)	7	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	J	150/160 (94%)	135 (90%)	15 (10%)	7	29
57	s8	150/160 (94%)	136 (91%)	14 (9%)	9	33
58	K	158/158 (100%)	129 (82%)	29 (18%)	1	9
58	s9	158/158 (100%)	137 (87%)	21 (13%)	4	17
59	L	77/98 (79%)	70 (91%)	7 (9%)	9	34
59	c0	73/98 (74%)	67 (92%)	6 (8%)	11	39
60	M	129/136 (95%)	108 (84%)	21 (16%)	2	11
60	c1	129/136 (95%)	110 (85%)	19 (15%)	3	15
61	N	88/119 (74%)	68 (77%)	20 (23%)	1	4
61	c2	88/119 (74%)	68 (77%)	20 (23%)	1	4
62	O	127/127 (100%)	106 (84%)	21 (16%)	2	11
62	c3	127/127 (100%)	110 (87%)	17 (13%)	4	17
63	P	81/97 (84%)	69 (85%)	12 (15%)	3	14
63	c4	97/97 (100%)	83 (86%)	14 (14%)	3	15
64	Q	101/111 (91%)	86 (85%)	15 (15%)	3	14
64	c5	103/111 (93%)	94 (91%)	9 (9%)	10	37
65	R	117/118 (99%)	100 (86%)	17 (14%)	3	15
65	c6	118/118 (100%)	102 (86%)	16 (14%)	3	17
66	S	94/113 (83%)	77 (82%)	17 (18%)	1	9
67	T	128/128 (100%)	104 (81%)	24 (19%)	1	8
67	c8	128/128 (100%)	111 (87%)	17 (13%)	4	17
68	U	115/115 (100%)	94 (82%)	21 (18%)	1	9
68	c9	115/115 (100%)	105 (91%)	10 (9%)	10	37
69	V	100/103 (97%)	84 (84%)	16 (16%)	2	12
69	d0	103/103 (100%)	89 (86%)	14 (14%)	3	17
70	W	74/74 (100%)	61 (82%)	13 (18%)	2	10
70	d1	74/74 (100%)	63 (85%)	11 (15%)	3	14
71	X	110/110 (100%)	91 (83%)	19 (17%)	2	10
71	d2	110/110 (100%)	99 (90%)	11 (10%)	7	29
72	Y	119/119 (100%)	101 (85%)	18 (15%)	3	14
72	d3	119/119 (100%)	106 (89%)	13 (11%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	Z	112/112 (100%)	99 (88%)	13 (12%)	5	23
73	d4	112/112 (100%)	101 (90%)	11 (10%)	8	30
74	a	61/61 (100%)	44 (72%)	17 (28%)	0	2
74	d5	61/61 (100%)	57 (93%)	4 (7%)	16	49
75	b	83/83 (100%)	73 (88%)	10 (12%)	5	22
75	d6	83/83 (100%)	77 (93%)	6 (7%)	14	45
76	c	70/70 (100%)	63 (90%)	7 (10%)	7	29
76	d7	70/70 (100%)	63 (90%)	7 (10%)	7	29
77	d	56/56 (100%)	49 (88%)	7 (12%)	4	20
77	d8	56/56 (100%)	50 (89%)	6 (11%)	6	26
78	d9	47/47 (100%)	37 (79%)	10 (21%)	1	5
78	e	47/47 (100%)	39 (83%)	8 (17%)	2	10
79	e0	53/53 (100%)	44 (83%)	9 (17%)	2	10
79	f	51/53 (96%)	44 (86%)	7 (14%)	3	17
80	g	62/62 (100%)	55 (89%)	7 (11%)	6	24
81	Rb	260/261 (100%)	243 (94%)	17 (6%)	17	50
81	h	259/261 (99%)	241 (93%)	18 (7%)	15	48
82	c7	92/110 (84%)	82 (89%)	10 (11%)	6	25
83	e1	43/43 (100%)	33 (77%)	10 (23%)	1	4
All	All	18683/19203 (97%)	16080 (86%)	2603 (14%)	3	16

All (2603) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	j	20	THR
4	j	32	LEU
4	j	44	ILE
4	j	45	VAL
4	j	62	VAL
4	j	71	LEU
4	j	72	ARG
4	j	74	GLU
4	j	96	LEU
4	j	101	VAL
4	j	104	LEU

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Mol	Chain	Res	Type
4	j	109	GLU
4	j	116	VAL
4	j	134	VAL
4	j	157	VAL
4	j	165	VAL
4	j	169	ILE
4	j	177	LYS
4	j	179	LEU
4	j	180	LEU
4	j	191	LEU
4	j	202	VAL
4	j	204	MET
4	j	207	VAL
4	j	219	ILE
4	j	226	SER
4	j	227	ARG
4	j	230	VAL
4	j	241	ARG
5	k	2	SER
5	k	4	ARG
5	k	5	LYS
5	k	7	GLU
5	k	10	ARG
5	k	17	LEU
5	k	25	ILE
5	k	37	ARG
5	k	47	LEU
5	k	56	ILE
5	k	79	VAL
5	k	84	VAL
5	k	85	VAL
5	k	90	VAL
5	k	103	THR
5	k	104	THR
5	k	114	VAL
5	k	134	SER
5	k	139	GLN
5	k	148	LEU
5	k	150	ARG
5	k	160	VAL
5	k	183	LEU
5	k	188	ILE

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Mol	Chain	Res	Type
5	k	192	VAL
5	k	196	ARG
5	k	202	THR
5	k	205	VAL
5	k	208	VAL
5	k	212	ASN
5	k	229	VAL
5	k	232	ARG
5	k	235	THR
5	k	236	LYS
5	k	238	LEU
5	k	241	LYS
5	k	244	ARG
5	k	247	ARG
5	k	252	ILE
5	k	264	VAL
5	k	277	SER
5	k	284	ARG
5	k	300	ARG
5	k	305	ILE
5	k	319	ASN
5	k	320	ASP
5	k	324	VAL
5	k	328	ILE
5	k	332	ARG
5	k	338	LEU
5	k	348	ARG
5	k	353	GLU
5	k	355	SER
5	k	380	MET
6	l	12	THR
6	l	71	VAL
6	l	74	ILE
6	l	85	SER
6	l	93	MET
6	l	110	ASN
6	l	133	SER
6	l	136	LEU
6	l	138	ARG
6	l	142	VAL
6	l	150	LEU
6	l	156	LEU

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Mol	Chain	Res	Type
6	l	172	VAL
6	l	176	SER
6	l	177	ASP
6	l	179	LEU
6	l	188	ARG
6	l	193	LYS
6	l	200	THR
6	l	203	ARG
6	l	206	LEU
6	l	220	ARG
6	l	222	VAL
6	l	230	VAL
6	l	233	LEU
6	l	246	ARG
6	l	258	LEU
6	l	266	THR
6	l	270	SER
6	l	287	THR
6	l	293	SER
6	l	295	ILE
6	l	297	SER
6	l	306	THR
6	l	307	GLN
6	l	313	LEU
6	l	323	VAL
6	l	327	LEU
6	l	332	LYS
6	l	338	LYS
6	l	339	LEU
6	l	347	THR
6	l	349	THR
6	l	354	VAL
6	l	356	THR
7	m	5	LYS
7	m	23	ARG
7	m	35	ARG
7	m	41	LYS
7	m	58	LYS
7	m	69	ILE
7	m	75	LEU
7	m	105	ILE
7	m	109	THR

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Mol	Chain	Res	Type
7	m	112	LYS
7	m	113	LEU
7	m	118	THR
7	m	122	VAL
7	m	131	LEU
7	m	136	GLU
7	m	137	ASP
7	m	140	ARG
7	m	146	LEU
7	m	148	ILE
7	m	151	GLN
7	m	152	ARG
7	m	155	THR
7	m	163	LEU
7	m	185	PHE
7	m	187	THR
7	m	214	ASP
7	m	216	GLU
7	m	217	GLU
7	m	222	LEU
7	m	231	ILE
7	m	234	ASP
7	m	236	LEU
7	m	254	LYS
7	m	258	LYS
7	m	259	LYS
7	m	273	ARG
7	m	293	LEU
8	n	2	SER
8	n	5	LYS
8	n	21	THR
8	n	22	ARG
8	n	35	VAL
8	n	48	ARG
8	n	52	VAL
8	n	64	LEU
8	n	65	ILE
8	n	78	ARG
8	n	79	VAL
8	n	84	VAL
8	n	89	THR
8	n	98	VAL

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Mol	Chain	Res	Type
8	n	129	GLU
8	n	134	ARG
8	n	152	THR
8	n	155	LEU
9	o	24	GLU
9	o	25	GLN
9	o	26	VAL
9	o	30	ARG
9	o	45	LEU
9	o	60	ARG
9	o	77	VAL
9	o	82	LYS
9	o	83	LEU
9	o	92	ILE
9	o	93	ASN
9	o	98	LYS
9	o	100	ARG
9	o	109	THR
9	o	121	LYS
9	o	143	THR
9	o	157	ASN
9	o	164	SER
9	o	175	LYS
9	o	179	LEU
9	o	184	LEU
9	o	239	LEU
10	p	26	LEU
10	p	27	THR
10	p	38	GLN
10	p	47	SER
10	p	50	VAL
10	p	57	ARG
10	p	63	LYS
10	p	65	LEU
10	p	69	LEU
10	p	71	VAL
10	p	74	THR
10	p	79	GLN
10	p	81	THR
10	p	84	ARG
10	p	101	THR
10	p	108	ARG

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Mol	Chain	Res	Type
10	p	110	THR
10	p	136	LEU
10	p	145	ASN
10	p	150	LEU
10	p	156	ASP
10	p	160	ILE
10	p	169	LEU
10	p	185	ARG
10	p	189	LEU
10	p	203	VAL
10	p	204	ARG
10	p	214	LEU
10	p	246	MET
10	p	248	LYS
11	q	4	ILE
11	q	5	GLN
11	q	6	THR
11	q	18	VAL
11	q	19	SER
11	q	22	SER
11	q	41	ILE
11	q	48	VAL
11	q	49	ASN
11	q	52	LEU
11	q	55	VAL
11	q	68	LEU
11	q	69	ARG
11	q	70	THR
11	q	82	VAL
11	q	135	GLU
11	q	138	THR
11	q	139	ASN
11	q	151	VAL
11	q	157	ASN
11	q	161	LEU
11	q	162	GLN
11	q	168	ARG
11	q	172	ILE
11	q	173	ARG
11	q	189	GLU
12	r	3	ARG
12	r	21	ARG

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Mol	Chain	Res	Type
12	r	24	ARG
12	r	26	VAL
12	r	30	LYS
12	r	32	ARG
12	r	42	THR
12	r	48	LEU
12	r	52	LEU
12	r	57	LEU
12	r	63	GLU
12	r	87	LEU
12	r	102	MET
12	r	130	ASP
12	r	133	GLN
12	r	138	VAL
12	r	139	ARG
12	r	140	THR
12	r	143	SER
12	r	163	GLN
12	r	165	ILE
12	r	177	ASP
12	r	185	ARG
12	r	191	LYS
12	r	203	LYS
12	r	207	GLU
13	s	9	MET
13	s	10	ARG
13	s	12	LEU
13	s	13	LYS
13	s	25	GLU
13	s	31	THR
13	s	40	LEU
13	s	44	THR
13	s	46	VAL
13	s	47	GLN
13	s	56	THR
13	s	65	ILE
13	s	70	THR
13	s	80	LEU
13	s	82	ARG
13	s	94	ARG
13	s	95	ASN
13	s	106	ILE

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Mol	Chain	Res	Type
13	s	107	ASP
13	s	112	LEU
13	s	130	VAL
13	s	140	ARG
13	s	142	LYS
13	s	158	ASP
13	s	173	ASP
14	t	13	HIS
14	t	23	LYS
14	t	24	VAL
14	t	35	ARG
14	t	41	THR
14	t	54	LEU
14	t	55	ARG
14	t	58	VAL
14	t	59	ARG
14	t	63	VAL
14	t	67	ARG
14	t	69	VAL
14	t	85	LEU
14	t	104	ARG
14	t	107	GLU
14	t	114	GLN
14	t	115	ARG
14	t	122	LYS
14	t	124	ILE
14	t	129	ASN
14	t	131	LYS
14	t	165	SER
14	t	168	ARG
14	t	174	ARG
15	u	8	LYS
15	u	11	ASN
15	u	27	GLN
15	u	38	ILE
15	u	50	LYS
15	u	53	VAL
15	u	63	VAL
15	u	72	LEU
15	u	90	VAL
15	u	91	CYS
15	u	92	GLU

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Mol	Chain	Res	Type
15	u	102	LYS
15	u	108	ARG
15	u	135	LEU
15	u	137	LYS
16	v	10	LEU
16	v	15	GLN
16	v	22	LEU
16	v	38	ARG
16	v	49	ARG
16	v	50	ARG
16	v	68	ARG
16	v	80	THR
16	v	85	THR
16	v	96	ARG
16	v	98	LEU
16	v	106	VAL
16	v	109	ARG
16	v	133	ILE
16	v	138	GLN
16	v	151	ILE
16	v	157	LYS
16	v	188	ARG
16	v	190	THR
17	w	33	ILE
17	w	59	ARG
17	w	68	ARG
17	w	78	ARG
17	w	82	LYS
17	w	84	LEU
17	w	85	ARG
17	w	106	GLU
17	w	115	LYS
17	w	116	LYS
17	w	117	ARG
17	w	124	LEU
17	w	128	ARG
17	w	129	LEU
17	w	143	THR
17	w	160	ARG
17	w	190	VAL
18	x	9	THR
18	x	24	VAL

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Mol	Chain	Res	Type
18	x	29	THR
18	x	32	THR
18	x	36	ILE
18	x	41	LEU
18	x	52	LEU
18	x	53	ASP
18	x	56	ARG
18	x	67	ILE
18	x	69	ARG
18	x	112	LEU
18	x	119	VAL
18	x	127	ARG
18	x	144	SER
18	x	168	LEU
18	x	180	LYS
18	x	181	ARG
19	y	3	ILE
19	y	17	THR
19	y	22	ASP
19	y	24	VAL
19	y	26	LEU
19	y	32	LEU
19	y	39	ARG
19	y	41	ASP
19	y	49	LEU
19	y	57	ILE
19	y	63	SER
19	y	64	VAL
19	y	66	ARG
19	y	69	ARG
19	y	74	GLU
19	y	80	THR
19	y	111	ARG
19	y	115	VAL
19	y	120	GLU
19	y	135	GLN
19	y	138	LEU
19	y	141	ARG
19	y	150	VAL
19	y	180	ARG
19	y	181	SER
20	z	8	LYS

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Mol	Chain	Res	Type
20	z	10	LEU
20	z	29	THR
20	z	41	ILE
20	z	43	LYS
20	z	44	LEU
20	z	51	VAL
20	z	55	VAL
20	z	91	SER
20	z	99	LEU
20	z	103	ARG
20	z	104	ARG
20	z	106	LEU
20	z	116	ASP
20	z	138	LEU
20	z	175	GLN
20	z	182	ASP
21	0	1	MET
21	0	24	LEU
21	0	40	ARG
21	0	45	LEU
21	0	51	VAL
21	0	61	ILE
21	0	64	ILE
21	0	79	VAL
21	0	80	ARG
21	0	87	THR
21	0	97	VAL
21	0	100	VAL
21	0	105	THR
21	0	115	ARG
21	0	117	ARG
21	0	132	THR
21	0	137	ARG
21	0	138	GLN
21	0	142	GLN
21	0	155	ARG
21	0	156	VAL
21	0	160	THR
21	0	162	THR
21	0	167	ARG
21	0	172	TYR
22	2	9	SER

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Mol	Chain	Res	Type
22	2	16	GLN
22	2	17	ARG
22	2	25	VAL
22	2	27	LEU
22	2	32	LYS
22	2	55	LYS
22	2	75	ILE
22	2	78	LYS
22	2	79	MET
22	2	80	VAL
22	2	83	ARG
22	2	88	ARG
22	2	89	LEU
22	2	96	ILE
22	2	102	ARG
22	2	104	GLU
22	2	106	LEU
22	2	126	VAL
22	2	127	GLN
22	2	128	LEU
22	2	139	ARG
22	2	141	VAL
22	2	143	THR
22	2	149	GLN
22	2	159	PHE
23	5	10	LYS
23	5	27	VAL
23	5	39	ASP
23	5	52	ASN
23	5	61	THR
23	5	66	VAL
23	5	88	GLN
23	5	93	ILE
23	5	99	LYS
23	5	100	THR
24	6	13	ILE
24	6	32	ARG
24	6	48	ARG
24	6	64	LYS
24	6	69	LEU
24	6	72	LYS
24	6	73	VAL

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Mol	Chain	Res	Type
24	6	74	MET
24	6	83	LYS
24	6	88	ARG
24	6	91	VAL
24	6	102	ILE
24	6	104	ASN
24	6	109	MET
24	6	115	THR
24	6	120	LYS
25	7	4	GLU
25	7	5	ILE
25	7	7	SER
25	7	19	THR
25	7	39	LEU
25	7	43	ARG
26	8	27	ARG
26	8	38	LEU
26	8	40	LEU
26	8	45	LYS
26	8	63	ILE
26	8	71	THR
26	8	86	VAL
26	8	92	LYS
26	8	104	GLU
26	8	108	LEU
26	8	109	LYS
26	8	115	ARG
26	8	125	ARG
26	8	133	LEU
26	8	135	ILE
26	8	137	ASN
26	8	142	ILE
27	9	8	VAL
27	9	13	ARG
27	9	26	GLN
27	9	37	LYS
27	9	45	ILE
27	9	50	ILE
27	9	51	ARG
27	9	56	VAL
27	9	57	LEU
27	9	60	ARG

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Mol	Chain	Res	Type
27	9	72	SER
27	9	74	TYR
27	9	76	LEU
27	9	80	VAL
27	9	94	SER
27	9	105	VAL
27	9	113	LYS
27	9	115	ARG
27	9	126	LEU
28	AA	24	VAL
28	AA	30	ASP
28	AA	46	ILE
28	AA	52	LYS
28	AA	66	THR
28	AA	75	VAL
28	AA	81	LEU
28	AA	83	THR
28	AA	86	THR
28	AA	89	VAL
28	AA	95	VAL
28	AA	102	GLU
28	AA	103	GLN
28	AA	107	ARG
28	AA	109	GLU
28	AA	134	LEU
28	AA	136	PHE
29	AB	4	ARG
29	AB	6	THR
29	AB	8	THR
29	AB	10	LYS
29	AB	32	ARG
29	AB	46	ASP
29	AB	56	VAL
29	AB	60	TYR
29	AB	76	ASP
29	AB	78	LEU
29	AB	80	THR
29	AB	88	ASP
29	AB	91	LEU
29	AB	92	LYS
29	AB	98	THR
29	AB	115	LYS

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Mol	Chain	Res	Type
29	AB	120	ASN
29	AB	130	VAL
29	AB	131	SER
29	AB	133	LEU
30	AC	23	LYS
30	AC	25	LYS
30	AC	28	LYS
30	AC	31	SER
30	AC	50	THR
30	AC	59	LYS
31	AD	16	LEU
31	AD	18	ILE
31	AD	34	LEU
31	AD	40	LYS
31	AD	41	LEU
31	AD	54	SER
31	AD	61	MET
31	AD	74	ASN
31	AD	76	GLU
31	AD	83	LYS
31	AD	87	VAL
31	AD	100	ILE
32	AE	6	ASP
32	AE	8	VAL
32	AE	13	THR
32	AE	16	LEU
32	AE	26	LYS
32	AE	31	ARG
32	AE	47	ASP
32	AE	64	VAL
32	AE	68	GLU
32	AE	79	ARG
32	AE	84	ASP
32	AE	106	THR
32	AE	110	GLU
33	AF	19	ARG
33	AF	31	ASN
33	AF	33	ARG
33	AF	34	LYS
33	AF	35	GLN
33	AF	51	SER
33	AF	54	LYS

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Mol	Chain	Res	Type
33	AF	61	LYS
33	AF	62	LYS
33	AF	73	THR
33	AF	75	LEU
33	AF	88	HIS
33	AF	106	VAL
33	AF	111	ARG
33	AF	125	ARG
34	AG	15	SER
34	AG	20	LYS
34	AG	59	VAL
34	AG	70	LYS
34	AG	81	VAL
34	AG	98	VAL
35	AH	5	VAL
35	AH	8	ARG
35	AH	20	ILE
35	AH	24	LYS
35	AH	29	ILE
35	AH	51	LEU
35	AH	56	THR
35	AH	58	ARG
35	AH	65	VAL
35	AH	71	THR
35	AH	79	SER
35	AH	81	CYS
35	AH	86	LYS
35	AH	104	VAL
35	AH	107	GLU
36	AI	15	GLU
36	AI	20	GLN
36	AI	21	LEU
36	AI	47	VAL
36	AI	48	ARG
36	AI	83	LYS
36	AI	85	THR
36	AI	89	ARG
36	AI	90	ARG
36	AI	92	LEU
36	AI	96	GLU
36	AI	101	THR
36	AI	104	GLN

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Mol	Chain	Res	Type
36	AI	107	LYS
36	AI	119	LYS
37	AJ	11	LEU
37	AJ	17	VAL
37	AJ	18	THR
37	AJ	21	THR
37	AJ	26	ILE
37	AJ	36	ARG
37	AJ	38	LYS
37	AJ	45	ARG
37	AJ	57	LEU
37	AJ	58	ILE
37	AJ	68	ARG
37	AJ	81	THR
37	AJ	88	GLU
37	AJ	90	MET
37	AJ	98	ARG
38	AK	17	THR
38	AK	24	ARG
38	AK	25	ARG
38	AK	33	THR
38	AK	34	CYS
38	AK	55	ARG
38	AK	59	THR
38	AK	65	ARG
38	AK	67	LEU
39	AL	24	THR
39	AL	32	ASN
39	AL	41	THR
39	AL	48	SER
39	AL	49	SER
39	AL	53	THR
39	AL	64	LYS
39	AL	65	LEU
39	AL	67	GLN
39	AL	72	THR
39	AL	77	ARG
40	AM	5	LYS
40	AM	10	LYS
40	AM	21	ARG
40	AM	29	LEU
40	AM	34	THR

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Mol	Chain	Res	Type
40	AM	45	ARG
40	AM	51	ILE
41	AN	78	ILE
41	AN	85	LEU
41	AN	92	ASP
41	AN	94	SER
41	AN	112	LYS
41	AN	113	ARG
41	AN	114	LYS
41	AN	126	LYS
41	AN	127	LEU
42	AO	5	TRP
42	AO	9	ARG
42	AO	11	ARG
42	AO	21	ARG
43	AP	4	VAL
43	AP	13	LYS
43	AP	35	LEU
43	AP	47	GLN
43	AP	78	LYS
43	AP	83	LEU
43	AP	84	THR
43	AP	85	LEU
43	AP	93	LEU
43	AP	99	GLN
44	AQ	7	LYS
44	AQ	11	THR
44	AQ	16	VAL
44	AQ	24	ARG
44	AQ	45	LYS
44	AQ	46	THR
44	AQ	49	ARG
44	AQ	56	THR
44	AQ	60	CYS
44	AQ	78	THR
44	AQ	82	THR
44	AQ	84	ARG
44	AQ	91	GLU
45	i	34	LYS
45	i	46	LYS
45	i	61	ILE
45	i	64	LYS

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Mol	Chain	Res	Type
45	i	68	ARG
45	i	74	LYS
45	i	77	THR
45	i	78	ASP
45	i	79	SER
45	i	84	LYS
45	i	91	THR
45	i	96	ARG
45	i	102	THR
45	i	116	GLU
45	i	130	GLU
45	i	131	ILE
4	CD	19	HIS
4	CD	32	LEU
4	CD	44	ILE
4	CD	45	VAL
4	CD	48	ILE
4	CD	49	VAL
4	CD	52	SER
4	CD	62	VAL
4	CD	73	GLU
4	CD	74	GLU
4	CD	96	LEU
4	CD	101	VAL
4	CD	116	VAL
4	CD	128	ARG
4	CD	137	ILE
4	CD	157	VAL
4	CD	158	ILE
4	CD	169	ILE
4	CD	179	LEU
4	CD	180	LEU
4	CD	204	MET
4	CD	207	VAL
4	CD	218	HIS
4	CD	225	ILE
4	CD	227	ARG
4	CD	230	VAL
4	CD	250	GLN
4	CD	252	THR
5	CE	2	SER
5	CE	10	ARG

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Mol	Chain	Res	Type
5	CE	17	LEU
5	CE	25	ILE
5	CE	30	LYS
5	CE	37	ARG
5	CE	43	LEU
5	CE	47	LEU
5	CE	56	ILE
5	CE	79	VAL
5	CE	84	VAL
5	CE	85	VAL
5	CE	100	ARG
5	CE	103	THR
5	CE	104	THR
5	CE	114	VAL
5	CE	120	LYS
5	CE	139	GLN
5	CE	148	LEU
5	CE	150	ARG
5	CE	156	SER
5	CE	157	VAL
5	CE	167	ARG
5	CE	169	THR
5	CE	183	LEU
5	CE	188	ILE
5	CE	192	VAL
5	CE	196	ARG
5	CE	200	GLU
5	CE	202	THR
5	CE	205	VAL
5	CE	208	VAL
5	CE	221	THR
5	CE	229	VAL
5	CE	232	ARG
5	CE	235	THR
5	CE	236	LYS
5	CE	238	LEU
5	CE	264	VAL
5	CE	284	ARG
5	CE	301	THR
5	CE	305	ILE
5	CE	308	MET
5	CE	317	ILE

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Mol	Chain	Res	Type
5	CE	324	VAL
5	CE	325	LYS
5	CE	328	ILE
5	CE	332	ARG
5	CE	338	LEU
5	CE	347	SER
5	CE	361	THR
6	CF	6	VAL
6	CF	47	ARG
6	CF	74	ILE
6	CF	93	MET
6	CF	118	LYS
6	CF	120	TYR
6	CF	122	THR
6	CF	138	ARG
6	CF	150	LEU
6	CF	153	SER
6	CF	156	LEU
6	CF	170	LYS
6	CF	176	SER
6	CF	179	LEU
6	CF	187	LEU
6	CF	188	ARG
6	CF	197	ARG
6	CF	200	THR
6	CF	203	ARG
6	CF	206	LEU
6	CF	220	ARG
6	CF	222	VAL
6	CF	230	VAL
6	CF	232	SER
6	CF	246	ARG
6	CF	265	GLU
6	CF	307	GLN
6	CF	313	LEU
6	CF	319	LYS
6	CF	323	VAL
6	CF	327	LEU
6	CF	332	LYS
6	CF	333	VAL
6	CF	343	LYS
6	CF	345	GLU

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Mol	Chain	Res	Type
6	CF	346	LYS
6	CF	349	THR
6	CF	354	VAL
6	CF	358	THR
7	CG	5	LYS
7	CG	8	LYS
7	CG	15	ARG
7	CG	22	ARG
7	CG	23	ARG
7	CG	35	ARG
7	CG	41	LYS
7	CG	69	ILE
7	CG	75	LEU
7	CG	89	THR
7	CG	92	LEU
7	CG	95	TRP
7	CG	105	ILE
7	CG	107	ARG
7	CG	110	LEU
7	CG	118	THR
7	CG	122	VAL
7	CG	124	GLU
7	CG	131	LEU
7	CG	132	THR
7	CG	140	ARG
7	CG	146	LEU
7	CG	148	ILE
7	CG	151	GLN
7	CG	152	ARG
7	CG	155	THR
7	CG	163	LEU
7	CG	177	GLU
7	CG	185	PHE
7	CG	187	THR
7	CG	188	GLU
7	CG	194	LEU
7	CG	211	LEU
7	CG	230	ASP
7	CG	236	LEU
7	CG	258	LYS
7	CG	277	LEU
7	CG	297	GLN

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Mol	Chain	Res	Type
8	CH	15	VAL
8	CH	21	THR
8	CH	31	ARG
8	CH	48	ARG
8	CH	52	VAL
8	CH	64	LEU
8	CH	65	ILE
8	CH	89	THR
8	CH	91	VAL
8	CH	93	VAL
8	CH	98	VAL
8	CH	129	GLU
8	CH	134	ARG
8	CH	152	THR
8	CH	155	LEU
9	CI	24	GLU
9	CI	25	GLN
9	CI	60	ARG
9	CI	77	VAL
9	CI	83	LEU
9	CI	89	ILE
9	CI	92	ILE
9	CI	98	LYS
9	CI	121	LYS
9	CI	124	LEU
9	CI	143	THR
9	CI	158	LYS
9	CI	173	LEU
9	CI	179	LEU
9	CI	181	ILE
9	CI	184	LEU
9	CI	239	LEU
10	CJ	27	THR
10	CJ	50	VAL
10	CJ	71	VAL
10	CJ	74	THR
10	CJ	79	GLN
10	CJ	84	ARG
10	CJ	124	ASP
10	CJ	132	VAL
10	CJ	136	LEU
10	CJ	150	LEU

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Mol	Chain	Res	Type
10	CJ	156	ASP
10	CJ	157	VAL
10	CJ	160	ILE
10	CJ	169	LEU
10	CJ	172	LYS
10	CJ	185	ARG
10	CJ	203	VAL
10	CJ	248	LYS
11	CK	5	GLN
11	CK	6	THR
11	CK	18	VAL
11	CK	19	SER
11	CK	22	SER
11	CK	33	THR
11	CK	41	ILE
11	CK	48	VAL
11	CK	52	LEU
11	CK	68	LEU
11	CK	69	ARG
11	CK	70	THR
11	CK	82	VAL
11	CK	121	LYS
11	CK	122	LYS
11	CK	133	THR
11	CK	139	ASN
11	CK	151	VAL
11	CK	152	GLU
11	CK	157	ASN
11	CK	161	LEU
11	CK	162	GLN
11	CK	164	ILE
11	CK	166	ARG
11	CK	190	ASP
12	CL	3	ARG
12	CL	24	ARG
12	CL	26	VAL
12	CL	32	ARG
12	CL	33	ILE
12	CL	36	LEU
12	CL	40	LYS
12	CL	42	THR
12	CL	44	ASP

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Mol	Chain	Res	Type
12	CL	48	LEU
12	CL	52	LEU
12	CL	63	GLU
12	CL	87	LEU
12	CL	129	VAL
12	CL	145	LYS
12	CL	163	GLN
12	CL	165	ILE
12	CL	174	THR
12	CL	197	VAL
12	CL	205	SER
13	CM	7	ASN
13	CM	9	MET
13	CM	10	ARG
13	CM	13	LYS
13	CM	23	VAL
13	CM	28	ASP
13	CM	29	ARG
13	CM	40	LEU
13	CM	44	THR
13	CM	56	THR
13	CM	63	GLU
13	CM	70	THR
13	CM	80	LEU
13	CM	95	ASN
13	CM	106	ILE
13	CM	107	ASP
13	CM	112	LEU
13	CM	115	LYS
13	CM	130	VAL
13	CM	137	ARG
13	CM	140	ARG
13	CM	158	ASP
13	CM	165	GLN
13	CM	173	ASP
14	CN	13	HIS
14	CN	23	LYS
14	CN	42	ARG
14	CN	54	LEU
14	CN	55	ARG
14	CN	58	VAL
14	CN	59	ARG

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Mol	Chain	Res	Type
14	CN	67	ARG
14	CN	69	VAL
14	CN	107	GLU
14	CN	122	LYS
14	CN	123	ILE
14	CN	124	ILE
14	CN	131	LYS
14	CN	134	GLU
14	CN	164	GLU
14	CN	165	SER
14	CN	168	ARG
14	CN	171	ARG
15	CO	5	SER
15	CO	15	VAL
15	CO	20	VAL
15	CO	38	ILE
15	CO	50	LYS
15	CO	64	VAL
15	CO	72	LEU
15	CO	90	VAL
15	CO	126	GLN
15	CO	130	THR
15	CO	137	LYS
16	CP	10	LEU
16	CP	15	GLN
16	CP	20	ARG
16	CP	22	LEU
16	CP	38	ARG
16	CP	68	ARG
16	CP	80	THR
16	CP	83	LYS
16	CP	85	THR
16	CP	92	LEU
16	CP	96	ARG
16	CP	104	GLU
16	CP	105	ARG
16	CP	106	VAL
16	CP	133	ILE
16	CP	138	GLN
16	CP	151	ILE
16	CP	153	ASP
16	CP	155	VAL

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Mol	Chain	Res	Type
16	CP	170	LYS
16	CP	183	THR
16	CP	190	THR
17	CQ	22	VAL
17	CQ	25	LYS
17	CQ	33	ILE
17	CQ	34	VAL
17	CQ	41	LEU
17	CQ	67	THR
17	CQ	78	ARG
17	CQ	85	ARG
17	CQ	106	GLU
17	CQ	117	ARG
17	CQ	124	LEU
17	CQ	128	ARG
17	CQ	152	VAL
17	CQ	160	ARG
17	CQ	175	THR
17	CQ	180	SER
17	CQ	184	THR
17	CQ	197	LEU
18	CR	3	ARG
18	CR	9	THR
18	CR	24	VAL
18	CR	32	THR
18	CR	36	ILE
18	CR	42	THR
18	CR	49	GLU
18	CR	52	LEU
18	CR	55	GLN
18	CR	69	ARG
18	CR	78	VAL
18	CR	89	LYS
18	CR	111	LYS
18	CR	112	LEU
18	CR	114	VAL
18	CR	119	VAL
18	CR	126	ARG
18	CR	128	ARG
18	CR	144	SER
18	CR	157	VAL
18	CR	168	LEU

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Mol	Chain	Res	Type
18	CR	169	THR
18	CR	171	ARG
18	CR	175	ARG
19	CS	3	ILE
19	CS	7	SER
19	CS	17	THR
19	CS	24	VAL
19	CS	26	LEU
19	CS	32	LEU
19	CS	34	THR
19	CS	41	ASP
19	CS	49	LEU
19	CS	59	ARG
19	CS	63	SER
19	CS	64	VAL
19	CS	66	ARG
19	CS	69	ARG
19	CS	80	THR
19	CS	81	VAL
19	CS	93	ILE
19	CS	100	THR
19	CS	113	LYS
19	CS	115	VAL
19	CS	135	GLN
19	CS	138	LEU
19	CS	168	THR
19	CS	170	ARG
19	CS	181	SER
20	CT	10	LEU
20	CT	24	LEU
20	CT	29	THR
20	CT	30	SER
20	CT	43	LYS
20	CT	44	LEU
20	CT	46	LYS
20	CT	52	LYS
20	CT	57	VAL
20	CT	74	ARG
20	CT	76	SER
20	CT	81	ARG
20	CT	91	SER
20	CT	98	ARG

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Mol	Chain	Res	Type
20	CT	99	LEU
20	CT	100	ARG
20	CT	103	ARG
20	CT	106	LEU
20	CT	134	HIS
20	CT	138	LEU
20	CT	144	GLN
20	CT	148	ASP
20	CT	152	GLU
20	CT	157	GLU
20	CT	158	GLU
20	CT	166	ASN
20	CT	167	ARG
20	CT	182	ASP
21	CU	8	GLN
21	CU	24	LEU
21	CU	40	ARG
21	CU	45	LEU
21	CU	50	LYS
21	CU	58	ILE
21	CU	61	ILE
21	CU	71	LYS
21	CU	80	ARG
21	CU	87	THR
21	CU	96	ASP
21	CU	97	VAL
21	CU	100	VAL
21	CU	104	GLU
21	CU	105	THR
21	CU	115	ARG
21	CU	117	ARG
21	CU	132	THR
21	CU	137	ARG
21	CU	149	LYS
21	CU	156	VAL
21	CU	160	THR
21	CU	162	THR
21	CU	172	TYR
22	CV	12	ARG
22	CV	21	LYS
22	CV	25	VAL
22	CV	26	HIS

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Mol	Chain	Res	Type
22	CV	27	LEU
22	CV	55	LYS
22	CV	71	SER
22	CV	75	ILE
22	CV	78	LYS
22	CV	79	MET
22	CV	80	VAL
22	CV	83	ARG
22	CV	88	ARG
22	CV	102	ARG
22	CV	103	GLN
22	CV	104	GLU
22	CV	106	LEU
22	CV	122	GLN
22	CV	124	VAL
22	CV	126	VAL
22	CV	127	GLN
22	CV	128	LEU
22	CV	139	ARG
22	CV	143	THR
22	CV	160	ILE
23	CW	10	LYS
23	CW	38	ILE
23	CW	43	VAL
23	CW	49	ASN
23	CW	52	ASN
23	CW	58	GLU
23	CW	61	THR
23	CW	72	SER
23	CW	75	TYR
23	CW	100	THR
23	CW	105	LEU
24	CX	13	ILE
24	CX	14	SER
24	CX	32	ARG
24	CX	48	ARG
24	CX	69	LEU
24	CX	73	VAL
24	CX	74	MET
24	CX	83	LYS
24	CX	88	ARG
24	CX	91	VAL

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Mol	Chain	Res	Type
24	CX	102	ILE
24	CX	115	THR
24	CX	120	LYS
25	CY	1	MET
25	CY	4	GLU
25	CY	17	ARG
25	CY	19	THR
25	CY	39	LEU
25	CY	54	LEU
26	CZ	27	ARG
26	CZ	37	THR
26	CZ	38	LEU
26	CZ	39	LYS
26	CZ	40	LEU
26	CZ	45	LYS
26	CZ	48	SER
26	CZ	63	ILE
26	CZ	65	GLN
26	CZ	71	THR
26	CZ	73	MET
26	CZ	106	ASP
26	CZ	108	LEU
26	CZ	115	ARG
26	CZ	125	ARG
26	CZ	135	ILE
26	CZ	139	ILE
26	CZ	142	ILE
27	DA	8	VAL
27	DA	13	ARG
27	DA	17	LYS
27	DA	37	LYS
27	DA	45	ILE
27	DA	50	ILE
27	DA	56	VAL
27	DA	57	LEU
27	DA	59	VAL
27	DA	71	SER
27	DA	74	TYR
27	DA	76	LEU
27	DA	105	VAL
27	DA	112	ASP
27	DA	125	LYS

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Mol	Chain	Res	Type
28	DB	14	VAL
28	DB	24	VAL
28	DB	26	VAL
28	DB	30	ASP
28	DB	81	LEU
28	DB	83	THR
28	DB	86	THR
28	DB	99	GLU
28	DB	102	GLU
28	DB	134	LEU
29	DC	4	ARG
29	DC	6	THR
29	DC	7	LYS
29	DC	8	THR
29	DC	9	ARG
29	DC	10	LYS
29	DC	25	HIS
29	DC	26	ARG
29	DC	42	ARG
29	DC	56	VAL
29	DC	60	TYR
29	DC	85	ASP
29	DC	91	LEU
29	DC	98	THR
29	DC	115	LYS
29	DC	133	LEU
30	DD	21	ILE
30	DD	22	LYS
30	DD	23	LYS
30	DD	26	THR
30	DD	31	SER
30	DD	50	THR
30	DD	59	LYS
31	DE	12	GLN
31	DE	34	LEU
31	DE	61	MET
31	DE	83	LYS
31	DE	87	VAL
31	DE	102	THR
32	DF	8	VAL
32	DF	13	THR
32	DF	16	LEU

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Mol	Chain	Res	Type
32	DF	18	LYS
32	DF	26	LYS
32	DF	28	ARG
32	DF	31	ARG
32	DF	46	THR
32	DF	64	VAL
32	DF	79	ARG
32	DF	83	GLU
32	DF	86	LYS
32	DF	91	SER
32	DF	98	VAL
32	DF	104	LEU
32	DF	105	GLN
32	DF	106	THR
32	DF	110	GLU
33	DG	8	LYS
33	DG	19	ARG
33	DG	33	ARG
33	DG	34	LYS
33	DG	41	VAL
33	DG	73	THR
33	DG	75	LEU
33	DG	82	LEU
33	DG	109	LEU
33	DG	111	ARG
33	DG	125	ARG
34	DH	4	SER
34	DH	10	LYS
34	DH	15	SER
34	DH	20	LYS
34	DH	21	ARG
34	DH	31	LYS
34	DH	59	VAL
34	DH	74	THR
34	DH	92	LYS
34	DH	98	VAL
35	DI	5	VAL
35	DI	20	ILE
35	DI	24	LYS
35	DI	29	ILE
35	DI	36	LYS
35	DI	58	ARG

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Mol	Chain	Res	Type
35	DI	65	VAL
35	DI	71	THR
35	DI	102	LYS
36	DJ	15	GLU
36	DJ	20	GLN
36	DJ	21	LEU
36	DJ	27	GLU
36	DJ	28	LEU
36	DJ	45	LYS
36	DJ	47	VAL
36	DJ	48	ARG
36	DJ	49	LYS
36	DJ	50	SER
36	DJ	62	GLN
36	DJ	69	LEU
36	DJ	71	LYS
36	DJ	73	LYS
36	DJ	81	ARG
36	DJ	84	LYS
36	DJ	85	THR
36	DJ	89	ARG
36	DJ	90	ARG
36	DJ	101	THR
36	DJ	104	GLN
36	DJ	107	LYS
36	DJ	119	LYS
37	DK	20	MET
37	DK	21	THR
37	DK	26	ILE
37	DK	29	LYS
37	DK	30	LYS
37	DK	35	ASN
37	DK	36	ARG
37	DK	37	THR
37	DK	43	LEU
37	DK	45	ARG
37	DK	68	ARG
37	DK	76	ARG
37	DK	79	SER
37	DK	81	THR
37	DK	99	ARG
37	DK	100	HIS

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Mol	Chain	Res	Type
38	DL	12	HIS
38	DL	17	THR
38	DL	21	ARG
38	DL	24	ARG
38	DL	25	ARG
38	DL	33	THR
38	DL	44	THR
38	DL	59	THR
38	DL	67	LEU
38	DL	72	ARG
38	DL	80	THR
39	DM	6	THR
39	DM	24	THR
39	DM	32	ASN
39	DM	41	THR
39	DM	45	VAL
39	DM	46	ARG
39	DM	53	THR
39	DM	58	ASP
39	DM	65	LEU
39	DM	69	LEU
39	DM	72	THR
39	DM	77	ARG
40	DN	4	GLN
40	DN	21	ARG
40	DN	29	LEU
40	DN	45	ARG
40	DN	51	ILE
41	DO	77	ILE
41	DO	85	LEU
41	DO	94	SER
41	DO	112	LYS
41	DO	113	ARG
41	DO	114	LYS
41	DO	127	LEU
42	DP	6	ARG
42	DP	9	ARG
42	DP	13	LEU
42	DP	15	ARG
43	DQ	6	LYS
43	DQ	7	THR
43	DQ	8	ARG

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Mol	Chain	Res	Type
43	DQ	22	GLN
43	DQ	35	LEU
43	DQ	45	ARG
43	DQ	48	SER
43	DQ	60	LYS
43	DQ	61	LYS
43	DQ	78	LYS
43	DQ	79	THR
43	DQ	83	LEU
43	DQ	84	THR
43	DQ	93	LEU
43	DQ	100	LYS
43	DQ	104	LEU
43	DQ	105	GLN
44	DR	11	THR
44	DR	20	SER
44	DR	25	GLN
44	DR	46	THR
44	DR	56	THR
44	DR	60	CYS
44	DR	73	THR
46	p0	4	ILE
46	p0	42	ARG
46	p0	44	GLU
46	p0	48	ARG
46	p0	51	VAL
46	p0	67	LEU
46	p0	69	ASP
46	p0	70	LEU
46	p0	72	ASP
46	p0	74	GLU
46	p0	76	LEU
46	p0	80	VAL
46	p0	84	VAL
46	p0	93	LEU
46	p0	97	LYS
46	p0	104	ARG
46	p0	192	ASP
47	sM	43	ASP
47	sM	49	LYS
47	sM	50	ASN
47	sM	68	ARG

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Mol	Chain	Res	Type
47	sM	74	LYS
47	sM	75	ASP
47	sM	77	THR
49	B	6	THR
49	B	8	ASP
49	B	37	VAL
49	B	59	LEU
49	B	62	ARG
49	B	84	ARG
49	B	87	LEU
49	B	88	LYS
49	B	154	GLU
49	B	157	ASP
49	B	172	LEU
49	B	185	ARG
49	B	188	LEU
49	B	198	MET
49	B	200	ASP
50	C	21	VAL
50	C	25	THR
50	C	29	TRP
50	C	30	PHE
50	C	46	THR
50	C	61	LEU
50	C	64	ARG
50	C	70	LEU
50	C	77	GLU
50	C	78	ASP
50	C	81	PHE
50	C	95	ASN
50	C	97	LEU
50	C	105	PHE
50	C	111	ARG
50	C	117	TRP
50	C	148	ASN
50	C	154	SER
50	C	177	GLN
50	C	180	THR
50	C	181	LEU
50	C	184	LEU
50	C	193	ILE
50	C	198	GLU

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Mol	Chain	Res	Type
50	C	202	LYS
50	C	214	LYS
50	C	215	VAL
50	C	218	LEU
50	C	220	GLN
50	C	222	LYS
50	C	223	PHE
51	D	40	LYS
51	D	53	ILE
51	D	69	ILE
51	D	70	ASP
51	D	72	LEU
51	D	73	LEU
51	D	76	LEU
51	D	77	GLN
51	D	80	VAL
51	D	89	GLN
51	D	91	ARG
51	D	94	GLN
51	D	95	ARG
51	D	96	THR
51	D	97	ARG
51	D	106	ASP
51	D	111	VAL
51	D	113	LEU
51	D	117	THR
51	D	134	LEU
51	D	140	ARG
51	D	141	ARG
51	D	148	LEU
51	D	153	SER
51	D	195	ASP
51	D	201	ASN
51	D	207	LEU
51	D	221	THR
51	D	222	TYR
51	D	225	LEU
51	D	226	THR
51	D	229	LEU
51	D	235	LEU
51	D	237	VAL
51	D	244	SER

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Mol	Chain	Res	Type
51	D	245	ASP
52	E	4	LEU
52	E	5	ILE
52	E	7	LYS
52	E	21	LEU
52	E	23	GLU
52	E	65	ARG
52	E	76	ARG
52	E	84	ILE
52	E	92	GLN
52	E	105	MET
52	E	111	ASN
52	E	120	TYR
52	E	127	MET
52	E	142	LEU
52	E	151	LYS
52	E	158	ILE
52	E	172	THR
52	E	175	VAL
52	E	176	LEU
52	E	178	ARG
52	E	181	VAL
52	E	182	LEU
52	E	196	ARG
52	E	217	ILE
52	E	224	ASP
53	F	6	LYS
53	F	7	LYS
53	F	9	LEU
53	F	38	LEU
53	F	70	VAL
53	F	77	ARG
53	F	105	VAL
53	F	115	THR
53	F	116	ASP
53	F	120	SER
53	F	126	VAL
53	F	131	LEU
53	F	133	LYS
53	F	180	LEU
53	F	181	VAL
53	F	182	TYR

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Mol	Chain	Res	Type
53	F	187	ARG
53	F	197	HIS
53	F	206	ASP
53	F	214	LEU
53	F	215	ASP
53	F	221	ARG
53	F	223	ASN
53	F	227	VAL
53	F	240	LYS
53	F	242	LYS
53	F	258	GLN
54	G	25	LEU
54	G	38	THR
54	G	43	PHE
54	G	45	LYS
54	G	65	ARG
54	G	76	ARG
54	G	79	ASN
54	G	94	THR
54	G	119	ASP
54	G	146	THR
54	G	147	THR
54	G	149	VAL
54	G	156	ARG
54	G	162	VAL
54	G	216	GLU
55	H	7	TYR
55	H	13	GLN
55	H	25	ARG
55	H	45	PHE
55	H	58	LYS
55	H	68	LEU
55	H	69	LEU
55	H	71	THR
55	H	79	LYS
55	H	81	VAL
55	H	82	SER
55	H	98	ARG
55	H	109	LEU
55	H	120	GLU
55	H	125	THR
55	H	126	ASP

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Mol	Chain	Res	Type
55	H	127	THR
55	H	128	THR
55	H	129	VAL
55	H	132	ARG
55	H	133	LEU
55	H	154	ARG
55	H	155	ASP
55	H	158	ILE
55	H	169	TYR
55	H	170	THR
55	H	175	ILE
55	H	193	LEU
55	H	212	LEU
56	I	15	GLU
56	I	28	GLU
56	I	29	ASN
56	I	38	LEU
56	I	50	ASP
56	I	70	PHE
56	I	77	LEU
56	I	85	PHE
56	I	87	ASP
56	I	97	ARG
56	I	110	GLN
56	I	114	ARG
56	I	116	ARG
56	I	117	THR
56	I	126	LEU
56	I	131	PHE
56	I	134	GLU
56	I	136	VAL
56	I	147	ASN
56	I	166	LEU
56	I	185	ILE
57	J	8	ARG
57	J	29	LEU
57	J	36	THR
57	J	46	VAL
57	J	49	ARG
57	J	58	LEU
57	J	74	LYS
57	J	121	LEU

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Mol	Chain	Res	Type
57	J	137	LYS
57	J	151	LYS
57	J	152	ILE
57	J	161	SER
57	J	164	ARG
57	J	184	LEU
57	J	196	LEU
58	K	3	ARG
58	K	6	ARG
58	K	7	THR
58	K	14	THR
58	K	21	SER
58	K	28	LEU
58	K	39	LYS
58	K	40	LYS
58	K	57	ARG
58	K	60	LEU
58	K	78	ARG
58	K	81	VAL
58	K	89	ASP
58	K	92	LYS
58	K	93	LEU
58	K	97	LEU
58	K	99	LEU
58	K	101	VAL
58	K	110	GLN
58	K	118	LEU
58	K	130	THR
58	K	138	LYS
58	K	149	ARG
58	K	150	LEU
58	K	161	THR
58	K	168	ARG
58	K	171	ARG
58	K	172	VAL
58	K	174	ARG
59	L	20	VAL
59	L	28	ASN
59	L	55	VAL
59	L	56	LYS
59	L	76	LEU
59	L	81	ASN

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Mol	Chain	Res	Type
59	L	82	LEU
60	M	5	LEU
60	M	21	ASN
60	M	29	LYS
60	M	37	ASN
60	M	40	LEU
60	M	44	THR
60	M	67	ARG
60	M	69	LYS
60	M	74	THR
60	M	79	LYS
60	M	80	MET
60	M	99	ARG
60	M	109	VAL
60	M	112	SER
60	M	118	GLN
60	M	123	VAL
60	M	127	GLN
60	M	128	CYS
60	M	136	ARG
60	M	140	VAL
60	M	141	LYS
61	N	28	LEU
61	N	33	ARG
61	N	36	LEU
61	N	37	VAL
61	N	43	ARG
61	N	50	LYS
61	N	58	LEU
61	N	61	VAL
61	N	66	VAL
61	N	71	ILE
61	N	74	LEU
61	N	81	ASP
61	N	85	LYS
61	N	103	LEU
61	N	116	VAL
61	N	126	TRP
61	N	129	GLU
61	N	132	GLU
61	N	133	LEU
61	N	140	PHE

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Mol	Chain	Res	Type
62	O	3	ARG
62	O	9	LYS
62	O	11	ILE
62	O	12	SER
62	O	21	ASN
62	O	27	LYS
62	O	39	LYS
62	O	42	ARG
62	O	45	LEU
62	O	48	SER
62	O	64	ARG
62	O	76	LYS
62	O	83	GLU
62	O	88	LEU
62	O	102	LEU
62	O	105	ASN
62	O	115	LEU
62	O	125	LEU
62	O	134	VAL
62	O	138	ASN
62	O	141	TYR
63	P	13	VAL
63	P	14	PHE
63	P	29	HIS
63	P	31	THR
63	P	39	ILE
63	P	43	THR
63	P	49	LYS
63	P	92	LYS
63	P	93	THR
63	P	103	ARG
63	P	118	VAL
63	P	137	LEU
64	Q	11	VAL
64	Q	22	LEU
64	Q	26	LEU
64	Q	28	MET
64	Q	31	GLU
64	Q	34	VAL
64	Q	36	LEU
64	Q	44	ARG
64	Q	47	ARG

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Mol	Chain	Res	Type
64	Q	50	THR
64	Q	52	LYS
64	Q	94	VAL
64	Q	110	GLU
64	Q	121	ILE
64	Q	124	THR
65	R	14	LYS
65	R	17	THR
65	R	29	ILE
65	R	42	GLU
65	R	43	ILE
65	R	47	LYS
65	R	53	LEU
65	R	57	LEU
65	R	66	ARG
65	R	69	VAL
65	R	98	ASP
65	R	114	ARG
65	R	116	LEU
65	R	123	ARG
65	R	127	LYS
65	R	128	LYS
65	R	137	ARG
66	S	3	ARG
66	S	6	THR
66	S	23	LYS
66	S	25	THR
66	S	26	LEU
66	S	34	LEU
66	S	38	ILE
66	S	46	LEU
66	S	62	GLN
66	S	69	ILE
66	S	71	PHE
66	S	72	LYS
66	S	83	GLN
66	S	84	TYR
66	S	105	GLN
66	S	113	LEU
66	S	115	LEU
67	T	3	LEU
67	T	5	VAL

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Mol	Chain	Res	Type
67	T	8	GLN
67	T	11	PHE
67	T	12	GLN
67	T	13	HIS
67	T	14	ILE
67	T	15	LEU
67	T	25	ASN
67	T	26	ILE
67	T	28	ILE
67	T	40	ARG
67	T	71	GLN
67	T	80	LYS
67	T	86	LEU
67	T	92	ILE
67	T	93	THR
67	T	110	ARG
67	T	116	LEU
67	T	132	ARG
67	T	136	GLN
67	T	138	THR
67	T	140	THR
67	T	143	ARG
68	U	6	VAL
68	U	22	LEU
68	U	28	LEU
68	U	30	VAL
68	U	33	TYR
68	U	35	ASP
68	U	36	ILE
68	U	57	ARG
68	U	63	ARG
68	U	67	MET
68	U	70	GLN
68	U	71	VAL
68	U	84	LYS
68	U	88	VAL
68	U	94	ILE
68	U	111	ILE
68	U	126	GLU
68	U	130	ARG
68	U	131	ASP
68	U	140	LEU

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Mol	Chain	Res	Type
68	U	144	GLU
69	V	15	GLN
69	V	23	ARG
69	V	27	THR
69	V	31	VAL
69	V	42	VAL
69	V	47	GLN
69	V	48	HIS
69	V	50	LEU
69	V	51	VAL
69	V	57	ARG
69	V	60	THR
69	V	61	LYS
69	V	74	GLU
69	V	81	THR
69	V	89	ARG
69	V	103	ILE
70	W	1	MET
70	W	5	LYS
70	W	11	LEU
70	W	25	LYS
70	W	32	VAL
70	W	41	GLU
70	W	49	GLU
70	W	52	THR
70	W	68	SER
70	W	69	LEU
70	W	76	ASP
70	W	78	LEU
70	W	80	LYS
71	X	22	LYS
71	X	23	ARG
71	X	24	GLN
71	X	25	VAL
71	X	27	ILE
71	X	30	SER
71	X	47	ILE
71	X	49	GLU
71	X	53	ILE
71	X	56	HIS
71	X	65	LEU
71	X	86	ILE

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Mol	Chain	Res	Type
71	X	87	GLU
71	X	93	LEU
71	X	98	GLN
71	X	103	ILE
71	X	119	LYS
71	X	121	VAL
71	X	125	ILE
72	Y	7	ARG
72	Y	9	LEU
72	Y	14	LYS
72	Y	18	HIS
72	Y	19	ARG
72	Y	40	SER
72	Y	69	ARG
72	Y	73	ARG
72	Y	77	ILE
72	Y	84	THR
72	Y	97	ASP
72	Y	103	LEU
72	Y	107	PHE
72	Y	114	LYS
72	Y	132	LEU
72	Y	138	GLU
72	Y	140	LYS
72	Y	144	ARG
73	Z	5	VAL
73	Z	17	LEU
73	Z	32	ARG
73	Z	47	VAL
73	Z	57	VAL
73	Z	62	THR
73	Z	75	VAL
73	Z	81	GLU
73	Z	84	LYS
73	Z	99	LYS
73	Z	102	LYS
73	Z	124	ARG
73	Z	127	LYS
74	a	37	GLN
74	a	40	VAL
74	a	42	LEU
74	a	44	GLN

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Mol	Chain	Res	Type
74	a	49	ARG
74	a	58	ARG
74	a	67	ASP
74	a	69	LEU
74	a	71	ILE
74	a	75	LEU
74	a	85	LYS
74	a	92	ILE
74	a	95	HIS
74	a	96	SER
74	a	97	LYS
74	a	100	ILE
74	a	102	THR
75	b	12	LYS
75	b	38	ARG
75	b	41	ILE
75	b	44	ILE
75	b	61	GLU
75	b	64	LEU
75	b	66	LYS
75	b	69	ASN
75	b	82	ARG
75	b	91	ASP
76	c	3	LEU
76	c	20	LYS
76	c	33	LEU
76	c	60	SER
76	c	61	THR
76	c	75	GLU
76	c	77	THR
77	d	19	THR
77	d	31	GLU
77	d	32	PHE
77	d	39	THR
77	d	49	ARG
77	d	58	GLU
77	d	64	ARG
78	e	8	PHE
78	e	12	ARG
78	e	19	ARG
78	e	28	THR
78	e	30	LEU

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Mol	Chain	Res	Type
78	e	32	ARG
78	e	36	LEU
78	e	49	ASP
79	f	21	VAL
79	f	28	LYS
79	f	29	LYS
79	f	39	LEU
79	f	42	ARG
79	f	43	ARG
79	f	56	MET
80	g	89	LYS
80	g	91	ILE
80	g	97	LYS
80	g	106	TYR
80	g	114	VAL
80	g	138	ARG
80	g	147	VAL
81	h	10	ARG
81	h	52	GLN
81	h	66	HIS
81	h	76	ASP
81	h	88	THR
81	h	106	HIS
81	h	116	ASP
81	h	117	LYS
81	h	136	ILE
81	h	141	LEU
81	h	145	LEU
81	h	165	ASP
81	h	193	ILE
81	h	238	ASP
81	h	265	LEU
81	h	292	LEU
81	h	300	THR
81	h	316	MET
81	Rb	16	HIS
81	Rb	29	GLN
81	Rb	52	GLN
81	Rb	58	VAL
81	Rb	64	HIS
81	Rb	66	HIS
81	Rb	76	ASP

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Mol	Chain	Res	Type
81	Rb	96	THR
81	Rb	106	HIS
81	Rb	133	VAL
81	Rb	145	LEU
81	Rb	149	ASP
81	Rb	159	ASN
81	Rb	202	LEU
81	Rb	245	PHE
81	Rb	275	ARG
81	Rb	297	ASP
49	s0	8	ASP
49	s0	9	LEU
49	s0	12	GLU
49	s0	28	ASN
49	s0	29	VAL
49	s0	41	ARG
49	s0	45	VAL
49	s0	59	LEU
49	s0	62	ARG
49	s0	87	LEU
49	s0	96	THR
49	s0	101	ARG
49	s0	111	ILE
49	s0	119	ARG
49	s0	131	GLN
49	s0	139	VAL
49	s0	154	GLU
49	s0	157	ASP
49	s0	164	ASN
49	s0	165	ARG
49	s0	172	LEU
49	s0	179	ARG
49	s0	185	ARG
49	s0	188	LEU
49	s0	191	ARG
49	s0	198	MET
50	s1	21	VAL
50	s1	37	THR
50	s1	47	LEU
50	s1	55	LYS
50	s1	61	LEU
50	s1	65	VAL

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Mol	Chain	Res	Type
50	s1	70	LEU
50	s1	73	LEU
50	s1	81	PHE
50	s1	83	LYS
50	s1	97	LEU
50	s1	105	PHE
50	s1	125	VAL
50	s1	126	THR
50	s1	129	THR
50	s1	131	ASP
50	s1	153	HIS
50	s1	173	THR
50	s1	181	LEU
50	s1	183	GLN
50	s1	193	ILE
50	s1	202	LYS
50	s1	212	VAL
50	s1	215	VAL
50	s1	223	PHE
50	s1	225	VAL
50	s1	231	LEU
50	s1	234	GLU
51	s2	41	LEU
51	s2	53	ILE
51	s2	55	GLU
51	s2	69	ILE
51	s2	70	ASP
51	s2	72	LEU
51	s2	73	LEU
51	s2	79	GLU
51	s2	80	VAL
51	s2	82	ASN
51	s2	83	ILE
51	s2	89	GLN
51	s2	91	ARG
51	s2	97	ARG
51	s2	111	VAL
51	s2	113	LEU
51	s2	117	THR
51	s2	140	ARG
51	s2	141	ARG
51	s2	146	THR

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Mol	Chain	Res	Type
51	s2	153	SER
51	s2	159	THR
51	s2	166	THR
51	s2	185	LYS
51	s2	194	GLU
51	s2	195	ASP
51	s2	206	THR
51	s2	208	GLU
51	s2	222	TYR
51	s2	225	LEU
51	s2	233	GLN
51	s2	237	VAL
51	s2	245	ASP
51	s2	246	GLU
51	s2	250	GLN
52	s3	4	LEU
52	s3	9	ARG
52	s3	57	ASP
52	s3	66	ILE
52	s3	69	LEU
52	s3	84	ILE
52	s3	90	ARG
52	s3	92	GLN
52	s3	115	ILE
52	s3	117	ARG
52	s3	120	TYR
52	s3	128	GLU
52	s3	142	LEU
52	s3	158	ILE
52	s3	164	VAL
52	s3	168	ILE
52	s3	169	ASP
52	s3	172	THR
52	s3	223	LYS
53	s4	6	LYS
53	s4	9	LEU
53	s4	11	ARG
53	s4	23	LEU
53	s4	30	ARG
53	s4	38	LEU
53	s4	42	LEU
53	s4	49	ARG

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Mol	Chain	Res	Type
53	s4	51	ARG
53	s4	70	VAL
53	s4	78	THR
53	s4	95	THR
53	s4	104	ASP
53	s4	128	LYS
53	s4	131	LEU
53	s4	160	VAL
53	s4	164	LEU
53	s4	176	ASP
53	s4	180	LEU
53	s4	181	VAL
53	s4	182	TYR
53	s4	194	THR
53	s4	195	ILE
53	s4	219	VAL
53	s4	221	ARG
53	s4	222	LEU
53	s4	227	VAL
53	s4	237	SER
53	s4	245	LYS
53	s4	254	ARG
54	s5	25	LEU
54	s5	27	THR
54	s5	38	THR
54	s5	43	PHE
54	s5	63	GLN
54	s5	68	ILE
54	s5	76	ARG
54	s5	79	ASN
54	s5	89	ILE
54	s5	93	LEU
54	s5	119	ASP
54	s5	125	THR
54	s5	146	THR
54	s5	157	ARG
54	s5	166	ARG
54	s5	194	LEU
54	s5	199	ILE
54	s5	203	LYS
54	s5	216	GLU
54	s5	225	ARG

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Mol	Chain	Res	Type
55	s6	31	ARG
55	s6	71	THR
55	s6	76	LEU
55	s6	78	THR
55	s6	98	ARG
55	s6	108	VAL
55	s6	109	LEU
55	s6	120	GLU
55	s6	121	LEU
55	s6	125	THR
55	s6	126	ASP
55	s6	127	THR
55	s6	128	THR
55	s6	129	VAL
55	s6	137	ARG
55	s6	151	ASP
55	s6	155	ASP
55	s6	177	ARG
55	s6	189	HIS
55	s6	193	LEU
55	s6	215	ARG
55	s6	216	LEU
56	s7	9	LEU
56	s7	33	GLU
56	s7	55	LYS
56	s7	64	VAL
56	s7	77	LEU
56	s7	79	ARG
56	s7	80	GLU
56	s7	86	GLN
56	s7	97	ARG
56	s7	101	LYS
56	s7	114	ARG
56	s7	116	ARG
56	s7	117	THR
56	s7	144	VAL
56	s7	159	VAL
56	s7	166	LEU
56	s7	185	ILE
57	s8	7	SER
57	s8	20	GLN
57	s8	29	LEU

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Mol	Chain	Res	Type
57	s8	36	THR
57	s8	46	VAL
57	s8	61	GLU
57	s8	74	LYS
57	s8	89	GLU
57	s8	138	ASN
57	s8	151	LYS
57	s8	155	SER
57	s8	179	CYS
57	s8	183	ILE
57	s8	184	LEU
58	s9	3	ARG
58	s9	6	ARG
58	s9	7	THR
58	s9	10	LYS
58	s9	17	ARG
58	s9	28	LEU
58	s9	33	GLU
58	s9	39	LYS
58	s9	49	LEU
58	s9	82	ARG
58	s9	93	LEU
58	s9	101	VAL
58	s9	109	LEU
58	s9	132	ARG
58	s9	134	ILE
58	s9	161	THR
58	s9	168	ARG
58	s9	172	VAL
58	s9	179	ARG
58	s9	180	LYS
58	s9	182	GLU
59	c0	3	MET
59	c0	15	LEU
59	c0	20	VAL
59	c0	28	ASN
59	c0	55	VAL
59	c0	71	GLU
60	c1	5	LEU
60	c1	6	THR
60	c1	8	GLN
60	c1	10	GLU

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Mol	Chain	Res	Type
60	c1	26	LYS
60	c1	27	THR
60	c1	31	THR
60	c1	40	LEU
60	c1	44	THR
60	c1	47	THR
60	c1	60	PHE
60	c1	67	ARG
60	c1	74	THR
60	c1	76	VAL
60	c1	83	THR
60	c1	109	VAL
60	c1	123	VAL
60	c1	129	ARG
60	c1	140	VAL
61	c2	28	LEU
61	c2	45	LEU
61	c2	52	LEU
61	c2	53	THR
61	c2	54	ARG
61	c2	58	LEU
61	c2	59	LEU
61	c2	61	VAL
61	c2	62	LEU
61	c2	71	ILE
61	c2	81	ASP
61	c2	83	GLU
61	c2	86	VAL
61	c2	89	ILE
61	c2	103	LEU
61	c2	131	ASP
61	c2	132	GLU
61	c2	133	LEU
61	c2	137	MET
61	c2	140	PHE
62	c3	6	SER
62	c3	12	SER
62	c3	14	SER
62	c3	16	ILE
62	c3	30	SER
62	c3	66	ILE
62	c3	76	LYS

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Mol	Chain	Res	Type
62	c3	80	LEU
62	c3	87	ASP
62	c3	102	LEU
62	c3	105	ASN
62	c3	115	LEU
62	c3	125	LEU
62	c3	127	ARG
62	c3	134	VAL
62	c3	138	ASN
62	c3	139	TRP
63	c4	20	TYR
63	c4	33	LEU
63	c4	51	ASP
63	c4	79	VAL
63	c4	81	VAL
63	c4	102	LEU
63	c4	107	ARG
63	c4	114	ARG
63	c4	118	VAL
63	c4	119	THR
63	c4	124	ASP
63	c4	133	ARG
63	c4	136	ARG
63	c4	137	LEU
64	c5	12	PHE
64	c5	27	GLU
64	c5	36	LEU
64	c5	40	ARG
64	c5	51	SER
64	c5	69	GLU
64	c5	110	GLU
64	c5	122	THR
64	c5	127	ARG
65	c6	17	THR
65	c6	23	LYS
65	c6	26	LYS
65	c6	28	LEU
65	c6	43	ILE
65	c6	48	VAL
65	c6	53	LEU
65	c6	54	LEU
65	c6	55	VAL

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Mol	Chain	Res	Type
65	c6	57	LEU
65	c6	68	ARG
65	c6	69	VAL
65	c6	110	THR
65	c6	113	ASP
65	c6	127	LYS
65	c6	137	ARG
82	c7	8	THR
82	c7	29	GLN
82	c7	34	LEU
82	c7	45	ARG
82	c7	46	LEU
82	c7	72	LYS
82	c7	83	GLN
82	c7	85	VAL
82	c7	104	ASN
82	c7	105	GLN
67	c8	4	VAL
67	c8	5	VAL
67	c8	6	GLN
67	c8	15	LEU
67	c8	25	ASN
67	c8	40	ARG
67	c8	61	LEU
67	c8	63	GLN
67	c8	85	PHE
67	c8	92	ILE
67	c8	94	ASP
67	c8	105	VAL
67	c8	116	LEU
67	c8	136	GLN
67	c8	138	THR
67	c8	143	ARG
67	c8	145	ARG
68	c9	6	VAL
68	c9	28	LEU
68	c9	57	ARG
68	c9	68	ARG
68	c9	71	VAL
68	c9	123	ARG
68	c9	131	ASP
68	c9	135	ILE

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Mol	Chain	Res	Type
68	c9	140	LEU
68	c9	142	GLU
69	d0	18	GLN
69	d0	23	ARG
69	d0	27	THR
69	d0	30	LYS
69	d0	34	LEU
69	d0	51	VAL
69	d0	57	ARG
69	d0	60	THR
69	d0	67	THR
69	d0	70	THR
69	d0	74	GLU
69	d0	103	ILE
69	d0	107	THR
69	d0	108	ILE
70	d1	2	GLU
70	d1	5	LYS
70	d1	11	LEU
70	d1	12	TYR
70	d1	32	VAL
70	d1	41	GLU
70	d1	44	ARG
70	d1	50	TYR
70	d1	52	THR
70	d1	68	SER
70	d1	78	LEU
71	d2	6	VAL
71	d2	7	LEU
71	d2	15	ASN
71	d2	23	ARG
71	d2	25	VAL
71	d2	26	LEU
71	d2	31	SER
71	d2	55	ASP
71	d2	65	LEU
71	d2	98	GLN
71	d2	103	ILE
72	d3	9	LEU
72	d3	16	ARG
72	d3	19	ARG
72	d3	23	ARG

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Mol	Chain	Res	Type
72	d3	40	SER
72	d3	55	GLU
72	d3	73	ARG
72	d3	84	THR
72	d3	96	VAL
72	d3	100	ASP
72	d3	103	LEU
72	d3	107	PHE
72	d3	121	ARG
73	d4	5	VAL
73	d4	26	ASP
73	d4	32	ARG
73	d4	43	LYS
73	d4	46	GLU
73	d4	47	VAL
73	d4	49	LYS
73	d4	52	LYS
73	d4	58	PHE
73	d4	62	THR
73	d4	88	THR
74	d5	51	LEU
74	d5	53	GLU
74	d5	57	TYR
74	d5	81	ARG
75	d6	11	ASN
75	d6	24	VAL
75	d6	53	LEU
75	d6	62	TYR
75	d6	82	ARG
75	d6	85	ARG
76	d7	3	LEU
76	d7	4	VAL
76	d7	43	ILE
76	d7	52	THR
76	d7	61	THR
76	d7	77	THR
76	d7	81	ARG
77	d8	16	LEU
77	d8	22	ARG
77	d8	32	PHE
77	d8	33	LEU
77	d8	48	VAL

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Mol	Chain	Res	Type
77	d8	64	ARG
78	d9	6	VAL
78	d9	19	ARG
78	d9	21	CYS
78	d9	23	VAL
78	d9	26	SER
78	d9	30	LEU
78	d9	32	ARG
78	d9	36	LEU
78	d9	53	ASN
78	d9	54	LYS
79	e0	4	VAL
79	e0	22	GLU
79	e0	26	LYS
79	e0	29	LYS
79	e0	39	LEU
79	e0	44	PHE
79	e0	46	ASN
79	e0	48	THR
79	e0	49	LEU
83	e1	103	LEU
83	e1	113	LYS
83	e1	120	GLU
83	e1	130	VAL
83	e1	135	HIS
83	e1	137	ASP
83	e1	147	VAL
83	e1	148	TYR
83	e1	150	VAL
83	e1	151	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
5	k	231	HIS
12	r	144	ASN
15	u	11	ASN
24	6	104	ASN
28	AA	29	HIS
11	CK	49	ASN
13	CM	95	ASN
22	CV	103	GLN

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Mol	Chain	Res	Type
29	DC	74	ASN
50	C	40	ASN
51	D	77	GLN
51	D	201	ASN
52	E	179	GLN
54	G	103	ASN
58	K	110	GLN
59	L	12	HIS
66	S	105	GLN
67	T	25	ASN
67	T	74	GLN
69	V	98	GLN
70	W	74	GLN
74	a	95	HIS
76	c	51	GLN
81	Rb	101	GLN
49	s0	32	HIS
50	s1	149	GLN
54	s5	104	ASN
56	s7	71	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3145/3149 (99%)	550 (17%)	62 (1%)
1	AR	3145/3149 (99%)	548 (17%)	63 (2%)
2	3	120/121 (99%)	14 (11%)	1 (0%)
2	AS	120/121 (99%)	14 (11%)	1 (0%)
3	4	157/158 (99%)	31 (19%)	3 (1%)
3	AT	157/158 (99%)	30 (19%)	3 (1%)
48	A	1778/1800 (98%)	417 (23%)	50 (2%)
48	sR	1780/1800 (98%)	372 (20%)	0
All	All	10402/10456 (99%)	1976 (18%)	183 (1%)

All (1976) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	26	A
1	1	40	A
1	1	49	A
1	1	59	G

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Mol	Chain	Res	Type
1	1	60	A
1	1	65	A
1	1	66	A
1	1	67	A
1	1	73	C
1	1	83	U
1	1	92	G
1	1	99	A
1	1	109	A
1	1	110	G
1	1	113	C
1	1	121	A
1	1	122	A
1	1	133	U
1	1	135	C
1	1	136	G
1	1	156	G
1	1	157	A
1	1	166	C
1	1	187	A
1	1	190	U
1	1	191	U
1	1	192	C
1	1	210	U
1	1	213	A
1	1	218	G
1	1	219	A
1	1	224	C
1	1	240	U
1	1	243	G
1	1	250	U
1	1	251	G
1	1	252	U
1	1	269	G
1	1	283	G
1	1	286	U
1	1	295	A
1	1	298	U
1	1	305	U
1	1	323	A
1	1	329	U
1	1	338	A

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Mol	Chain	Res	Type
1	1	339	C
1	1	349	A
1	1	350	C
1	1	351	A
1	1	352	A
1	1	376	G
1	1	398	A
1	1	399	A
1	1	401	U
1	1	402	A
1	1	403	C
1	1	421	G
1	1	422	A
1	1	438	A
1	1	439	C
1	1	440	A
1	1	495	G
1	1	498	A
1	1	507	U
1	1	520	U
1	1	521	A
1	1	535	G
1	1	544	C
1	1	546	C
1	1	547	G
1	1	548	G
1	1	551	A
1	1	552	G
1	1	555	U
1	1	557	A
1	1	558	U
1	1	559	A
1	1	578	A
1	1	579	G
1	1	592	A
1	1	604	G
1	1	607	A
1	1	609	G
1	1	611	A
1	1	619	A
1	1	620	U
1	1	621	A

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Mol	Chain	Res	Type
1	1	622	A
1	1	636	C
1	1	637	C
1	1	638	C
1	1	644	G
1	1	649	A
1	1	660	A
1	1	661	G
1	1	677	A
1	1	681	U
1	1	691	A
1	1	705	A
1	1	712	G
1	1	715	A
1	1	716	A
1	1	764	U
1	1	766	U
1	1	767	U
1	1	776	U
1	1	777	U
1	1	780	A
1	1	781	G
1	1	785	G
1	1	806	A
1	1	817	A
1	1	830	A
1	1	849	C
1	1	851	C
1	1	861	C
1	1	874	U
1	1	879	U
1	1	890	C
1	1	896	A
1	1	907	G
1	1	908	G
1	1	914	A
1	1	916	G
1	1	917	A
1	1	923	C
1	1	924	G
1	1	937	G
1	1	944	C

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Mol	Chain	Res	Type
1	1	959	C
1	1	960	U
1	1	974	G
1	1	979	U
1	1	980	A
1	1	981	U
1	1	982	C
1	1	994	G
1	1	1000	C
1	1	1001	G
1	1	1002	A
1	1	1006	A
1	1	1010	G
1	1	1017	C
1	1	1018	G
1	1	1020	G
1	1	1021	G
1	1	1024	G
1	1	1025	A
1	1	1029	G
1	1	1036	A
1	1	1047	A
1	1	1049	C
1	1	1063	G
1	1	1064	A
1	1	1065	A
1	1	1072	G
1	1	1079	A
1	1	1081	U
1	1	1082	U
1	1	1083	G
1	1	1093	A
1	1	1094	U
1	1	1095	U
1	1	1097	G
1	1	1098	A
1	1	1103	A
1	1	1104	G
1	1	1117	G
1	1	1131	G
1	1	1153	A
1	1	1159	A

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Mol	Chain	Res	Type
1	1	1160	C
1	1	1180	A
1	1	1181	U
1	1	1182	A
1	1	1185	C
1	1	1190	A
1	1	1191	U
1	1	1192	C
1	1	1201	C
1	1	1209	G
1	1	1216	C
1	1	1217	A
1	1	1222	G
1	1	1225	A
1	1	1227	C
1	1	1232	C
1	1	1233	G
1	1	1235	U
1	1	1236	G
1	1	1237	G
1	1	1239	C
1	1	1241	U
1	1	1243	G
1	1	1245	A
1	1	1246	G
1	1	1248	C
1	1	1249	G
1	1	1258	U
1	1	1262	G
1	1	1263	A
1	1	1264	G
1	1	1266	G
1	1	1269	U
1	1	1270	A
1	1	1271	A
1	1	1274	A
1	1	1278	A
1	1	1279	C
1	1	1285	G
1	1	1286	A
1	1	1287	A
1	1	1292	C

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Mol	Chain	Res	Type
1	1	1307	G
1	1	1308	A
1	1	1309	U
1	1	1313	G
1	1	1330	A
1	1	1333	C
1	1	1348	U
1	1	1349	G
1	1	1351	U
1	1	1352	A
1	1	1353	U
1	1	1355	A
1	1	1356	U
1	1	1357	G
1	1	1380	G
1	1	1386	A
1	1	1399	A
1	1	1400	G
1	1	1418	A
1	1	1419	A
1	1	1425	U
1	1	1433	A
1	1	1434	G
1	1	1437	C
1	1	1446	A
1	1	1450	G
1	1	1481	A
1	1	1482	A
1	1	1484	U
1	1	1485	G
1	1	1503	A
1	1	1508	C
1	1	1527	C
1	1	1536	G
1	1	1556	C
1	1	1560	G
1	1	1561	G
1	1	1562	C
1	1	1563	C
1	1	1564	U
1	1	1566	A
1	1	1567	U

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Mol	Chain	Res	Type
1	1	1568	U
1	1	1569	U
1	1	1570	U
1	1	1576	G
1	1	1580	A
1	1	1582	C
1	1	1583	A
1	1	1587	A
1	1	1589	A
1	1	1593	A
1	1	1605	A
1	1	1607	U
1	1	1620	U
1	1	1629	U
1	1	1643	A
1	1	1657	C
1	1	1683	A
1	1	1716	U
1	1	1717	U
1	1	1724	U
1	1	1725	C
1	1	1736	G
1	1	1741	A
1	1	1742	U
1	1	1750	A
1	1	1751	G
1	1	1760	A
1	1	1762	C
1	1	1765	U
1	1	1766	G
1	1	1769	G
1	1	1770	G
1	1	1780	G
1	1	1797	A
1	1	1810	A
1	1	1812	G
1	1	1814	A
1	1	1815	U
1	1	1816	A
1	1	1817	G
1	1	1819	U
1	1	1820	U

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Mol	Chain	Res	Type
1	1	1821	U
1	1	1835	A
1	1	1839	A
1	1	1842	A
1	1	1845	G
1	1	1846	C
1	1	1849	C
1	1	1850	A
1	1	1866	C
1	1	1871	U
1	1	1879	A
1	1	1906	G
1	1	1948	G
1	1	1951	C
1	1	1952	G
1	1	1954	G
1	1	2094	C
1	1	2101	C
1	1	2102	U
1	1	2111	G
1	1	2112	U
1	1	2113	A
1	1	2114	C
1	1	2121	G
1	1	2122	G
1	1	2131	A
1	1	2140	U
1	1	2158	A
1	1	2169	G
1	1	2177	G
1	1	2188	A
1	1	2192	C
1	1	2205	U
1	1	2208	A
1	1	2210	G
1	1	2223	A
1	1	2225	U
1	1	2228	A
1	1	2244	A
1	1	2249	G
1	1	2250	G
1	1	2255	A

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Mol	Chain	Res	Type
1	1	2256	A
1	1	2272	G
1	1	2273	G
1	1	2279	A
1	1	2281	A
1	1	2282	U
1	1	2288	G
1	1	2307	G
1	1	2310	U
1	1	2313	A
1	1	2314	U
1	1	2315	G
1	1	2334	U
1	1	2336	U
1	1	2373	A
1	1	2374	C
1	1	2375	G
1	1	2385	G
1	1	2388	U
1	1	2393	G
1	1	2397	A
1	1	2401	A
1	1	2402	A
1	1	2403	G
1	1	2411	U
1	1	2418	G
1	1	2419	A
1	1	2435	G
1	1	2444	C
1	1	2445	A
1	1	2502	A
1	1	2503	G
1	1	2514	U
1	1	2515	A
1	1	2522	G
1	1	2523	A
1	1	2532	U
1	1	2533	G
1	1	2537	U
1	1	2538	U
1	1	2539	C
1	1	2540	A

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Mol	Chain	Res	Type
1	1	2541	U
1	1	2542	U
1	1	2543	U
1	1	2547	A
1	1	2548	C
1	1	2549	G
1	1	2551	U
1	1	2552	C
1	1	2555	G
1	1	2561	A
1	1	2568	C
1	1	2569	A
1	1	2570	U
1	1	2571	U
1	1	2572	C
1	1	2573	G
1	1	2581	U
1	1	2585	G
1	1	2593	A
1	1	2594	C
1	1	2606	G
1	1	2607	G
1	1	2614	G
1	1	2637	A
1	1	2652	U
1	1	2656	A
1	1	2672	G
1	1	2674	A
1	1	2677	G
1	1	2689	A
1	1	2691	A
1	1	2694	A
1	1	2696	A
1	1	2705	A
1	1	2714	G
1	1	2728	G
1	1	2729	U
1	1	2752	U
1	1	2753	G
1	1	2755	C
1	1	2762	A
1	1	2772	C

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Mol	Chain	Res	Type
1	1	2777	G
1	1	2778	G
1	1	2779	A
1	1	2796	G
1	1	2799	A
1	1	2800	G
1	1	2801	A
1	1	2802	A
1	1	2810	C
1	1	2814	G
1	1	2816	G
1	1	2817	A
1	1	2818	U
1	1	2842	U
1	1	2843	U
1	1	2845	A
1	1	2849	C
1	1	2860	U
1	1	2867	C
1	1	2871	G
1	1	2872	A
1	1	2875	U
1	1	2876	C
1	1	2887	A
1	1	2889	C
1	1	2896	A
1	1	2897	A
1	1	2898	G
1	1	2899	C
1	1	2910	A
1	1	2914	G
1	1	2923	U
1	1	2935	U
1	1	2936	A
1	1	2942	C
1	1	2947	G
1	1	2954	U
1	1	2971	A
1	1	2983	C
1	1	2990	G
1	1	2996	U
1	1	2997	G

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Mol	Chain	Res	Type
1	1	3012	A
1	1	3057	U
1	1	3059	G
1	1	3078	U
1	1	3079	U
1	1	3086	A
1	1	3087	A
1	1	3092	C
1	1	3113	A
1	1	3119	U
1	1	3122	A
1	1	3130	A
1	1	3131	U
1	1	3142	A
1	1	3143	C
1	1	3151	U
1	1	3153	U
1	1	3154	C
1	1	3155	U
1	1	3156	U
1	1	3157	U
1	1	3164	C
1	1	3165	A
1	1	3168	A
1	1	3170	A
1	1	3171	U
1	1	3173	G
1	1	3174	A
1	1	3176	G
1	1	3179	U
1	1	3181	C
1	1	3187	A
1	1	3196	U
1	1	3199	G
1	1	3207	U
1	1	3210	A
1	1	3217	C
1	1	3218	A
1	1	3219	G
1	1	3228	C
1	1	3229	G
1	1	3243	A

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Mol	Chain	Res	Type
1	1	3245	A
1	1	3246	G
1	1	3247	G
1	1	3259	U
1	1	3269	U
1	1	3270	U
1	1	3272	C
1	1	3276	G
1	1	3281	U
1	1	3286	G
1	1	3287	U
1	1	3288	G
1	1	3289	G
1	1	3294	A
1	1	3295	A
1	1	3304	U
1	1	3313	U
1	1	3316	A
1	1	3317	U
1	1	3318	G
1	1	3319	U
1	1	3320	A
1	1	3341	U
1	1	3342	A
1	1	3345	G
1	1	3347	A
1	1	3350	C
1	1	3351	U
1	1	3352	U
1	1	3353	G
1	1	3354	U
1	1	3355	U
1	1	3356	G
1	1	3369	G
1	1	3375	A
1	1	3376	A
1	1	3378	C
1	1	3382	U
1	1	3383	G
1	1	3389	U
1	1	3390	G
1	1	3396	U

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Mol	Chain	Res	Type
2	3	7	G
2	3	13	A
2	3	14	U
2	3	22	A
2	3	26	C
2	3	54	U
2	3	65	G
2	3	73	C
2	3	74	C
2	3	76	A
2	3	95	A
2	3	102	A
2	3	112	G
2	3	121	U
3	4	2	A
3	4	34	U
3	4	35	C
3	4	48	A
3	4	52	A
3	4	53	A
3	4	59	A
3	4	62	C
3	4	63	G
3	4	79	A
3	4	80	A
3	4	81	U
3	4	82	U
3	4	83	C
3	4	86	U
3	4	87	G
3	4	90	U
3	4	95	G
3	4	104	A
3	4	105	A
3	4	106	C
3	4	111	A
3	4	113	U
3	4	125	U
3	4	126	A
3	4	128	U
3	4	138	A
3	4	148	G

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Mol	Chain	Res	Type
3	4	152	G
3	4	155	A
3	4	158	U
1	AR	24	G
1	AR	26	A
1	AR	40	A
1	AR	49	A
1	AR	59	G
1	AR	60	A
1	AR	65	A
1	AR	66	A
1	AR	76	G
1	AR	83	U
1	AR	92	G
1	AR	99	A
1	AR	109	A
1	AR	110	G
1	AR	111	C
1	AR	116	A
1	AR	121	A
1	AR	122	A
1	AR	133	U
1	AR	135	C
1	AR	136	G
1	AR	156	G
1	AR	157	A
1	AR	165	A
1	AR	166	C
1	AR	172	G
1	AR	173	G
1	AR	174	C
1	AR	180	C
1	AR	187	A
1	AR	190	U
1	AR	191	U
1	AR	192	C
1	AR	210	U
1	AR	211	A
1	AR	218	G
1	AR	219	A
1	AR	231	G
1	AR	234	G

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Mol	Chain	Res	Type
1	AR	240	U
1	AR	241	G
1	AR	243	G
1	AR	249	U
1	AR	250	U
1	AR	251	G
1	AR	252	U
1	AR	269	G
1	AR	286	U
1	AR	295	A
1	AR	298	U
1	AR	315	C
1	AR	323	A
1	AR	329	U
1	AR	339	C
1	AR	349	A
1	AR	350	C
1	AR	351	A
1	AR	370	U
1	AR	375	A
1	AR	376	G
1	AR	398	A
1	AR	401	U
1	AR	402	A
1	AR	403	C
1	AR	421	G
1	AR	422	A
1	AR	436	A
1	AR	439	C
1	AR	440	A
1	AR	495	G
1	AR	521	A
1	AR	535	G
1	AR	543	C
1	AR	544	C
1	AR	546	C
1	AR	547	G
1	AR	548	G
1	AR	551	A
1	AR	552	G
1	AR	555	U
1	AR	557	A

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Mol	Chain	Res	Type
1	AR	559	A
1	AR	578	A
1	AR	579	G
1	AR	592	A
1	AR	600	G
1	AR	604	G
1	AR	609	G
1	AR	611	A
1	AR	620	U
1	AR	621	A
1	AR	622	A
1	AR	636	C
1	AR	649	A
1	AR	660	A
1	AR	677	A
1	AR	681	U
1	AR	691	A
1	AR	705	A
1	AR	712	G
1	AR	715	A
1	AR	716	A
1	AR	726	G
1	AR	727	G
1	AR	764	U
1	AR	765	C
1	AR	766	U
1	AR	767	U
1	AR	776	U
1	AR	777	U
1	AR	781	G
1	AR	785	G
1	AR	806	A
1	AR	817	A
1	AR	830	A
1	AR	849	C
1	AR	861	C
1	AR	871	U
1	AR	874	U
1	AR	879	U
1	AR	896	A
1	AR	897	U
1	AR	907	G

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Mol	Chain	Res	Type
1	AR	908	G
1	AR	910	G
1	AR	914	A
1	AR	916	G
1	AR	917	A
1	AR	921	A
1	AR	923	C
1	AR	924	G
1	AR	937	G
1	AR	944	C
1	AR	959	C
1	AR	960	U
1	AR	974	G
1	AR	979	U
1	AR	980	A
1	AR	981	U
1	AR	982	C
1	AR	994	G
1	AR	1001	G
1	AR	1002	A
1	AR	1003	A
1	AR	1010	G
1	AR	1017	C
1	AR	1018	G
1	AR	1020	G
1	AR	1021	G
1	AR	1024	G
1	AR	1029	G
1	AR	1036	A
1	AR	1037	C
1	AR	1047	A
1	AR	1049	C
1	AR	1052	U
1	AR	1064	A
1	AR	1065	A
1	AR	1071	U
1	AR	1072	G
1	AR	1081	U
1	AR	1082	U
1	AR	1093	A
1	AR	1094	U
1	AR	1095	U

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Mol	Chain	Res	Type
1	AR	1096	U
1	AR	1097	G
1	AR	1098	A
1	AR	1103	A
1	AR	1104	G
1	AR	1117	G
1	AR	1131	G
1	AR	1152	G
1	AR	1153	A
1	AR	1159	A
1	AR	1160	C
1	AR	1180	A
1	AR	1181	U
1	AR	1182	A
1	AR	1191	U
1	AR	1192	C
1	AR	1201	C
1	AR	1202	A
1	AR	1209	G
1	AR	1217	A
1	AR	1222	G
1	AR	1235	U
1	AR	1236	G
1	AR	1237	G
1	AR	1239	C
1	AR	1241	U
1	AR	1242	G
1	AR	1245	A
1	AR	1246	G
1	AR	1258	U
1	AR	1262	G
1	AR	1263	A
1	AR	1264	G
1	AR	1265	U
1	AR	1266	G
1	AR	1285	G
1	AR	1292	C
1	AR	1307	G
1	AR	1309	U
1	AR	1313	G
1	AR	1330	A
1	AR	1331	U

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Mol	Chain	Res	Type
1	AR	1345	G
1	AR	1348	U
1	AR	1349	G
1	AR	1351	U
1	AR	1352	A
1	AR	1353	U
1	AR	1356	U
1	AR	1357	G
1	AR	1380	G
1	AR	1385	C
1	AR	1386	A
1	AR	1399	A
1	AR	1400	G
1	AR	1418	A
1	AR	1419	A
1	AR	1421	G
1	AR	1431	G
1	AR	1434	G
1	AR	1437	C
1	AR	1446	A
1	AR	1450	G
1	AR	1481	A
1	AR	1482	A
1	AR	1490	A
1	AR	1496	C
1	AR	1502	C
1	AR	1508	C
1	AR	1536	G
1	AR	1539	A
1	AR	1555	U
1	AR	1556	C
1	AR	1560	G
1	AR	1561	G
1	AR	1562	C
1	AR	1563	C
1	AR	1564	U
1	AR	1566	A
1	AR	1567	U
1	AR	1568	U
1	AR	1569	U
1	AR	1570	U
1	AR	1572	U

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Mol	Chain	Res	Type
1	AR	1576	G
1	AR	1578	C
1	AR	1579	C
1	AR	1580	A
1	AR	1581	C
1	AR	1582	C
1	AR	1583	A
1	AR	1587	A
1	AR	1589	A
1	AR	1593	A
1	AR	1620	U
1	AR	1629	U
1	AR	1639	C
1	AR	1643	A
1	AR	1645	U
1	AR	1657	C
1	AR	1658	G
1	AR	1683	A
1	AR	1716	U
1	AR	1717	U
1	AR	1724	U
1	AR	1725	C
1	AR	1735	G
1	AR	1736	G
1	AR	1741	A
1	AR	1742	U
1	AR	1750	A
1	AR	1751	G
1	AR	1760	A
1	AR	1761	C
1	AR	1762	C
1	AR	1765	U
1	AR	1766	G
1	AR	1770	G
1	AR	1780	G
1	AR	1797	A
1	AR	1810	A
1	AR	1814	A
1	AR	1816	A
1	AR	1817	G
1	AR	1819	U
1	AR	1820	U

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Mol	Chain	Res	Type
1	AR	1821	U
1	AR	1839	A
1	AR	1841	A
1	AR	1842	A
1	AR	1846	C
1	AR	1849	C
1	AR	1850	A
1	AR	1871	U
1	AR	1879	A
1	AR	1893	A
1	AR	1895	A
1	AR	1906	G
1	AR	1908	A
1	AR	1952	G
1	AR	1953	G
1	AR	1954	G
1	AR	2094	C
1	AR	2101	C
1	AR	2102	U
1	AR	2111	G
1	AR	2112	U
1	AR	2113	A
1	AR	2114	C
1	AR	2121	G
1	AR	2122	G
1	AR	2131	A
1	AR	2158	A
1	AR	2169	G
1	AR	2198	A
1	AR	2205	U
1	AR	2210	G
1	AR	2223	A
1	AR	2225	U
1	AR	2228	A
1	AR	2244	A
1	AR	2252	A
1	AR	2253	G
1	AR	2254	U
1	AR	2255	A
1	AR	2256	A
1	AR	2261	G
1	AR	2264	U

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Mol	Chain	Res	Type
1	AR	2269	U
1	AR	2270	A
1	AR	2271	A
1	AR	2273	G
1	AR	2279	A
1	AR	2282	U
1	AR	2288	G
1	AR	2298	U
1	AR	2307	G
1	AR	2310	U
1	AR	2313	A
1	AR	2314	U
1	AR	2315	G
1	AR	2334	U
1	AR	2335	G
1	AR	2336	U
1	AR	2373	A
1	AR	2374	C
1	AR	2375	G
1	AR	2385	G
1	AR	2393	G
1	AR	2394	G
1	AR	2397	A
1	AR	2401	A
1	AR	2402	A
1	AR	2403	G
1	AR	2404	A
1	AR	2405	C
1	AR	2411	U
1	AR	2418	G
1	AR	2419	A
1	AR	2443	A
1	AR	2444	C
1	AR	2445	A
1	AR	2502	A
1	AR	2503	G
1	AR	2504	U
1	AR	2508	U
1	AR	2514	U
1	AR	2515	A
1	AR	2522	G
1	AR	2523	A

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Mol	Chain	Res	Type
1	AR	2531	C
1	AR	2532	U
1	AR	2533	G
1	AR	2538	U
1	AR	2539	C
1	AR	2540	A
1	AR	2541	U
1	AR	2542	U
1	AR	2543	U
1	AR	2544	U
1	AR	2547	A
1	AR	2549	G
1	AR	2552	C
1	AR	2555	G
1	AR	2561	A
1	AR	2568	C
1	AR	2569	A
1	AR	2570	U
1	AR	2571	U
1	AR	2572	C
1	AR	2573	G
1	AR	2581	U
1	AR	2585	G
1	AR	2587	U
1	AR	2593	A
1	AR	2594	C
1	AR	2595	A
1	AR	2606	G
1	AR	2607	G
1	AR	2614	G
1	AR	2637	A
1	AR	2639	G
1	AR	2652	U
1	AR	2656	A
1	AR	2674	A
1	AR	2677	G
1	AR	2681	U
1	AR	2689	A
1	AR	2690	G
1	AR	2691	A
1	AR	2694	A
1	AR	2696	A

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Mol	Chain	Res	Type
1	AR	2714	G
1	AR	2728	G
1	AR	2729	U
1	AR	2752	U
1	AR	2753	G
1	AR	2755	C
1	AR	2762	A
1	AR	2771	U
1	AR	2772	C
1	AR	2777	G
1	AR	2778	G
1	AR	2779	A
1	AR	2796	G
1	AR	2799	A
1	AR	2800	G
1	AR	2801	A
1	AR	2802	A
1	AR	2810	C
1	AR	2817	A
1	AR	2818	U
1	AR	2842	U
1	AR	2843	U
1	AR	2845	A
1	AR	2860	U
1	AR	2861	U
1	AR	2871	G
1	AR	2872	A
1	AR	2873	U
1	AR	2875	U
1	AR	2887	A
1	AR	2889	C
1	AR	2896	A
1	AR	2899	C
1	AR	2923	U
1	AR	2928	C
1	AR	2935	U
1	AR	2936	A
1	AR	2942	C
1	AR	2947	G
1	AR	2957	G
1	AR	2971	A
1	AR	2983	C

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Mol	Chain	Res	Type
1	AR	2990	G
1	AR	2992	U
1	AR	2996	U
1	AR	2997	G
1	AR	3012	A
1	AR	3028	G
1	AR	3033	A
1	AR	3056	U
1	AR	3057	U
1	AR	3059	G
1	AR	3078	U
1	AR	3079	U
1	AR	3086	A
1	AR	3087	A
1	AR	3092	C
1	AR	3119	U
1	AR	3122	A
1	AR	3130	A
1	AR	3131	U
1	AR	3142	A
1	AR	3143	C
1	AR	3151	U
1	AR	3153	U
1	AR	3154	C
1	AR	3155	U
1	AR	3156	U
1	AR	3157	U
1	AR	3164	C
1	AR	3165	A
1	AR	3167	A
1	AR	3173	G
1	AR	3174	A
1	AR	3176	G
1	AR	3179	U
1	AR	3181	C
1	AR	3187	A
1	AR	3195	U
1	AR	3197	G
1	AR	3199	G
1	AR	3207	U
1	AR	3209	A
1	AR	3217	C

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Mol	Chain	Res	Type
1	AR	3218	A
1	AR	3219	G
1	AR	3223	A
1	AR	3224	G
1	AR	3228	C
1	AR	3229	G
1	AR	3243	A
1	AR	3245	A
1	AR	3246	G
1	AR	3247	G
1	AR	3253	G
1	AR	3259	U
1	AR	3265	C
1	AR	3270	U
1	AR	3276	G
1	AR	3281	U
1	AR	3286	G
1	AR	3287	U
1	AR	3289	G
1	AR	3294	A
1	AR	3295	A
1	AR	3304	U
1	AR	3316	A
1	AR	3317	U
1	AR	3318	G
1	AR	3319	U
1	AR	3320	A
1	AR	3341	U
1	AR	3342	A
1	AR	3345	G
1	AR	3347	A
1	AR	3350	C
1	AR	3351	U
1	AR	3352	U
1	AR	3353	G
1	AR	3355	U
1	AR	3356	G
1	AR	3359	A
1	AR	3360	C
1	AR	3369	G
1	AR	3375	A
1	AR	3376	A

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Mol	Chain	Res	Type
1	AR	3378	C
1	AR	3383	G
1	AR	3389	U
1	AR	3390	G
1	AR	3396	U
2	AS	7	G
2	AS	22	A
2	AS	52	G
2	AS	53	U
2	AS	54	U
2	AS	55	A
2	AS	65	G
2	AS	73	C
2	AS	74	C
2	AS	95	A
2	AS	101	G
2	AS	102	A
2	AS	112	G
2	AS	121	U
3	AT	34	U
3	AT	35	C
3	AT	48	A
3	AT	51	G
3	AT	53	A
3	AT	59	A
3	AT	62	C
3	AT	63	G
3	AT	79	A
3	AT	80	A
3	AT	81	U
3	AT	82	U
3	AT	83	C
3	AT	84	C
3	AT	85	G
3	AT	86	U
3	AT	87	G
3	AT	90	U
3	AT	95	G
3	AT	104	A
3	AT	105	A
3	AT	106	C
3	AT	111	A

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Mol	Chain	Res	Type
3	AT	113	U
3	AT	125	U
3	AT	126	A
3	AT	151	C
3	AT	152	G
3	AT	155	A
3	AT	158	U
48	A	2	A
48	A	4	C
48	A	17	C
48	A	25	C
48	A	26	A
48	A	27	U
48	A	34	G
48	A	42	G
48	A	45	U
48	A	47	A
48	A	57	G
48	A	60	U
48	A	67	A
48	A	68	A
48	A	69	G
48	A	72	A
48	A	73	U
48	A	74	U
48	A	75	U
48	A	77	U
48	A	104	A
48	A	114	C
48	A	131	C
48	A	132	U
48	A	133	U
48	A	134	U
48	A	135	A
48	A	136	C
48	A	137	U
48	A	140	A
48	A	141	U
48	A	144	U
48	A	145	A
48	A	146	U
48	A	153	G

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Mol	Chain	Res	Type
48	A	158	U
48	A	159	U
48	A	176	C
48	A	178	U
48	A	179	A
48	A	185	U
48	A	186	C
48	A	187	G
48	A	188	A
48	A	190	C
48	A	191	C
48	A	192	U
48	A	193	U
48	A	194	U
48	A	195	G
48	A	196	G
48	A	197	A
48	A	200	A
48	A	215	A
48	A	217	A
48	A	218	A
48	A	219	A
48	A	226	A
48	A	227	U
48	A	228	G
48	A	233	C
48	A	234	G
48	A	235	G
48	A	238	U
48	A	239	C
48	A	240	U
48	A	241	U
48	A	250	C
48	A	261	U
48	A	262	U
48	A	265	A
48	A	271	A
48	A	272	U
48	A	274	G
48	A	275	C
48	A	276	C
48	A	277	U

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Mol	Chain	Res	Type
48	A	278	U
48	A	279	G
48	A	280	U
48	A	281	G
48	A	288	A
48	A	290	G
48	A	299	A
48	A	308	C
48	A	314	C
48	A	316	A
48	A	319	U
48	A	321	C
48	A	337	G
48	A	338	C
48	A	352	A
48	A	359	A
48	A	360	A
48	A	361	C
48	A	397	A
48	A	400	A
48	A	402	C
48	A	403	G
48	A	404	G
48	A	416	A
48	A	418	G
48	A	419	G
48	A	424	C
48	A	425	A
48	A	426	G
48	A	428	A
48	A	434	G
48	A	439	U
48	A	444	C
48	A	448	C
48	A	468	A
48	A	470	A
48	A	477	A
48	A	480	G
48	A	484	C
48	A	485	A
48	A	488	G
48	A	493	U

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Mol	Chain	Res	Type
48	A	494	U
48	A	495	C
48	A	496	G
48	A	497	G
48	A	498	G
48	A	499	U
48	A	500	C
48	A	502	U
48	A	504	U
48	A	505	A
48	A	506	A
48	A	507	U
48	A	510	G
48	A	511	A
48	A	512	A
48	A	513	U
48	A	515	A
48	A	516	G
48	A	527	A
48	A	532	U
48	A	538	A
48	A	539	G
48	A	540	G
48	A	541	A
48	A	542	A
48	A	543	C
48	A	544	A
48	A	555	A
48	A	556	A
48	A	557	G
48	A	558	U
48	A	559	C
48	A	565	C
48	A	579	A
48	A	580	A
48	A	582	U
48	A	594	A
48	A	595	G
48	A	606	A
48	A	611	U
48	A	619	A
48	A	620	A

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Mol	Chain	Res	Type
48	A	622	A
48	A	623	A
48	A	639	U
48	A	640	U
48	A	650	U
48	A	653	C
48	A	654	C
48	A	656	G
48	A	658	C
48	A	677	G
48	A	679	U
48	A	680	U
48	A	682	C
48	A	684	A
48	A	685	A
48	A	686	C
48	A	694	U
48	A	696	C
48	A	697	C
48	A	700	C
48	A	702	G
48	A	703	G
48	A	704	C
48	A	705	U
48	A	706	A
48	A	707	A
48	A	709	C
48	A	710	U
48	A	712	G
48	A	713	A
48	A	714	G
48	A	717	C
48	A	718	U
48	A	719	U
48	A	720	G
48	A	721	U
48	A	722	G
48	A	723	G
48	A	725	U
48	A	727	U
48	A	728	U
48	A	730	G

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Mol	Chain	Res	Type
48	A	731	C
48	A	732	G
48	A	733	A
48	A	734	A
48	A	735	C
48	A	736	C
48	A	737	A
48	A	738	G
48	A	742	U
48	A	743	U
48	A	754	A
48	A	755	A
48	A	756	A
48	A	765	G
48	A	766	U
48	A	774	A
48	A	775	G
48	A	778	G
48	A	780	A
48	A	781	U
48	A	782	U
48	A	783	G
48	A	784	C
48	A	787	G
48	A	789	A
48	A	793	A
48	A	794	U
48	A	795	U
48	A	812	A
48	A	815	G
48	A	816	G
48	A	818	C
48	A	819	G
48	A	820	U
48	A	821	U
48	A	822	U
48	A	823	G
48	A	824	G
48	A	830	U
48	A	831	U
48	A	833	U
48	A	846	G

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Mol	Chain	Res	Type
48	A	856	A
48	A	863	A
48	A	864	U
48	A	886	U
48	A	898	A
48	A	912	U
48	A	913	G
48	A	914	G
48	A	915	A
48	A	933	A
48	A	935	U
48	A	942	G
48	A	951	A
48	A	960	U
48	A	966	A
48	A	988	A
48	A	992	A
48	A	993	A
48	A	997	G
48	A	1003	A
48	A	1004	U
48	A	1005	A
48	A	1020	A
48	A	1021	C
48	A	1026	A
48	A	1028	C
48	A	1039	A
48	A	1040	G
48	A	1052	U
48	A	1053	G
48	A	1058	U
48	A	1060	U
48	A	1061	A
48	A	1074	G
48	A	1079	U
48	A	1082	C
48	A	1086	A
48	A	1092	A
48	A	1093	A
48	A	1096	C
48	A	1097	U
48	A	1100	G

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Mol	Chain	Res	Type
48	A	1111	G
48	A	1138	A
48	A	1146	G
48	A	1150	G
48	A	1151	A
48	A	1157	A
48	A	1158	C
48	A	1160	A
48	A	1167	G
48	A	1185	U
48	A	1191	U
48	A	1194	A
48	A	1196	A
48	A	1197	C
48	A	1199	G
48	A	1200	G
48	A	1202	A
48	A	1207	C
48	A	1217	A
48	A	1218	G
48	A	1227	A
48	A	1228	G
48	A	1229	G
48	A	1244	A
48	A	1245	G
48	A	1250	U
48	A	1251	U
48	A	1257	U
48	A	1258	U
48	A	1286	U
48	A	1314	U
48	A	1315	U
48	A	1321	A
48	A	1324	G
48	A	1339	C
48	A	1340	U
48	A	1341	A
48	A	1344	A
48	A	1345	A
48	A	1357	A
48	A	1361	U
48	A	1362	U

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Mol	Chain	Res	Type
48	A	1363	U
48	A	1364	G
48	A	1370	U
48	A	1371	A
48	A	1390	U
48	A	1398	U
48	A	1399	C
48	A	1400	A
48	A	1412	G
48	A	1413	U
48	A	1415	U
48	A	1427	A
48	A	1428	G
48	A	1431	C
48	A	1446	A
48	A	1457	C
48	A	1458	G
48	A	1459	C
48	A	1461	C
48	A	1471	A
48	A	1473	U
48	A	1474	G
48	A	1475	A
48	A	1477	G
48	A	1482	C
48	A	1486	G
48	A	1487	A
48	A	1489	U
48	A	1490	C
48	A	1491	U
48	A	1492	A
48	A	1493	A
48	A	1506	G
48	A	1515	A
48	A	1516	A
48	A	1517	U
48	A	1521	G
48	A	1523	G
48	A	1524	A
48	A	1526	A
48	A	1535	U
48	A	1536	G

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Mol	Chain	Res	Type
48	A	1537	C
48	A	1538	U
48	A	1557	U
48	A	1559	A
48	A	1560	U
48	A	1569	A
48	A	1574	G
48	A	1584	G
48	A	1590	G
48	A	1601	G
48	A	1614	A
48	A	1616	G
48	A	1624	C
48	A	1626	U
48	A	1631	A
48	A	1635	A
48	A	1657	U
48	A	1658	G
48	A	1680	G
48	A	1683	C
48	A	1684	U
48	A	1686	C
48	A	1697	G
48	A	1698	G
48	A	1699	G
48	A	1700	C
48	A	1701	A
48	A	1702	A
48	A	1703	C
48	A	1711	C
48	A	1712	A
48	A	1713	G
48	A	1731	A
48	A	1756	A
48	A	1760	G
48	A	1762	A
48	A	1766	A
48	A	1769	U
48	A	1780	G
48	A	1782	A
48	A	1783	C
48	A	1792	G

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Mol	Chain	Res	Type
48	A	1793	G
48	A	1794	A
48	A	1795	U
48	A	1796	C
48	sR	2	A
48	sR	4	C
48	sR	17	C
48	sR	25	C
48	sR	26	A
48	sR	27	U
48	sR	34	G
48	sR	42	G
48	sR	44	U
48	sR	47	A
48	sR	57	G
48	sR	60	U
48	sR	61	A
48	sR	68	A
48	sR	69	G
48	sR	72	A
48	sR	73	U
48	sR	75	U
48	sR	76	A
48	sR	77	U
48	sR	104	A
48	sR	114	C
48	sR	116	U
48	sR	132	U
48	sR	137	U
48	sR	138	A
48	sR	140	A
48	sR	141	U
48	sR	144	U
48	sR	145	A
48	sR	146	U
48	sR	159	U
48	sR	166	C
48	sR	178	U
48	sR	185	U
48	sR	188	A
48	sR	190	C
48	sR	191	C

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Mol	Chain	Res	Type
48	sR	192	U
48	sR	193	U
48	sR	194	U
48	sR	195	G
48	sR	197	A
48	sR	200	A
48	sR	215	A
48	sR	216	U
48	sR	218	A
48	sR	219	A
48	sR	220	A
48	sR	227	U
48	sR	228	G
48	sR	230	C
48	sR	232	U
48	sR	233	C
48	sR	240	U
48	sR	241	U
48	sR	250	C
48	sR	261	U
48	sR	265	A
48	sR	271	A
48	sR	272	U
48	sR	273	G
48	sR	275	C
48	sR	277	U
48	sR	278	U
48	sR	280	U
48	sR	299	A
48	sR	308	C
48	sR	314	C
48	sR	316	A
48	sR	319	U
48	sR	321	C
48	sR	322	G
48	sR	333	A
48	sR	337	G
48	sR	338	C
48	sR	352	A
48	sR	359	A
48	sR	360	A
48	sR	361	C

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Mol	Chain	Res	Type
48	sR	381	C
48	sR	400	A
48	sR	401	A
48	sR	402	C
48	sR	404	G
48	sR	416	A
48	sR	418	G
48	sR	424	C
48	sR	425	A
48	sR	426	G
48	sR	434	G
48	sR	437	A
48	sR	439	U
48	sR	444	C
48	sR	445	A
48	sR	448	C
48	sR	454	U
48	sR	468	A
48	sR	477	A
48	sR	480	G
48	sR	486	G
48	sR	488	G
48	sR	489	C
48	sR	490	C
48	sR	492	A
48	sR	493	U
48	sR	494	U
48	sR	496	G
48	sR	497	G
48	sR	500	C
48	sR	501	U
48	sR	504	U
48	sR	505	A
48	sR	506	A
48	sR	507	U
48	sR	510	G
48	sR	511	A
48	sR	513	U
48	sR	519	C
48	sR	527	A
48	sR	538	A
48	sR	539	G

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Mol	Chain	Res	Type
48	sR	540	G
48	sR	541	A
48	sR	542	A
48	sR	543	C
48	sR	544	A
48	sR	548	G
48	sR	555	A
48	sR	557	G
48	sR	558	U
48	sR	559	C
48	sR	565	C
48	sR	566	C
48	sR	570	A
48	sR	574	G
48	sR	579	A
48	sR	580	A
48	sR	582	U
48	sR	594	A
48	sR	595	G
48	sR	611	U
48	sR	619	A
48	sR	620	A
48	sR	622	A
48	sR	623	A
48	sR	624	G
48	sR	639	U
48	sR	640	U
48	sR	650	U
48	sR	652	G
48	sR	653	C
48	sR	658	C
48	sR	676	G
48	sR	679	U
48	sR	680	U
48	sR	681	U
48	sR	682	C
48	sR	683	C
48	sR	684	A
48	sR	685	A
48	sR	691	C
48	sR	696	C
48	sR	709	C

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Mol	Chain	Res	Type
48	sR	710	U
48	sR	711	U
48	sR	714	G
48	sR	718	U
48	sR	719	U
48	sR	720	G
48	sR	721	U
48	sR	722	G
48	sR	723	G
48	sR	730	G
48	sR	742	U
48	sR	754	A
48	sR	755	A
48	sR	756	A
48	sR	765	G
48	sR	766	U
48	sR	774	A
48	sR	775	G
48	sR	780	A
48	sR	781	U
48	sR	782	U
48	sR	783	G
48	sR	787	G
48	sR	789	A
48	sR	793	A
48	sR	794	U
48	sR	811	A
48	sR	812	A
48	sR	815	G
48	sR	816	G
48	sR	821	U
48	sR	823	G
48	sR	825	U
48	sR	829	A
48	sR	830	U
48	sR	831	U
48	sR	832	U
48	sR	834	G
48	sR	835	U
48	sR	863	A
48	sR	873	U
48	sR	876	G

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Mol	Chain	Res	Type
48	sR	898	A
48	sR	906	A
48	sR	913	G
48	sR	914	G
48	sR	916	U
48	sR	933	A
48	sR	935	U
48	sR	942	G
48	sR	959	U
48	sR	960	U
48	sR	966	A
48	sR	970	A
48	sR	971	A
48	sR	992	A
48	sR	997	G
48	sR	1003	A
48	sR	1004	U
48	sR	1005	A
48	sR	1021	C
48	sR	1026	A
48	sR	1028	C
48	sR	1039	A
48	sR	1040	G
48	sR	1052	U
48	sR	1053	G
48	sR	1057	U
48	sR	1058	U
48	sR	1059	U
48	sR	1060	U
48	sR	1072	C
48	sR	1082	C
48	sR	1092	A
48	sR	1094	G
48	sR	1096	C
48	sR	1097	U
48	sR	1098	U
48	sR	1100	G
48	sR	1101	G
48	sR	1109	G
48	sR	1138	A
48	sR	1150	G
48	sR	1151	A

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Mol	Chain	Res	Type
48	sR	1155	G
48	sR	1158	C
48	sR	1159	C
48	sR	1160	A
48	sR	1167	G
48	sR	1185	U
48	sR	1194	A
48	sR	1196	A
48	sR	1197	C
48	sR	1199	G
48	sR	1200	G
48	sR	1202	A
48	sR	1208	A
48	sR	1217	A
48	sR	1218	G
48	sR	1225	U
48	sR	1226	A
48	sR	1228	G
48	sR	1229	G
48	sR	1230	A
48	sR	1241	G
48	sR	1243	G
48	sR	1244	A
48	sR	1245	G
48	sR	1246	C
48	sR	1255	G
48	sR	1256	A
48	sR	1257	U
48	sR	1258	U
48	sR	1259	U
48	sR	1286	U
48	sR	1288	G
48	sR	1291	G
48	sR	1314	U
48	sR	1315	U
48	sR	1316	G
48	sR	1321	A
48	sR	1341	A
48	sR	1344	A
48	sR	1345	A
48	sR	1346	A
48	sR	1354	G

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Mol	Chain	Res	Type
48	sR	1361	U
48	sR	1363	U
48	sR	1364	G
48	sR	1371	A
48	sR	1388	A
48	sR	1390	U
48	sR	1398	U
48	sR	1399	C
48	sR	1400	A
48	sR	1402	G
48	sR	1413	U
48	sR	1414	U
48	sR	1415	U
48	sR	1427	A
48	sR	1428	G
48	sR	1433	G
48	sR	1445	G
48	sR	1446	A
48	sR	1448	G
48	sR	1458	G
48	sR	1459	C
48	sR	1460	A
48	sR	1461	C
48	sR	1471	A
48	sR	1481	C
48	sR	1482	C
48	sR	1490	C
48	sR	1491	U
48	sR	1492	A
48	sR	1493	A
48	sR	1506	G
48	sR	1514	U
48	sR	1516	A
48	sR	1521	G
48	sR	1523	G
48	sR	1524	A
48	sR	1535	U
48	sR	1536	G
48	sR	1537	C
48	sR	1538	U
48	sR	1540	G
48	sR	1554	U

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Mol	Chain	Res	Type
48	sR	1557	U
48	sR	1559	A
48	sR	1569	A
48	sR	1573	A
48	sR	1574	G
48	sR	1575	G
48	sR	1584	G
48	sR	1590	G
48	sR	1601	G
48	sR	1616	G
48	sR	1621	U
48	sR	1622	G
48	sR	1634	C
48	sR	1656	U
48	sR	1657	U
48	sR	1658	G
48	sR	1698	G
48	sR	1699	G
48	sR	1700	C
48	sR	1701	A
48	sR	1702	A
48	sR	1703	C
48	sR	1710	U
48	sR	1712	A
48	sR	1716	C
48	sR	1717	G
48	sR	1731	A
48	sR	1760	G
48	sR	1766	A
48	sR	1767	G
48	sR	1769	U
48	sR	1780	G
48	sR	1782	A
48	sR	1783	C
48	sR	1792	G
48	sR	1793	G
48	sR	1794	A
48	sR	1796	C
48	sR	1799	U
48	sR	1800	A

All (183) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	43	A
1	1	65	A
1	1	223	U
1	1	239	G
1	1	282	G
1	1	547	G
1	1	588	G
1	1	594	U
1	1	637	C
1	1	715	A
1	1	763	G
1	1	873	C
1	1	916	G
1	1	979	U
1	1	981	U
1	1	993	G
1	1	1064	A
1	1	1094	U
1	1	1097	G
1	1	1103	A
1	1	1273	A
1	1	1307	G
1	1	1329	U
1	1	1331	U
1	1	1352	A
1	1	1355	A
1	1	1484	U
1	1	1562	C
1	1	1568	U
1	1	1589	A
1	1	1716	U
1	1	1816	A
1	1	1820	U
1	1	1841	A
1	1	2101	C
1	1	2112	U
1	1	2209	U
1	1	2227	C
1	1	2249	G
1	1	2418	G
1	1	2537	U
1	1	2541	U
1	1	2585	G

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Mol	Chain	Res	Type
1	1	2593	A
1	1	2728	G
1	1	2801	A
1	1	2818	U
1	1	2896	A
1	1	3056	U
1	1	3078	U
1	1	3121	U
1	1	3195	U
1	1	3217	C
1	1	3218	A
1	1	3228	C
1	1	3269	U
1	1	3275	U
1	1	3319	U
1	1	3350	C
1	1	3351	U
1	1	3353	G
1	1	3375	A
2	3	13	A
3	4	85	G
3	4	111	A
3	4	125	U
1	AR	43	A
1	AR	65	A
1	AR	210	U
1	AR	547	G
1	AR	588	G
1	AR	715	A
1	AR	763	G
1	AR	873	C
1	AR	896	A
1	AR	916	G
1	AR	979	U
1	AR	981	U
1	AR	993	G
1	AR	1064	A
1	AR	1097	G
1	AR	1103	A
1	AR	1238	C
1	AR	1241	U
1	AR	1284	C

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Mol	Chain	Res	Type
1	AR	1317	A
1	AR	1329	U
1	AR	1331	U
1	AR	1352	A
1	AR	1355	A
1	AR	1554	U
1	AR	1562	C
1	AR	1589	A
1	AR	1716	U
1	AR	1815	U
1	AR	1816	A
1	AR	1820	U
1	AR	1846	C
1	AR	2101	C
1	AR	2112	U
1	AR	2209	U
1	AR	2227	C
1	AR	2252	A
1	AR	2255	A
1	AR	2260	U
1	AR	2269	U
1	AR	2281	A
1	AR	2373	A
1	AR	2374	C
1	AR	2418	G
1	AR	2537	U
1	AR	2541	U
1	AR	2586	G
1	AR	2593	A
1	AR	2728	G
1	AR	2801	A
1	AR	2818	U
1	AR	2896	A
1	AR	3078	U
1	AR	3121	U
1	AR	3218	A
1	AR	3228	C
1	AR	3242	G
1	AR	3269	U
1	AR	3316	A
1	AR	3317	U
1	AR	3319	U

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Mol	Chain	Res	Type
1	AR	3350	C
1	AR	3375	A
2	AS	52	G
3	AT	82	U
3	AT	85	G
3	AT	125	U
48	A	25	C
48	A	45	U
48	A	68	A
48	A	73	U
48	A	130	C
48	A	131	C
48	A	139	C
48	A	158	U
48	A	187	G
48	A	218	A
48	A	240	U
48	A	278	U
48	A	280	U
48	A	417	A
48	A	497	G
48	A	499	U
48	A	501	U
48	A	503	G
48	A	510	G
48	A	512	A
48	A	555	A
48	A	558	U
48	A	685	A
48	A	704	C
48	A	720	G
48	A	721	U
48	A	755	A
48	A	781	U
48	A	782	U
48	A	811	A
48	A	829	A
48	A	913	G
48	A	1051	G
48	A	1081	A
48	A	1157	A
48	A	1196	A

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Mol	Chain	Res	Type
48	A	1226	A
48	A	1244	A
48	A	1250	U
48	A	1339	C
48	A	1344	A
48	A	1370	U
48	A	1481	C
48	A	1489	U
48	A	1568	C
48	A	1573	A
48	A	1615	C
48	A	1657	U
48	A	1698	G
48	A	1761	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2486 ligands modelled in this entry, 1 is modelled with single atom and 1410 are monoatomic - leaving 1075 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	$\# Z > 2$
84	OHX	A	1983	-	0,6,6	0.00	-	-		
84	OHX	1	3645	-	0,6,6	0.00	-	-		
84	OHX	AR	3587	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3438	-	0,6,6	0.00	-	-		
84	OHX	1	3705	84	0,6,6	0.00	-	-		
84	OHX	1	3427	-	0,6,6	0.00	-	-		
84	OHX	A	1993	-	0,6,6	0.00	-	-		
84	OHX	sR	1965	-	0,6,6	0.00	-	-		
84	OHX	AR	3476	-	0,6,6	0.00	-	-		
84	OHX	O	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3630	-	0,6,6	0.00	-	-		
84	OHX	1	3449	-	0,6,6	0.00	-	-		
84	OHX	A	1904	-	0,6,6	0.00	-	-		
84	OHX	A	1901	-	0,6,6	0.00	-	-		
84	OHX	1	3706	-	0,6,6	0.00	-	-		
84	OHX	1	3459	-	0,6,6	0.00	-	-		
84	OHX	1	3546	-	0,6,6	0.00	-	-		
84	OHX	1	3500	-	0,6,6	0.00	-	-		
84	OHX	h	401	-	0,6,6	0.00	-	-		
84	OHX	1	3547	-	0,6,6	0.00	-	-		
84	OHX	AR	3726	-	0,6,6	0.00	-	-		
84	OHX	AR	3680	-	0,6,6	0.00	-	-		
84	OHX	A	1936	-	0,6,6	0.00	-	-		
84	OHX	1	3493	-	0,6,6	0.00	-	-		
84	OHX	1	3644	-	0,6,6	0.00	-	-		
84	OHX	1	3589	-	0,6,6	0.00	-	-		
84	OHX	3	204	-	0,6,6	0.00	-	-		
84	OHX	AR	3710	-	0,6,6	0.00	-	-		
84	OHX	AR	3436	-	0,6,6	0.00	-	-		
84	OHX	AR	3558	-	0,6,6	0.00	-	-		
84	OHX	1	3447	-	0,6,6	0.00	-	-		
84	OHX	1	3620	-	0,6,6	0.00	-	-		
84	OHX	A	1922	-	0,6,6	0.00	-	-		
84	OHX	1	3628	-	0,6,6	0.00	-	-		
84	OHX	AR	3691	-	0,6,6	0.00	-	-		
84	OHX	1	3601	-	0,6,6	0.00	-	-		
84	OHX	AR	3730	-	0,6,6	0.00	-	-		
84	OHX	sR	1940	-	0,6,6	0.00	-	-		
84	OHX	sR	2040	-	0,6,6	0.00	-	-		
84	OHX	1	3487	-	0,6,6	0.00	-	-		
84	OHX	1	3498	-	0,6,6	0.00	-	-		
84	OHX	AR	3741	-	0,6,6	0.00	-	-		
84	OHX	sR	1984	-	0,6,6	0.00	-	-		
84	OHX	AR	3556	-	0,6,6	0.00	-	-		
84	OHX	1	3602	-	0,6,6	0.00	-	-		
84	OHX	AR	3422	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3503	-	0,6,6	0.00	-	-		
84	OHX	1	3456	-	0,6,6	0.00	-	-		
84	OHX	CX	202	-	0,6,6	0.00	-	-		
84	OHX	AT	206	-	0,6,6	0.00	-	-		
84	OHX	3	207	-	0,6,6	0.00	-	-		
84	OHX	1	3477	-	0,6,6	0.00	-	-		
84	OHX	1	3489	-	0,6,6	0.00	-	-		
84	OHX	1	3603	-	0,6,6	0.00	-	-		
84	OHX	A	2021	-	0,6,6	0.00	-	-		
84	OHX	AR	3543	-	0,6,6	0.00	-	-		
84	OHX	1	3414	-	0,6,6	0.00	-	-		
84	OHX	A	2020	-	0,6,6	0.00	-	-		
84	OHX	1	3436	-	0,6,6	0.00	-	-		
84	OHX	1	3615	-	0,6,6	0.00	-	-		
84	OHX	1	3709	-	0,6,6	0.00	-	-		
84	OHX	1	3692	-	0,6,6	0.00	-	-		
84	OHX	sR	2002	-	0,6,6	0.00	-	-		
84	OHX	CM	201	-	0,6,6	0.00	-	-		
84	OHX	sR	1960	-	0,6,6	0.00	-	-		
84	OHX	AR	3438	-	0,6,6	0.00	-	-		
84	OHX	1	3496	-	0,6,6	0.00	-	-		
84	OHX	AR	3504	-	0,6,6	0.00	-	-		
84	OHX	1	3418	-	0,6,6	0.00	-	-		
84	OHX	1	3452	-	0,6,6	0.00	-	-		
84	OHX	1	3529	-	0,6,6	0.00	-	-		
84	OHX	AR	3732	-	0,6,6	0.00	-	-		
84	OHX	AR	3586	-	0,6,6	0.00	-	-		
84	OHX	1	3441	-	0,6,6	0.00	-	-		
84	OHX	AR	3549	-	0,6,6	0.00	-	-		
84	OHX	AR	3490	-	0,6,6	0.00	-	-		
84	OHX	A	1985	-	0,6,6	0.00	-	-		
84	OHX	sR	1955	-	0,6,6	0.00	-	-		
84	OHX	AR	3624	-	0,6,6	0.00	-	-		
84	OHX	AR	3489	-	0,6,6	0.00	-	-		
84	OHX	c3	201	-	0,6,6	0.00	-	-		
84	OHX	1	3573	-	0,6,6	0.00	-	-		
84	OHX	1	3510	-	0,6,6	0.00	-	-		
84	OHX	d4	201	-	0,6,6	0.00	-	-		
84	OHX	A	1987	-	0,6,6	0.00	-	-		
84	OHX	AR	3506	-	0,6,6	0.00	-	-		
84	OHX	1	3649	-	0,6,6	0.00	-	-		
84	OHX	1	3406	-	0,6,6	0.00	-	-		
84	OHX	1	3585	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3502	-	0,6,6	0.00	-	-		
84	OHX	AR	3581	-	0,6,6	0.00	-	-		
84	OHX	AR	3406	-	0,6,6	0.00	-	-		
84	OHX	A	1931	-	0,6,6	0.00	-	-		
84	OHX	AR	3403	-	0,6,6	0.00	-	-		
84	OHX	AR	3554	-	0,6,6	0.00	-	-		
84	OHX	A	1934	-	0,6,6	0.00	-	-		
84	OHX	A	1994	-	0,6,6	0.00	-	-		
84	OHX	A	2042	-	0,6,6	0.00	-	-		
84	OHX	AR	3513	-	0,6,6	0.00	-	-		
84	OHX	AR	3725	-	0,6,6	0.00	-	-		
86	7AL	1	4210	-	28,28,28	0.38	0	35,45,45	0.68	1 (2%)
84	OHX	A	2038	-	0,6,6	0.00	-	-		
84	OHX	1	3691	-	0,6,6	0.00	-	-		
84	OHX	AR	3706	-	0,6,6	0.00	-	-		
84	OHX	A	2032	-	0,6,6	0.00	-	-		
84	OHX	1	3650	-	0,6,6	0.00	-	-		
84	OHX	sR	2046	-	0,6,6	0.00	-	-		
84	OHX	sR	1970	-	0,6,6	0.00	-	-		
84	OHX	sR	2026	-	0,6,6	0.00	-	-		
84	OHX	AR	3417	-	0,6,6	0.00	-	-		
84	OHX	AR	3656	-	0,6,6	0.00	-	-		
84	OHX	A	1933	-	0,6,6	0.00	-	-		
84	OHX	A	1958	-	0,6,6	0.00	-	-		
84	OHX	1	3671	-	0,6,6	0.00	-	-		
84	OHX	1	3533	-	0,6,6	0.00	-	-		
84	OHX	1	3539	-	0,6,6	0.00	-	-		
84	OHX	A	1925	-	0,6,6	0.00	-	-		
84	OHX	1	3614	-	0,6,6	0.00	-	-		
84	OHX	AR	3488	-	0,6,6	0.00	-	-		
84	OHX	1	3558	-	0,6,6	0.00	-	-		
84	OHX	AR	3475	-	0,6,6	0.00	-	-		
84	OHX	AR	3548	-	0,6,6	0.00	-	-		
84	OHX	AT	205	-	0,6,6	0.00	-	-		
84	OHX	1	3636	-	0,6,6	0.00	-	-		
84	OHX	AR	3687	-	0,6,6	0.00	-	-		
84	OHX	1	3731	-	0,6,6	0.00	-	-		
84	OHX	CG	301	-	0,6,6	0.00	-	-		
84	OHX	4	211	-	0,6,6	0.00	-	-		
84	OHX	AR	3482	-	0,6,6	0.00	-	-		
84	OHX	sR	2042	-	0,6,6	0.00	-	-		
84	OHX	AR	3651	-	0,6,6	0.00	-	-		
84	OHX	AR	3605	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3504	-	0,6,6	0.00	-	-		
84	OHX	AR	3470	-	0,6,6	0.00	-	-		
84	OHX	sR	1985	-	0,6,6	0.00	-	-		
84	OHX	1	3422	-	0,6,6	0.00	-	-		
84	OHX	AR	3448	-	0,6,6	0.00	-	-		
84	OHX	AR	3493	-	0,6,6	0.00	-	-		
84	OHX	1	3566	-	0,6,6	0.00	-	-		
84	OHX	AR	3647	-	0,6,6	0.00	-	-		
84	OHX	AR	3509	-	0,6,6	0.00	-	-		
84	OHX	AR	3690	-	0,6,6	0.00	-	-		
84	OHX	1	3491	-	0,6,6	0.00	-	-		
84	OHX	v	301	-	0,6,6	0.00	-	-		
84	OHX	AR	3451	-	0,6,6	0.00	-	-		
84	OHX	1	3506	-	0,6,6	0.00	-	-		
84	OHX	1	3658	-	0,6,6	0.00	-	-		
84	OHX	AT	211	-	0,6,6	0.00	-	-		
84	OHX	sR	2025	-	0,6,6	0.00	-	-		
84	OHX	A	1945	-	0,6,6	0.00	-	-		
84	OHX	AR	3542	-	0,6,6	0.00	-	-		
84	OHX	sR	1903	-	0,6,6	0.00	-	-		
84	OHX	AR	3519	-	0,6,6	0.00	-	-		
84	OHX	1	3647	-	0,6,6	0.00	-	-		
84	OHX	DQ	201	-	0,6,6	0.00	-	-		
84	OHX	A	1950	-	0,6,6	0.00	-	-		
84	OHX	AR	3697	-	0,6,6	0.00	-	-		
84	OHX	AS	209	-	0,6,6	0.00	-	-		
84	OHX	A	2015	-	0,6,6	0.00	-	-		
84	OHX	1	3424	-	0,6,6	0.00	-	-		
84	OHX	1	3638	-	0,6,6	0.00	-	-		
84	OHX	sR	1939	-	0,6,6	0.00	-	-		
84	OHX	AR	3574	-	0,6,6	0.00	-	-		
84	OHX	AR	3477	-	0,6,6	0.00	-	-		
84	OHX	1	3722	-	0,6,6	0.00	-	-		
84	OHX	sR	1968	-	0,6,6	0.00	-	-		
84	OHX	sR	1983	-	0,6,6	0.00	-	-		
84	OHX	AR	3430	-	0,6,6	0.00	-	-		
84	OHX	CE	402	-	0,6,6	0.00	-	-		
84	OHX	1	3440	-	0,6,6	0.00	-	-		
84	OHX	AR	3402	-	0,6,6	0.00	-	-		
84	OHX	1	3444	-	0,6,6	0.00	-	-		
84	OHX	AR	3627	-	0,6,6	0.00	-	-		
84	OHX	AR	3539	-	0,6,6	0.00	-	-		
84	OHX	AT	204	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3531	-	0,6,6	0.00	-	-		
84	OHX	AR	3456	-	0,6,6	0.00	-	-		
84	OHX	AR	3593	-	0,6,6	0.00	-	-		
84	OHX	AR	3600	-	0,6,6	0.00	-	-		
84	OHX	A	2030	-	0,6,6	0.00	-	-		
84	OHX	A	1955	-	0,6,6	0.00	-	-		
84	OHX	1	3624	-	0,6,6	0.00	-	-		
84	OHX	AR	3560	-	0,6,6	0.00	-	-		
84	OHX	AR	3469	-	0,6,6	0.00	-	-		
84	OHX	AR	3607	-	0,6,6	0.00	-	-		
84	OHX	AR	3474	-	0,6,6	0.00	-	-		
84	OHX	sR	1956	-	0,6,6	0.00	-	-		
84	OHX	AR	3502	-	0,6,6	0.00	-	-		
84	OHX	A	1969	-	0,6,6	0.00	-	-		
84	OHX	AR	3705	-	0,6,6	0.00	-	-		
84	OHX	1	3557	-	0,6,6	0.00	-	-		
84	OHX	sR	1981	-	0,6,6	0.00	-	-		
84	OHX	A	1974	-	0,6,6	0.00	-	-		
84	OHX	1	3619	-	0,6,6	0.00	-	-		
84	OHX	AR	3668	-	0,6,6	0.00	-	-		
84	OHX	A	2006	-	0,6,6	0.00	-	-		
84	OHX	1	3634	-	0,6,6	0.00	-	-		
84	OHX	1	3714	-	0,6,6	0.00	-	-		
84	OHX	AR	3743	-	0,6,6	0.00	-	-		
84	OHX	1	3642	-	0,6,6	0.00	-	-		
84	OHX	1	3643	-	0,6,6	0.00	-	-		
84	OHX	1	3445	-	0,6,6	0.00	-	-		
84	OHX	sR	1963	-	0,6,6	0.00	-	-		
84	OHX	1	3659	-	0,6,6	0.00	-	-		
84	OHX	sR	1991	-	0,6,6	0.00	-	-		
84	OHX	A	1963	-	0,6,6	0.00	-	-		
84	OHX	AR	3455	-	0,6,6	0.00	-	-		
84	OHX	3	208	-	0,6,6	0.00	-	-		
84	OHX	A	1910	-	0,6,6	0.00	-	-		
84	OHX	1	3702	-	0,6,6	0.00	-	-		
84	OHX	1	3521	-	0,6,6	0.00	-	-		
84	OHX	sR	2012	-	0,6,6	0.00	-	-		
84	OHX	AR	3515	-	0,6,6	0.00	-	-		
84	OHX	1	3607	-	0,6,6	0.00	-	-		
84	OHX	A	1908	-	0,6,6	0.00	-	-		
84	OHX	sR	1973	-	0,6,6	0.00	-	-		
84	OHX	1	3556	-	0,6,6	0.00	-	-		
84	OHX	AR	3570	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	sR	1982	-	0,6,6	0.00	-	-		
84	OHX	1	3666	-	0,6,6	0.00	-	-		
84	OHX	1	3417	-	0,6,6	0.00	-	-		
84	OHX	1	3419	-	0,6,6	0.00	-	-		
84	OHX	sR	2029	-	0,6,6	0.00	-	-		
84	OHX	AR	3584	-	0,6,6	0.00	-	-		
84	OHX	sR	1997	-	0,6,6	0.00	-	-		
84	OHX	AR	3487	-	0,6,6	0.00	-	-		
84	OHX	1	3609	-	0,6,6	0.00	-	-		
84	OHX	AR	3692	-	0,6,6	0.00	-	-		
84	OHX	A	1916	-	0,6,6	0.00	-	-		
84	OHX	1	3446	-	0,6,6	0.00	-	-		
84	OHX	AR	3625	-	0,6,6	0.00	-	-		
84	OHX	sR	1901	-	0,6,6	0.00	-	-		
84	OHX	AT	203	-	0,6,6	0.00	-	-		
84	OHX	sR	1930	-	0,6,6	0.00	-	-		
84	OHX	sR	2048	-	0,6,6	0.00	-	-		
84	OHX	1	3678	-	0,6,6	0.00	-	-		
84	OHX	sR	2021	-	0,6,6	0.00	-	-		
84	OHX	1	3411	-	0,6,6	0.00	-	-		
84	OHX	AR	3685	-	0,6,6	0.00	-	-		
84	OHX	1	3711	-	0,6,6	0.00	-	-		
84	OHX	AR	3623	-	0,6,6	0.00	-	-		
84	OHX	AR	3671	-	0,6,6	0.00	-	-		
84	OHX	AR	3738	-	0,6,6	0.00	-	-		
84	OHX	1	3622	-	0,6,6	0.00	-	-		
84	OHX	AR	3678	-	0,6,6	0.00	-	-		
84	OHX	A	1928	-	0,6,6	0.00	-	-		
84	OHX	A	1918	-	0,6,6	0.00	-	-		
84	OHX	AR	3640	-	0,6,6	0.00	-	-		
84	OHX	1	3518	-	0,6,6	0.00	-	-		
84	OHX	s8	301	-	0,6,6	0.00	-	-		
84	OHX	AR	3717	-	0,6,6	0.00	-	-		
84	OHX	AR	3650	-	0,6,6	0.00	-	-		
84	OHX	4	215	-	0,6,6	0.00	-	-		
84	OHX	sR	2019	-	0,6,6	0.00	-	-		
84	OHX	sR	2044	-	0,6,6	0.00	-	-		
84	OHX	3	203	-	0,6,6	0.00	-	-		
84	OHX	A	2031	-	0,6,6	0.00	-	-		
84	OHX	1	3707	-	0,6,6	0.00	-	-		
84	OHX	1	3693	-	0,6,6	0.00	-	-		
84	OHX	1	3429	-	0,6,6	0.00	-	-		
84	OHX	sR	2031	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3534	-	0,6,6	0.00	-	-		
84	OHX	sR	2000	-	0,6,6	0.00	-	-		
84	OHX	AR	3527	-	0,6,6	0.00	-	-		
84	OHX	AR	3446	-	0,6,6	0.00	-	-		
84	OHX	sR	1924	-	0,6,6	0.00	-	-		
84	OHX	1	3724	-	0,6,6	0.00	-	-		
84	OHX	1	3584	-	0,6,6	0.00	-	-		
84	OHX	1	3681	-	0,6,6	0.00	-	-		
84	OHX	sR	2037	-	0,6,6	0.00	-	-		
84	OHX	1	3468	-	0,6,6	0.00	-	-		
84	OHX	A	1926	-	0,6,6	0.00	-	-		
84	OHX	AR	3592	-	0,6,6	0.00	-	-		
84	OHX	AR	3562	-	0,6,6	0.00	-	-		
84	OHX	x	202	-	0,6,6	0.00	-	-		
84	OHX	AR	3708	-	0,6,6	0.00	-	-		
84	OHX	1	3604	-	0,6,6	0.00	-	-		
84	OHX	AT	208	-	0,6,6	0.00	-	-		
84	OHX	A	1956	-	0,6,6	0.00	-	-		
84	OHX	1	3530	-	0,6,6	0.00	-	-		
84	OHX	1	3434	-	0,6,6	0.00	-	-		
84	OHX	1	3431	-	0,6,6	0.00	-	-		
84	OHX	AR	3525	-	0,6,6	0.00	-	-		
84	OHX	1	3616	-	0,6,6	0.00	-	-		
84	OHX	A	2019	-	0,6,6	0.00	-	-		
84	OHX	AR	3672	-	0,6,6	0.00	-	-		
84	OHX	x	201	-	0,6,6	0.00	-	-		
84	OHX	AT	216	-	0,6,6	0.00	-	-		
84	OHX	A	2022	-	0,6,6	0.00	-	-		
84	OHX	4	201	-	0,6,6	0.00	-	-		
84	OHX	A	1978	-	0,6,6	0.00	-	-		
84	OHX	AR	3480	-	0,6,6	0.00	-	-		
84	OHX	AR	3521	-	0,6,6	0.00	-	-		
84	OHX	AR	3485	-	0,6,6	0.00	-	-		
84	OHX	A	1988	-	0,6,6	0.00	-	-		
84	OHX	A	1919	-	0,6,6	0.00	-	-		
84	OHX	sR	1962	-	0,6,6	0.00	-	-		
84	OHX	AR	3551	-	0,6,6	0.00	-	-		
84	OHX	A	1902	-	0,6,6	0.00	-	-		
84	OHX	AR	3628	-	0,6,6	0.00	-	-		
84	OHX	AR	3435	-	0,6,6	0.00	-	-		
84	OHX	AR	3411	-	0,6,6	0.00	-	-		
84	OHX	1	3717	-	0,6,6	0.00	-	-		
84	OHX	A	1976	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3652	-	0,6,6	0.00	-	-		
84	OHX	sR	1994	-	0,6,6	0.00	-	-		
84	OHX	sR	1957	-	0,6,6	0.00	-	-		
84	OHX	1	3527	-	0,6,6	0.00	-	-		
84	OHX	1	3698	-	0,6,6	0.00	-	-		
84	OHX	1	3723	-	0,6,6	0.00	-	-		
84	OHX	sR	2028	-	0,6,6	0.00	-	-		
84	OHX	1	3687	-	0,6,6	0.00	-	-		
84	OHX	AR	3416	-	0,6,6	0.00	-	-		
84	OHX	AR	3679	-	0,6,6	0.00	-	-		
84	OHX	sR	1980	-	0,6,6	0.00	-	-		
84	OHX	1	3490	-	0,6,6	0.00	-	-		
84	OHX	1	3472	-	0,6,6	0.00	-	-		
84	OHX	AR	3491	-	0,6,6	0.00	-	-		
84	OHX	A	1930	-	0,6,6	0.00	-	-		
84	OHX	AR	3563	-	0,6,6	0.00	-	-		
84	OHX	1	3592	-	0,6,6	0.00	-	-		
84	OHX	1	3721	-	0,6,6	0.00	-	-		
84	OHX	1	3720	-	0,6,6	0.00	-	-		
84	OHX	1	3689	-	0,6,6	0.00	-	-		
84	OHX	sR	2039	-	0,6,6	0.00	-	-		
84	OHX	AR	3606	-	0,6,6	0.00	-	-		
84	OHX	AR	3580	-	0,6,6	0.00	-	-		
84	OHX	sR	1954	-	0,6,6	0.00	-	-		
84	OHX	AR	3405	-	0,6,6	0.00	-	-		
84	OHX	CF	402	-	0,6,6	0.00	-	-		
84	OHX	1	3669	-	0,6,6	0.00	-	-		
84	OHX	1	3480	-	0,6,6	0.00	-	-		
84	OHX	1	3648	-	0,6,6	0.00	-	-		
84	OHX	1	3660	-	0,6,6	0.00	-	-		
84	OHX	AR	3572	-	0,6,6	0.00	-	-		
84	OHX	AR	3505	-	0,6,6	0.00	-	-		
84	OHX	AR	3520	-	0,6,6	0.00	-	-		
84	OHX	1	3495	-	0,6,6	0.00	-	-		
84	OHX	1	3588	-	0,6,6	0.00	-	-		
84	OHX	1	3475	-	0,6,6	0.00	-	-		
84	OHX	CL	302	-	0,6,6	0.00	-	-		
84	OHX	A	2002	-	0,6,6	0.00	-	-		
84	OHX	A	1980	-	0,6,6	0.00	-	-		
84	OHX	AR	3616	-	0,6,6	0.00	-	-		
84	OHX	sR	1975	-	0,6,6	0.00	-	-		
84	OHX	sR	2045	-	0,6,6	0.00	-	-		
84	OHX	AR	3582	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AR	3457	-	0,6,6	0.00	-	-		
86	7AL	AR	4246	-	28,28,28	0.37	0	35,45,45	0.36	0
84	OHX	A	2033	-	0,6,6	0.00	-	-		
84	OHX	1	3464	-	0,6,6	0.00	-	-		
84	OHX	1	3483	-	0,6,6	0.00	-	-		
84	OHX	1	3581	-	0,6,6	0.00	-	-		
84	OHX	1	3416	-	0,6,6	0.00	-	-		
84	OHX	1	3486	-	0,6,6	0.00	-	-		
84	OHX	AR	3718	-	0,6,6	0.00	-	-		
84	OHX	1	3651	-	0,6,6	0.00	-	-		
84	OHX	AR	3589	-	0,6,6	0.00	-	-		
84	OHX	AR	3742	-	0,6,6	0.00	-	-		
84	OHX	1	3608	-	0,6,6	0.00	-	-		
84	OHX	AR	3569	-	0,6,6	0.00	-	-		
84	OHX	AR	3466	-	0,6,6	0.00	-	-		
84	OHX	1	3471	-	0,6,6	0.00	-	-		
84	OHX	AR	3429	-	0,6,6	0.00	-	-		
84	OHX	1	3515	-	0,6,6	0.00	-	-		
84	OHX	1	3525	-	0,6,6	0.00	-	-		
84	OHX	sR	2024	-	0,6,6	0.00	-	-		
84	OHX	AR	3734	-	0,6,6	0.00	-	-		
84	OHX	1	3586	-	0,6,6	0.00	-	-		
84	OHX	A	1913	-	0,6,6	0.00	-	-		
84	OHX	AR	3557	-	0,6,6	0.00	-	-		
84	OHX	A	1998	48	0,6,6	0.00	-	-		
84	OHX	AR	3688	-	0,6,6	0.00	-	-		
84	OHX	sR	1935	-	0,6,6	0.00	-	-		
84	OHX	c5	201	-	0,6,6	0.00	-	-		
84	OHX	sR	2043	-	0,6,6	0.00	-	-		
84	OHX	AR	3443	-	0,6,6	0.00	-	-		
84	OHX	3	202	-	0,6,6	0.00	-	-		
84	OHX	A	2040	-	0,6,6	0.00	-	-		
84	OHX	AR	3673	-	0,6,6	0.00	-	-		
84	OHX	AR	3409	-	0,6,6	0.00	-	-		
84	OHX	A	1921	-	0,6,6	0.00	-	-		
84	OHX	sR	2005	-	0,6,6	0.00	-	-		
84	OHX	1	3465	-	0,6,6	0.00	-	-		
84	OHX	AR	3613	-	0,6,6	0.00	-	-		
84	OHX	4	209	-	0,6,6	0.00	-	-		
84	OHX	AR	3496	-	0,6,6	0.00	-	-		
84	OHX	CX	201	-	0,6,6	0.00	-	-		
84	OHX	A	1920	-	0,6,6	0.00	-	-		
84	OHX	A	1903	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3403	-	0,6,6	0.00	-	-		
84	OHX	sR	1925	-	0,6,6	0.00	-	-		
84	OHX	AR	3615	-	0,6,6	0.00	-	-		
84	OHX	AR	3514	-	0,6,6	0.00	-	-		
84	OHX	1	3467	-	0,6,6	0.00	-	-		
84	OHX	A	1986	-	0,6,6	0.00	-	-		
84	OHX	A	2010	-	0,6,6	0.00	-	-		
84	OHX	AR	3686	-	0,6,6	0.00	-	-		
84	OHX	sR	1904	-	0,6,6	0.00	-	-		
84	OHX	sR	1999	-	0,6,6	0.00	-	-		
84	OHX	AR	3571	-	0,6,6	0.00	-	-		
84	OHX	AR	3652	-	0,6,6	0.00	-	-		
84	OHX	AR	3675	-	0,6,6	0.00	-	-		
84	OHX	A	2024	-	0,6,6	0.00	-	-		
84	OHX	4	203	-	0,6,6	0.00	-	-		
84	OHX	sR	1978	-	0,6,6	0.00	-	-		
84	OHX	1	3686	-	0,6,6	0.00	-	-		
84	OHX	sR	1907	-	0,6,6	0.00	-	-		
84	OHX	AS	208	-	0,6,6	0.00	-	-		
84	OHX	AR	3703	84	0,6,6	0.00	-	-		
84	OHX	1	3599	-	0,6,6	0.00	-	-		
84	OHX	AR	3626	-	0,6,6	0.00	-	-		
84	OHX	A	1992	-	0,6,6	0.00	-	-		
84	OHX	1	3623	-	0,6,6	0.00	-	-		
84	OHX	e	101	-	0,6,6	0.00	-	-		
84	OHX	1	3564	-	0,6,6	0.00	-	-		
84	OHX	1	3420	-	0,6,6	0.00	-	-		
84	OHX	1	3404	-	0,6,6	0.00	-	-		
84	OHX	sR	1986	-	0,6,6	0.00	-	-		
84	OHX	sR	2033	-	0,6,6	0.00	-	-		
84	OHX	A	2025	-	0,6,6	0.00	-	-		
84	OHX	1	3492	-	0,6,6	0.00	-	-		
84	OHX	sR	1944	-	0,6,6	0.00	-	-		
84	OHX	AR	3664	-	0,6,6	0.00	-	-		
84	OHX	AR	3609	-	0,6,6	0.00	-	-		
84	OHX	AR	3479	-	0,6,6	0.00	-	-		
84	OHX	T	201	-	0,6,6	0.00	-	-		
84	OHX	sR	1908	-	0,6,6	0.00	-	-		
84	OHX	1	3591	-	0,6,6	0.00	-	-		
84	OHX	AR	3414	-	0,6,6	0.00	-	-		
84	OHX	AR	3428	-	0,6,6	0.00	-	-		
84	OHX	sR	1953	-	0,6,6	0.00	-	-		
84	OHX	AR	3500	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AR	3677	-	0,6,6	0.00	-	-		
84	OHX	1	3461	-	0,6,6	0.00	-	-		
84	OHX	sR	2015	-	0,6,6	0.00	-	-		
84	OHX	AR	3541	-	0,6,6	0.00	-	-		
84	OHX	A	2007	-	0,6,6	0.00	-	-		
84	OHX	1	3540	84	0,6,6	0.00	-	-		
84	OHX	1	3672	-	0,6,6	0.00	-	-		
84	OHX	1	3526	-	0,6,6	0.00	-	-		
84	OHX	1	3631	-	0,6,6	0.00	-	-		
84	OHX	AR	3603	-	0,6,6	0.00	-	-		
84	OHX	1	3683	-	0,6,6	0.00	-	-		
84	OHX	AR	3632	-	0,6,6	0.00	-	-		
84	OHX	AR	3659	-	0,6,6	0.00	-	-		
84	OHX	AR	3585	-	0,6,6	0.00	-	-		
84	OHX	sR	2008	-	0,6,6	0.00	-	-		
84	OHX	AS	202	-	0,6,6	0.00	-	-		
84	OHX	1	3715	-	0,6,6	0.00	-	-		
84	OHX	A	2026	-	0,6,6	0.00	-	-		
84	OHX	1	3675	-	0,6,6	0.00	-	-		
84	OHX	AR	3468	-	0,6,6	0.00	-	-		
84	OHX	1	3725	-	0,6,6	0.00	-	-		
84	OHX	1	3443	-	0,6,6	0.00	-	-		
84	OHX	1	3679	-	0,6,6	0.00	-	-		
84	OHX	AR	3611	-	0,6,6	0.00	-	-		
84	OHX	sR	2013	-	0,6,6	0.00	-	-		
84	OHX	AR	3649	-	0,6,6	0.00	-	-		
84	OHX	1	3598	-	0,6,6	0.00	-	-		
84	OHX	A	1935	-	0,6,6	0.00	-	-		
84	OHX	1	3621	-	0,6,6	0.00	-	-		
84	OHX	AR	3674	-	0,6,6	0.00	-	-		
84	OHX	AS	210	-	0,6,6	0.00	-	-		
84	OHX	A	1941	-	0,6,6	0.00	-	-		
84	OHX	Q	201	-	0,6,6	0.00	-	-		
84	OHX	1	3653	-	0,6,6	0.00	-	-		
84	OHX	sR	1996	-	0,6,6	0.00	-	-		
84	OHX	1	3505	-	0,6,6	0.00	-	-		
84	OHX	AR	3526	-	0,6,6	0.00	-	-		
84	OHX	AR	3667	-	0,6,6	0.00	-	-		
84	OHX	AS	204	-	0,6,6	0.00	-	-		
84	OHX	AR	3552	-	0,6,6	0.00	-	-		
84	OHX	v	302	-	0,6,6	0.00	-	-		
84	OHX	sR	2007	-	0,6,6	0.00	-	-		
84	OHX	sR	1920	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	sR	1946	-	0,6,6	0.00	-	-		
84	OHX	1	3680	-	0,6,6	0.00	-	-		
84	OHX	1	3519	-	0,6,6	0.00	-	-		
84	OHX	1	3655	-	0,6,6	0.00	-	-		
84	OHX	1	3513	-	0,6,6	0.00	-	-		
84	OHX	sR	2049	-	0,6,6	0.00	-	-		
84	OHX	A	1917	-	0,6,6	0.00	-	-		
84	OHX	1	3451	-	0,6,6	0.00	-	-		
84	OHX	1	3629	-	0,6,6	0.00	-	-		
84	OHX	sR	1951	-	0,6,6	0.00	-	-		
84	OHX	AR	3465	-	0,6,6	0.00	-	-		
84	OHX	AR	3660	-	0,6,6	0.00	-	-		
84	OHX	sR	1937	-	0,6,6	0.00	-	-		
84	OHX	z	201	-	0,6,6	0.00	-	-		
84	OHX	1	3432	-	0,6,6	0.00	-	-		
84	OHX	sR	2050	-	0,6,6	0.00	-	-		
84	OHX	1	3514	-	0,6,6	0.00	-	-		
84	OHX	AR	3739	-	0,6,6	0.00	-	-		
84	OHX	sR	1947	-	0,6,6	0.00	-	-		
84	OHX	AR	3698	-	0,6,6	0.00	-	-		
84	OHX	r	301	-	0,6,6	0.00	-	-		
84	OHX	AR	3720	-	0,6,6	0.00	-	-		
84	OHX	AR	3669	-	0,6,6	0.00	-	-		
84	OHX	A	1927	-	0,6,6	0.00	-	-		
84	OHX	4	202	-	0,6,6	0.00	-	-		
84	OHX	AR	3704	-	0,6,6	0.00	-	-		
84	OHX	AR	3683	-	0,6,6	0.00	-	-		
84	OHX	A	2037	-	0,6,6	0.00	-	-		
84	OHX	AR	3617	-	0,6,6	0.00	-	-		
84	OHX	AR	3531	-	0,6,6	0.00	-	-		
84	OHX	AR	3736	-	0,6,6	0.00	-	-		
84	OHX	AR	3415	-	0,6,6	0.00	-	-		
84	OHX	A	2041	-	0,6,6	0.00	-	-		
84	OHX	1	3448	-	0,6,6	0.00	-	-		
84	OHX	AR	3631	-	0,6,6	0.00	-	-		
84	OHX	sR	1931	-	0,6,6	0.00	-	-		
84	OHX	AR	3681	-	0,6,6	0.00	-	-		
84	OHX	AR	3629	-	0,6,6	0.00	-	-		
84	OHX	1	3703	-	0,6,6	0.00	-	-		
84	OHX	AR	3716	-	0,6,6	0.00	-	-		
84	OHX	sR	1989	-	0,6,6	0.00	-	-		
84	OHX	A	2009	-	0,6,6	0.00	-	-		
84	OHX	A	1966	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AR	3467	-	0,6,6	0.00	-	-		
84	OHX	A	1909	-	0,6,6	0.00	-	-		
84	OHX	3	205	-	0,6,6	0.00	-	-		
84	OHX	sR	1915	-	0,6,6	0.00	-	-		
84	OHX	A	1915	-	0,6,6	0.00	-	-		
84	OHX	1	3524	-	0,6,6	0.00	-	-		
84	OHX	AR	3534	-	0,6,6	0.00	-	-		
84	OHX	1	3469	-	0,6,6	0.00	-	-		
84	OHX	1	3606	-	0,6,6	0.00	-	-		
84	OHX	A	1937	-	0,6,6	0.00	-	-		
84	OHX	1	3415	-	0,6,6	0.00	-	-		
84	OHX	sR	1990	-	0,6,6	0.00	-	-		
84	OHX	1	3479	-	0,6,6	0.00	-	-		
84	OHX	A	1947	-	0,6,6	0.00	-	-		
84	OHX	AR	3431	-	0,6,6	0.00	-	-		
84	OHX	AR	3594	-	0,6,6	0.00	-	-		
84	OHX	A	1911	-	0,6,6	0.00	-	-		
84	OHX	1	3641	-	0,6,6	0.00	-	-		
84	OHX	AS	211	-	0,6,6	0.00	-	-		
84	OHX	A	1995	-	0,6,6	0.00	-	-		
84	OHX	sR	2047	-	0,6,6	0.00	-	-		
84	OHX	1	3562	-	0,6,6	0.00	-	-		
84	OHX	1	3730	-	0,6,6	0.00	-	-		
84	OHX	AK	102	-	0,6,6	0.00	-	-		
84	OHX	sR	1992	-	0,6,6	0.00	-	-		
84	OHX	A	1964	-	0,6,6	0.00	-	-		
84	OHX	AR	3578	-	0,6,6	0.00	-	-		
84	OHX	A	2018	-	0,6,6	0.00	-	-		
84	OHX	1	3553	-	0,6,6	0.00	-	-		
84	OHX	A	1939	-	0,6,6	0.00	-	-		
84	OHX	AR	3432	-	0,6,6	0.00	-	-		
84	OHX	AR	3715	-	0,6,6	0.00	-	-		
84	OHX	1	3538	-	0,6,6	0.00	-	-		
84	OHX	sR	2051	-	0,6,6	0.00	-	-		
84	OHX	1	3523	-	0,6,6	0.00	-	-		
84	OHX	1	3632	-	0,6,6	0.00	-	-		
84	OHX	AR	3481	84	0,6,6	0.00	-	-		
84	OHX	sR	1941	-	0,6,6	0.00	-	-		
84	OHX	AR	3433	-	0,6,6	0.00	-	-		
84	OHX	AR	3658	-	0,6,6	0.00	-	-		
84	OHX	1	3537	-	0,6,6	0.00	-	-		
84	OHX	1	3667	-	0,6,6	0.00	-	-		
84	OHX	1	3637	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	H	301	-	0,6,6	0.00	-	-		
84	OHX	AT	212	84	0,6,6	0.00	-	-		
84	OHX	A	2039	-	0,6,6	0.00	-	-		
84	OHX	AR	3425	-	0,6,6	0.00	-	-		
84	OHX	AR	3684	-	0,6,6	0.00	-	-		
84	OHX	AR	3724	-	0,6,6	0.00	-	-		
84	OHX	AR	3483	-	0,6,6	0.00	-	-		
84	OHX	AR	3410	-	0,6,6	0.00	-	-		
84	OHX	A	1912	-	0,6,6	0.00	-	-		
84	OHX	1	3719	-	0,6,6	0.00	-	-		
84	OHX	sR	1910	-	0,6,6	0.00	-	-		
84	OHX	1	3712	-	0,6,6	0.00	-	-		
84	OHX	AR	3641	-	0,6,6	0.00	-	-		
84	OHX	AS	207	-	0,6,6	0.00	-	-		
84	OHX	1	3590	-	0,6,6	0.00	-	-		
84	OHX	AR	3622	-	0,6,6	0.00	-	-		
84	OHX	A	1997	-	0,6,6	0.00	-	-		
84	OHX	A	2028	-	0,6,6	0.00	-	-		
84	OHX	AR	3540	-	0,6,6	0.00	-	-		
84	OHX	AR	3655	-	0,6,6	0.00	-	-		
84	OHX	AR	3419	-	0,6,6	0.00	-	-		
84	OHX	AR	3676	-	0,6,6	0.00	-	-		
84	OHX	1	3462	-	0,6,6	0.00	-	-		
84	OHX	AR	3702	-	0,6,6	0.00	-	-		
84	OHX	1	3611	-	0,6,6	0.00	-	-		
84	OHX	AR	3566	-	0,6,6	0.00	-	-		
84	OHX	1	3454	-	0,6,6	0.00	-	-		
84	OHX	1	3576	-	0,6,6	0.00	-	-		
84	OHX	AR	3637	-	0,6,6	0.00	-	-		
84	OHX	4	212	-	0,6,6	0.00	-	-		
84	OHX	1	3565	-	0,6,6	0.00	-	-		
84	OHX	A	1971	-	0,6,6	0.00	-	-		
84	OHX	4	208	-	0,6,6	0.00	-	-		
84	OHX	1	3688	-	0,6,6	0.00	-	-		
84	OHX	AR	3700	-	0,6,6	0.00	-	-		
84	OHX	1	3593	-	0,6,6	0.00	-	-		
84	OHX	AR	3619	-	0,6,6	0.00	-	-		
84	OHX	1	3701	-	0,6,6	0.00	-	-		
84	OHX	1	3450	-	0,6,6	0.00	-	-		
84	OHX	AR	3714	-	0,6,6	0.00	-	-		
84	OHX	AR	3727	-	0,6,6	0.00	-	-		
84	OHX	1	3549	-	0,6,6	0.00	-	-		
84	OHX	A	1961	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	sR	1972	-	0,6,6	0.00	-	-		
84	OHX	1	3460	-	0,6,6	0.00	-	-		
84	OHX	sR	1977	-	0,6,6	0.00	-	-		
84	OHX	A	2036	-	0,6,6	0.00	-	-		
84	OHX	1	3704	-	0,6,6	0.00	-	-		
84	OHX	AR	3731	-	0,6,6	0.00	-	-		
84	OHX	sR	1969	-	0,6,6	0.00	-	-		
84	OHX	1	3661	-	0,6,6	0.00	-	-		
84	OHX	AR	3598	-	0,6,6	0.00	-	-		
84	OHX	sR	2038	-	0,6,6	0.00	-	-		
84	OHX	AR	3595	-	0,6,6	0.00	-	-		
84	OHX	1	3517	-	0,6,6	0.00	-	-		
84	OHX	1	3499	-	0,6,6	0.00	-	-		
84	OHX	AR	3709	-	0,6,6	0.00	-	-		
84	OHX	A	1981	-	0,6,6	0.00	-	-		
84	OHX	sR	1909	-	0,6,6	0.00	-	-		
84	OHX	1	3428	-	0,6,6	0.00	-	-		
84	OHX	1	3664	-	0,6,6	0.00	-	-		
84	OHX	sR	2036	-	0,6,6	0.00	-	-		
84	OHX	1	3555	-	0,6,6	0.00	-	-		
84	OHX	AR	3666	-	0,6,6	0.00	-	-		
84	OHX	AR	3404	-	0,6,6	0.00	-	-		
84	OHX	1	3405	-	0,6,6	0.00	-	-		
84	OHX	AR	3746	-	0,6,6	0.00	-	-		
84	OHX	sR	1967	-	0,6,6	0.00	-	-		
84	OHX	sR	1932	-	0,6,6	0.00	-	-		
84	OHX	1	3674	-	0,6,6	0.00	-	-		
84	OHX	sR	1988	-	0,6,6	0.00	-	-		
84	OHX	sR	1902	-	0,6,6	0.00	-	-		
84	OHX	AR	3565	-	0,6,6	0.00	-	-		
84	OHX	A	1989	-	0,6,6	0.00	-	-		
84	OHX	AR	3546	-	0,6,6	0.00	-	-		
84	OHX	1	3696	-	0,6,6	0.00	-	-		
84	OHX	CV	201	-	0,6,6	0.00	-	-		
84	OHX	sR	1950	-	0,6,6	0.00	-	-		
84	OHX	1	3577	-	0,6,6	0.00	-	-		
84	OHX	1	3618	-	0,6,6	0.00	-	-		
84	OHX	AR	3661	-	0,6,6	0.00	-	-		
84	OHX	1	3663	-	0,6,6	0.00	-	-		
84	OHX	AR	3427	-	0,6,6	0.00	-	-		
84	OHX	AR	3682	-	0,6,6	0.00	-	-		
84	OHX	A	1932	-	0,6,6	0.00	-	-		
84	OHX	A	1951	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	sR	1995	-	0,6,6	0.00	-	-		
84	OHX	AR	3529	84	0,6,6	0.00	-	-		
84	OHX	1	3474	-	0,6,6	0.00	-	-		
84	OHX	1	3435	-	0,6,6	0.00	-	-		
84	OHX	AR	3499	-	0,6,6	0.00	-	-		
84	OHX	sR	2034	-	0,6,6	0.00	-	-		
84	OHX	sR	2052	-	0,6,6	0.00	-	-		
84	OHX	AR	3612	-	0,6,6	0.00	-	-		
84	OHX	1	3630	-	0,6,6	0.00	-	-		
84	OHX	1	3567	-	0,6,6	0.00	-	-		
84	OHX	1	3716	-	0,6,6	0.00	-	-		
84	OHX	1	3494	-	0,6,6	0.00	-	-		
84	OHX	4	213	-	0,6,6	0.00	-	-		
84	OHX	1	3673	-	0,6,6	0.00	-	-		
84	OHX	AR	3463	-	0,6,6	0.00	-	-		
84	OHX	AR	3723	-	0,6,6	0.00	-	-		
84	OHX	AR	3665	-	0,6,6	0.00	-	-		
84	OHX	AR	3590	-	0,6,6	0.00	-	-		
84	OHX	A	2005	-	0,6,6	0.00	-	-		
84	OHX	AT	202	84	0,6,6	0.00	-	-		
84	OHX	1	3662	-	0,6,6	0.00	-	-		
84	OHX	sR	2027	-	0,6,6	0.00	-	-		
84	OHX	A	1959	-	0,6,6	0.00	-	-		
84	OHX	1	3727	-	0,6,6	0.00	-	-		
84	OHX	AR	3464	-	0,6,6	0.00	-	-		
84	OHX	AR	3596	-	0,6,6	0.00	-	-		
84	OHX	AR	3573	-	0,6,6	0.00	-	-		
84	OHX	1	3568	-	0,6,6	0.00	-	-		
84	OHX	A	2003	-	0,6,6	0.00	-	-		
84	OHX	AR	3614	-	0,6,6	0.00	-	-		
84	OHX	AR	3440	-	0,6,6	0.00	-	-		
84	OHX	1	3635	-	0,6,6	0.00	-	-		
84	OHX	A	1957	-	0,6,6	0.00	-	-		
84	OHX	A	1943	-	0,6,6	0.00	-	-		
84	OHX	1	3481	-	0,6,6	0.00	-	-		
84	OHX	1	3509	-	0,6,6	0.00	-	-		
84	OHX	AR	3421	-	0,6,6	0.00	-	-		
84	OHX	AT	215	-	0,6,6	0.00	-	-		
84	OHX	1	3600	-	0,6,6	0.00	-	-		
84	OHX	Rb	401	-	0,6,6	0.00	-	-		
84	OHX	AR	3642	-	0,6,6	0.00	-	-		
84	OHX	A	2029	-	0,6,6	0.00	-	-		
84	OHX	AP	502	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3507	-	0,6,6	0.00	-	-		
84	OHX	DD	102	-	0,6,6	0.00	-	-		
84	OHX	sR	1976	-	0,6,6	0.00	-	-		
84	OHX	sR	1979	-	0,6,6	0.00	-	-		
84	OHX	1	3457	-	0,6,6	0.00	-	-		
84	OHX	AK	103	-	0,6,6	0.00	-	-		
84	OHX	AR	3699	-	0,6,6	0.00	-	-		
84	OHX	1	3488	-	0,6,6	0.00	-	-		
84	OHX	1	3626	-	0,6,6	0.00	-	-		
84	OHX	sR	1916	-	0,6,6	0.00	-	-		
84	OHX	A	2035	-	0,6,6	0.00	-	-		
84	OHX	4	205	-	0,6,6	0.00	-	-		
84	OHX	1	3430	-	0,6,6	0.00	-	-		
84	OHX	A	1944	-	0,6,6	0.00	-	-		
84	OHX	1	3437	-	0,6,6	0.00	-	-		
84	OHX	AR	3670	-	0,6,6	0.00	-	-		
84	OHX	AR	3576	-	0,6,6	0.00	-	-		
84	OHX	A	1970	-	0,6,6	0.00	-	-		
84	OHX	AR	3454	-	0,6,6	0.00	-	-		
84	OHX	1	3657	-	0,6,6	0.00	-	-		
84	OHX	A	1929	-	0,6,6	0.00	-	-		
84	OHX	AT	207	-	0,6,6	0.00	-	-		
84	OHX	1	3710	-	0,6,6	0.00	-	-		
84	OHX	1	3466	-	0,6,6	0.00	-	-		
84	OHX	A	2017	-	0,6,6	0.00	-	-		
84	OHX	AR	3461	-	0,6,6	0.00	-	-		
84	OHX	AR	3657	-	0,6,6	0.00	-	-		
84	OHX	AR	3472	-	0,6,6	0.00	-	-		
84	OHX	A	1973	-	0,6,6	0.00	-	-		
84	OHX	1	3482	-	0,6,6	0.00	-	-		
84	OHX	1	3612	-	0,6,6	0.00	-	-		
84	OHX	AR	3547	-	0,6,6	0.00	-	-		
84	OHX	1	3594	-	0,6,6	0.00	-	-		
84	OHX	AR	3722	-	0,6,6	0.00	-	-		
84	OHX	A	1982	-	0,6,6	0.00	-	-		
84	OHX	4	207	-	0,6,6	0.00	-	-		
84	OHX	A	2023	-	0,6,6	0.00	-	-		
84	OHX	AR	3745	-	0,6,6	0.00	-	-		
84	OHX	1	3640	-	0,6,6	0.00	-	-		
84	OHX	1	3516	-	0,6,6	0.00	-	-		
84	OHX	CO	201	-	0,6,6	0.00	-	-		
84	OHX	sR	1943	-	0,6,6	0.00	-	-		
84	OHX	AR	3733	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3541	-	0,6,6	0.00	-	-		
84	OHX	sR	1993	-	0,6,6	0.00	-	-		
84	OHX	sR	1938	-	0,6,6	0.00	-	-		
84	OHX	sR	1919	-	0,6,6	0.00	-	-		
84	OHX	1	3551	-	0,6,6	0.00	-	-		
84	OHX	AR	3460	-	0,6,6	0.00	-	-		
84	OHX	AR	3511	-	0,6,6	0.00	-	-		
84	OHX	1	3485	-	0,6,6	0.00	-	-		
84	OHX	1	3560	-	0,6,6	0.00	-	-		
84	OHX	1	3408	-	0,6,6	0.00	-	-		
84	OHX	1	3544	-	0,6,6	0.00	-	-		
84	OHX	s4	301	-	0,6,6	0.00	-	-		
84	OHX	AR	3728	-	0,6,6	0.00	-	-		
84	OHX	1	3625	-	0,6,6	0.00	-	-		
84	OHX	1	3708	-	0,6,6	0.00	-	-		
84	OHX	AR	3424	-	0,6,6	0.00	-	-		
84	OHX	1	3685	-	0,6,6	0.00	-	-		
84	OHX	sR	2041	-	0,6,6	0.00	-	-		
84	OHX	AR	3437	-	0,6,6	0.00	-	-		
84	OHX	AR	3413	-	0,6,6	0.00	-	-		
84	OHX	J	301	-	0,6,6	0.00	-	-		
84	OHX	AR	3634	-	0,6,6	0.00	-	-		
84	OHX	1	3442	-	0,6,6	0.00	-	-		
84	OHX	AR	3426	-	0,6,6	0.00	-	-		
84	OHX	sR	2009	-	0,6,6	0.00	-	-		
84	OHX	M	201	-	0,6,6	0.00	-	-		
84	OHX	A	1905	-	0,6,6	0.00	-	-		
84	OHX	AR	3471	-	0,6,6	0.00	-	-		
84	OHX	AR	3524	-	0,6,6	0.00	-	-		
84	OHX	y	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3694	-	0,6,6	0.00	-	-		
84	OHX	sR	1952	-	0,6,6	0.00	-	-		
84	OHX	1	3670	-	0,6,6	0.00	-	-		
84	OHX	AS	205	-	0,6,6	0.00	-	-		
84	OHX	AS	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3662	-	0,6,6	0.00	-	-		
84	OHX	A	1967	-	0,6,6	0.00	-	-		
84	OHX	AR	3646	-	0,6,6	0.00	-	-		
84	OHX	A	2014	-	0,6,6	0.00	-	-		
84	OHX	sR	1998	-	0,6,6	0.00	-	-		
84	OHX	CG	303	-	0,6,6	0.00	-	-		
84	OHX	1	3578	-	0,6,6	0.00	-	-		
84	OHX	AR	3654	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AR	3439	-	0,6,6	0.00	-	-		
84	OHX	A	2004	-	0,6,6	0.00	-	-		
84	OHX	AR	3407	-	0,6,6	0.00	-	-		
84	OHX	1	3484	-	0,6,6	0.00	-	-		
84	OHX	1	3690	-	0,6,6	0.00	-	-		
84	OHX	1	3455	-	0,6,6	0.00	-	-		
84	OHX	AR	3523	-	0,6,6	0.00	-	-		
84	OHX	AR	3530	-	0,6,6	0.00	-	-		
84	OHX	1	3522	-	0,6,6	0.00	-	-		
84	OHX	sR	1945	-	0,6,6	0.00	-	-		
84	OHX	sR	1918	-	0,6,6	0.00	-	-		
84	OHX	AR	3693	-	0,6,6	0.00	-	-		
84	OHX	AR	3740	-	0,6,6	0.00	-	-		
84	OHX	1	3410	-	0,6,6	0.00	-	-		
84	OHX	1	3478	-	0,6,6	0.00	-	-		
84	OHX	4	204	-	0,6,6	0.00	-	-		
84	OHX	AR	3533	-	0,6,6	0.00	-	-		
84	OHX	A	2013	-	0,6,6	0.00	-	-		
84	OHX	AR	3507	-	0,6,6	0.00	-	-		
84	OHX	1	3402	-	0,6,6	0.00	-	-		
84	OHX	1	3453	-	0,6,6	0.00	-	-		
84	OHX	1	3697	-	0,6,6	0.00	-	-		
84	OHX	AR	3695	-	0,6,6	0.00	-	-		
84	OHX	AR	3537	-	0,6,6	0.00	-	-		
84	OHX	AR	3452	-	0,6,6	0.00	-	-		
84	OHX	AR	3561	-	0,6,6	0.00	-	-		
84	OHX	1	3579	-	0,6,6	0.00	-	-		
84	OHX	AR	3478	-	0,6,6	0.00	-	-		
84	OHX	AR	3445	-	0,6,6	0.00	-	-		
84	OHX	A	1979	-	0,6,6	0.00	-	-		
84	OHX	1	3570	-	0,6,6	0.00	-	-		
84	OHX	1	3548	-	0,6,6	0.00	-	-		
84	OHX	AR	3553	-	0,6,6	0.00	-	-		
84	OHX	sR	1949	-	0,6,6	0.00	-	-		
84	OHX	1	3501	-	0,6,6	0.00	-	-		
84	OHX	AR	3567	-	0,6,6	0.00	-	-		
84	OHX	AR	3633	-	0,6,6	0.00	-	-		
84	OHX	sR	2018	-	0,6,6	0.00	-	-		
84	OHX	AR	3545	-	0,6,6	0.00	-	-		
84	OHX	AR	3447	-	0,6,6	0.00	-	-		
84	OHX	AR	3532	-	0,6,6	0.00	-	-		
84	OHX	1	3677	-	0,6,6	0.00	-	-		
84	OHX	1	3726	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	A	2000	-	0,6,6	0.00	-	-		
84	OHX	AR	3719	-	0,6,6	0.00	-	-		
84	OHX	A	2001	-	0,6,6	0.00	-	-		
84	OHX	sR	2003	-	0,6,6	0.00	-	-		
84	OHX	1	3554	-	0,6,6	0.00	-	-		
84	OHX	1	3476	-	0,6,6	0.00	-	-		
84	OHX	4	206	-	0,6,6	0.00	-	-		
84	OHX	AR	3555	-	0,6,6	0.00	-	-		
84	OHX	sR	2016	-	0,6,6	0.00	-	-		
84	OHX	AR	3494	-	0,6,6	0.00	-	-		
84	OHX	AS	203	-	0,6,6	0.00	-	-		
84	OHX	AR	3711	-	0,6,6	0.00	-	-		
84	OHX	sR	2023	-	0,6,6	0.00	-	-		
84	OHX	A	2008	-	0,6,6	0.00	-	-		
84	OHX	1	3473	-	0,6,6	0.00	-	-		
84	OHX	AR	3712	-	0,6,6	0.00	-	-		
84	OHX	AR	3434	-	0,6,6	0.00	-	-		
84	OHX	AR	3575	-	0,6,6	0.00	-	-		
84	OHX	1	3656	-	0,6,6	0.00	-	-		
84	OHX	AR	3644	-	0,6,6	0.00	-	-		
84	OHX	AR	3459	-	0,6,6	0.00	-	-		
84	OHX	AR	3721	84	0,6,6	0.00	-	-		
84	OHX	AR	3604	-	0,6,6	0.00	-	-		
84	OHX	1	3684	-	0,6,6	0.00	-	-		
84	OHX	A	1948	-	0,6,6	0.00	-	-		
84	OHX	AR	3601	-	0,6,6	0.00	-	-		
84	OHX	sR	2020	-	0,6,6	0.00	-	-		
84	OHX	1	3676	-	0,6,6	0.00	-	-		
84	OHX	sR	2001	-	0,6,6	0.00	-	-		
84	OHX	k	401	-	0,6,6	0.00	-	-		
84	OHX	1	3575	-	0,6,6	0.00	-	-		
84	OHX	sR	2004	-	0,6,6	0.00	-	-		
84	OHX	1	3729	-	0,6,6	0.00	-	-		
84	OHX	AR	3544	-	0,6,6	0.00	-	-		
84	OHX	A	1990	-	0,6,6	0.00	-	-		
84	OHX	AT	210	-	0,6,6	0.00	-	-		
84	OHX	AR	3412	-	0,6,6	0.00	-	-		
84	OHX	1	3668	-	0,6,6	0.00	-	-		
84	OHX	sR	1958	-	0,6,6	0.00	-	-		
84	OHX	AR	3689	-	0,6,6	0.00	-	-		
84	OHX	1	3654	-	0,6,6	0.00	-	-		
84	OHX	1	3536	-	0,6,6	0.00	-	-		
84	OHX	1	3596	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	sR	1936	-	0,6,6	0.00	-	-		
84	OHX	1	3511	-	0,6,6	0.00	-	-		
84	OHX	AR	3518	-	0,6,6	0.00	-	-		
84	OHX	1	3552	-	0,6,6	0.00	-	-		
84	OHX	1	3572	-	0,6,6	0.00	-	-		
84	OHX	1	3605	-	0,6,6	0.00	-	-		
84	OHX	sR	1912	-	0,6,6	0.00	-	-		
84	OHX	sR	1961	-	0,6,6	0.00	-	-		
84	OHX	AR	3517	-	0,6,6	0.00	-	-		
84	OHX	AR	3501	-	0,6,6	0.00	-	-		
84	OHX	AR	3441	-	0,6,6	0.00	-	-		
84	OHX	1	3613	-	0,6,6	0.00	-	-		
84	OHX	1	3700	-	0,6,6	0.00	-	-		
84	OHX	CL	301	-	0,6,6	0.00	-	-		
84	OHX	AR	3663	-	0,6,6	0.00	-	-		
84	OHX	sR	2010	-	0,6,6	0.00	-	-		
84	OHX	sR	1917	-	0,6,6	0.00	-	-		
84	OHX	l	401	-	0,6,6	0.00	-	-		
84	OHX	AR	3462	-	0,6,6	0.00	-	-		
84	OHX	AR	3618	-	0,6,6	0.00	-	-		
84	OHX	1	3463	-	0,6,6	0.00	-	-		
84	OHX	1	3583	-	0,6,6	0.00	-	-		
84	OHX	1	3401	-	0,6,6	0.00	-	-		
84	OHX	c8	201	-	0,6,6	0.00	-	-		
84	OHX	A	2027	-	0,6,6	0.00	-	-		
84	OHX	1	3508	-	0,6,6	0.00	-	-		
84	OHX	1	3610	-	0,6,6	0.00	-	-		
84	OHX	sR	1971	-	0,6,6	0.00	-	-		
84	OHX	1	3407	-	0,6,6	0.00	-	-		
84	OHX	1	3633	-	0,6,6	0.00	-	-		
84	OHX	AR	3550	-	0,6,6	0.00	-	-		
84	OHX	3	201	-	0,6,6	0.00	-	-		
84	OHX	sR	1906	-	0,6,6	0.00	-	-		
84	OHX	AR	3735	-	0,6,6	0.00	-	-		
84	OHX	AR	3559	-	0,6,6	0.00	-	-		
84	OHX	sR	2006	-	0,6,6	0.00	-	-		
84	OHX	1	3532	-	0,6,6	0.00	-	-		
84	OHX	1	3563	-	0,6,6	0.00	-	-		
84	OHX	AR	3713	-	0,6,6	0.00	-	-		
84	OHX	1	3713	-	0,6,6	0.00	-	-		
84	OHX	1	3458	-	0,6,6	0.00	-	-		
84	OHX	AR	3648	-	0,6,6	0.00	-	-		
84	OHX	sR	1913	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	1	3582	-	0,6,6	0.00	-	-		
84	OHX	AC	101	-	0,6,6	0.00	-	-		
84	OHX	1	3587	-	0,6,6	0.00	-	-		
84	OHX	AT	209	-	0,6,6	0.00	-	-		
84	OHX	AR	3653	-	0,6,6	0.00	-	-		
84	OHX	CF	401	-	0,6,6	0.00	-	-		
84	OHX	AR	3707	-	0,6,6	0.00	-	-		
84	OHX	1	3426	-	0,6,6	0.00	-	-		
84	OHX	1	3694	-	0,6,6	0.00	-	-		
84	OHX	AR	3401	-	0,6,6	0.00	-	-		
84	OHX	1	3512	-	0,6,6	0.00	-	-		
84	OHX	d9	101	-	0,6,6	0.00	-	-		
84	OHX	1	3627	-	0,6,6	0.00	-	-		
84	OHX	sR	1905	-	0,6,6	0.00	-	-		
84	OHX	AR	3579	-	0,6,6	0.00	-	-		
84	OHX	sR	2030	-	0,6,6	0.00	-	-		
84	OHX	sR	1974	-	0,6,6	0.00	-	-		
84	OHX	1	3569	-	0,6,6	0.00	-	-		
84	OHX	AR	3583	-	0,6,6	0.00	-	-		
84	OHX	sR	2022	-	0,6,6	0.00	-	-		
84	OHX	AR	3538	-	0,6,6	0.00	-	-		
84	OHX	3	206	-	0,6,6	0.00	-	-		
84	OHX	AR	3588	-	0,6,6	0.00	-	-		
84	OHX	1	3580	-	0,6,6	0.00	-	-		
84	OHX	A	1907	-	0,6,6	0.00	-	-		
84	OHX	AR	3535	-	0,6,6	0.00	-	-		
84	OHX	1	3597	-	0,6,6	0.00	-	-		
84	OHX	AR	3744	-	0,6,6	0.00	-	-		
84	OHX	A	1991	-	0,6,6	0.00	-	-		
84	OHX	A	2012	-	0,6,6	0.00	-	-		
84	OHX	A	1938	-	0,6,6	0.00	-	-		
84	OHX	AR	3444	-	0,6,6	0.00	-	-		
84	OHX	AR	3473	-	0,6,6	0.00	-	-		
84	OHX	AR	3458	-	0,6,6	0.00	-	-		
84	OHX	AS	206	-	0,6,6	0.00	-	-		
84	OHX	A	1968	-	0,6,6	0.00	-	-		
84	OHX	A	1923	-	0,6,6	0.00	-	-		
84	OHX	AR	3591	-	0,6,6	0.00	-	-		
84	OHX	A	1977	-	0,6,6	0.00	-	-		
84	OHX	AR	3450	-	0,6,6	0.00	-	-		
84	OHX	AT	218	-	0,6,6	0.00	-	-		
84	OHX	AR	3635	-	0,6,6	0.00	-	-		
84	OHX	AR	3568	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	AR	3484	-	0,6,6	0.00	-	-		
84	OHX	A	2016	-	0,6,6	0.00	-	-		
84	OHX	AR	3497	-	0,6,6	0.00	-	-		
84	OHX	1	3423	-	0,6,6	0.00	-	-		
84	OHX	1	3543	-	0,6,6	0.00	-	-		
84	OHX	1	3412	-	0,6,6	0.00	-	-		
84	OHX	sR	2035	-	0,6,6	0.00	-	-		
84	OHX	AR	3645	-	0,6,6	0.00	-	-		
84	OHX	sR	1922	-	0,6,6	0.00	-	-		
84	OHX	sR	1959	-	0,6,6	0.00	-	-		
84	OHX	AR	3639	-	0,6,6	0.00	-	-		
84	OHX	4	214	-	0,6,6	0.00	-	-		
84	OHX	1	3409	-	0,6,6	0.00	-	-		
84	OHX	1	3425	-	0,6,6	0.00	-	-		
84	OHX	AR	3423	-	0,6,6	0.00	-	-		
84	OHX	AR	3599	-	0,6,6	0.00	-	-		
84	OHX	AR	3701	-	0,6,6	0.00	-	-		
84	OHX	AR	3597	-	0,6,6	0.00	-	-		
84	OHX	A	1946	-	0,6,6	0.00	-	-		
84	OHX	A	1952	-	0,6,6	0.00	-	-		
84	OHX	1	3528	-	0,6,6	0.00	-	-		
84	OHX	AR	3729	-	0,6,6	0.00	-	-		
84	OHX	sR	1966	-	0,6,6	0.00	-	-		
84	OHX	sR	2011	-	0,6,6	0.00	-	-		
84	OHX	1	3571	-	0,6,6	0.00	-	-		
84	OHX	A	1984	-	0,6,6	0.00	-	-		
84	OHX	1	3574	-	0,6,6	0.00	-	-		
84	OHX	AR	3643	-	0,6,6	0.00	-	-		
84	OHX	AT	217	-	0,6,6	0.00	-	-		
84	OHX	sR	1934	-	0,6,6	0.00	-	-		
84	OHX	AR	3492	-	0,6,6	0.00	-	-		
84	OHX	AR	3737	-	0,6,6	0.00	-	-		
84	OHX	AR	3453	-	0,6,6	0.00	-	-		
84	OHX	AR	3516	-	0,6,6	0.00	-	-		
84	OHX	AR	3608	-	0,6,6	0.00	-	-		
84	OHX	AR	3610	-	0,6,6	0.00	-	-		
84	OHX	CE	401	-	0,6,6	0.00	-	-		
84	OHX	1	3550	-	0,6,6	0.00	-	-		
84	OHX	A	2034	-	0,6,6	0.00	-	-		
84	OHX	AR	3510	-	0,6,6	0.00	-	-		
84	OHX	sR	1914	-	0,6,6	0.00	-	-		
84	OHX	sR	2032	-	0,6,6	0.00	-	-		
84	OHX	A	1924	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	sR	1942	-	0,6,6	0.00	-	-		
84	OHX	1	3439	-	0,6,6	0.00	-	-		
84	OHX	A	1953	-	0,6,6	0.00	-	-		
84	OHX	A	1972	-	0,6,6	0.00	-	-		
84	OHX	sR	1964	-	0,6,6	0.00	-	-		
84	OHX	A	1906	-	0,6,6	0.00	-	-		
84	OHX	1	3617	-	0,6,6	0.00	-	-		
84	OHX	1	3470	-	0,6,6	0.00	-	-		
84	OHX	AR	3528	-	0,6,6	0.00	-	-		
84	OHX	s1	301	-	0,6,6	0.00	-	-		
84	OHX	AR	3418	-	0,6,6	0.00	-	-		
84	OHX	AR	3508	-	0,6,6	0.00	-	-		
84	OHX	1	3695	-	0,6,6	0.00	-	-		
84	OHX	1	3682	-	0,6,6	0.00	-	-		
84	OHX	A	1999	-	0,6,6	0.00	-	-		
84	OHX	sR	1911	-	0,6,6	0.00	-	-		
84	OHX	DL	101	-	0,6,6	0.00	-	-		
84	OHX	A	1949	-	0,6,6	0.00	-	-		
84	OHX	1	3718	-	0,6,6	0.00	-	-		
84	OHX	CK	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3449	-	0,6,6	0.00	-	-		
84	OHX	1	3433	-	0,6,6	0.00	-	-		
84	OHX	1	3646	-	0,6,6	0.00	-	-		
84	OHX	sR	2014	-	0,6,6	0.00	-	-		
84	OHX	1	3639	-	0,6,6	0.00	-	-		
84	OHX	1	3413	-	0,6,6	0.00	-	-		
84	OHX	1	3535	-	0,6,6	0.00	-	-		
84	OHX	1	3561	-	0,6,6	0.00	-	-		
84	OHX	A	1940	-	0,6,6	0.00	-	-		
84	OHX	AR	3503	-	0,6,6	0.00	-	-		
84	OHX	AR	3522	-	0,6,6	0.00	-	-		
84	OHX	1	3520	-	0,6,6	0.00	-	-		
84	OHX	AR	3564	-	0,6,6	0.00	-	-		
84	OHX	A	1996	-	0,6,6	0.00	-	-		
84	OHX	sR	1933	-	0,6,6	0.00	-	-		
84	OHX	AR	3696	-	0,6,6	0.00	-	-		
84	OHX	A	1954	-	0,6,6	0.00	-	-		
84	OHX	1	3421	-	0,6,6	0.00	-	-		
84	OHX	1	3545	-	0,6,6	0.00	-	-		
84	OHX	sR	1928	-	0,6,6	0.00	-	-		
84	OHX	AR	3638	-	0,6,6	0.00	-	-		
84	OHX	1	3595	-	0,6,6	0.00	-	-		
84	OHX	4	210	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	OHX	A	1960	-	0,6,6	0.00	-	-		
84	OHX	sR	1923	-	0,6,6	0.00	-	-		
84	OHX	A	1965	-	0,6,6	0.00	-	-		
84	OHX	sR	1929	-	0,6,6	0.00	-	-		
84	OHX	sR	1926	-	0,6,6	0.00	-	-		
84	OHX	AR	3442	-	0,6,6	0.00	-	-		
84	OHX	1	3665	-	0,6,6	0.00	-	-		
84	OHX	DH	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3495	-	0,6,6	0.00	-	-		
84	OHX	CG	302	-	0,6,6	0.00	-	-		
84	OHX	AR	3498	-	0,6,6	0.00	-	-		
84	OHX	A	2011	-	0,6,6	0.00	-	-		
84	OHX	AR	3408	-	0,6,6	0.00	-	-		
84	OHX	AR	3512	-	0,6,6	0.00	-	-		
84	OHX	A	1942	-	0,6,6	0.00	-	-		
84	OHX	sR	1927	-	0,6,6	0.00	-	-		
84	OHX	AR	3486	-	0,6,6	0.00	-	-		
84	OHX	AR	3636	-	0,6,6	0.00	-	-		
84	OHX	AT	213	-	0,6,6	0.00	-	-		
84	OHX	1	3542	-	0,6,6	0.00	-	-		
84	OHX	sR	2017	-	0,6,6	0.00	-	-		
84	OHX	AR	3620	-	0,6,6	0.00	-	-		
84	OHX	AR	3536	-	0,6,6	0.00	-	-		
84	OHX	A	1962	-	0,6,6	0.00	-	-		
84	OHX	1	3728	-	0,6,6	0.00	-	-		
84	OHX	AR	3621	-	0,6,6	0.00	-	-		
84	OHX	A	1975	-	0,6,6	0.00	-	-		
84	OHX	AR	3420	-	0,6,6	0.00	-	-		
84	OHX	sR	1921	-	0,6,6	0.00	-	-		
84	OHX	A	1914	-	0,6,6	0.00	-	-		
84	OHX	CP	501	-	0,6,6	0.00	-	-		
84	OHX	AT	214	-	0,6,6	0.00	-	-		
84	OHX	1	3497	-	0,6,6	0.00	-	-		
84	OHX	1	3559	-	0,6,6	0.00	-	-		
84	OHX	sR	1948	-	0,6,6	0.00	-	-		
84	OHX	AR	3602	-	0,6,6	0.00	-	-		
84	OHX	1	3699	-	0,6,6	0.00	-	-		
84	OHX	sR	1987	-	0,6,6	0.00	-	-		
84	OHX	AG	201	-	0,6,6	0.00	-	-		
84	OHX	AR	3577	-	0,6,6	0.00	-	-		

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
86	7AL	AR	4246	-	-	2/8/60/60	0/3/3/3
86	7AL	1	4210	-	-	2/8/60/60	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	1	4210	7AL	O4-C8-C7	2.33	114.89	109.92

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	1	4210	7AL	C10-C14-C15-C16
86	AR	4246	7AL	C10-C14-C15-C16
86	1	4210	7AL	C10-C14-C15-O1
86	AR	4246	7AL	C10-C14-C15-O1

There are no ring outliers.

514 monomers are involved in 753 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3587	OHX	2	0
84	1	3705	OHX	5	0
84	1	3427	OHX	3	0
84	O	201	OHX	1	0
84	A	1904	OHX	1	0
84	A	1901	OHX	2	0
84	1	3459	OHX	1	0
84	1	3546	OHX	1	0
84	1	3500	OHX	2	0
84	AR	3726	OHX	1	0
84	A	1936	OHX	1	0
84	1	3493	OHX	3	0
84	1	3644	OHX	1	0
84	3	204	OHX	1	0
84	1	3620	OHX	1	0
84	A	1922	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3691	OHX	1	0
84	1	3601	OHX	1	0
84	AR	3730	OHX	2	0
84	AR	3741	OHX	1	0
84	AR	3556	OHX	1	0
84	1	3503	OHX	2	0
84	CX	202	OHX	2	0
84	AT	206	OHX	2	0
84	1	3489	OHX	1	0
84	1	3603	OHX	1	0
84	A	2021	OHX	1	0
84	1	3414	OHX	2	0
84	1	3436	OHX	2	0
84	1	3692	OHX	1	0
84	CM	201	OHX	1	0
84	AR	3504	OHX	1	0
84	1	3418	OHX	2	0
84	AR	3732	OHX	1	0
84	AR	3586	OHX	2	0
84	1	3441	OHX	1	0
84	AR	3490	OHX	1	0
84	A	1985	OHX	1	0
84	AR	3624	OHX	1	0
84	AR	3489	OHX	1	0
84	1	3510	OHX	1	0
84	A	1987	OHX	1	0
84	AR	3506	OHX	2	0
84	1	3406	OHX	4	0
84	1	3502	OHX	2	0
84	AR	3406	OHX	1	0
84	A	1931	OHX	1	0
84	AR	3403	OHX	1	0
84	AR	3554	OHX	1	0
84	A	2042	OHX	1	0
84	AR	3513	OHX	3	0
84	A	2038	OHX	1	0
84	AR	3706	OHX	2	0
84	A	2032	OHX	1	0
84	AR	3417	OHX	1	0
84	AR	3656	OHX	2	0
84	1	3671	OHX	2	0
84	1	3539	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	A	1925	OHX	2	0
84	1	3614	OHX	1	0
84	AR	3488	OHX	1	0
84	AR	3475	OHX	2	0
84	AR	3548	OHX	1	0
84	AR	3687	OHX	1	0
84	AR	3605	OHX	1	0
84	1	3504	OHX	1	0
84	AR	3470	OHX	1	0
84	1	3422	OHX	1	0
84	AR	3448	OHX	1	0
84	AR	3647	OHX	2	0
84	AR	3690	OHX	1	0
84	AR	3451	OHX	1	0
84	AT	211	OHX	1	0
84	AR	3519	OHX	1	0
84	DQ	201	OHX	3	0
84	AR	3697	OHX	2	0
84	1	3424	OHX	1	0
84	AR	3574	OHX	1	0
84	AR	3477	OHX	1	0
84	1	3722	OHX	1	0
84	CE	402	OHX	1	0
84	AR	3402	OHX	1	0
84	1	3444	OHX	1	0
84	AR	3627	OHX	1	0
84	AR	3539	OHX	2	0
84	AT	204	OHX	1	0
84	AR	3456	OHX	1	0
84	AR	3593	OHX	1	0
84	AR	3600	OHX	1	0
84	A	2030	OHX	3	0
84	1	3624	OHX	1	0
84	AR	3469	OHX	1	0
84	AR	3502	OHX	1	0
84	AR	3705	OHX	4	0
84	AR	3743	OHX	1	0
84	1	3642	OHX	1	0
84	1	3445	OHX	1	0
84	A	1963	OHX	2	0
84	AR	3455	OHX	1	0
84	A	1910	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3556	OHX	2	0
84	AR	3570	OHX	1	0
84	1	3666	OHX	1	0
84	1	3417	OHX	2	0
84	1	3419	OHX	2	0
84	AR	3584	OHX	1	0
84	1	3609	OHX	1	0
84	AR	3692	OHX	1	0
84	A	1916	OHX	2	0
84	1	3446	OHX	1	0
84	AR	3625	OHX	1	0
84	AT	203	OHX	1	0
84	1	3411	OHX	1	0
84	AR	3685	OHX	1	0
84	1	3711	OHX	3	0
84	AR	3623	OHX	1	0
84	AR	3738	OHX	7	0
84	1	3622	OHX	1	0
84	AR	3678	OHX	1	0
84	A	1928	OHX	2	0
84	A	1918	OHX	1	0
84	AR	3640	OHX	1	0
84	1	3518	OHX	1	0
84	4	215	OHX	1	0
84	3	203	OHX	1	0
84	1	3429	OHX	1	0
84	1	3534	OHX	1	0
84	AR	3446	OHX	1	0
84	1	3724	OHX	1	0
84	1	3584	OHX	1	0
84	1	3468	OHX	3	0
84	AR	3592	OHX	1	0
84	AR	3562	OHX	2	0
84	1	3604	OHX	1	0
84	A	1956	OHX	1	0
84	1	3616	OHX	1	0
84	A	2019	OHX	1	0
84	AT	216	OHX	2	0
84	A	2022	OHX	1	0
84	4	201	OHX	1	0
84	AR	3521	OHX	1	0
84	A	1988	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	A	1919	OHX	1	0
84	AR	3551	OHX	1	0
84	A	1902	OHX	1	0
84	AR	3435	OHX	1	0
84	AR	3411	OHX	1	0
84	1	3652	OHX	2	0
84	1	3687	OHX	1	0
84	AR	3416	OHX	1	0
84	1	3490	OHX	1	0
84	1	3592	OHX	4	0
84	1	3721	OHX	1	0
84	1	3689	OHX	1	0
84	AR	3606	OHX	1	0
84	AR	3580	OHX	1	0
84	AR	3405	OHX	1	0
84	CF	402	OHX	1	0
84	1	3648	OHX	1	0
84	AR	3572	OHX	1	0
84	AR	3520	OHX	1	0
84	1	3588	OHX	1	0
84	AR	3582	OHX	1	0
84	AR	3457	OHX	1	0
86	AR	4246	7AL	1	0
84	1	3483	OHX	2	0
84	1	3581	OHX	1	0
84	AR	3718	OHX	2	0
84	AR	3569	OHX	1	0
84	1	3471	OHX	1	0
84	1	3515	OHX	1	0
84	AR	3734	OHX	2	0
84	1	3586	OHX	1	0
84	A	1913	OHX	2	0
84	A	1998	OHX	2	0
84	AR	3688	OHX	2	0
84	AR	3443	OHX	1	0
84	3	202	OHX	1	0
84	AR	3409	OHX	1	0
84	1	3465	OHX	1	0
84	AR	3613	OHX	2	0
84	AR	3496	OHX	1	0
84	A	1920	OHX	1	0
84	A	1903	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3403	OHX	1	0
84	AR	3615	OHX	1	0
84	AR	3514	OHX	1	0
84	A	1986	OHX	1	0
84	AR	3686	OHX	1	0
84	AR	3571	OHX	2	0
84	A	2024	OHX	6	0
84	1	3686	OHX	1	0
84	AS	208	OHX	1	0
84	AR	3703	OHX	5	0
84	1	3420	OHX	2	0
84	1	3404	OHX	1	0
84	1	3492	OHX	2	0
84	AR	3664	OHX	2	0
84	T	201	OHX	1	0
84	1	3591	OHX	2	0
84	AR	3677	OHX	4	0
84	1	3461	OHX	2	0
84	AR	3541	OHX	1	0
84	A	2007	OHX	2	0
84	1	3540	OHX	5	0
84	1	3526	OHX	1	0
84	AR	3603	OHX	1	0
84	1	3683	OHX	1	0
84	AR	3659	OHX	1	0
84	AR	3585	OHX	1	0
84	AS	202	OHX	2	0
84	1	3675	OHX	1	0
84	AR	3468	OHX	1	0
84	1	3725	OHX	2	0
84	1	3679	OHX	2	0
84	AR	3611	OHX	2	0
84	AR	3649	OHX	2	0
84	1	3598	OHX	1	0
84	AR	3674	OHX	1	0
84	AS	210	OHX	1	0
84	Q	201	OHX	2	0
84	1	3653	OHX	1	0
84	AR	3526	OHX	6	0
84	AR	3667	OHX	2	0
84	AS	204	OHX	1	0
84	AR	3552	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3680	OHX	1	0
84	1	3519	OHX	2	0
84	1	3513	OHX	1	0
84	A	1917	OHX	1	0
84	1	3451	OHX	1	0
84	1	3629	OHX	1	0
84	AR	3465	OHX	4	0
84	AR	3660	OHX	2	0
84	AR	3720	OHX	1	0
84	4	202	OHX	1	0
84	A	2037	OHX	1	0
84	AR	3736	OHX	1	0
84	AR	3415	OHX	2	0
84	1	3448	OHX	1	0
84	AR	3629	OHX	1	0
84	AR	3716	OHX	1	0
84	A	2009	OHX	4	0
84	A	1966	OHX	1	0
84	AR	3467	OHX	1	0
84	A	1909	OHX	8	0
84	3	205	OHX	1	0
84	A	1915	OHX	2	0
84	1	3524	OHX	1	0
84	1	3469	OHX	1	0
84	1	3606	OHX	1	0
84	A	1937	OHX	1	0
84	1	3479	OHX	1	0
84	A	1947	OHX	1	0
84	AR	3594	OHX	1	0
84	A	1911	OHX	2	0
84	1	3562	OHX	1	0
84	1	3730	OHX	5	0
84	AK	102	OHX	3	0
84	A	1964	OHX	2	0
84	A	1939	OHX	2	0
84	AR	3715	OHX	1	0
84	1	3538	OHX	3	0
84	1	3632	OHX	1	0
84	AR	3481	OHX	3	0
84	1	3667	OHX	1	0
84	1	3637	OHX	1	0
84	AT	212	OHX	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3684	OHX	1	0
84	AR	3483	OHX	1	0
84	AR	3410	OHX	3	0
84	A	1912	OHX	1	0
84	1	3719	OHX	1	0
84	1	3712	OHX	1	0
84	A	1997	OHX	1	0
84	AR	3655	OHX	1	0
84	AR	3419	OHX	2	0
84	1	3462	OHX	1	0
84	AR	3702	OHX	2	0
84	1	3611	OHX	1	0
84	4	208	OHX	1	0
84	1	3688	OHX	2	0
84	1	3593	OHX	1	0
84	AR	3619	OHX	1	0
84	1	3701	OHX	2	0
84	1	3450	OHX	1	0
84	1	3460	OHX	2	0
84	1	3661	OHX	2	0
84	AR	3598	OHX	1	0
84	1	3517	OHX	1	0
84	AR	3709	OHX	1	0
84	1	3428	OHX	1	0
84	1	3664	OHX	3	0
84	1	3405	OHX	1	0
84	CV	201	OHX	1	0
84	1	3577	OHX	1	0
84	AR	3661	OHX	1	0
84	AR	3427	OHX	2	0
84	AR	3682	OHX	1	0
84	A	1932	OHX	2	0
84	A	1951	OHX	2	0
84	AR	3529	OHX	2	0
84	1	3474	OHX	4	0
84	AR	3612	OHX	3	0
84	1	3630	OHX	1	0
84	1	3567	OHX	1	0
84	1	3716	OHX	2	0
84	1	3494	OHX	3	0
84	4	213	OHX	1	0
84	AR	3463	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3590	OHX	1	0
84	A	2005	OHX	1	0
84	AT	202	OHX	1	0
84	AR	3464	OHX	2	0
84	AR	3573	OHX	1	0
84	A	2003	OHX	1	0
84	1	3635	OHX	1	0
84	A	1943	OHX	3	0
84	1	3509	OHX	1	0
84	AR	3421	OHX	1	0
84	1	3600	OHX	1	0
84	AR	3642	OHX	1	0
84	A	2029	OHX	1	0
84	AP	502	OHX	5	0
84	1	3507	OHX	1	0
84	DD	102	OHX	1	0
84	1	3457	OHX	1	0
84	1	3626	OHX	1	0
84	A	2035	OHX	1	0
84	1	3430	OHX	1	0
84	A	1944	OHX	1	0
84	1	3437	OHX	4	0
84	A	1970	OHX	1	0
84	AR	3454	OHX	2	0
84	AT	207	OHX	2	0
84	1	3466	OHX	1	0
84	AR	3461	OHX	1	0
84	AR	3472	OHX	2	0
84	A	1973	OHX	2	0
84	1	3482	OHX	1	0
84	1	3612	OHX	1	0
84	1	3594	OHX	1	0
84	4	207	OHX	1	0
84	A	2023	OHX	1	0
84	1	3640	OHX	1	0
84	AR	3733	OHX	1	0
84	AR	3460	OHX	2	0
84	AR	3511	OHX	1	0
84	1	3485	OHX	1	0
84	1	3408	OHX	2	0
84	1	3544	OHX	1	0
84	AR	3728	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3424	OHX	1	0
84	AR	3437	OHX	2	0
84	AR	3413	OHX	1	0
84	J	301	OHX	1	0
84	1	3442	OHX	1	0
84	AR	3426	OHX	1	0
84	M	201	OHX	1	0
84	AR	3524	OHX	2	0
84	AR	3694	OHX	2	0
84	1	3670	OHX	1	0
84	AS	205	OHX	1	0
84	AS	201	OHX	1	0
84	CG	303	OHX	1	0
84	1	3578	OHX	1	0
84	AR	3439	OHX	1	0
84	A	2004	OHX	1	0
84	AR	3407	OHX	2	0
84	1	3690	OHX	1	0
84	AR	3530	OHX	1	0
84	1	3522	OHX	1	0
84	4	204	OHX	1	0
84	AR	3533	OHX	2	0
84	A	2013	OHX	1	0
84	AR	3507	OHX	4	0
84	1	3402	OHX	1	0
84	1	3453	OHX	1	0
84	1	3697	OHX	4	0
84	AR	3695	OHX	3	0
84	AR	3537	OHX	1	0
84	AR	3561	OHX	2	0
84	AR	3445	OHX	8	0
84	1	3570	OHX	2	0
84	AR	3553	OHX	1	0
84	1	3501	OHX	1	0
84	AR	3567	OHX	1	0
84	AR	3633	OHX	1	0
84	AR	3545	OHX	3	0
84	AR	3447	OHX	1	0
84	AR	3532	OHX	2	0
84	1	3554	OHX	2	0
84	1	3476	OHX	1	0
84	4	206	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3711	OHX	1	0
84	A	2008	OHX	2	0
84	1	3473	OHX	1	0
84	AR	3434	OHX	1	0
84	AR	3575	OHX	1	0
84	1	3656	OHX	1	0
84	AR	3459	OHX	2	0
84	AR	3721	OHX	7	0
84	1	3684	OHX	1	0
84	1	3575	OHX	1	0
84	AT	210	OHX	1	0
84	AR	3412	OHX	1	0
84	1	3668	OHX	1	0
84	AR	3689	OHX	2	0
84	1	3654	OHX	1	0
84	1	3536	OHX	1	0
84	1	3596	OHX	1	0
84	1	3511	OHX	2	0
84	AR	3518	OHX	1	0
84	1	3552	OHX	1	0
84	AR	3517	OHX	1	0
84	AR	3441	OHX	1	0
84	CL	301	OHX	5	0
84	AR	3663	OHX	1	0
84	AR	3462	OHX	1	0
84	AR	3618	OHX	1	0
84	1	3463	OHX	1	0
84	1	3401	OHX	1	0
84	A	2027	OHX	1	0
84	1	3508	OHX	1	0
84	1	3610	OHX	1	0
84	AR	3735	OHX	1	0
84	1	3532	OHX	1	0
84	1	3563	OHX	1	0
84	AR	3713	OHX	2	0
84	1	3713	OHX	4	0
84	AC	101	OHX	2	0
84	AT	209	OHX	2	0
84	AR	3653	OHX	1	0
84	CF	401	OHX	3	0
84	1	3426	OHX	1	0
84	1	3694	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3401	OHX	1	0
84	1	3627	OHX	1	0
84	1	3569	OHX	2	0
84	AR	3583	OHX	1	0
84	3	206	OHX	1	0
84	1	3580	OHX	4	0
84	A	1907	OHX	1	0
84	AR	3535	OHX	1	0
84	AR	3744	OHX	1	0
84	A	2012	OHX	1	0
84	A	1938	OHX	1	0
84	AR	3444	OHX	2	0
84	AR	3473	OHX	1	0
84	AR	3458	OHX	2	0
84	A	1968	OHX	3	0
84	A	1923	OHX	1	0
84	AR	3450	OHX	1	0
84	AT	218	OHX	1	0
84	AR	3635	OHX	2	0
84	AR	3568	OHX	1	0
84	AR	3497	OHX	1	0
84	1	3543	OHX	1	0
84	1	3409	OHX	1	0
84	1	3425	OHX	1	0
84	AR	3599	OHX	5	0
84	AR	3597	OHX	3	0
84	A	1952	OHX	1	0
84	A	1984	OHX	1	0
84	AR	3643	OHX	1	0
84	AT	217	OHX	1	0
84	AR	3492	OHX	2	0
84	AR	3453	OHX	1	0
84	AR	3516	OHX	5	0
84	AR	3608	OHX	3	0
84	CE	401	OHX	3	0
84	AR	3510	OHX	2	0
84	A	1953	OHX	1	0
84	A	1972	OHX	1	0
84	AR	3528	OHX	2	0
84	AR	3418	OHX	1	0
84	AR	3508	OHX	2	0
84	1	3695	OHX	1	0

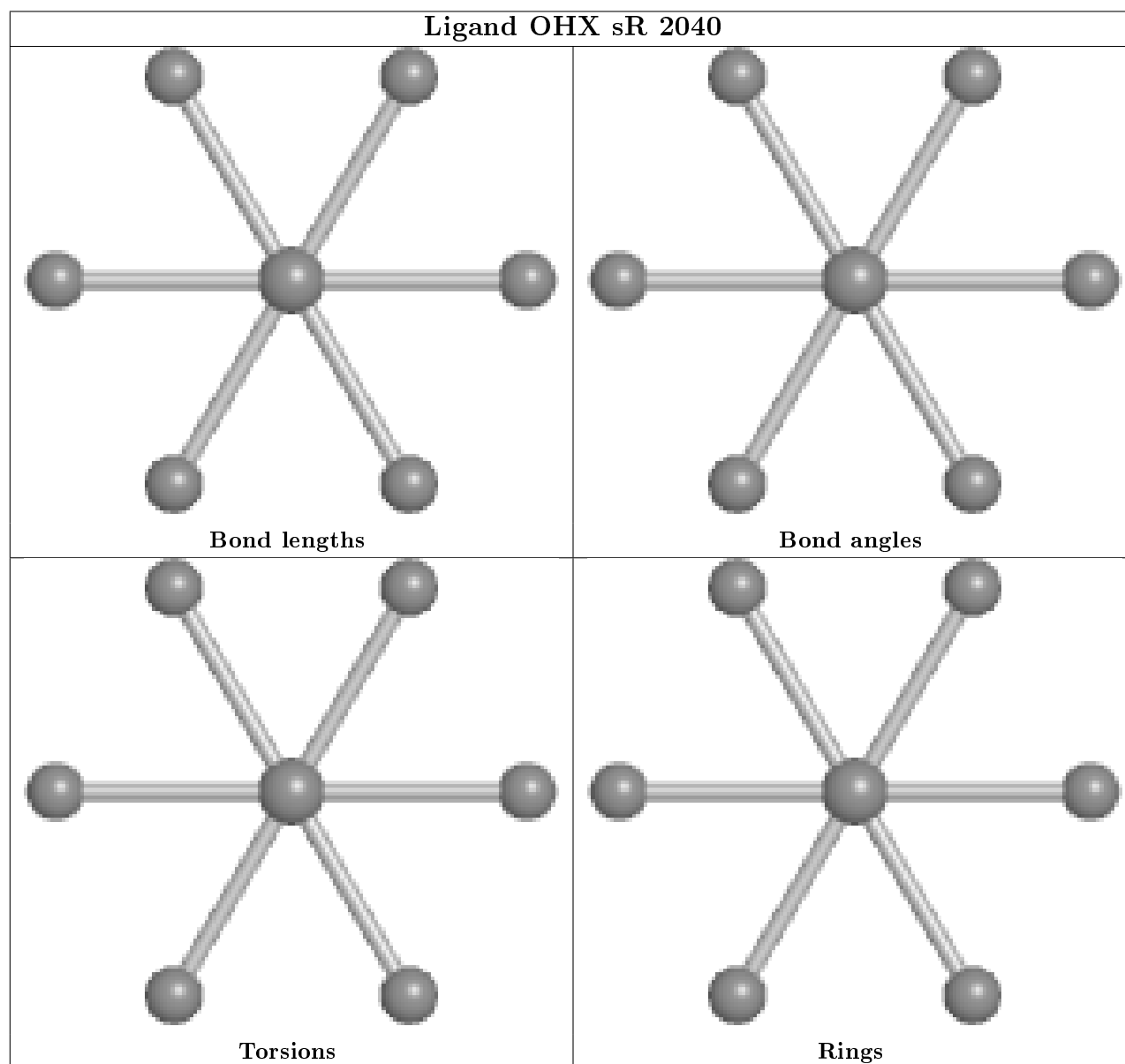
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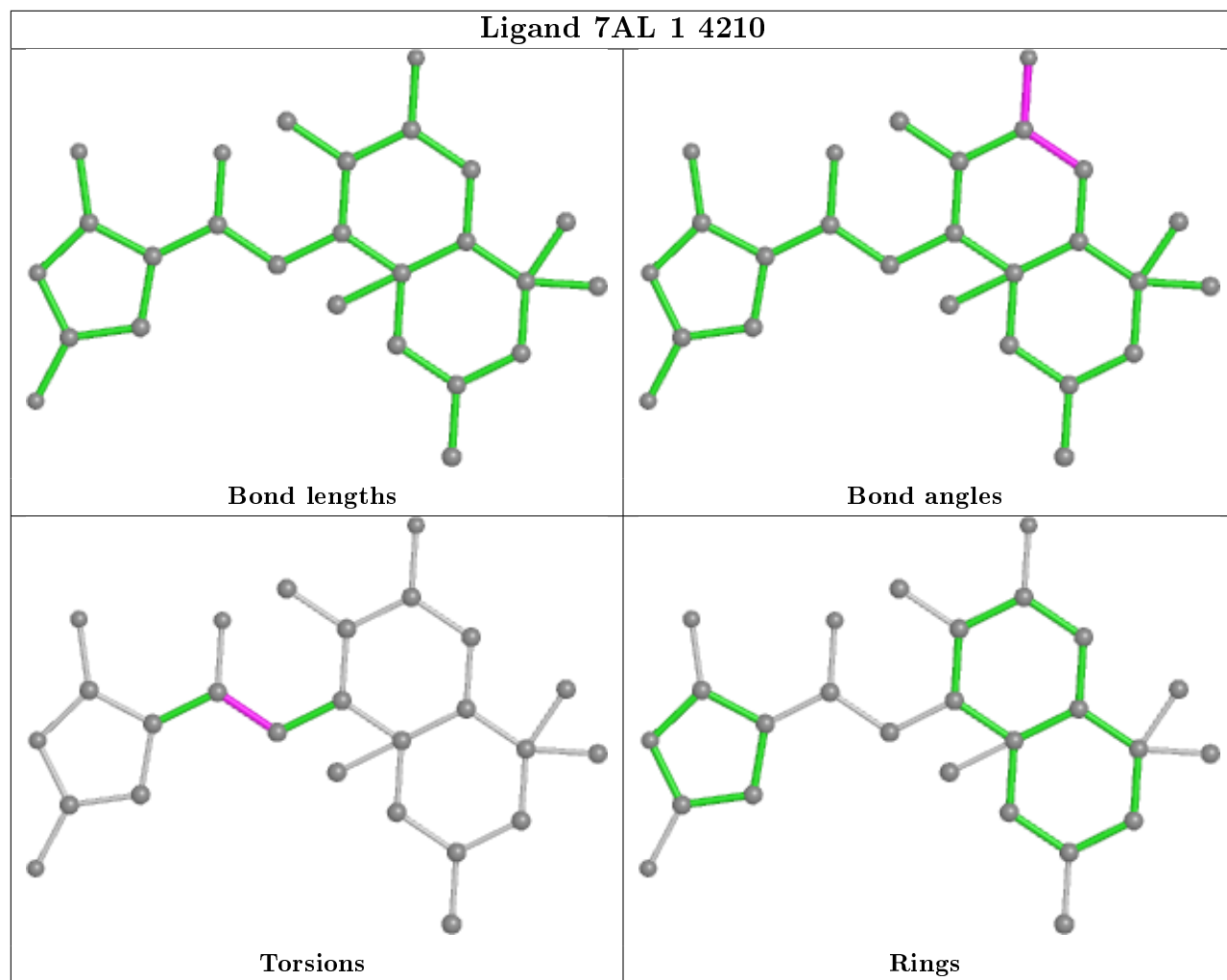
Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3682	OHX	3	0
84	A	1999	OHX	1	0
84	DL	101	OHX	2	0
84	AR	3449	OHX	1	0
84	1	3646	OHX	1	0
84	1	3639	OHX	1	0
84	1	3535	OHX	2	0
84	1	3561	OHX	2	0
84	A	1940	OHX	1	0
84	AR	3503	OHX	1	0
84	1	3520	OHX	2	0
84	AR	3564	OHX	1	0
84	AR	3696	OHX	2	0
84	A	1954	OHX	3	0
84	1	3545	OHX	1	0
84	AR	3638	OHX	2	0
84	1	3595	OHX	1	0
84	1	3665	OHX	3	0
84	AR	3495	OHX	3	0
84	CG	302	OHX	3	0
84	AR	3408	OHX	2	0
84	AR	3512	OHX	1	0
84	A	1942	OHX	1	0
84	AR	3486	OHX	2	0
84	AR	3636	OHX	1	0
84	1	3542	OHX	1	0
84	AR	3620	OHX	1	0
84	AR	3536	OHX	1	0
84	A	1962	OHX	3	0
84	AR	3420	OHX	1	0
84	A	1914	OHX	1	0
84	CP	501	OHX	1	0
84	AT	214	OHX	2	0
84	AR	3602	OHX	1	0
84	AG	201	OHX	1	0
84	AR	3577	OHX	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

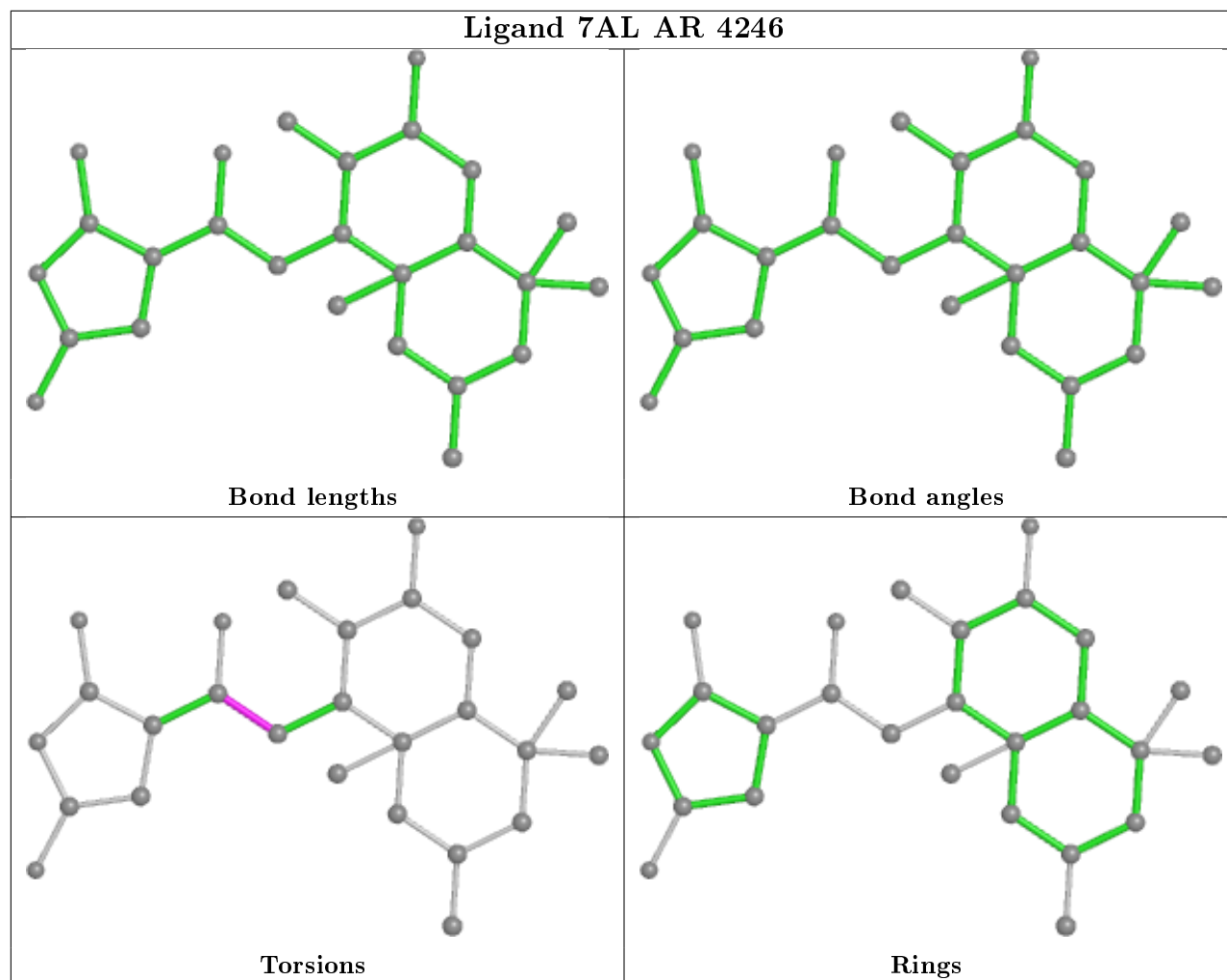
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

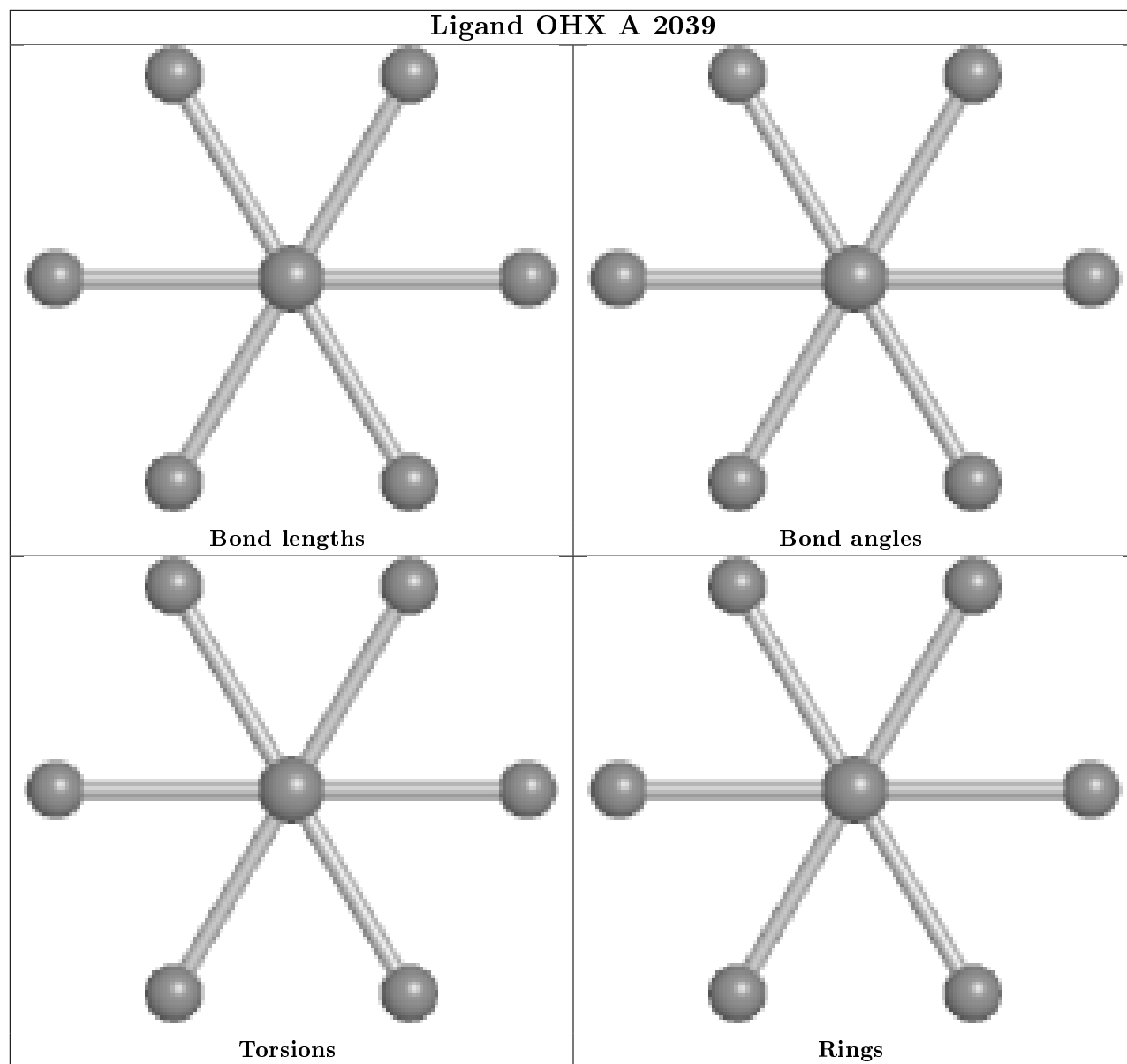


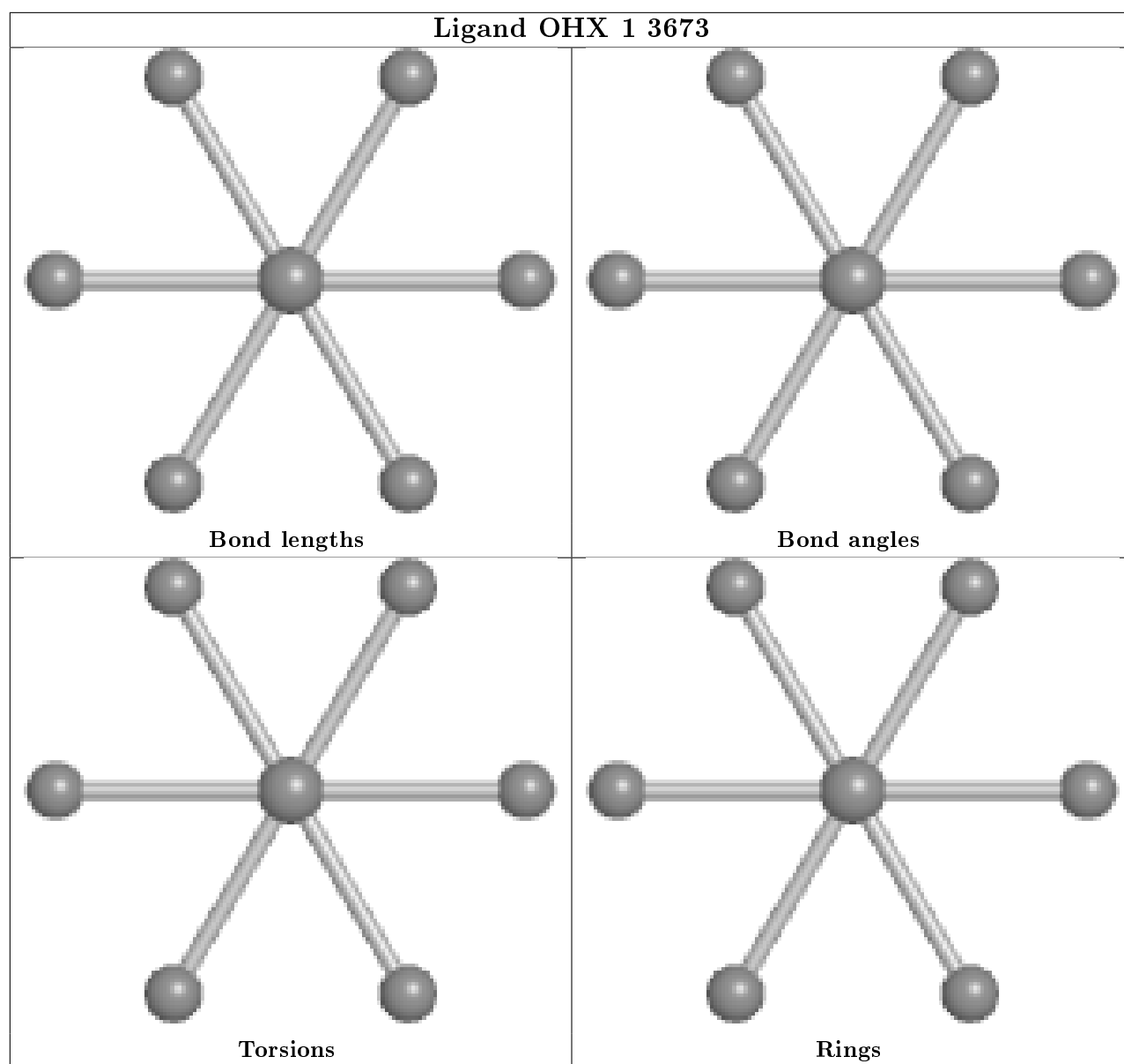
Ligand 7AL 1 4210

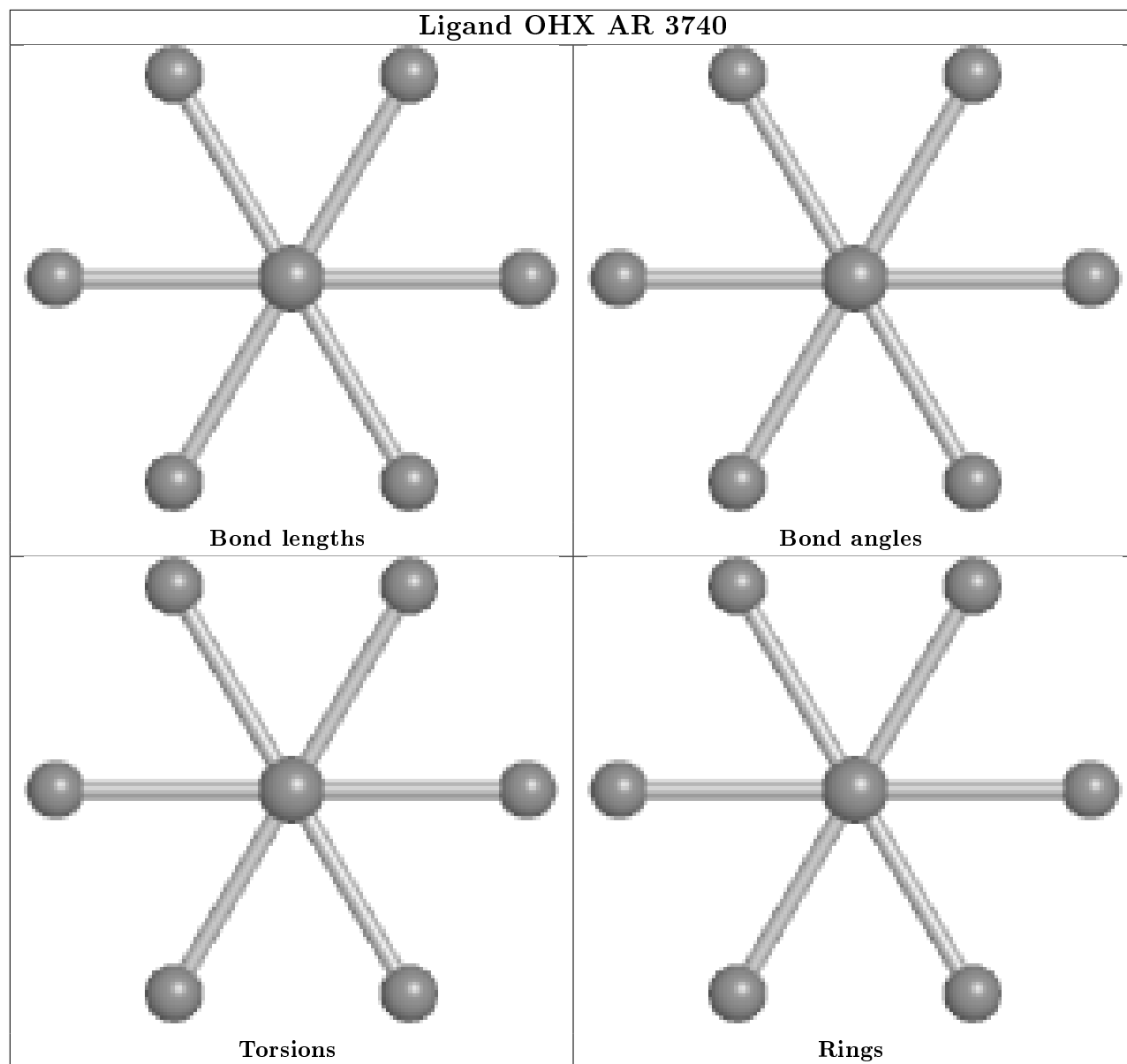


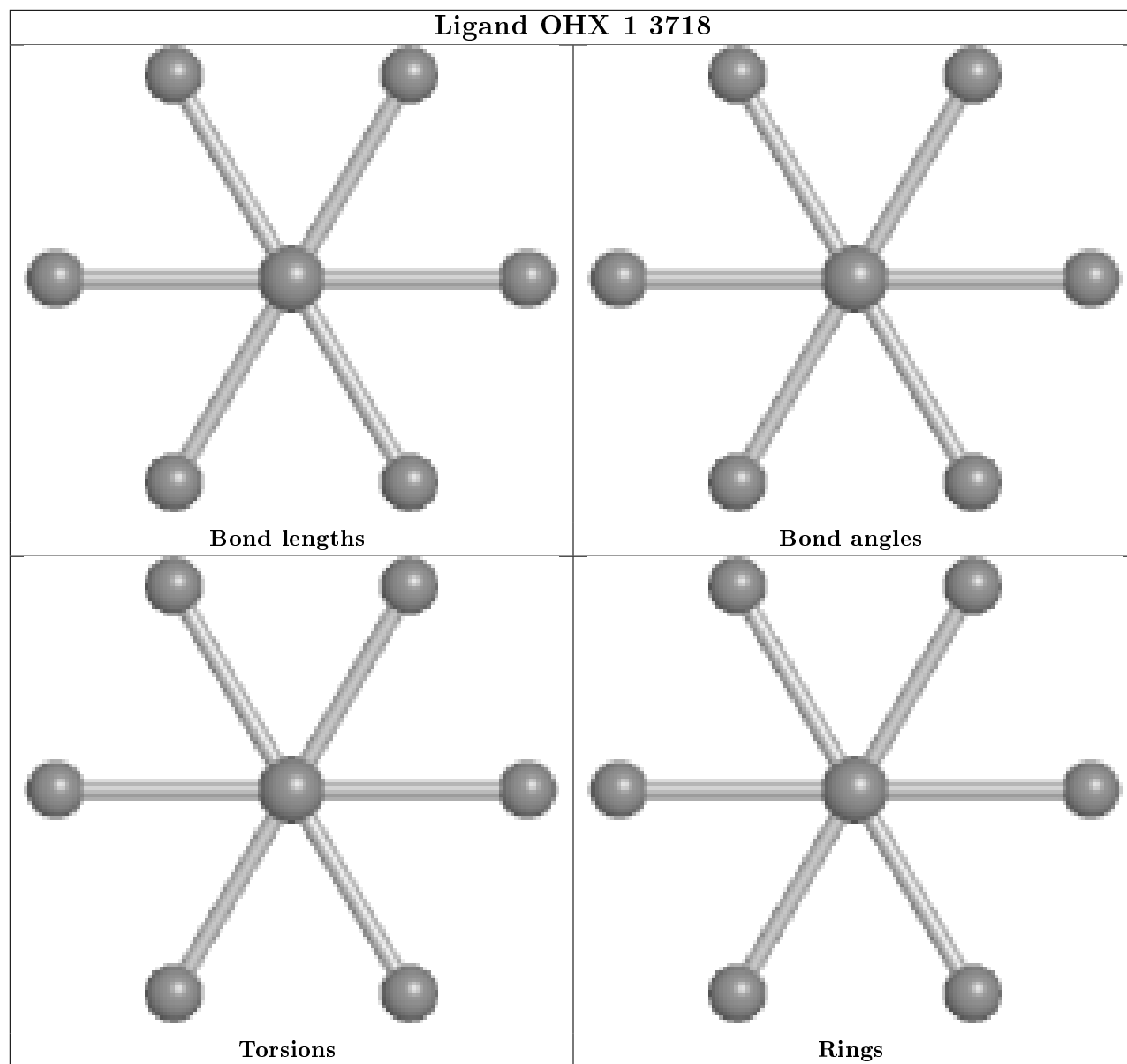
Ligand 7AL AR 4246











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AR	3
1	1	3
47	sM	2

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Mol	Chain	Number of breaks
48	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	85:SER	C	119:UNK	N	43.91
1	sM	139:UNK	C	155:UNK	N	37.53
1	1	1955:U	O3'	2093:A	P	25.84
1	AR	1955:U	O3'	2093:A	P	24.08
1	1	2445:A	O3'	2501:U	P	15.80
1	AR	2445:A	O3'	2501:U	P	15.47
1	AR	440:A	O3'	494:G	P	14.11
1	1	440:A	O3'	494:G	P	13.47
1	A	1716:C	O3'	1717:G	P	3.73

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	1	3149/3149 (100%)	-0.02	78 (2%)	57	29	23, 45, 148, 258	0
1	AR	3149/3149 (100%)	-0.00	87 (2%)	53	25	24, 48, 147, 276	0
2	3	121/121 (100%)	-0.34	0	100	100	33, 61, 76, 92	0
2	AS	121/121 (100%)	-0.33	0	100	100	30, 54, 69, 103	0
3	4	158/158 (100%)	-0.10	1 (0%)	89	72	28, 46, 98, 165	0
3	AT	158/158 (100%)	-0.06	2 (1%)	77	51	35, 57, 112, 166	0
4	CD	252/252 (100%)	-0.27	2 (0%)	86	65	31, 51, 76, 131	0
4	j	252/252 (100%)	-0.27	0	100	100	26, 45, 64, 113	0
5	CE	386/386 (100%)	-0.35	2 (0%)	91	75	24, 42, 66, 121	0
5	k	386/386 (100%)	-0.36	1 (0%)	94	84	26, 49, 69, 116	0
6	CF	361/361 (100%)	-0.33	0	100	100	28, 48, 75, 107	0
6	l	361/361 (100%)	-0.34	0	100	100	24, 43, 72, 92	0
7	CG	296/296 (100%)	-0.14	4 (1%)	75	49	40, 56, 94, 133	0
7	m	296/296 (100%)	0.09	6 (2%)	65	36	42, 70, 104, 152	0
8	CH	156/175 (89%)	-0.25	3 (1%)	66	37	36, 47, 85, 108	0
8	n	156/175 (89%)	-0.34	0	100	100	33, 44, 74, 119	0
9	CI	222/222 (100%)	-0.30	3 (1%)	75	49	28, 38, 86, 165	0
9	o	222/222 (100%)	-0.33	2 (0%)	84	63	28, 38, 75, 155	0
10	CJ	233/233 (100%)	0.73	22 (9%)	8	3	65, 82, 141, 172	0
10	p	233/233 (100%)	0.18	4 (1%)	70	41	50, 68, 138, 161	0
11	CK	191/191 (100%)	-0.22	3 (1%)	72	44	36, 47, 78, 142	0
11	q	191/191 (100%)	-0.31	1 (0%)	91	75	41, 56, 75, 141	0
12	CL	211/220 (95%)	0.02	6 (2%)	53	25	29, 55, 91, 155	0
12	r	211/220 (95%)	-0.24	0	100	100	28, 48, 95, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	CM	169/169 (100%)	-0.21	1 (0%) 89 72	42, 62, 82, 103	0
13	s	169/169 (100%)	-0.04	1 (0%) 89 72	50, 73, 91, 114	0
14	CN	193/193 (100%)	0.10	5 (2%) 56 27	31, 61, 121, 150	0
14	t	193/193 (100%)	-0.16	2 (1%) 82 59	25, 51, 110, 138	0
15	CO	136/136 (100%)	-0.42	1 (0%) 87 69	35, 43, 72, 91	0
15	u	136/136 (100%)	-0.42	0 100 100	38, 46, 70, 86	0
16	CP	203/203 (100%)	-0.22	0 100 100	34, 52, 67, 70	0
16	v	203/203 (100%)	-0.36	0 100 100	26, 42, 54, 71	0
17	CQ	197/197 (100%)	-0.26	3 (1%) 73 46	24, 35, 75, 89	0
17	w	197/197 (100%)	-0.37	0 100 100	27, 38, 65, 71	0
18	CR	183/183 (100%)	1.09	29 (15%) 2 1	27, 40, 169, 211	0
18	x	183/183 (100%)	0.18	14 (7%) 13 4	30, 39, 137, 171	0
19	CS	185/185 (100%)	-0.35	0 100 100	31, 45, 60, 78	0
19	y	185/185 (100%)	-0.29	0 100 100	30, 42, 79, 117	0
20	CT	188/188 (100%)	0.12	11 (5%) 22 7	44, 63, 165, 184	0
20	z	188/188 (100%)	0.19	13 (6%) 16 5	44, 60, 163, 180	0
21	0	172/172 (100%)	-0.30	2 (1%) 79 54	33, 43, 64, 89	0
21	CU	172/172 (100%)	-0.38	2 (1%) 79 54	29, 40, 62, 77	0
22	2	159/159 (100%)	-0.20	2 (1%) 77 51	29, 44, 105, 121	0
22	CV	159/159 (100%)	-0.21	0 100 100	29, 42, 100, 120	0
23	5	100/100 (100%)	0.72	11 (11%) 5 2	76, 99, 124, 160	0
23	CW	100/100 (100%)	1.19	19 (19%) 1 0	74, 95, 120, 141	0
24	6	136/136 (100%)	-0.15	1 (0%) 87 69	33, 46, 73, 108	0
24	CX	136/136 (100%)	0.02	3 (2%) 62 33	28, 42, 67, 92	0
25	7	98/98 (100%)	1.70	32 (32%) 0 0	42, 58, 175, 180	0
25	CY	98/98 (100%)	1.01	17 (17%) 1 0	39, 54, 177, 215	0
26	8	121/121 (100%)	-0.14	0 100 100	40, 57, 79, 136	0
26	CZ	121/121 (100%)	-0.01	2 (1%) 70 41	46, 63, 89, 142	0
27	9	126/126 (100%)	-0.15	1 (0%) 86 65	33, 50, 69, 92	0
27	DA	126/126 (100%)	-0.02	2 (1%) 72 44	37, 55, 79, 96	0
28	AA	135/135 (100%)	0.66	6 (4%) 34 13	65, 80, 103, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DB	135/135 (100%)	0.65	9 (6%) 17 5	75, 97, 119, 125	0
29	AB	148/148 (100%)	-0.22	0 100 100	24, 42, 79, 92	0
29	DC	148/148 (100%)	-0.15	0 100 100	26, 49, 78, 89	0
30	AC	58/58 (100%)	-0.20	0 100 100	27, 47, 111, 141	0
30	DD	58/58 (100%)	-0.21	1 (1%) 70 41	30, 53, 92, 108	0
31	AD	97/97 (100%)	0.27	3 (3%) 49 21	62, 75, 101, 127	0
31	DE	97/97 (100%)	0.35	5 (5%) 27 10	69, 84, 117, 131	0
32	AE	109/109 (100%)	-0.06	3 (2%) 53 25	40, 58, 116, 136	0
32	DF	109/109 (100%)	-0.02	5 (4%) 32 12	39, 53, 120, 142	0
33	AF	127/127 (100%)	-0.14	2 (1%) 72 44	24, 37, 56, 121	0
33	DG	127/127 (100%)	-0.05	3 (2%) 59 30	25, 41, 59, 125	0
34	AG	106/106 (100%)	-0.42	0 100 100	28, 36, 62, 95	0
34	DH	106/106 (100%)	-0.34	0 100 100	28, 36, 68, 120	0
35	AH	112/112 (100%)	-0.01	4 (3%) 42 17	39, 59, 119, 136	0
35	DI	112/112 (100%)	-0.00	2 (1%) 68 40	44, 67, 126, 145	0
36	AI	119/119 (100%)	-0.06	1 (0%) 86 65	36, 59, 75, 83	0
36	DJ	119/119 (100%)	-0.06	2 (1%) 70 41	45, 68, 84, 91	0
37	AJ	99/99 (100%)	0.07	6 (6%) 21 7	46, 60, 108, 143	0
37	DK	99/99 (100%)	0.41	6 (6%) 21 7	59, 72, 112, 151	0
38	AK	87/87 (100%)	-0.11	2 (2%) 60 31	29, 36, 59, 115	0
38	DL	87/87 (100%)	0.05	2 (2%) 60 31	34, 43, 74, 156	0
39	AL	77/77 (100%)	0.43	1 (1%) 77 51	64, 84, 120, 132	0
39	DM	77/77 (100%)	1.47	20 (25%) 0 0	67, 91, 127, 132	0
40	AM	50/50 (100%)	-0.25	1 (2%) 65 36	33, 47, 58, 65	0
40	DN	50/50 (100%)	-0.26	0 100 100	42, 52, 65, 77	0
41	AN	52/52 (100%)	-0.22	1 (1%) 66 37	36, 45, 69, 100	0
41	DO	52/52 (100%)	-0.37	0 100 100	30, 36, 59, 92	0
42	AO	25/25 (100%)	-0.14	0 100 100	50, 55, 64, 71	0
42	DP	25/25 (100%)	-0.17	0 100 100	45, 53, 65, 76	0
43	AP	105/105 (100%)	0.04	2 (1%) 66 37	28, 49, 81, 150	0
43	DQ	105/105 (100%)	-0.10	1 (0%) 82 59	33, 50, 81, 142	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
44	AQ	91/91 (100%)	-0.31	0	100	100	36, 49, 81, 96	0
44	DR	91/91 (100%)	-0.31	0	100	100	36, 54, 76, 84	0
45	i	159/168 (94%)	0.90	25 (15%)	2	1	49, 98, 163, 168	0
46	p0	143/219 (65%)	1.32	37 (25%)	0	0	85, 106, 174, 178	0
47	sM	63/104 (60%)	0.89	12 (19%)	1	0	55, 105, 131, 138	0
48	A	1781/1800 (98%)	0.16	89 (4%)	28	10	45, 85, 220, 289	0
48	sR	1783/1800 (99%)	0.14	88 (4%)	29	11	39, 76, 187, 269	0
49	B	206/206 (100%)	0.73	24 (11%)	4	1	90, 114, 140, 174	0
49	s0	206/206 (100%)	0.47	14 (6%)	17	5	76, 100, 125, 142	0
50	C	214/216 (99%)	1.23	44 (20%)	1	0	93, 128, 163, 175	0
50	s1	216/216 (100%)	0.54	12 (5%)	24	8	66, 85, 121, 152	0
51	D	217/217 (100%)	0.13	4 (1%)	68	40	71, 90, 113, 136	0
51	s2	217/217 (100%)	0.16	6 (2%)	53	25	59, 79, 101, 128	0
52	E	223/223 (100%)	0.48	13 (5%)	23	7	74, 93, 131, 173	0
52	s3	223/223 (100%)	0.42	10 (4%)	33	12	73, 106, 139, 159	0
53	F	260/260 (100%)	0.41	8 (3%)	49	21	65, 85, 104, 157	0
53	s4	260/260 (100%)	0.19	6 (2%)	60	31	54, 80, 100, 152	0
54	G	206/206 (100%)	0.96	30 (14%)	2	1	89, 114, 139, 171	0
54	s5	206/206 (100%)	0.94	27 (13%)	3	1	78, 106, 139, 163	0
55	H	226/226 (100%)	0.50	17 (7%)	14	4	61, 95, 135, 168	0
55	s6	218/226 (96%)	0.29	13 (5%)	21	7	49, 80, 118, 141	0
56	I	184/186 (98%)	0.85	24 (13%)	3	1	81, 117, 151, 173	0
56	s7	186/186 (100%)	0.91	25 (13%)	3	1	74, 111, 152, 173	0
57	J	188/199 (94%)	0.17	6 (3%)	47	20	47, 65, 105, 130	0
57	s8	188/199 (94%)	0.35	9 (4%)	30	11	43, 71, 119, 137	0
58	K	185/185 (100%)	0.79	20 (10%)	5	2	81, 98, 138, 175	0
58	s9	185/185 (100%)	0.49	10 (5%)	25	9	67, 83, 126, 178	0
59	L	96/105 (91%)	0.55	1 (1%)	82	59	74, 102, 139, 163	0
59	c0	96/105 (91%)	1.48	24 (25%)	0	0	92, 127, 157, 175	0
60	M	155/155 (100%)	0.57	18 (11%)	4	1	52, 65, 151, 176	0
60	c1	146/155 (94%)	0.35	10 (6%)	17	5	49, 68, 116, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
61	N	124/143 (86%)	1.78	50 (40%) 0 0	124, 148, 177, 187	0
61	c2	124/143 (86%)	2.68	77 (62%) 0 0	167, 178, 203, 219	0
62	O	150/150 (100%)	0.20	4 (2%) 54 26	58, 84, 107, 127	0
62	c3	150/150 (100%)	-0.07	0 100 100	56, 77, 102, 126	0
63	P	127/128 (99%)	1.28	31 (24%) 0 0	67, 131, 155, 163	0
63	c4	128/128 (100%)	0.66	12 (9%) 8 3	53, 87, 102, 110	0
64	Q	124/135 (91%)	0.49	6 (4%) 30 11	69, 86, 147, 175	0
64	c5	135/135 (100%)	0.75	16 (11%) 4 1	77, 100, 139, 149	0
65	R	141/142 (99%)	0.80	19 (13%) 3 1	76, 104, 114, 121	0
65	c6	142/142 (100%)	0.66	13 (9%) 9 3	65, 99, 118, 149	0
66	S	120/125 (96%)	0.40	11 (9%) 9 3	83, 111, 155, 165	0
67	T	145/145 (100%)	0.56	15 (10%) 6 2	66, 100, 134, 148	0
67	c8	145/145 (100%)	0.50	13 (8%) 9 3	78, 95, 133, 156	0
68	U	143/143 (100%)	0.53	10 (6%) 16 5	78, 99, 125, 149	0
68	c9	143/143 (100%)	0.53	12 (8%) 11 3	71, 93, 120, 146	0
69	V	107/110 (97%)	1.02	24 (22%) 0 0	66, 107, 159, 169	0
69	d0	110/110 (100%)	1.34	28 (25%) 0 0	68, 113, 164, 172	0
70	W	87/87 (100%)	0.56	7 (8%) 12 4	89, 98, 123, 140	0
70	d1	87/87 (100%)	0.29	5 (5%) 23 8	70, 83, 115, 137	0
71	X	129/129 (100%)	0.20	1 (0%) 86 65	64, 80, 92, 97	0
71	d2	129/129 (100%)	-0.19	0 100 100	54, 68, 77, 86	0
72	Y	144/144 (100%)	-0.06	0 100 100	52, 62, 77, 113	0
72	d3	144/144 (100%)	-0.11	1 (0%) 87 69	43, 52, 71, 108	0
73	Z	134/134 (100%)	0.58	7 (5%) 27 10	63, 97, 136, 156	0
73	d4	134/134 (100%)	0.18	5 (3%) 41 17	58, 86, 117, 146	0
74	a	70/70 (100%)	1.49	23 (32%) 0 0	110, 129, 149, 159	0
74	d5	69/70 (98%)	1.45	22 (31%) 0 0	90, 122, 141, 152	0
75	b	97/97 (100%)	0.86	15 (15%) 2 1	73, 101, 162, 171	0
75	d6	97/97 (100%)	0.15	2 (2%) 63 34	55, 76, 112, 124	0
76	c	81/81 (100%)	0.86	10 (12%) 4 1	77, 96, 147, 155	0
76	d7	81/81 (100%)	0.69	12 (14%) 2 1	68, 84, 146, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
77	d	63/63 (100%)	1.22	11 (17%) 1 0	106, 124, 145, 152	0
77	d8	63/63 (100%)	1.59	20 (31%) 0 0	94, 117, 146, 163	0
78	d9	53/53 (100%)	0.40	2 (3%) 40 16	68, 80, 127, 157	0
78	e	53/53 (100%)	-0.08	1 (1%) 66 37	68, 75, 95, 120	0
79	e0	62/62 (100%)	0.71	6 (9%) 7 2	55, 83, 146, 149	0
79	f	60/62 (96%)	1.21	8 (13%) 3 1	55, 92, 162, 167	0
80	g	71/71 (100%)	1.15	15 (21%) 1 0	100, 130, 157, 167	0
81	Rb	318/318 (100%)	1.31	80 (25%) 0 0	103, 125, 145, 164	0
81	h	318/318 (100%)	0.89	43 (13%) 3 1	92, 114, 155, 188	0
82	c7	117/121 (96%)	0.32	6 (5%) 28 10	76, 101, 137, 150	0
83	e1	51/51 (100%)	1.49	15 (29%) 0 0	145, 158, 171, 177	0
All	All	33004/33349 (98%)	0.19	1773 (5%) 25 9	23, 66, 144, 289	0

All (1773) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	CR	161	ALA	21.9
18	CR	160	ALA	18.7
25	7	76	VAL	16.1
25	7	75	THR	15.5
18	CR	162	GLU	15.3
18	CR	178	ALA	13.8
18	CR	179	GLN	13.3
18	CR	158	ALA	13.3
18	CR	165	VAL	13.2
48	A	1702	A	13.0
18	CR	176	ILE	12.3
60	c1	3	THR	12.1
18	CR	159	LYS	11.9
25	7	86	SER	11.6
1	AR	1569	U	11.5
18	x	161	ALA	11.4
48	A	1709	C	11.3
48	A	1694	A	11.2
60	M	152	GLN	10.7
25	CY	69	LYS	10.6
25	CY	95	SER	10.5
48	A	1699	G	10.4

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Mol	Chain	Res	Type	RSRZ
60	M	146	ALA	10.4
25	7	88	ASP	10.4
48	A	1693	A	10.2
18	CR	184	ALA	10.1
48	A	1711	C	9.9
27	DA	127	GLU	9.8
54	G	37	GLN	9.7
48	A	1700	C	9.7
18	CR	157	VAL	9.7
25	CY	97	LYS	9.5
45	i	88	ARG	9.4
18	CR	174	GLY	9.4
54	s5	151	GLY	9.3
60	M	147	GLY	9.1
25	CY	96	LEU	8.8
25	CY	81	PRO	8.7
48	A	1708	U	8.5
48	A	238	U	8.5
48	A	1692	G	8.5
59	c0	98	THR	8.5
18	CR	167	ARG	8.5
45	i	87	THR	8.4
1	1	1955	U	8.3
60	M	2	SER	8.2
25	7	81	PRO	8.2
25	7	77	LYS	8.0
1	1	1952	G	8.0
38	DL	88	ALA	8.0
79	e0	63	GLN	8.0
54	G	153	GLY	8.0
12	CL	219	ALA	7.9
25	CY	67	VAL	7.9
69	d0	18	GLN	7.8
25	7	87	LEU	7.8
1	1	1570	U	7.7
54	G	152	GLY	7.6
45	i	85	SER	7.5
1	AR	1351	U	7.4
48	sR	718	U	7.3
60	M	145	ALA	7.3
25	7	84	GLY	7.3
25	7	69	LYS	7.2

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Mol	Chain	Res	Type	RSRZ
1	1	1569	U	7.2
63	P	15	GLY	7.2
81	Rb	121	MET	7.2
18	x	162	GLU	7.1
48	A	1698	G	7.1
33	DG	128	LEU	7.1
1	1	1568	U	7.0
60	c1	2	SER	7.0
60	c1	5	LEU	7.0
61	c2	63	VAL	7.0
48	sR	658	C	6.9
18	CR	177	ALA	6.9
69	d0	121	ASN	6.9
60	M	3	THR	6.9
54	s5	37	GLN	6.9
54	G	151	GLY	6.8
48	A	1690	G	6.8
79	f	52	GLY	6.8
61	c2	20	ALA	6.8
54	s5	152	GLY	6.8
18	CR	170	SER	6.7
48	A	1696	G	6.7
25	CY	66	GLU	6.7
50	C	54	LEU	6.7
48	A	913	G	6.7
37	DK	100	HIS	6.6
1	AR	2535	A	6.6
61	c2	30	VAL	6.6
48	A	1703	C	6.6
58	K	182	GLU	6.5
1	1	1762	C	6.5
48	A	1704	U	6.5
25	CY	94	ARG	6.4
18	CR	168	LEU	6.4
33	AF	128	LEU	6.4
81	h	52	GLN	6.4
25	CY	68	ALA	6.4
79	f	53	LYS	6.4
1	1	2539	C	6.4
60	M	148	LYS	6.4
18	CR	180	LYS	6.3
67	T	2	SER	6.3

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Mol	Chain	Res	Type	RSRZ
18	CR	163	LYS	6.3
79	f	48	THR	6.3
56	s7	52	ALA	6.2
61	c2	105	LYS	6.2
20	CT	183	ALA	6.2
25	7	85	ALA	6.2
64	c5	134	THR	6.2
25	CY	65	GLU	6.1
1	AR	2539	C	6.1
10	CJ	254	ASP	6.1
54	G	36	ALA	6.1
20	CT	182	ASP	6.1
45	i	89	ARG	6.1
48	sR	676	G	6.0
61	c2	133	LEU	6.0
36	DJ	120	ALA	6.0
1	1	1571	A	6.0
56	s7	3	ALA	6.0
56	s7	2	SER	6.0
48	A	1701	A	6.0
48	sR	1710	U	6.0
54	s5	153	GLY	5.9
25	7	90	ILE	5.9
61	N	88	LEU	5.9
37	DK	96	ALA	5.9
78	d9	4	GLU	5.9
48	A	1712	A	5.9
50	C	55	LYS	5.9
18	x	163	LYS	5.9
46	p0	192	ASP	5.9
65	R	57	LEU	5.9
1	AR	1570	U	5.9
69	d0	100	VAL	5.8
65	R	66	ARG	5.8
48	sR	194	U	5.8
61	c2	22	VAL	5.8
61	c2	28	LEU	5.7
45	i	16	ASP	5.7
18	x	160	ALA	5.7
9	CI	26	VAL	5.7
25	7	89	LEU	5.7
25	7	78	ALA	5.7

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Mol	Chain	Res	Type	RSRZ
61	c2	136	ILE	5.7
18	CR	183	ALA	5.7
77	d	43	ASN	5.7
48	A	1697	G	5.6
50	C	20	VAL	5.6
25	7	68	ALA	5.6
55	H	226	ILE	5.6
58	K	181	ALA	5.6
54	s5	154	ALA	5.6
48	sR	678	A	5.6
1	1	1764	U	5.6
18	CR	175	ARG	5.5
54	s5	150	GLY	5.5
48	A	239	C	5.5
76	c	38	PRO	5.5
61	c2	132	GLU	5.5
83	e1	146	SER	5.5
1	AR	2445	A	5.5
25	CY	98	PRO	5.5
5	k	387	LEU	5.5
48	A	1710	U	5.5
61	c2	23	THR	5.5
1	1	1763	U	5.4
48	sR	1699	G	5.4
43	AP	106	PHE	5.4
61	c2	64	SER	5.4
48	A	715	U	5.4
18	x	184	ALA	5.4
69	d0	17	GLN	5.4
54	G	41	LYS	5.4
18	CR	166	VAL	5.3
64	c5	135	THR	5.3
1	AR	1352	A	5.3
81	Rb	303	ALA	5.3
61	c2	126	TRP	5.3
48	A	718	U	5.3
66	S	125	SER	5.3
63	P	16	VAL	5.3
45	i	19	VAL	5.3
61	c2	59	LEU	5.3
48	A	1707	A	5.3
46	p0	205	THR	5.2

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Mol	Chain	Res	Type	RSRZ
61	c2	123	VAL	5.2
59	c0	37	THR	5.2
25	7	82	ILE	5.2
48	sR	1700	C	5.2
61	c2	56	GLU	5.2
48	A	194	U	5.2
79	e0	49	LEU	5.1
1	1	1351	U	5.1
48	A	719	U	5.1
81	h	4	ASN	5.1
52	E	44	THR	5.1
45	i	84	LYS	5.1
48	sR	1701	A	5.1
48	sR	229	U	5.1
48	sR	1694	A	5.0
45	i	18	VAL	5.0
18	CR	173	ARG	5.0
48	A	1687	U	5.0
48	A	135	A	5.0
48	A	1695	G	5.0
63	P	40	ALA	5.0
64	c5	4	ALA	5.0
1	AR	1028	U	5.0
48	sR	232	U	5.0
48	A	232	U	5.0
81	Rb	314	GLN	5.0
11	CK	190	ASP	5.0
1	1	1243	G	5.0
79	e0	62	VAL	5.0
1	AR	1016	C	5.0
20	CT	185	LEU	4.9
18	CR	169	THR	4.9
61	N	111	ASN	4.9
74	d5	86	GLU	4.9
81	h	79	TYR	4.9
20	z	187	GLU	4.9
18	x	164	LYS	4.9
69	V	105	GLN	4.9
25	7	70	LYS	4.9
20	z	188	ASP	4.9
69	V	104	THR	4.9
39	DM	34	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
61	N	112	ALA	4.9
18	CR	172	GLN	4.9
18	x	159	LYS	4.9
18	CR	164	LYS	4.9
60	M	156	PHE	4.8
39	DM	32	ASN	4.8
68	U	5	SER	4.8
10	CJ	253	SER	4.8
77	d	44	VAL	4.8
48	sR	1711	C	4.8
65	c6	141	SER	4.8
1	1	1349	G	4.8
79	f	54	ARG	4.8
48	sR	1712	A	4.8
60	M	151	LYS	4.8
45	i	15	ALA	4.8
1	AR	1025	A	4.8
48	sR	506	A	4.8
61	c2	21	GLU	4.8
11	CK	191	LEU	4.8
10	p	116	VAL	4.8
45	i	17	VAL	4.8
48	A	1713	G	4.8
69	d0	98	GLN	4.8
49	B	28	ASN	4.7
47	sM	84	LYS	4.7
38	AK	87	SER	4.7
75	b	65	PRO	4.7
48	sR	1702	A	4.7
61	c2	92	ALA	4.7
63	P	79	VAL	4.7
48	A	1686	C	4.7
35	AH	109	THR	4.7
51	s2	90	THR	4.7
17	CQ	182	ASN	4.7
50	s1	227	ALA	4.7
60	M	154	ALA	4.7
1	1	1352	A	4.7
1	1	1572	U	4.7
48	sR	493	U	4.7
48	A	1691	A	4.7
1	AR	2536	A	4.7

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Mol	Chain	Res	Type	RSRZ
69	V	121	ASN	4.7
45	i	173	GLU	4.7
61	N	67	THR	4.6
25	7	72	SER	4.6
48	A	658	C	4.6
60	c1	4	GLU	4.6
65	c6	142	TYR	4.6
81	Rb	25	THR	4.6
7	CG	296	GLN	4.6
61	c2	57	ALA	4.6
10	CJ	121	SER	4.6
1	1	1567	U	4.6
74	a	88	ILE	4.6
25	7	73	ARG	4.6
10	CJ	107	GLU	4.6
50	C	26	ARG	4.6
3	4	158	U	4.6
48	A	491	C	4.6
61	N	62	LEU	4.5
1	AR	1567	U	4.5
60	M	153	PHE	4.5
73	Z	2	SER	4.5
77	d8	65	ARG	4.5
48	A	656	G	4.5
81	Rb	138	GLY	4.5
81	h	3	SER	4.5
18	x	157	VAL	4.5
63	P	29	HIS	4.5
23	5	27	VAL	4.5
48	sR	677	G	4.4
65	R	21	HIS	4.4
65	c6	19	VAL	4.4
31	DE	105	ALA	4.4
81	Rb	167	VAL	4.4
60	M	149	ALA	4.4
74	a	48	ASP	4.4
79	f	49	LEU	4.4
60	M	155	LYS	4.4
1	AR	2502	A	4.4
61	N	63	VAL	4.4
20	z	181	ARG	4.4
1	1	1350	A	4.4

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Mol	Chain	Res	Type	RSRZ
1	AR	3352	U	4.4
21	0	1	MET	4.4
58	K	186	GLU	4.4
48	A	1705	C	4.4
68	U	6	VAL	4.4
69	d0	104	THR	4.4
69	d0	107	THR	4.4
1	1	1095	U	4.4
48	A	134	U	4.4
61	N	68	GLU	4.4
50	C	47	LEU	4.4
54	G	161	ASP	4.4
81	Rb	72	THR	4.4
60	M	4	GLU	4.3
81	Rb	244	ALA	4.3
1	1	1566	A	4.3
48	sR	1707	A	4.3
61	c2	128	ALA	4.3
54	s5	35	GLN	4.3
76	d7	57	GLU	4.3
45	i	175	ASP	4.3
81	Rb	214	ALA	4.3
1	1	1240	A	4.3
27	DA	126	LEU	4.3
1	1	1239	C	4.3
48	sR	234	G	4.3
48	sR	239	C	4.3
81	Rb	168	THR	4.3
1	AR	3154	C	4.3
61	N	32	LEU	4.3
18	CR	182	ILE	4.3
48	sR	719	U	4.2
58	K	180	LYS	4.2
35	DI	113	LYS	4.2
81	h	283	LYS	4.2
58	K	106	GLU	4.2
61	c2	112	ALA	4.2
61	c2	125	ASN	4.2
32	DF	82	GLU	4.2
69	d0	95	ALA	4.2
18	x	158	ALA	4.2
61	N	85	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
48	A	488	G	4.2
12	CL	220	GLN	4.2
48	sR	240	U	4.2
74	a	69	LEU	4.2
81	Rb	165	ASP	4.2
69	d0	103	ILE	4.2
1	1	1951	C	4.2
46	p0	218	SER	4.2
64	Q	12	PHE	4.2
64	c5	10	ARG	4.2
46	p0	197	PHE	4.2
1	AR	2506	U	4.2
48	sR	1696	G	4.2
45	i	86	ASN	4.2
63	P	78	ALA	4.2
66	S	123	ASN	4.2
25	7	74	LYS	4.2
50	C	29	TRP	4.1
48	sR	1491	U	4.1
73	d4	135	ASP	4.1
23	CW	52	ASN	4.1
59	c0	64	TYR	4.1
61	c2	80	ASN	4.1
65	R	92	TYR	4.1
81	Rb	51	ASP	4.1
59	c0	95	ARG	4.1
64	c5	5	VAL	4.1
48	A	506	A	4.1
1	1	2205	U	4.1
48	A	730	G	4.1
48	sR	679	U	4.1
1	AR	546	C	4.1
77	d8	13	ILE	4.1
25	CY	77	LYS	4.1
81	h	115	ILE	4.1
72	d3	145	SER	4.1
1	AR	2537	U	4.1
57	s8	200	LYS	4.1
48	sR	656	G	4.1
80	g	109	ASP	4.1
53	F	167	GLY	4.1
45	i	83	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
48	A	493	U	4.1
74	d5	89	ILE	4.1
61	c2	85	LYS	4.1
48	sR	1692	G	4.1
69	d0	97	VAL	4.0
1	AR	544	C	4.0
1	AR	2504	U	4.0
1	AR	3275	U	4.0
61	c2	75	VAL	4.0
1	AR	1350	A	4.0
59	c0	94	GLU	4.0
48	sR	1695	G	4.0
69	d0	99	ILE	4.0
47	sM	78	ASP	4.0
64	Q	50	THR	4.0
1	AR	1581	C	4.0
50	C	94	LYS	4.0
52	E	213	GLU	4.0
69	V	97	VAL	4.0
50	C	100	PHE	4.0
37	AJ	98	ARG	4.0
76	c	37	CYS	4.0
69	d0	105	GLN	4.0
50	C	25	THR	3.9
50	C	96	LEU	3.9
54	s5	156	ARG	3.9
1	AR	1574	C	3.9
50	C	45	LYS	3.9
64	Q	51	SER	3.9
70	W	69	LEU	3.9
74	d5	105	THR	3.9
33	AF	127	ALA	3.9
52	s3	145	ALA	3.9
74	a	89	ILE	3.9
69	d0	102	ARG	3.9
1	AR	1571	A	3.9
49	B	166	GLY	3.9
50	C	46	THR	3.9
52	s3	44	THR	3.9
45	i	174	LEU	3.9
49	s0	173	ILE	3.9
50	s1	234	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	1	2095	G	3.9
48	sR	721	U	3.9
61	c2	29	LYS	3.9
81	Rb	313	TRP	3.9
25	7	79	GLN	3.9
31	AD	105	ALA	3.9
50	C	91	VAL	3.9
75	d6	98	PRO	3.9
50	C	28	GLU	3.9
8	CH	130	ILE	3.8
64	c5	133	ALA	3.8
54	s5	129	PRO	3.8
20	z	178	ALA	3.8
65	R	20	ALA	3.8
80	g	86	THR	3.8
1	1	2207	A	3.8
52	E	218	LEU	3.8
54	G	20	PHE	3.8
81	h	212	ALA	3.8
61	N	136	ILE	3.8
81	Rb	52	GLN	3.8
82	c7	87	GLU	3.8
55	s6	217	SER	3.8
3	AT	81	U	3.8
1	AR	1566	A	3.8
24	CX	3	GLY	3.8
28	DB	2	ALA	3.8
65	c6	90	VAL	3.8
59	c0	79	TYR	3.8
81	Rb	48	THR	3.8
49	s0	24	LEU	3.8
55	H	148	SER	3.8
83	e1	102	VAL	3.8
1	AR	1349	G	3.8
48	sR	1698	G	3.8
47	sM	85	SER	3.8
75	d6	45	VAL	3.8
56	I	74	GLN	3.7
50	C	42	ASN	3.7
80	g	85	TYR	3.7
25	7	67	VAL	3.7
48	sR	487	G	3.7

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Mol	Chain	Res	Type	RSRZ
75	b	60	PRO	3.7
46	p0	212	HIS	3.7
20	z	186	LYS	3.7
56	I	52	ALA	3.7
69	V	120	SER	3.7
74	a	97	LYS	3.7
1	AR	1954	G	3.7
61	N	91	VAL	3.7
59	c0	36	ASP	3.7
48	sR	1800	A	3.7
60	M	150	ASN	3.7
23	5	89	LEU	3.7
74	d5	50	ILE	3.7
23	CW	13	LYS	3.7
63	P	14	PHE	3.7
49	s0	19	ALA	3.7
18	CR	181	ARG	3.7
48	sR	1693	A	3.7
56	I	20	VAL	3.7
1	AR	1572	U	3.7
1	AR	2505	U	3.7
65	R	143	ARG	3.7
81	Rb	301	LEU	3.7
64	c5	6	ASN	3.7
64	c5	132	GLY	3.6
56	I	38	LEU	3.6
76	d7	38	PRO	3.6
25	7	80	ARG	3.6
37	AJ	99	ARG	3.6
76	c	33	LEU	3.6
48	sR	1228	G	3.6
64	c5	136	SER	3.6
1	1	3155	U	3.6
23	CW	56	VAL	3.6
81	Rb	315	VAL	3.6
32	DF	112	ASP	3.6
39	DM	71	PRO	3.6
5	CE	387	LEU	3.6
37	DK	98	ARG	3.6
63	P	41	ARG	3.6
61	c2	74	LEU	3.6
80	g	87	THR	3.6

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Mol	Chain	Res	Type	RSRZ
83	e1	145	HIS	3.6
69	V	20	ILE	3.6
50	C	233	GLY	3.6
69	V	96	PRO	3.6
48	sR	225	A	3.6
48	sR	1059	U	3.6
61	c2	104	GLY	3.6
81	Rb	123	ILE	3.6
45	i	176	ALA	3.6
1	AR	2538	U	3.6
48	A	720	G	3.6
1	1	1269	U	3.6
1	1	3154	C	3.6
48	sR	675	U	3.6
75	b	55	GLU	3.6
63	P	27	PHE	3.5
69	V	101	LYS	3.5
1	1	1573	G	3.5
1	AR	2503	G	3.5
61	N	108	ARG	3.5
48	A	1688	U	3.5
49	B	97	PRO	3.5
81	Rb	177	MET	3.5
48	A	492	A	3.5
63	P	13	VAL	3.5
23	5	9	GLN	3.5
9	CI	27	ALA	3.5
81	Rb	157	VAL	3.5
50	C	31	ASP	3.5
68	U	108	LEU	3.5
79	f	61	SER	3.5
49	s0	20	ALA	3.5
52	E	179	GLN	3.5
1	1	1765	U	3.5
1	AR	1764	U	3.5
61	c2	26	ASP	3.5
54	G	24	VAL	3.5
50	C	130	SER	3.5
68	c9	55	TYR	3.5
56	s7	48	GLU	3.5
77	d	26	THR	3.5
67	T	22	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
81	Rb	134	TRP	3.5
69	d0	93	LEU	3.5
76	c	39	GLY	3.5
50	C	95	ASN	3.4
25	7	96	LEU	3.4
59	c0	76	LEU	3.4
65	R	54	LEU	3.4
63	P	94	PRO	3.4
81	Rb	53	LYS	3.4
1	AR	1815	U	3.4
48	A	132	U	3.4
23	CW	9	GLN	3.4
48	A	240	U	3.4
66	S	126	ALA	3.4
61	c2	58	LEU	3.4
23	CW	11	ILE	3.4
1	AR	2546	C	3.4
79	f	60	PRO	3.4
81	Rb	319	ASN	3.4
48	sR	1697	G	3.4
9	CI	25	GLN	3.4
43	AP	104	LEU	3.4
81	Rb	309	VAL	3.4
38	DL	87	SER	3.4
61	N	20	ALA	3.4
81	Rb	166	SER	3.4
81	Rb	186	PHE	3.4
48	sR	490	C	3.4
52	s3	42	THR	3.4
61	c2	113	ARG	3.4
50	C	93	GLY	3.4
1	AR	252	U	3.4
58	K	111	THR	3.4
58	K	185	GLY	3.4
76	d7	58	SER	3.4
1	AR	3157	U	3.4
22	2	124	VAL	3.4
48	sR	494	U	3.4
1	1	1577	G	3.4
11	CK	189	GLU	3.4
61	c2	96	GLN	3.4
25	CY	70	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
77	d8	5	THR	3.4
48	A	794	U	3.3
48	sR	75	U	3.3
77	d	35	ASP	3.3
46	p0	104	ARG	3.3
61	c2	65	SER	3.3
61	N	41	LEU	3.3
61	c2	121	VAL	3.3
81	Rb	83	ALA	3.3
20	z	182	ASP	3.3
81	Rb	118	LYS	3.3
69	d0	14	GLN	3.3
56	s7	93	LEU	3.3
74	a	82	HIS	3.3
74	d5	102	THR	3.3
48	sR	495	C	3.3
52	E	217	ILE	3.3
55	H	149	LYS	3.3
77	d8	61	ARG	3.3
61	N	86	VAL	3.3
76	c	59	CYS	3.3
14	CN	129	ASN	3.3
28	DB	92	PHE	3.3
35	AH	113	LYS	3.3
49	B	198	MET	3.3
54	G	150	GLY	3.3
46	p0	25	LEU	3.3
50	C	131	ASP	3.3
52	E	45	LYS	3.3
48	A	1059	U	3.3
50	C	60	ALA	3.3
54	s5	68	ILE	3.3
77	d8	43	ASN	3.3
12	CL	112	GLN	3.3
74	a	83	LEU	3.3
1	AR	2444	C	3.3
1	AR	1568	U	3.3
81	Rb	26	SER	3.3
74	d5	88	ILE	3.3
45	i	98	GLY	3.3
81	Rb	24	ALA	3.3
61	c2	87	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
67	T	3	LEU	3.3
81	h	252	LEU	3.3
64	c5	50	THR	3.3
81	Rb	300	THR	3.3
5	CE	386	ASP	3.3
70	W	10	GLU	3.3
52	E	214	GLU	3.3
54	s5	155	ALA	3.3
48	A	235	G	3.3
54	G	222	LYS	3.3
39	DM	72	THR	3.3
58	s9	182	GLU	3.3
81	Rb	294	TRP	3.3
63	P	74	VAL	3.3
48	sR	492	A	3.2
37	AJ	97	SER	3.2
48	A	261	U	3.2
46	p0	29	GLY	3.2
51	D	145	GLY	3.2
48	A	914	G	3.2
49	B	24	LEU	3.2
10	CJ	182	GLY	3.2
81	h	43	ILE	3.2
23	5	10	LYS	3.2
31	AD	104	LEU	3.2
48	A	1706	C	3.2
51	s2	91	ARG	3.2
61	c2	122	VAL	3.2
56	s7	187	SER	3.2
67	T	17	LEU	3.2
23	CW	27	VAL	3.2
1	1	1574	C	3.2
25	7	71	ARG	3.2
48	sR	1703	C	3.2
24	6	4	ASN	3.2
56	s7	58	LEU	3.2
69	V	111	GLY	3.2
12	CL	186	GLU	3.2
20	CT	157	GLU	3.2
1	AR	3276	G	3.2
77	d8	10	ALA	3.2
1	AR	1026	A	3.2

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Mol	Chain	Res	Type	RSRZ
81	Rb	46	LYS	3.2
81	h	253	ALA	3.2
54	G	70	VAL	3.2
66	S	86	PRO	3.2
75	b	62	TYR	3.2
1	1	3286	G	3.2
73	d4	2	SER	3.2
74	a	65	LEU	3.2
55	s6	214	LYS	3.2
47	sM	52	PRO	3.2
61	c2	43	ARG	3.2
1	1	1242	G	3.2
81	h	146	GLY	3.2
81	Rb	117	LYS	3.2
81	h	25	THR	3.2
1	AR	2507	C	3.2
48	sR	231	U	3.2
26	CZ	142	ILE	3.2
65	c6	89	LEU	3.2
79	e0	51	ASN	3.2
83	e1	134	ASN	3.2
55	s6	218	GLU	3.2
1	AR	1103	A	3.2
1	AR	2540	A	3.2
48	sR	673	A	3.2
39	DM	69	LEU	3.1
52	s3	144	ALA	3.1
54	G	154	ALA	3.1
63	P	80	HIS	3.1
81	h	265	LEU	3.1
81	Rb	32	LEU	3.1
48	A	714	G	3.1
61	c2	55	GLY	3.1
56	I	43	PHE	3.1
69	V	100	VAL	3.1
47	sM	75	ASP	3.1
57	s8	67	TRP	3.1
81	h	313	TRP	3.1
1	1	1094	U	3.1
10	p	121	SER	3.1
24	CX	4	ASN	3.1
59	c0	65	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
46	p0	204	ILE	3.1
56	s7	4	PRO	3.1
61	N	49	THR	3.1
61	N	110	GLY	3.1
62	O	61	THR	3.1
1	1	2501	U	3.1
50	C	41	ARG	3.1
48	A	1689	A	3.1
1	1	1761	C	3.1
77	d8	9	LEU	3.1
1	1	1237	G	3.1
25	7	98	PRO	3.1
45	i	137	GLU	3.1
81	h	2	ALA	3.1
83	e1	106	TYR	3.1
23	5	11	ILE	3.1
50	C	32	ILE	3.1
61	N	50	LYS	3.1
14	t	192	GLU	3.1
53	s4	253	ASP	3.1
20	CT	181	ARG	3.1
51	s2	247	ALA	3.1
50	C	207	LEU	3.1
1	AR	1955	U	3.1
49	B	39	ASN	3.1
1	1	1238	C	3.1
69	d0	101	LYS	3.1
74	d5	37	GLN	3.1
46	p0	103	ASN	3.1
58	K	87	SER	3.1
57	s8	148	ALA	3.1
60	c1	145	ALA	3.1
61	N	109	GLU	3.1
46	p0	221	ALA	3.1
61	N	26	ASP	3.1
69	V	93	LEU	3.1
61	N	126	TRP	3.1
50	C	23	PRO	3.1
58	s9	184	SER	3.1
81	Rb	102	ARG	3.1
61	N	127	GLY	3.1
69	V	107	THR	3.1

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Mol	Chain	Res	Type	RSRZ
81	Rb	316	MET	3.1
49	B	41	ARG	3.1
68	c9	24	ARG	3.1
12	CL	221	ALA	3.1
59	c0	96	ASN	3.0
7	CG	297	GLN	3.0
20	z	185	LEU	3.0
48	sR	235	G	3.0
50	s1	54	LEU	3.0
52	E	88	ALA	3.0
75	b	56	ALA	3.0
49	B	170	ILE	3.0
81	Rb	50	ASP	3.0
59	c0	67	THR	3.0
67	c8	5	VAL	3.0
9	o	23	ALA	3.0
48	A	729	G	3.0
61	N	106	ILE	3.0
68	U	72	GLY	3.0
48	sR	1227	A	3.0
23	5	108	TYR	3.0
80	g	124	PRO	3.0
64	c5	11	VAL	3.0
1	1	547	G	3.0
11	q	191	LEU	3.0
39	DM	31	LEU	3.0
76	c	41	LEU	3.0
1	1	1241	U	3.0
50	s1	235	GLY	3.0
78	d9	5	ASN	3.0
22	2	121	ALA	3.0
46	p0	94	THR	3.0
48	A	1716	C	3.0
48	sR	230	C	3.0
48	sR	651	G	3.0
56	I	34	LEU	3.0
7	CG	295	GLY	3.0
14	CN	132	ALA	3.0
20	CT	189	ALA	3.0
83	e1	113	LYS	3.0
1	1	439	C	3.0
1	1	1581	C	3.0

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Mol	Chain	Res	Type	RSRZ
1	AR	3156	U	3.0
46	p0	217	VAL	3.0
64	c5	109	PRO	3.0
69	d0	96	PRO	3.0
32	DF	86	LYS	3.0
49	B	196	SER	3.0
53	F	123	LEU	3.0
1	AR	3153	U	3.0
14	t	130	GLY	3.0
18	x	183	ALA	3.0
24	CX	2	SER	3.0
37	AJ	64	SER	3.0
54	s5	36	ALA	3.0
74	d5	104	ALA	3.0
52	E	41	VAL	3.0
63	P	42	VAL	3.0
1	AR	1765	U	3.0
48	A	1362	U	3.0
54	G	31	GLU	3.0
52	E	54	ARG	3.0
10	CJ	249	ARG	3.0
49	s0	184	LEU	3.0
55	s6	212	LEU	3.0
65	R	28	LEU	3.0
33	DG	2	ALA	2.9
58	K	178	ALA	2.9
55	H	217	SER	2.9
1	1	2502	A	2.9
50	s1	53	GLY	2.9
55	s6	166	GLU	2.9
69	V	54	GLY	2.9
69	d0	115	GLU	2.9
70	d1	42	GLU	2.9
61	c2	124	LYS	2.9
77	d8	44	VAL	2.9
80	g	152	ALA	2.9
82	c7	88	VAL	2.9
48	A	234	G	2.9
48	sR	1704	U	2.9
7	m	231	ILE	2.9
10	CJ	106	LYS	2.9
48	sR	654	C	2.9

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Mol	Chain	Res	Type	RSRZ
63	c4	62	LEU	2.9
81	h	81	LEU	2.9
48	A	912	U	2.9
47	sM	49	LYS	2.9
58	s9	186	GLU	2.9
10	CJ	252	ASN	2.9
81	Rb	3	SER	2.9
81	Rb	302	PHE	2.9
1	AR	3350	C	2.9
39	DM	29	LYS	2.9
81	Rb	253	ALA	2.9
10	CJ	251	LYS	2.9
74	a	56	THR	2.9
1	AR	1762	C	2.9
53	F	261	LEU	2.9
53	s4	261	LEU	2.9
55	H	153	VAL	2.9
68	c9	4	VAL	2.9
1	1	1580	A	2.9
43	DQ	106	PHE	2.9
51	s2	92	ALA	2.9
46	p0	190	VAL	2.9
48	A	490	C	2.9
58	K	95	TYR	2.9
69	d0	106	ILE	2.9
61	c2	142	GLN	2.9
81	h	254	ALA	2.9
47	sM	79	SER	2.9
56	I	187	SER	2.9
1	1	1950	U	2.9
83	e1	147	VAL	2.9
52	E	87	TYR	2.9
75	b	61	GLU	2.9
35	DI	27	GLY	2.9
10	CJ	245	LYS	2.9
81	Rb	183	LEU	2.9
25	7	95	SER	2.8
36	AI	120	ALA	2.8
67	T	8	GLN	2.8
81	Rb	311	ARG	2.8
74	d5	52	LYS	2.8
48	sR	226	A	2.8

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Mol	Chain	Res	Type	RSRZ
58	K	105	LEU	2.8
61	N	52	LEU	2.8
81	Rb	33	LEU	2.8
58	s9	148	VAL	2.8
61	N	37	VAL	2.8
18	CR	156	ALA	2.8
20	CT	175	GLN	2.8
20	CT	187	GLU	2.8
75	b	46	GLU	2.8
77	d8	63	ALA	2.8
81	h	284	ALA	2.8
50	C	75	GLY	2.8
61	c2	78	LEU	2.8
46	p0	50	VAL	2.8
69	d0	114	VAL	2.8
55	s6	169	TYR	2.8
56	I	11	GLN	2.8
56	I	17	GLU	2.8
63	c4	63	ALA	2.8
63	P	102	LEU	2.8
10	CJ	116	VAL	2.8
37	DK	58	ILE	2.8
48	sR	491	C	2.8
61	c2	91	VAL	2.8
21	CU	1	MET	2.8
54	s5	30	PRO	2.8
25	7	92	GLU	2.8
61	N	64	SER	2.8
70	d1	75	ASN	2.8
1	AR	547	G	2.8
49	B	44	GLY	2.8
64	Q	10	ARG	2.8
1	AR	1763	U	2.8
35	AH	110	GLU	2.8
49	s0	54	TRP	2.8
58	K	183	ALA	2.8
49	B	201	LEU	2.8
61	c2	86	VAL	2.8
27	9	127	GLU	2.8
48	sR	489	C	2.8
61	c2	127	GLY	2.8
61	c2	143	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
54	s5	48	PHE	2.8
67	c8	14	ILE	2.8
61	N	21	GLU	2.8
48	sR	238	U	2.8
61	N	33	ARG	2.8
61	c2	114	LYS	2.8
64	Q	101	ALA	2.8
81	Rb	185	GLN	2.8
49	s0	185	ARG	2.8
80	g	148	TYR	2.8
28	DB	4	PHE	2.8
52	s3	25	PHE	2.8
52	s3	40	ARG	2.8
23	CW	14	THR	2.8
39	DM	73	LEU	2.8
61	c2	27	ALA	2.8
65	R	11	GLY	2.8
81	Rb	163	ASP	2.8
48	A	136	C	2.8
81	Rb	252	LEU	2.8
10	CJ	120	LYS	2.8
14	CN	131	LYS	2.8
31	DE	67	VAL	2.8
74	d5	41	ILE	2.8
48	A	494	U	2.8
48	A	1370	U	2.8
61	N	36	LEU	2.8
67	c8	19	ASN	2.8
81	Rb	243	LEU	2.8
20	CT	186	LYS	2.8
46	p0	87	VAL	2.8
48	sR	653	C	2.8
56	I	16	LEU	2.7
79	e0	2	ALA	2.7
69	V	48	HIS	2.7
23	CW	44	GLU	2.7
76	c	40	CYS	2.7
3	AT	158	U	2.7
26	CZ	23	ALA	2.7
61	c2	115	VAL	2.7
63	c4	50	ALA	2.7
14	CN	93	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
75	b	69	ASN	2.7
47	sM	83	LYS	2.7
1	AR	1353	U	2.7
23	CW	28	PHE	2.7
57	s8	117	TYR	2.7
61	c2	60	VAL	2.7
69	V	51	VAL	2.7
10	CJ	137	ASN	2.7
61	N	105	LYS	2.7
1	AR	440	A	2.7
1	AR	621	A	2.7
52	E	37	VAL	2.7
55	H	225	GLU	2.7
55	H	80	ASN	2.7
25	7	83	THR	2.7
1	1	1025	A	2.7
28	AA	92	PHE	2.7
48	sR	722	G	2.7
61	N	40	GLY	2.7
74	a	36	ALA	2.7
66	S	75	GLU	2.7
76	d7	59	CYS	2.7
81	Rb	172	ALA	2.7
53	F	168	LYS	2.7
61	c2	106	ILE	2.7
77	d	67	ARG	2.7
1	AR	3155	U	2.7
37	AJ	100	HIS	2.7
45	i	151	LEU	2.7
56	s7	31	SER	2.7
57	s8	121	LEU	2.7
81	Rb	116	ASP	2.7
61	c2	47	GLU	2.7
65	c6	29	ILE	2.7
64	Q	28	MET	2.7
81	Rb	126	SER	2.7
1	1	3351	U	2.7
23	5	29	ASP	2.7
57	J	106	ALA	2.7
80	g	115	THR	2.7
39	DM	54	LEU	2.7
77	d	54	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
10	CJ	111	LYS	2.7
25	CY	91	LYS	2.7
54	G	22	PRO	2.7
1	1	545	U	2.7
54	s5	225	ARG	2.7
67	T	5	VAL	2.7
48	A	717	C	2.7
53	F	54	TYR	2.7
56	s7	49	ILE	2.7
61	c2	140	PHE	2.7
77	d8	57	MET	2.7
79	f	56	MET	2.7
69	V	103	ILE	2.7
81	Rb	317	THR	2.7
65	R	26	LYS	2.7
61	N	137	MET	2.7
28	AA	95	VAL	2.7
54	G	33	VAL	2.7
81	Rb	49	GLY	2.7
1	1	440	A	2.7
49	s0	17	LEU	2.7
81	Rb	159	ASN	2.7
77	d	5	THR	2.7
1	1	1579	C	2.7
39	DM	11	PHE	2.7
48	A	696	C	2.7
48	sR	1709	C	2.7
1	1	1954	G	2.7
59	c0	97	PRO	2.7
69	V	110	PRO	2.7
81	h	34	LEU	2.6
25	CY	75	THR	2.6
61	c2	61	VAL	2.6
61	c2	116	VAL	2.6
48	A	716	C	2.6
65	R	29	ILE	2.6
81	h	261	LYS	2.6
50	C	230	ALA	2.6
10	CJ	255	SER	2.6
55	H	152	ASP	2.6
4	CD	252	THR	2.6
4	CD	253	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
18	x	165	VAL	2.6
50	C	53	GLY	2.6
61	c2	25	GLU	2.6
83	e1	114	VAL	2.6
48	sR	236	A	2.6
55	H	224	ALA	2.6
81	Rb	120	SER	2.6
1	AR	1573	G	2.6
32	AE	6	ASP	2.6
49	B	95	ALA	2.6
56	s7	57	ALA	2.6
59	c0	35	ILE	2.6
69	V	19	ILE	2.6
56	I	4	PRO	2.6
10	CJ	195	SER	2.6
48	A	131	C	2.6
66	S	124	VAL	2.6
66	S	101	ASN	2.6
1	1	1815	U	2.6
1	AR	246	U	2.6
45	i	172	VAL	2.6
48	sR	483	A	2.6
58	K	184	SER	2.6
1	1	2772	C	2.6
81	h	314	GLN	2.6
81	Rb	292	LEU	2.6
33	DG	127	ALA	2.6
39	DM	33	LYS	2.6
1	1	2538	U	2.6
1	1	1576	G	2.6
1	AR	1029	G	2.6
1	AR	1354	G	2.6
50	s1	233	GLY	2.6
54	s5	127	GLN	2.6
74	a	93	SER	2.6
69	d0	20	ILE	2.6
74	d5	44	GLN	2.6
75	b	41	ILE	2.6
37	DK	99	ARG	2.6
48	sR	484	C	2.6
56	s7	24	PHE	2.6
49	B	199	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
48	A	133	U	2.6
57	J	200	LYS	2.6
67	c8	10	SER	2.6
81	h	33	LEU	2.6
54	G	155	ALA	2.6
1	1	1270	A	2.6
1	AR	543	C	2.6
25	7	93	ARG	2.6
23	5	31	ALA	2.6
69	V	92	ASP	2.6
23	CW	101	ASN	2.6
61	c2	76	GLU	2.6
61	c2	84	ASN	2.6
68	c9	127	ASN	2.6
52	s3	43	PRO	2.6
73	Z	6	THR	2.6
1	AR	1816	A	2.6
56	s7	16	LEU	2.6
61	N	89	ILE	2.6
61	c2	46	ARG	2.6
48	A	820	U	2.6
50	s1	89	ASP	2.6
67	T	10	SER	2.6
68	c9	128	GLY	2.6
55	s6	215	ARG	2.6
57	J	104	ILE	2.6
69	d0	19	ILE	2.6
69	V	98	GLN	2.6
48	sR	74	U	2.6
61	c2	93	ASP	2.6
67	c8	4	VAL	2.6
77	d8	56	LEU	2.6
56	s7	60	ILE	2.6
67	T	55	HIS	2.6
80	g	93	HIS	2.6
20	z	189	ALA	2.5
54	s5	61	TYR	2.5
63	P	99	GLN	2.5
1	1	1260	A	2.5
1	AR	243	G	2.5
61	N	55	GLY	2.5
66	S	107	SER	2.5

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Mol	Chain	Res	Type	RSRZ
23	CW	98	THR	2.5
56	I	165	LYS	2.5
53	s4	259	GLN	2.5
1	AR	1356	U	2.5
49	B	9	LEU	2.5
54	s5	145	ASP	2.5
65	R	60	PHE	2.5
50	C	232	HIS	2.5
74	d5	38	HIS	2.5
81	h	248	ASN	2.5
36	DJ	119	LYS	2.5
59	c0	1	MET	2.5
48	sR	1371	A	2.5
10	CJ	256	ALA	2.5
83	e1	148	TYR	2.5
49	B	25	GLY	2.5
61	N	66	VAL	2.5
61	N	28	LEU	2.5
81	Rb	263	PHE	2.5
48	sR	1058	U	2.5
48	sR	1708	U	2.5
23	CW	108	TYR	2.5
62	O	57	ALA	2.5
63	P	101	ALA	2.5
1	1	2096	A	2.5
7	CG	5	LYS	2.5
39	DM	74	LYS	2.5
50	C	50	LYS	2.5
54	s5	20	PHE	2.5
54	G	71	ALA	2.5
54	G	210	ALA	2.5
63	c4	67	VAL	2.5
1	1	2445	A	2.5
48	sR	674	C	2.5
61	c2	135	MET	2.5
45	i	171	LYS	2.5
64	c5	9	LYS	2.5
76	c	75	GLU	2.5
51	s2	78	ASP	2.5
1	1	1268	G	2.5
81	Rb	180	ALA	2.5
50	s1	232	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
69	d0	52	LYS	2.5
15	CO	9	ALA	2.5
46	p0	211	SER	2.5
49	B	162	CYS	2.5
54	G	25	LEU	2.5
67	T	146	ALA	2.5
74	a	101	TYR	2.5
81	h	32	LEU	2.5
49	B	23	HIS	2.5
54	s5	137	ILE	2.5
20	CT	152	GLU	2.5
52	s3	41	VAL	2.5
58	s9	181	ALA	2.5
61	N	78	LEU	2.5
51	D	248	SER	2.5
74	a	38	HIS	2.5
76	d7	37	CYS	2.5
80	g	104	SER	2.5
65	R	40	GLU	2.5
58	s9	185	GLY	2.5
81	Rb	151	VAL	2.5
55	H	156	PHE	2.5
68	U	2	PRO	2.5
79	e0	53	LYS	2.5
46	p0	219	THR	2.5
47	sM	50	ASN	2.5
13	CM	174	LYS	2.5
48	sR	228	G	2.5
59	c0	70	GLU	2.5
74	a	78	ILE	2.5
1	1	1255	C	2.4
50	C	229	MET	2.4
50	C	21	VAL	2.4
58	K	138	LYS	2.4
69	V	31	VAL	2.4
48	A	231	U	2.4
23	CW	18	ASP	2.4
61	c2	107	ASP	2.4
1	1	1256	G	2.4
58	K	141	VAL	2.4
10	CJ	115	ALA	2.4
1	1	1353	U	2.4

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Mol	Chain	Res	Type	RSRZ
37	AJ	56	ARG	2.4
28	AA	46	ILE	2.4
56	s7	11	GLN	2.4
61	c2	24	ILE	2.4
74	d5	46	LYS	2.4
74	d5	85	LYS	2.4
23	CW	89	LEU	2.4
17	CQ	183	ALA	2.4
68	c9	17	ALA	2.4
1	AR	1031	C	2.4
7	m	189	GLU	2.4
54	s5	130	ILE	2.4
56	s7	7	LYS	2.4
56	s7	22	GLN	2.4
10	CJ	250	ALA	2.4
46	p0	18	TYR	2.4
50	C	56	SER	2.4
68	c9	136	ALA	2.4
25	CY	82	ILE	2.4
50	s1	183	GLN	2.4
63	P	76	ILE	2.4
55	s6	216	LEU	2.4
61	c2	44	GLY	2.4
67	T	13	HIS	2.4
68	c9	32	GLY	2.4
54	s5	96	SER	2.4
63	c4	55	SER	2.4
59	c0	78	GLU	2.4
80	g	151	ASN	2.4
28	AA	5	LEU	2.4
61	c2	82	PRO	2.4
81	Rb	125	GLY	2.4
1	AR	545	U	2.4
45	i	75	ASP	2.4
48	A	1363	U	2.4
48	sR	227	U	2.4
53	s4	93	ASP	2.4
1	1	1278	A	2.4
23	CW	33	TYR	2.4
64	c5	7	ALA	2.4
46	p0	96	ILE	2.4
25	CY	71	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
77	d8	67	ARG	2.4
35	AH	112	ALA	2.4
46	p0	48	ARG	2.4
48	A	495	C	2.4
61	c2	71	ILE	2.4
74	d5	103	ARG	2.4
76	c	58	SER	2.4
1	1	1103	A	2.4
1	1	1251	A	2.4
61	N	90	LYS	2.4
54	s5	44	ASN	2.4
62	O	151	ASN	2.4
81	Rb	224	ASN	2.4
63	c4	58	TYR	2.4
48	sR	501	U	2.4
46	p0	24	SER	2.4
56	I	7	LYS	2.4
81	Rb	254	ALA	2.4
1	AR	2095	G	2.4
23	5	93	ILE	2.4
48	sR	655	G	2.4
61	c2	39	ASP	2.4
63	P	83	ILE	2.4
81	h	114	ASP	2.4
46	p0	184	GLY	2.4
49	s0	186	GLY	2.4
52	E	221	SER	2.4
63	P	113	GLY	2.4
1	1	3285	C	2.4
1	1	2208	A	2.4
73	Z	34	ASN	2.4
18	x	182	ILE	2.4
31	DE	100	ILE	2.4
56	s7	20	VAL	2.4
61	N	120	VAL	2.4
48	A	280	U	2.4
63	c4	97	GLY	2.4
70	d1	48	GLY	2.4
53	F	252	ARG	2.4
61	N	141	SER	2.4
59	c0	74	GLU	2.4
1	AR	439	C	2.4

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Mol	Chain	Res	Type	RSRZ
61	N	84	ASN	2.4
76	d7	62	ILE	2.4
61	c2	45	LEU	2.4
81	Rb	13	LEU	2.4
81	Rb	47	LEU	2.4
1	1	1271	A	2.3
54	s5	43	PHE	2.3
74	a	67	ASP	2.3
81	Rb	61	PHE	2.3
82	c7	64	GLY	2.3
1	1	979	U	2.3
48	sR	241	U	2.3
55	s6	164	LYS	2.3
80	g	83	LYS	2.3
81	h	246	SER	2.3
81	Rb	82	SER	2.3
38	AK	86	ALA	2.3
41	AN	77	ILE	2.3
48	sR	496	G	2.3
58	K	116	LEU	2.3
60	c1	21	ASN	2.3
61	c2	41	LEU	2.3
81	h	71	CYS	2.3
70	d1	39	VAL	2.3
74	d5	87	GLY	2.3
25	7	66	GLU	2.3
1	1	252	U	2.3
75	b	57	SER	2.3
54	G	162	VAL	2.3
81	h	6	VAL	2.3
1	AR	1563	C	2.3
67	c8	6	GLN	2.3
46	p0	188	VAL	2.3
46	p0	202	LEU	2.3
23	CW	54	VAL	2.3
32	AE	79	ARG	2.3
54	G	21	THR	2.3
74	d5	68	ARG	2.3
63	P	19	ILE	2.3
69	d0	21	LYS	2.3
1	1	1272	C	2.3
48	sR	1690	G	2.3

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Mol	Chain	Res	Type	RSRZ
48	sR	1687	U	2.3
60	c1	116	ARG	2.3
76	d7	33	LEU	2.3
17	CQ	187	GLU	2.3
65	c6	5	PRO	2.3
68	U	141	GLU	2.3
31	DE	22	LYS	2.3
48	A	657	U	2.3
20	CT	178	ALA	2.3
53	F	228	ILE	2.3
67	T	14	ILE	2.3
48	sR	198	A	2.3
71	X	55	ASP	2.3
81	h	263	PHE	2.3
32	AE	82	GLU	2.3
45	i	49	LYS	2.3
73	Z	46	GLU	2.3
81	Rb	205	SER	2.3
1	AR	1579	C	2.3
18	x	168	LEU	2.3
48	A	489	C	2.3
56	I	5	GLN	2.3
61	c2	62	LEU	2.3
20	z	163	ARG	2.3
1	1	1565	G	2.3
50	C	226	GLY	2.3
74	a	53	GLU	2.3
52	s3	195	SER	2.3
65	R	141	SER	2.3
49	B	203	PHE	2.3
56	I	24	PHE	2.3
59	c0	41	TYR	2.3
1	1	1016	C	2.3
1	AR	1951	C	2.3
48	A	320	U	2.3
48	A	499	U	2.3
56	I	75	THR	2.3
81	Rb	135	THR	2.3
51	D	151	PRO	2.3
48	A	793	A	2.3
67	c8	15	LEU	2.3
54	G	35	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
58	s9	179	ARG	2.3
81	h	310	ILE	2.3
70	W	53	TYR	2.3
76	d7	82	LYS	2.3
65	R	56	GLY	2.3
67	T	20	THR	2.3
76	c	44	THR	2.3
1	1	1252	A	2.3
13	s	90	GLN	2.3
61	c2	120	VAL	2.3
63	c4	28	VAL	2.3
74	a	98	GLN	2.3
56	I	80	GLU	2.2
56	s7	53	GLY	2.2
49	s0	9	LEU	2.2
54	s5	161	ASP	2.2
65	R	64	ASP	2.2
69	V	89	ARG	2.2
81	h	72	THR	2.2
81	h	182	ASN	2.2
1	AR	1582	C	2.2
25	7	91	LYS	2.2
48	sR	224	C	2.2
68	c9	113	ILE	2.2
81	h	206	PRO	2.2
56	s7	51	VAL	2.2
55	H	146	GLY	2.2
67	c8	146	ALA	2.2
81	Rb	27	ALA	2.2
81	Rb	80	ALA	2.2
23	CW	92	TRP	2.2
83	e1	111	GLU	2.2
49	B	113	ARG	2.2
10	CJ	132	VAL	2.2
1	AR	2572	C	2.2
9	o	25	GLN	2.2
48	A	230	C	2.2
48	A	237	C	2.2
58	K	177	ALA	2.2
61	N	138	GLU	2.2
61	c2	40	GLY	2.2
59	L	76	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
83	e1	149	LYS	2.2
48	sR	1714	A	2.2
68	c9	35	ASP	2.2
70	W	40	ASP	2.2
20	z	177	VAL	2.2
1	1	2206	G	2.2
1	AR	245	U	2.2
10	p	115	ALA	2.2
48	A	723	G	2.2
48	A	899	G	2.2
56	s7	184	GLU	2.2
57	s8	141	ARG	2.2
66	S	74	GLN	2.2
55	H	124	LEU	2.2
59	c0	22	VAL	2.2
65	c6	64	ASP	2.2
68	U	131	ASP	2.2
14	CN	130	GLY	2.2
75	b	82	ARG	2.2
28	AA	2	ALA	2.2
46	p0	216	ALA	2.2
57	J	167	ALA	2.2
61	N	128	ALA	2.2
1	AR	3277	U	2.2
69	d0	120	SER	2.2
81	Rb	213	SER	2.2
68	U	71	VAL	2.2
31	DE	59	TYR	2.2
56	I	76	LYS	2.2
61	N	125	ASN	2.2
61	c2	94	ALA	2.2
63	P	12	GLN	2.2
73	Z	125	LEU	2.2
82	c7	113	LEU	2.2
20	z	167	ARG	2.2
55	H	12	SER	2.2
59	c0	48	SER	2.2
66	S	71	PHE	2.2
61	N	22	VAL	2.2
76	d7	35	VAL	2.2
81	h	211	ILE	2.2
81	Rb	124	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	AR	1577	G	2.2
57	s8	118	GLY	2.2
21	0	2	ALA	2.2
54	G	26	ALA	2.2
70	W	37	ALA	2.2
74	d5	57	TYR	2.2
65	c6	52	LEU	2.2
1	AR	2541	U	2.2
74	d5	82	HIS	2.2
50	C	193	ILE	2.2
56	I	33	GLU	2.2
73	Z	101	GLU	2.2
54	G	56	ALA	2.2
67	c8	8	GLN	2.2
67	c8	18	LEU	2.2
74	a	58	ARG	2.2
58	s9	146	PHE	2.2
49	B	32	HIS	2.2
74	a	71	ILE	2.2
48	sR	794	U	2.2
46	p0	191	TYR	2.2
75	b	48	ALA	2.2
25	7	94	ARG	2.2
31	AD	12	GLN	2.2
45	i	14	ASP	2.2
56	I	63	PRO	2.2
23	5	28	PHE	2.2
53	F	57	ASN	2.2
54	G	140	THR	2.2
57	J	72	ILE	2.2
60	M	6	THR	2.2
49	B	139	VAL	2.2
74	a	60	VAL	2.2
80	g	145	HIS	2.2
7	m	127	GLY	2.2
68	c9	112	GLY	2.2
69	d0	111	GLY	2.2
20	z	174	ALA	2.2
21	CU	2	ALA	2.2
48	sR	705	U	2.2
61	c2	103	LEU	2.2
12	CL	217	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
54	G	48	PHE	2.2
58	K	89	ASP	2.2
67	c8	11	PHE	2.2
56	I	26	GLU	2.2
58	s9	111	THR	2.2
67	c8	20	THR	2.2
63	c4	45	GLY	2.2
7	m	236	LEU	2.2
40	AM	2	ALA	2.2
61	c2	79	ALA	2.2
63	c4	125	SER	2.2
46	p0	206	ASP	2.2
47	sM	43	ASP	2.2
49	B	125	ASP	2.2
52	s3	128	GLU	2.2
54	G	52	GLU	2.2
56	I	87	ASP	2.2
61	c2	77	GLY	2.2
62	O	59	GLY	2.2
63	P	114	ARG	2.2
77	d	45	LYS	2.2
81	h	77	GLY	2.2
82	c7	90	ALA	2.1
81	h	22	SER	2.1
81	h	262	VAL	2.1
83	e1	124	PRO	2.1
20	z	170	ARG	2.1
46	p0	186	THR	2.1
54	s5	128	ASN	2.1
73	d4	34	ASN	2.1
77	d8	66	LEU	2.1
46	p0	213	PHE	2.1
81	Rb	54	PHE	2.1
37	DK	97	SER	2.1
50	C	114	VAL	2.1
65	c6	143	ARG	2.1
75	b	44	ILE	2.1
76	d7	36	LYS	2.1
77	d8	31	GLU	2.1
81	h	205	SER	2.1
81	Rb	129	LYS	2.1
61	c2	117	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	AR	3286	G	2.1
77	d8	32	PHE	2.1
81	Rb	103	PHE	2.1
28	DB	6	LYS	2.1
28	DB	21	LYS	2.1
48	sR	579	A	2.1
61	N	87	PRO	2.1
63	c4	15	GLY	2.1
77	d8	37	SER	2.1
80	g	146	SER	2.1
81	h	213	SER	2.1
48	sR	192	U	2.1
48	sR	1686	C	2.1
64	c5	32	ASP	2.1
74	a	42	LEU	2.1
32	DF	79	ARG	2.1
54	G	139	ASN	2.1
49	B	50	VAL	2.1
53	s4	162	ILE	2.1
10	CJ	119	GLY	2.1
48	A	486	G	2.1
48	sR	1691	A	2.1
61	N	113	ARG	2.1
63	P	82	LYS	2.1
69	V	45	ALA	2.1
73	d4	134	ALA	2.1
81	h	296	ALA	2.1
49	s0	162	CYS	2.1
56	I	8	ILE	2.1
55	H	165	GLY	2.1
65	R	5	PRO	2.1
66	S	120	SER	2.1
1	AR	1565	G	2.1
46	p0	69	ASP	2.1
49	B	43	ASP	2.1
54	G	43	PHE	2.1
75	b	85	ARG	2.1
28	DB	120	GLU	2.1
39	DM	27	ILE	2.1
46	p0	101	VAL	2.1
63	P	38	THR	2.1
65	c6	63	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
8	CH	8	LYS	2.1
46	p0	81	LYS	2.1
58	K	29	LYS	2.1
63	c4	46	MET	2.1
67	c8	17	LEU	2.1
74	a	49	ARG	2.1
60	c1	144	ALA	2.1
48	A	713	A	2.1
1	AR	3349	C	2.1
49	s0	41	ARG	2.1
58	K	86	LEU	2.1
69	d0	16	GLN	2.1
77	d	57	MET	2.1
39	DM	70	PRO	2.1
39	AL	34	ALA	2.1
58	s9	183	ALA	2.1
81	h	264	SER	2.1
49	s0	86	VAL	2.1
7	m	295	GLY	2.1
18	CR	171	ARG	2.1
76	d7	80	ARG	2.1
48	A	137	U	2.1
81	Rb	141	LEU	2.1
55	s6	10	ASN	2.1
83	e1	115	THR	2.1
1	AR	1032	C	2.1
1	AR	2545	C	2.1
30	DD	58	LYS	2.1
39	DM	64	LYS	2.1
47	sM	68	ARG	2.1
50	C	137	ILE	2.1
70	W	82	VAL	2.1
77	d8	55	VAL	2.1
81	h	234	LEU	2.1
68	U	138	GLN	2.1
77	d	27	GLN	2.1
10	p	122	LYS	2.1
32	DF	111	GLU	2.1
39	DM	37	PRO	2.1
82	c7	86	PRO	2.1
55	H	67	VAL	2.1
56	s7	90	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
83	e1	110	ALA	2.1
48	A	500	C	2.1
50	C	140	ILE	2.1
65	R	65	ILE	2.1
10	CJ	247	ASP	2.1
48	sR	720	G	2.1
81	Rb	210	LEU	2.1
51	s2	64	LYS	2.1
73	d4	99	LYS	2.1
1	AR	250	U	2.1
1	AR	1094	U	2.1
77	d8	64	ARG	2.1
83	e1	123	ASN	2.1
23	CW	22	PRO	2.1
28	DB	75	VAL	2.1
45	i	54	PRO	2.1
60	c1	146	ALA	2.1
61	N	51	ALA	2.1
63	P	30	VAL	2.1
48	sR	485	A	2.1
65	c6	85	ILE	2.1
7	m	297	GLN	2.0
55	H	155	ASP	2.1
55	s6	156	PHE	2.0
57	s8	111	GLN	2.0
67	T	6	GLN	2.0
1	AR	1024	G	2.0
1	AR	1952	G	2.0
50	C	133	TYR	2.0
73	Z	98	GLU	2.0
77	d8	58	GLU	2.0
81	Rb	160	GLU	2.0
23	CW	61	THR	2.0
28	DB	7	ALA	2.0
49	s0	21	ASN	2.0
46	p0	220	ILE	2.0
48	A	781	U	2.0
48	sR	193	U	2.0
81	Rb	88	THR	2.0
75	b	53	LEU	2.0
50	C	30	PHE	2.0
60	M	26	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
63	P	11	SER	2.0
74	d5	58	ARG	2.0
81	h	192	PHE	2.0
50	C	132	ASP	2.0
50	s1	132	ASP	2.0
18	x	177	ALA	2.0
57	s8	150	ALA	2.0
59	c0	66	TYR	2.0
61	c2	31	VAL	2.0
63	P	28	VAL	2.0
69	V	116	VAL	2.0
23	5	87	ASN	2.0
47	sM	44	PRO	2.0
50	C	98	THR	2.0
61	c2	88	LEU	2.0
63	P	110	LEU	2.0
63	P	115	ILE	2.0
64	c5	68	PRO	2.0
77	d8	6	PRO	2.0
1	AR	1950	U	2.0
55	s6	143	LYS	2.0
56	s7	175	LYS	2.0
60	c1	30	ARG	2.0
65	c6	60	PHE	2.0
59	c0	7	ASP	2.0
61	N	119	SER	2.0
69	d0	92	ASP	2.0
77	d	59	SER	2.0
78	e	4	GLU	2.0
55	H	221	ALA	2.0
74	a	47	TYR	2.0
28	DB	56	LYS	2.0
46	p0	100	ILE	2.0
51	D	190	LEU	2.0
68	U	135	ILE	2.0
28	AA	4	PHE	2.0
39	DM	16	ARG	2.0
46	p0	82	GLY	2.0
46	p0	92	PRO	2.0
70	d1	43	GLY	2.0
74	d5	70	LYS	2.0
1	1	3287	U	2.0

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Mol	Chain	Res	Type	RSRZ
50	C	103	MET	2.0
39	DM	67	GLN	2.0
39	DM	7	ASP	2.0
48	A	228	G	2.0
59	c0	26	ASP	2.0
74	d5	43	ASP	2.0
56	s7	34	LEU	2.0
57	J	199	LYS	2.0
60	M	144	ALA	2.0
80	g	99	LYS	2.0
81	Rb	81	LEU	2.0
39	DM	35	GLY	2.0
56	I	78	THR	2.0
63	P	77	THR	2.0
65	R	62	ASN	2.0
67	T	44	ASN	2.0
76	d7	40	CYS	2.0
53	s4	258	GLN	2.0
50	s1	73	LEU	2.0
50	s1	224	ASP	2.0
54	s5	133	VAL	2.0
56	s7	157	LYS	2.0
70	W	36	VAL	2.0
61	N	94	ALA	2.0
68	c9	19	ALA	2.0
55	s6	173	PRO	2.0
8	CH	129	GLU	2.0
59	c0	20	VAL	2.0
67	T	61	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
85	MG	AR	3834	1/1	0.28	0.47	61,61,61,61	0
85	MG	1	4165	1/1	0.32	0.36	153,153,153,153	0
85	MG	AR	4138	1/1	0.39	0.48	75,75,75,75	0
85	MG	AR	4055	1/1	0.40	0.54	72,72,72,72	0
85	MG	1	3970	1/1	0.41	0.29	82,82,82,82	0
85	MG	sR	2066	1/1	0.41	0.43	73,73,73,73	0
85	MG	AR	4156	1/1	0.43	0.66	56,56,56,56	0
85	MG	sR	2157	1/1	0.47	0.66	71,71,71,71	0
85	MG	4	229	1/1	0.47	0.37	55,55,55,55	0
85	MG	3	210	1/1	0.52	0.45	46,46,46,46	0
85	MG	AR	4006	1/1	0.53	0.20	54,54,54,54	0
85	MG	1	3822	1/1	0.55	0.73	69,69,69,69	0
85	MG	AR	4102	1/1	0.56	0.69	53,53,53,53	0
85	MG	AR	4126	1/1	0.57	0.79	46,46,46,46	0
85	MG	3	216	1/1	0.57	0.49	78,78,78,78	0
85	MG	AR	4230	1/1	0.58	0.40	59,59,59,59	0
85	MG	AR	4113	1/1	0.59	0.52	63,63,63,63	0
85	MG	sR	2142	1/1	0.59	0.28	65,65,65,65	0
85	MG	AR	3957	1/1	0.59	0.30	57,57,57,57	0
85	MG	A	2119	1/1	0.59	0.67	66,66,66,66	0
84	OHX	AR	3742	7/7	0.60	0.35	225,225,226,226	0
85	MG	AR	4004	1/1	0.60	0.36	68,68,68,68	0
85	MG	1	4076	1/1	0.61	0.34	82,82,82,82	0
85	MG	1	4116	1/1	0.61	0.51	52,52,52,52	0
85	MG	l	404	1/1	0.61	0.57	44,44,44,44	0
85	MG	sR	2185	1/1	0.61	0.60	68,68,68,68	0
85	MG	s	300	1/1	0.62	0.18	63,63,63,63	0
85	MG	1	4115	1/1	0.62	0.31	60,60,60,60	0
85	MG	AR	4236	1/1	0.62	0.53	58,58,58,58	0
84	OHX	CG	302	7/7	0.64	0.33	208,208,209,209	0
85	MG	AR	4091	1/1	0.64	0.49	70,70,70,70	0
85	MG	sR	2082	1/1	0.64	0.60	63,63,63,63	0
85	MG	AR	4085	1/1	0.65	0.41	73,73,73,73	0
85	MG	A	2098	1/1	0.65	0.21	96,96,96,96	0
85	MG	1	4155	1/1	0.65	0.68	71,71,71,71	0
85	MG	AR	4186	1/1	0.65	0.45	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	4038	1/1	0.65	0.47	57,57,57,57	0
85	MG	A	2068	1/1	0.65	0.44	73,73,73,73	0
85	MG	x	206	1/1	0.65	0.56	47,47,47,47	0
85	MG	sR	2151	1/1	0.66	0.40	63,63,63,63	0
85	MG	A	2113	1/1	0.66	0.41	78,78,78,78	0
85	MG	AR	4059	1/1	0.66	0.19	68,68,68,68	0
85	MG	AR	3817	1/1	0.66	0.18	106,106,106,106	0
85	MG	1	3979	1/1	0.67	0.35	59,59,59,59	0
85	MG	sR	2170	1/1	0.67	0.39	59,59,59,59	0
85	MG	1	3802	1/1	0.67	0.47	52,52,52,52	0
85	MG	AR	4183	1/1	0.67	0.14	102,102,102,102	0
85	MG	AR	3777	1/1	0.67	0.25	78,78,78,78	0
85	MG	AR	4130	1/1	0.67	0.24	64,64,64,64	0
85	MG	1	3921	1/1	0.68	0.39	39,39,39,39	0
85	MG	A	2115	1/1	0.68	0.34	69,69,69,69	0
85	MG	AR	4048	1/1	0.68	0.33	68,68,68,68	0
85	MG	AR	3908	1/1	0.68	0.39	41,41,41,41	0
84	OHX	AR	3740	7/7	0.68	0.55	212,212,213,213	0
85	MG	1	4033	1/1	0.68	0.32	73,73,73,73	0
85	MG	AR	4145	1/1	0.68	0.27	48,48,48,48	0
85	MG	d3	202	1/1	0.69	0.30	59,59,59,59	0
85	MG	1	4045	1/1	0.69	0.26	58,58,58,58	0
85	MG	AR	4037	1/1	0.69	0.30	70,70,70,70	0
85	MG	AR	4027	1/1	0.70	0.12	105,105,105,105	0
85	MG	AR	4124	1/1	0.70	0.17	73,73,73,73	0
84	OHX	sR	2041	7/7	0.70	0.30	238,238,239,240	0
85	MG	A	2104	1/1	0.71	0.59	67,67,67,67	0
85	MG	sR	2121	1/1	0.71	0.32	69,69,69,69	0
85	MG	AR	4049	1/1	0.71	0.20	52,52,52,52	0
85	MG	AR	4227	1/1	0.71	0.60	78,78,78,78	0
85	MG	1	4104	1/1	0.71	0.57	47,47,47,47	0
85	MG	AR	3796	1/1	0.71	0.34	62,62,62,62	0
85	MG	1	3994	1/1	0.72	0.59	45,45,45,45	0
85	MG	1	4183	1/1	0.72	0.14	67,67,67,67	0
85	MG	AR	4169	1/1	0.72	0.99	101,101,101,101	0
85	MG	sR	2069	1/1	0.72	0.33	53,53,53,53	0
85	MG	AR	4014	1/1	0.72	0.19	53,53,53,53	0
85	MG	AR	3972	1/1	0.72	0.64	52,52,52,52	0
85	MG	A	2110	1/1	0.73	0.25	78,78,78,78	0
85	MG	AR	4110	1/1	0.73	0.30	56,56,56,56	0
85	MG	sR	2187	1/1	0.73	0.59	70,70,70,70	0
85	MG	AR	4155	1/1	0.73	0.35	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	A	2046	1/1	0.73	0.27	55,55,55,55	0
85	MG	AR	3989	1/1	0.73	0.72	58,58,58,58	0
85	MG	DA	201	1/1	0.73	0.22	52,52,52,52	0
85	MG	A	2150	1/1	0.73	0.39	51,51,51,51	0
85	MG	1	3834	1/1	0.73	0.45	42,42,42,42	0
84	OHX	1	3673	7/7	0.74	0.47	183,183,183,183	0
85	MG	AR	4176	1/1	0.74	0.22	60,60,60,60	0
85	MG	1	4138	1/1	0.74	0.35	44,44,44,44	0
85	MG	1	4125	1/1	0.74	0.38	49,49,49,49	0
85	MG	AR	3974	1/1	0.74	0.41	71,71,71,71	0
85	MG	1	4003	1/1	0.74	0.43	62,62,62,62	0
85	MG	1	3988	1/1	0.74	0.44	44,44,44,44	0
85	MG	1	4032	1/1	0.74	0.58	66,66,66,66	0
85	MG	A	2134	1/1	0.75	0.55	53,53,53,53	0
84	OHX	AR	3746	7/7	0.75	0.20	269,269,270,270	0
85	MG	1	4100	1/1	0.75	0.28	46,46,46,46	0
85	MG	AT	221	1/1	0.75	0.77	57,57,57,57	0
85	MG	sR	2074	1/1	0.75	0.37	51,51,51,51	0
85	MG	A	2138	1/1	0.76	0.33	74,74,74,74	0
85	MG	AR	3966	1/1	0.76	0.55	55,55,55,55	0
85	MG	1	4152	1/1	0.76	0.35	37,37,37,37	0
84	OHX	AR	3735	7/7	0.76	0.34	208,208,208,209	0
85	MG	A	2097	1/1	0.76	0.25	75,75,75,75	0
84	OHX	sR	2052	7/7	0.76	0.22	208,209,210,210	0
85	MG	1	4187	1/1	0.76	0.33	52,52,52,52	0
85	MG	AR	4171	1/1	0.76	0.45	50,50,50,50	0
85	MG	1	402	1/1	0.76	0.20	39,39,39,39	0
85	MG	1	3772	1/1	0.76	0.43	50,50,50,50	0
85	MG	1	3790	1/1	0.76	0.79	72,72,72,72	0
85	MG	A	2082	1/1	0.76	0.26	69,69,69,69	0
85	MG	1	4167	1/1	0.76	0.24	57,57,57,57	0
84	OHX	1	3718	7/7	0.77	0.42	254,254,255,255	0
85	MG	AR	4157	1/1	0.77	0.44	62,62,62,62	0
85	MG	AR	4161	1/1	0.77	0.27	52,52,52,52	0
85	MG	1	3824	1/1	0.77	0.34	53,53,53,53	0
85	MG	1	3875	1/1	0.77	0.28	32,32,32,32	0
85	MG	sR	2094	1/1	0.77	0.29	33,33,33,33	0
85	MG	J	302	1/1	0.77	0.30	55,55,55,55	0
85	MG	AR	4233	1/1	0.77	0.44	54,54,54,54	0
85	MG	sR	2159	1/1	0.77	0.63	58,58,58,58	0
85	MG	DC	205	1/1	0.77	0.40	34,34,34,34	0
85	MG	1	4093	1/1	0.77	0.13	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	sR	2132	1/1	0.77	0.21	59,59,59,59	0
85	MG	CP	504	1/1	0.77	0.40	51,51,51,51	0
85	MG	1	4184	1/1	0.78	0.26	48,48,48,48	0
85	MG	e	102	1/1	0.78	0.17	81,81,81,81	0
85	MG	AR	4187	1/1	0.78	0.29	50,50,50,50	0
84	OHX	A	2039	7/7	0.78	0.40	234,235,236,236	0
85	MG	1	4162	1/1	0.78	0.49	32,32,32,32	0
85	MG	1	4088	1/1	0.78	0.28	53,53,53,53	0
85	MG	1	3866	1/1	0.78	0.41	44,44,44,44	0
85	MG	l	403	1/1	0.78	0.45	63,63,63,63	0
85	MG	1	4130	1/1	0.78	0.33	69,69,69,69	0
85	MG	1	3985	1/1	0.78	0.46	85,85,85,85	0
85	MG	w	201	1/1	0.78	0.40	54,54,54,54	0
85	MG	1	3784	1/1	0.78	0.39	54,54,54,54	0
85	MG	1	3785	1/1	0.78	0.37	30,30,30,30	0
85	MG	AR	4118	1/1	0.78	0.15	55,55,55,55	0
85	MG	6	202	1/1	0.78	0.30	67,67,67,67	0
85	MG	sR	2076	1/1	0.78	0.37	77,77,77,77	0
85	MG	A	2087	1/1	0.78	0.30	70,70,70,70	0
84	OHX	AR	3670	7/7	0.78	0.37	245,245,245,245	0
85	MG	AR	3803	1/1	0.78	0.51	43,43,43,43	0
85	MG	AR	4150	1/1	0.78	0.31	63,63,63,63	0
85	MG	l	406	1/1	0.78	0.81	72,72,72,72	0
85	MG	AT	224	1/1	0.78	0.29	70,70,70,70	0
85	MG	1	3787	1/1	0.79	0.49	63,63,63,63	0
85	MG	AR	4029	1/1	0.79	0.16	51,51,51,51	0
85	MG	A	2051	1/1	0.79	0.35	69,69,69,69	0
85	MG	AT	225	1/1	0.79	0.71	72,72,72,72	0
84	OHX	1	3698	7/7	0.79	0.29	245,245,246,246	0
84	OHX	sR	2040	7/7	0.79	0.42	165,166,166,167	0
84	OHX	AR	3693	7/7	0.79	0.30	221,222,222,223	0
85	MG	1	4004	1/1	0.79	0.13	66,66,66,66	0
85	MG	1	4094	1/1	0.79	0.32	59,59,59,59	0
85	MG	A	2124	1/1	0.79	0.25	67,67,67,67	0
85	MG	1	4001	1/1	0.79	0.58	61,61,61,61	0
85	MG	sR	2158	1/1	0.79	0.20	62,62,62,62	0
85	MG	AR	4100	1/1	0.79	0.32	63,63,63,63	0
85	MG	1	4123	1/1	0.79	0.28	53,53,53,53	0
84	OHX	AR	3725	7/7	0.79	0.37	178,178,178,178	0
85	MG	sR	2188	1/1	0.79	0.43	62,62,62,62	0
85	MG	1	3878	1/1	0.79	0.49	53,53,53,53	0
85	MG	A	2084	1/1	0.79	0.28	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	sR	2086	1/1	0.80	0.28	81,81,81,81	0
85	MG	1	3913	1/1	0.80	0.44	40,40,40,40	0
85	MG	sR	2087	1/1	0.80	0.33	53,53,53,53	0
85	MG	A	2102	1/1	0.80	0.61	75,75,75,75	0
85	MG	4	232	1/1	0.80	0.17	52,52,52,52	0
85	MG	AR	3983	1/1	0.80	0.28	71,71,71,71	0
85	MG	AR	4234	1/1	0.80	0.40	59,59,59,59	0
85	MG	1	3871	1/1	0.80	0.33	70,70,70,70	0
85	MG	1	4005	1/1	0.80	0.30	49,49,49,49	0
85	MG	AR	4182	1/1	0.80	0.28	40,40,40,40	0
85	MG	1	4194	1/1	0.80	0.41	29,29,29,29	0
85	MG	1	4108	1/1	0.80	0.51	69,69,69,69	0
85	MG	1	4110	1/1	0.80	0.34	76,76,76,76	0
84	OHX	1	3682	7/7	0.80	0.28	179,179,180,180	0
85	MG	A	2106	1/1	0.81	0.47	71,71,71,71	0
85	MG	3	219	1/1	0.81	0.16	68,68,68,68	0
84	OHX	4	215	7/7	0.81	0.27	167,168,168,168	0
85	MG	AR	4194	1/1	0.81	0.29	54,54,54,54	0
85	MG	AR	3751	1/1	0.81	0.50	33,33,33,33	0
85	MG	1	3738	1/1	0.81	0.40	36,36,36,36	0
85	MG	A	2132	1/1	0.81	0.23	68,68,68,68	0
85	MG	AR	4162	1/1	0.81	0.40	69,69,69,69	0
85	MG	AR	4043	1/1	0.81	0.39	45,45,45,45	0
85	MG	AR	3899	1/1	0.81	0.43	32,32,32,32	0
85	MG	1	4132	1/1	0.81	0.36	54,54,54,54	0
85	MG	1	4192	1/1	0.81	0.20	32,32,32,32	0
85	MG	AR	4082	1/1	0.81	0.23	37,37,37,37	0
85	MG	1	4185	1/1	0.81	0.35	42,42,42,42	0
85	MG	AT	227	1/1	0.81	0.79	75,75,75,75	0
85	MG	A	2129	1/1	0.81	0.61	65,65,65,65	0
85	MG	1	4047	1/1	0.81	0.65	63,63,63,63	0
85	MG	CE	403	1/1	0.81	0.39	31,31,31,31	0
85	MG	1	4176	1/1	0.81	0.32	66,66,66,66	0
85	MG	CF	403	1/1	0.81	0.38	37,37,37,37	0
85	MG	AR	3985	1/1	0.81	0.37	61,61,61,61	0
85	MG	1	3935	1/1	0.81	0.26	38,38,38,38	0
85	MG	A	2069	1/1	0.81	0.53	65,65,65,65	0
84	OHX	A	2015	7/7	0.81	0.46	213,214,216,216	0
85	MG	sR	2161	1/1	0.81	0.35	58,58,58,58	0
84	OHX	sR	2051	7/7	0.81	0.29	196,196,197,198	0
85	MG	1	3762	1/1	0.81	0.50	45,45,45,45	0
84	OHX	AR	3669	7/7	0.81	0.21	188,189,189,189	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	sR	2180	1/1	0.81	0.46	68,68,68,68	0
85	MG	sR	2141	1/1	0.81	0.15	62,62,62,62	0
85	MG	AR	4235	1/1	0.81	0.37	66,66,66,66	0
85	MG	sR	2179	1/1	0.81	0.45	64,64,64,64	0
85	MG	1	3960	1/1	0.82	0.64	47,47,47,47	0
85	MG	AR	4046	1/1	0.82	0.46	63,63,63,63	0
85	MG	sR	2085	1/1	0.82	0.68	64,64,64,64	0
85	MG	d6	102	1/1	0.82	0.40	59,59,59,59	0
85	MG	1	3984	1/1	0.82	0.36	54,54,54,54	0
85	MG	AR	4200	1/1	0.82	0.36	46,46,46,46	0
85	MG	AR	3876	1/1	0.82	0.20	50,50,50,50	0
85	MG	AR	3774	1/1	0.82	0.34	48,48,48,48	0
85	MG	AR	4202	1/1	0.82	0.42	50,50,50,50	0
85	MG	CM	202	1/1	0.82	0.17	60,60,60,60	0
85	MG	AR	4207	1/1	0.82	0.23	54,54,54,54	0
85	MG	x	203	1/1	0.82	0.43	65,65,65,65	0
85	MG	A	2061	1/1	0.82	0.44	68,68,68,68	0
85	MG	4	226	1/1	0.82	0.36	55,55,55,55	0
85	MG	AR	4222	1/1	0.82	0.33	73,73,73,73	0
85	MG	1	3971	1/1	0.82	0.23	41,41,41,41	0
85	MG	AR	3982	1/1	0.82	0.30	45,45,45,45	0
85	MG	1	4020	1/1	0.82	0.24	62,62,62,62	0
85	MG	sR	2110	1/1	0.82	0.48	61,61,61,61	0
84	OHX	A	2034	7/7	0.82	0.16	261,262,263,263	0
85	MG	DC	204	1/1	0.82	0.62	47,47,47,47	0
85	MG	1	3808	1/1	0.82	0.32	52,52,52,52	0
85	MG	1	3952	1/1	0.82	0.45	75,75,75,75	0
85	MG	AR	3980	1/1	0.82	0.41	66,66,66,66	0
84	OHX	1	3704	7/7	0.82	0.45	181,181,181,181	0
85	MG	1	4181	1/1	0.83	0.16	50,50,50,50	0
85	MG	AR	3778	1/1	0.83	0.39	52,52,52,52	0
85	MG	A	2053	1/1	0.83	0.50	49,49,49,49	0
85	MG	sR	2116	1/1	0.83	0.32	64,64,64,64	0
85	MG	1	4062	1/1	0.83	0.37	47,47,47,47	0
85	MG	4	230	1/1	0.83	0.50	60,60,60,60	0
85	MG	sR	2138	1/1	0.83	0.26	65,65,65,65	0
85	MG	AR	4238	1/1	0.83	0.39	54,54,54,54	0
85	MG	AR	3819	1/1	0.83	0.37	56,56,56,56	0
85	MG	sR	2183	1/1	0.83	0.58	68,68,68,68	0
85	MG	sR	2124	1/1	0.83	0.52	54,54,54,54	0
85	MG	1	4180	1/1	0.83	0.20	58,58,58,58	0
85	MG	AR	4140	1/1	0.83	0.26	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	4022	1/1	0.83	0.42	36,36,36,36	0
85	MG	1	4051	1/1	0.83	0.32	44,44,44,44	0
85	MG	sR	2191	1/1	0.83	0.16	67,67,67,67	0
85	MG	n	201	1/1	0.83	0.21	48,48,48,48	0
84	OHX	1	3719	7/7	0.83	0.28	176,176,177,177	0
84	OHX	AS	209	7/7	0.83	0.25	182,183,183,184	0
85	MG	AR	3968	1/1	0.83	0.31	47,47,47,47	0
85	MG	1	4160	1/1	0.83	0.22	51,51,51,51	0
84	OHX	CM	201	7/7	0.83	0.31	200,200,201,201	0
85	MG	A	2088	1/1	0.83	0.28	55,55,55,55	0
85	MG	1	3981	1/1	0.83	0.25	49,49,49,49	0
85	MG	AR	4165	1/1	0.84	0.34	43,43,43,43	0
85	MG	AR	3830	1/1	0.84	0.24	47,47,47,47	0
85	MG	AR	4122	1/1	0.84	0.47	62,62,62,62	0
85	MG	1	4021	1/1	0.84	0.39	46,46,46,46	0
85	MG	1	4195	1/1	0.84	0.39	25,25,25,25	0
85	MG	AR	4197	1/1	0.84	0.17	82,82,82,82	0
85	MG	1	4122	1/1	0.84	0.24	51,51,51,51	0
85	MG	A	2070	1/1	0.84	0.41	70,70,70,70	0
84	OHX	A	2041	7/7	0.84	0.45	182,182,183,183	0
85	MG	A	2135	1/1	0.84	0.56	70,70,70,70	0
85	MG	t	203	1/1	0.84	0.66	41,41,41,41	0
84	OHX	AR	3653	7/7	0.84	0.32	167,167,168,168	0
84	OHX	A	1971	7/7	0.84	0.18	164,165,166,166	0
85	MG	sR	2122	1/1	0.84	0.23	71,71,71,71	0
84	OHX	AR	3732	7/7	0.84	0.27	227,228,228,228	0
84	OHX	AR	3711	7/7	0.84	0.29	180,181,181,181	0
85	MG	1	4109	1/1	0.84	0.36	40,40,40,40	0
85	MG	k	403	1/1	0.84	0.37	37,37,37,37	0
85	MG	AR	4087	1/1	0.84	0.28	72,72,72,72	0
85	MG	AR	4172	1/1	0.84	0.17	73,73,73,73	0
85	MG	AR	4023	1/1	0.84	0.29	73,73,73,73	0
85	MG	AR	4245	1/1	0.84	0.26	56,56,56,56	0
85	MG	AR	4149	1/1	0.84	0.29	53,53,53,53	0
85	MG	AR	4196	1/1	0.84	0.20	72,72,72,72	0
85	MG	AR	4134	1/1	0.84	0.35	46,46,46,46	0
85	MG	1	4058	1/1	0.84	0.25	45,45,45,45	0
85	MG	1	4178	1/1	0.84	0.33	39,39,39,39	0
85	MG	1	4097	1/1	0.84	0.25	55,55,55,55	0
85	MG	k	402	1/1	0.84	0.25	57,57,57,57	0
85	MG	sR	2172	1/1	0.84	0.39	101,101,101,101	0
85	MG	1	3757	1/1	0.84	0.16	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	4061	1/1	0.84	0.44	55,55,55,55	0
85	MG	sR	2176	1/1	0.84	0.32	64,64,64,64	0
85	MG	d5	201	1/1	0.84	0.08	74,74,74,74	0
85	MG	1	4066	1/1	0.84	0.27	45,45,45,45	0
85	MG	AR	3828	1/1	0.84	0.74	64,64,64,64	0
85	MG	AR	3842	1/1	0.84	0.20	42,42,42,42	0
85	MG	1	3896	1/1	0.84	0.56	35,35,35,35	0
85	MG	AR	4166	1/1	0.84	0.11	91,91,91,91	0
85	MG	AR	3753	1/1	0.84	0.27	39,39,39,39	0
84	OHX	A	2040	7/7	0.84	0.27	215,216,216,216	0
84	OHX	z	201	7/7	0.84	0.39	229,229,229,230	0
85	MG	AR	4053	1/1	0.84	0.14	47,47,47,47	0
85	MG	CG	304	1/1	0.84	0.20	59,59,59,59	0
85	MG	AR	4079	1/1	0.85	0.10	57,57,57,57	0
84	OHX	AS	211	7/7	0.85	0.25	190,191,192,192	0
85	MG	1	3753	1/1	0.85	0.39	30,30,30,30	0
85	MG	A	2133	1/1	0.85	0.24	68,68,68,68	0
85	MG	AR	4247	1/1	0.85	0.30	31,31,31,31	0
85	MG	DD	101	1/1	0.85	0.47	41,41,41,41	0
85	MG	d6	101	1/1	0.85	0.62	50,50,50,50	0
85	MG	AR	4052	1/1	0.85	0.46	42,42,42,42	0
85	MG	AR	3920	1/1	0.85	0.56	27,27,27,27	0
84	OHX	sR	2022	7/7	0.85	0.22	215,216,217,218	0
85	MG	1	4154	1/1	0.85	0.31	69,69,69,69	0
85	MG	1	3954	1/1	0.85	0.32	38,38,38,38	0
85	MG	1	3880	1/1	0.85	0.59	48,48,48,48	0
85	MG	3	220	1/1	0.85	0.23	58,58,58,58	0
85	MG	1	4103	1/1	0.85	0.24	48,48,48,48	0
85	MG	AR	4104	1/1	0.85	0.26	49,49,49,49	0
85	MG	AR	3996	1/1	0.85	0.20	63,63,63,63	0
85	MG	AR	4028	1/1	0.85	0.23	48,48,48,48	0
85	MG	1	3780	1/1	0.85	0.23	43,43,43,43	0
85	MG	1	3987	1/1	0.85	0.23	51,51,51,51	0
85	MG	A	2105	1/1	0.85	0.40	58,58,58,58	0
84	OHX	A	1946	7/7	0.85	0.16	181,182,183,183	0
85	MG	AR	4081	1/1	0.85	0.15	107,107,107,107	0
85	MG	sR	2117	1/1	0.85	0.16	88,88,88,88	0
84	OHX	1	3709	7/7	0.85	0.33	189,190,190,190	0
85	MG	A	2131	1/1	0.85	0.20	90,90,90,90	0
84	OHX	4	214	7/7	0.85	0.33	187,187,187,187	0
85	MG	1	4083	1/1	0.85	0.43	56,56,56,56	0
84	OHX	1	3697	7/7	0.85	0.40	154,155,155,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	CR	203	1/1	0.85	0.37	112,112,112,112	0
85	MG	AR	4089	1/1	0.85	0.31	52,52,52,52	0
85	MG	AR	4012	1/1	0.85	0.37	60,60,60,60	0
85	MG	AR	4036	1/1	0.85	0.30	61,61,61,61	0
85	MG	A	2109	1/1	0.85	0.53	60,60,60,60	0
85	MG	1	4046	1/1	0.85	0.11	48,48,48,48	0
85	MG	AR	4061	1/1	0.85	0.22	56,56,56,56	0
85	MG	CE	404	1/1	0.85	0.32	31,31,31,31	0
85	MG	j	301	1/1	0.85	0.36	33,33,33,33	0
84	OHX	sR	2050	7/7	0.85	0.31	224,224,225,225	0
85	MG	A	2085	1/1	0.85	0.15	75,75,75,75	0
85	MG	AR	3835	1/1	0.85	0.63	58,58,58,58	0
85	MG	1	3855	1/1	0.85	0.26	31,31,31,31	0
85	MG	1	4029	1/1	0.85	0.36	46,46,46,46	0
85	MG	AR	3759	1/1	0.85	0.38	50,50,50,50	0
85	MG	1	3982	1/1	0.85	0.24	46,46,46,46	0
85	MG	1	4065	1/1	0.85	0.20	46,46,46,46	0
85	MG	1	3949	1/1	0.85	0.20	46,46,46,46	0
85	MG	AR	4056	1/1	0.85	0.25	55,55,55,55	0
85	MG	1	4073	1/1	0.85	0.63	47,47,47,47	0
85	MG	AR	4163	1/1	0.85	0.18	50,50,50,50	0
84	OHX	s1	301	7/7	0.85	0.41	188,189,190,190	0
85	MG	AS	228	1/1	0.85	0.07	72,72,72,72	0
85	MG	sR	2079	1/1	0.85	0.40	46,46,46,46	0
85	MG	AR	3921	1/1	0.85	0.57	31,31,31,31	0
85	MG	1	4161	1/1	0.85	0.29	54,54,54,54	0
85	MG	1	4098	1/1	0.85	0.44	50,50,50,50	0
85	MG	1	3820	1/1	0.85	0.29	51,51,51,51	0
85	MG	AB	204	1/1	0.86	0.24	35,35,35,35	0
85	MG	sR	2080	1/1	0.86	0.52	70,70,70,70	0
85	MG	AR	3789	1/1	0.86	0.38	25,25,25,25	0
85	MG	AR	3826	1/1	0.86	0.35	69,69,69,69	0
84	OHX	A	2024	7/7	0.86	0.51	164,165,166,166	0
85	MG	1	3966	1/1	0.86	0.20	70,70,70,70	0
85	MG	AR	4129	1/1	0.86	0.26	91,91,91,91	0
84	OHX	A	2029	7/7	0.86	0.18	219,220,221,221	0
85	MG	1	4027	1/1	0.86	0.43	41,41,41,41	0
85	MG	AR	3909	1/1	0.86	0.30	22,22,22,22	0
85	MG	1	4030	1/1	0.86	0.35	60,60,60,60	0
85	MG	1	4036	1/1	0.86	0.59	55,55,55,55	0
85	MG	A	2086	1/1	0.86	0.23	50,50,50,50	0
85	MG	AR	4024	1/1	0.86	0.55	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3726	7/7	0.86	0.33	214,215,215,216	0
85	MG	1	4163	1/1	0.86	0.22	45,45,45,45	0
85	MG	sR	2083	1/1	0.86	0.47	69,69,69,69	0
84	OHX	CO	201	7/7	0.86	0.25	244,244,245,245	0
85	MG	A	2081	1/1	0.86	0.42	61,61,61,61	0
85	MG	1	3806	1/1	0.86	0.23	77,77,77,77	0
85	MG	1	4117	1/1	0.86	0.34	60,60,60,60	0
85	MG	AR	4168	1/1	0.86	0.30	44,44,44,44	0
85	MG	AR	4008	1/1	0.86	0.43	58,58,58,58	0
85	MG	sR	2118	1/1	0.86	0.28	72,72,72,72	0
85	MG	AR	4051	1/1	0.86	0.39	43,43,43,43	0
85	MG	AR	4003	1/1	0.86	0.26	45,45,45,45	0
85	MG	sR	2070	1/1	0.86	0.41	65,65,65,65	0
85	MG	AR	4034	1/1	0.86	0.12	52,52,52,52	0
85	MG	4	231	1/1	0.86	0.28	66,66,66,66	0
84	OHX	AR	3652	7/7	0.86	0.28	140,141,141,141	0
85	MG	AR	3869	1/1	0.86	0.48	28,28,28,28	0
85	MG	AS	217	1/1	0.86	0.32	50,50,50,50	0
84	OHX	A	2042	7/7	0.86	0.19	211,213,213,214	0
85	MG	sR	2123	1/1	0.86	0.31	65,65,65,65	0
84	OHX	A	2036	7/7	0.86	0.13	277,278,279,279	0
85	MG	AR	3916	1/1	0.86	0.46	49,49,49,49	0
85	MG	AR	4131	1/1	0.86	0.13	65,65,65,65	0
85	MG	1	3859	1/1	0.86	0.33	43,43,43,43	0
85	MG	sR	2102	1/1	0.86	0.44	45,45,45,45	0
85	MG	sR	2186	1/1	0.86	0.33	86,86,86,86	0
85	MG	1	3831	1/1	0.86	0.77	66,66,66,66	0
85	MG	AR	3911	1/1	0.86	0.67	35,35,35,35	0
85	MG	sR	2160	1/1	0.86	0.30	51,51,51,51	0
85	MG	AR	3976	1/1	0.86	0.45	39,39,39,39	0
85	MG	sR	2068	1/1	0.86	0.41	60,60,60,60	0
85	MG	A	2094	1/1	0.86	0.46	62,62,62,62	0
85	MG	1	3939	1/1	0.86	0.43	55,55,55,55	0
85	MG	AR	3772	1/1	0.86	0.24	36,36,36,36	0
85	MG	A	2064	1/1	0.86	0.24	69,69,69,69	0
84	OHX	1	3727	7/7	0.87	0.38	167,168,168,168	0
85	MG	1	4172	1/1	0.87	0.26	44,44,44,44	0
85	MG	A	2089	1/1	0.87	0.43	72,72,72,72	0
84	OHX	AR	3637	7/7	0.87	0.16	213,213,213,214	0
84	OHX	1	3710	7/7	0.87	0.18	243,243,244,244	0
84	OHX	c3	201	7/7	0.87	0.21	189,190,191,191	0
85	MG	AR	3762	1/1	0.87	0.31	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	3941	1/1	0.87	0.18	44,44,44,44	0
85	MG	AR	4112	1/1	0.87	0.33	54,54,54,54	0
85	MG	CX	204	1/1	0.87	0.18	57,57,57,57	0
85	MG	A	2137	1/1	0.87	0.33	60,60,60,60	0
84	OHX	AR	3607	7/7	0.87	0.19	168,169,169,169	0
85	MG	1	4050	1/1	0.87	0.20	55,55,55,55	0
85	MG	A	2076	1/1	0.87	0.50	72,72,72,72	0
85	MG	sR	2064	1/1	0.87	0.77	60,60,60,60	0
85	MG	1	3944	1/1	0.87	0.29	46,46,46,46	0
85	MG	A	2127	1/1	0.87	0.25	72,72,72,72	0
85	MG	sR	2164	1/1	0.87	0.23	107,107,107,107	0
85	MG	AR	4224	1/1	0.87	0.20	79,79,79,79	0
84	OHX	AR	3687	7/7	0.87	0.23	167,168,168,168	0
84	OHX	1	3726	7/7	0.87	0.45	182,183,183,183	0
84	OHX	1	3729	7/7	0.87	0.46	178,179,179,179	0
85	MG	1	4149	1/1	0.87	0.41	27,27,27,27	0
85	MG	1	3754	1/1	0.87	0.48	50,50,50,50	0
85	MG	AR	4042	1/1	0.87	0.36	58,58,58,58	0
84	OHX	AR	3646	7/7	0.87	0.28	162,162,163,163	0
84	OHX	AR	3744	7/7	0.87	0.51	196,196,197,197	0
85	MG	z	202	1/1	0.87	0.27	63,63,63,63	0
85	MG	1	4151	1/1	0.87	0.24	51,51,51,51	0
84	OHX	AR	3676	7/7	0.87	0.21	193,193,193,193	0
85	MG	1	4038	1/1	0.87	0.30	47,47,47,47	0
85	MG	1	4055	1/1	0.87	0.17	41,41,41,41	0
84	OHX	AS	210	7/7	0.87	0.34	153,153,154,154	0
85	MG	1	4191	1/1	0.87	0.09	52,52,52,52	0
85	MG	3	218	1/1	0.87	0.24	64,64,64,64	0
85	MG	1	3948	1/1	0.87	0.18	50,50,50,50	0
85	MG	AR	4067	1/1	0.87	0.29	51,51,51,51	0
85	MG	AR	4088	1/1	0.87	0.34	46,46,46,46	0
84	OHX	AR	3569	7/7	0.87	0.19	143,143,144,144	0
85	MG	AR	4248	1/1	0.87	0.73	45,45,45,45	0
85	MG	AR	3783	1/1	0.87	0.34	33,33,33,33	0
85	MG	1	3967	1/1	0.87	0.44	53,53,53,53	0
85	MG	c8	202	1/1	0.87	0.30	80,80,80,80	0
85	MG	1	4173	1/1	0.87	0.34	51,51,51,51	0
85	MG	AR	3768	1/1	0.87	0.38	40,40,40,40	0
85	MG	AR	3902	1/1	0.87	0.49	44,44,44,44	0
85	MG	A	2146	1/1	0.87	0.62	50,50,50,50	0
85	MG	1	4024	1/1	0.87	0.41	43,43,43,43	0
84	OHX	x	201	7/7	0.87	0.46	143,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3718	7/7	0.87	0.44	158,158,159,159	0
85	MG	sR	2140	1/1	0.87	0.23	69,69,69,69	0
85	MG	1	3884	1/1	0.87	0.25	45,45,45,45	0
85	MG	sR	2060	1/1	0.87	0.41	46,46,46,46	0
85	MG	AR	4209	1/1	0.87	0.31	58,58,58,58	0
85	MG	AR	4090	1/1	0.87	0.46	50,50,50,50	0
85	MG	AR	4244	1/1	0.87	0.21	52,52,52,52	0
85	MG	CP	502	1/1	0.87	0.34	49,49,49,49	0
85	MG	O	202	1/1	0.87	0.47	55,55,55,55	0
85	MG	AR	3812	1/1	0.87	0.53	39,39,39,39	0
84	OHX	sR	1960	7/7	0.87	0.21	140,140,141,141	0
85	MG	x	204	1/1	0.87	0.37	33,33,33,33	0
84	OHX	AR	3720	7/7	0.88	0.37	169,170,170,170	0
85	MG	AR	4214	1/1	0.88	0.26	50,50,50,50	0
87	ZN	e1	501	1/1	0.88	0.03	156,156,156,156	0
84	OHX	AR	3677	7/7	0.88	0.36	146,146,147,147	0
85	MG	1	3829	1/1	0.88	0.42	41,41,41,41	0
85	MG	AR	3815	1/1	0.88	0.35	35,35,35,35	0
85	MG	sR	2071	1/1	0.88	0.43	38,38,38,38	0
85	MG	1	3852	1/1	0.88	0.43	73,73,73,73	0
85	MG	AR	3797	1/1	0.88	0.47	56,56,56,56	0
85	MG	AR	4215	1/1	0.88	0.54	38,38,38,38	0
85	MG	1	4064	1/1	0.88	0.20	57,57,57,57	0
85	MG	A	2056	1/1	0.88	0.38	47,47,47,47	0
85	MG	AT	223	1/1	0.88	0.70	58,58,58,58	0
85	MG	AR	4210	1/1	0.88	0.32	44,44,44,44	0
85	MG	v	304	1/1	0.88	0.47	46,46,46,46	0
85	MG	1	4011	1/1	0.88	0.54	53,53,53,53	0
85	MG	CJ	301	1/1	0.88	0.28	75,75,75,75	0
85	MG	A	2147	1/1	0.88	0.19	103,103,103,103	0
85	MG	1	3733	1/1	0.88	0.80	50,50,50,50	0
85	MG	AR	4075	1/1	0.88	0.23	58,58,58,58	0
85	MG	1	3786	1/1	0.88	0.40	44,44,44,44	0
85	MG	AR	4065	1/1	0.88	0.55	45,45,45,45	0
85	MG	sR	2174	1/1	0.88	0.29	53,53,53,53	0
85	MG	AR	3851	1/1	0.88	0.51	50,50,50,50	0
85	MG	1	4124	1/1	0.88	0.33	71,71,71,71	0
85	MG	AR	3977	1/1	0.88	0.23	24,24,24,24	0
85	MG	1	4182	1/1	0.88	0.55	75,75,75,75	0
85	MG	1	4015	1/1	0.88	0.21	56,56,56,56	0
85	MG	1	4010	1/1	0.88	0.57	51,51,51,51	0
85	MG	sR	2137	1/1	0.88	0.15	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	sR	2092	1/1	0.88	0.45	77,77,77,77	0
84	OHX	1	3617	7/7	0.88	0.33	165,165,166,166	0
85	MG	1	4111	1/1	0.88	0.29	50,50,50,50	0
85	MG	AR	4181	1/1	0.88	0.47	51,51,51,51	0
85	MG	CR	202	1/1	0.88	0.35	39,39,39,39	0
84	OHX	1	3708	7/7	0.88	0.31	195,196,197,197	0
85	MG	1	3888	1/1	0.88	0.10	54,54,54,54	0
85	MG	1	3877	1/1	0.88	0.25	56,56,56,56	0
85	MG	A	2052	1/1	0.88	0.51	53,53,53,53	0
85	MG	1	4146	1/1	0.88	0.24	76,76,76,76	0
85	MG	1	3775	1/1	0.88	0.18	72,72,72,72	0
85	MG	AR	4167	1/1	0.88	0.30	44,44,44,44	0
85	MG	AR	4018	1/1	0.88	0.53	50,50,50,50	0
85	MG	A	2060	1/1	0.88	0.56	45,45,45,45	0
85	MG	AR	3766	1/1	0.88	0.32	58,58,58,58	0
85	MG	AT	219	1/1	0.88	0.39	38,38,38,38	0
85	MG	AR	3953	1/1	0.88	0.58	48,48,48,48	0
85	MG	AP	503	1/1	0.88	0.14	68,68,68,68	0
85	MG	CR	206	1/1	0.88	0.29	46,46,46,46	0
85	MG	1	3978	1/1	0.88	0.38	47,47,47,47	0
85	MG	AR	4069	1/1	0.88	0.43	51,51,51,51	0
85	MG	sR	2096	1/1	0.88	0.51	60,60,60,60	0
85	MG	AR	3814	1/1	0.88	0.33	82,82,82,82	0
85	MG	1	4127	1/1	0.88	0.20	64,64,64,64	0
87	ZN	c	101	1/1	0.88	0.39	190,190,190,190	0
85	MG	1	3963	1/1	0.88	0.29	33,33,33,33	0
84	OHX	AR	3674	7/7	0.88	0.23	153,153,153,154	0
85	MG	1	4081	1/1	0.88	0.34	52,52,52,52	0
85	MG	AR	4094	1/1	0.88	0.29	56,56,56,56	0
85	MG	AR	4026	1/1	0.88	0.24	46,46,46,46	0
85	MG	s8	302	1/1	0.88	0.31	54,54,54,54	0
84	OHX	AR	3713	7/7	0.88	0.29	164,164,164,164	0
85	MG	1	4054	1/1	0.88	0.44	45,45,45,45	0
85	MG	AR	4031	1/1	0.88	0.24	73,73,73,73	0
84	OHX	AR	3743	7/7	0.88	0.16	160,161,161,162	0
85	MG	AR	3840	1/1	0.88	0.29	68,68,68,68	0
85	MG	sR	2126	1/1	0.88	0.36	58,58,58,58	0
85	MG	1	4016	1/1	0.88	0.34	51,51,51,51	0
84	OHX	CF	402	7/7	0.88	0.51	190,191,192,192	0
85	MG	1	3977	1/1	0.88	0.21	48,48,48,48	0
84	OHX	AT	218	7/7	0.88	0.34	162,162,163,163	0
85	MG	AR	4041	1/1	0.88	0.45	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	3	208	7/7	0.88	0.18	190,190,191,191	0
84	OHX	1	3607	7/7	0.88	0.23	152,152,153,153	0
85	MG	1	3848	1/1	0.88	0.44	43,43,43,43	0
84	OHX	1	3720	7/7	0.88	0.45	163,163,163,163	0
85	MG	AR	4057	1/1	0.88	0.12	50,50,50,50	0
85	MG	AR	4030	1/1	0.88	0.21	34,34,34,34	0
85	MG	d3	201	1/1	0.88	0.30	55,55,55,55	0
84	OHX	1	3721	7/7	0.88	0.42	172,172,173,173	0
85	MG	1	4200	1/1	0.88	0.61	49,49,49,49	0
84	OHX	AR	3522	7/7	0.88	0.17	164,165,165,165	0
84	OHX	AR	3730	7/7	0.88	0.17	207,207,208,208	0
85	MG	AR	4219	1/1	0.88	0.21	40,40,40,40	0
85	MG	1	3746	1/1	0.88	0.31	46,46,46,46	0
84	OHX	1	3716	7/7	0.88	0.39	164,164,165,165	0
85	MG	AR	3905	1/1	0.88	0.56	49,49,49,49	0
85	MG	AR	4035	1/1	0.88	0.19	38,38,38,38	0
85	MG	AR	4148	1/1	0.89	0.42	50,50,50,50	0
85	MG	AR	3963	1/1	0.89	0.14	34,34,34,34	0
84	OHX	1	3713	7/7	0.89	0.27	138,139,139,139	0
85	MG	AR	4141	1/1	0.89	0.50	81,81,81,81	0
84	OHX	AT	213	7/7	0.89	0.29	187,187,187,187	0
84	OHX	AR	3729	7/7	0.89	0.31	177,177,178,178	0
85	MG	1	3749	1/1	0.89	0.54	41,41,41,41	0
84	OHX	1	3648	7/7	0.89	0.20	195,195,195,196	0
85	MG	1	4000	1/1	0.89	0.32	60,60,60,60	0
84	OHX	AR	3739	7/7	0.89	0.45	190,191,191,191	0
84	OHX	AR	3736	7/7	0.89	0.32	154,155,155,156	0
85	MG	AR	3776	1/1	0.89	0.22	31,31,31,31	0
85	MG	AR	4178	1/1	0.89	0.06	94,94,94,94	0
84	OHX	1	3730	7/7	0.89	0.36	159,160,160,160	0
85	MG	4	222	1/1	0.89	0.47	40,40,40,40	0
84	OHX	sR	2042	7/7	0.89	0.29	179,180,180,181	0
85	MG	AR	4226	1/1	0.89	0.28	38,38,38,38	0
84	OHX	AR	3602	7/7	0.89	0.27	173,174,174,175	0
84	OHX	1	3699	7/7	0.89	0.32	151,151,152,152	0
84	OHX	sR	2047	7/7	0.89	0.26	195,195,196,196	0
85	MG	AR	3927	1/1	0.89	0.48	36,36,36,36	0
85	MG	1	3938	1/1	0.89	0.45	52,52,52,52	0
84	OHX	sR	2046	7/7	0.89	0.40	178,178,178,179	0
84	OHX	AR	3702	7/7	0.89	0.33	156,156,157,157	0
84	OHX	1	3724	7/7	0.89	0.47	186,186,187,188	0
84	OHX	A	2011	7/7	0.89	0.22	182,183,183,183	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3981	1/1	0.89	0.45	39,39,39,39	0
85	MG	1	4216	1/1	0.89	0.12	53,53,53,53	0
85	MG	AR	4107	1/1	0.89	0.28	38,38,38,38	0
84	OHX	A	2007	7/7	0.89	0.19	220,222,222,223	0
84	OHX	AR	3708	7/7	0.89	0.34	181,182,182,182	0
85	MG	AR	4137	1/1	0.89	0.33	61,61,61,61	0
85	MG	sR	2136	1/1	0.89	0.33	71,71,71,71	0
85	MG	1	3773	1/1	0.89	0.44	28,28,28,28	0
85	MG	1	3943	1/1	0.89	0.36	40,40,40,40	0
85	MG	AR	4237	1/1	0.89	0.71	59,59,59,59	0
85	MG	AR	3944	1/1	0.89	0.55	41,41,41,41	0
85	MG	A	2103	1/1	0.89	0.40	89,89,89,89	0
84	OHX	sR	2003	7/7	0.89	0.21	188,188,189,189	0
85	MG	AR	4013	1/1	0.89	0.60	52,52,52,52	0
85	MG	1	4199	1/1	0.89	0.40	31,31,31,31	0
85	MG	AR	3965	1/1	0.89	0.19	46,46,46,46	0
85	MG	1	3750	1/1	0.89	0.21	57,57,57,57	0
85	MG	AR	4105	1/1	0.89	0.33	51,51,51,51	0
85	MG	1	3764	1/1	0.89	0.53	47,47,47,47	0
85	MG	c6	201	1/1	0.89	0.23	82,82,82,82	0
85	MG	AR	3893	1/1	0.89	0.39	32,32,32,32	0
85	MG	1	4107	1/1	0.89	0.19	43,43,43,43	0
85	MG	sR	2145	1/1	0.89	0.36	58,58,58,58	0
85	MG	AR	3951	1/1	0.89	0.12	39,39,39,39	0
84	OHX	1	3671	7/7	0.89	0.44	152,153,154,154	0
85	MG	1	4044	1/1	0.89	0.25	39,39,39,39	0
85	MG	1	3758	1/1	0.89	0.31	41,41,41,41	0
85	MG	sR	2133	1/1	0.89	0.30	50,50,50,50	0
85	MG	1	4140	1/1	0.89	0.44	56,56,56,56	0
84	OHX	AR	3688	7/7	0.89	0.42	182,182,182,183	0
84	OHX	A	2030	7/7	0.89	0.33	163,164,165,165	0
85	MG	AR	4211	1/1	0.89	0.41	69,69,69,69	0
84	OHX	A	2038	7/7	0.89	0.52	164,164,166,166	0
85	MG	1	3942	1/1	0.89	0.27	44,44,44,44	0
85	MG	AR	3884	1/1	0.89	0.24	46,46,46,46	0
85	MG	1	4019	1/1	0.89	0.45	53,53,53,53	0
85	MG	AT	222	1/1	0.89	0.72	48,48,48,48	0
85	MG	1	4075	1/1	0.89	0.26	75,75,75,75	0
84	OHX	sR	1991	7/7	0.89	0.31	174,175,175,176	0
85	MG	AR	4173	1/1	0.89	0.26	54,54,54,54	0
85	MG	AR	4019	1/1	0.89	0.25	35,35,35,35	0
85	MG	1	3889	1/1	0.89	0.40	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	b	101	1/1	0.89	0.22	75,75,75,75	0
85	MG	CM	203	1/1	0.89	0.14	60,60,60,60	0
85	MG	u	201	1/1	0.89	0.19	62,62,62,62	0
85	MG	sR	2154	1/1	0.89	0.14	72,72,72,72	0
85	MG	1	3816	1/1	0.89	0.31	47,47,47,47	0
85	MG	AR	3757	1/1	0.89	0.33	29,29,29,29	0
85	MG	1	4025	1/1	0.89	0.22	36,36,36,36	0
84	OHX	AR	3733	7/7	0.89	0.38	153,153,154,154	0
85	MG	AR	4193	1/1	0.89	0.28	57,57,57,57	0
85	MG	1	4114	1/1	0.89	0.75	57,57,57,57	0
85	MG	sR	2155	1/1	0.89	0.22	67,67,67,67	0
85	MG	AR	3755	1/1	0.89	0.33	49,49,49,49	0
85	MG	1	4128	1/1	0.89	0.30	53,53,53,53	0
85	MG	AS	218	1/1	0.89	0.25	60,60,60,60	0
84	OHX	AR	3724	7/7	0.89	0.39	217,218,219,219	0
85	MG	1	3832	1/1	0.89	0.44	57,57,57,57	0
85	MG	AR	3978	1/1	0.89	0.21	55,55,55,55	0
85	MG	1	3957	1/1	0.89	0.21	56,56,56,56	0
84	OHX	AR	3737	7/7	0.89	0.26	189,189,190,190	0
85	MG	A	2054	1/1	0.89	0.31	61,61,61,61	0
85	MG	AR	4251	1/1	0.89	0.09	45,45,45,45	0
85	MG	AR	4083	1/1	0.89	0.16	57,57,57,57	0
85	MG	AR	4198	1/1	0.89	0.55	54,54,54,54	0
85	MG	1	4186	1/1	0.89	0.32	59,59,59,59	0
85	MG	1	4022	1/1	0.89	0.31	42,42,42,42	0
85	MG	1	3741	1/1	0.89	0.34	43,43,43,43	0
85	MG	AR	3818	1/1	0.89	0.33	32,32,32,32	0
85	MG	Y	201	1/1	0.89	0.17	55,55,55,55	0
84	OHX	1	3728	7/7	0.89	0.33	211,212,212,212	0
85	MG	4	216	1/1	0.89	0.62	55,55,55,55	0
84	OHX	AR	3723	7/7	0.89	0.34	168,168,168,169	0
85	MG	AR	3994	1/1	0.90	0.57	49,49,49,49	0
85	MG	AR	3780	1/1	0.90	0.35	76,76,76,76	0
85	MG	AS	220	1/1	0.90	0.24	70,70,70,70	0
84	OHX	AR	3681	7/7	0.90	0.26	165,165,166,166	0
85	MG	1	4164	1/1	0.90	0.38	34,34,34,34	0
85	MG	1	3874	1/1	0.90	0.43	36,36,36,36	0
85	MG	1	3969	1/1	0.90	0.24	66,66,66,66	0
84	OHX	1	3703	7/7	0.90	0.36	209,209,210,210	0
85	MG	1	3825	1/1	0.90	0.25	75,75,75,75	0
85	MG	AS	227	1/1	0.90	0.30	57,57,57,57	0
85	MG	1	4034	1/1	0.90	0.22	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	A	2022	7/7	0.90	0.29	194,195,195,196	0
85	MG	A	2128	1/1	0.90	0.35	63,63,63,63	0
85	MG	AR	3785	1/1	0.90	0.29	60,60,60,60	0
85	MG	1	3879	1/1	0.90	0.46	43,43,43,43	0
85	MG	AR	4120	1/1	0.90	0.27	45,45,45,45	0
85	MG	A	2140	1/1	0.90	0.49	57,57,57,57	0
85	MG	AR	3878	1/1	0.90	0.41	51,51,51,51	0
84	OHX	A	2025	7/7	0.90	0.27	202,203,204,204	0
84	OHX	1	3696	7/7	0.90	0.39	213,214,214,214	0
85	MG	AR	3940	1/1	0.90	0.34	28,28,28,28	0
84	OHX	A	1997	7/7	0.90	0.27	179,180,180,180	0
85	MG	DC	201	1/1	0.90	0.47	44,44,44,44	0
85	MG	A	2080	1/1	0.90	0.44	59,59,59,59	0
85	MG	1	3958	1/1	0.90	0.39	71,71,71,71	0
85	MG	AR	4040	1/1	0.90	0.19	53,53,53,53	0
85	MG	1	4135	1/1	0.90	0.47	44,44,44,44	0
84	OHX	AR	3727	7/7	0.90	0.31	174,174,174,175	0
85	MG	AR	4177	1/1	0.90	0.19	45,45,45,45	0
84	OHX	sR	1969	7/7	0.90	0.17	155,155,156,156	0
85	MG	sR	2105	1/1	0.90	0.46	56,56,56,56	0
85	MG	AR	3924	1/1	0.90	0.36	35,35,35,35	0
85	MG	AR	4032	1/1	0.90	0.34	40,40,40,40	0
85	MG	AR	4044	1/1	0.90	0.17	44,44,44,44	0
84	OHX	AT	217	7/7	0.90	0.28	153,153,153,153	0
84	OHX	AR	3715	7/7	0.90	0.26	139,139,139,139	0
85	MG	1	3843	1/1	0.90	0.40	34,34,34,34	0
85	MG	AR	3988	1/1	0.90	0.31	54,54,54,54	0
84	OHX	sR	2009	7/7	0.90	0.14	175,176,176,177	0
85	MG	A	2111	1/1	0.90	0.52	86,86,86,86	0
84	OHX	AR	3614	7/7	0.90	0.32	151,152,152,152	0
85	MG	1	3821	1/1	0.90	0.25	27,27,27,27	0
85	MG	1	4159	1/1	0.90	0.34	54,54,54,54	0
85	MG	sR	2153	1/1	0.90	0.33	63,63,63,63	0
85	MG	1	4002	1/1	0.90	0.38	38,38,38,38	0
85	MG	A	2063	1/1	0.90	0.44	44,44,44,44	0
85	MG	sR	2062	1/1	0.90	0.41	47,47,47,47	0
85	MG	1	3811	1/1	0.90	0.24	77,77,77,77	0
85	MG	AR	3843	1/1	0.90	0.39	41,41,41,41	0
85	MG	AR	4174	1/1	0.90	0.21	60,60,60,60	0
84	OHX	AR	3734	7/7	0.90	0.17	240,241,242,242	0
85	MG	AR	3813	1/1	0.90	0.22	60,60,60,60	0
85	MG	CQ	201	1/1	0.90	0.34	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	4072	1/1	0.90	0.23	44,44,44,44	0
85	MG	v	303	1/1	0.90	0.47	45,45,45,45	0
85	MG	AR	3771	1/1	0.90	0.47	49,49,49,49	0
85	MG	1	4060	1/1	0.90	0.23	47,47,47,47	0
84	OHX	DL	101	7/7	0.90	0.34	167,167,167,167	0
85	MG	AR	3993	1/1	0.90	0.20	41,41,41,41	0
84	OHX	sR	2044	7/7	0.90	0.27	194,194,195,195	0
85	MG	sR	2184	1/1	0.90	0.25	55,55,55,55	0
85	MG	AR	3795	1/1	0.90	0.24	39,39,39,39	0
85	MG	sR	2169	1/1	0.90	0.70	55,55,55,55	0
85	MG	1	4134	1/1	0.90	0.24	43,43,43,43	0
84	OHX	AR	3701	7/7	0.90	0.24	168,168,169,169	0
85	MG	AR	4011	1/1	0.90	0.41	30,30,30,30	0
85	MG	1	4179	1/1	0.90	0.19	52,52,52,52	0
85	MG	1	3965	1/1	0.90	0.37	42,42,42,42	0
85	MG	1	4126	1/1	0.90	0.41	54,54,54,54	0
84	OHX	AR	3719	7/7	0.90	0.21	227,227,228,228	0
85	MG	1	4074	1/1	0.90	0.30	53,53,53,53	0
84	OHX	1	3693	7/7	0.90	0.38	183,184,184,184	0
84	OHX	1	3654	7/7	0.90	0.22	159,159,159,159	0
85	MG	AR	4070	1/1	0.90	0.51	63,63,63,63	0
85	MG	d9	102	1/1	0.90	0.13	94,94,94,94	0
84	OHX	sR	2020	7/7	0.90	0.31	174,175,176,176	0
84	OHX	sR	2034	7/7	0.90	0.30	177,178,179,179	0
85	MG	1	3867	1/1	0.90	0.60	58,58,58,58	0
85	MG	1	3947	1/1	0.90	0.41	40,40,40,40	0
85	MG	AR	3794	1/1	0.90	0.40	43,43,43,43	0
85	MG	AR	4084	1/1	0.90	0.25	50,50,50,50	0
85	MG	sR	2059	1/1	0.90	0.42	63,63,63,63	0
85	MG	3	209	1/1	0.90	0.31	49,49,49,49	0
84	OHX	1	3725	7/7	0.90	0.11	188,189,189,189	0
85	MG	1	3991	1/1	0.90	0.62	44,44,44,44	0
85	MG	AR	4073	1/1	0.90	0.14	62,62,62,62	0
85	MG	AR	4111	1/1	0.90	0.09	41,41,41,41	0
84	OHX	sR	1998	7/7	0.90	0.21	190,191,192,192	0
84	OHX	A	2012	7/7	0.90	0.26	162,162,163,163	0
85	MG	1	4113	1/1	0.90	0.30	43,43,43,43	0
85	MG	AR	4160	1/1	0.90	0.34	52,52,52,52	0
85	MG	sR	2143	1/1	0.90	0.14	51,51,51,51	0
85	MG	AR	3992	1/1	0.90	0.22	50,50,50,50	0
85	MG	AR	4116	1/1	0.90	0.47	65,65,65,65	0
84	OHX	sR	2049	7/7	0.90	0.20	217,218,219,219	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	1	3631	7/7	0.90	0.23	170,170,171,172	0
85	MG	AR	3832	1/1	0.90	0.17	53,53,53,53	0
84	OHX	AR	3659	7/7	0.90	0.31	144,144,145,145	0
85	MG	1	4096	1/1	0.90	0.34	45,45,45,45	0
85	MG	AR	3809	1/1	0.90	0.49	43,43,43,43	0
85	MG	1	3929	1/1	0.90	0.67	42,42,42,42	0
85	MG	1	3895	1/1	0.90	0.58	50,50,50,50	0
84	OHX	1	3678	7/7	0.90	0.23	189,189,190,190	0
84	OHX	1	3629	7/7	0.90	0.19	163,163,163,163	0
85	MG	AT	201	1/1	0.91	0.29	57,57,57,57	0
85	MG	AR	4017	1/1	0.91	0.35	31,31,31,31	0
85	MG	AR	3754	1/1	0.91	0.29	23,23,23,23	0
85	MG	3	213	1/1	0.91	0.50	32,32,32,32	0
84	OHX	sR	2031	7/7	0.91	0.25	134,134,135,135	0
85	MG	1	4082	1/1	0.91	0.41	58,58,58,58	0
85	MG	4	217	1/1	0.91	0.55	47,47,47,47	0
85	MG	1	4141	1/1	0.91	0.42	53,53,53,53	0
85	MG	AR	3971	1/1	0.91	0.28	42,42,42,42	0
85	MG	sR	2091	1/1	0.91	0.36	56,56,56,56	0
84	OHX	A	2023	7/7	0.91	0.28	178,179,180,180	0
85	MG	AR	4109	1/1	0.91	0.53	50,50,50,50	0
85	MG	AR	3954	1/1	0.91	0.50	48,48,48,48	0
85	MG	AR	4062	1/1	0.91	0.20	64,64,64,64	0
85	MG	A	2117	1/1	0.91	0.53	69,69,69,69	0
85	MG	1	3956	1/1	0.91	0.44	53,53,53,53	0
85	MG	CU	201	1/1	0.91	0.36	48,48,48,48	0
84	OHX	1	3619	7/7	0.91	0.20	179,180,180,181	0
85	MG	DC	203	1/1	0.91	0.32	57,57,57,57	0
85	MG	sR	2067	1/1	0.91	0.33	56,56,56,56	0
85	MG	sR	2072	1/1	0.91	0.87	70,70,70,70	0
85	MG	1	4018	1/1	0.91	0.22	43,43,43,43	0
84	OHX	AR	3645	7/7	0.91	0.20	165,165,166,166	0
85	MG	AR	3833	1/1	0.91	0.32	56,56,56,56	0
85	MG	AR	4097	1/1	0.91	0.26	37,37,37,37	0
85	MG	AS	221	1/1	0.91	0.17	50,50,50,50	0
84	OHX	1	3702	7/7	0.91	0.48	192,192,193,193	0
84	OHX	sR	2007	7/7	0.91	0.20	185,186,187,187	0
84	OHX	AR	3745	7/7	0.91	0.23	208,208,209,209	0
84	OHX	A	1993	7/7	0.91	0.42	172,173,174,174	0
85	MG	1	3907	1/1	0.91	0.47	30,30,30,30	0
84	OHX	1	3598	7/7	0.91	0.39	180,180,180,180	0
85	MG	AR	3889	1/1	0.91	0.48	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	sR	2036	7/7	0.91	0.34	173,173,174,175	0
85	MG	AR	3847	1/1	0.91	0.50	52,52,52,52	0
85	MG	A	2095	1/1	0.91	0.37	79,79,79,79	0
85	MG	1	4201	1/1	0.91	0.71	47,47,47,47	0
84	OHX	1	3623	7/7	0.91	0.23	148,148,148,148	0
84	OHX	AR	3511	7/7	0.91	0.21	126,127,127,127	0
84	OHX	A	1981	7/7	0.91	0.11	215,217,217,217	0
85	MG	AR	4009	1/1	0.91	0.57	35,35,35,35	0
84	OHX	1	3555	7/7	0.91	0.19	153,153,154,154	0
84	OHX	1	3564	7/7	0.91	0.21	142,142,143,143	0
84	OHX	1	3665	7/7	0.91	0.38	150,150,151,151	0
84	OHX	1	3622	7/7	0.91	0.21	151,151,152,152	0
84	OHX	1	3731	7/7	0.91	0.20	165,166,167,168	0
85	MG	A	2114	1/1	0.91	0.31	55,55,55,55	0
85	MG	AR	3897	1/1	0.91	0.57	55,55,55,55	0
85	MG	AR	3781	1/1	0.91	0.26	72,72,72,72	0
85	MG	A	2047	1/1	0.91	0.69	55,55,55,55	0
85	MG	AR	4213	1/1	0.91	0.18	52,52,52,52	0
84	OHX	AR	3741	7/7	0.91	0.26	172,173,173,173	0
85	MG	AR	4188	1/1	0.91	0.15	46,46,46,46	0
85	MG	AR	4152	1/1	0.91	0.36	69,69,69,69	0
84	OHX	1	3692	7/7	0.91	0.50	183,183,184,184	0
84	OHX	H	301	7/7	0.91	0.35	182,183,184,184	0
85	MG	1	4166	1/1	0.91	0.23	70,70,70,70	0
85	MG	1	3794	1/1	0.91	0.42	23,23,23,23	0
84	OHX	1	3618	7/7	0.91	0.23	161,161,161,162	0
84	OHX	AR	3692	7/7	0.91	0.49	146,146,146,146	0
84	OHX	1	3606	7/7	0.91	0.35	141,142,142,143	0
85	MG	1	3946	1/1	0.91	0.56	44,44,44,44	0
85	MG	AR	3955	1/1	0.91	0.13	36,36,36,36	0
84	OHX	A	2026	7/7	0.91	0.38	150,150,151,151	0
85	MG	1	3997	1/1	0.91	0.15	52,52,52,52	0
85	MG	sR	2134	1/1	0.91	0.32	58,58,58,58	0
85	MG	1	3992	1/1	0.91	0.60	56,56,56,56	0
85	MG	A	2057	1/1	0.91	0.50	58,58,58,58	0
85	MG	A	2112	1/1	0.91	0.30	91,91,91,91	0
85	MG	1	4041	1/1	0.91	0.38	43,43,43,43	0
85	MG	1	3760	1/1	0.91	0.51	49,49,49,49	0
85	MG	AR	4010	1/1	0.91	0.38	62,62,62,62	0
85	MG	1	3774	1/1	0.91	0.27	72,72,72,72	0
85	MG	AR	4159	1/1	0.91	0.63	51,51,51,51	0
84	OHX	AR	3728	7/7	0.91	0.45	172,172,173,173	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	4095	1/1	0.91	0.39	46,46,46,46	0
85	MG	AR	3882	1/1	0.91	0.45	50,50,50,50	0
85	MG	AR	4071	1/1	0.91	0.25	46,46,46,46	0
85	MG	1	4204	1/1	0.91	0.38	42,42,42,42	0
85	MG	1	4209	1/1	0.91	0.23	42,42,42,42	0
85	MG	AR	4001	1/1	0.91	0.69	65,65,65,65	0
85	MG	AR	4076	1/1	0.91	0.20	43,43,43,43	0
85	MG	AR	3865	1/1	0.91	0.27	39,39,39,39	0
84	OHX	AR	3650	7/7	0.91	0.24	157,158,158,159	0
85	MG	sR	2165	1/1	0.91	0.65	59,59,59,59	0
85	MG	sR	2144	1/1	0.91	0.93	85,85,85,85	0
85	MG	1	4057	1/1	0.91	0.31	68,68,68,68	0
85	MG	1	4023	1/1	0.91	0.83	58,58,58,58	0
84	OHX	sR	2030	7/7	0.91	0.28	190,190,191,192	0
85	MG	AR	3752	1/1	0.91	0.21	38,38,38,38	0
85	MG	1	4196	1/1	0.91	0.21	68,68,68,68	0
85	MG	1	3813	1/1	0.91	0.53	36,36,36,36	0
85	MG	AR	4058	1/1	0.91	0.25	48,48,48,48	0
85	MG	A	2048	1/1	0.91	0.28	45,45,45,45	0
85	MG	A	2101	1/1	0.91	0.64	63,63,63,63	0
85	MG	4	220	1/1	0.91	0.52	54,54,54,54	0
85	MG	A	2071	1/1	0.91	0.34	53,53,53,53	0
85	MG	AR	4133	1/1	0.91	0.14	97,97,97,97	0
84	OHX	sR	2019	7/7	0.91	0.19	222,223,224,225	0
84	OHX	AR	3722	7/7	0.91	0.23	188,188,188,189	0
85	MG	1	4067	1/1	0.91	0.21	64,64,64,64	0
84	OHX	sR	2023	7/7	0.91	0.33	153,154,155,155	0
85	MG	AR	4033	1/1	0.91	0.38	44,44,44,44	0
85	MG	t	202	1/1	0.91	0.39	86,86,86,86	0
84	OHX	1	3717	7/7	0.91	0.33	188,189,189,189	0
85	MG	1	4136	1/1	0.91	0.29	58,58,58,58	0
84	OHX	AR	3606	7/7	0.91	0.30	145,146,146,146	0
85	MG	1	4091	1/1	0.91	0.29	48,48,48,48	0
85	MG	1	3751	1/1	0.91	0.32	74,74,74,74	0
85	MG	AR	4068	1/1	0.91	0.43	57,57,57,57	0
85	MG	sR	2146	1/1	0.91	0.22	40,40,40,40	0
84	OHX	d9	101	7/7	0.91	0.39	182,183,183,184	0
85	MG	1	4153	1/1	0.91	0.30	52,52,52,52	0
85	MG	AR	3969	1/1	0.91	0.71	57,57,57,57	0
85	MG	1	4039	1/1	0.91	0.39	57,57,57,57	0
84	OHX	CG	301	7/7	0.91	0.19	174,175,176,176	0
85	MG	AR	4080	1/1	0.91	0.46	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	DR	503	1/1	0.91	0.33	80,80,80,80	0
85	MG	DH	202	1/1	0.91	0.23	51,51,51,51	0
85	MG	CD	302	1/1	0.91	0.47	46,46,46,46	0
85	MG	1	4079	1/1	0.91	0.21	55,55,55,55	0
85	MG	AR	3973	1/1	0.91	0.34	44,44,44,44	0
85	MG	1	3788	1/1	0.91	0.39	26,26,26,26	0
85	MG	AR	4154	1/1	0.91	0.34	47,47,47,47	0
84	OHX	1	3647	7/7	0.91	0.39	147,148,148,148	0
84	OHX	1	3656	7/7	0.91	0.32	137,137,137,137	0
84	OHX	AR	3604	7/7	0.91	0.19	156,157,157,157	0
85	MG	sR	2131	1/1	0.91	0.51	53,53,53,53	0
85	MG	A	2139	1/1	0.91	0.20	65,65,65,65	0
85	MG	1	4143	1/1	0.91	0.36	47,47,47,47	0
84	OHX	A	2028	7/7	0.91	0.21	186,187,187,188	0
84	OHX	AR	3621	7/7	0.91	0.31	159,159,160,160	0
85	MG	A	2072	1/1	0.91	0.29	60,60,60,60	0
85	MG	o	301	1/1	0.92	0.20	44,44,44,44	0
84	OHX	1	3560	7/7	0.92	0.16	169,169,170,170	0
85	MG	AR	3995	1/1	0.92	0.23	42,42,42,42	0
85	MG	AR	3852	1/1	0.92	0.31	45,45,45,45	0
85	MG	A	2125	1/1	0.92	0.60	52,52,52,52	0
84	OHX	AR	3699	7/7	0.92	0.28	202,202,203,203	0
84	OHX	sR	2048	7/7	0.92	0.27	188,189,190,190	0
85	MG	1	3912	1/1	0.92	0.30	39,39,39,39	0
84	OHX	AR	3658	7/7	0.92	0.34	146,146,146,146	0
84	OHX	AR	3697	7/7	0.92	0.44	157,158,158,159	0
85	MG	AR	4217	1/1	0.92	0.56	43,43,43,43	0
85	MG	AR	3888	1/1	0.92	0.61	37,37,37,37	0
85	MG	AR	3883	1/1	0.92	0.35	47,47,47,47	0
85	MG	1	3783	1/1	0.92	0.29	30,30,30,30	0
85	MG	AR	3962	1/1	0.92	0.30	46,46,46,46	0
85	MG	DR	502	1/1	0.92	0.18	61,61,61,61	0
84	OHX	A	2037	7/7	0.92	0.34	188,189,189,189	0
84	OHX	AR	3714	7/7	0.92	0.26	169,170,170,170	0
85	MG	1	3747	1/1	0.92	0.43	31,31,31,31	0
85	MG	1	3810	1/1	0.92	0.49	45,45,45,45	0
85	MG	AR	3885	1/1	0.92	0.56	41,41,41,41	0
84	OHX	1	3557	7/7	0.92	0.20	145,145,145,145	0
84	OHX	1	3668	7/7	0.92	0.26	120,121,121,121	0
85	MG	AR	4218	1/1	0.92	0.40	60,60,60,60	0
85	MG	1	4144	1/1	0.92	0.51	34,34,34,34	0
84	OHX	sR	2027	7/7	0.92	0.24	177,177,178,178	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3930	1/1	0.92	0.36	38,38,38,38	0
84	OHX	1	3657	7/7	0.92	0.20	166,167,167,167	0
84	OHX	AR	3680	7/7	0.92	0.38	170,170,171,171	0
85	MG	1	4215	1/1	0.92	0.48	40,40,40,40	0
85	MG	1	3950	1/1	0.92	0.40	51,51,51,51	0
84	OHX	1	3663	7/7	0.92	0.22	169,169,170,170	0
84	OHX	AT	216	7/7	0.92	0.39	154,155,155,155	0
85	MG	A	2121	1/1	0.92	0.25	73,73,73,73	0
84	OHX	1	3681	7/7	0.92	0.24	160,161,162,162	0
85	MG	AS	213	1/1	0.92	0.51	31,31,31,31	0
85	MG	AR	4232	1/1	0.92	0.18	41,41,41,41	0
84	OHX	sR	2039	7/7	0.92	0.41	197,198,198,198	0
85	MG	1	3796	1/1	0.92	0.47	59,59,59,59	0
85	MG	1	3891	1/1	0.92	0.41	36,36,36,36	0
84	OHX	A	2035	7/7	0.92	0.36	148,149,150,150	0
85	MG	AR	3984	1/1	0.92	0.27	48,48,48,48	0
85	MG	1	4150	1/1	0.92	0.84	36,36,36,36	0
85	MG	A	2067	1/1	0.92	0.86	73,73,73,73	0
85	MG	AR	4240	1/1	0.92	0.79	66,66,66,66	0
84	OHX	1	3679	7/7	0.92	0.38	165,166,166,166	0
85	MG	AR	3931	1/1	0.92	0.33	30,30,30,30	0
85	MG	AB	202	1/1	0.92	0.26	62,62,62,62	0
85	MG	1	3737	1/1	0.92	0.27	32,32,32,32	0
85	MG	1	4053	1/1	0.92	0.26	55,55,55,55	0
85	MG	AR	3904	1/1	0.92	0.55	29,29,29,29	0
85	MG	1	3959	1/1	0.92	0.27	29,29,29,29	0
85	MG	AR	3862	1/1	0.92	0.19	26,26,26,26	0
84	OHX	1	3652	7/7	0.92	0.42	154,155,155,155	0
85	MG	A	2149	1/1	0.92	0.20	73,73,73,73	0
85	MG	A	2130	1/1	0.92	0.36	58,58,58,58	0
85	MG	AR	3836	1/1	0.92	0.26	52,52,52,52	0
84	OHX	AR	3707	7/7	0.92	0.44	177,177,177,178	0
85	MG	AR	4050	1/1	0.92	0.25	48,48,48,48	0
85	MG	1	3953	1/1	0.92	0.07	63,63,63,63	0
85	MG	AR	4101	1/1	0.92	0.14	52,52,52,52	0
84	OHX	A	1966	7/7	0.92	0.17	146,147,147,148	0
84	OHX	sR	2014	7/7	0.92	0.33	141,141,142,142	0
84	OHX	1	3660	7/7	0.92	0.42	177,177,178,178	0
84	OHX	sR	2038	7/7	0.92	0.39	167,167,168,169	0
85	MG	1	3973	1/1	0.92	0.19	55,55,55,55	0
85	MG	1	3795	1/1	0.92	0.35	50,50,50,50	0
84	OHX	CL	302	7/7	0.92	0.16	142,142,143,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3533	7/7	0.92	0.22	114,114,114,114	0
85	MG	A	2062	1/1	0.92	0.58	58,58,58,58	0
85	MG	1	3972	1/1	0.92	0.19	42,42,42,42	0
85	MG	AR	3804	1/1	0.92	0.51	30,30,30,30	0
85	MG	AR	4098	1/1	0.92	0.25	65,65,65,65	0
84	OHX	A	1959	7/7	0.92	0.16	165,166,167,167	0
85	MG	1	4069	1/1	0.92	0.40	95,95,95,95	0
84	OHX	A	2021	7/7	0.92	0.41	158,159,160,160	0
85	MG	AR	4074	1/1	0.92	0.27	53,53,53,53	0
85	MG	AR	3756	1/1	0.92	0.32	48,48,48,48	0
85	MG	s1	302	1/1	0.92	0.13	63,63,63,63	0
85	MG	AR	4206	1/1	0.92	0.35	44,44,44,44	0
85	MG	1	3968	1/1	0.92	0.18	48,48,48,48	0
84	OHX	AR	3710	7/7	0.92	0.45	180,180,181,181	0
85	MG	AR	3868	1/1	0.92	0.65	28,28,28,28	0
85	MG	1	3789	1/1	0.92	0.34	36,36,36,36	0
85	MG	AS	219	1/1	0.92	0.39	52,52,52,52	0
85	MG	AR	3820	1/1	0.92	0.26	40,40,40,40	0
85	MG	AR	4072	1/1	0.92	0.17	73,73,73,73	0
84	OHX	A	1977	7/7	0.92	0.27	175,176,177,177	0
85	MG	AR	4225	1/1	0.92	0.10	82,82,82,82	0
84	OHX	1	3489	7/7	0.92	0.22	107,108,108,108	0
85	MG	CQ	202	1/1	0.92	0.45	40,40,40,40	0
84	OHX	1	3608	7/7	0.92	0.26	173,173,173,173	0
85	MG	D	301	1/1	0.92	0.64	72,72,72,72	0
85	MG	1	4077	1/1	0.92	0.21	58,58,58,58	0
85	MG	AR	3854	1/1	0.92	0.58	39,39,39,39	0
85	MG	A	2122	1/1	0.92	0.17	87,87,87,87	0
85	MG	A	2066	1/1	0.92	0.68	76,76,76,76	0
85	MG	AR	3769	1/1	0.92	0.16	39,39,39,39	0
85	MG	AR	3767	1/1	0.92	0.20	65,65,65,65	0
84	OHX	1	3625	7/7	0.92	0.17	156,157,158,158	0
84	OHX	AR	3609	7/7	0.92	0.15	171,171,172,172	0
84	OHX	A	2017	7/7	0.92	0.26	186,187,188,188	0
85	MG	4	233	1/1	0.92	0.34	44,44,44,44	0
84	OHX	1	3646	7/7	0.92	0.29	168,169,169,169	0
85	MG	1	4014	1/1	0.92	0.48	63,63,63,63	0
85	MG	A	2144	1/1	0.92	0.36	61,61,61,61	0
84	OHX	A	1985	7/7	0.92	0.22	146,147,148,148	0
84	OHX	A	2018	7/7	0.92	0.31	190,191,191,192	0
85	MG	1	3980	1/1	0.92	0.37	37,37,37,37	0
84	OHX	1	3649	7/7	0.92	0.26	154,155,156,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3979	1/1	0.92	0.20	56,56,56,56	0
85	MG	AR	3822	1/1	0.92	0.66	55,55,55,55	0
85	MG	1	3873	1/1	0.92	0.57	33,33,33,33	0
85	MG	c1	201	1/1	0.92	0.47	69,69,69,69	0
85	MG	1	3894	1/1	0.93	0.33	45,45,45,45	0
85	MG	DC	202	1/1	0.93	0.38	27,27,27,27	0
85	MG	1	4212	1/1	0.93	0.19	25,25,25,25	0
85	MG	AR	4119	1/1	0.93	0.18	47,47,47,47	0
85	MG	AR	3991	1/1	0.93	0.20	38,38,38,38	0
84	OHX	1	3630	7/7	0.93	0.28	149,149,150,150	0
85	MG	AR	3939	1/1	0.93	0.42	30,30,30,30	0
85	MG	A	2065	1/1	0.93	0.62	49,49,49,49	0
84	OHX	AR	3684	7/7	0.93	0.39	171,171,172,172	0
84	OHX	A	2009	7/7	0.93	0.35	156,157,157,158	0
84	OHX	AR	3664	7/7	0.93	0.29	143,144,144,144	0
85	MG	sR	2090	1/1	0.93	0.61	44,44,44,44	0
84	OHX	A	2001	7/7	0.93	0.20	169,170,171,171	0
85	MG	1	3778	1/1	0.93	0.32	43,43,43,43	0
84	OHX	1	3674	7/7	0.93	0.44	151,151,151,151	0
85	MG	sR	2104	1/1	0.93	0.22	68,68,68,68	0
85	MG	1	4040	1/1	0.93	0.75	61,61,61,61	0
85	MG	1	3777	1/1	0.93	0.08	38,38,38,38	0
85	MG	AR	3875	1/1	0.93	0.54	29,29,29,29	0
85	MG	AT	229	1/1	0.93	0.49	65,65,65,65	0
85	MG	1	3742	1/1	0.93	0.46	39,39,39,39	0
84	OHX	AR	3712	7/7	0.93	0.20	171,171,172,172	0
85	MG	A	2100	1/1	0.93	0.60	54,54,54,54	0
85	MG	6	201	1/1	0.93	0.44	27,27,27,27	0
84	OHX	1	3568	7/7	0.93	0.15	152,153,153,154	0
84	OHX	A	2005	7/7	0.93	0.33	157,157,158,158	0
85	MG	AR	3891	1/1	0.93	0.54	27,27,27,27	0
85	MG	AR	4212	1/1	0.93	0.24	36,36,36,36	0
85	MG	1	3803	1/1	0.93	0.51	46,46,46,46	0
84	OHX	AR	3628	7/7	0.93	0.23	163,164,164,164	0
85	MG	1	3799	1/1	0.93	0.15	37,37,37,37	0
84	OHX	AR	3717	7/7	0.93	0.29	201,201,202,202	0
85	MG	1	4059	1/1	0.93	0.23	40,40,40,40	0
85	MG	1	3798	1/1	0.93	0.14	44,44,44,44	0
84	OHX	sR	2037	7/7	0.93	0.35	174,174,175,175	0
85	MG	AR	4216	1/1	0.93	0.17	29,29,29,29	0
85	MG	AR	3792	1/1	0.93	0.29	33,33,33,33	0
85	MG	AT	226	1/1	0.93	0.17	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	DO	202	1/1	0.93	0.15	45,45,45,45	0
84	OHX	AR	3532	7/7	0.93	0.19	129,129,130,130	0
84	OHX	1	3589	7/7	0.93	0.17	151,151,152,152	0
85	MG	AR	4021	1/1	0.93	0.46	53,53,53,53	0
85	MG	sR	2173	1/1	0.93	0.21	77,77,77,77	0
85	MG	1	3745	1/1	0.93	0.42	32,32,32,32	0
85	MG	AR	4136	1/1	0.93	0.26	64,64,64,64	0
85	MG	1	3993	1/1	0.93	0.96	52,52,52,52	0
84	OHX	AR	3709	7/7	0.93	0.36	174,174,174,174	0
84	OHX	1	3638	7/7	0.93	0.16	167,167,168,168	0
85	MG	1	3732	1/1	0.93	0.47	39,39,39,39	0
85	MG	1	3781	1/1	0.93	0.26	43,43,43,43	0
84	OHX	sR	2033	7/7	0.93	0.45	154,155,155,156	0
85	MG	1	4049	1/1	0.93	0.20	38,38,38,38	0
85	MG	1	3830	1/1	0.93	0.38	32,32,32,32	0
85	MG	c7	201	1/1	0.93	0.52	71,71,71,71	0
84	OHX	1	3690	7/7	0.93	0.35	173,173,174,174	0
85	MG	1	4193	1/1	0.93	0.58	45,45,45,45	0
85	MG	1	4131	1/1	0.93	0.22	52,52,52,52	0
85	MG	A	2142	1/1	0.93	0.15	70,70,70,70	0
84	OHX	AR	3640	7/7	0.93	0.28	136,136,136,136	0
85	MG	1	3955	1/1	0.93	0.26	44,44,44,44	0
85	MG	1	3951	1/1	0.93	0.27	52,52,52,52	0
85	MG	1	3923	1/1	0.93	0.36	42,42,42,42	0
85	MG	4	228	1/1	0.93	0.18	52,52,52,52	0
84	OHX	sR	2025	7/7	0.93	0.29	173,173,174,175	0
84	OHX	AR	3662	7/7	0.93	0.27	164,164,165,165	0
84	OHX	A	1974	7/7	0.93	0.13	168,169,170,170	0
85	MG	1	4013	1/1	0.93	0.26	37,37,37,37	0
85	MG	1	4188	1/1	0.93	0.20	54,54,54,54	0
85	MG	AR	3949	1/1	0.93	0.12	31,31,31,31	0
84	OHX	1	3695	7/7	0.93	0.48	190,190,190,190	0
84	OHX	3	205	7/7	0.93	0.15	133,134,135,135	0
84	OHX	A	1964	7/7	0.93	0.28	139,139,140,140	0
84	OHX	CS	201	1/7	0.93	0.09	173,173,173,173	0
84	OHX	sR	2016	7/7	0.93	0.30	158,158,159,159	0
84	OHX	s4	301	7/7	0.93	0.18	178,179,179,180	0
84	OHX	A	1958	7/7	0.93	0.17	191,191,193,193	0
84	OHX	1	3666	7/7	0.93	0.22	134,134,134,135	0
84	OHX	sR	2002	7/7	0.93	0.37	139,140,141,141	0
84	OHX	sR	2029	7/7	0.93	0.34	157,157,157,158	0
85	MG	AR	3748	1/1	0.93	0.29	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
85	MG	AR	4099	1/1	0.93	0.27	41,41,41,41	0
85	MG	CQ	203	1/1	0.93	0.23	55,55,55,55	0
85	MG	AS	225	1/1	0.93	0.17	54,54,54,54	0
85	MG	A	2126	1/1	0.93	0.34	77,77,77,77	0
85	MG	sR	2100	1/1	0.93	0.49	35,35,35,35	0
85	MG	1	3846	1/1	0.93	0.45	33,33,33,33	0
84	OHX	1	3628	7/7	0.93	0.19	163,164,164,164	0
85	MG	AR	3857	1/1	0.93	0.67	36,36,36,36	0
84	OHX	1	3715	7/7	0.93	0.24	173,173,174,174	0
85	MG	sR	2063	1/1	0.93	0.39	81,81,81,81	0
84	OHX	A	2032	7/7	0.93	0.21	185,186,186,187	0
85	MG	sR	2103	1/1	0.93	0.42	57,57,57,57	0
85	MG	AR	3802	1/1	0.93	0.22	51,51,51,51	0
85	MG	1	3827	1/1	0.93	0.46	49,49,49,49	0
84	OHX	1	3712	7/7	0.93	0.38	176,177,177,177	0
85	MG	CR	204	1/1	0.93	0.31	59,59,59,59	0
84	OHX	sR	1932	7/7	0.93	0.21	125,125,126,126	0
84	OHX	4	213	7/7	0.93	0.26	142,142,143,143	0
84	OHX	A	2033	7/7	0.93	0.22	178,179,179,179	0
85	MG	sR	2107	1/1	0.93	0.56	40,40,40,40	0
84	OHX	sR	2032	7/7	0.93	0.28	149,150,150,151	0
84	OHX	AR	3655	7/7	0.93	0.31	177,177,177,177	0
85	MG	AR	4128	1/1	0.93	0.39	46,46,46,46	0
84	OHX	1	3676	7/7	0.93	0.23	134,134,135,135	0
85	MG	1	4043	1/1	0.93	0.31	39,39,39,39	0
85	MG	sR	2129	1/1	0.93	0.32	36,36,36,36	0
85	MG	AR	3901	1/1	0.93	0.59	37,37,37,37	0
85	MG	A	2148	1/1	0.93	0.33	86,86,86,86	0
84	OHX	CE	402	7/7	0.93	0.40	187,187,188,188	0
85	MG	sR	2167	1/1	0.93	0.43	47,47,47,47	0
85	MG	1	3844	1/1	0.93	0.67	35,35,35,35	0
85	MG	AR	3903	1/1	0.93	0.82	42,42,42,42	0
84	OHX	A	2031	7/7	0.93	0.24	199,200,201,202	0
85	MG	1	4198	1/1	0.93	0.57	32,32,32,32	0
85	MG	AR	3765	1/1	0.93	0.40	31,31,31,31	0
84	OHX	AR	3683	7/7	0.93	0.35	136,136,136,137	0
84	OHX	1	3694	7/7	0.93	0.23	160,161,161,161	0
84	OHX	AR	3679	7/7	0.93	0.19	147,148,148,148	0
84	OHX	sR	2008	7/7	0.93	0.17	175,175,176,177	0
84	OHX	sR	2035	7/7	0.93	0.19	179,179,181,181	0
85	MG	AR	3827	1/1	0.93	0.52	56,56,56,56	0
85	MG	AR	4223	1/1	0.93	0.58	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	4108	1/1	0.93	0.42	52,52,52,52	0
85	MG	1	3864	1/1	0.93	0.31	32,32,32,32	0
85	MG	AR	3808	1/1	0.93	0.30	33,33,33,33	0
85	MG	AR	3970	1/1	0.93	0.15	97,97,97,97	0
85	MG	1	4101	1/1	0.93	0.31	27,27,27,27	0
84	OHX	AR	3700	7/7	0.93	0.38	183,183,184,184	0
85	MG	1	3756	1/1	0.93	0.27	32,32,32,32	0
84	OHX	sR	2043	7/7	0.93	0.26	197,198,198,199	0
84	OHX	AR	3666	7/7	0.93	0.31	146,146,147,147	0
85	MG	sR	2163	1/1	0.93	0.33	62,62,62,62	0
85	MG	AR	3816	1/1	0.93	0.28	37,37,37,37	0
84	OHX	sR	2024	7/7	0.93	0.28	188,189,190,191	0
84	OHX	AR	3731	7/7	0.93	0.34	162,163,163,164	0
85	MG	CD	301	1/1	0.93	0.77	52,52,52,52	0
85	MG	1	3765	1/1	0.93	0.22	33,33,33,33	0
85	MG	1	4112	1/1	0.93	0.17	52,52,52,52	0
84	OHX	A	2002	7/7	0.93	0.19	177,179,179,179	0
85	MG	sR	2101	1/1	0.93	0.55	55,55,55,55	0
85	MG	1	4006	1/1	0.93	0.77	70,70,70,70	0
84	OHX	CK	201	7/7	0.93	0.21	150,151,151,151	0
85	MG	sR	2114	1/1	0.93	0.31	77,77,77,77	0
84	OHX	1	3675	7/7	0.93	0.37	169,169,170,170	0
85	MG	1	4008	1/1	0.93	0.29	22,22,22,22	0
85	MG	sR	2148	1/1	0.93	0.20	58,58,58,58	0
85	MG	AR	3887	1/1	0.93	0.44	44,44,44,44	0
85	MG	AR	3845	1/1	0.93	0.29	31,31,31,31	0
85	MG	AR	4005	1/1	0.93	0.38	68,68,68,68	0
84	OHX	sR	2012	7/7	0.93	0.25	167,168,168,169	0
84	OHX	sR	1950	7/7	0.93	0.17	145,145,146,147	0
85	MG	AR	3749	1/1	0.93	0.40	49,49,49,49	0
85	MG	1	4007	1/1	0.93	0.33	59,59,59,59	0
85	MG	1	4208	1/1	0.93	0.24	26,26,26,26	0
85	MG	1	3776	1/1	0.93	0.44	34,34,34,34	0
85	MG	sR	2056	1/1	0.94	0.26	67,67,67,67	0
84	OHX	1	3655	7/7	0.94	0.17	165,165,166,166	0
84	OHX	AR	3675	7/7	0.94	0.12	200,201,201,201	0
85	MG	AR	3926	1/1	0.94	0.36	47,47,47,47	0
84	OHX	1	3672	7/7	0.94	0.31	154,155,155,156	0
85	MG	AR	3791	1/1	0.94	0.33	21,21,21,21	0
85	MG	AR	4086	1/1	0.94	0.36	41,41,41,41	0
84	OHX	AR	3618	7/7	0.94	0.28	128,129,129,129	0
84	OHX	1	3662	7/7	0.94	0.27	187,188,188,189	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3626	7/7	0.94	0.28	172,173,173,174	0
85	MG	AR	3950	1/1	0.94	0.11	39,39,39,39	0
85	MG	A	2090	1/1	0.94	0.39	55,55,55,55	0
84	OHX	1	3486	7/7	0.94	0.17	120,121,121,121	0
84	OHX	A	2020	7/7	0.94	0.15	156,157,157,157	0
84	OHX	AR	3690	7/7	0.94	0.40	145,146,146,146	0
84	OHX	1	3545	7/7	0.94	0.15	142,143,143,143	0
85	MG	AR	3821	1/1	0.94	0.38	51,51,51,51	0
85	MG	AR	3894	1/1	0.94	0.35	61,61,61,61	0
84	OHX	AR	3526	7/7	0.94	0.28	124,125,125,126	0
84	OHX	AR	3716	7/7	0.94	0.21	162,162,163,163	0
84	OHX	1	3664	7/7	0.94	0.28	188,189,190,190	0
84	OHX	sR	2001	7/7	0.94	0.14	160,160,161,161	0
84	OHX	sR	2017	7/7	0.94	0.28	150,150,151,151	0
84	OHX	AR	3620	7/7	0.94	0.24	133,133,133,134	0
84	OHX	AR	3605	7/7	0.94	0.24	145,146,146,146	0
84	OHX	A	1915	7/7	0.94	0.17	133,134,135,135	0
85	MG	AR	4077	1/1	0.94	0.28	43,43,43,43	0
85	MG	AT	230	1/1	0.94	0.79	49,49,49,49	0
85	MG	AR	3943	1/1	0.94	0.47	30,30,30,30	0
85	MG	AR	3844	1/1	0.94	0.39	28,28,28,28	0
84	OHX	1	3707	7/7	0.94	0.41	174,175,175,175	0
85	MG	1	4197	1/1	0.94	0.42	68,68,68,68	0
85	MG	sR	2125	1/1	0.94	0.21	52,52,52,52	0
84	OHX	sR	1940	7/7	0.94	0.13	162,163,164,164	0
84	OHX	sR	2021	7/7	0.94	0.13	162,162,163,164	0
84	OHX	AK	102	7/7	0.94	0.14	114,114,114,114	0
85	MG	AR	4000	1/1	0.94	0.11	64,64,64,64	0
85	MG	1	4017	1/1	0.94	0.34	41,41,41,41	0
85	MG	sR	2135	1/1	0.94	0.12	82,82,82,82	0
85	MG	1	3734	1/1	0.94	0.40	37,37,37,37	0
84	OHX	AR	3691	7/7	0.94	0.26	149,149,150,150	0
85	MG	AR	3960	1/1	0.94	0.37	34,34,34,34	0
84	OHX	AR	3663	7/7	0.94	0.28	161,161,162,162	0
84	OHX	sR	1966	7/7	0.94	0.16	146,146,147,147	0
85	MG	1	3876	1/1	0.94	0.48	61,61,61,61	0
85	MG	sR	2130	1/1	0.94	0.12	83,83,83,83	0
85	MG	1	3853	1/1	0.94	0.61	34,34,34,34	0
85	MG	1	3999	1/1	0.94	0.43	47,47,47,47	0
85	MG	4	225	1/1	0.94	0.23	59,59,59,59	0
84	OHX	1	3446	7/7	0.94	0.25	99,99,100,100	0
85	MG	1	4071	1/1	0.94	0.25	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	1	3667	7/7	0.94	0.25	142,142,142,143	0
85	MG	sR	2139	1/1	0.94	0.19	54,54,54,54	0
85	MG	AR	3784	1/1	0.94	0.43	41,41,41,41	0
84	OHX	sR	2006	7/7	0.94	0.25	148,149,150,150	0
85	MG	sR	2168	1/1	0.94	0.34	47,47,47,47	0
85	MG	1	3814	1/1	0.94	0.22	21,21,21,21	0
85	MG	AS	223	1/1	0.94	0.30	75,75,75,75	0
84	OHX	1	3593	7/7	0.94	0.31	147,147,148,148	0
84	OHX	AT	215	7/7	0.94	0.21	157,157,157,158	0
84	OHX	AR	3641	7/7	0.94	0.20	164,164,165,165	0
84	OHX	sR	2026	7/7	0.94	0.47	143,144,144,144	0
84	OHX	AR	3639	7/7	0.94	0.17	153,154,154,154	0
85	MG	AR	3811	1/1	0.94	0.41	53,53,53,53	0
85	MG	1	4105	1/1	0.94	0.28	41,41,41,41	0
84	OHX	AR	3595	7/7	0.94	0.38	135,135,136,136	0
85	MG	1	3983	1/1	0.94	0.26	47,47,47,47	0
87	ZN	d7	101	1/1	0.94	0.45	180,180,180,180	0
85	MG	AR	4143	1/1	0.94	0.21	55,55,55,55	0
84	OHX	1	3502	7/7	0.94	0.18	123,123,124,124	0
84	OHX	A	1918	7/7	0.94	0.18	108,109,109,109	0
84	OHX	AR	3682	7/7	0.94	0.26	153,154,154,154	0
84	OHX	1	3611	7/7	0.94	0.25	141,141,141,141	0
85	MG	CP	505	1/1	0.94	0.85	106,106,106,106	0
85	MG	3	214	1/1	0.94	0.48	30,30,30,30	0
85	MG	AB	203	1/1	0.94	0.56	44,44,44,44	0
84	OHX	AR	3499	7/7	0.94	0.17	127,128,128,128	0
84	OHX	AR	3590	7/7	0.94	0.12	153,154,155,155	0
85	MG	1	3924	1/1	0.94	0.42	49,49,49,49	0
85	MG	AR	4054	1/1	0.94	0.34	35,35,35,35	0
84	OHX	AR	3665	7/7	0.94	0.29	161,162,162,162	0
85	MG	AR	4063	1/1	0.94	0.41	49,49,49,49	0
85	MG	4	234	1/1	0.94	0.66	52,52,52,52	0
84	OHX	1	3616	7/7	0.94	0.36	146,147,147,148	0
85	MG	1	3904	1/1	0.94	0.52	32,32,32,32	0
84	OHX	AR	3541	7/7	0.94	0.17	148,148,149,149	0
85	MG	AR	3947	1/1	0.94	0.55	34,34,34,34	0
84	OHX	1	3722	7/7	0.94	0.26	176,176,177,177	0
85	MG	AR	3879	1/1	0.94	0.39	30,30,30,30	0
85	MG	sR	2115	1/1	0.94	0.28	59,59,59,59	0
84	OHX	sR	1976	7/7	0.94	0.15	170,171,172,172	0
84	OHX	AR	3647	7/7	0.94	0.34	156,156,157,157	0
85	MG	AR	4096	1/1	0.94	0.34	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	3976	1/1	0.94	0.43	52,52,52,52	0
85	MG	sR	2088	1/1	0.94	0.45	74,74,74,74	0
85	MG	1	3911	1/1	0.94	0.38	44,44,44,44	0
85	MG	A	2075	1/1	0.94	0.45	61,61,61,61	0
85	MG	A	2120	1/1	0.94	0.38	49,49,49,49	0
84	OHX	AR	3633	7/7	0.94	0.26	151,151,151,151	0
84	OHX	AR	3560	7/7	0.94	0.23	122,122,122,122	0
85	MG	A	2059	1/1	0.94	0.55	60,60,60,60	0
84	OHX	sR	1919	7/7	0.94	0.18	107,107,108,108	0
85	MG	1	4203	1/1	0.94	0.60	45,45,45,45	0
85	MG	AR	3758	1/1	0.94	0.46	42,42,42,42	0
85	MG	sR	2097	1/1	0.94	0.49	48,48,48,48	0
84	OHX	AR	3643	7/7	0.94	0.33	158,159,159,159	0
85	MG	AR	4060	1/1	0.94	0.36	47,47,47,47	0
85	MG	1	4190	1/1	0.94	0.33	18,18,18,18	0
85	MG	A	2077	1/1	0.94	0.39	53,53,53,53	0
85	MG	sR	2054	1/1	0.94	0.39	57,57,57,57	0
85	MG	sR	2156	1/1	0.94	0.27	62,62,62,62	0
84	OHX	sR	1981	7/7	0.94	0.33	127,128,129,129	0
85	MG	AR	4020	1/1	0.94	0.37	43,43,43,43	0
84	OHX	AR	3705	7/7	0.94	0.43	142,142,142,143	0
84	OHX	1	3635	7/7	0.94	0.26	142,143,143,143	0
85	MG	sR	2055	1/1	0.94	0.75	54,54,54,54	0
84	OHX	A	2013	7/7	0.94	0.27	154,155,155,155	0
85	MG	1	4070	1/1	0.94	0.28	47,47,47,47	0
84	OHX	AR	3695	7/7	0.94	0.24	160,161,161,162	0
84	OHX	1	3670	7/7	0.94	0.31	151,152,152,152	0
85	MG	1	3928	1/1	0.94	0.55	23,23,23,23	0
85	MG	1	3779	1/1	0.94	0.38	39,39,39,39	0
85	MG	AR	3958	1/1	0.94	0.40	24,24,24,24	0
84	OHX	AR	3642	7/7	0.94	0.51	153,154,154,154	0
85	MG	1	3801	1/1	0.94	0.37	49,49,49,49	0
85	MG	1	4168	1/1	0.94	0.27	34,34,34,34	0
84	OHX	AR	3613	7/7	0.94	0.33	154,155,155,155	0
85	MG	1	4148	1/1	0.94	0.19	53,53,53,53	0
84	OHX	AR	3627	7/7	0.94	0.34	164,164,165,165	0
85	MG	d4	202	1/1	0.94	0.32	60,60,60,60	0
84	OHX	sR	2045	7/7	0.94	0.38	163,164,164,165	0
85	MG	3	215	1/1	0.94	0.37	53,53,53,53	0
84	OHX	sR	1979	7/7	0.94	0.26	160,160,161,161	0
85	MG	AR	3890	1/1	0.94	0.47	25,25,25,25	0
84	OHX	AR	3601	7/7	0.94	0.18	150,150,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AK	104	1/1	0.94	0.83	59,59,59,59	0
84	OHX	1	3626	7/7	0.94	0.25	182,182,183,183	0
85	MG	1	3766	1/1	0.94	0.49	44,44,44,44	0
85	MG	sR	2078	1/1	0.94	0.54	48,48,48,48	0
84	OHX	s8	301	7/7	0.94	0.32	194,195,195,196	0
85	MG	A	2074	1/1	0.94	0.52	44,44,44,44	0
85	MG	1	4177	1/1	0.94	0.48	80,80,80,80	0
85	MG	sR	2081	1/1	0.94	0.34	59,59,59,59	0
84	OHX	1	3706	7/7	0.94	0.25	194,194,195,195	0
85	MG	1	3823	1/1	0.94	0.46	29,29,29,29	0
85	MG	4	221	1/1	0.94	0.42	36,36,36,36	0
84	OHX	sR	2005	7/7	0.94	0.28	176,176,177,178	0
85	MG	CX	203	1/1	0.94	0.43	30,30,30,30	0
85	MG	AR	3941	1/1	0.94	0.59	47,47,47,47	0
85	MG	1	3763	1/1	0.94	0.43	46,46,46,46	0
84	OHX	1	3604	7/7	0.94	0.24	145,146,146,146	0
85	MG	AR	4127	1/1	0.94	0.28	43,43,43,43	0
85	MG	4	227	1/1	0.94	0.45	39,39,39,39	0
85	MG	AT	228	1/1	0.94	0.35	43,43,43,43	0
84	OHX	x	202	7/7	0.94	0.33	176,176,176,176	0
85	MG	AR	3907	1/1	0.94	0.59	30,30,30,30	0
84	OHX	A	1991	7/7	0.94	0.15	183,184,185,185	0
84	OHX	1	3659	7/7	0.94	0.28	169,169,169,169	0
85	MG	1	4087	1/1	0.94	0.25	40,40,40,40	0
84	OHX	A	2019	7/7	0.94	0.21	210,210,212,212	0
85	MG	AR	3824	1/1	0.94	0.23	24,24,24,24	0
85	MG	AR	3853	1/1	0.94	0.27	43,43,43,43	0
84	OHX	AR	3570	7/7	0.94	0.15	169,170,170,171	0
85	MG	1	3809	1/1	0.94	0.48	49,49,49,49	0
85	MG	CR	205	1/1	0.94	0.37	44,44,44,44	0
85	MG	AR	3932	1/1	0.94	0.45	34,34,34,34	0
85	MG	A	2118	1/1	0.94	0.13	67,67,67,67	0
84	OHX	AR	3657	7/7	0.94	0.21	165,165,166,166	0
84	OHX	O	201	7/7	0.94	0.15	198,199,199,199	0
84	OHX	1	3645	7/7	0.94	0.29	162,162,163,163	0
84	OHX	sR	1961	7/7	0.94	0.16	135,136,136,137	0
84	OHX	AR	3548	7/7	0.94	0.22	142,142,142,143	0
84	OHX	sR	2028	7/7	0.94	0.35	184,184,185,185	0
84	OHX	1	3511	7/7	0.94	0.21	118,118,119,119	0
84	OHX	sR	2000	7/7	0.94	0.22	162,163,163,164	0
85	MG	1	3885	1/1	0.94	0.52	36,36,36,36	0
85	MG	AH	201	1/1	0.94	0.17	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AT	214	7/7	0.94	0.24	153,153,153,153	0
84	OHX	sR	1978	7/7	0.94	0.21	126,126,127,127	0
84	OHX	A	1953	7/7	0.94	0.27	164,165,166,166	0
84	OHX	AR	3508	7/7	0.94	0.15	117,118,119,119	0
85	MG	CX	205	1/1	0.94	0.19	48,48,48,48	0
85	MG	1	4080	1/1	0.94	0.19	30,30,30,30	0
85	MG	sR	2120	1/1	0.94	0.40	70,70,70,70	0
84	OHX	A	1980	7/7	0.94	0.22	166,166,167,167	0
84	OHX	1	3463	7/7	0.94	0.21	104,104,105,105	0
84	OHX	sR	1971	7/7	0.94	0.19	151,151,152,152	0
84	OHX	AR	3685	7/7	0.94	0.25	182,182,183,183	0
84	OHX	AR	3611	7/7	0.94	0.27	136,136,137,137	0
84	OHX	A	2010	7/7	0.94	0.19	171,173,173,174	0
85	MG	AR	3859	1/1	0.94	0.40	39,39,39,39	0
84	OHX	AR	3623	7/7	0.94	0.28	147,148,148,148	0
85	MG	1	4084	1/1	0.94	0.29	52,52,52,52	0
84	OHX	sR	1996	7/7	0.94	0.17	184,184,185,186	0
85	MG	AR	4015	1/1	0.94	0.59	49,49,49,49	0
85	MG	sR	2190	1/1	0.94	0.38	57,57,57,57	0
85	MG	AR	3986	1/1	0.94	0.07	63,63,63,63	0
85	MG	1	3743	1/1	0.95	0.59	42,42,42,42	0
85	MG	A	2083	1/1	0.95	0.34	53,53,53,53	0
85	MG	sR	2077	1/1	0.95	0.52	41,41,41,41	0
84	OHX	AR	3558	7/7	0.95	0.25	121,121,121,122	0
84	OHX	1	3562	7/7	0.95	0.18	141,141,141,142	0
84	OHX	sR	2015	7/7	0.95	0.31	158,159,159,160	0
85	MG	AR	3871	1/1	0.95	0.78	44,44,44,44	0
84	OHX	sR	1985	7/7	0.95	0.17	137,137,138,138	0
85	MG	1	3839	1/1	0.95	0.58	28,28,28,28	0
85	MG	A	2055	1/1	0.95	0.40	61,61,61,61	0
84	OHX	AR	3518	7/7	0.95	0.11	163,164,165,165	0
85	MG	sR	2089	1/1	0.95	0.51	44,44,44,44	0
85	MG	1	3759	1/1	0.95	0.33	55,55,55,55	0
85	MG	1	4028	1/1	0.95	0.42	61,61,61,61	0
84	OHX	1	3621	7/7	0.95	0.11	200,201,201,201	0
85	MG	AR	3945	1/1	0.95	0.40	43,43,43,43	0
84	OHX	AR	3600	7/7	0.95	0.25	157,158,158,159	0
84	OHX	1	3470	7/7	0.95	0.19	108,109,109,109	0
84	OHX	AT	206	7/7	0.95	0.15	128,128,128,128	0
85	MG	1	3861	1/1	0.95	0.30	44,44,44,44	0
84	OHX	AR	3738	7/7	0.95	0.26	129,130,130,130	0
84	OHX	1	3537	7/7	0.95	0.23	127,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3831	1/1	0.95	0.64	34,34,34,34	0
85	MG	4	223	1/1	0.95	0.58	50,50,50,50	0
85	MG	A	2136	1/1	0.95	0.12	96,96,96,96	0
85	MG	AR	3849	1/1	0.95	0.40	40,40,40,40	0
84	OHX	Q	201	7/7	0.95	0.19	187,187,188,188	0
84	OHX	AR	3536	7/7	0.95	0.13	139,139,139,139	0
84	OHX	1	3651	7/7	0.95	0.21	149,149,150,150	0
84	OHX	A	1963	7/7	0.95	0.22	165,166,167,167	0
85	MG	1	4147	1/1	0.95	0.14	62,62,62,62	0
85	MG	AS	224	1/1	0.95	0.15	88,88,88,88	0
85	MG	1	3815	1/1	0.95	0.49	47,47,47,47	0
84	OHX	1	3701	7/7	0.95	0.33	147,148,148,148	0
84	OHX	1	3597	7/7	0.95	0.11	158,158,158,159	0
85	MG	AR	3837	1/1	0.95	0.64	25,25,25,25	0
84	OHX	1	3547	7/7	0.95	0.15	147,147,148,148	0
85	MG	AR	4201	1/1	0.95	0.66	40,40,40,40	0
85	MG	1	4142	1/1	0.95	0.19	47,47,47,47	0
84	OHX	AR	3610	7/7	0.95	0.13	155,155,156,156	0
84	OHX	sR	2018	7/7	0.95	0.27	157,158,158,159	0
84	OHX	AT	212	7/7	0.95	0.26	152,152,152,152	0
84	OHX	1	3661	7/7	0.95	0.21	145,145,146,146	0
84	OHX	1	3714	7/7	0.95	0.40	163,164,164,165	0
84	OHX	AT	211	7/7	0.95	0.15	163,163,164,164	0
85	MG	AR	4125	1/1	0.95	0.85	32,32,32,32	0
84	OHX	A	1995	7/7	0.95	0.11	177,178,179,179	0
84	OHX	1	3643	7/7	0.95	0.25	157,158,158,158	0
85	MG	AR	3918	1/1	0.95	0.42	24,24,24,24	0
85	MG	AR	4132	1/1	0.95	0.24	37,37,37,37	0
84	OHX	1	3711	7/7	0.95	0.42	157,157,158,158	0
85	MG	sR	2189	1/1	0.95	0.25	58,58,58,58	0
85	MG	AR	4229	1/1	0.95	0.64	92,92,92,92	0
84	OHX	A	1998	7/7	0.95	0.23	178,179,180,181	0
85	MG	1	3755	1/1	0.95	0.29	40,40,40,40	0
84	OHX	CX	202	7/7	0.95	0.20	131,132,132,132	0
85	MG	AR	3896	1/1	0.95	0.71	46,46,46,46	0
85	MG	AR	3823	1/1	0.95	0.12	80,80,80,80	0
84	OHX	AS	207	7/7	0.95	0.10	152,153,154,154	0
85	MG	AR	3873	1/1	0.95	0.41	47,47,47,47	0
84	OHX	A	1978	7/7	0.95	0.17	167,168,169,169	0
85	MG	A	2143	1/1	0.95	0.11	115,115,115,115	0
84	OHX	AR	3580	7/7	0.95	0.19	132,132,133,133	0
85	MG	1	3869	1/1	0.95	0.51	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	sR	1995	7/7	0.95	0.19	159,160,161,161	0
84	OHX	AR	3543	7/7	0.95	0.16	137,138,138,139	0
85	MG	sR	2112	1/1	0.95	0.23	62,62,62,62	0
85	MG	3	217	1/1	0.95	0.21	47,47,47,47	0
85	MG	AR	4115	1/1	0.95	0.14	53,53,53,53	0
84	OHX	sR	1973	7/7	0.95	0.17	145,145,146,147	0
84	OHX	1	3637	7/7	0.95	0.26	143,144,144,144	0
84	OHX	1	3609	7/7	0.95	0.17	134,135,135,135	0
84	OHX	sR	1977	7/7	0.95	0.12	159,160,161,161	0
85	MG	AR	4092	1/1	0.95	0.31	41,41,41,41	0
84	OHX	AR	3667	7/7	0.95	0.41	143,143,143,143	0
85	MG	1	4171	1/1	0.95	0.37	44,44,44,44	0
84	OHX	AR	3553	7/7	0.95	0.15	136,136,137,137	0
84	OHX	AR	3625	7/7	0.95	0.26	147,148,148,149	0
84	OHX	sR	1988	7/7	0.95	0.22	173,173,174,174	0
85	MG	1	3945	1/1	0.95	0.36	34,34,34,34	0
84	OHX	AR	3706	7/7	0.95	0.29	146,146,146,147	0
84	OHX	A	2003	7/7	0.95	0.26	153,154,155,155	0
85	MG	AR	4205	1/1	0.95	0.14	36,36,36,36	0
84	OHX	AR	3656	7/7	0.95	0.37	152,152,153,153	0
85	MG	AR	4078	1/1	0.95	0.54	34,34,34,34	0
84	OHX	AR	3564	7/7	0.95	0.14	149,149,149,150	0
84	OHX	1	3600	7/7	0.95	0.27	154,154,155,155	0
84	OHX	AR	3624	7/7	0.95	0.18	139,139,140,140	0
84	OHX	1	3636	7/7	0.95	0.27	194,194,195,195	0
84	OHX	AR	3644	7/7	0.95	0.32	156,157,157,157	0
84	OHX	1	3620	7/7	0.95	0.17	148,148,149,149	0
84	OHX	AR	3573	7/7	0.95	0.12	145,145,145,145	0
85	MG	1	3961	1/1	0.95	0.37	67,67,67,67	0
84	OHX	AR	3549	7/7	0.95	0.16	137,138,138,138	0
85	MG	1	4106	1/1	0.95	0.15	37,37,37,37	0
84	OHX	AR	3458	7/7	0.95	0.18	109,110,110,110	0
85	MG	1	3857	1/1	0.95	0.48	33,33,33,33	0
84	OHX	1	3482	7/7	0.95	0.17	99,99,100,100	0
85	MG	AR	4142	1/1	0.95	0.09	69,69,69,69	0
85	MG	1	4133	1/1	0.95	0.43	74,74,74,74	0
84	OHX	1	3640	7/7	0.95	0.25	145,145,146,146	0
84	OHX	1	3680	7/7	0.95	0.29	180,180,181,181	0
85	MG	DH	203	1/1	0.95	0.38	39,39,39,39	0
85	MG	A	2045	1/1	0.95	0.56	45,45,45,45	0
84	OHX	AR	3577	7/7	0.95	0.16	156,156,157,157	0
85	MG	1	4095	1/1	0.95	0.14	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	4185	1/1	0.95	0.49	53,53,53,53	0
85	MG	1	3882	1/1	0.95	0.42	22,22,22,22	0
85	MG	1	3886	1/1	0.95	0.63	31,31,31,31	0
85	MG	A	2093	1/1	0.95	0.33	54,54,54,54	0
85	MG	AR	3999	1/1	0.95	0.23	42,42,42,42	0
85	MG	1	3986	1/1	0.95	0.29	66,66,66,66	0
84	OHX	1	3612	7/7	0.95	0.17	149,150,151,151	0
84	OHX	AR	3612	7/7	0.95	0.24	139,140,140,140	0
84	OHX	1	3691	7/7	0.95	0.28	152,152,153,153	0
85	MG	1	3934	1/1	0.95	0.14	34,34,34,34	0
84	OHX	CG	303	7/7	0.95	0.35	158,159,159,160	0
84	OHX	4	211	7/7	0.95	0.16	160,160,160,160	0
84	OHX	1	3515	7/7	0.95	0.18	124,124,124,125	0
84	OHX	AR	3694	7/7	0.95	0.38	147,148,148,149	0
85	MG	AR	4189	1/1	0.95	0.34	46,46,46,46	0
84	OHX	A	2004	7/7	0.95	0.22	167,168,169,169	0
85	MG	AR	3800	1/1	0.95	0.63	48,48,48,48	0
84	OHX	A	2006	7/7	0.95	0.18	162,163,164,164	0
84	OHX	AR	3668	7/7	0.95	0.21	136,136,136,136	0
84	OHX	c5	201	7/7	0.95	0.26	179,180,181,181	0
84	OHX	1	3455	7/7	0.95	0.16	110,111,111,111	0
84	OHX	3	207	7/7	0.95	0.16	158,158,159,159	0
84	OHX	1	3685	7/7	0.95	0.26	172,172,173,173	0
84	OHX	3	203	7/7	0.95	0.16	113,114,114,114	0
85	MG	AR	3987	1/1	0.95	0.30	45,45,45,45	0
85	MG	AR	4007	1/1	0.95	0.45	52,52,52,52	0
85	MG	sR	2095	1/1	0.95	0.46	36,36,36,36	0
84	OHX	sR	1982	7/7	0.95	0.31	140,140,140,140	0
85	MG	1	3840	1/1	0.95	0.61	22,22,22,22	0
84	OHX	AR	3634	7/7	0.95	0.27	173,173,174,174	0
84	OHX	AR	3598	7/7	0.95	0.23	137,138,138,138	0
84	OHX	l	401	7/7	0.95	0.30	163,163,164,164	0
85	MG	1	3919	1/1	0.95	0.66	23,23,23,23	0
85	MG	AR	3855	1/1	0.95	0.35	56,56,56,56	0
85	MG	AS	214	1/1	0.95	0.35	57,57,57,57	0
84	OHX	A	2000	7/7	0.95	0.20	167,168,168,168	0
84	OHX	1	3519	7/7	0.95	0.17	110,110,111,111	0
85	MG	1	3793	1/1	0.95	0.47	25,25,25,25	0
85	MG	AR	4199	1/1	0.95	0.27	54,54,54,54	0
84	OHX	AR	3661	7/7	0.95	0.43	164,165,165,166	0
85	MG	1	3996	1/1	0.95	0.30	46,46,46,46	0
85	MG	1	4085	1/1	0.95	0.17	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	A	2014	7/7	0.95	0.37	154,155,155,155	0
85	MG	A	2116	1/1	0.95	0.45	76,76,76,76	0
85	MG	1	4207	1/1	0.95	0.42	35,35,35,35	0
85	MG	AR	3961	1/1	0.95	0.27	28,28,28,28	0
84	OHX	AR	3696	7/7	0.95	0.30	145,146,147,147	0
84	OHX	1	3615	7/7	0.95	0.22	151,151,152,153	0
85	MG	AR	3942	1/1	0.95	0.66	34,34,34,34	0
84	OHX	sR	1999	7/7	0.95	0.25	161,161,162,162	0
84	OHX	AR	3477	7/7	0.95	0.17	120,120,121,121	0
84	OHX	AR	3689	7/7	0.95	0.34	152,153,153,153	0
85	MG	1	405	1/1	0.95	0.34	40,40,40,40	0
85	MG	sR	2099	1/1	0.95	0.38	42,42,42,42	0
84	OHX	AR	3704	7/7	0.95	0.24	136,136,136,137	0
85	MG	AS	222	1/1	0.95	0.32	34,34,34,34	0
85	MG	AR	4228	1/1	0.95	0.35	62,62,62,62	0
84	OHX	1	3686	7/7	0.95	0.24	154,154,155,155	0
85	MG	AR	4220	1/1	0.95	0.35	47,47,47,47	0
85	MG	sR	2128	1/1	0.95	0.31	38,38,38,38	0
84	OHX	1	3633	7/7	0.95	0.23	178,179,179,180	0
84	OHX	AR	3672	7/7	0.95	0.16	159,160,160,160	0
85	MG	A	2043	1/1	0.95	0.37	55,55,55,55	0
84	OHX	CF	401	7/7	0.95	0.30	165,166,166,167	0
85	MG	1	3887	1/1	0.95	0.45	31,31,31,31	0
85	MG	4	218	1/1	0.95	0.61	48,48,48,48	0
84	OHX	1	3700	7/7	0.95	0.24	149,149,150,150	0
84	OHX	A	1947	7/7	0.95	0.17	124,125,125,125	0
84	OHX	sR	2013	7/7	0.95	0.15	170,170,171,171	0
85	MG	CN	201	1/1	0.95	0.17	72,72,72,72	0
85	MG	CP	503	1/1	0.95	0.30	42,42,42,42	0
84	OHX	1	3677	7/7	0.95	0.16	196,197,197,198	0
85	MG	AR	3799	1/1	0.95	0.36	46,46,46,46	0
84	OHX	A	2027	7/7	0.95	0.20	197,198,199,199	0
84	OHX	A	1968	7/7	0.95	0.28	146,147,147,148	0
85	MG	A	2151	1/1	0.95	0.14	67,67,67,67	0
85	MG	AR	3886	1/1	0.95	0.45	28,28,28,28	0
85	MG	1	3736	1/1	0.95	0.34	53,53,53,53	0
84	OHX	AR	3559	7/7	0.95	0.17	115,116,116,116	0
85	MG	1	3768	1/1	0.95	0.30	28,28,28,28	0
85	MG	sR	2053	1/1	0.95	0.65	49,49,49,49	0
85	MG	AR	4158	1/1	0.95	0.23	52,52,52,52	0
84	OHX	1	3582	7/7	0.95	0.29	125,125,126,126	0
85	MG	sR	2181	1/1	0.95	0.13	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3750	1/1	0.95	0.12	39,39,39,39	0
85	MG	1	3989	1/1	0.95	0.22	45,45,45,45	0
84	OHX	AR	3542	7/7	0.95	0.14	145,146,147,147	0
84	OHX	sR	1987	7/7	0.95	0.27	144,145,146,146	0
85	MG	1	4052	1/1	0.95	0.17	51,51,51,51	0
84	OHX	AR	3597	7/7	0.95	0.34	126,127,127,127	0
84	OHX	1	3554	7/7	0.95	0.14	145,146,146,146	0
84	OHX	1	3669	7/7	0.95	0.24	150,150,151,151	0
85	MG	sR	2127	1/1	0.95	0.28	65,65,65,65	0
85	MG	1	3835	1/1	0.95	0.42	25,25,25,25	0
85	MG	1	3998	1/1	0.95	0.18	54,54,54,54	0
85	MG	AR	3938	1/1	0.95	0.54	52,52,52,52	0
87	ZN	g	501	1/1	0.95	0.05	121,121,121,121	0
84	OHX	1	3613	7/7	0.95	0.35	140,141,141,141	0
84	OHX	1	3599	7/7	0.95	0.35	146,146,146,147	0
85	MG	1	3812	1/1	0.95	0.50	60,60,60,60	0
84	OHX	A	1999	7/7	0.95	0.21	169,170,170,171	0
84	OHX	AR	3616	7/7	0.95	0.32	156,157,158,158	0
84	OHX	1	3689	7/7	0.95	0.31	131,132,132,132	0
85	MG	AR	4153	1/1	0.95	0.34	36,36,36,36	0
84	OHX	AR	3503	7/7	0.95	0.14	118,119,119,120	0
84	OHX	sR	2011	7/7	0.95	0.26	172,172,173,173	0
84	OHX	AR	3629	7/7	0.95	0.24	157,157,158,158	0
84	OHX	1	3658	7/7	0.95	0.12	173,174,174,175	0
85	MG	1	3770	1/1	0.95	0.62	42,42,42,42	0
84	OHX	AR	3686	7/7	0.95	0.32	173,174,175,175	0
85	MG	sR	2149	1/1	0.95	0.51	59,59,59,59	0
85	MG	1	4211	1/1	0.95	0.29	22,22,22,22	0
85	MG	AR	4123	1/1	0.95	0.15	40,40,40,40	0
85	MG	AR	4164	1/1	0.95	0.11	152,152,152,152	0
85	MG	AS	216	1/1	0.95	0.55	26,26,26,26	0
84	OHX	AR	3635	7/7	0.95	0.15	158,159,159,159	0
84	OHX	sR	1954	7/7	0.95	0.09	176,177,178,179	0
85	MG	AR	3838	1/1	0.95	0.28	27,27,27,27	0
85	MG	sR	2113	1/1	0.95	0.39	52,52,52,52	0
85	MG	1	4078	1/1	0.95	0.26	38,38,38,38	0
84	OHX	sR	1986	7/7	0.96	0.16	172,173,174,174	0
84	OHX	AR	3622	7/7	0.96	0.30	127,127,127,128	0
85	MG	AR	3858	1/1	0.96	0.49	29,29,29,29	0
84	OHX	sR	1992	7/7	0.96	0.29	144,144,145,145	0
84	OHX	CL	301	7/7	0.96	0.16	151,151,151,152	0
85	MG	1	3872	1/1	0.96	0.34	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	1	3553	7/7	0.96	0.09	170,170,171,171	0
84	OHX	1	3504	7/7	0.96	0.10	137,137,138,138	0
84	OHX	AR	3585	7/7	0.96	0.24	156,156,156,156	0
85	MG	1	3791	1/1	0.96	0.55	37,37,37,37	0
85	MG	1	4205	1/1	0.96	0.42	58,58,58,58	0
84	OHX	c8	201	7/7	0.96	0.14	166,166,167,167	0
85	MG	AT	220	1/1	0.96	0.58	52,52,52,52	0
85	MG	1	3863	1/1	0.96	0.49	42,42,42,42	0
84	OHX	1	3540	7/7	0.96	0.21	130,131,131,131	0
84	OHX	1	3499	7/7	0.96	0.15	106,107,107,107	0
85	MG	1	4175	1/1	0.96	0.38	54,54,54,54	0
84	OHX	1	3526	7/7	0.96	0.25	118,119,119,119	0
84	OHX	1	3650	7/7	0.96	0.18	148,149,149,149	0
85	MG	1	3932	1/1	0.96	0.43	22,22,22,22	0
85	MG	AR	3964	1/1	0.96	0.25	38,38,38,38	0
84	OHX	A	1973	7/7	0.96	0.20	167,168,169,170	0
85	MG	1	4174	1/1	0.96	0.27	60,60,60,60	0
85	MG	AR	4093	1/1	0.96	0.30	33,33,33,33	0
84	OHX	AR	3550	7/7	0.96	0.19	117,117,118,118	0
84	OHX	A	1996	7/7	0.96	0.25	162,162,163,163	0
85	MG	1	4170	1/1	0.96	0.13	50,50,50,50	0
84	OHX	1	3538	7/7	0.96	0.20	114,114,114,115	0
84	OHX	1	3539	7/7	0.96	0.13	130,131,131,132	0
84	OHX	1	3614	7/7	0.96	0.19	133,133,134,134	0
84	OHX	1	3523	7/7	0.96	0.12	131,131,132,132	0
85	MG	AR	4103	1/1	0.96	0.28	38,38,38,38	0
84	OHX	AR	3721	7/7	0.96	0.27	125,126,126,126	0
84	OHX	AT	205	7/7	0.96	0.12	136,137,137,137	0
85	MG	DP	101	1/1	0.96	0.34	52,52,52,52	0
84	OHX	A	1948	7/7	0.96	0.12	140,141,141,142	0
84	OHX	sR	1952	7/7	0.96	0.10	159,159,160,160	0
85	MG	AR	3998	1/1	0.96	0.16	48,48,48,48	0
84	OHX	y	201	7/7	0.96	0.18	151,152,153,154	0
84	OHX	1	3512	7/7	0.96	0.16	107,107,108,108	0
85	MG	1	3936	1/1	0.96	0.12	40,40,40,40	0
85	MG	1	4139	1/1	0.96	0.48	35,35,35,35	0
85	MG	AR	3790	1/1	0.96	0.41	40,40,40,40	0
84	OHX	1	3549	7/7	0.96	0.12	147,147,147,148	0
84	OHX	1	3602	7/7	0.96	0.10	168,168,169,169	0
85	MG	1	3836	1/1	0.96	0.30	36,36,36,36	0
85	MG	sR	2108	1/1	0.96	0.34	55,55,55,55	0
85	MG	1	3868	1/1	0.96	0.60	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	3915	1/1	0.96	0.31	39,39,39,39	0
85	MG	3	211	1/1	0.96	0.48	33,33,33,33	0
84	OHX	1	3653	7/7	0.96	0.28	133,133,133,134	0
84	OHX	1	3605	7/7	0.96	0.13	141,142,142,142	0
84	OHX	A	1921	7/7	0.96	0.14	124,125,126,126	0
84	OHX	AR	3582	7/7	0.96	0.33	145,145,146,146	0
84	OHX	AR	3531	7/7	0.96	0.14	121,121,122,122	0
85	MG	1	4214	1/1	0.96	0.42	36,36,36,36	0
85	MG	sR	2057	1/1	0.96	0.50	56,56,56,56	0
84	OHX	sR	1967	7/7	0.96	0.15	142,143,144,144	0
85	MG	AR	4047	1/1	0.96	0.23	45,45,45,45	0
84	OHX	1	3603	7/7	0.96	0.25	136,136,137,137	0
86	7AL	1	4210	26/26	0.96	0.23	31,31,32,32	0
84	OHX	sR	1989	7/7	0.96	0.15	151,151,152,152	0
85	MG	1	3964	1/1	0.96	0.38	43,43,43,43	0
84	OHX	AS	208	7/7	0.96	0.24	135,135,136,136	0
84	OHX	AR	3535	7/7	0.96	0.20	107,107,108,108	0
85	MG	1	3800	1/1	0.96	0.50	62,62,62,62	0
84	OHX	AR	3476	7/7	0.96	0.21	84,84,85,85	0
84	OHX	sR	1994	7/7	0.96	0.17	157,158,159,159	0
84	OHX	A	1932	7/7	0.96	0.14	143,144,144,145	0
84	OHX	AR	3671	7/7	0.96	0.26	161,161,161,161	0
84	OHX	AR	3648	7/7	0.96	0.30	152,152,153,153	0
84	OHX	sR	1956	7/7	0.96	0.10	175,176,177,178	0
84	OHX	1	3634	7/7	0.96	0.27	128,128,129,129	0
85	MG	AR	4190	1/1	0.96	0.24	48,48,48,48	0
84	OHX	AT	209	7/7	0.96	0.20	133,133,134,134	0
84	OHX	1	3641	7/7	0.96	0.14	154,155,156,156	0
84	OHX	sR	1975	7/7	0.96	0.39	135,135,136,136	0
85	MG	A	2044	1/1	0.96	0.64	40,40,40,40	0
85	MG	1	3838	1/1	0.96	0.82	49,49,49,49	0
85	MG	sR	2162	1/1	0.96	0.40	50,50,50,50	0
84	OHX	1	3521	7/7	0.96	0.17	134,134,135,135	0
85	MG	1	3933	1/1	0.96	0.26	32,32,32,32	0
84	OHX	A	2016	7/7	0.96	0.18	161,162,162,163	0
84	OHX	1	3723	7/7	0.96	0.23	157,158,158,159	0
85	MG	AR	3910	1/1	0.96	0.49	38,38,38,38	0
85	MG	AR	4242	1/1	0.96	0.51	36,36,36,36	0
85	MG	AR	4114	1/1	0.96	0.51	37,37,37,37	0
85	MG	AR	3959	1/1	0.96	0.36	30,30,30,30	0
85	MG	1	3902	1/1	0.96	0.69	37,37,37,37	0
84	OHX	sR	1984	7/7	0.96	0.12	158,159,159,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	sR	2119	1/1	0.96	0.46	67,67,67,67	0
84	OHX	1	3592	7/7	0.96	0.21	118,119,119,119	0
84	OHX	1	3528	7/7	0.96	0.15	138,139,139,139	0
85	MG	AR	3801	1/1	0.96	0.68	41,41,41,41	0
85	MG	1	3909	1/1	0.96	0.46	27,27,27,27	0
84	OHX	1	3591	7/7	0.96	0.15	169,170,171,171	0
84	OHX	1	3481	7/7	0.96	0.13	120,120,121,121	0
85	MG	1	4120	1/1	0.96	0.35	42,42,42,42	0
84	OHX	AR	3537	7/7	0.96	0.12	142,142,143,143	0
84	OHX	AR	3592	7/7	0.96	0.20	147,148,148,149	0
84	OHX	AR	3678	7/7	0.96	0.34	123,124,124,124	0
84	OHX	Rb	401	7/7	0.96	0.16	195,195,197,197	0
84	OHX	1	3576	7/7	0.96	0.24	130,130,130,131	0
84	OHX	AR	3638	7/7	0.96	0.25	130,130,130,130	0
85	MG	A	2073	1/1	0.96	0.72	75,75,75,75	0
85	MG	1	4056	1/1	0.96	0.42	50,50,50,50	0
85	MG	1	3771	1/1	0.96	0.65	41,41,41,41	0
84	OHX	1	3488	7/7	0.96	0.15	111,112,112,112	0
85	MG	1	3937	1/1	0.96	0.15	50,50,50,50	0
84	OHX	AR	3561	7/7	0.96	0.18	122,123,123,123	0
85	MG	1	3841	1/1	0.96	0.33	40,40,40,40	0
85	MG	A	2049	1/1	0.96	0.57	48,48,48,48	0
84	OHX	AR	3563	7/7	0.96	0.12	143,144,144,144	0
84	OHX	AR	3554	7/7	0.96	0.16	125,125,125,126	0
85	MG	1	3940	1/1	0.96	0.41	52,52,52,52	0
84	OHX	1	3432	7/7	0.96	0.23	84,85,85,85	0
84	OHX	A	1960	7/7	0.96	0.13	167,168,168,169	0
85	MG	1	3962	1/1	0.96	0.22	93,93,93,93	0
84	OHX	1	3552	7/7	0.96	0.21	130,131,132,132	0
85	MG	1	3862	1/1	0.96	0.39	21,21,21,21	0
84	OHX	AT	207	7/7	0.96	0.21	135,135,135,135	0
84	OHX	AR	3587	7/7	0.96	0.20	120,121,121,121	0
85	MG	AR	3779	1/1	0.96	0.27	49,49,49,49	0
85	MG	AR	4151	1/1	0.96	0.36	49,49,49,49	0
85	MG	sR	2147	1/1	0.96	0.21	67,67,67,67	0
85	MG	AR	3906	1/1	0.96	0.78	47,47,47,47	0
84	OHX	sR	1933	7/7	0.96	0.17	106,106,107,107	0
85	MG	AR	3786	1/1	0.96	0.35	40,40,40,40	0
84	OHX	1	3596	7/7	0.96	0.14	146,147,147,147	0
85	MG	1	3899	1/1	0.96	0.32	22,22,22,22	0
85	MG	1	3865	1/1	0.96	0.67	29,29,29,29	0
85	MG	x	207	1/1	0.96	0.33	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	sR	2010	7/7	0.96	0.17	138,139,140,140	0
84	OHX	AR	3649	7/7	0.96	0.23	145,146,146,147	0
85	MG	AR	3956	1/1	0.96	0.32	41,41,41,41	0
84	OHX	h	401	7/7	0.96	0.12	193,195,196,196	0
84	OHX	AR	3619	7/7	0.96	0.24	138,139,139,139	0
84	OHX	1	3705	7/7	0.96	0.25	123,124,124,125	0
84	OHX	1	3574	7/7	0.96	0.12	152,152,153,153	0
85	MG	1	4012	1/1	0.96	0.25	49,49,49,49	0
85	MG	AR	4170	1/1	0.96	0.27	55,55,55,55	0
84	OHX	1	3595	7/7	0.96	0.14	183,183,184,185	0
85	MG	1	3805	1/1	0.96	0.53	21,21,21,21	0
84	OHX	1	3627	7/7	0.96	0.18	134,135,135,135	0
85	MG	1	4026	1/1	0.96	0.67	47,47,47,47	0
85	MG	AR	3782	1/1	0.96	0.26	28,28,28,28	0
84	OHX	AR	3608	7/7	0.96	0.17	128,128,128,128	0
84	OHX	AR	3583	7/7	0.96	0.11	170,170,171,171	0
84	OHX	1	3580	7/7	0.96	0.18	117,117,118,118	0
84	OHX	AR	3581	7/7	0.96	0.25	131,132,132,132	0
85	MG	A	2096	1/1	0.96	0.17	91,91,91,91	0
84	OHX	AR	3603	7/7	0.96	0.16	142,143,143,143	0
84	OHX	AR	3698	7/7	0.96	0.31	147,148,148,148	0
85	MG	1	3990	1/1	0.96	0.31	31,31,31,31	0
85	MG	AR	3914	1/1	0.96	0.57	31,31,31,31	0
85	MG	AR	3810	1/1	0.96	0.54	25,25,25,25	0
85	MG	sM	201	1/1	0.96	0.25	44,44,44,44	0
85	MG	1	3807	1/1	0.96	0.25	33,33,33,33	0
84	OHX	AR	3547	7/7	0.96	0.11	157,157,158,158	0
84	OHX	AT	210	7/7	0.96	0.19	136,136,137,137	0
84	OHX	1	3683	7/7	0.96	0.27	135,136,136,137	0
84	OHX	AR	3632	7/7	0.96	0.23	151,151,151,151	0
85	MG	AR	3761	1/1	0.96	0.15	56,56,56,56	0
84	OHX	AR	3571	7/7	0.96	0.21	129,130,130,130	0
85	MG	AR	4239	1/1	0.96	0.29	38,38,38,38	0
84	OHX	AR	3568	7/7	0.96	0.16	147,147,148,148	0
84	OHX	AR	3519	7/7	0.96	0.17	108,108,109,109	0
84	OHX	AR	3594	7/7	0.96	0.22	137,138,138,138	0
84	OHX	AR	3576	7/7	0.96	0.21	138,139,139,140	0
84	OHX	AR	3538	7/7	0.96	0.15	124,124,124,124	0
84	OHX	1	3687	7/7	0.96	0.32	149,150,150,150	0
84	OHX	A	1965	7/7	0.96	0.12	148,149,150,150	0
84	OHX	1	3583	7/7	0.96	0.19	139,140,140,140	0
85	MG	1	3828	1/1	0.96	0.29	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	4203	1/1	0.96	0.22	40,40,40,40	0
84	OHX	sR	1943	7/7	0.96	0.12	131,132,132,132	0
84	OHX	AR	3673	7/7	0.96	0.25	179,180,181,181	0
86	7AL	AR	4246	26/26	0.96	0.20	33,33,33,33	0
84	OHX	sR	1990	7/7	0.96	0.11	159,159,160,161	0
85	MG	1	3905	1/1	0.96	0.41	36,36,36,36	0
85	MG	AR	4191	1/1	0.96	0.19	26,26,26,26	0
85	MG	1	4217	1/1	0.96	0.14	36,36,36,36	0
85	MG	1	3735	1/1	0.96	0.47	50,50,50,50	0
85	MG	sR	2093	1/1	0.96	0.28	50,50,50,50	0
85	MG	AR	4192	1/1	0.96	0.49	47,47,47,47	0
84	OHX	1	3541	7/7	0.96	0.15	141,141,142,142	0
84	OHX	d4	201	7/7	0.96	0.22	171,172,172,172	0
85	MG	AB	201	1/1	0.96	0.36	26,26,26,26	0
85	MG	AR	3829	1/1	0.96	0.42	38,38,38,38	0
84	OHX	sR	1955	7/7	0.96	0.11	168,169,170,171	0
85	MG	AR	3841	1/1	0.96	0.32	53,53,53,53	0
85	MG	1	3850	1/1	0.96	0.62	40,40,40,40	0
85	MG	1	3797	1/1	0.96	0.59	54,54,54,54	0
84	OHX	sR	1929	7/7	0.96	0.15	154,154,155,156	0
85	MG	AR	3863	1/1	0.96	0.23	49,49,49,49	0
85	MG	AR	4144	1/1	0.96	0.45	30,30,30,30	0
84	OHX	AR	3617	7/7	0.96	0.15	146,146,147,147	0
85	MG	AR	3764	1/1	0.96	0.54	15,15,15,15	0
84	OHX	AR	3478	7/7	0.96	0.19	99,99,100,100	0
85	MG	sR	2058	1/1	0.96	0.36	51,51,51,51	0
84	OHX	A	1975	7/7	0.96	0.10	169,171,172,172	0
84	OHX	AR	3459	7/7	0.96	0.17	100,101,101,102	0
85	MG	AR	3825	1/1	0.96	0.39	27,27,27,27	0
84	OHX	AP	502	7/7	0.96	0.20	102,102,103,104	0
85	MG	1	3908	1/1	0.96	0.29	21,21,21,21	0
84	OHX	sR	1921	7/7	0.96	0.15	124,125,126,127	0
84	OHX	e	101	7/7	0.96	0.33	167,168,169,169	0
84	OHX	AR	3630	7/7	0.96	0.20	173,173,174,174	0
84	OHX	A	1936	7/7	0.96	0.14	127,128,128,128	0
84	OHX	AR	3447	7/7	0.97	0.16	87,87,88,88	0
84	OHX	sR	1941	7/7	0.97	0.17	110,111,111,112	0
84	OHX	sR	1963	7/7	0.97	0.12	126,126,127,127	0
84	OHX	1	3533	7/7	0.97	0.11	160,161,162,162	0
84	OHX	4	210	7/7	0.97	0.20	123,123,123,123	0
84	OHX	1	3566	7/7	0.97	0.17	143,143,143,143	0
84	OHX	1	3503	7/7	0.97	0.17	109,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	3916	1/1	0.97	0.41	43,43,43,43	0
85	MG	AR	4139	1/1	0.97	0.13	51,51,51,51	0
84	OHX	AS	203	7/7	0.97	0.18	114,115,115,115	0
85	MG	1	3975	1/1	0.97	0.45	43,43,43,43	0
84	OHX	1	3588	7/7	0.97	0.20	152,152,153,153	0
84	OHX	v	302	7/7	0.97	0.15	121,122,122,122	0
85	MG	AR	3898	1/1	0.97	0.29	45,45,45,45	0
85	MG	1	3818	1/1	0.97	0.49	44,44,44,44	0
84	OHX	A	1944	7/7	0.97	0.13	135,136,136,137	0
84	OHX	AR	3631	7/7	0.97	0.26	164,164,164,164	0
85	MG	AR	4175	1/1	0.97	0.28	47,47,47,47	0
85	MG	A	2092	1/1	0.97	0.19	80,80,80,80	0
85	MG	1	3826	1/1	0.97	0.22	38,38,38,38	0
85	MG	AR	3881	1/1	0.97	0.67	28,28,28,28	0
85	MG	AR	4039	1/1	0.97	0.34	47,47,47,47	0
85	MG	AR	3807	1/1	0.97	0.50	32,32,32,32	0
84	OHX	1	3578	7/7	0.97	0.19	129,130,130,131	0
85	MG	AR	3806	1/1	0.97	0.33	76,76,76,76	0
84	OHX	AR	3429	7/7	0.97	0.21	81,81,81,81	0
85	MG	AR	3763	1/1	0.97	0.17	25,25,25,25	0
85	MG	1	4129	1/1	0.97	0.46	26,26,26,26	0
85	MG	1	3767	1/1	0.97	0.28	39,39,39,39	0
84	OHX	AR	3578	7/7	0.97	0.20	132,133,133,134	0
85	MG	1	3858	1/1	0.97	0.65	37,37,37,37	0
84	OHX	AR	3589	7/7	0.97	0.15	121,122,122,122	0
84	OHX	A	1939	7/7	0.97	0.10	143,144,145,145	0
84	OHX	AR	3488	7/7	0.97	0.20	100,100,101,101	0
84	OHX	AR	3654	7/7	0.97	0.37	148,148,149,149	0
85	MG	1	3748	1/1	0.97	0.34	39,39,39,39	0
84	OHX	k	401	7/7	0.97	0.18	123,123,124,124	0
84	OHX	1	3496	7/7	0.97	0.14	115,116,116,116	0
85	MG	A	2058	1/1	0.97	0.54	49,49,49,49	0
84	OHX	AR	3540	7/7	0.97	0.15	104,104,105,105	0
85	MG	1	3739	1/1	0.97	0.45	31,31,31,31	0
85	MG	t	201	1/1	0.97	0.14	44,44,44,44	0
85	MG	1	3901	1/1	0.97	0.46	18,18,18,18	0
84	OHX	J	301	7/7	0.97	0.27	177,178,179,179	0
84	OHX	M	201	7/7	0.97	0.30	145,146,147,147	0
84	OHX	AR	3524	7/7	0.97	0.18	117,117,117,117	0
84	OHX	AR	3492	7/7	0.97	0.12	127,128,128,129	0
84	OHX	1	3449	7/7	0.97	0.19	91,91,92,92	0
85	MG	AR	3880	1/1	0.97	0.44	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3856	1/1	0.97	0.47	34,34,34,34	0
84	OHX	4	207	7/7	0.97	0.17	130,131,131,132	0
84	OHX	1	3688	7/7	0.97	0.23	122,122,123,123	0
84	OHX	A	1910	7/7	0.97	0.20	102,103,104,104	0
84	OHX	A	1967	7/7	0.97	0.13	136,137,137,138	0
84	OHX	AR	3557	7/7	0.97	0.29	129,130,130,130	0
84	OHX	AR	3591	7/7	0.97	0.20	141,141,142,142	0
85	MG	AR	3915	1/1	0.97	0.38	28,28,28,28	0
84	OHX	sR	1972	7/7	0.97	0.33	168,169,170,170	0
84	OHX	AR	3484	7/7	0.97	0.16	105,105,106,106	0
84	OHX	1	3594	7/7	0.97	0.27	138,138,139,139	0
85	MG	A	2079	1/1	0.97	0.58	53,53,53,53	0
85	MG	4	219	1/1	0.97	0.37	43,43,43,43	0
84	OHX	A	1945	7/7	0.97	0.12	160,161,162,162	0
85	MG	AR	3948	1/1	0.97	0.50	37,37,37,37	0
84	OHX	1	3451	7/7	0.97	0.17	101,101,102,102	0
85	MG	sR	2111	1/1	0.97	0.52	43,43,43,43	0
84	OHX	1	3472	7/7	0.97	0.18	97,98,98,98	0
85	MG	sR	2175	1/1	0.97	0.25	36,36,36,36	0
85	MG	1	3761	1/1	0.97	0.58	44,44,44,44	0
84	OHX	sR	1983	7/7	0.97	0.20	155,155,156,156	0
85	MG	1	3804	1/1	0.97	0.26	21,21,21,21	0
85	MG	AR	3892	1/1	0.97	0.41	36,36,36,36	0
84	OHX	AR	3546	7/7	0.97	0.15	138,139,139,139	0
85	MG	AR	3967	1/1	0.97	0.34	38,38,38,38	0
85	MG	1	3860	1/1	0.97	0.49	31,31,31,31	0
84	OHX	1	3532	7/7	0.97	0.19	113,114,114,114	0
84	OHX	AR	3586	7/7	0.97	0.14	128,129,129,129	0
85	MG	4	224	1/1	0.97	0.24	44,44,44,44	0
85	MG	1	3927	1/1	0.97	0.61	20,20,20,20	0
84	OHX	AR	3490	7/7	0.97	0.16	95,95,96,96	0
85	MG	AR	4250	1/1	0.97	0.43	28,28,28,28	0
84	OHX	AR	3469	7/7	0.97	0.14	101,102,102,103	0
85	MG	sR	2106	1/1	0.97	0.29	41,41,41,41	0
84	OHX	1	3484	7/7	0.97	0.12	113,113,114,114	0
84	OHX	1	3544	7/7	0.97	0.23	120,121,121,121	0
85	MG	AR	3913	1/1	0.97	0.71	36,36,36,36	0
84	OHX	AR	3575	7/7	0.97	0.17	161,161,161,161	0
84	OHX	1	3624	7/7	0.97	0.18	103,103,103,103	0
84	OHX	AR	3660	7/7	0.97	0.17	131,132,133,133	0
85	MG	AS	212	1/1	0.97	0.40	40,40,40,40	0
85	MG	1	3925	1/1	0.97	0.54	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	A	1952	7/7	0.97	0.21	139,140,140,141	0
84	OHX	sR	1938	7/7	0.97	0.12	121,121,122,122	0
84	OHX	A	1986	7/7	0.97	0.28	169,171,172,173	0
84	OHX	A	1969	7/7	0.97	0.21	158,158,159,159	0
84	OHX	A	1970	7/7	0.97	0.19	136,136,137,137	0
84	OHX	AR	3482	7/7	0.97	0.18	102,102,102,102	0
85	MG	1	4206	1/1	0.97	0.60	25,25,25,25	0
85	MG	AR	3975	1/1	0.97	0.33	31,31,31,31	0
85	MG	AR	4002	1/1	0.97	0.35	27,27,27,27	0
84	OHX	1	3550	7/7	0.97	0.17	134,134,135,135	0
84	OHX	AR	3466	7/7	0.97	0.16	97,98,98,98	0
85	MG	AR	3872	1/1	0.97	0.42	29,29,29,29	0
85	MG	1	3856	1/1	0.97	0.40	23,23,23,23	0
85	MG	AR	3850	1/1	0.97	0.36	21,21,21,21	0
84	OHX	1	3468	7/7	0.97	0.16	109,110,110,111	0
84	OHX	1	3642	7/7	0.97	0.22	128,129,130,130	0
84	OHX	1	3567	7/7	0.97	0.26	116,117,117,118	0
85	MG	1	3917	1/1	0.97	0.51	46,46,46,46	0
84	OHX	AT	204	7/7	0.97	0.13	116,116,116,116	0
84	OHX	sR	1974	7/7	0.97	0.14	129,129,130,130	0
85	MG	AR	3922	1/1	0.97	0.59	41,41,41,41	0
84	OHX	AR	3529	7/7	0.97	0.22	127,128,128,128	0
84	OHX	AR	3544	7/7	0.97	0.12	140,140,141,142	0
85	MG	1	3918	1/1	0.97	0.50	33,33,33,33	0
84	OHX	sR	1947	7/7	0.97	0.12	124,124,125,125	0
85	MG	sR	2178	1/1	0.97	0.17	78,78,78,78	0
84	OHX	AR	3444	7/7	0.97	0.16	91,91,92,92	0
84	OHX	AS	206	7/7	0.97	0.12	114,114,115,115	0
84	OHX	1	3458	7/7	0.97	0.19	83,83,83,83	0
84	OHX	AR	3574	7/7	0.97	0.20	114,115,115,116	0
84	OHX	1	3518	7/7	0.97	0.16	109,110,110,111	0
85	MG	1	3837	1/1	0.97	0.33	33,33,33,33	0
84	OHX	AR	3443	7/7	0.97	0.14	105,105,106,106	0
84	OHX	1	3476	7/7	0.97	0.15	107,107,108,108	0
84	OHX	AT	202	7/7	0.97	0.14	134,134,134,134	0
85	MG	1	3974	1/1	0.97	0.09	59,59,59,59	0
84	OHX	1	3575	7/7	0.97	0.19	134,135,135,135	0
84	OHX	1	3522	7/7	0.97	0.13	128,129,130,130	0
84	OHX	AR	3463	7/7	0.97	0.18	85,86,86,86	0
84	OHX	A	1927	7/7	0.97	0.12	130,130,131,131	0
84	OHX	1	3473	7/7	0.97	0.18	99,99,99,100	0
84	OHX	r	301	7/7	0.97	0.17	105,105,105,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	3870	1/1	0.97	0.56	27,27,27,27	0
84	OHX	A	1928	7/7	0.97	0.12	128,129,130,130	0
85	MG	sR	2073	1/1	0.97	0.61	58,58,58,58	0
84	OHX	1	3610	7/7	0.97	0.20	136,137,137,137	0
84	OHX	A	1933	7/7	0.97	0.16	119,120,120,120	0
85	MG	AR	4117	1/1	0.97	0.07	41,41,41,41	0
84	OHX	AR	3445	7/7	0.97	0.16	106,106,107,107	0
85	MG	AR	3877	1/1	0.97	0.75	36,36,36,36	0
84	OHX	1	3546	7/7	0.97	0.13	145,145,146,146	0
84	OHX	A	1979	7/7	0.97	0.17	154,155,156,157	0
84	OHX	1	3570	7/7	0.97	0.21	125,126,126,126	0
85	MG	AR	3775	1/1	0.97	0.19	38,38,38,38	0
84	OHX	A	1951	7/7	0.97	0.17	152,152,153,154	0
84	OHX	1	3563	7/7	0.97	0.12	135,135,135,136	0
84	OHX	A	1931	7/7	0.97	0.11	133,134,135,135	0
84	OHX	1	3464	7/7	0.97	0.15	108,108,109,109	0
85	MG	1	3833	1/1	0.97	0.44	23,23,23,23	0
85	MG	1	3769	1/1	0.97	0.31	50,50,50,50	0
84	OHX	1	3509	7/7	0.97	0.12	124,124,125,125	0
85	MG	1	4102	1/1	0.97	0.26	66,66,66,66	0
85	MG	1	3740	1/1	0.97	0.49	27,27,27,27	0
85	MG	1	3819	1/1	0.97	0.28	35,35,35,35	0
85	MG	AR	3997	1/1	0.97	0.34	37,37,37,37	0
84	OHX	A	1937	7/7	0.97	0.13	134,135,136,136	0
85	MG	AR	3860	1/1	0.97	0.43	26,26,26,26	0
85	MG	1	4037	1/1	0.97	0.28	55,55,55,55	0
85	MG	AR	4135	1/1	0.97	0.23	35,35,35,35	0
84	OHX	A	1956	7/7	0.97	0.12	145,146,147,147	0
85	MG	1	4048	1/1	0.97	0.58	37,37,37,37	0
84	OHX	1	3639	7/7	0.97	0.25	140,141,141,141	0
85	MG	1	3845	1/1	0.97	0.54	22,22,22,22	0
85	MG	1	4145	1/1	0.97	0.08	44,44,44,44	0
85	MG	AS	226	1/1	0.97	0.35	50,50,50,50	0
84	OHX	4	206	7/7	0.97	0.13	129,129,129,129	0
85	MG	1	3897	1/1	0.97	0.47	39,39,39,39	0
84	OHX	AR	3651	7/7	0.97	0.36	150,151,151,151	0
85	MG	1	4035	1/1	0.97	0.08	91,91,91,91	0
84	OHX	A	1943	7/7	0.97	0.15	119,120,120,121	0
85	MG	AR	3923	1/1	0.97	0.50	32,32,32,32	0
84	OHX	A	1994	7/7	0.97	0.17	158,159,160,160	0
84	OHX	1	3572	7/7	0.97	0.21	104,105,105,105	0
84	OHX	1	3585	7/7	0.97	0.19	128,128,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3866	1/1	0.97	0.45	30,30,30,30	0
84	OHX	1	3573	7/7	0.97	0.19	144,144,145,145	0
84	OHX	A	1976	7/7	0.97	0.24	135,135,136,136	0
85	MG	1	4009	1/1	0.97	0.18	64,64,64,64	0
84	OHX	1	3542	7/7	0.97	0.18	123,124,125,125	0
84	OHX	AR	3572	7/7	0.97	0.17	130,130,131,131	0
84	OHX	AR	3480	7/7	0.97	0.17	103,104,104,104	0
84	OHX	AR	3636	7/7	0.97	0.14	127,127,128,128	0
84	OHX	sR	1980	7/7	0.97	0.31	161,162,163,163	0
84	OHX	1	3579	7/7	0.97	0.19	115,115,116,116	0
85	MG	1	4092	1/1	0.97	0.40	46,46,46,46	0
84	OHX	A	1988	7/7	0.97	0.18	132,133,133,134	0
84	OHX	1	3587	7/7	0.97	0.13	142,142,143,143	0
84	OHX	1	3535	7/7	0.97	0.21	126,126,126,126	0
84	OHX	1	3590	7/7	0.97	0.17	125,126,126,126	0
84	OHX	A	1982	7/7	0.97	0.28	135,136,136,137	0
84	OHX	1	3586	7/7	0.97	0.16	132,132,132,132	0
84	OHX	sR	1905	7/7	0.97	0.25	96,97,97,97	0
84	OHX	AR	3579	7/7	0.97	0.16	134,134,135,135	0
84	OHX	AR	3523	7/7	0.97	0.13	127,128,128,129	0
85	MG	AR	3788	1/1	0.97	0.57	39,39,39,39	0
84	OHX	sR	1964	7/7	0.97	0.12	137,137,138,138	0
84	OHX	AR	3588	7/7	0.97	0.28	124,124,125,125	0
84	OHX	AR	3528	7/7	0.97	0.11	115,115,115,116	0
84	OHX	1	3495	7/7	0.97	0.13	119,119,119,120	0
85	MG	A	2108	1/1	0.97	0.30	79,79,79,79	0
84	OHX	1	3498	7/7	0.97	0.12	127,128,129,129	0
84	OHX	sR	1993	7/7	0.97	0.19	141,142,142,143	0
85	MG	1	3817	1/1	0.97	0.28	39,39,39,39	0
85	MG	1	4213	1/1	0.97	0.08	72,72,72,72	0
84	OHX	4	212	7/7	0.97	0.21	144,144,145,145	0
84	OHX	1	3485	7/7	0.97	0.11	121,121,122,122	0
84	OHX	1	3684	7/7	0.97	0.10	145,145,145,146	0
84	OHX	AR	3516	7/7	0.97	0.28	114,115,115,115	0
84	OHX	A	1940	7/7	0.97	0.19	126,127,127,128	0
85	MG	AR	3874	1/1	0.97	0.43	34,34,34,34	0
85	MG	sR	2109	1/1	0.97	0.53	48,48,48,48	0
84	OHX	1	3534	7/7	0.97	0.12	161,161,162,162	0
84	OHX	sR	1939	7/7	0.97	0.11	130,131,131,132	0
84	OHX	AR	3512	7/7	0.97	0.11	133,134,134,134	0
84	OHX	4	209	7/7	0.97	0.17	129,130,130,130	0
85	MG	A	2145	1/1	0.97	0.27	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3517	7/7	0.97	0.17	116,116,117,117	0
84	OHX	1	3490	7/7	0.97	0.16	101,102,102,102	0
84	OHX	1	3543	7/7	0.97	0.15	113,114,114,114	0
85	MG	A	2099	1/1	0.97	0.32	50,50,50,50	0
84	OHX	1	3584	7/7	0.97	0.18	149,149,150,150	0
85	MG	AR	4106	1/1	0.97	0.22	47,47,47,47	0
84	OHX	sR	1959	7/7	0.97	0.14	141,142,143,143	0
84	OHX	1	3507	7/7	0.97	0.26	118,118,118,119	0
84	OHX	AR	3562	7/7	0.97	0.16	120,121,121,121	0
85	MG	1	4202	1/1	0.97	0.49	36,36,36,36	0
84	OHX	AR	3703	7/7	0.97	0.22	106,106,107,107	0
85	MG	AR	3805	1/1	0.97	0.60	38,38,38,38	0
84	OHX	AT	208	7/7	0.97	0.14	138,138,139,139	0
85	MG	AR	3846	1/1	0.97	0.46	40,40,40,40	0
84	OHX	AR	3551	7/7	0.97	0.19	136,136,137,137	0
84	OHX	AR	3453	7/7	0.97	0.18	86,87,87,87	0
85	MG	1	3883	1/1	0.97	0.59	30,30,30,30	0
84	OHX	sR	1965	7/7	0.97	0.21	124,125,125,125	0
85	MG	sR	2065	1/1	0.97	0.55	42,42,42,42	0
85	MG	AR	3848	1/1	0.97	0.29	29,29,29,29	0
85	MG	1	4090	1/1	0.97	0.09	43,43,43,43	0
84	OHX	AR	3500	7/7	0.97	0.24	108,109,109,109	0
84	OHX	AG	201	7/7	0.97	0.21	127,127,128,128	0
84	OHX	A	1983	7/7	0.97	0.17	161,162,163,163	0
84	OHX	1	3632	7/7	0.97	0.17	172,173,173,174	0
84	OHX	A	1909	7/7	0.97	0.17	116,116,118,118	0
85	MG	AR	3990	1/1	0.97	0.73	48,48,48,48	0
85	MG	sR	2061	1/1	0.97	0.32	84,84,84,84	0
84	OHX	AR	3539	7/7	0.97	0.20	120,120,120,120	0
85	MG	sR	2098	1/1	0.97	0.49	62,62,62,62	0
84	OHX	A	1911	7/7	0.97	0.18	110,111,112,112	0
84	OHX	AR	3593	7/7	0.97	0.14	137,137,138,138	0
84	OHX	A	1935	7/7	0.97	0.18	149,150,150,150	0
84	OHX	1	3520	7/7	0.97	0.18	113,113,114,114	0
85	MG	AR	4121	1/1	0.97	0.18	50,50,50,50	0
85	MG	AR	4016	1/1	0.97	0.29	28,28,28,28	0
84	OHX	1	3565	7/7	0.97	0.24	155,155,155,156	0
85	MG	AR	4249	1/1	0.97	0.18	38,38,38,38	0
84	OHX	1	3510	7/7	0.97	0.15	118,118,119,119	0
84	OHX	1	3508	7/7	0.97	0.13	116,116,117,117	0
84	OHX	AR	3498	7/7	0.97	0.13	146,147,147,147	0
84	OHX	A	1955	7/7	0.97	0.11	132,133,134,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AS	204	7/7	0.97	0.13	109,110,110,110	0
84	OHX	AR	3552	7/7	0.97	0.20	109,109,109,110	0
84	OHX	1	3441	7/7	0.97	0.17	88,88,89,89	0
84	OHX	1	3474	7/7	0.97	0.17	118,119,119,119	0
85	MG	r	302	1/1	0.97	0.26	35,35,35,35	0
84	OHX	3	206	7/7	0.97	0.11	137,138,138,139	0
85	MG	AR	3798	1/1	0.97	0.32	30,30,30,30	0
84	OHX	sR	1957	7/7	0.97	0.13	125,126,126,127	0
84	OHX	1	3493	7/7	0.97	0.12	107,107,108,108	0
84	OHX	sR	1911	7/7	0.97	0.21	98,98,98,99	0
84	OHX	sR	1946	7/7	0.97	0.10	135,136,137,137	0
84	OHX	3	202	7/7	0.97	0.12	122,122,123,123	0
84	OHX	A	1972	7/7	0.98	0.12	163,164,165,165	0
85	MG	A	2078	1/1	0.98	0.53	43,43,43,43	0
85	MG	sR	2075	1/1	0.98	0.16	63,63,63,63	0
84	OHX	A	1957	7/7	0.98	0.21	139,140,140,141	0
84	OHX	A	1941	7/7	0.98	0.15	146,146,147,147	0
85	MG	3	212	1/1	0.98	0.42	47,47,47,47	0
85	MG	AR	3937	1/1	0.98	0.38	25,25,25,25	0
85	MG	1	3893	1/1	0.98	0.55	28,28,28,28	0
84	OHX	sR	1948	7/7	0.98	0.13	118,119,119,120	0
84	OHX	sR	1918	7/7	0.98	0.14	93,94,94,94	0
84	OHX	A	1934	7/7	0.98	0.13	138,139,140,140	0
84	OHX	4	205	7/7	0.98	0.13	111,111,111,111	0
85	MG	AR	4243	1/1	0.98	0.26	27,27,27,27	0
85	MG	1	3931	1/1	0.98	0.14	29,29,29,29	0
84	OHX	AR	3449	7/7	0.98	0.17	82,82,82,82	0
85	MG	AR	3919	1/1	0.98	0.47	34,34,34,34	0
85	MG	AR	4066	1/1	0.98	0.20	71,71,71,71	0
85	MG	AR	3793	1/1	0.98	0.48	53,53,53,53	0
84	OHX	A	1929	7/7	0.98	0.16	113,113,114,114	0
84	OHX	sR	1934	7/7	0.98	0.12	123,123,124,124	0
84	OHX	1	3505	7/7	0.98	0.14	108,108,109,109	0
84	OHX	AR	3505	7/7	0.98	0.14	121,121,121,122	0
85	MG	sR	2182	1/1	0.98	0.20	60,60,60,60	0
84	OHX	AR	3525	7/7	0.98	0.20	119,120,120,120	0
84	OHX	AR	3506	7/7	0.98	0.26	117,118,118,118	0
84	OHX	AR	3596	7/7	0.98	0.14	109,110,110,110	0
85	MG	sR	2084	1/1	0.98	0.31	52,52,52,52	0
84	OHX	A	1992	7/7	0.98	0.19	142,143,143,144	0
84	OHX	AR	3474	7/7	0.98	0.14	97,97,97,97	0
84	OHX	AR	3510	7/7	0.98	0.14	117,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	AR	3934	1/1	0.98	0.49	38,38,38,38	0
84	OHX	AR	3440	7/7	0.98	0.17	79,79,79,79	0
85	MG	AR	3760	1/1	0.98	0.57	33,33,33,33	0
84	OHX	4	201	7/7	0.98	0.28	79,80,80,80	0
84	OHX	1	3559	7/7	0.98	0.13	156,156,157,157	0
85	MG	AR	3900	1/1	0.98	0.42	35,35,35,35	0
84	OHX	AR	3515	7/7	0.98	0.12	116,116,116,117	0
85	MG	1	3892	1/1	0.98	0.68	34,34,34,34	0
85	MG	AR	3933	1/1	0.98	0.57	42,42,42,42	0
85	MG	AR	4045	1/1	0.98	0.23	74,74,74,74	0
84	OHX	AS	202	7/7	0.98	0.17	91,92,93,93	0
85	MG	AR	3787	1/1	0.98	0.55	31,31,31,31	0
84	OHX	AR	3434	7/7	0.98	0.20	85,85,85,85	0
84	OHX	1	3516	7/7	0.98	0.12	102,102,102,102	0
85	MG	sR	2166	1/1	0.98	0.09	59,59,59,59	0
84	OHX	1	3480	7/7	0.98	0.15	95,96,96,96	0
84	OHX	CE	401	7/7	0.98	0.12	110,110,111,111	0
84	OHX	1	3527	7/7	0.98	0.21	124,124,124,124	0
85	MG	1	4068	1/1	0.98	0.62	33,33,33,33	0
84	OHX	AR	3467	7/7	0.98	0.15	84,84,84,84	0
84	OHX	AR	3455	7/7	0.98	0.13	110,111,111,111	0
84	OHX	1	3551	7/7	0.98	0.15	122,123,123,123	0
84	OHX	1	3417	7/7	0.98	0.23	85,85,86,86	0
84	OHX	AR	3413	7/7	0.98	0.25	77,78,78,78	0
85	MG	AR	4025	1/1	0.98	0.19	36,36,36,36	0
85	MG	AR	3864	1/1	0.98	0.61	27,27,27,27	0
85	MG	1	3903	1/1	0.98	0.38	29,29,29,29	0
84	OHX	sR	1924	7/7	0.98	0.12	111,111,112,112	0
84	OHX	AR	3472	7/7	0.98	0.13	102,103,103,103	0
85	MG	AR	4195	1/1	0.98	0.12	81,81,81,81	0
84	OHX	3	204	7/7	0.98	0.13	119,119,120,120	0
84	OHX	AR	3565	7/7	0.98	0.19	128,128,128,128	0
84	OHX	A	1930	7/7	0.98	0.14	120,121,121,121	0
84	OHX	sR	2004	7/7	0.98	0.14	124,125,126,126	0
85	MG	1	4086	1/1	0.98	0.08	40,40,40,40	0
85	MG	1	3849	1/1	0.98	0.40	27,27,27,27	0
85	MG	AR	3936	1/1	0.98	0.71	22,22,22,22	0
85	MG	r	303	1/1	0.98	0.12	43,43,43,43	0
84	OHX	AR	3487	7/7	0.98	0.25	110,110,110,110	0
84	OHX	A	1990	7/7	0.98	0.21	150,151,152,152	0
84	OHX	1	3459	7/7	0.98	0.16	93,94,94,94	0
85	MG	AR	3952	1/1	0.98	0.13	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	sR	1958	7/7	0.98	0.14	119,119,120,120	0
85	MG	A	2107	1/1	0.98	0.10	147,147,147,147	0
84	OHX	4	204	7/7	0.98	0.14	103,103,103,104	0
84	OHX	1	3581	7/7	0.98	0.30	120,120,121,121	0
84	OHX	AR	3507	7/7	0.98	0.18	90,90,91,91	0
84	OHX	1	3467	7/7	0.98	0.15	102,102,103,103	0
85	MG	1	3752	1/1	0.98	0.50	36,36,36,36	0
84	OHX	AR	3485	7/7	0.98	0.14	98,98,98,98	0
85	MG	1	3782	1/1	0.98	0.47	35,35,35,35	0
85	MG	1	3898	1/1	0.98	0.39	29,29,29,29	0
84	OHX	1	3525	7/7	0.98	0.16	112,112,113,113	0
85	MG	1	3922	1/1	0.98	0.46	34,34,34,34	0
84	OHX	A	1984	7/7	0.98	0.13	130,131,131,132	0
84	OHX	1	3447	7/7	0.98	0.12	93,93,93,94	0
84	OHX	A	1913	7/7	0.98	0.15	114,114,115,115	0
84	OHX	AR	3452	7/7	0.98	0.13	107,107,108,108	0
85	MG	CR	201	1/1	0.98	0.60	35,35,35,35	0
84	OHX	AR	3545	7/7	0.98	0.21	104,105,105,105	0
84	OHX	1	3644	7/7	0.98	0.22	144,145,145,145	0
84	OHX	sR	1931	7/7	0.98	0.12	115,115,116,116	0
84	OHX	1	3601	7/7	0.98	0.28	118,118,119,119	0
85	MG	1	4119	1/1	0.98	0.10	69,69,69,69	0
84	OHX	AR	3514	7/7	0.98	0.11	110,110,110,111	0
84	OHX	sR	1949	7/7	0.98	0.12	144,145,146,146	0
84	OHX	AR	3555	7/7	0.98	0.14	116,116,117,117	0
84	OHX	1	3475	7/7	0.98	0.14	105,105,106,106	0
84	OHX	AR	3446	7/7	0.98	0.16	88,88,88,88	0
85	MG	A	2091	1/1	0.98	0.69	56,56,56,56	0
84	OHX	AR	3567	7/7	0.98	0.20	111,112,112,112	0
84	OHX	1	3448	7/7	0.98	0.14	89,89,90,90	0
84	OHX	AR	3457	7/7	0.98	0.16	100,101,101,101	0
84	OHX	1	3461	7/7	0.98	0.16	103,103,104,104	0
84	OHX	1	3487	7/7	0.98	0.14	90,91,91,92	0
84	OHX	sR	1916	7/7	0.98	0.15	93,93,94,94	0
84	OHX	1	3483	7/7	0.98	0.20	117,118,118,119	0
85	MG	1	4042	1/1	0.98	0.08	57,57,57,57	0
84	OHX	AR	3556	7/7	0.98	0.11	142,142,143,143	0
85	MG	AR	3946	1/1	0.98	0.48	21,21,21,21	0
84	OHX	sR	1937	7/7	0.98	0.13	110,110,111,111	0
84	OHX	1	3569	7/7	0.98	0.28	122,122,123,123	0
84	OHX	A	2008	7/7	0.98	0.16	132,133,133,133	0
84	OHX	AR	3479	7/7	0.98	0.13	110,111,111,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	T	201	7/7	0.98	0.15	115,116,117,117	0
84	OHX	AR	3461	7/7	0.98	0.15	95,95,95,96	0
85	MG	1	3906	1/1	0.98	0.65	23,23,23,23	0
84	OHX	A	1987	7/7	0.98	0.16	146,146,147,147	0
85	MG	1	3792	1/1	0.98	0.50	20,20,20,20	0
84	OHX	3	201	7/7	0.98	0.15	95,95,96,96	0
84	OHX	sR	1936	7/7	0.98	0.16	101,101,101,102	0
85	MG	AR	3925	1/1	0.98	0.53	32,32,32,32	0
84	OHX	sR	1944	7/7	0.98	0.09	145,146,147,147	0
84	OHX	A	1922	7/7	0.98	0.13	110,111,111,111	0
85	MG	AR	3917	1/1	0.98	0.62	34,34,34,34	0
84	OHX	1	3548	7/7	0.98	0.09	124,125,126,126	0
84	OHX	DH	201	7/7	0.98	0.15	119,119,120,120	0
84	OHX	sR	1997	7/7	0.98	0.19	151,152,153,153	0
85	MG	1	3881	1/1	0.98	0.31	29,29,29,29	0
84	OHX	1	3530	7/7	0.98	0.19	114,115,115,115	0
84	OHX	sR	1913	7/7	0.98	0.17	97,98,98,98	0
84	OHX	A	1926	7/7	0.98	0.12	122,123,123,123	0
84	OHX	1	3556	7/7	0.98	0.17	127,127,127,128	0
85	MG	1	4089	1/1	0.98	0.45	23,23,23,23	0
84	OHX	sR	1970	7/7	0.98	0.15	135,135,136,136	0
85	MG	AS	215	1/1	0.98	0.57	77,77,77,77	0
84	OHX	1	3452	7/7	0.98	0.16	99,99,99,100	0
84	OHX	1	3529	7/7	0.98	0.12	131,132,132,132	0
84	OHX	sR	1920	7/7	0.98	0.14	114,115,116,116	0
84	OHX	AR	3481	7/7	0.98	0.21	96,97,97,97	0
84	OHX	AR	3509	7/7	0.98	0.16	97,97,97,97	0
85	MG	AR	3861	1/1	0.98	0.53	30,30,30,30	0
84	OHX	1	3513	7/7	0.98	0.19	104,105,105,105	0
84	OHX	AK	103	7/7	0.98	0.14	100,100,101,101	0
85	MG	1	3900	1/1	0.98	0.50	25,25,25,25	0
84	OHX	sR	1942	7/7	0.98	0.13	130,131,131,132	0
84	OHX	A	1949	7/7	0.98	0.09	144,146,146,146	0
84	OHX	AR	3470	7/7	0.98	0.15	95,96,96,96	0
84	OHX	sR	1951	7/7	0.98	0.13	137,138,139,139	0
84	OHX	AR	3432	7/7	0.98	0.17	79,80,80,80	0
84	OHX	AR	3435	7/7	0.98	0.17	90,90,91,91	0
85	MG	1	3854	1/1	0.98	0.60	29,29,29,29	0
84	OHX	AR	3483	7/7	0.98	0.14	102,102,102,102	0
84	OHX	1	3477	7/7	0.98	0.14	103,103,104,104	0
84	OHX	AR	3450	7/7	0.98	0.17	92,93,93,93	0
84	OHX	1	3506	7/7	0.98	0.14	120,120,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	DQ	201	7/7	0.98	0.14	107,107,107,108	0
84	OHX	sR	1909	7/7	0.98	0.18	102,103,103,104	0
85	MG	AR	3895	1/1	0.98	0.31	25,25,25,25	0
84	OHX	1	3514	7/7	0.98	0.12	116,117,117,117	0
84	OHX	AR	3491	7/7	0.98	0.16	103,103,104,104	0
84	OHX	sR	1907	7/7	0.98	0.24	98,99,99,100	0
85	MG	1	3914	1/1	0.98	0.56	31,31,31,31	0
85	MG	1	3847	1/1	0.98	0.55	38,38,38,38	0
84	OHX	sR	1968	7/7	0.98	0.22	132,133,134,134	0
87	ZN	AQ	501	1/1	0.98	0.11	60,60,60,60	0
85	MG	AR	3747	1/1	0.98	0.19	46,46,46,46	0
84	OHX	4	208	7/7	0.98	0.23	126,126,126,126	0
84	OHX	AR	3527	7/7	0.98	0.11	120,121,121,122	0
84	OHX	A	1989	7/7	0.98	0.27	183,183,184,184	0
84	OHX	1	3536	7/7	0.98	0.16	100,100,101,101	0
84	OHX	AR	3584	7/7	0.98	0.14	109,109,110,110	0
84	OHX	AR	3520	7/7	0.98	0.15	112,112,113,113	0
84	OHX	1	3501	7/7	0.98	0.14	106,107,107,108	0
85	MG	AR	3935	1/1	0.98	0.60	35,35,35,35	0
85	MG	DC	206	1/1	0.98	0.15	38,38,38,38	0
85	MG	sR	2171	1/1	0.98	0.15	101,101,101,101	0
84	OHX	1	3426	7/7	0.98	0.19	79,79,80,80	0
84	OHX	AR	3475	7/7	0.98	0.15	90,91,91,91	0
84	OHX	AR	3454	7/7	0.98	0.15	109,110,110,110	0
84	OHX	AR	3451	7/7	0.98	0.13	103,103,104,104	0
84	OHX	1	3531	7/7	0.98	0.11	124,125,126,126	0
84	OHX	AR	3496	7/7	0.98	0.14	106,107,107,107	0
84	OHX	A	1903	7/7	0.98	0.26	107,108,108,108	0
85	MG	1	3920	1/1	0.98	0.38	25,25,25,25	0
84	OHX	AR	3501	7/7	0.98	0.09	133,134,134,135	0
84	OHX	AR	3504	7/7	0.98	0.19	106,106,106,107	0
84	OHX	A	1923	7/7	0.98	0.14	115,116,116,116	0
84	OHX	AR	3495	7/7	0.98	0.13	99,100,100,100	0
84	OHX	A	1912	7/7	0.98	0.13	105,105,106,106	0
85	MG	1	4137	1/1	0.98	0.13	62,62,62,62	0
85	MG	1	3890	1/1	0.98	0.43	27,27,27,27	0
84	OHX	AR	3497	7/7	0.98	0.20	104,104,105,105	0
84	OHX	A	1906	7/7	0.98	0.17	102,103,104,104	0
84	OHX	A	1942	7/7	0.98	0.17	127,128,128,129	0
84	OHX	A	1938	7/7	0.98	0.15	121,122,122,123	0
84	OHX	1	3577	7/7	0.98	0.14	146,147,147,148	0
84	OHX	1	3462	7/7	0.98	0.13	92,92,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3521	7/7	0.98	0.14	112,112,113,113	0
84	OHX	sR	1930	7/7	0.98	0.16	98,99,99,100	0
84	OHX	1	3561	7/7	0.98	0.15	116,116,116,116	0
85	MG	AR	3839	1/1	0.98	0.54	45,45,45,45	0
84	OHX	1	3436	7/7	0.98	0.18	87,88,88,88	0
85	MG	A	2050	1/1	0.98	0.45	66,66,66,66	0
84	OHX	AS	205	7/7	0.98	0.11	112,113,113,113	0
84	OHX	sR	1953	7/7	0.98	0.12	132,133,134,134	0
84	OHX	AR	3599	7/7	0.98	0.19	130,130,131,131	0
84	OHX	1	3571	7/7	0.98	0.09	155,155,155,155	0
84	OHX	sR	1926	7/7	0.98	0.12	114,115,115,116	0
85	MG	1	4031	1/1	0.98	0.19	33,33,33,33	0
84	OHX	1	3558	7/7	0.98	0.19	127,127,128,128	0
84	OHX	1	3456	7/7	0.98	0.14	96,97,97,97	0
84	OHX	AR	3462	7/7	0.98	0.21	83,83,83,84	0
84	OHX	A	1961	7/7	0.98	0.11	154,155,156,157	0
84	OHX	sR	1962	7/7	0.98	0.20	148,148,149,149	0
85	MG	1	4157	1/1	0.98	0.10	57,57,57,57	0
84	OHX	AR	3566	7/7	0.98	0.09	156,156,157,157	0
84	OHX	AR	3534	7/7	0.98	0.13	104,104,105,105	0
84	OHX	sR	1928	7/7	0.98	0.12	126,127,127,127	0
87	ZN	DQ	202	1/1	0.98	0.04	82,82,82,82	0
85	MG	AR	3870	1/1	0.98	0.35	35,35,35,35	0
84	OHX	A	1962	7/7	0.98	0.15	133,134,135,135	0
85	MG	A	2123	1/1	0.98	0.46	50,50,50,50	0
84	OHX	1	3453	7/7	0.98	0.13	101,102,102,102	0
84	OHX	CP	501	7/7	0.98	0.18	137,137,138,138	0
85	MG	1	3995	1/1	0.98	0.12	29,29,29,29	0
85	MG	AR	4147	1/1	0.98	0.08	55,55,55,55	0
84	OHX	1	3497	7/7	0.98	0.14	104,105,105,105	0
84	OHX	DD	102	7/7	0.99	0.23	82,82,83,83	0
84	OHX	AC	101	7/7	0.99	0.24	84,84,84,85	0
84	OHX	AR	3402	7/7	0.99	0.31	82,82,82,82	0
84	OHX	1	3439	7/7	0.99	0.18	86,86,86,86	0
85	MG	sR	2152	1/1	0.99	0.08	110,110,110,110	0
84	OHX	AR	3464	7/7	0.99	0.11	98,98,98,99	0
84	OHX	A	1905	7/7	0.99	0.18	93,94,94,94	0
84	OHX	AR	3420	7/7	0.99	0.23	84,84,84,84	0
84	OHX	1	3437	7/7	0.99	0.20	85,85,85,85	0
84	OHX	AR	3473	7/7	0.99	0.13	103,103,104,104	0
84	OHX	AR	3428	7/7	0.99	0.20	81,81,81,81	0
84	OHX	AR	3427	7/7	0.99	0.17	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	1	3471	7/7	0.99	0.12	98,99,99,99	0
84	OHX	A	1950	7/7	0.99	0.14	116,117,117,118	0
84	OHX	A	1914	7/7	0.99	0.15	101,102,103,103	0
84	OHX	1	3440	7/7	0.99	0.17	82,83,83,83	0
84	OHX	1	3442	7/7	0.99	0.15	88,89,89,89	0
84	OHX	AR	3513	7/7	0.99	0.15	81,81,81,82	0
84	OHX	1	3443	7/7	0.99	0.15	89,90,90,91	0
84	OHX	sR	1927	7/7	0.99	0.15	100,100,101,101	0
84	OHX	1	3410	7/7	0.99	0.24	82,83,83,83	0
84	OHX	A	1954	7/7	0.99	0.15	129,130,130,130	0
85	MG	1	3744	1/1	0.99	0.76	52,52,52,52	0
84	OHX	AR	3401	7/7	0.99	0.34	88,88,88,88	0
84	OHX	1	3444	7/7	0.99	0.18	90,90,91,91	0
84	OHX	sR	1904	7/7	0.99	0.19	90,90,90,91	0
84	OHX	1	3402	7/7	0.99	0.30	84,84,84,84	0
84	OHX	AR	3422	7/7	0.99	0.22	83,84,84,84	0
84	OHX	sR	1901	7/7	0.99	0.27	87,87,87,87	0
84	OHX	1	3416	7/7	0.99	0.18	80,80,80,80	0
84	OHX	AR	3493	7/7	0.99	0.19	83,83,83,83	0
87	ZN	AP	501	1/1	0.99	0.03	75,75,75,75	0
84	OHX	AR	3530	7/7	0.99	0.07	128,129,129,130	0
84	OHX	1	3450	7/7	0.99	0.14	97,98,99,99	0
84	OHX	1	3478	7/7	0.99	0.15	93,93,93,94	0
84	OHX	AR	3486	7/7	0.99	0.16	87,87,88,88	0
84	OHX	A	1901	7/7	0.99	0.21	92,93,93,93	0
85	MG	AR	3867	1/1	0.99	0.34	37,37,37,37	0
84	OHX	AR	3433	7/7	0.99	0.19	80,80,80,80	0
84	OHX	1	3454	7/7	0.99	0.13	90,91,91,91	0
84	OHX	sR	1925	7/7	0.99	0.16	101,101,102,102	0
85	MG	AR	3929	1/1	0.99	0.49	31,31,31,31	0
84	OHX	AR	3412	7/7	0.99	0.26	80,80,80,80	0
84	OHX	AR	3441	7/7	0.99	0.16	87,87,87,88	0
85	MG	1	4121	1/1	0.99	0.18	66,66,66,66	0
84	OHX	1	3435	7/7	0.99	0.20	92,92,93,93	0
84	OHX	A	1904	7/7	0.99	0.17	97,97,97,97	0
84	OHX	AR	3426	7/7	0.99	0.20	82,82,83,83	0
84	OHX	AR	3410	7/7	0.99	0.24	78,79,79,79	0
84	OHX	sR	1910	7/7	0.99	0.20	87,88,88,88	0
84	OHX	1	3419	7/7	0.99	0.20	79,79,79,79	0
84	OHX	AR	3407	7/7	0.99	0.25	80,80,80,80	0
84	OHX	1	3438	7/7	0.99	0.18	85,86,86,86	0
84	OHX	sR	1922	7/7	0.99	0.16	103,103,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3409	7/7	0.99	0.24	82,82,83,83	0
84	OHX	1	3427	7/7	0.99	0.20	88,88,89,89	0
85	MG	1	4189	1/1	0.99	0.14	46,46,46,46	0
85	MG	1	4156	1/1	0.99	0.12	83,83,83,83	0
84	OHX	1	3445	7/7	0.99	0.17	85,85,85,85	0
84	OHX	A	1920	7/7	0.99	0.12	102,102,103,103	0
84	OHX	A	1924	7/7	0.99	0.08	121,121,122,123	0
85	MG	AR	3773	1/1	0.99	0.59	43,43,43,43	0
84	OHX	sR	1915	7/7	0.99	0.16	92,93,93,94	0
84	OHX	1	3500	7/7	0.99	0.13	81,82,82,82	0
84	OHX	1	3469	7/7	0.99	0.23	85,85,85,86	0
84	OHX	AR	3442	7/7	0.99	0.12	95,96,96,97	0
84	OHX	1	3403	7/7	0.99	0.30	83,83,83,83	0
84	OHX	1	3492	7/7	0.99	0.11	106,106,107,107	0
84	OHX	AR	3431	7/7	0.99	0.17	81,81,82,82	0
84	OHX	AR	3615	7/7	0.99	0.18	107,107,107,107	0
85	MG	1	3851	1/1	0.99	0.17	38,38,38,38	0
84	OHX	A	1908	7/7	0.99	0.17	103,104,105,105	0
84	OHX	AR	3439	7/7	0.99	0.17	79,79,79,79	0
85	MG	A	2141	1/1	0.99	0.28	78,78,78,78	0
85	MG	AR	4231	1/1	0.99	0.14	80,80,80,80	0
84	OHX	AR	3468	7/7	0.99	0.11	101,101,102,102	0
84	OHX	sR	1935	7/7	0.99	0.13	109,109,110,110	0
84	OHX	1	3517	7/7	0.99	0.11	117,117,118,118	0
84	OHX	1	3429	7/7	0.99	0.20	93,93,94,94	0
84	OHX	CX	201	7/7	0.99	0.15	93,94,94,94	0
84	OHX	1	3405	7/7	0.99	0.28	91,91,91,91	0
84	OHX	1	3460	7/7	0.99	0.13	82,82,83,83	0
85	MG	x	205	1/1	0.99	0.63	31,31,31,31	0
84	OHX	1	3479	7/7	0.99	0.11	108,108,109,109	0
84	OHX	1	3433	7/7	0.99	0.18	86,86,87,87	0
84	OHX	sR	1906	7/7	0.99	0.20	90,90,90,90	0
84	OHX	AR	3425	7/7	0.99	0.21	81,81,81,82	0
87	ZN	DR	501	1/1	0.99	0.11	62,62,62,62	0
84	OHX	4	202	7/7	0.99	0.24	83,83,83,83	0
84	OHX	CV	201	7/7	0.99	0.26	85,85,85,85	0
84	OHX	1	3420	7/7	0.99	0.21	86,86,86,87	0
84	OHX	1	3466	7/7	0.99	0.13	94,95,95,95	0
84	OHX	sR	1902	7/7	0.99	0.24	98,99,99,99	0
84	OHX	AR	3424	7/7	0.99	0.23	82,82,82,82	0
85	MG	AR	4184	1/1	0.99	0.14	43,43,43,43	0
85	MG	AR	4146	1/1	0.99	0.07	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	ZN	DL	102	1/1	0.99	0.18	44,44,44,44	0
84	OHX	1	3434	7/7	0.99	0.18	86,87,87,87	0
84	OHX	1	3414	7/7	0.99	0.20	80,81,81,81	0
87	ZN	AK	101	1/1	0.99	0.16	39,39,39,39	0
84	OHX	1	3401	7/7	0.99	0.30	84,84,84,85	0
84	OHX	1	3465	7/7	0.99	0.14	93,93,94,94	0
84	OHX	AR	3489	7/7	0.99	0.15	95,95,95,96	0
85	MG	1	3930	1/1	0.99	0.52	26,26,26,26	0
84	OHX	1	3418	7/7	0.99	0.21	84,84,84,84	0
84	OHX	A	1902	7/7	0.99	0.18	88,89,89,89	0
87	ZN	b	102	1/1	0.99	0.10	84,84,84,84	0
85	MG	sR	2177	1/1	0.99	0.15	84,84,84,84	0
85	MG	1	3910	1/1	0.99	0.44	31,31,31,31	0
85	MG	1	3842	1/1	0.99	0.44	27,27,27,27	0
84	OHX	1	3494	7/7	0.99	0.14	89,90,90,90	0
85	MG	1	3926	1/1	0.99	0.63	23,23,23,23	0
84	OHX	sR	1917	7/7	0.99	0.13	98,99,100,100	0
84	OHX	AR	3456	7/7	0.99	0.15	83,83,83,83	0
85	MG	AR	4221	1/1	0.99	0.15	40,40,40,40	0
84	OHX	AR	3421	7/7	0.99	0.20	89,89,89,89	0
84	OHX	AR	3494	7/7	0.99	0.10	106,107,107,107	0
85	MG	1	4118	1/1	0.99	0.16	100,100,100,100	0
84	OHX	AR	3423	7/7	0.99	0.20	82,82,82,82	0
84	OHX	1	3524	7/7	0.99	0.14	107,107,108,108	0
84	OHX	AR	3406	7/7	0.99	0.26	82,82,82,82	0
84	OHX	AR	3404	7/7	0.99	0.29	81,81,82,82	0
84	OHX	AS	201	7/7	0.99	0.17	88,88,88,89	0
84	OHX	1	3412	7/7	0.99	0.24	83,83,84,84	0
84	OHX	AR	3403	7/7	0.99	0.29	80,80,80,80	0
84	OHX	1	3428	7/7	0.99	0.18	83,83,83,83	0
85	MG	AR	4179	1/1	0.99	0.14	70,70,70,70	0
87	ZN	e	103	1/1	0.99	0.09	82,82,82,82	0
84	OHX	1	3406	7/7	0.99	0.26	79,79,79,79	0
84	OHX	A	1917	7/7	0.99	0.12	105,106,106,107	0
84	OHX	1	3407	7/7	0.99	0.23	78,78,78,78	0
84	OHX	1	3415	7/7	0.99	0.24	90,90,91,91	0
84	OHX	AR	3419	7/7	0.99	0.20	81,82,82,82	0
84	OHX	1	3408	7/7	0.99	0.27	83,83,83,83	0
85	MG	AR	4180	1/1	0.99	0.15	66,66,66,66	0
85	MG	AR	4241	1/1	0.99	0.67	41,41,41,41	0
84	OHX	A	1907	7/7	0.99	0.15	99,100,100,101	0
84	OHX	AR	3460	7/7	0.99	0.12	90,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3418	7/7	0.99	0.17	84,84,84,84	0
84	OHX	sR	1945	7/7	0.99	0.12	118,119,119,120	0
84	OHX	4	203	7/7	0.99	0.14	83,83,84,84	0
84	OHX	AR	3416	7/7	0.99	0.21	82,82,82,82	0
84	OHX	AR	3448	7/7	0.99	0.16	86,86,86,87	0
84	OHX	1	3431	7/7	0.99	0.15	81,81,82,82	0
84	OHX	1	3430	7/7	0.99	0.13	86,86,86,86	0
84	OHX	AR	3417	7/7	0.99	0.22	79,80,80,80	0
84	OHX	AR	3471	7/7	0.99	0.14	90,91,91,92	0
85	MG	AR	3770	1/1	0.99	0.29	55,55,55,55	0
85	MG	1	4169	1/1	0.99	0.16	39,39,39,39	0
84	OHX	AR	3408	7/7	0.99	0.24	77,77,77,77	0
84	OHX	1	3423	7/7	0.99	0.18	88,88,88,88	0
84	OHX	A	1925	7/7	0.99	0.11	135,135,136,136	0
84	OHX	AR	3465	7/7	0.99	0.11	102,103,103,103	0
84	OHX	1	3413	7/7	0.99	0.24	82,83,83,83	0
84	OHX	1	3457	7/7	0.99	0.14	94,95,95,95	0
85	MG	AR	4064	1/1	0.99	0.12	84,84,84,84	0
84	OHX	AT	203	7/7	0.99	0.13	104,104,104,104	0
85	MG	1	4063	1/1	0.99	0.52	35,35,35,35	0
84	OHX	1	3425	7/7	0.99	0.21	87,88,88,88	0
84	OHX	A	1919	7/7	0.99	0.13	100,100,101,101	0
84	OHX	1	3422	7/7	0.99	0.20	85,86,86,86	0
84	OHX	sR	1923	7/7	0.99	0.14	92,93,93,94	0
84	OHX	AR	3502	7/7	0.99	0.12	112,112,113,113	0
84	OHX	sR	1912	7/7	0.99	0.16	89,89,90,90	0
85	MG	AR	3928	1/1	0.99	0.67	42,42,42,42	0
84	OHX	AR	3405	7/7	0.99	0.27	86,86,87,87	0
85	MG	sR	2150	1/1	0.99	0.09	76,76,76,76	0
84	OHX	AR	3414	7/7	0.99	0.24	80,80,80,80	0
84	OHX	1	3409	7/7	0.99	0.25	85,86,86,86	0
84	OHX	sR	1903	7/7	0.99	0.21	86,86,86,87	0
84	OHX	AR	3415	7/7	0.99	0.21	78,78,79,79	0
84	OHX	sR	1908	7/7	0.99	0.18	87,88,88,88	0
84	OHX	AR	3438	7/7	0.99	0.14	84,84,85,85	0
84	OHX	AR	3411	7/7	0.99	0.26	87,87,88,88	0
84	OHX	A	1916	7/7	0.99	0.13	106,107,108,108	0
84	OHX	1	3424	7/7	0.99	0.16	84,84,84,84	0
84	OHX	AR	3436	7/7	0.99	0.15	80,81,81,81	0
84	OHX	1	3491	7/7	0.99	0.14	97,97,98,98	0
84	OHX	v	301	7/7	0.99	0.15	92,92,92,93	0
84	OHX	AR	3437	7/7	0.99	0.14	83,83,83,84	0

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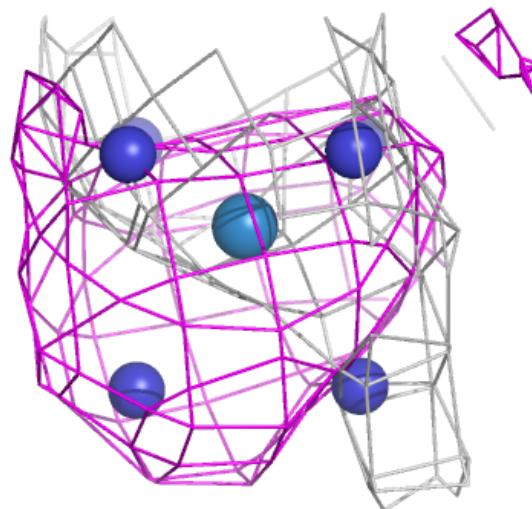
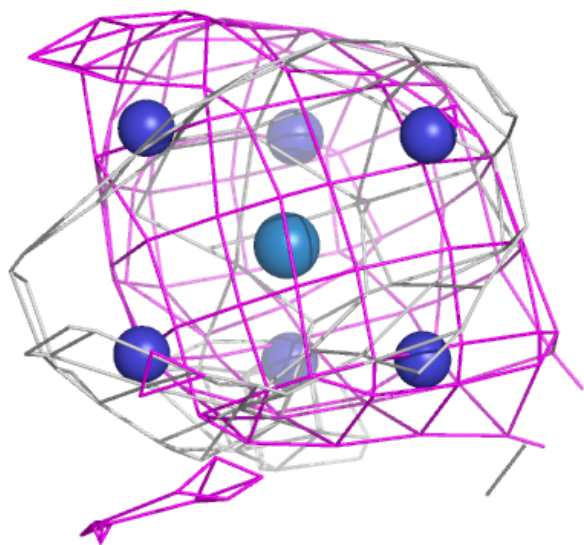
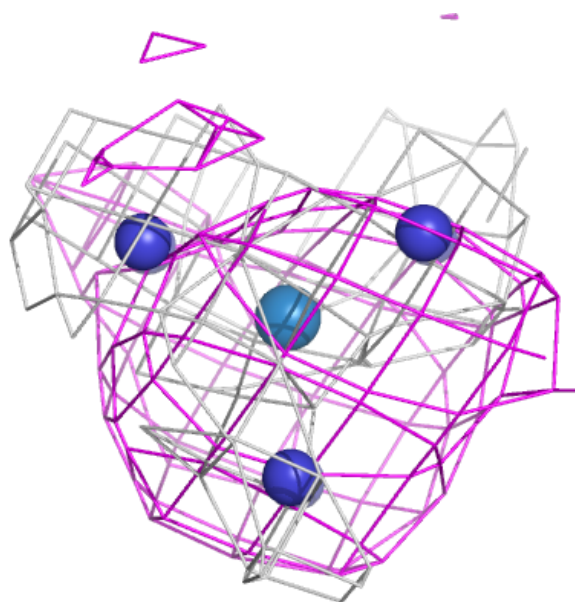
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	OHX	AR	3430	7/7	0.99	0.15	84,84,85,85	0
84	OHX	1	3404	7/7	0.99	0.29	89,89,89,89	0
84	OHX	sR	1914	7/7	0.99	0.15	104,104,105,106	0
87	ZN	AN	500	1/1	1.00	0.15	43,43,43,43	0
85	MG	AR	4208	1/1	1.00	0.17	73,73,73,73	0
87	ZN	d6	103	1/1	1.00	0.12	68,68,68,68	0
87	ZN	d9	103	1/1	1.00	0.12	81,81,81,81	0
85	MG	1	4099	1/1	1.00	0.17	68,68,68,68	0
87	ZN	DO	201	1/1	1.00	0.16	29,29,29,29	0
85	MG	AR	3912	1/1	1.00	0.58	29,29,29,29	0
85	MG	1	4158	1/1	1.00	0.15	57,57,57,57	0
84	OHX	1	3411	7/7	1.00	0.22	81,82,82,82	0
84	OHX	1	3421	7/7	1.00	0.21	84,84,85,85	0
85	MG	AR	4204	1/1	1.00	0.17	63,63,63,63	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

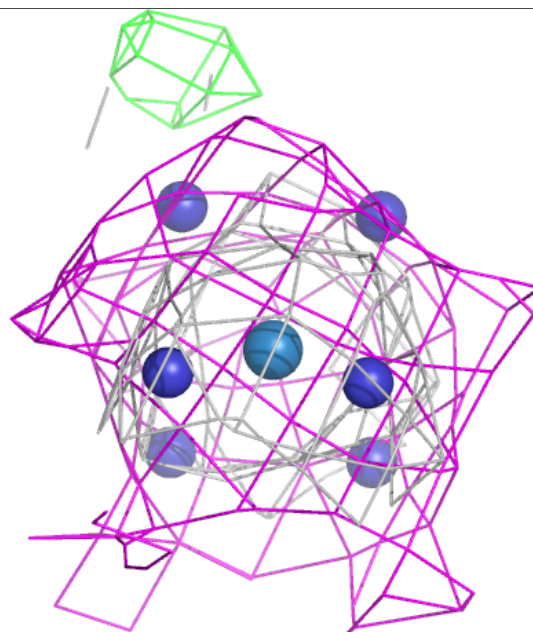
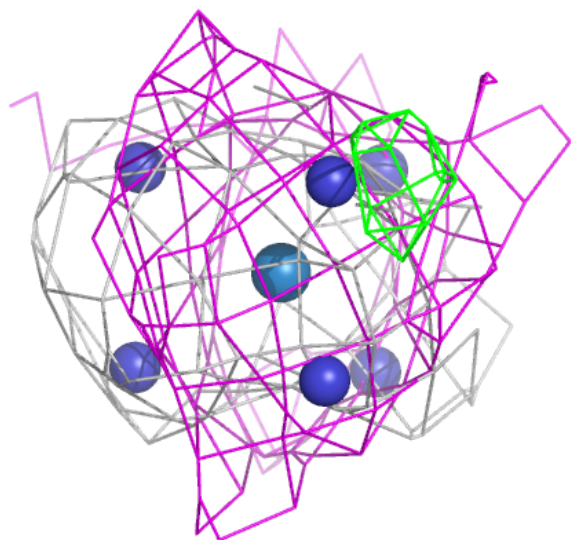
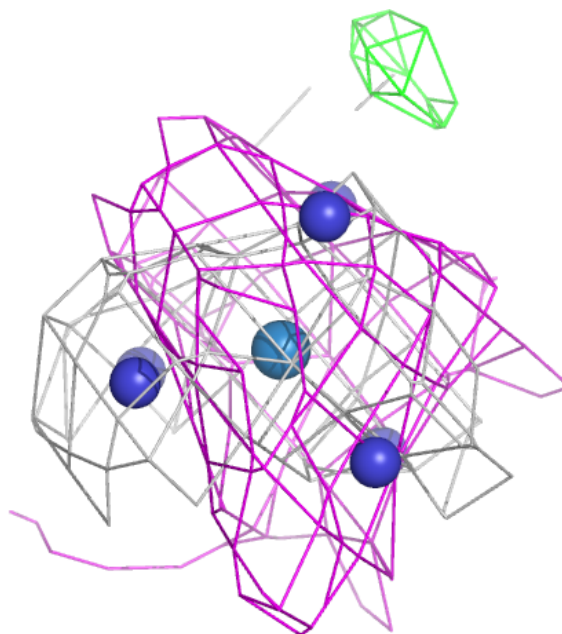
Electron density around OHX AR 3740:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



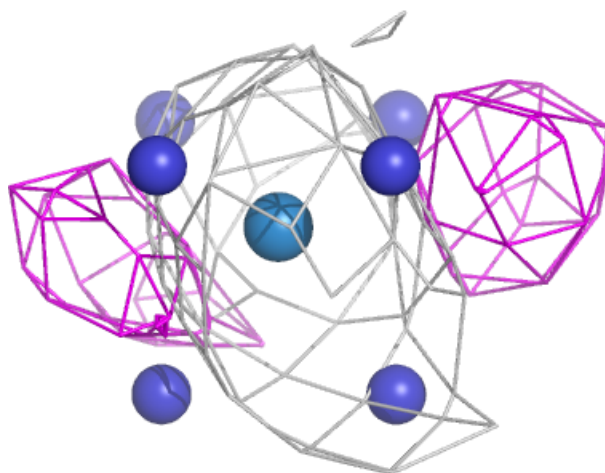
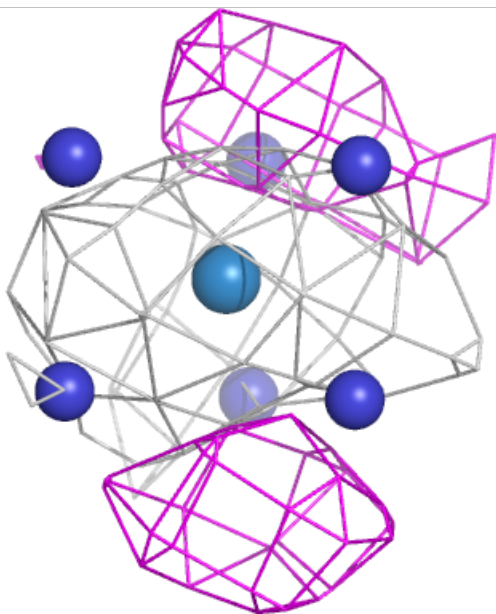
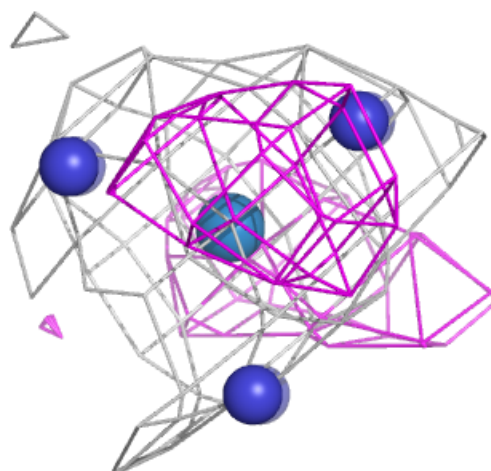
Electron density around OHX 1 3673:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



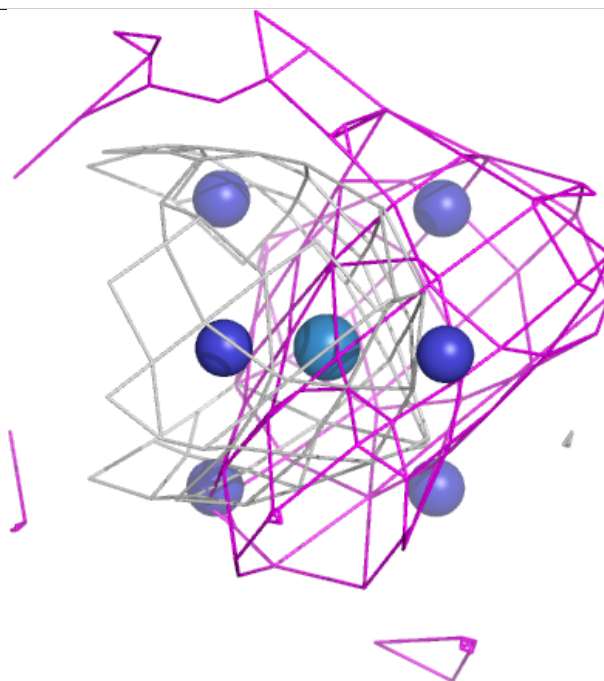
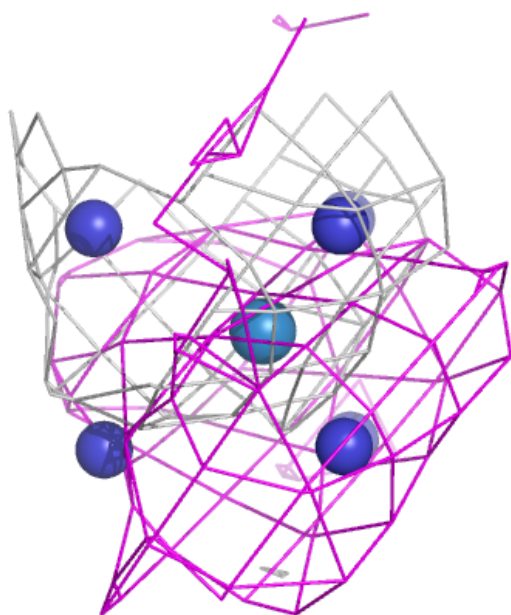
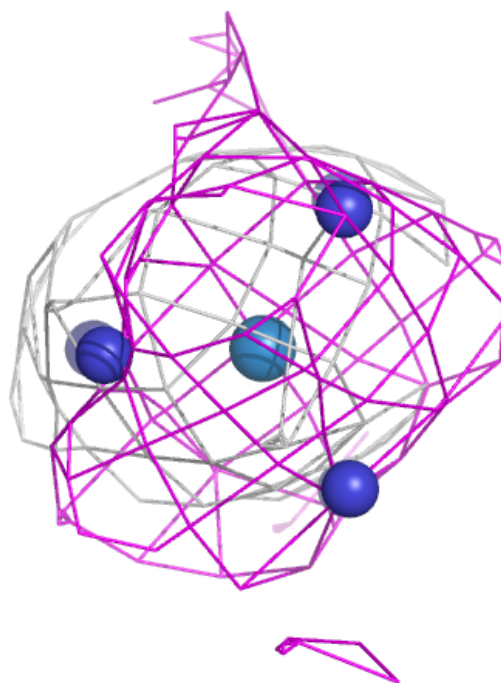
Electron density around OHX 1 3718:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



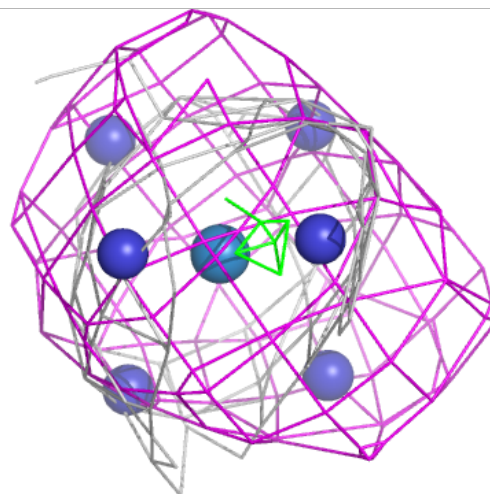
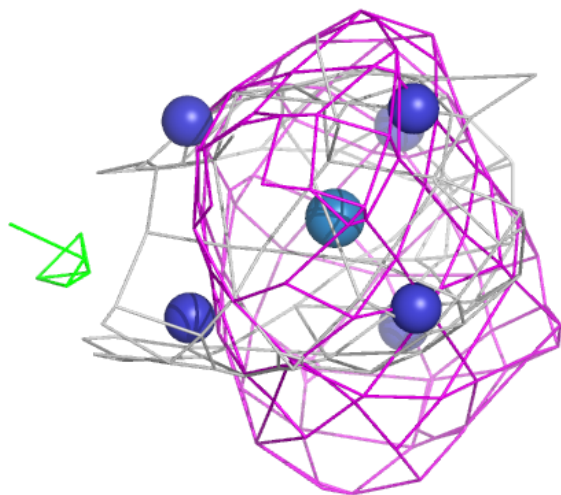
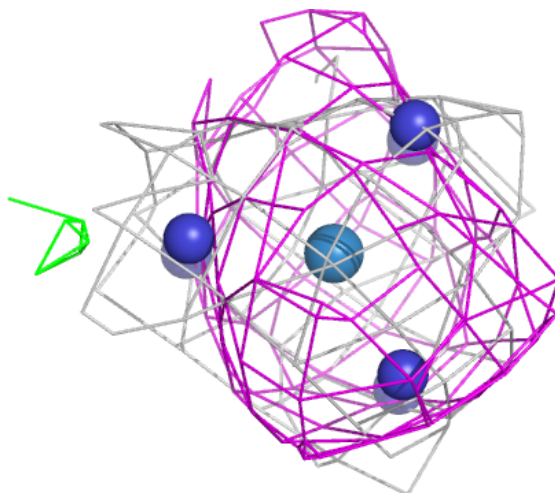
Electron density around OHX A 2039:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



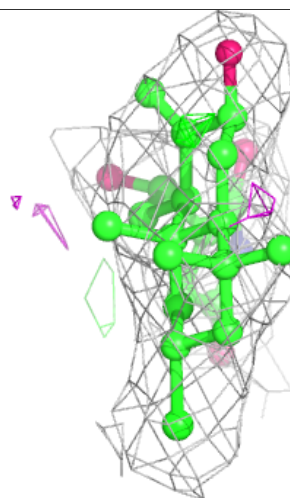
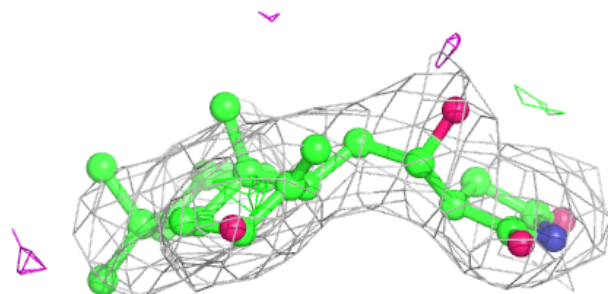
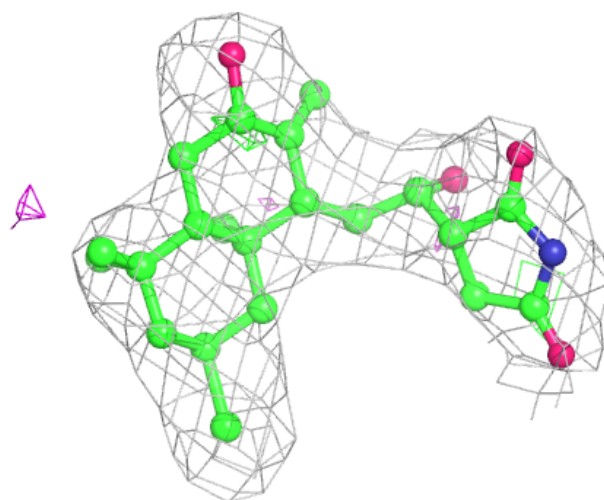
Electron density around OHX sR 2040:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



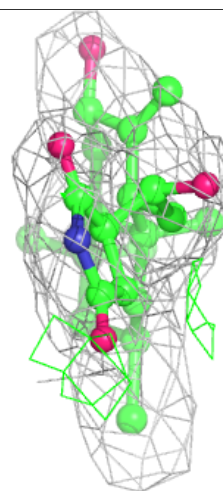
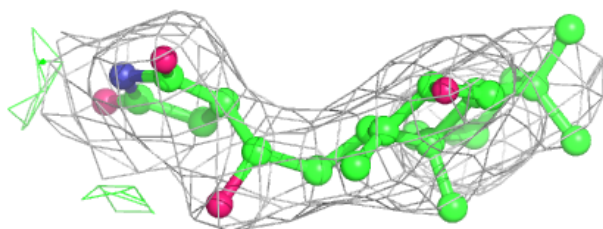
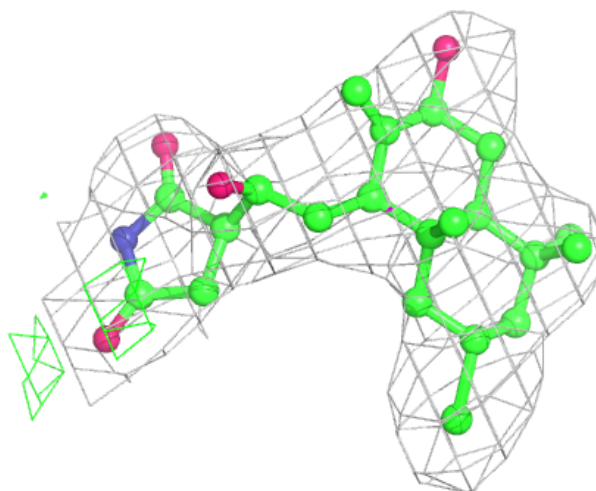
Electron density around 7AL 1 4210:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 7AL AR 4246:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.