



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 04:01 PM EST

PDB ID : 5ON6  
Title : Crystal structure of haemanthamine bound to the 80S ribosome  
Authors : Pellegrino, S.; Meyer, M.; Yusupova, G.; Yusupov, M.  
Deposited on : 2017-08-03  
Resolution : 3.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

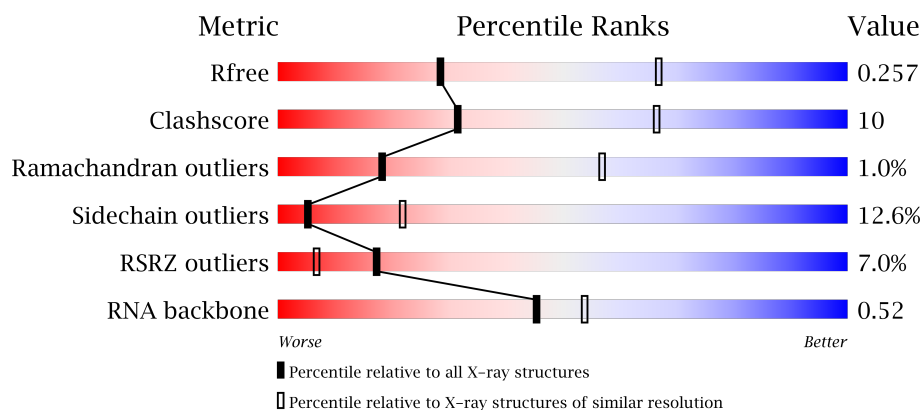
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

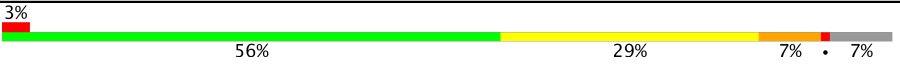



The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)
RNA backbone	2435	1112 (3.50-2.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	3396	
1	AR	3396	
2	3	121	
2	AS	121	

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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	CX	136	
24	IR	136	
25	6	1800	
25	A	1800	
26	7	98	
26	CY	98	
27	8	121	
27	CZ	121	

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Mol	Chain	Length	Quality of chain
28	9	126	
28	DA	126	
29	AA	135	
29	DB	135	
30	AB	148	
30	DC	148	
31	AC	58	
31	DD	58	
32	AD	97	
32	DE	97	
33	AE	109	
33	DF	109	
34	AF	127	
34	DG	127	
35	AG	106	
35	DH	106	
36	AH	112	
36	DI	112	
37	AI	119	
37	DJ	119	
38	AJ	99	
38	DK	99	
39	AK	87	
39	DL	87	
40	AL	77	

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Mol	Chain	Length	Quality of chain
40	DM	77	
41	AM	50	
41	DN	50	
42	AN	52	
42	DO	52	
43	AO	25	
43	DP	25	
44	AP	105	
44	DQ	105	
45	AQ	91	
45	DR	91	
46	i	272	
47	m2	150	
48	sM	104	
49	p0	311	
50	B	206	
50	s0	206	
51	C	216	
51	s1	216	
52	D	217	
52	s2	217	
53	E	223	
53	s3	223	
54	F	260	
54	s4	260	

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Mol	Chain	Length	Quality of chain
55	G	206	
55	s5	206	
56	H	226	
56	s6	226	
57	I	186	
57	s7	186	
58	J	199	
58	s8	199	
59	K	185	
59	s9	185	
60	L	105	
60	c0	105	
61	M	155	
61	c1	155	
62	N	124	
62	c2	124	
63	O	150	
63	c3	150	
64	P	128	
64	c4	128	
65	Q	141	
65	c5	141	
66	R	142	
66	c6	142	
67	S	125	

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Mol	Chain	Length	Quality of chain
67	c7	125	
68	T	145	
68	c8	145	
69	U	143	
69	c9	143	
70	V	110	
70	d0	110	
71	W	87	
71	d1	87	
72	X	129	
72	d2	129	
73	Y	144	
73	d3	144	
74	Z	134	
74	d4	134	
75	a	70	
75	d5	70	
76	b	97	
76	d6	97	
77	c	81	
77	d7	81	
78	d	63	
78	d8	63	
79	d9	53	
79	e	53	

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Mol	Chain	Length	Quality of chain
80	e0	62	
80	f	62	
81	g	71	
82	h	318	
82	sR	318	
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	3401	-	-	-	X
84	OHX	1	3402	-	-	-	X
84	OHX	1	3403	-	-	-	X
84	OHX	1	3404	-	-	-	X
84	OHX	1	3405	-	-	-	X
84	OHX	1	3406	-	-	-	X
84	OHX	1	3407	-	-	-	X
84	OHX	1	3408	-	-	-	X
84	OHX	1	3409	-	-	-	X
84	OHX	1	3410	-	-	-	X
84	OHX	1	3411	-	-	-	X
84	OHX	1	3412	-	-	-	X
84	OHX	1	3413	-	-	-	X
84	OHX	1	3414	-	-	-	X
84	OHX	1	3415	-	-	-	X
84	OHX	1	3416	-	-	-	X
84	OHX	1	3417	-	-	-	X
84	OHX	1	3418	-	-	-	X
84	OHX	1	3419	-	-	-	X
84	OHX	1	3420	-	-	-	X
84	OHX	1	3421	-	-	-	X
84	OHX	1	3422	-	-	-	X
84	OHX	1	3423	-	-	-	X
84	OHX	1	3425	-	-	-	X
84	OHX	1	3426	-	-	-	X
84	OHX	1	3427	-	-	-	X
84	OHX	1	3428	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	1	3431	-	-	-	X
84	OHX	1	3432	-	-	-	X
84	OHX	1	3433	-	-	-	X
84	OHX	1	3436	-	-	-	X
84	OHX	1	3437	-	-	-	X
84	OHX	1	3438	-	-	-	X
84	OHX	1	3442	-	-	-	X
84	OHX	1	3445	-	-	-	X
84	OHX	1	3449	-	-	-	X
84	OHX	1	3462	-	-	-	X
84	OHX	1	3473	-	-	X	-
84	OHX	1	3506	-	-	-	X
84	OHX	1	3507	-	-	-	X
84	OHX	1	3539	-	-	-	X
84	OHX	1	3541	-	-	-	X
84	OHX	1	3543	-	-	-	X
84	OHX	1	3551	-	-	-	X
84	OHX	1	3556	-	-	-	X
84	OHX	1	3572	-	-	-	X
84	OHX	1	3575	-	-	-	X
84	OHX	1	3577	-	-	-	X
84	OHX	1	3582	-	-	-	X
84	OHX	1	3584	-	-	-	X
84	OHX	1	3591	-	-	-	X
84	OHX	1	3592	-	-	-	X
84	OHX	1	3596	-	-	-	X
84	OHX	1	3599	-	-	-	X
84	OHX	1	3601	-	-	-	X
84	OHX	1	3604	-	-	-	X
84	OHX	1	3605	-	-	-	X
84	OHX	1	3606	-	-	-	X
84	OHX	1	3608	-	-	-	X
84	OHX	1	3609	-	-	-	X
84	OHX	1	3612	-	-	-	X
84	OHX	1	3613	-	-	-	X
84	OHX	1	3616	-	-	-	X
84	OHX	1	3620	-	-	-	X
84	OHX	1	3623	-	-	-	X
84	OHX	1	3626	-	-	-	X
84	OHX	1	3629	-	-	-	X
84	OHX	1	3631	-	-	-	X
84	OHX	1	3636	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	1	3638	-	-	-	X
84	OHX	1	3640	-	-	-	X
84	OHX	1	3641	-	-	-	X
84	OHX	1	3642	-	-	-	X
84	OHX	1	3643	-	-	-	X
84	OHX	1	3645	-	-	-	X
84	OHX	1	3646	-	-	-	X
84	OHX	1	3649	-	-	-	X
84	OHX	1	3650	-	-	-	X
84	OHX	1	3653	-	-	-	X
84	OHX	1	3655	-	-	-	X
84	OHX	1	3657	-	-	-	X
84	OHX	1	3659	-	-	-	X
84	OHX	1	3661	-	-	-	X
84	OHX	1	3662	-	-	-	X
84	OHX	1	3665	-	-	-	X
84	OHX	1	3666	-	-	-	X
84	OHX	1	3672	-	-	-	X
84	OHX	1	3673	-	-	-	X
84	OHX	1	3675	-	-	-	X
84	OHX	1	3676	-	-	-	X
84	OHX	1	3677	-	-	-	X
84	OHX	1	3679	-	-	-	X
84	OHX	1	3680	-	-	-	X
84	OHX	1	3683	-	-	-	X
84	OHX	1	3685	-	-	-	X
84	OHX	1	3687	-	-	-	X
84	OHX	1	3690	-	-	-	X
84	OHX	1	3692	-	-	-	X
84	OHX	1	3694	-	-	-	X
84	OHX	1	3695	-	-	-	X
84	OHX	1	3697	-	-	-	X
84	OHX	1	3699	-	-	-	X
84	OHX	1	3701	-	-	-	X
84	OHX	1	3703	-	-	-	X
84	OHX	1	3704	-	-	-	X
84	OHX	1	3705	-	-	-	X
84	OHX	1	3707	-	-	-	X
84	OHX	1	3708	-	-	-	X
84	OHX	1	3711	-	-	-	X
84	OHX	1	3717	-	-	-	X
84	OHX	1	3719	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	1	3720	-	-	X	-
84	OHX	1	3721	-	-	-	X
84	OHX	1	3723	-	-	-	X
84	OHX	2	201	-	-	-	X
84	OHX	3	208	-	-	-	X
84	OHX	4	201	-	-	-	X
84	OHX	4	202	-	-	-	X
84	OHX	4	208	-	-	-	X
84	OHX	4	209	-	-	-	X
84	OHX	4	210	-	-	-	X
84	OHX	4	212	-	-	-	X
84	OHX	4	213	-	-	-	X
84	OHX	4	214	-	-	-	X
84	OHX	4	215	-	-	-	X
84	OHX	4	216	-	-	-	X
84	OHX	6	1901	-	-	-	X
84	OHX	6	1902	-	-	-	X
84	OHX	6	1903	-	-	-	X
84	OHX	6	1904	-	-	-	X
84	OHX	6	1906	-	-	-	X
84	OHX	6	1907	-	-	-	X
84	OHX	6	1909	-	-	-	X
84	OHX	6	1910	-	-	-	X
84	OHX	6	1968	-	-	-	X
84	OHX	6	1971	-	-	-	X
84	OHX	6	1972	-	-	-	X
84	OHX	6	1975	-	-	X	-
84	OHX	6	1978	-	-	-	X
84	OHX	6	1979	-	-	-	X
84	OHX	6	1980	-	-	-	X
84	OHX	6	1986	-	-	-	X
84	OHX	6	1987	-	-	-	X
84	OHX	6	1989	-	-	-	X
84	OHX	6	1991	-	-	-	X
84	OHX	6	1992	-	-	-	X
84	OHX	6	1993	-	-	-	X
84	OHX	6	1994	-	-	-	X
84	OHX	6	2001	-	-	X	X
84	OHX	6	2005	-	-	-	X
84	OHX	6	2011	-	-	-	X
84	OHX	6	2013	-	-	-	X
84	OHX	6	2015	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	6	2019	-	-	-	X
84	OHX	6	2025	-	-	X	X
84	OHX	6	2027	-	-	-	X
84	OHX	6	2028	-	-	-	X
84	OHX	6	2029	-	-	-	X
84	OHX	6	2030	-	-	-	X
84	OHX	6	2031	-	-	-	X
84	OHX	6	2032	-	-	-	X
84	OHX	6	2033	-	-	-	X
84	OHX	6	2035	-	-	-	X
84	OHX	6	2038	-	-	-	X
84	OHX	6	2039	-	-	-	X
84	OHX	6	2041	-	-	-	X
84	OHX	6	2043	-	-	-	X
84	OHX	6	2044	-	-	-	X
84	OHX	6	2046	-	-	-	X
84	OHX	6	2050	-	-	-	X
84	OHX	6	2051	-	-	-	X
84	OHX	6	2052	-	-	-	X
84	OHX	A	1901	-	-	-	X
84	OHX	A	1902	-	-	-	X
84	OHX	A	1903	-	-	-	X
84	OHX	A	1905	-	-	-	X
84	OHX	A	1908	-	-	-	X
84	OHX	A	1909	-	-	X	-
84	OHX	A	1918	-	-	-	X
84	OHX	A	1940	-	-	-	X
84	OHX	A	1947	-	-	-	X
84	OHX	A	1953	-	-	-	X
84	OHX	A	1964	-	-	-	X
84	OHX	A	1970	-	-	-	X
84	OHX	A	1979	-	-	-	X
84	OHX	A	1980	-	-	-	X
84	OHX	A	1982	-	-	-	X
84	OHX	A	1985	-	-	-	X
84	OHX	A	1990	-	-	-	X
84	OHX	A	1994	-	-	-	X
84	OHX	A	1996	-	-	-	X
84	OHX	A	1997	-	-	-	X
84	OHX	A	2003	-	-	-	X
84	OHX	A	2006	-	-	-	X
84	OHX	A	2009	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	A	2012	-	-	-	X
84	OHX	A	2013	-	-	-	X
84	OHX	A	2014	-	-	-	X
84	OHX	A	2015	-	-	-	X
84	OHX	A	2017	-	-	-	X
84	OHX	A	2018	-	-	-	X
84	OHX	A	2021	-	-	-	X
84	OHX	A	2024	-	-	X	-
84	OHX	A	2026	-	-	-	X
84	OHX	A	2030	-	-	-	X
84	OHX	A	2031	-	-	-	X
84	OHX	A	2035	-	-	-	X
84	OHX	A	2040	-	-	-	X
84	OHX	AC	101	-	-	-	X
84	OHX	AH	201	-	-	-	X
84	OHX	AM	101	-	-	-	X
84	OHX	AR	3401	-	-	-	X
84	OHX	AR	3402	-	-	-	X
84	OHX	AR	3403	-	-	-	X
84	OHX	AR	3404	-	-	-	X
84	OHX	AR	3405	-	-	-	X
84	OHX	AR	3406	-	-	-	X
84	OHX	AR	3407	-	-	-	X
84	OHX	AR	3408	-	-	-	X
84	OHX	AR	3409	-	-	-	X
84	OHX	AR	3410	-	-	-	X
84	OHX	AR	3411	-	-	-	X
84	OHX	AR	3412	-	-	-	X
84	OHX	AR	3413	-	-	-	X
84	OHX	AR	3414	-	-	-	X
84	OHX	AR	3415	-	-	-	X
84	OHX	AR	3416	-	-	-	X
84	OHX	AR	3417	-	-	-	X
84	OHX	AR	3418	-	-	-	X
84	OHX	AR	3420	-	-	-	X
84	OHX	AR	3421	-	-	-	X
84	OHX	AR	3422	-	-	-	X
84	OHX	AR	3423	-	-	-	X
84	OHX	AR	3424	-	-	-	X
84	OHX	AR	3425	-	-	-	X
84	OHX	AR	3426	-	-	-	X
84	OHX	AR	3427	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	AR	3431	-	-	-	X
84	OHX	AR	3432	-	-	-	X
84	OHX	AR	3439	-	-	-	X
84	OHX	AR	3443	-	-	X	-
84	OHX	AR	3455	-	-	-	X
84	OHX	AR	3459	-	-	-	X
84	OHX	AR	3493	-	-	-	X
84	OHX	AR	3496	-	-	-	X
84	OHX	AR	3501	-	-	-	X
84	OHX	AR	3511	-	-	X	-
84	OHX	AR	3520	-	-	-	X
84	OHX	AR	3521	-	-	X	X
84	OHX	AR	3524	-	-	-	X
84	OHX	AR	3543	-	-	-	X
84	OHX	AR	3547	-	-	-	X
84	OHX	AR	3552	-	-	-	X
84	OHX	AR	3561	-	-	-	X
84	OHX	AR	3566	-	-	-	X
84	OHX	AR	3568	-	-	-	X
84	OHX	AR	3570	-	-	-	X
84	OHX	AR	3573	-	-	-	X
84	OHX	AR	3575	-	-	-	X
84	OHX	AR	3576	-	-	-	X
84	OHX	AR	3579	-	-	-	X
84	OHX	AR	3582	-	-	-	X
84	OHX	AR	3588	-	-	-	X
84	OHX	AR	3590	-	-	-	X
84	OHX	AR	3592	-	-	-	X
84	OHX	AR	3596	-	-	-	X
84	OHX	AR	3599	-	-	-	X
84	OHX	AR	3600	-	-	-	X
84	OHX	AR	3601	-	-	-	X
84	OHX	AR	3603	-	-	-	X
84	OHX	AR	3606	-	-	-	X
84	OHX	AR	3607	-	-	-	X
84	OHX	AR	3610	-	-	-	X
84	OHX	AR	3612	-	-	-	X
84	OHX	AR	3613	-	-	-	X
84	OHX	AR	3616	-	-	-	X
84	OHX	AR	3617	-	-	-	X
84	OHX	AR	3619	-	-	-	X
84	OHX	AR	3625	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	AR	3626	-	-	-	X
84	OHX	AR	3632	-	-	-	X
84	OHX	AR	3636	-	-	-	X
84	OHX	AR	3638	-	-	-	X
84	OHX	AR	3640	-	-	-	X
84	OHX	AR	3641	-	-	-	X
84	OHX	AR	3643	-	-	-	X
84	OHX	AR	3644	-	-	-	X
84	OHX	AR	3645	-	-	-	X
84	OHX	AR	3646	-	-	-	X
84	OHX	AR	3648	-	-	-	X
84	OHX	AR	3652	-	-	-	X
84	OHX	AR	3653	-	-	-	X
84	OHX	AR	3654	-	-	-	X
84	OHX	AR	3657	-	-	-	X
84	OHX	AR	3658	-	-	-	X
84	OHX	AR	3659	-	-	-	X
84	OHX	AR	3660	-	-	-	X
84	OHX	AR	3661	-	-	-	X
84	OHX	AR	3663	-	-	-	X
84	OHX	AR	3667	-	-	-	X
84	OHX	AR	3668	-	-	-	X
84	OHX	AR	3671	-	-	-	X
84	OHX	AR	3672	-	-	-	X
84	OHX	AR	3677	-	-	-	X
84	OHX	AR	3683	-	-	-	X
84	OHX	AR	3684	-	-	-	X
84	OHX	AR	3685	-	-	-	X
84	OHX	AR	3688	-	-	-	X
84	OHX	AR	3689	-	-	-	X
84	OHX	AR	3690	-	-	-	X
84	OHX	AR	3691	-	-	-	X
84	OHX	AR	3693	-	-	-	X
84	OHX	AR	3695	-	-	-	X
84	OHX	AR	3696	-	-	X	-
84	OHX	AR	3698	-	-	X	X
84	OHX	AR	3699	-	-	-	X
84	OHX	AR	3700	-	-	-	X
84	OHX	AR	3703	-	-	-	X
84	OHX	AR	3705	-	-	-	X
84	OHX	AR	3709	-	-	-	X
84	OHX	AR	3712	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	AR	3714	-	-	-	X
84	OHX	AR	3715	-	-	X	X
84	OHX	AR	3717	-	-	-	X
84	OHX	AR	3721	-	-	-	X
84	OHX	AR	3722	-	-	-	X
84	OHX	AR	3726	-	-	-	X
84	OHX	AR	3728	-	-	-	X
84	OHX	AR	3729	-	-	-	X
84	OHX	AR	3731	-	-	X	-
84	OHX	AR	3732	-	-	-	X
84	OHX	AR	3735	-	-	-	X
84	OHX	AR	3736	-	-	-	X
84	OHX	AR	3737	-	-	-	X
84	OHX	AR	3743	-	-	-	X
84	OHX	AS	203	-	-	X	-
84	OHX	AS	210	-	-	X	-
84	OHX	AS	211	-	-	-	X
84	OHX	AT	201	-	-	-	X
84	OHX	AT	202	-	-	-	X
84	OHX	AT	208	-	-	-	X
84	OHX	AT	214	-	-	-	X
84	OHX	CV	201	-	-	-	X
84	OHX	K	201	-	-	-	X
84	OHX	M	201	-	-	-	X
84	OHX	c1	201	-	-	-	X
84	OHX	c4	201	-	-	-	X
84	OHX	d9	101	-	-	-	X
84	OHX	e	101	-	-	-	X
84	OHX	l	401	-	-	-	X
84	OHX	x	201	-	-	-	X
84	OHX	x	202	-	-	-	X
84	OHX	y	201	-	-	-	X
85	MG	1	3725	-	-	-	X
85	MG	1	3730	-	-	-	X
85	MG	1	3731	-	-	-	X
85	MG	1	3732	-	-	-	X
85	MG	1	3734	-	-	-	X
85	MG	1	3738	-	-	-	X
85	MG	1	3739	-	-	-	X
85	MG	1	3740	-	-	-	X
85	MG	1	3741	-	-	-	X
85	MG	1	3746	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	1	3748	-	-	-	X
85	MG	1	3756	-	-	-	X
85	MG	1	3760	-	-	-	X
85	MG	1	3764	-	-	-	X
85	MG	1	3778	-	-	-	X
85	MG	1	3779	-	-	-	X
85	MG	1	3783	-	-	-	X
85	MG	1	3793	-	-	-	X
85	MG	1	3795	-	-	-	X
85	MG	1	3796	-	-	-	X
85	MG	1	3798	-	-	-	X
85	MG	1	3799	-	-	-	X
85	MG	1	3801	-	-	-	X
85	MG	1	3809	-	-	-	X
85	MG	1	3819	-	-	-	X
85	MG	1	3822	-	-	-	X
85	MG	1	3823	-	-	-	X
85	MG	1	3828	-	-	-	X
85	MG	1	3829	-	-	-	X
85	MG	1	3833	-	-	-	X
85	MG	1	3836	-	-	-	X
85	MG	1	3837	-	-	-	X
85	MG	1	3841	-	-	-	X
85	MG	1	3843	-	-	-	X
85	MG	1	3845	-	-	-	X
85	MG	1	3846	-	-	-	X
85	MG	1	3856	-	-	-	X
85	MG	1	3858	-	-	-	X
85	MG	1	3859	-	-	-	X
85	MG	1	3860	-	-	-	X
85	MG	1	3866	-	-	-	X
85	MG	1	3867	-	-	-	X
85	MG	1	3868	-	-	-	X
85	MG	1	3869	-	-	-	X
85	MG	1	3871	-	-	-	X
85	MG	1	3875	-	-	-	X
85	MG	1	3876	-	-	-	X
85	MG	1	3879	-	-	-	X
85	MG	1	3882	-	-	-	X
85	MG	1	3884	-	-	-	X
85	MG	1	3885	-	-	-	X
85	MG	1	3886	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	1	3887	-	-	-	X
85	MG	1	3889	-	-	-	X
85	MG	1	3890	-	-	-	X
85	MG	1	3891	-	-	-	X
85	MG	1	3892	-	-	-	X
85	MG	1	3894	-	-	-	X
85	MG	1	3899	-	-	-	X
85	MG	1	3900	-	-	-	X
85	MG	1	3901	-	-	-	X
85	MG	1	3902	-	-	-	X
85	MG	1	3904	-	-	-	X
85	MG	1	3905	-	-	-	X
85	MG	1	3909	-	-	-	X
85	MG	1	3911	-	-	-	X
85	MG	1	3912	-	-	-	X
85	MG	1	3914	-	-	-	X
85	MG	1	3916	-	-	-	X
85	MG	1	3917	-	-	-	X
85	MG	1	3924	-	-	-	X
85	MG	1	3939	-	-	-	X
85	MG	1	3946	-	-	-	X
85	MG	1	3959	-	-	-	X
85	MG	1	3962	-	-	-	X
85	MG	1	3978	-	-	-	X
85	MG	1	3990	-	-	-	X
85	MG	1	4027	-	-	-	X
85	MG	1	4031	-	-	-	X
85	MG	1	4048	-	-	-	X
85	MG	1	4052	-	-	-	X
85	MG	1	4064	-	-	-	X
85	MG	1	4066	-	-	-	X
85	MG	1	4078	-	-	-	X
85	MG	1	4083	-	-	-	X
85	MG	1	4084	-	-	-	X
85	MG	1	4096	-	-	-	X
85	MG	1	4100	-	-	-	X
85	MG	1	4125	-	-	-	X
85	MG	1	4126	-	-	-	X
85	MG	1	4127	-	-	-	X
85	MG	1	4135	-	-	-	X
85	MG	1	4142	-	-	-	X
85	MG	1	4167	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	1	4168	-	-	-	X
85	MG	1	4186	-	-	-	X
85	MG	1	4188	-	-	-	X
85	MG	1	4189	-	-	-	X
85	MG	1	4193	-	-	-	X
85	MG	1	4195	-	-	-	X
85	MG	1	4196	-	-	-	X
85	MG	1	4204	-	-	-	X
85	MG	1	4207	-	-	-	X
85	MG	1	4208	-	-	-	X
85	MG	1	4215	-	-	-	X
85	MG	1	4222	-	-	-	X
85	MG	4	221	-	-	-	X
85	MG	4	224	-	-	-	X
85	MG	4	225	-	-	-	X
85	MG	4	227	-	-	-	X
85	MG	6	2053	-	-	-	X
85	MG	6	2057	-	-	-	X
85	MG	6	2059	-	-	-	X
85	MG	6	2061	-	-	-	X
85	MG	6	2068	-	-	-	X
85	MG	6	2071	-	-	-	X
85	MG	6	2077	-	-	-	X
85	MG	6	2078	-	-	-	X
85	MG	6	2082	-	-	-	X
85	MG	6	2086	-	-	-	X
85	MG	6	2088	-	-	-	X
85	MG	6	2091	-	-	-	X
85	MG	6	2093	-	-	-	X
85	MG	6	2098	-	-	-	X
85	MG	6	2099	-	-	-	X
85	MG	6	2103	-	-	-	X
85	MG	6	2107	-	-	-	X
85	MG	6	2108	-	-	-	X
85	MG	6	2116	-	-	-	X
85	MG	6	2122	-	-	-	X
85	MG	6	2125	-	-	-	X
85	MG	6	2140	-	-	-	X
85	MG	6	2144	-	-	-	X
85	MG	6	2154	-	-	-	X
85	MG	6	2155	-	-	-	X
85	MG	6	2158	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	6	2161	-	-	-	X
85	MG	6	2197	-	-	-	X
85	MG	A	2047	-	-	-	X
85	MG	A	2052	-	-	-	X
85	MG	A	2053	-	-	-	X
85	MG	A	2055	-	-	-	X
85	MG	A	2056	-	-	-	X
85	MG	A	2057	-	-	-	X
85	MG	A	2061	-	-	-	X
85	MG	A	2062	-	-	-	X
85	MG	A	2064	-	-	-	X
85	MG	A	2066	-	-	-	X
85	MG	A	2072	-	-	-	X
85	MG	A	2077	-	-	-	X
85	MG	A	2078	-	-	-	X
85	MG	A	2079	-	-	-	X
85	MG	A	2080	-	-	-	X
85	MG	A	2088	-	-	-	X
85	MG	A	2095	-	-	-	X
85	MG	A	2100	-	-	-	X
85	MG	A	2101	-	-	-	X
85	MG	A	2105	-	-	-	X
85	MG	A	2108	-	-	-	X
85	MG	A	2109	-	-	-	X
85	MG	A	2115	-	-	-	X
85	MG	A	2119	-	-	-	X
85	MG	A	2126	-	-	-	X
85	MG	A	2129	-	-	-	X
85	MG	A	2131	-	-	-	X
85	MG	A	2138	-	-	-	X
85	MG	A	2147	-	-	-	X
85	MG	A	2153	-	-	-	X
85	MG	A	2155	-	-	-	X
85	MG	AB	203	-	-	-	X
85	MG	AB	206	-	-	-	X
85	MG	AF	202	-	-	-	X
85	MG	AK	103	-	-	-	X
85	MG	AR	3747	-	-	-	X
85	MG	AR	3750	-	-	-	X
85	MG	AR	3751	-	-	-	X
85	MG	AR	3753	-	-	-	X
85	MG	AR	3756	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	AR	3757	-	-	-	X
85	MG	AR	3763	-	-	-	X
85	MG	AR	3764	-	-	-	X
85	MG	AR	3767	-	-	-	X
85	MG	AR	3772	-	-	-	X
85	MG	AR	3786	-	-	-	X
85	MG	AR	3790	-	-	-	X
85	MG	AR	3794	-	-	-	X
85	MG	AR	3801	-	-	-	X
85	MG	AR	3804	-	-	-	X
85	MG	AR	3809	-	-	-	X
85	MG	AR	3810	-	-	-	X
85	MG	AR	3814	-	-	-	X
85	MG	AR	3816	-	-	-	X
85	MG	AR	3819	-	-	-	X
85	MG	AR	3825	-	-	-	X
85	MG	AR	3826	-	-	-	X
85	MG	AR	3833	-	-	-	X
85	MG	AR	3841	-	-	-	X
85	MG	AR	3844	-	-	-	X
85	MG	AR	3848	-	-	-	X
85	MG	AR	3850	-	-	-	X
85	MG	AR	3853	-	-	-	X
85	MG	AR	3857	-	-	-	X
85	MG	AR	3859	-	-	-	X
85	MG	AR	3860	-	-	-	X
85	MG	AR	3863	-	-	-	X
85	MG	AR	3864	-	-	-	X
85	MG	AR	3865	-	-	-	X
85	MG	AR	3871	-	-	-	X
85	MG	AR	3873	-	-	-	X
85	MG	AR	3874	-	-	-	X
85	MG	AR	3879	-	-	-	X
85	MG	AR	3888	-	-	-	X
85	MG	AR	3893	-	-	-	X
85	MG	AR	3895	-	-	-	X
85	MG	AR	3896	-	-	-	X
85	MG	AR	3897	-	-	-	X
85	MG	AR	3901	-	-	-	X
85	MG	AR	3904	-	-	-	X
85	MG	AR	3905	-	-	-	X
85	MG	AR	3906	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	AR	3909	-	-	-	X
85	MG	AR	3910	-	-	-	X
85	MG	AR	3912	-	-	-	X
85	MG	AR	3913	-	-	-	X
85	MG	AR	3914	-	-	-	X
85	MG	AR	3915	-	-	-	X
85	MG	AR	3918	-	-	-	X
85	MG	AR	3919	-	-	-	X
85	MG	AR	3926	-	-	-	X
85	MG	AR	3930	-	-	-	X
85	MG	AR	3933	-	-	-	X
85	MG	AR	3934	-	-	-	X
85	MG	AR	3936	-	-	-	X
85	MG	AR	3937	-	-	-	X
85	MG	AR	3938	-	-	-	X
85	MG	AR	3939	-	-	-	X
85	MG	AR	3940	-	-	-	X
85	MG	AR	3941	-	-	-	X
85	MG	AR	3942	-	-	-	X
85	MG	AR	3950	-	-	-	X
85	MG	AR	3961	-	-	-	X
85	MG	AR	3964	-	-	-	X
85	MG	AR	3966	-	-	-	X
85	MG	AR	3977	-	-	-	X
85	MG	AR	3978	-	-	-	X
85	MG	AR	3985	-	-	-	X
85	MG	AR	3987	-	-	-	X
85	MG	AR	3993	-	-	-	X
85	MG	AR	3994	-	-	-	X
85	MG	AR	4002	-	-	-	X
85	MG	AR	4007	-	-	-	X
85	MG	AR	4012	-	-	-	X
85	MG	AR	4019	-	-	-	X
85	MG	AR	4024	-	-	-	X
85	MG	AR	4034	-	-	-	X
85	MG	AR	4038	-	-	-	X
85	MG	AR	4041	-	-	-	X
85	MG	AR	4051	-	-	-	X
85	MG	AR	4075	-	-	-	X
85	MG	AR	4080	-	-	-	X
85	MG	AR	4082	-	-	-	X
85	MG	AR	4083	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	AR	4090	-	-	-	X
85	MG	AR	4091	-	-	-	X
85	MG	AR	4102	-	-	-	X
85	MG	AR	4111	-	-	-	X
85	MG	AR	4114	-	-	-	X
85	MG	AR	4138	-	-	-	X
85	MG	AR	4140	-	-	-	X
85	MG	AR	4141	-	-	-	X
85	MG	AR	4155	-	-	-	X
85	MG	AR	4161	-	-	-	X
85	MG	AR	4169	-	-	-	X
85	MG	AR	4179	-	-	-	X
85	MG	AR	4188	-	-	-	X
85	MG	AR	4189	-	-	-	X
85	MG	AR	4198	-	-	-	X
85	MG	AR	4202	-	-	-	X
85	MG	AR	4203	-	-	-	X
85	MG	AR	4206	-	-	-	X
85	MG	AR	4226	-	-	-	X
85	MG	AR	4227	-	-	-	X
85	MG	AR	4228	-	-	-	X
85	MG	AR	4230	-	-	-	X
85	MG	AR	4241	-	-	-	X
85	MG	AR	4247	-	-	-	X
85	MG	AR	4249	-	-	-	X
85	MG	AR	4252	-	-	-	X
85	MG	AT	218	-	-	-	X
85	MG	AT	221	-	-	-	X
85	MG	AT	230	-	-	-	X
85	MG	CD	301	-	-	-	X
85	MG	CD	302	-	-	-	X
85	MG	CE	404	-	-	-	X
85	MG	CE	405	-	-	-	X
85	MG	CE	407	-	-	-	X
85	MG	CI	301	-	-	-	X
85	MG	CP	502	-	-	-	X
85	MG	CQ	202	-	-	-	X
85	MG	CR	201	-	-	-	X
85	MG	CR	205	-	-	-	X
85	MG	CU	201	-	-	-	X
85	MG	CX	203	-	-	-	X
85	MG	DC	202	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	DH	203	-	-	-	X
85	MG	F	301	-	-	-	X
85	MG	b	101	-	-	-	X
85	MG	c1	202	-	-	-	X
85	MG	c8	202	-	-	-	X
85	MG	d3	202	-	-	-	X
85	MG	d6	102	-	-	-	X
85	MG	k	404	-	-	-	X
85	MG	l	404	-	-	-	X
85	MG	r	302	-	-	-	X
85	MG	s8	302	-	-	-	X
85	MG	sM	202	-	-	-	X
85	MG	v	302	-	-	-	X
85	MG	w	202	-	-	-	X
85	MG	x	204	-	-	-	X
85	MG	x	205	-	-	-	X
85	MG	x	208	-	-	-	X
85	MG	x	209	-	-	-	X
86	HN8	1	4223	-	-	-	X
86	HN8	AR	4263	-	-	-	X
87	GOL	A	2160	-	-	-	X
87	GOL	AR	4261	-	-	-	X
87	GOL	v	305	-	-	-	X
88	ZN	d7	101	-	-	-	X

## 2 Entry composition [i](#)

There are 88 unique types of molecules in this entry. The entry contains 410383 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	IR	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 RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	6	1783	Total	C	N	O	P	0	0	0
			37990	16984	6723	12500	1783			
25	A	1781	Total	C	N	O	P	0	0	0
			37948	16965	6715	12487	1781			

- Molecule 26 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	7	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			

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

- Molecule 27 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	8	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			
27	CZ	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			

- Molecule 28 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	9	126	Total	C	N	O		0	0	0
			993	625	192	176				
28	DA	126	Total	C	N	O		0	0	0
			993	625	192	176				

- Molecule 29 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 30 is a protein called 60S ribosomal protein L28.

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

- Molecule 31 is a protein called 60S ribosomal protein L29.

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

- Molecule 32 is a protein called 60S ribosomal protein L30.

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

- Molecule 33 is a protein called 60S ribosomal protein L31-A.

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

- Molecule 34 is a protein called 60S ribosomal protein L32.

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

- Molecule 35 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 36 is a protein called 60S ribosomal protein L34-A.

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

- Molecule 37 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 38 is a protein called 60S ribosomal protein L36-A.

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

- Molecule 39 is a protein called 60S ribosomal protein L37-A.

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

- Molecule 40 is a protein called 60S ribosomal protein L38.

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

- Molecule 41 is a protein called 60S ribosomal protein L39.

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

- Molecule 42 is a protein called Ubiquitin-60S ribosomal protein L40.

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

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

- Molecule 43 is a protein called 60S ribosomal protein L41-B.

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

- Molecule 44 is a protein called 60S ribosomal protein L42-A.

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

- Molecule 45 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 46 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	i	159	Total	C	N	O	0	0	0
			1104	652	221	231			

- Molecule 47 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	m2	150	Total	C	N	O	0	0	0
			750	450	150	150			

- Molecule 48 is a protein called Suppressor protein STM1,Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	sM	104	Total	C	N	O			
			680	403	140	137	0	0	0

- Molecule 49 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	p0	143	Total	C	N	O	S			
			1076	686	192	195	3	0	0	0

- Molecule 50 is a protein called 40S ribosomal protein S0-A.

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

- Molecule 51 is a protein called 40S ribosomal protein S1-A.

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

- Molecule 52 is a protein called 40S ribosomal protein S2.

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

- Molecule 53 is a protein called 40S ribosomal protein S3.

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

- Molecule 54 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 55 is a protein called 40S ribosomal protein S5.

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

- Molecule 56 is a protein called 40S ribosomal protein S6-A.

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

- Molecule 57 is a protein called 40S ribosomal protein S7-A.

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

- Molecule 58 is a protein called 40S ribosomal protein S8-A.

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

- Molecule 59 is a protein called 40S ribosomal protein S9-A.

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

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

- Molecule 60 is a protein called 40S ribosomal protein S10-A.

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

- Molecule 61 is a protein called 40S ribosomal protein S11-A.

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

- Molecule 62 is a protein called 40S ribosomal protein S12.

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

- Molecule 63 is a protein called 40S ribosomal protein S13.

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

- Molecule 64 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	P	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			
64	c4	128	Total	C	N	O	S	0	0	0
			949	582	188	176	3			

- Molecule 65 is a protein called 40S ribosomal protein S15.

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

- Molecule 66 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 67 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	S	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			
67	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

- Molecule 68 is a protein called 40S ribosomal protein S18-A.

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

- Molecule 69 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 70 is a protein called 40S ribosomal protein S20.

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

- Molecule 71 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 72 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 73 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 74 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 75 is a protein called 40S ribosomal protein S25-A.

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

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

- Molecule 76 is a protein called 40S ribosomal protein S26-B.

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

- Molecule 77 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 78 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 79 is a protein called 40S ribosomal protein S29-A.

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

- Molecule 80 is a protein called 40S ribosomal protein S30-A.

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

- Molecule 81 is a protein called Ubiquitin-40S ribosomal protein S31.

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

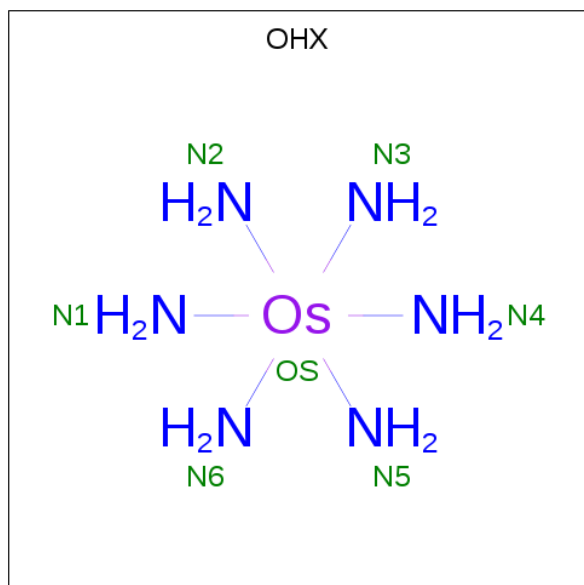
- Molecule 82 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	h	318	Total	C	N	O	S	0	0	0
			2441	1544	419	470	8			
82	sR	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- 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		

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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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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		
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
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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
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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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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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			7	6	1		
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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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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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
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84	4	1	Total	N	Os	0	0
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84	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	2	1	Total	N	Os	0	0
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84	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	6	1	Total	N	Os	0	0
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84	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	6	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	6	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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84	AP	1	Total	N	Os	0	0
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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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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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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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84	AR	1	Total	N	Os	0	0
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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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84	AR	1	Total	N	Os	0	0
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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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84	AR	1	Total	N	Os	0	0
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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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84	AR	1	Total	N	Os	0	0
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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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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
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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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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	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
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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
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			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
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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		

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AR	1	Total	N	Os	0	0
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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
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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
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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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			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
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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		
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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
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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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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	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
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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
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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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84	AR	1	Total	N	Os	0	0
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			7	6	1		
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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		
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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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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
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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		
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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		
84	AS	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
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84	AS	1	Total	N	Os	0	0
			7	6	1		
84	AS	1	Total	N	Os	0	0
			7	6	1		
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84	AS	1	Total	N	Os	0	0
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84	AS	1	Total	N	Os	0	0
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84	AT	1	Total	N	Os	0	0
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84	AT	1	Total	N	Os	0	0
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84	AT	1	Total	N	Os	0	0
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			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	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
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84	AT	1	Total	N	Os	0	0
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84	CE	1	Total	N	Os	0	0
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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
			7	6	1		
84	CG	1	Total	N	Os	0	0
			7	6	1		
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	CM	1	Total	N	Os	0	0
			7	6	1		
84	CP	1	Total	N	Os	0	0
			7	6	1		
84	CV	1	Total	N	Os	0	0
			7	6	1		
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	DQ	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		
84	A	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			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		

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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	J	1	Total	N	Os	0	0
			7	6	1		
84	K	1	Total	N	Os	0	0
			7	6	1		
84	M	1	Total	N	Os	0	0
			7	6	1		
84	O	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	Q	1	Total	N	Os	0	0
			7	6	1		
84	T	1	Total	N	Os	0	0
			7	6	1		
84	e	1	Total	N	Os	0	0
			7	6	1		
84	h	1	Total	N	Os	0	0
			7	6	1		
84	s8	1	Total	N	Os	0	0
			7	6	1		
84	c1	1	Total	N	Os	0	0
			7	6	1		
84	c3	1	Total	N	Os	0	0
			7	6	1		
84	c4	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		
84	d9	1	Total	N	Os	0	0
			7	6	1		
84	sR	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	DQ	2	Total	Mg	0	0
			2	2		
85	AB	7	Total	Mg	0	0
			7	7		
85	c6	1	Total	Mg	0	0
			1	1		
85	6	146	Total	Mg	0	0
			146	146		
85	DO	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	sM	2	Total 2	Mg 2	0	0
85	d5	1	Total 1	Mg 1	0	0
85	t	3	Total 3	Mg 3	0	0
85	CD	2	Total 2	Mg 2	0	0
85	lR	1	Total 1	Mg 1	0	0
85	CR	5	Total 5	Mg 5	0	0
85	o	2	Total 2	Mg 2	0	0
85	DC	4	Total 4	Mg 4	0	0
85	AS	20	Total 20	Mg 20	0	0
85	DH	2	Total 2	Mg 2	0	0
85	c9	1	Total 1	Mg 1	0	0
85	k	3	Total 3	Mg 3	0	0
85	CO	1	Total 1	Mg 1	0	0
85	CU	1	Total 1	Mg 1	0	0
85	b	1	Total 1	Mg 1	0	0
85	DL	1	Total 1	Mg 1	0	0
85	V	1	Total 1	Mg 1	0	0
85	c8	1	Total 1	Mg 1	0	0
85	w	2	Total 2	Mg 2	0	0
85	CK	1	Total 1	Mg 1	0	0
85	CQ	4	Total 4	Mg 4	0	0

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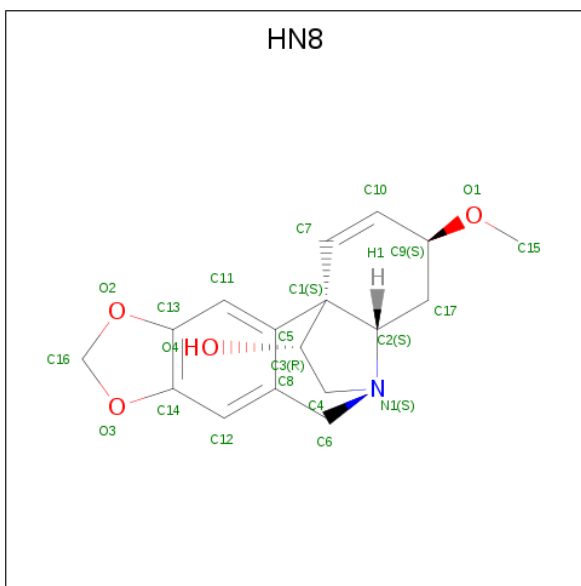
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	n	1	Total 1	Mg 1	0	0
85	x	7	Total 7	Mg 7	0	0
85	T	1	Total 1	Mg 1	0	0
85	AR	515	Total 515	Mg 515	0	0
85	d6	2	Total 2	Mg 2	0	0
85	s6	1	Total 1	Mg 1	0	0
85	s	1	Total 1	Mg 1	0	0
85	DI	2	Total 2	Mg 2	0	0
85	CG	2	Total 2	Mg 2	0	0
85	j	2	Total 2	Mg 2	0	0
85	1	498	Total 498	Mg 498	0	0
85	D	1	Total 1	Mg 1	0	0
85	CM	2	Total 2	Mg 2	0	0
85	d3	2	Total 2	Mg 2	0	0
85	c1	1	Total 1	Mg 1	0	0
85	v	3	Total 3	Mg 3	0	0
85	CJ	1	Total 1	Mg 1	0	0
85	A	116	Total 116	Mg 116	0	0
85	CP	4	Total 4	Mg 4	0	0
85	4	25	Total 25	Mg 25	0	0
85	DA	2	Total 2	Mg 2	0	0

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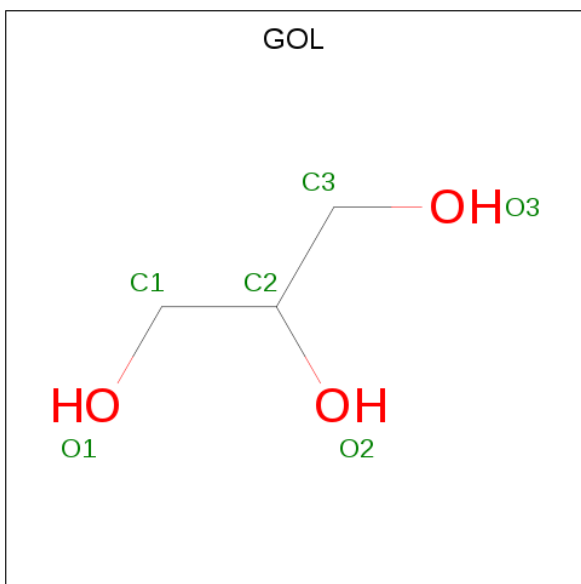
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	U	1	Total 1	Mg 1	0	0
85	r	1	Total 1	Mg 1	0	0
85	CF	1	Total 1	Mg 1	0	0
85	CX	2	Total 2	Mg 2	0	0
85	AG	1	Total 1	Mg 1	0	0
85	DE	1	Total 1	Mg 1	0	0
85	AH	1	Total 1	Mg 1	0	0
85	F	1	Total 1	Mg 1	0	0
85	s8	1	Total 1	Mg 1	0	0
85	CI	1	Total 1	Mg 1	0	0
85	d4	1	Total 1	Mg 1	0	0
85	H	1	Total 1	Mg 1	0	0
85	z	1	Total 1	Mg 1	0	0
85	AT	14	Total 14	Mg 14	0	0
85	CL	1	Total 1	Mg 1	0	0
85	s4	1	Total 1	Mg 1	0	0
85	CE	5	Total 5	Mg 5	0	0
85	Y	1	Total 1	Mg 1	0	0
85	l	3	Total 3	Mg 3	0	0
85	3	13	Total 13	Mg 13	0	0
85	AF	2	Total 2	Mg 2	0	0

- Molecule 86 is Haemanthamine (three-letter code: HN8) (formula:  $C_{17}H_{19}NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
86	1	1	Total	C	N	O	0	0
			22	17	1	4		
86	AR	1	Total	C	N	O	0	0
			22	17	1	4		

- Molecule 87 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	v	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	6	1	Total	C	O	0	0
			6	3	3		
87	AR	1	Total	C	O	0	0
			6	3	3		
87	AR	1	Total	C	O	0	0
			6	3	3		
87	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	AP	1	Total	Zn	0	0
			1	1		
88	g	1	Total	Zn	0	0
			1	1		
88	AQ	1	Total	Zn	0	0
			1	1		
88	AK	1	Total	Zn	0	0
			1	1		
88	DQ	1	Total	Zn	0	0
			1	1		
88	e	1	Total	Zn	0	0
			1	1		
88	b	1	Total	Zn	0	0
			1	1		
88	e1	1	Total	Zn	0	0
			1	1		
88	c	1	Total	Zn	0	0
			1	1		
88	DL	1	Total	Zn	0	0
			1	1		
88	d9	1	Total	Zn	0	0
			1	1		
88	DR	1	Total	Zn	0	0
			1	1		
88	DO	1	Total	Zn	0	0
			1	1		
88	AN	1	Total	Zn	0	0
			1	1		
88	d7	1	Total	Zn	0	0
			1	1		

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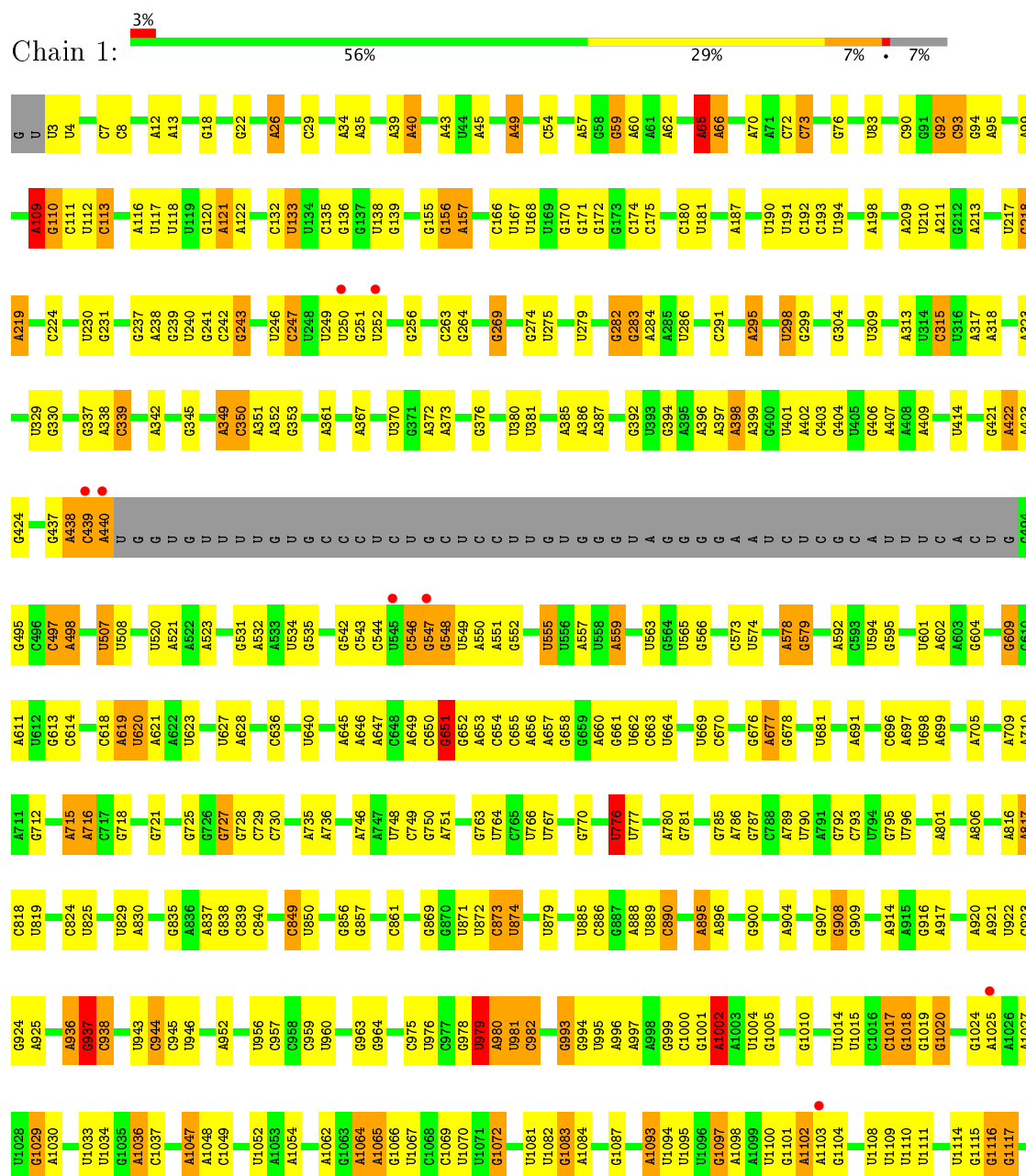
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	d6	1	Total	Zn	0	0
			1	1		

### 3 Residue-property plots [i](#)

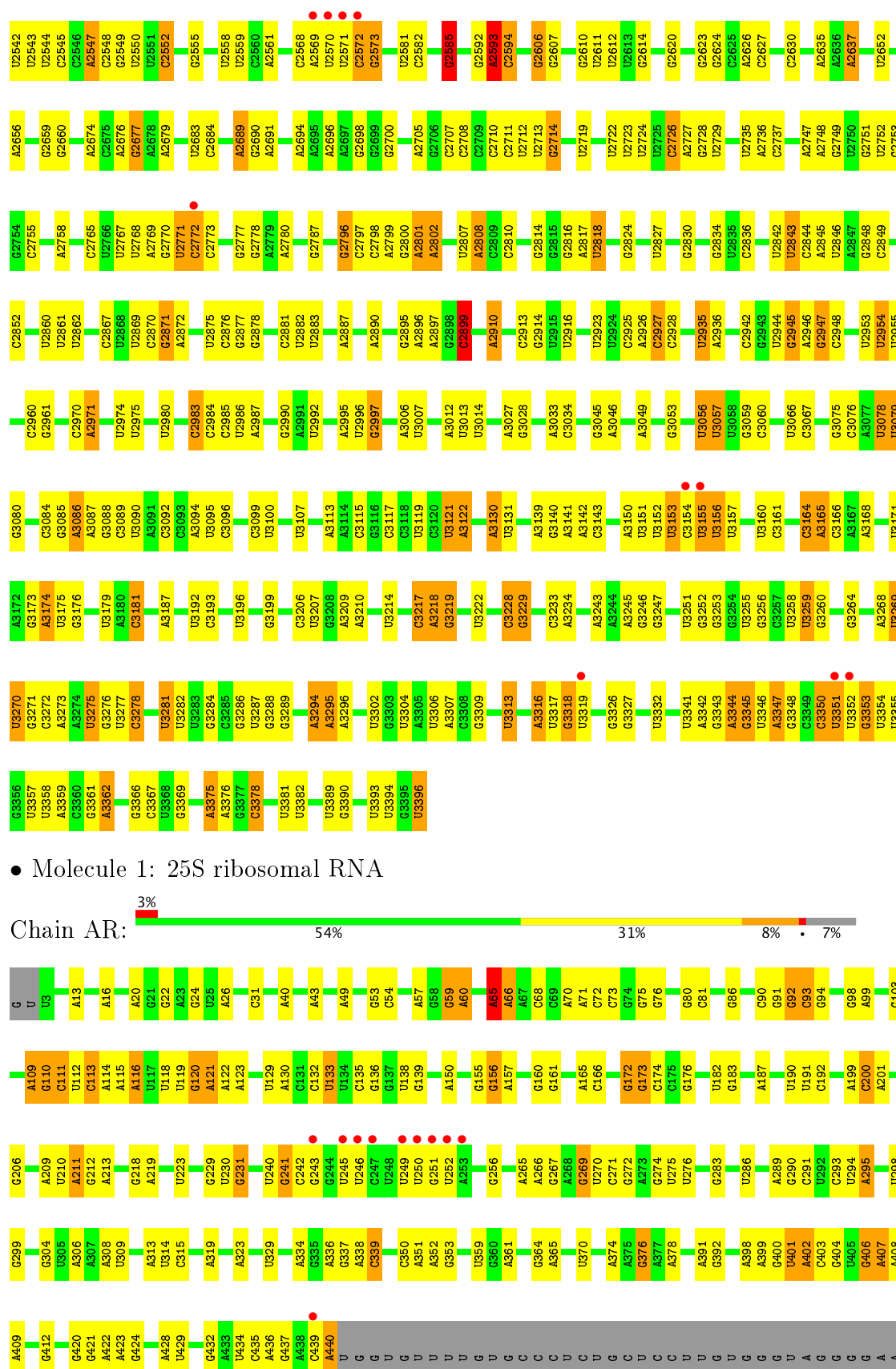
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



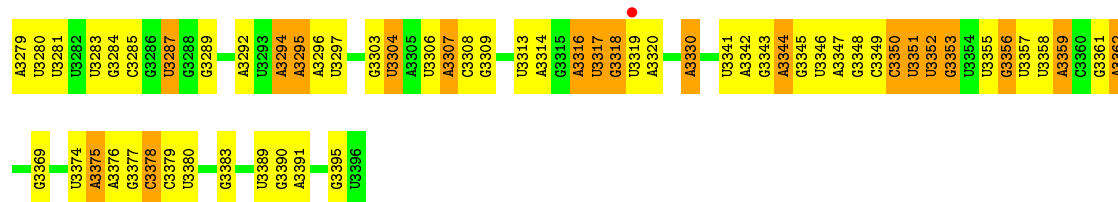






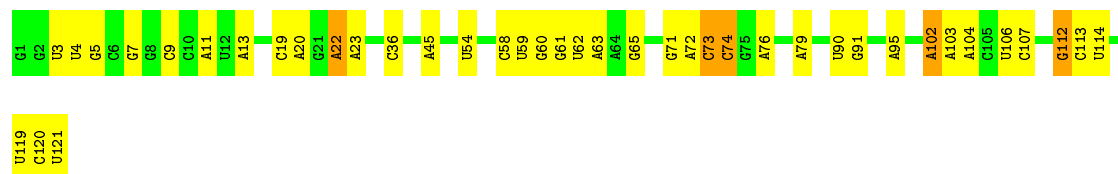
G1838	U1742	U1641	G1561	U1436	G1145	U1039	U956	G867	C758	G644	U558	U
A1839	U1746	A1642	C1562	C1437	G1149	A1040	C957	C868	G763	C548	A559	C
U1840	U1750	A1643	U1564	U1439	A1150	U1042	C958	C873	U764	A649	U563	U
A1841	A1751	U1645	G1565	U1445	U1151	C1043	U960	U874	C765	C850	U567	G
A1842	G1751	C1657	A1566	A1446	G1152	A1047	G964	G878	U766	G651	G567	C
C1846	G1758	G1658	U1567	G1447	A1153	A1048	U976	U879	U767	G652	G568	A
A1847	C1759	U1659	U1568	G1448	A1154	C1049	U977	G880	U776	A653	U578	U
C1848	U1762	C1660	U1570	G1450	G1155	U1049	C977	C881	U777	C854	G579	U
A1858	U1763	G1661	A1571	U1451	U1156	A1062	G978	G887	U778	A656	A585	C
U1861	U1764	G1662	U1572	A1452	A1157	G1063	U979	A888	G779	G657	C586	A
U1862	U1765	C1663	G1573	U1453	A1158	A1064	A980	A889	A780	G658	U587	C
U1863	G1766	G1674	C1574	A1456	A1159	A1065	U981	G894	G781	G659	G588	U
G1866	C1767	A1676	A1575	G1464	G1171	G1066	C982	G895	U782	A660	A589	G
A1874	G1769	A1677	G1576	G1465	G1172	A1072	A983	A896	G785	U662	G495	G
U1878	G1770	U1682	U1577	U1471	G1174	C1076	U984	A897	A786	C663	C496	C
A1879	G1780	U1688	C1578	U1472	G1178	U1080	U985	U898	G787	U664	C497	C
A1886	U1783	U1689	U1579	U1473	A1179	A1082	U986	U899	G788	A665	A498	C
U1887	G1784	A1689	A1580	U1474	U1181	A1083	U990	G900	U790	C670	G594	G
U1888	U1785	A1696	A1581	G1374	A1184	U1084	G993	A904	U794	U673	G600	U
G1889	G1786	U1697	U1582	G1375	C1185	A1093	G994	U905	G795	A677	U601	U
U1893	A1787	U1702	G1583	U1367	A1190	U1094	U995	G907	G799	A678	A602	G
U1894	C1788	U1703	U1584	U1368	U1191	U1095	A996	G908	G800	U681	A603	U
A1895	G1794	U1704	C1585	U1369	C1192	G1097	U997	G910	G805	U682	U508	U
U1906	U1797	C1706	A1586	A1366	A1193	A1098	C1000	G912	A806	G685	A607	U
C1907	A1798	A1707	G1587	A1367	C1196	G1101	G1001	A913	U814	G686	A608	U
A1908	U1799	U1708	U1588	U1368	U1197	A1102	A1002	A914	U815	U687	G609	A
U1909	G1800	U1709	A1589	U1369	C1201	A1103	A1003	A915	G816	A692	G610	G
A1910	A1801	G1712	A1590	A1370	A1202	G1104	A1006	A917	A817	U705	A611	U
U1911	U1802	U1713	G1591	G1306	G1209	U1108	G1010	A821	C818	A709	G617	U
U1912	A1803	A1714	U1592	G1307	A1212	U1109	U1014	U922	U819	U709	C618	U
A1913	U1804	A1715	C1593	A1308	G1213	U1110	U1015	C923	C823	A619	U620	U
G1914	U1805	U1716	A1594	U1309	U1214	U1111	C1016	G924	C824	G712	A621	U
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U1916	G1807	G1718	G1596	G1311	C1216	G1117	G1018	A926	U826	A716	U623	U
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C1932	A1814	A1720	C1598	A1317	G1221	U1129	G1020	A836	U836	G718	G625	G
A1933	U1815	U1721	U1599	A1318	G1222	A1130	G1021	A837	U837	G721	U626	U
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U1937	U1817	U1726	U1601	U1320	C1232	G1132	A1025	U939	U839	U723	U629	U
G1940	U1820	G1727	G1543	U1329	U1235	G1133	U1028	G940	A847	A630	G547	U
U1941	A1821	U1728	U1544	U1330	G1236	A1134	G1029	G941	A848	C634	G548	U
U1942	G1827	U1729	U1545	U1331	G1237	A1135	U1030	U942	U850	G635	U549	U
U1943	A1828	U1730	C1546	U1332	C1238	A1136	C1031	U943	C851	C636	A550	U
U1944	G1833	U1731	U1547	A1337	G1239	G1139	U1032	C945	C734	C637	A551	U
A1945	U1834	U1732	U1548	U1338	A1240	U1140	U1033	U946	A735	G638	G552	U
U1946	U1835	A1741	U1549	G1340	U1241	C1141	A1036	G953	G860	C743	U555	U
			U1550	U1341	G1242	A1142	C1037	U954	C861	A744	U556	U
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			U1560	G1345	A1244	U1144						





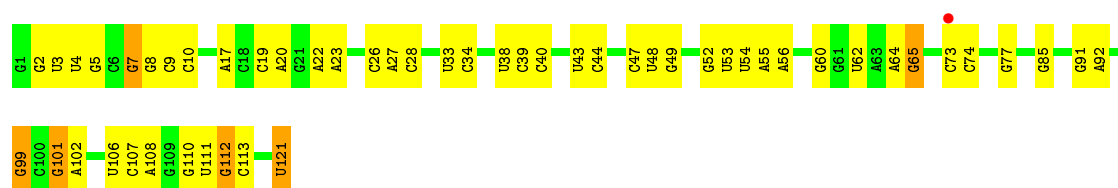
• Molecule 2: 5S ribosomal RNA

Chain 3: 66% 30% .



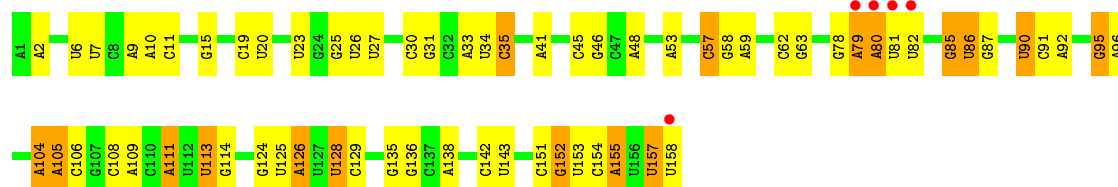
• Molecule 2: 5S ribosomal RNA

Chain AS: 57% 38% 5%



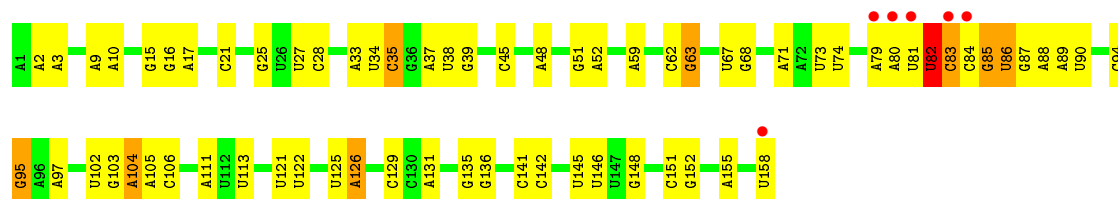
• Molecule 3: 5.8S ribosomal RNA

Chain 4: 58% 31% 11%



• Molecule 3: 5.8S ribosomal RNA

Chain AT: 57% 37% 5%

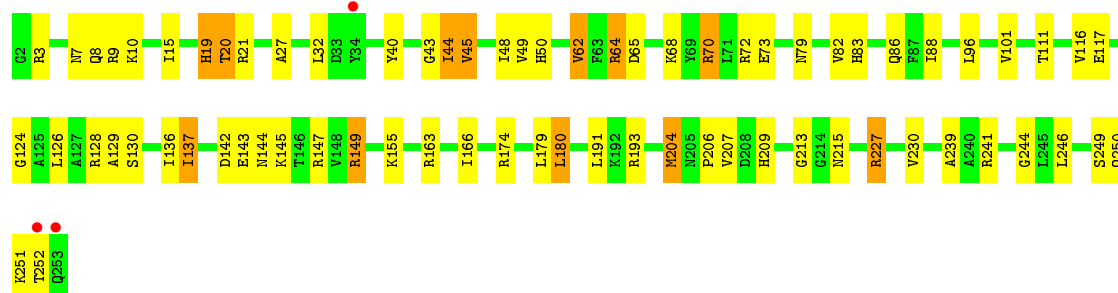
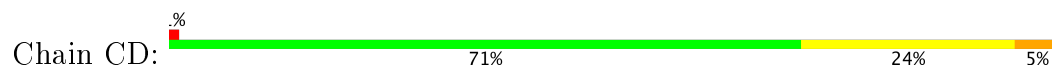


• Molecule 4: 60S ribosomal protein L2-A

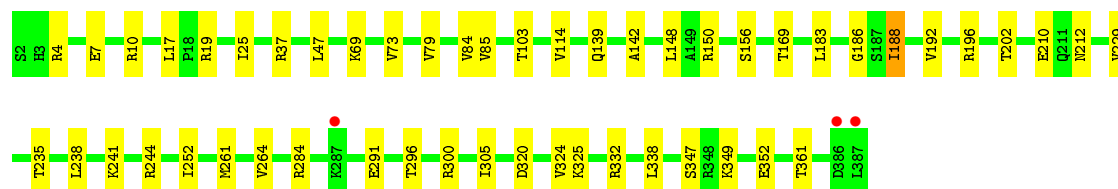
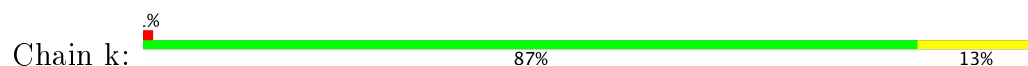
Chain j: 89% 11%



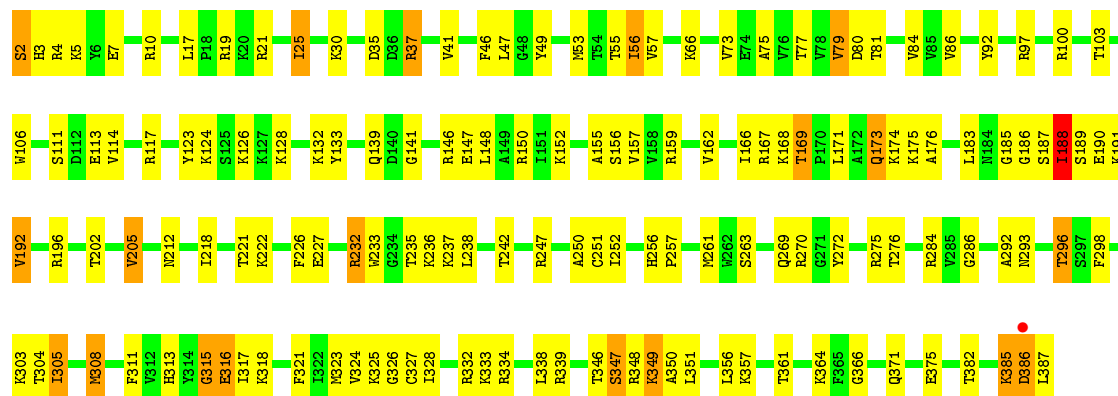
- Molecule 4: 60S ribosomal protein L2-A



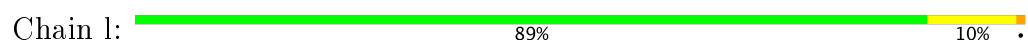
- Molecule 5: 60S ribosomal protein L3



- Molecule 5: 60S ribosomal protein L3



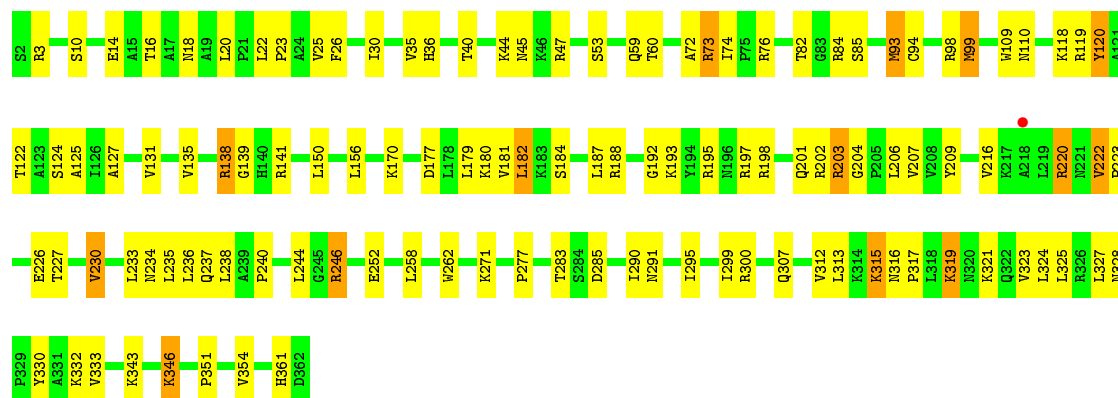
- Molecule 6: 60S ribosomal protein L4-A





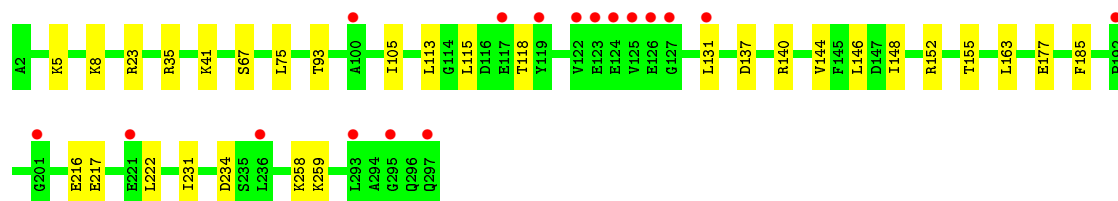
• Molecule 6: 60S ribosomal protein L4-A

Chain CF: 68% 29%



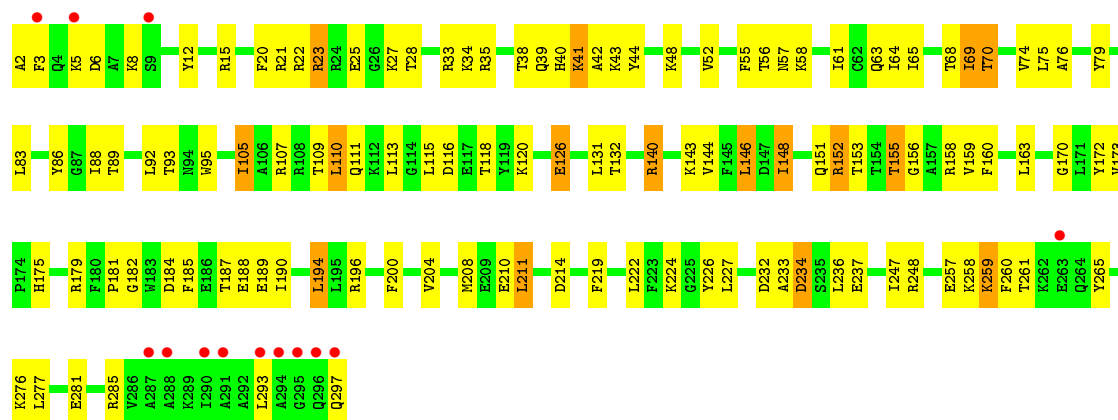
• Molecule 7: 60S ribosomal protein L5

Chain m: 6% 90% 10%



• Molecule 7: 60S ribosomal protein L5

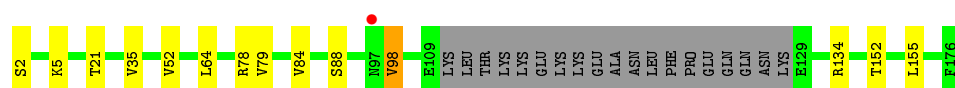
Chain CG: 4% 59% 35% 5%



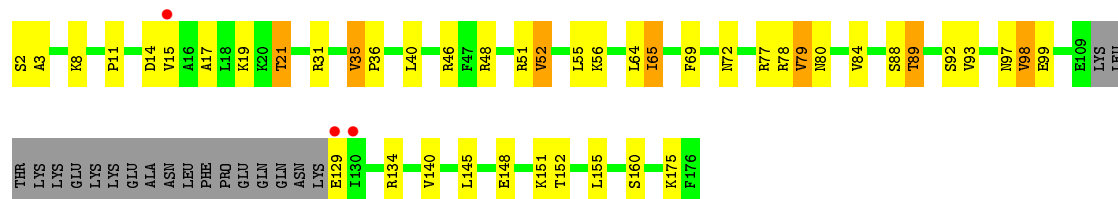
• Molecule 8: 60S ribosomal protein L6-A

Chain n: 81% 7% 11%

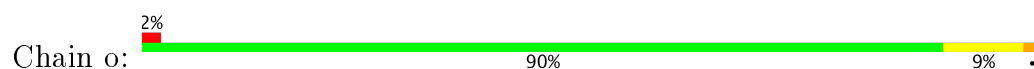




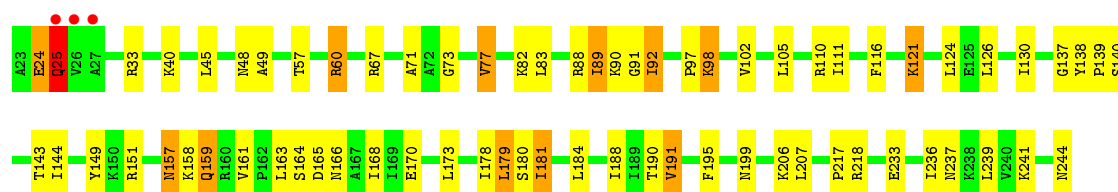
- Molecule 8: 60S ribosomal protein L6-A



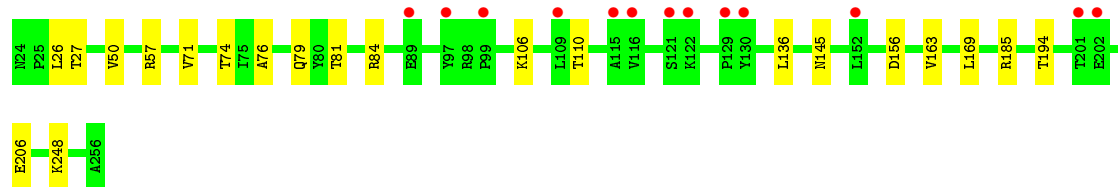
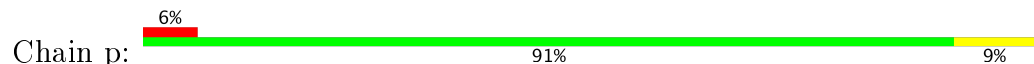
- Molecule 9: 60S ribosomal protein L7-A



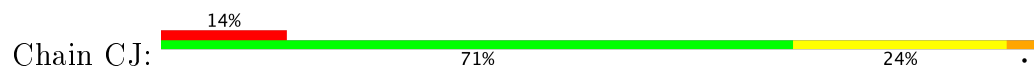
- Molecule 9: 60S ribosomal protein L7-A

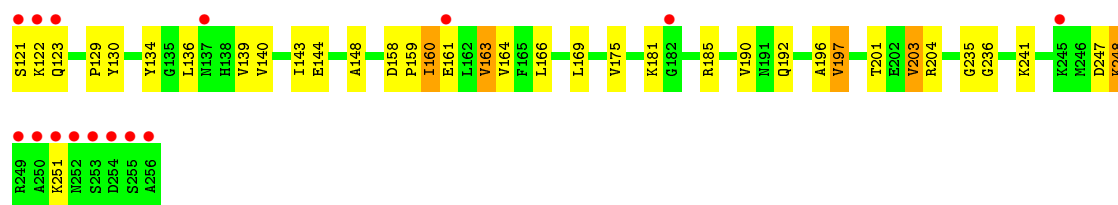


- Molecule 10: 60S ribosomal protein L8-A



- Molecule 10: 60S ribosomal protein L8-A





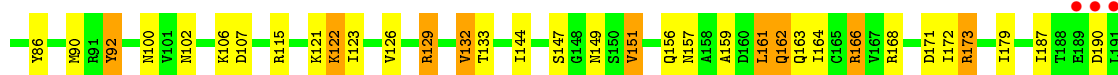
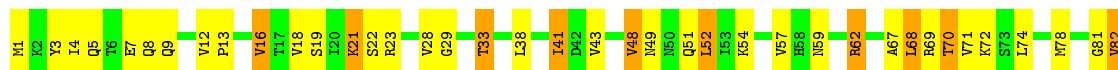
- Molecule 11: 60S ribosomal protein L9-A

Chain q: 87% 13%



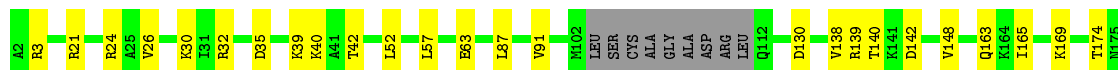
- Molecule 11: 60S ribosomal protein L9-A

Chain CK: 2% 62% 28% 10%



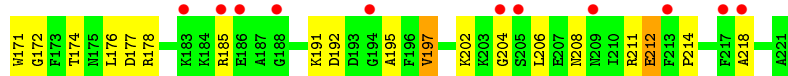
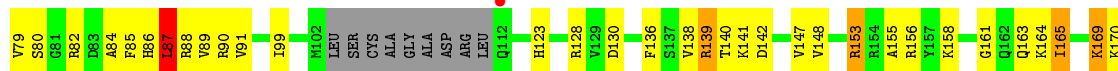
- Molecule 12: 60S ribosomal protein L10

Chain r: 82% 14%



- Molecule 12: 60S ribosomal protein L10

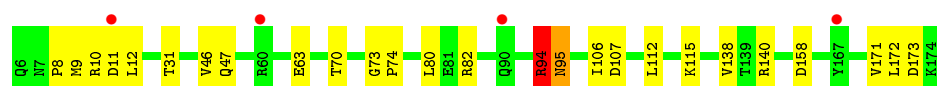
Chain CL: 5% 55% 34% 6%



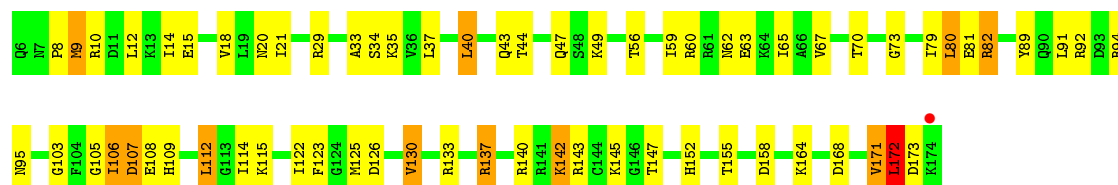
- Molecule 13: 60S ribosomal protein L11-B

Chain s: 2% 85% 14%

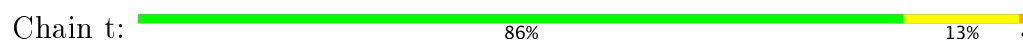




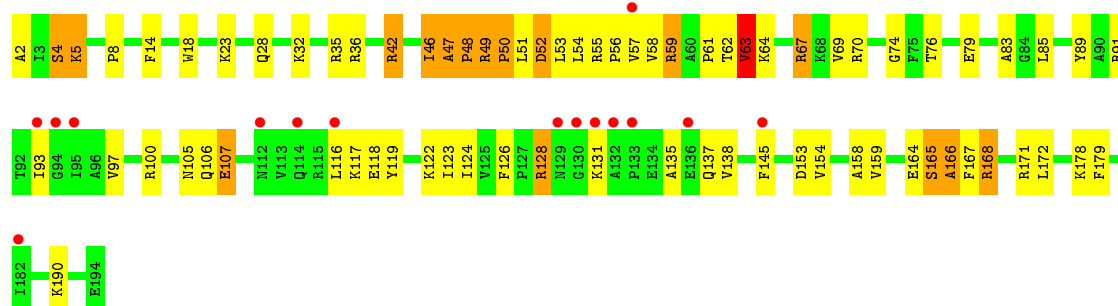
- Molecule 13: 60S ribosomal protein L11-B



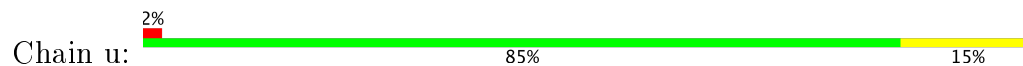
- Molecule 14: 60S ribosomal protein L13-A



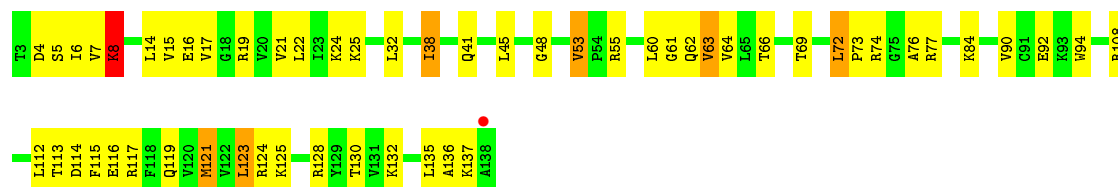
- Molecule 14: 60S ribosomal protein L13-A



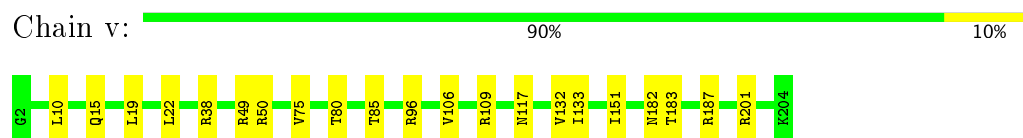
- Molecule 15: 60S ribosomal protein L14-A



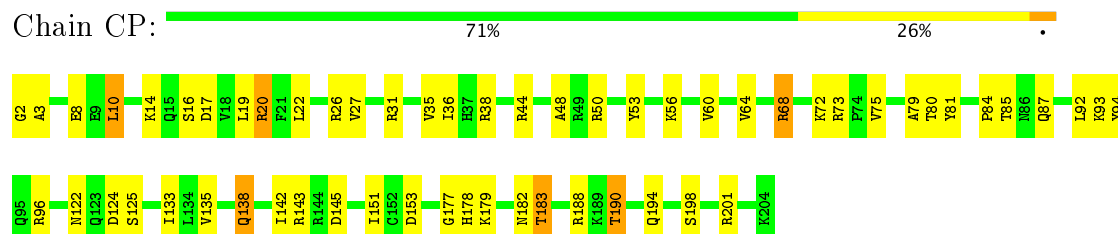
- Molecule 15: 60S ribosomal protein L14-A



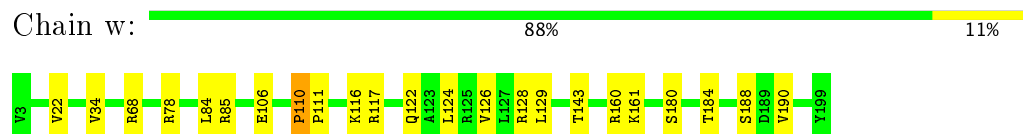
- Molecule 16: 60S ribosomal protein L15-A



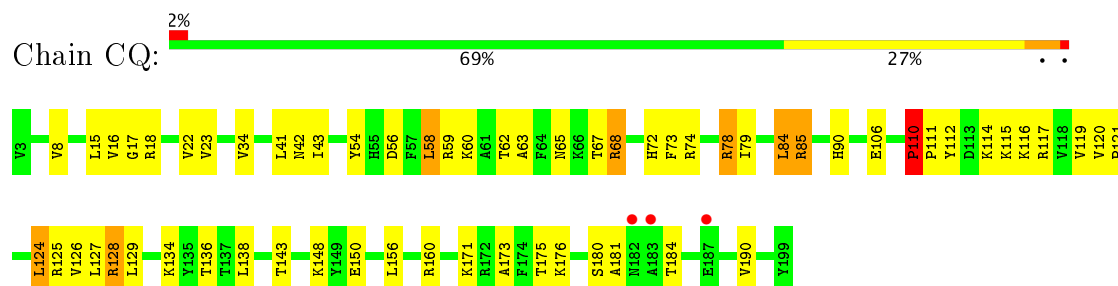
- Molecule 16: 60S ribosomal protein L15-A



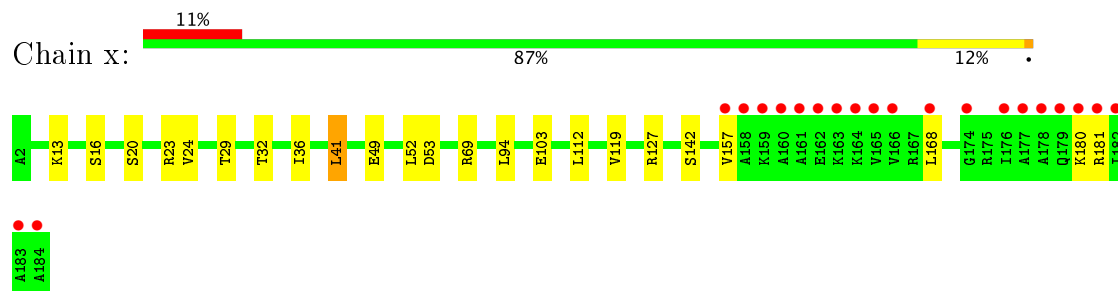
- Molecule 17: 60S ribosomal protein L16-A



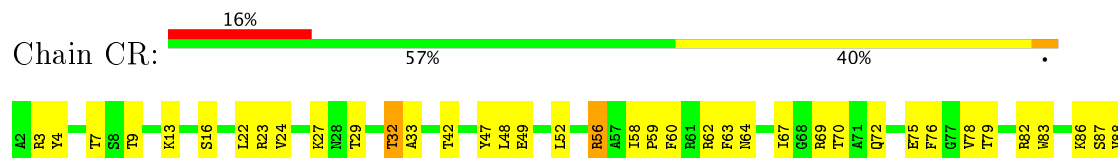
- Molecule 17: 60S ribosomal protein L16-A

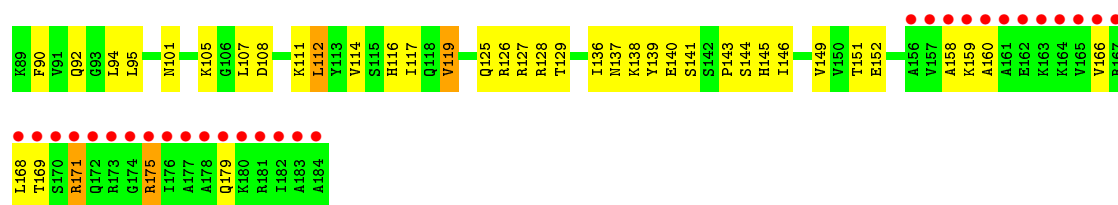


- Molecule 18: 60S ribosomal protein L17-A



- Molecule 18: 60S ribosomal protein L17-A





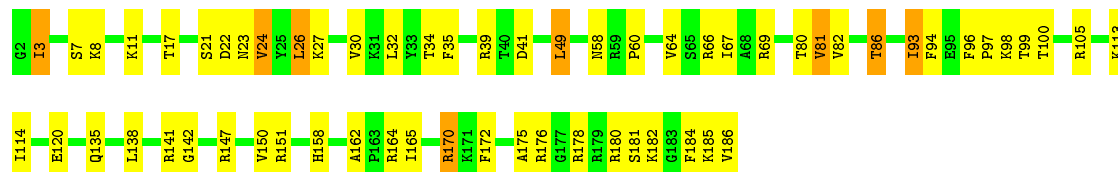
• Molecule 19: 60S ribosomal protein L18-A

Chain y: 89% 10% .



• Molecule 19: 60S ribosomal protein L18-A

Chain CS: 67% 29% .



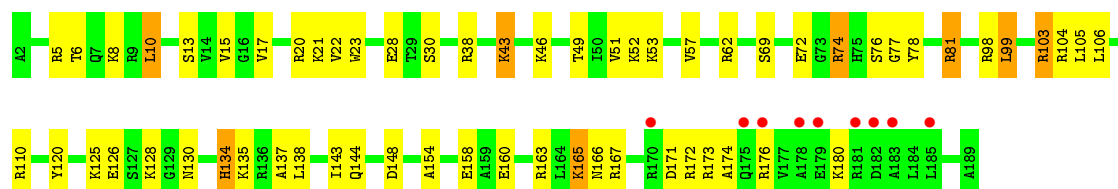
• Molecule 20: 60S ribosomal protein L19-A

Chain z: 4% 93% 7% .



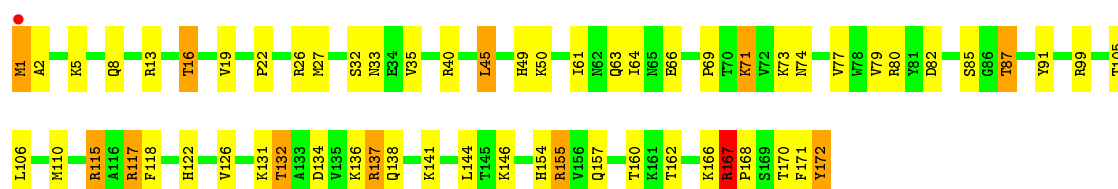
• Molecule 20: 60S ribosomal protein L19-A

Chain CT: 5% 68% 28% .

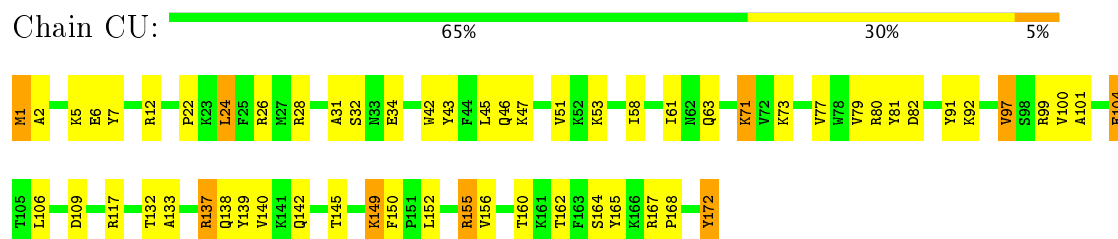


• Molecule 21: 60S ribosomal protein L20-A

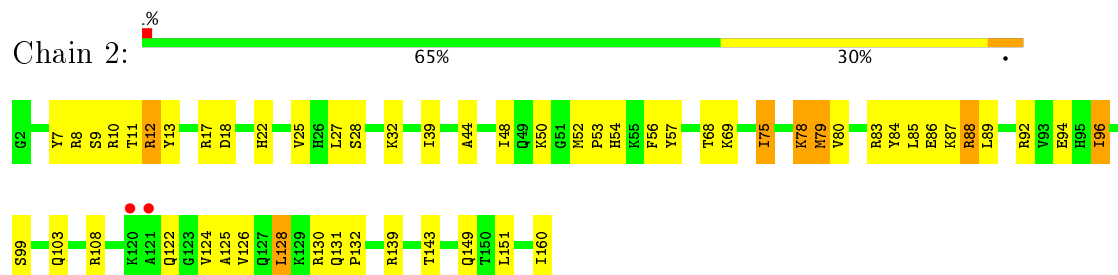
Chain 0: 65% 28% 6% .



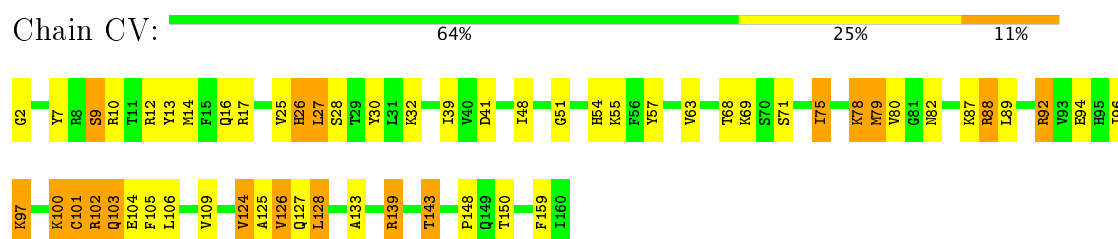
- Molecule 21: 60S ribosomal protein L20-A



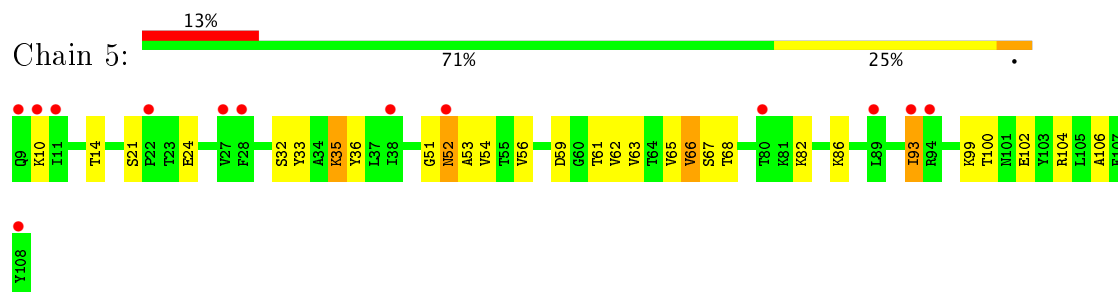
- Molecule 22: 60S ribosomal protein L21-A



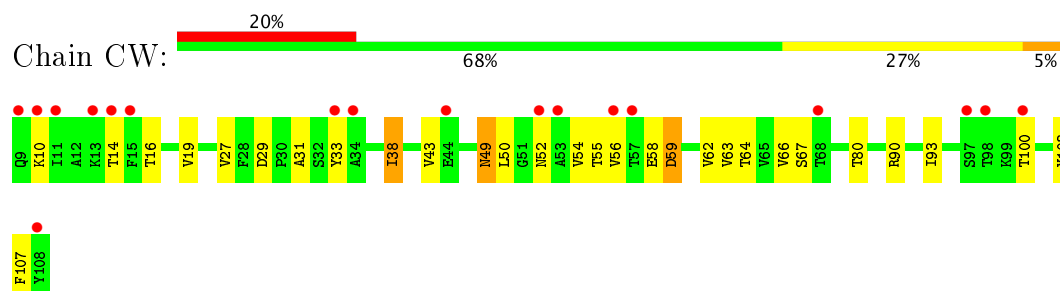
- Molecule 22: 60S ribosomal protein L21-A



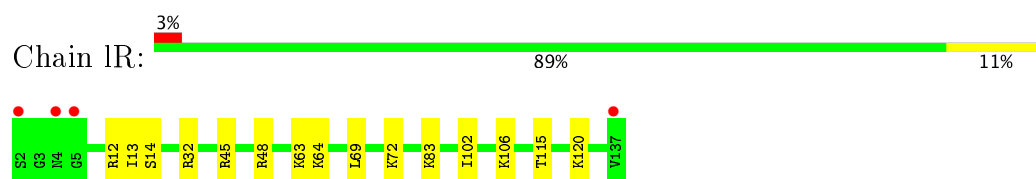
- Molecule 23: 60S ribosomal protein L22-A



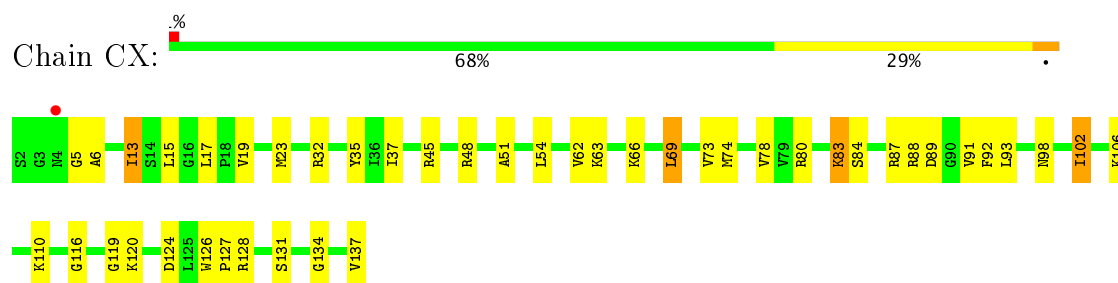
- Molecule 23: 60S ribosomal protein L22-A



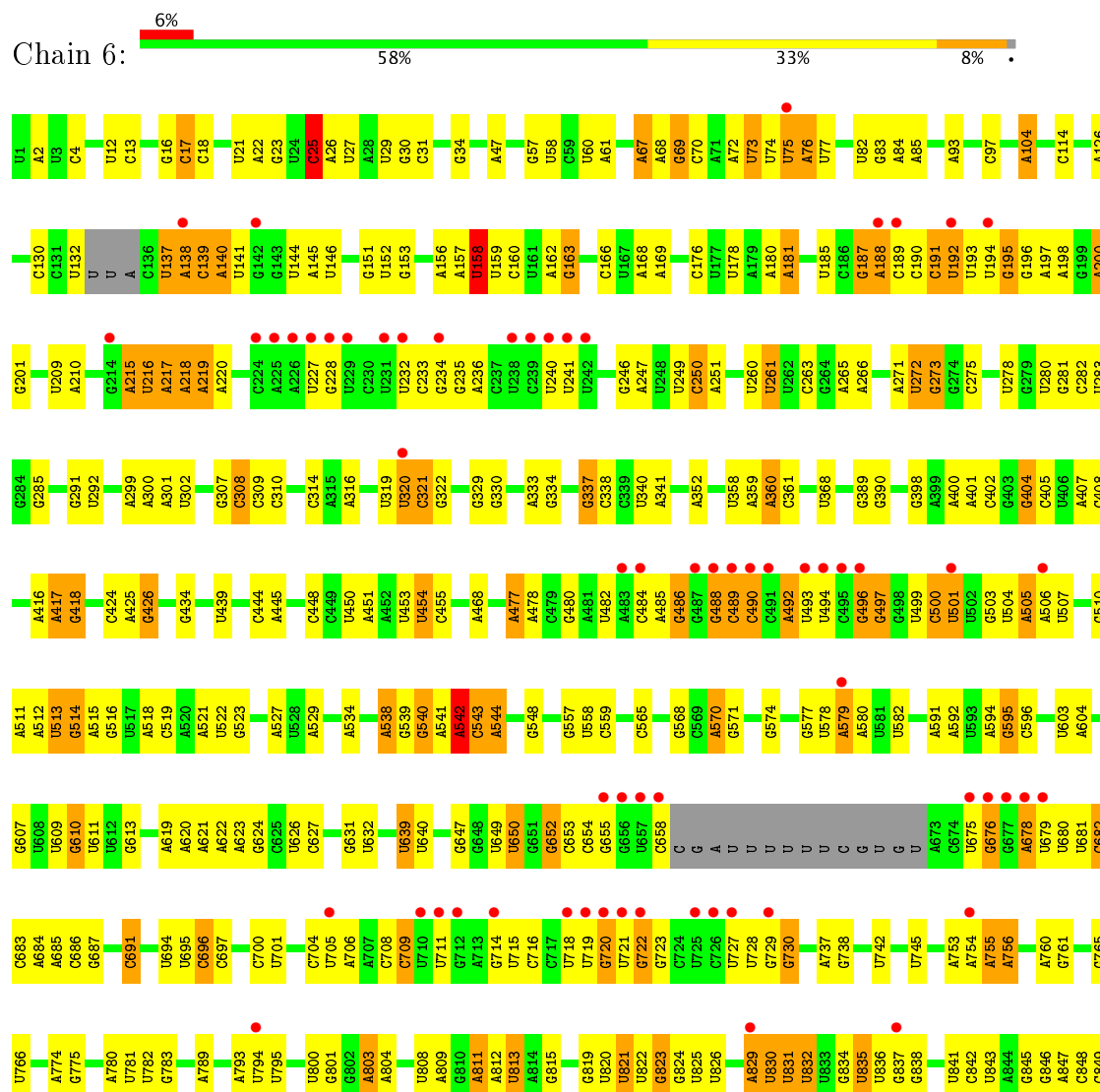
• Molecule 24: 60S ribosomal protein L23-A

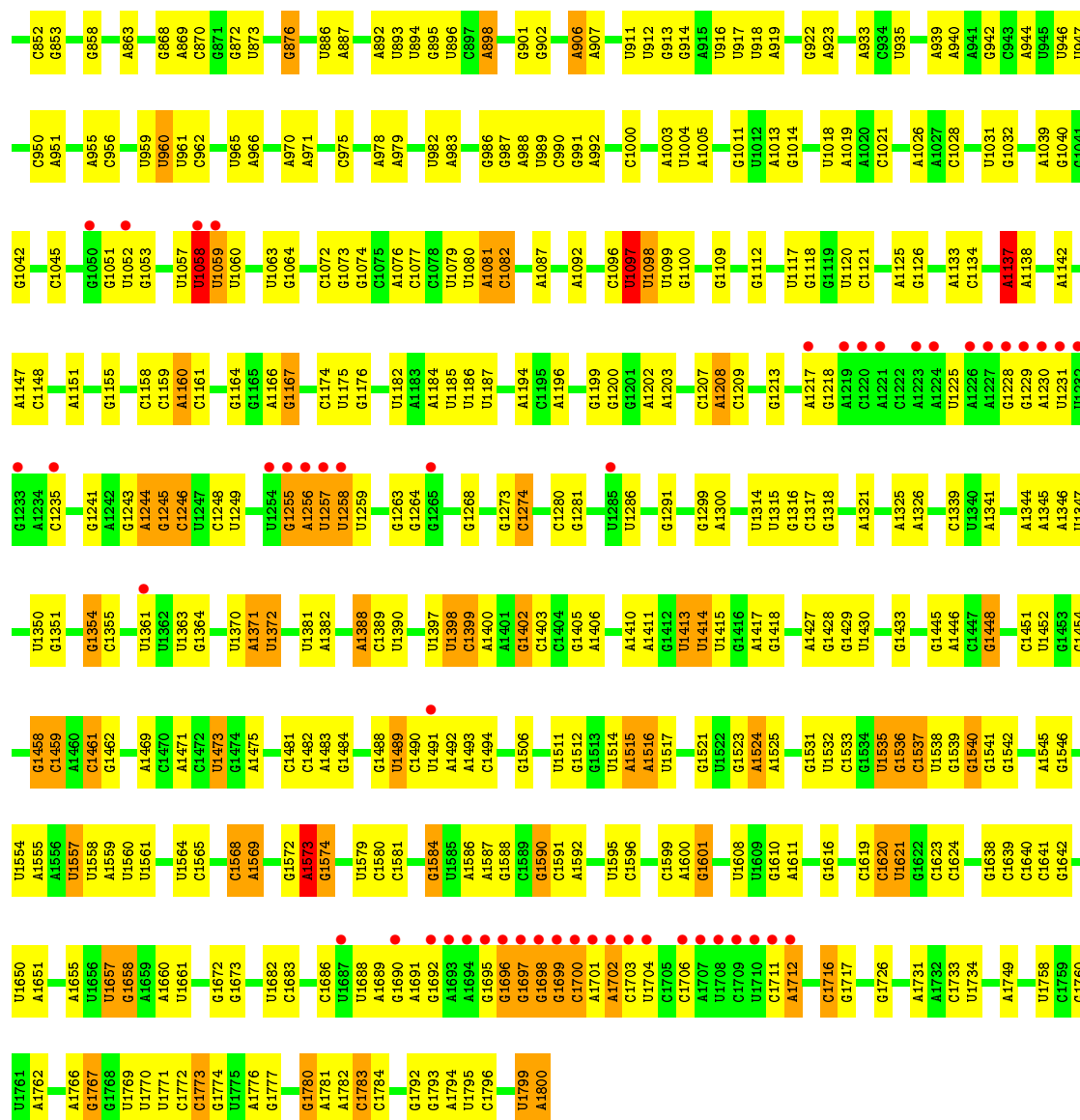


• Molecule 24: 60S ribosomal protein L23-A

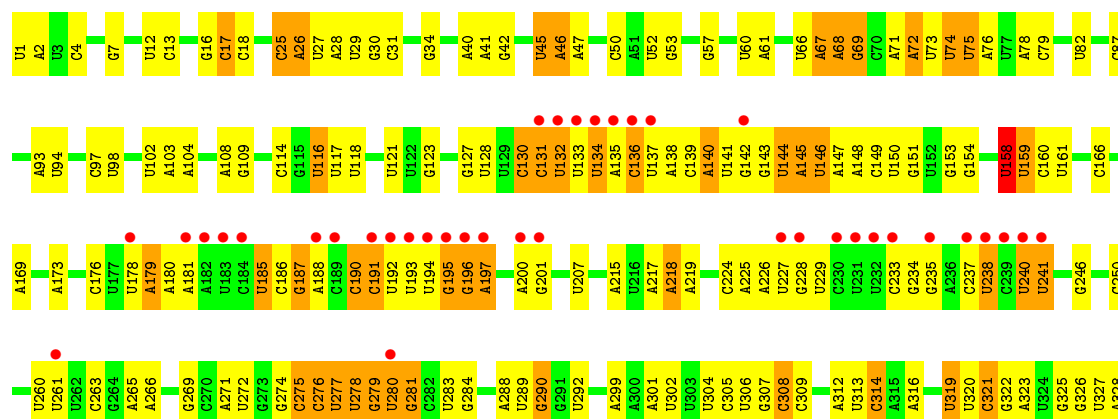


• Molecule 25: 18S ribosomal RNA

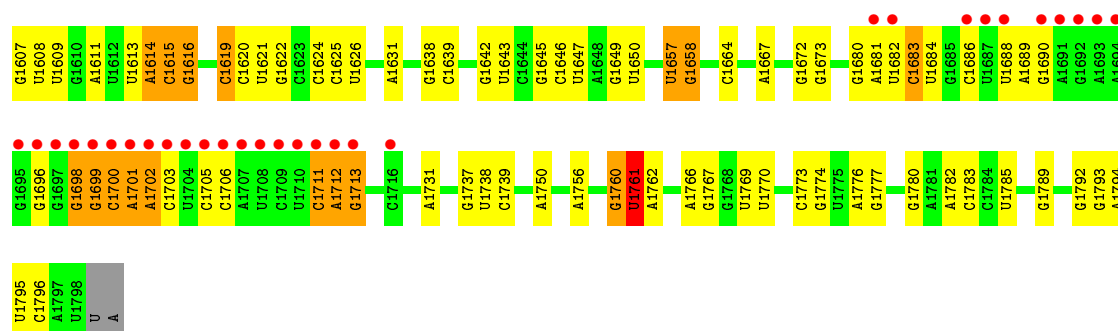




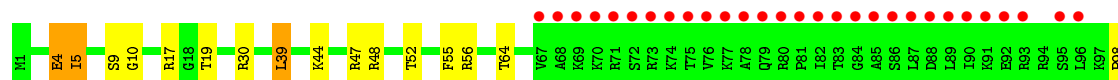
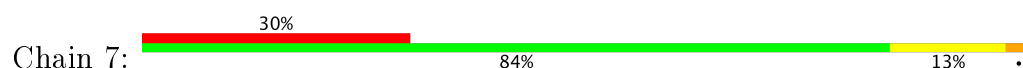
• Molecule 25: 18S ribosomal RNA



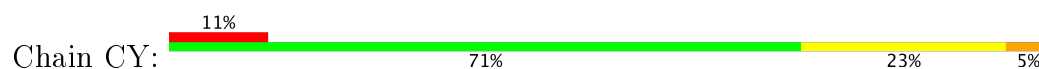
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C1535	C1456	C1359	A1256	C1172	U1079	U989	U887	U812	A734	U	U603	U507	A438	A331
G1536	G1457	C1360	U1257	C1173	U1080	C990	U888	U813	C735	G	A604	U509	U439	G337
C1537	G1458	U1361	U1258	C1174	A1081	G991	A892	A814	C736	A	A605	G510	C338	C338
U1538	C1459	U1362	G1261	U1175	C1082	A992	U893	G815	A737	U	A606	A511	C444	C339
G1539	A1460	U1363	U1262	C1176	G1083	A993	U894	U816	G738	C	G607	A512	A445	
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G1541	G1462	G1366	G1268	G1179	A1088	U996	G896	G819	C741		U609	G514	U447	A452
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	A1475	U1372	G1278	U1190	U1097	U1012	U914	U826	A684		U618	A520	U456	A360
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			U1314	A1211	G1130	A1027	U933	G845	U700		U632	A542	U475	G389
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			G1316	A1217	A1132	U1031	U935	C848	A774		A635	C544	U477	C393
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			C1339	G1149	G1150	G1052	A956	A862	A789		U653	C565	U488	U406
			U1340	A1151	A1151	G1053	C959	A863	U790		U654	C566	U489	C406
			A1341	A1152	A1152	U1058	U959	U864	U791		U655	A567	U490	U413
			A1344	A1157	A1159	U1059	U960	A865	A793		U656	G577	U491	C414
			A1345	C1158	C1159	U1060	A966	G866	U794		U657	U578	U494	C415
			A1346	A1160	A1160	A1062	A967	G867	U795		U658	A579	U495	A416
			G1349	G1164	G1164	C1067	U968	G868	A799		C	U580	U496	A417
			U1350	G1165	G1165	C1068	A969	G869	U800		G	U581	U497	G418
			G1351	A1166	A1166	C1068	U974	C870	G801		A	U582	U498	C424
			U1251	G1167	G1167	C1068	U975	G872	U802		U	C583	U499	A425
			G1354	U1168	U1168	G1073	U976	U873	A804		U	U500	C500	C426
						C1075	U986	G876	U808		U	A591	U501	G427
									U809		U	A592	U502	A428
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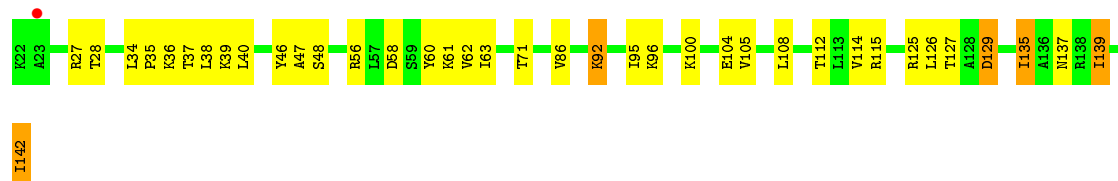
- Molecule 26: 60S ribosomal protein L24-A



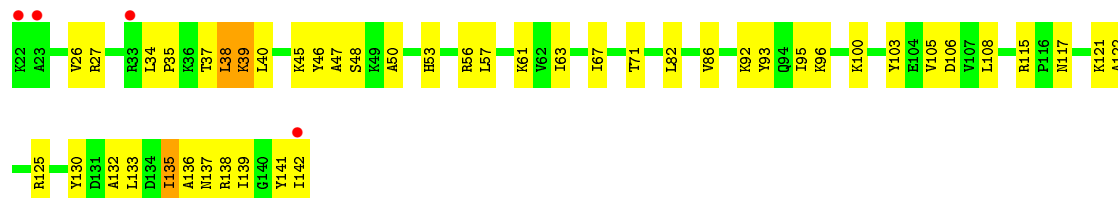
- Molecule 26: 60S ribosomal protein L24-A



- Molecule 27: 60S ribosomal protein L25



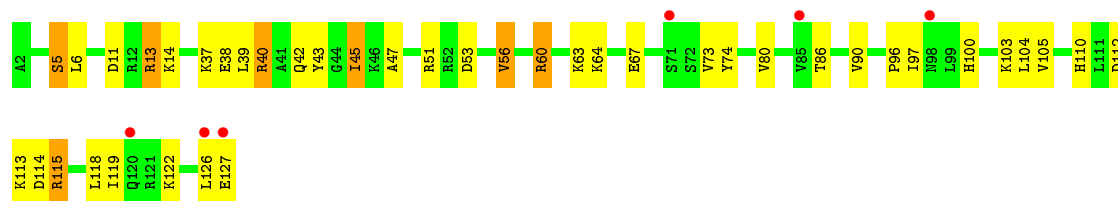
- Molecule 27: 60S ribosomal protein L25



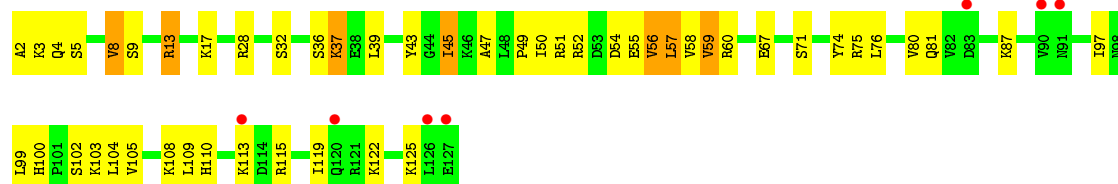
- Molecule 28: 60S ribosomal protein L26-A



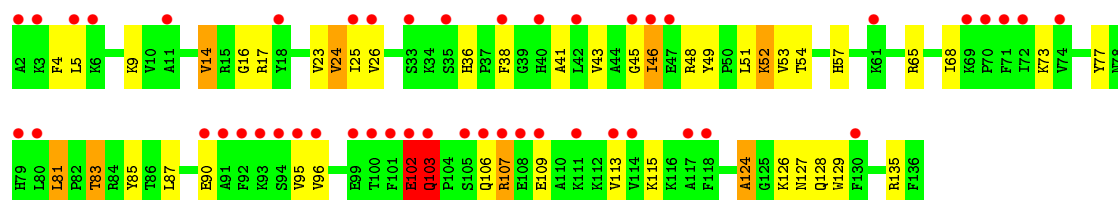




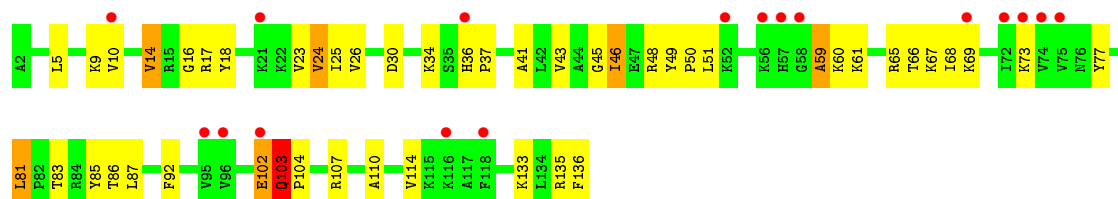
- Molecule 28: 60S ribosomal protein L26-A



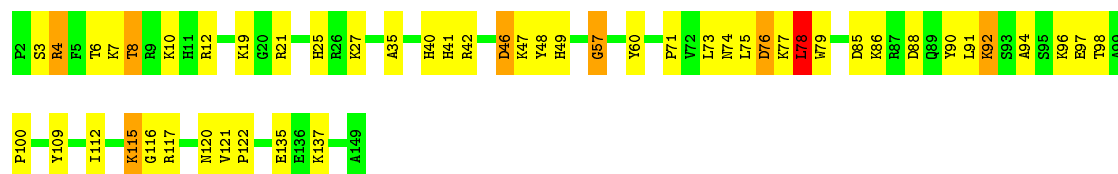
- Molecule 29: 60S ribosomal protein L27-A



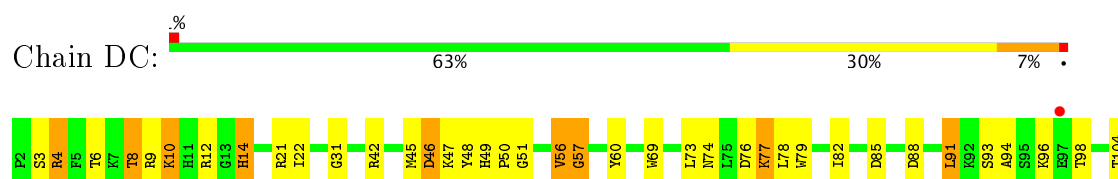
- Molecule 29: 60S ribosomal protein L27-A



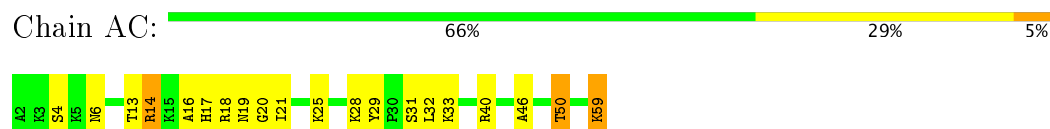
- Molecule 30: 60S ribosomal protein L28



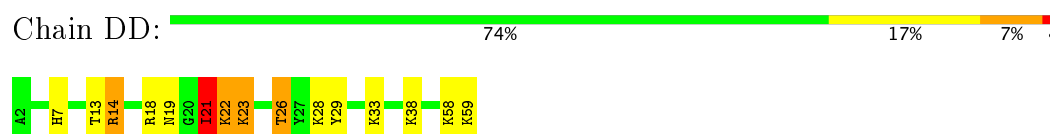
- Molecule 30: 60S ribosomal protein L28



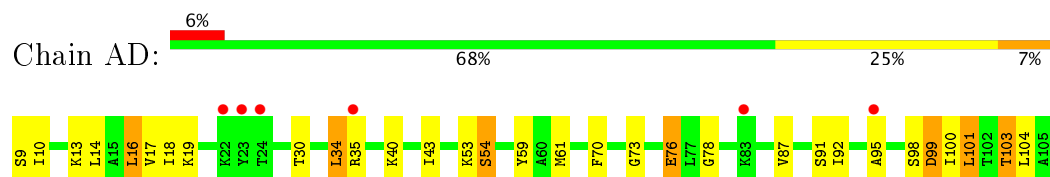
- Molecule 31: 60S ribosomal protein L29



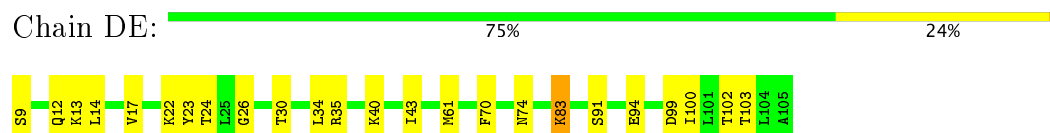
- Molecule 31: 60S ribosomal protein L29



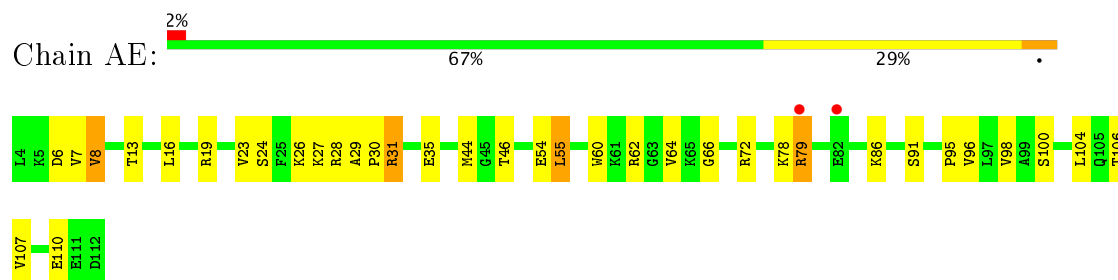
- Molecule 32: 60S ribosomal protein L30



- Molecule 32: 60S ribosomal protein L30



- Molecule 33: 60S ribosomal protein L31-A

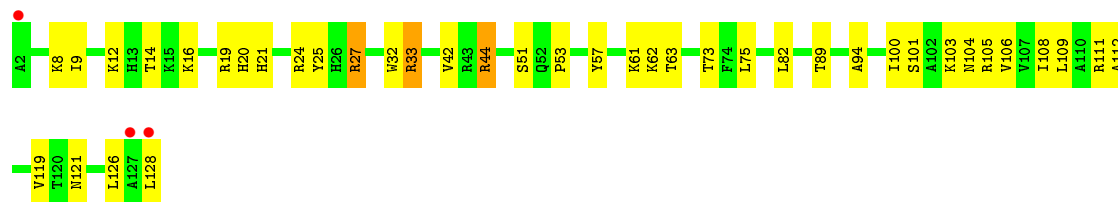


- Molecule 33: 60S ribosomal protein L31-A

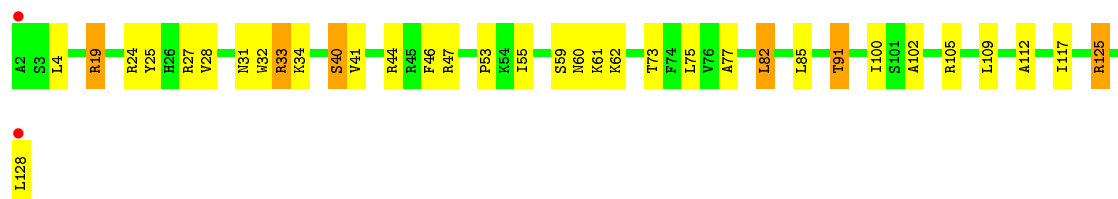
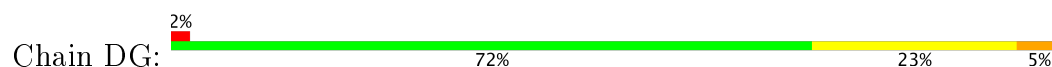




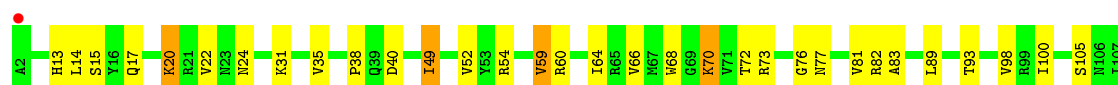
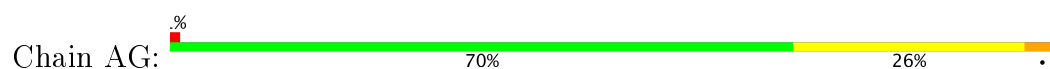
- Molecule 34: 60S ribosomal protein L32



- Molecule 34: 60S ribosomal protein L32



- Molecule 35: 60S ribosomal protein L33-A



- Molecule 35: 60S ribosomal protein L33-A

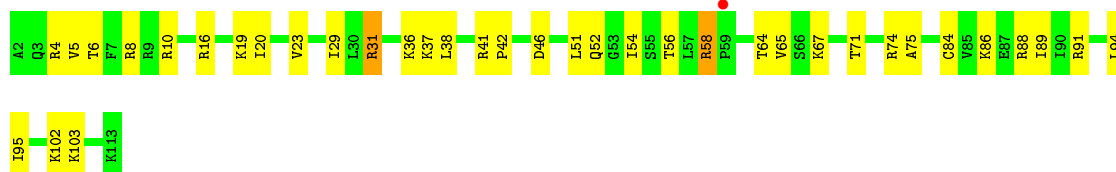


- Molecule 36: 60S ribosomal protein L34-A

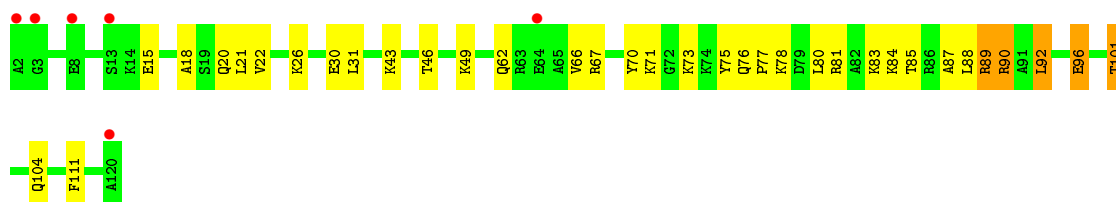




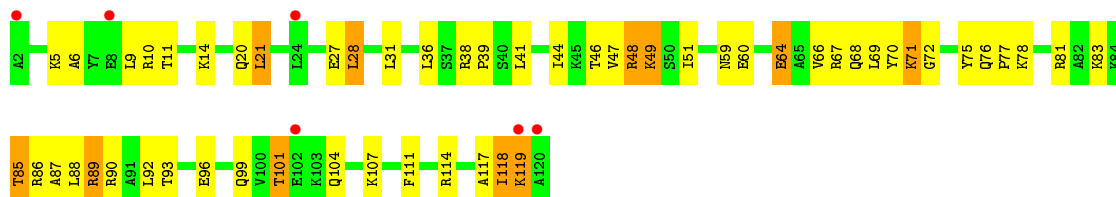
- Molecule 36: 60S ribosomal protein L34-A



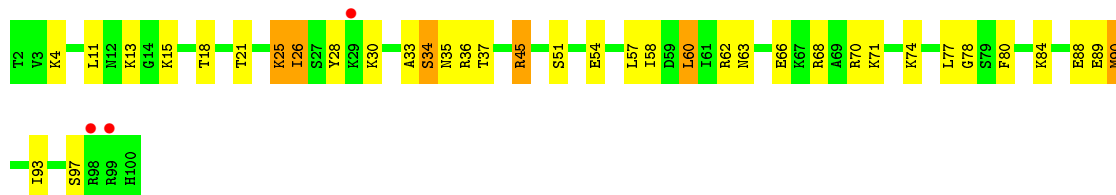
- Molecule 37: 60S ribosomal protein L35-A



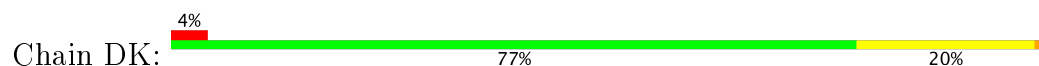
- Molecule 37: 60S ribosomal protein L35-A

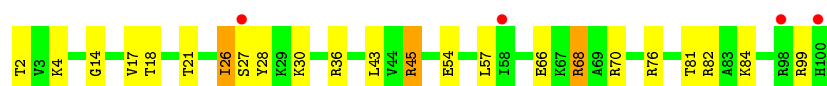


- Molecule 38: 60S ribosomal protein L36-A



- Molecule 38: 60S ribosomal protein L36-A

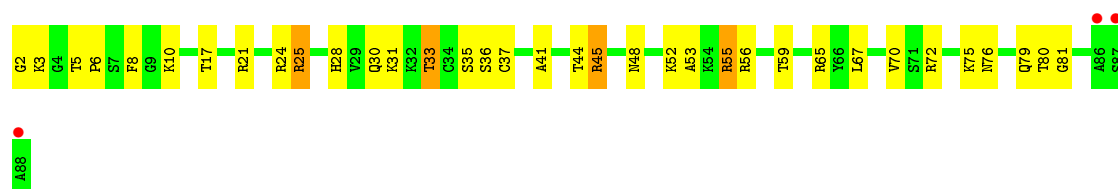




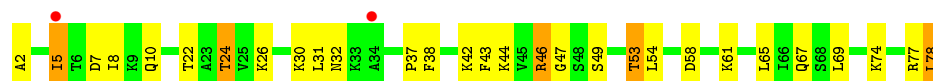
- Molecule 39: 60S ribosomal protein L37-A



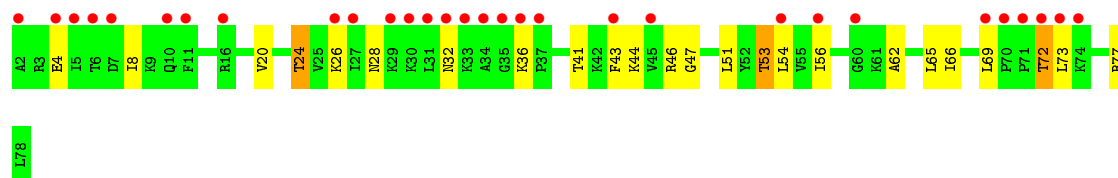
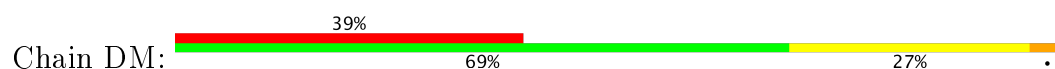
- Molecule 39: 60S ribosomal protein L37-A



- Molecule 40: 60S ribosomal protein L38



- Molecule 40: 60S ribosomal protein L38



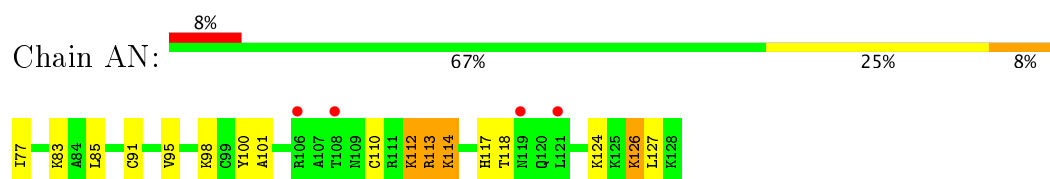
- Molecule 41: 60S ribosomal protein L39



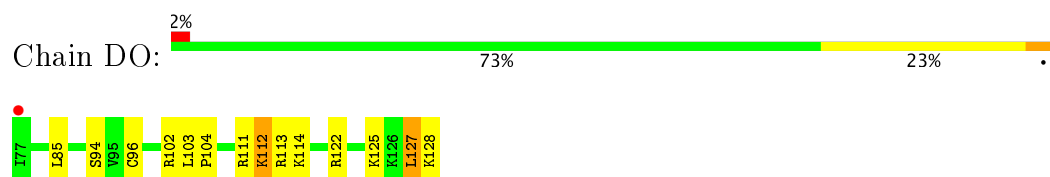
- Molecule 41: 60S ribosomal protein L39



- Molecule 42: Ubiquitin-60S ribosomal protein L40



- Molecule 42: Ubiquitin-60S ribosomal protein L40



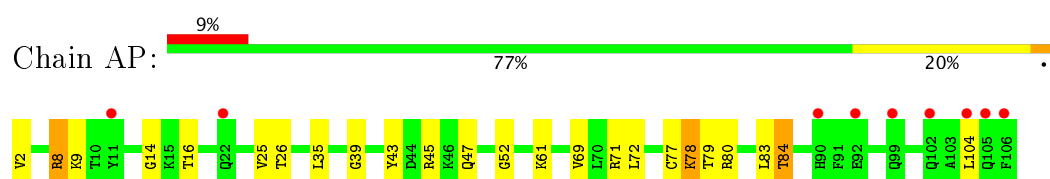
- Molecule 43: 60S ribosomal protein L41-B



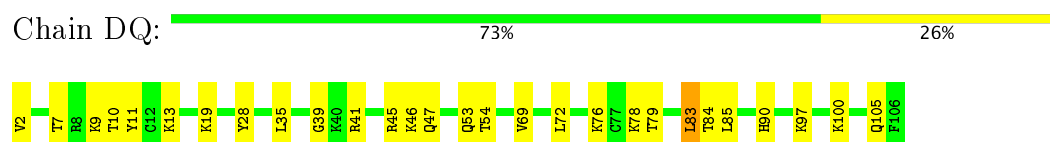
- Molecule 43: 60S ribosomal protein L41-B



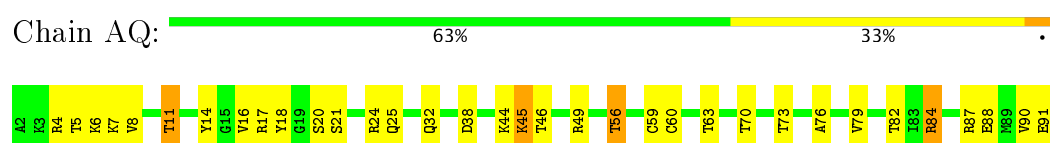
- Molecule 44: 60S ribosomal protein L42-A



- Molecule 44: 60S ribosomal protein L42-A



- Molecule 45: 60S ribosomal protein L43-A



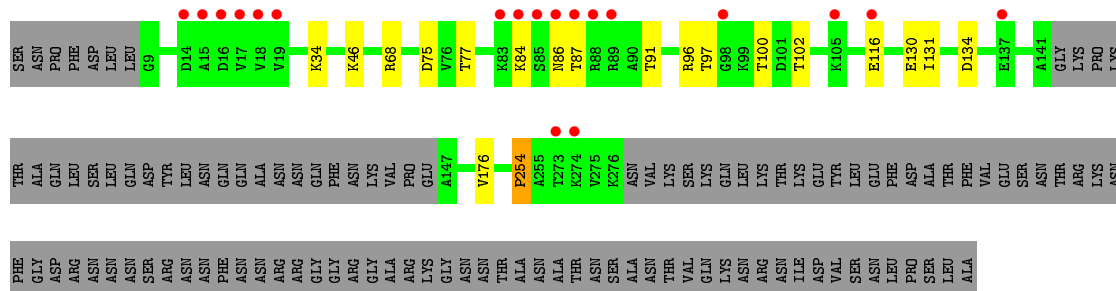
- Molecule 45: 60S ribosomal protein L43-A

Chain DR:  71% 24% .

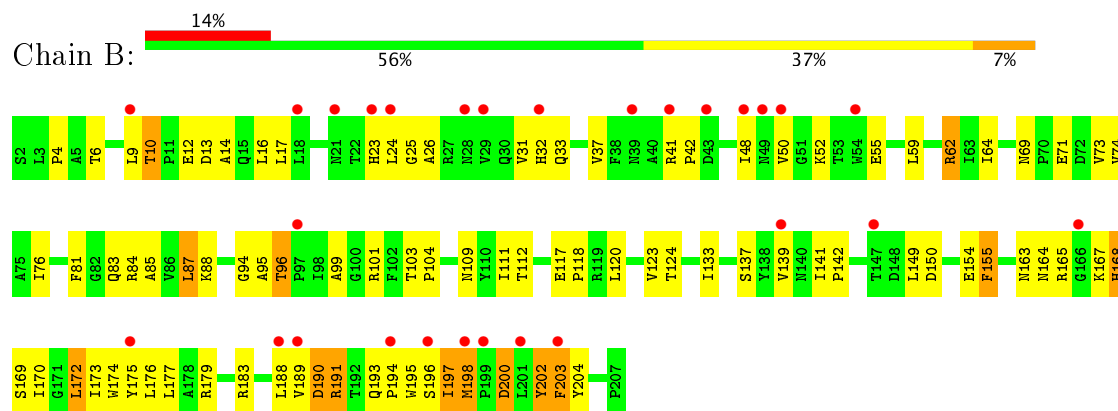


- Molecule 46: Suppressor protein STM1

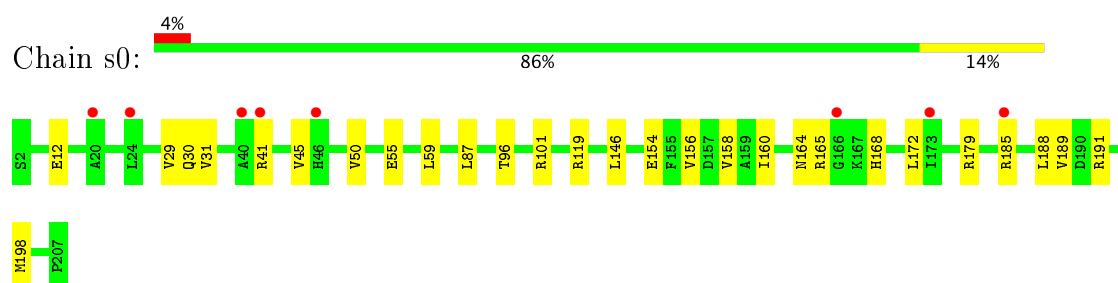
Chain i:  7% 51% 7% 42%



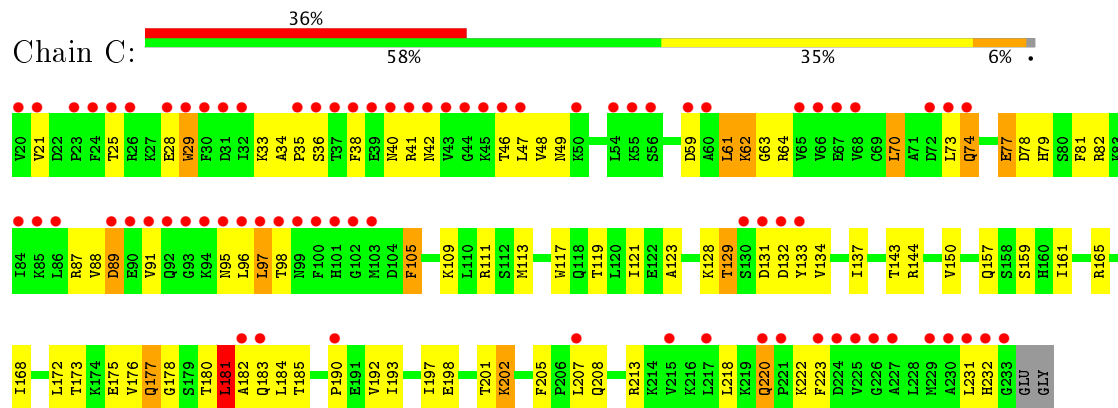
- Molecule 50: 40S ribosomal protein S0-A



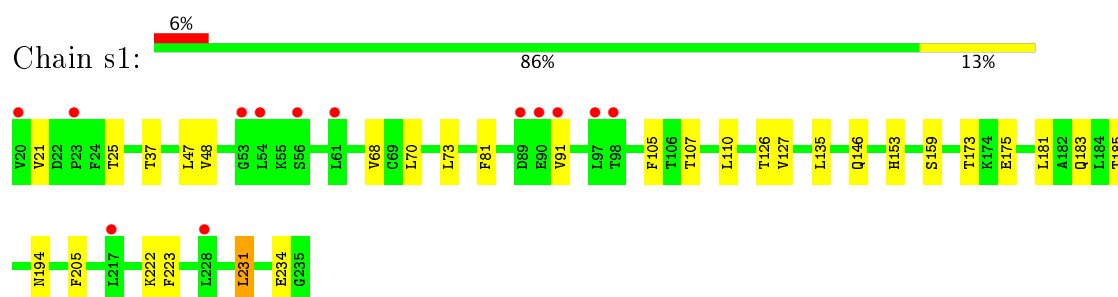
- Molecule 50: 40S ribosomal protein S0-A



- Molecule 51: 40S ribosomal protein S1-A

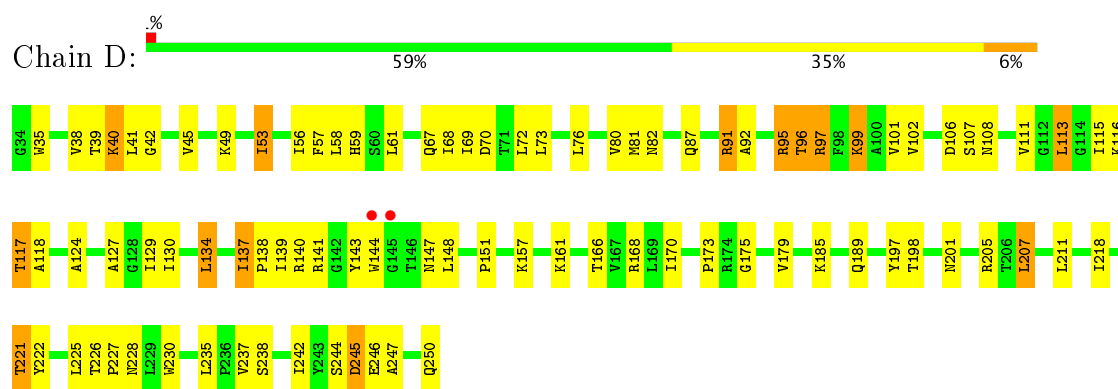


- Molecule 51: 40S ribosomal protein S1-A

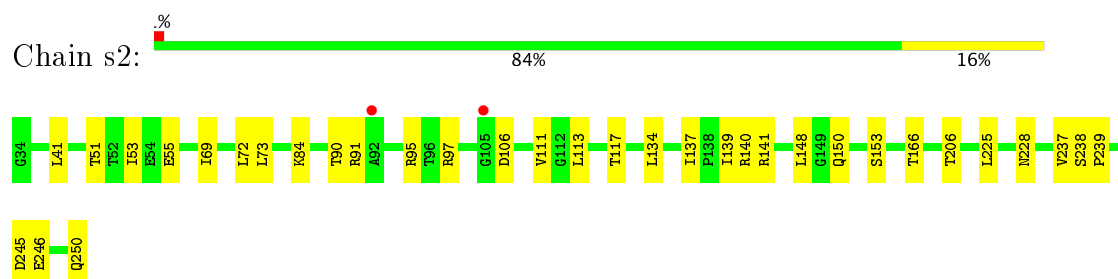


- Molecule 52: 40S ribosomal protein S2

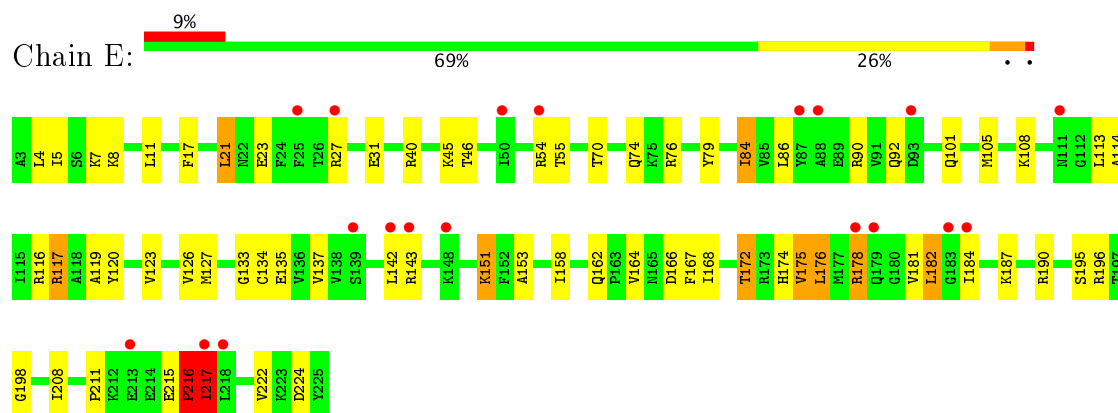




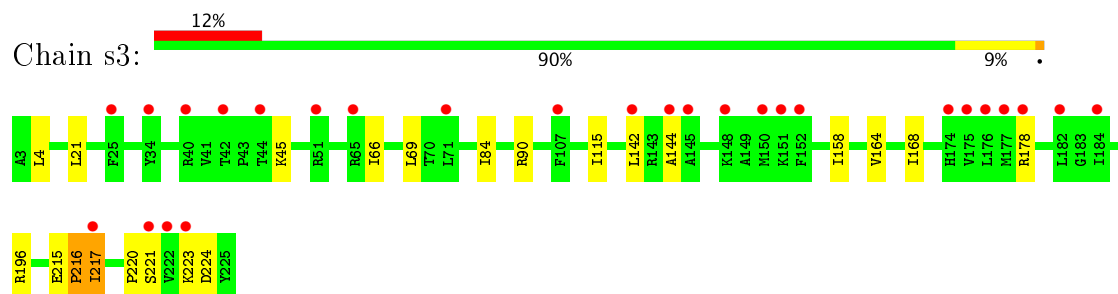
• Molecule 52: 40S ribosomal protein S2



• Molecule 53: 40S ribosomal protein S3

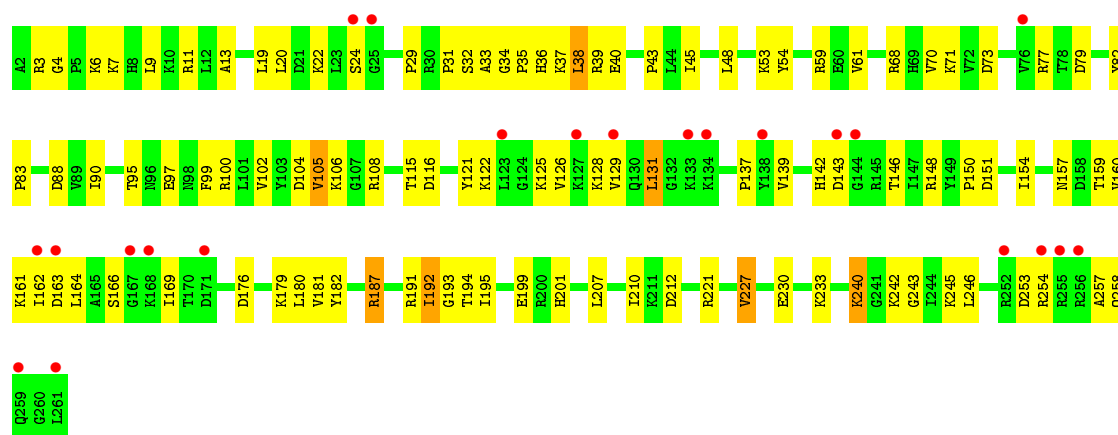


• Molecule 53: 40S ribosomal protein S3



• Molecule 54: 40S ribosomal protein S4-A

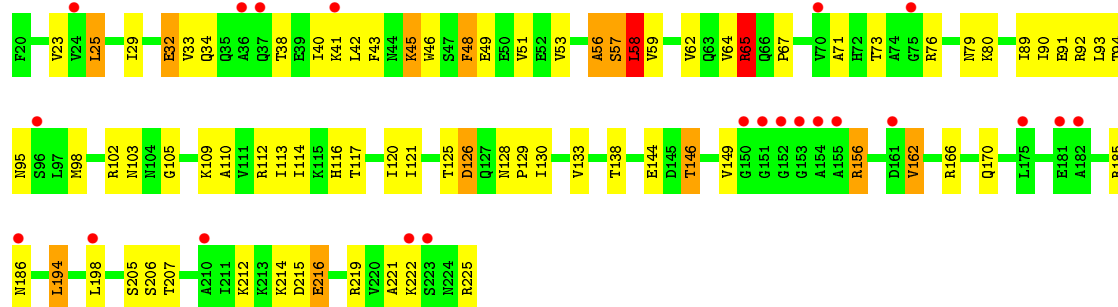




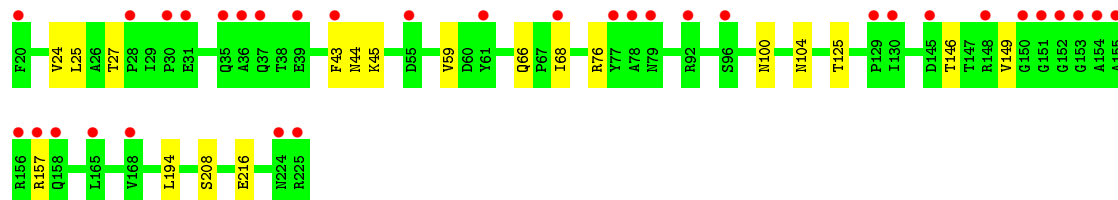
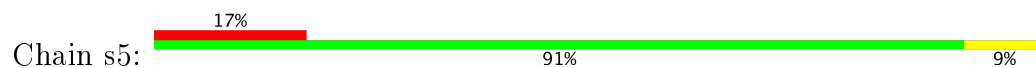
- Molecule 54: 40S ribosomal protein S4-A



- Molecule 55: 40S ribosomal protein S5

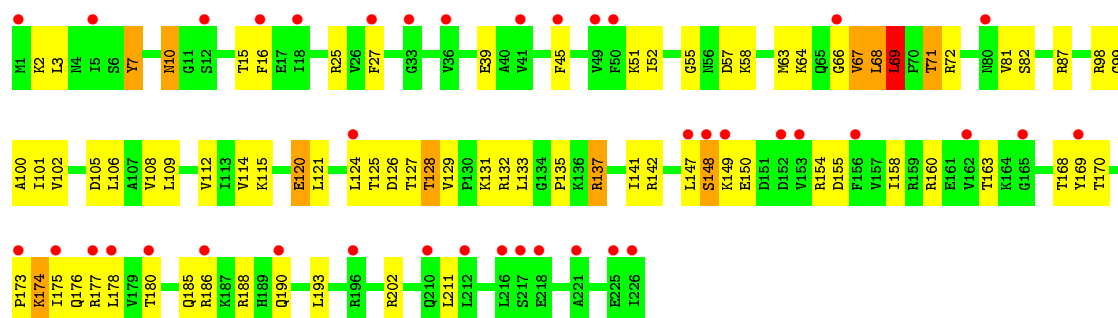


- Molecule 55: 40S ribosomal protein S5

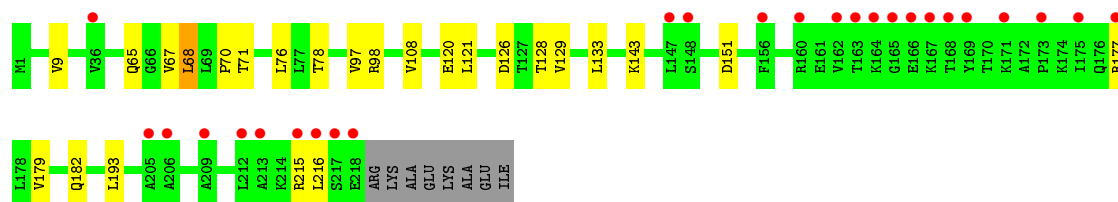
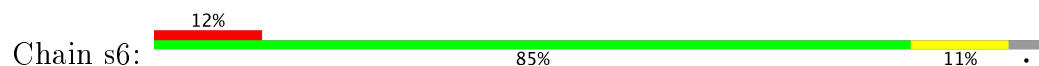


- Molecule 56: 40S ribosomal protein S6-A

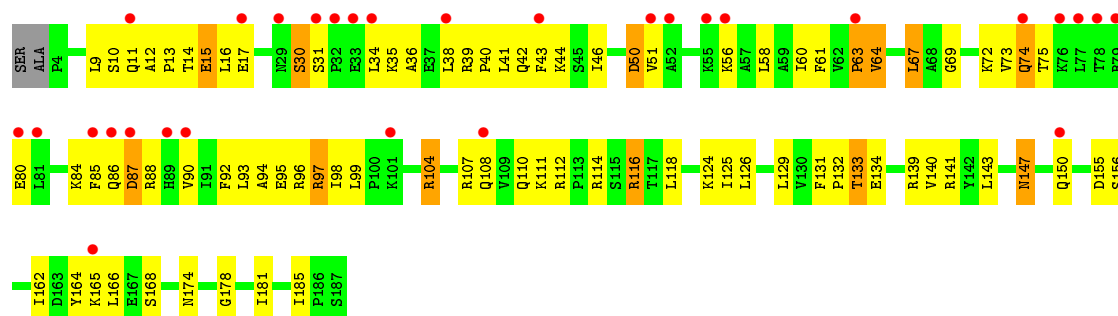




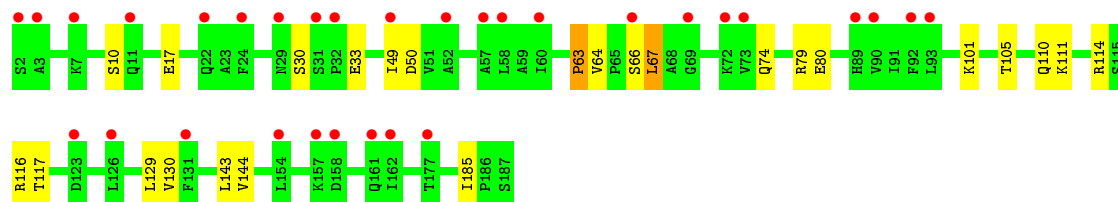
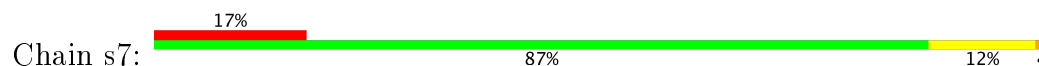
- Molecule 56: 40S ribosomal protein S6-A



- Molecule 57: 40S ribosomal protein S7-A

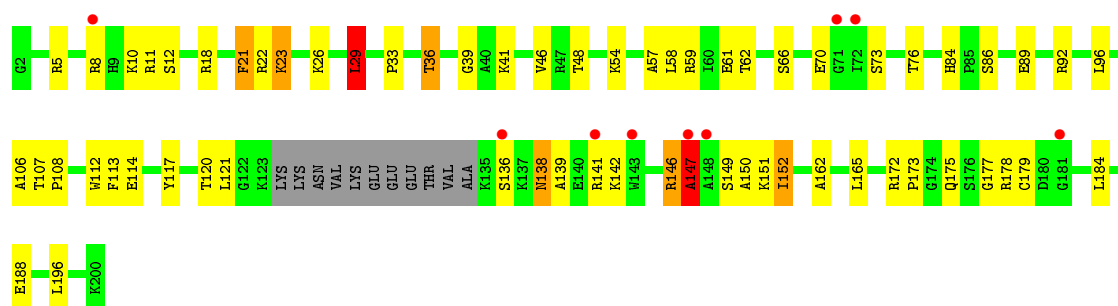


- Molecule 57: 40S ribosomal protein S7-A

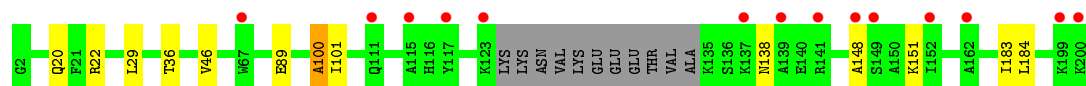
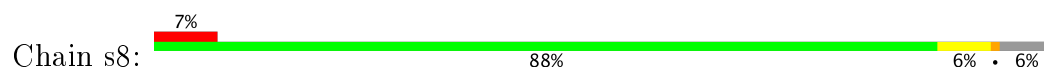


- Molecule 58: 40S ribosomal protein S8-A

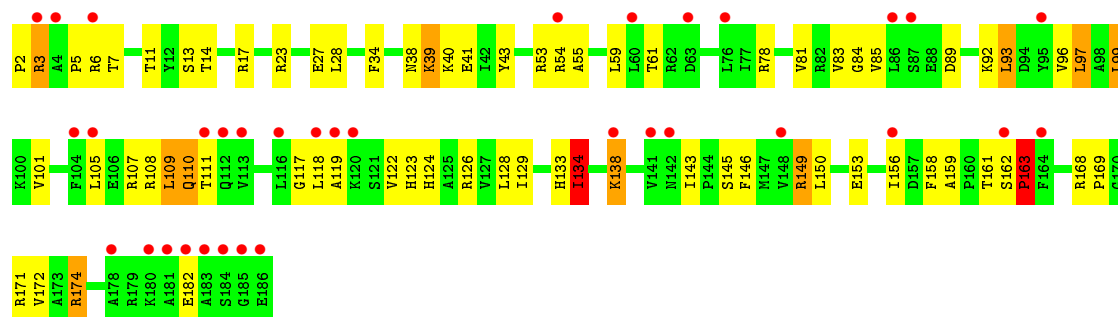




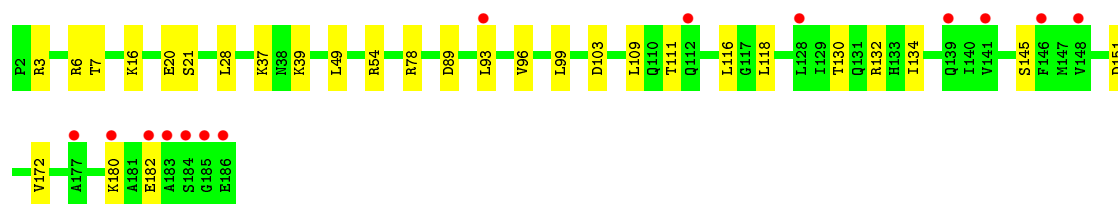
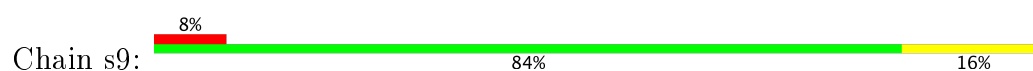
- Molecule 58: 40S ribosomal protein S8-A



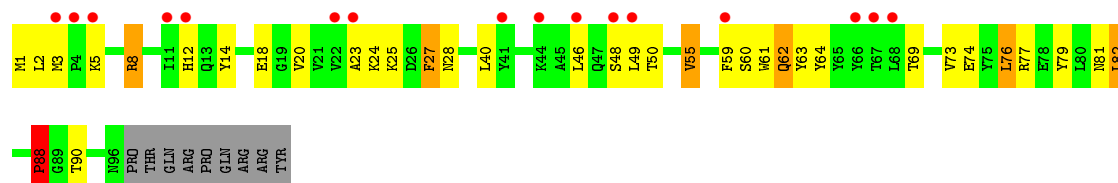
- Molecule 59: 40S ribosomal protein S9-A



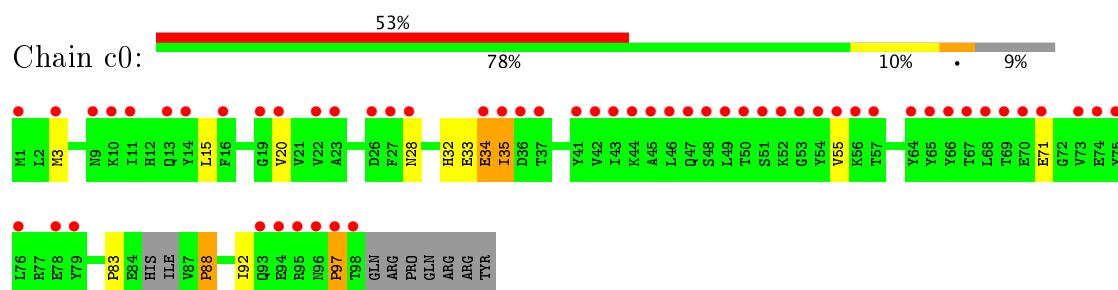
- Molecule 59: 40S ribosomal protein S9-A



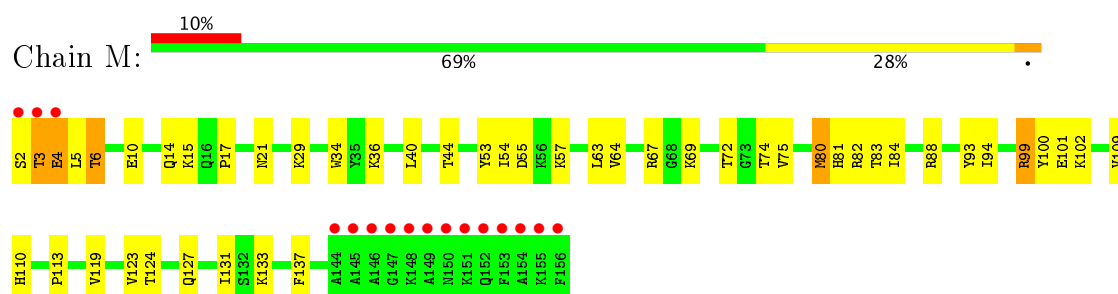
- Molecule 60: 40S ribosomal protein S10-A



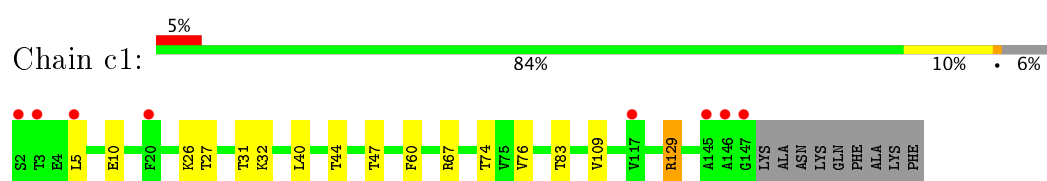
- Molecule 60: 40S ribosomal protein S10-A



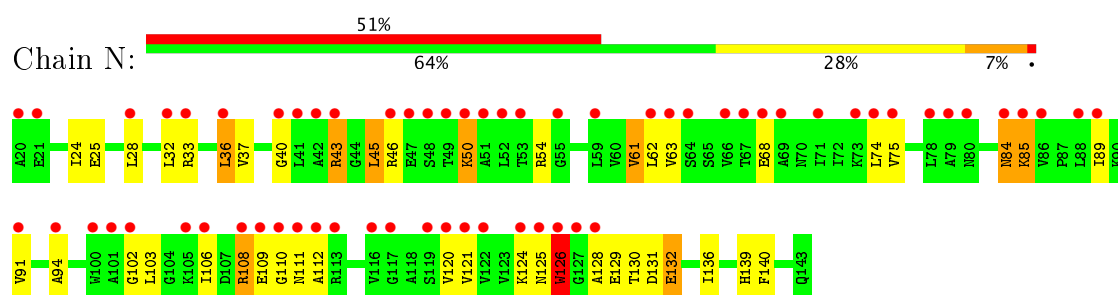
- Molecule 61: 40S ribosomal protein S11-A



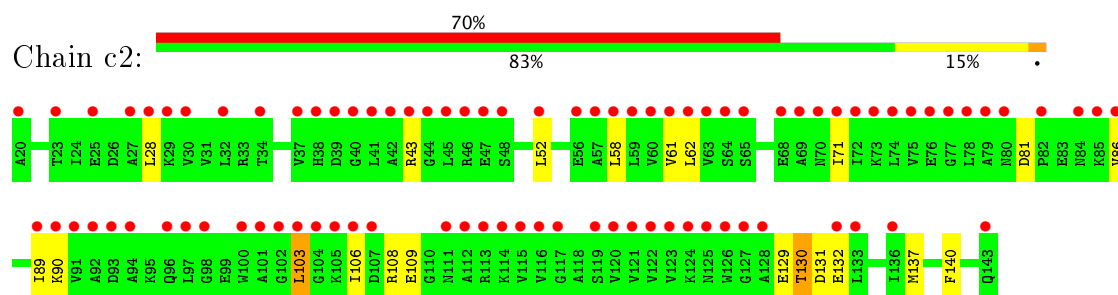
- Molecule 61: 40S ribosomal protein S11-A



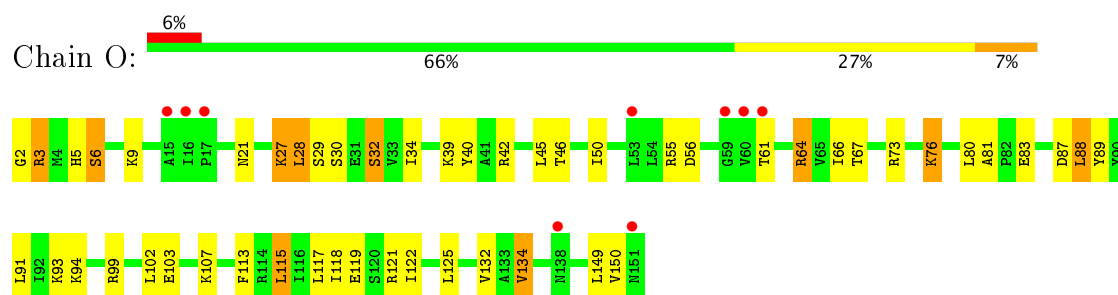
- Molecule 62: 40S ribosomal protein S12



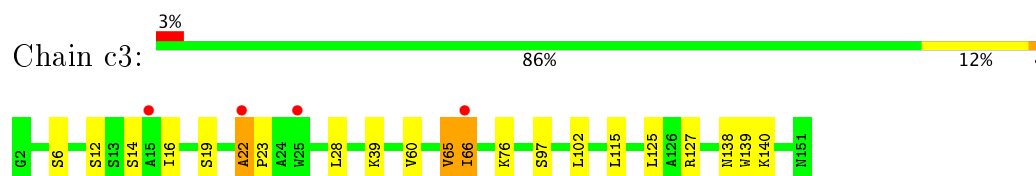
- Molecule 62: 40S ribosomal protein S12



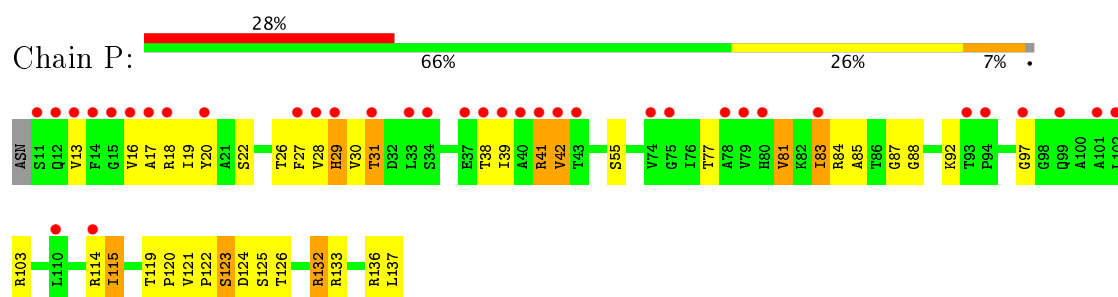
- Molecule 63: 40S ribosomal protein S13



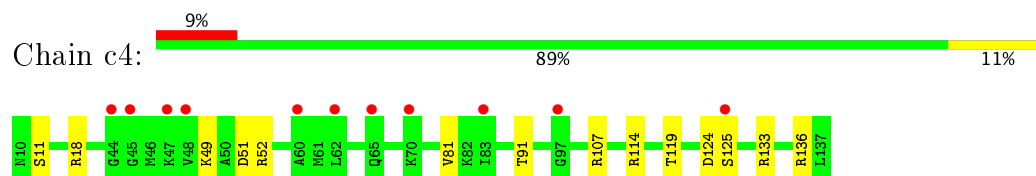
- Molecule 63: 40S ribosomal protein S13



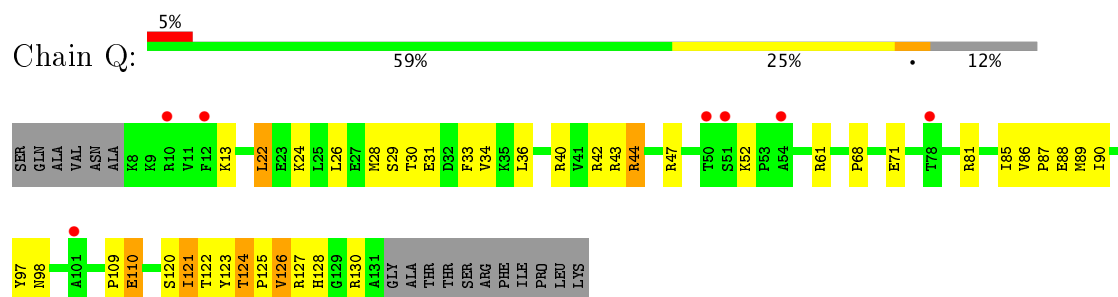
- Molecule 64: 40S ribosomal protein S14-B



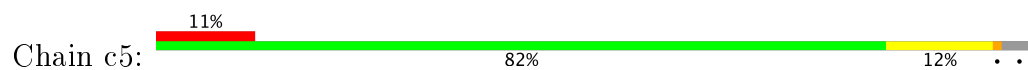
- Molecule 64: 40S ribosomal protein S14-B

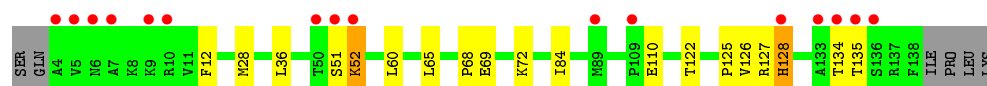


- Molecule 65: 40S ribosomal protein S15

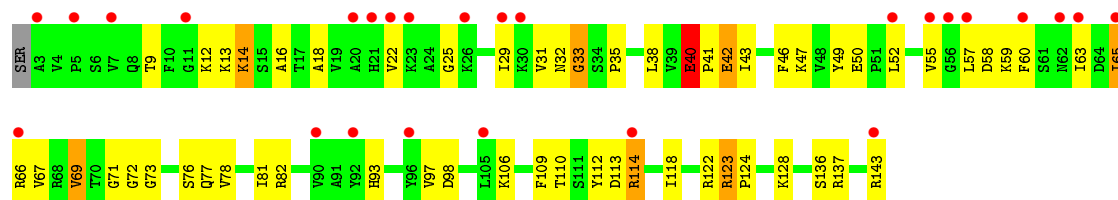


- Molecule 65: 40S ribosomal protein S15

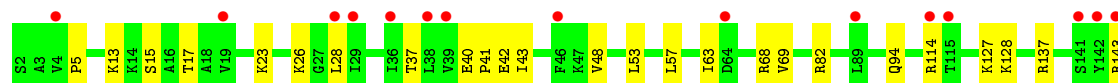
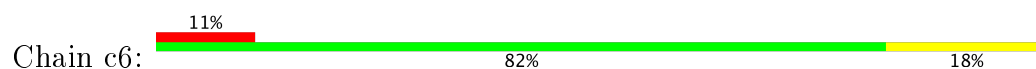




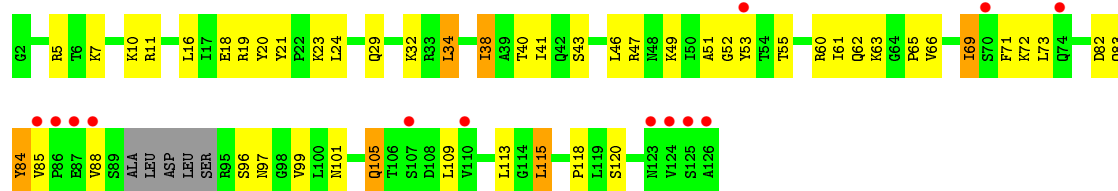
- Molecule 66: 40S ribosomal protein S16-A



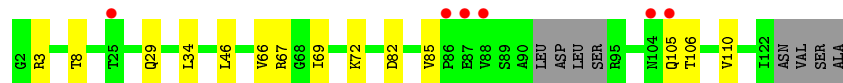
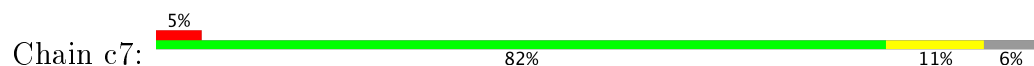
- Molecule 66: 40S ribosomal protein S16-A



- Molecule 67: 40S ribosomal protein S17-A



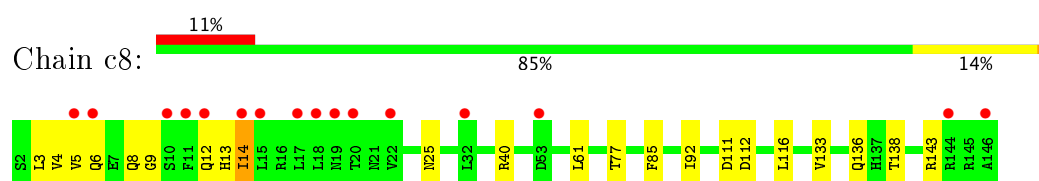
- Molecule 67: 40S ribosomal protein S17-A



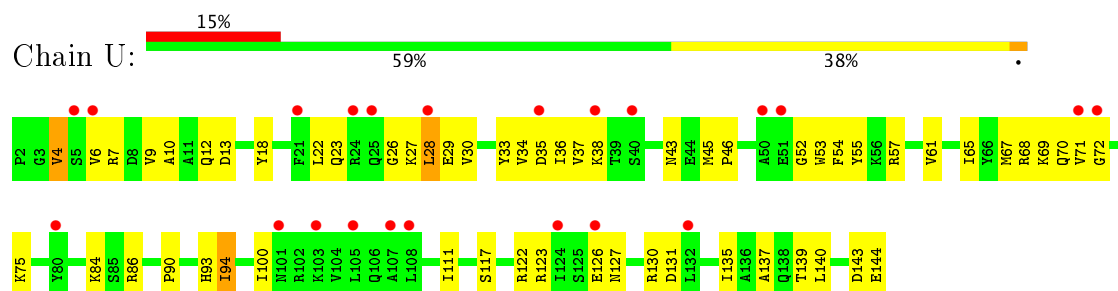
- Molecule 68: 40S ribosomal protein S18-A



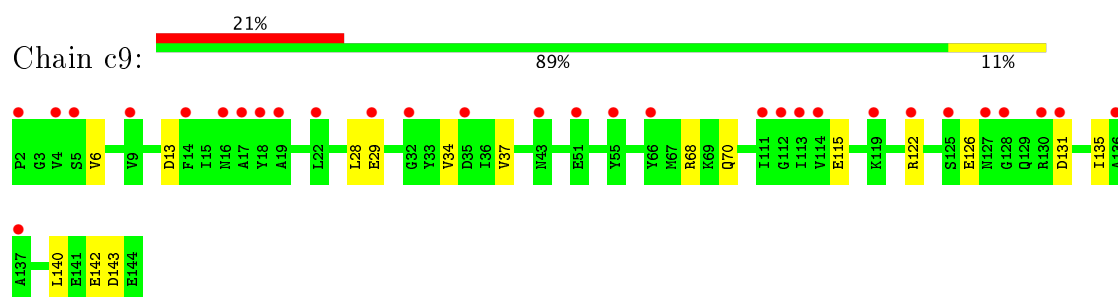
- Molecule 68: 40S ribosomal protein S18-A



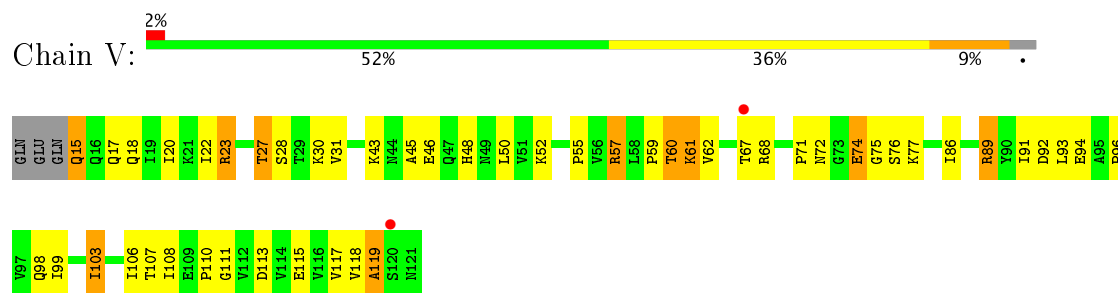
- Molecule 69: 40S ribosomal protein S19-A



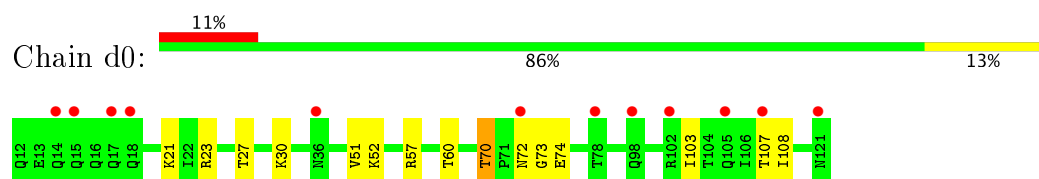
- Molecule 69: 40S ribosomal protein S19-A



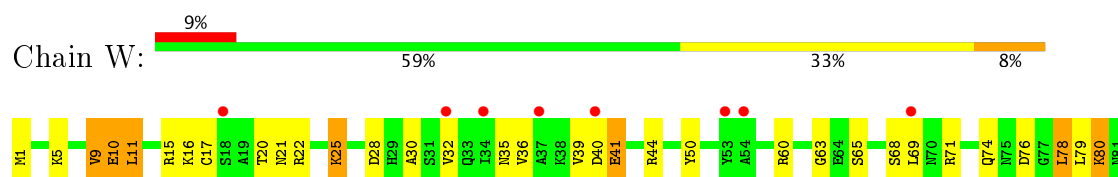
- Molecule 70: 40S ribosomal protein S20



- Molecule 70: 40S ribosomal protein S20



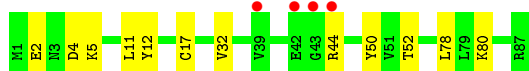
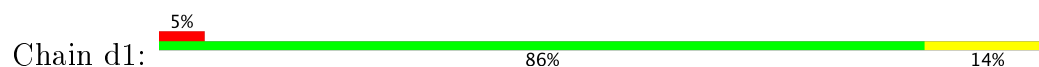
- Molecule 71: 40S ribosomal protein S21-A







- Molecule 71: 40S ribosomal protein S21-A



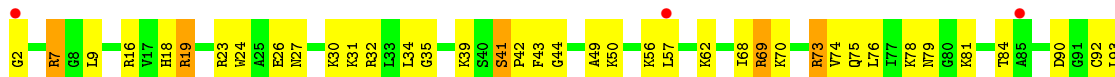
- Molecule 72: 40S ribosomal protein S22-A



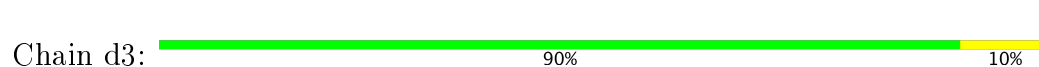
- Molecule 72: 40S ribosomal protein S22-A



- Molecule 73: 40S ribosomal protein S23-A

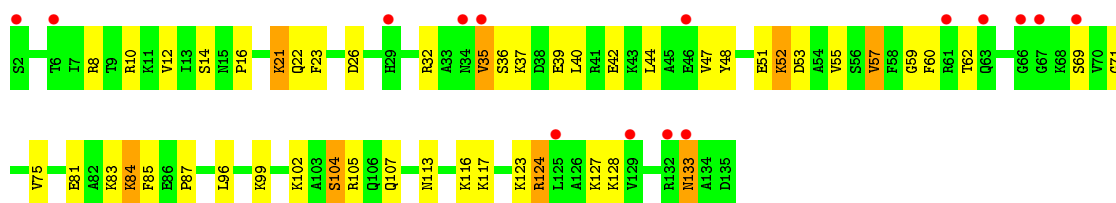


- Molecule 73: 40S ribosomal protein S23-A

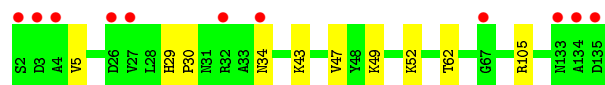


- Molecule 74: 40S ribosomal protein S24-A

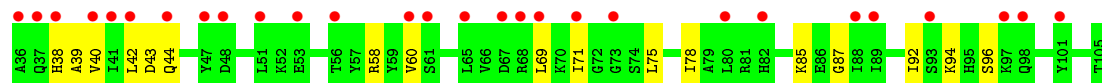
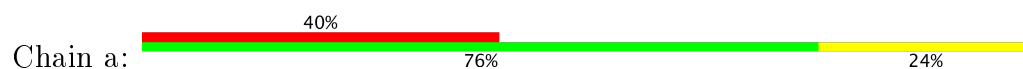




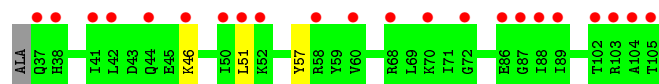
- Molecule 74: 40S ribosomal protein S24-A



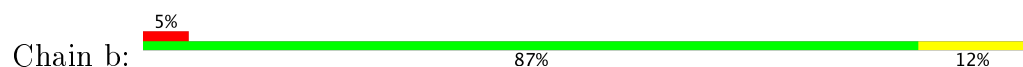
- Molecule 75: 40S ribosomal protein S25-A



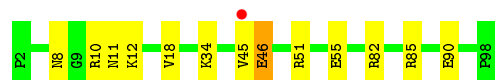
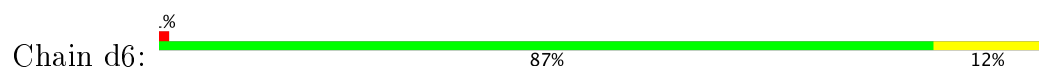
- Molecule 75: 40S ribosomal protein S25-A



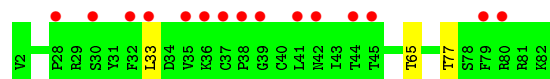
- Molecule 76: 40S ribosomal protein S26-B



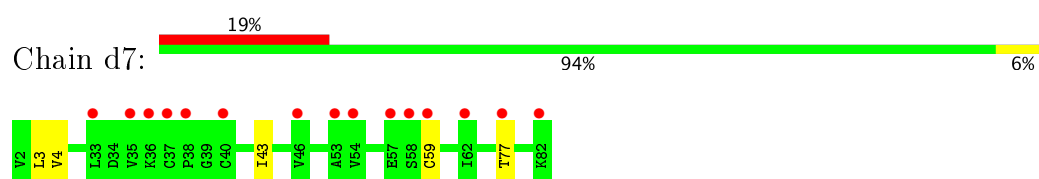
- Molecule 76: 40S ribosomal protein S26-B



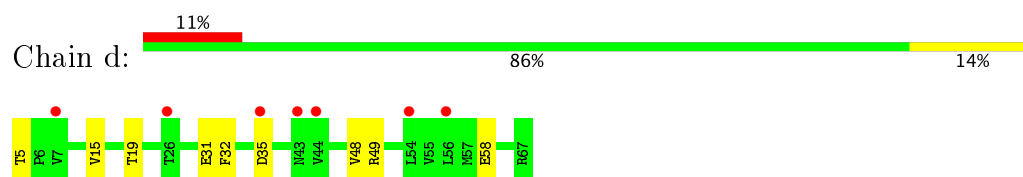
- Molecule 77: 40S ribosomal protein S27-A



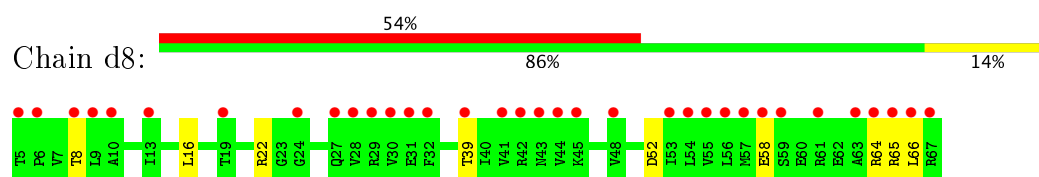
- Molecule 77: 40S ribosomal protein S27-A



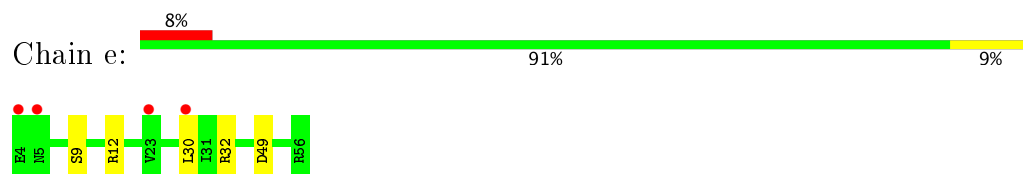
- Molecule 78: 40S ribosomal protein S28-A



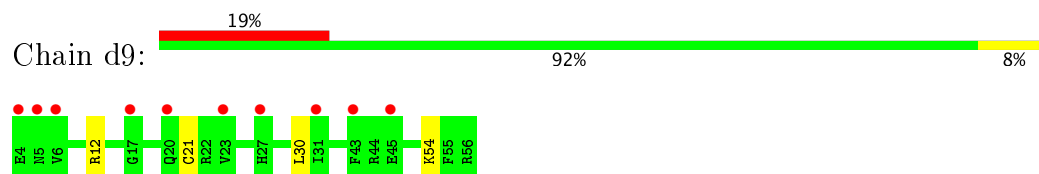
- Molecule 78: 40S ribosomal protein S28-A



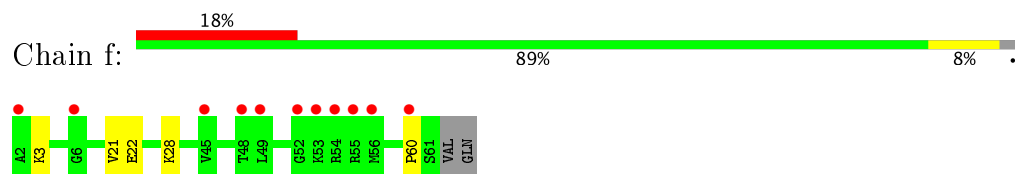
- Molecule 79: 40S ribosomal protein S29-A



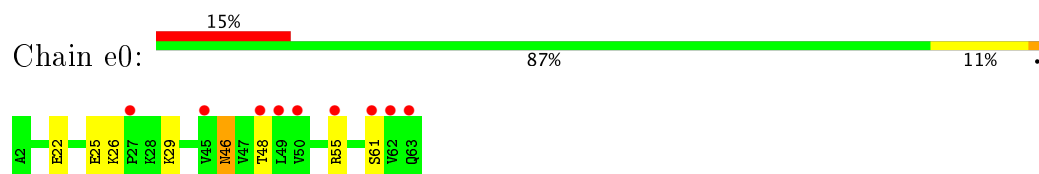
- Molecule 79: 40S ribosomal protein S29-A



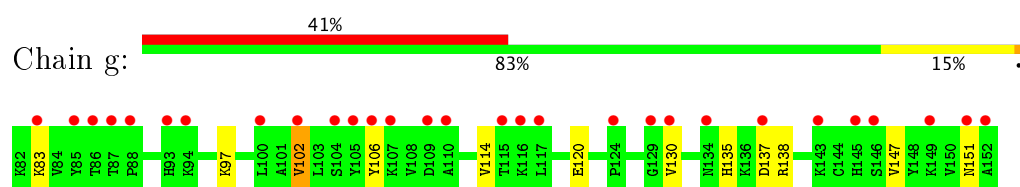
- Molecule 80: 40S ribosomal protein S30-A



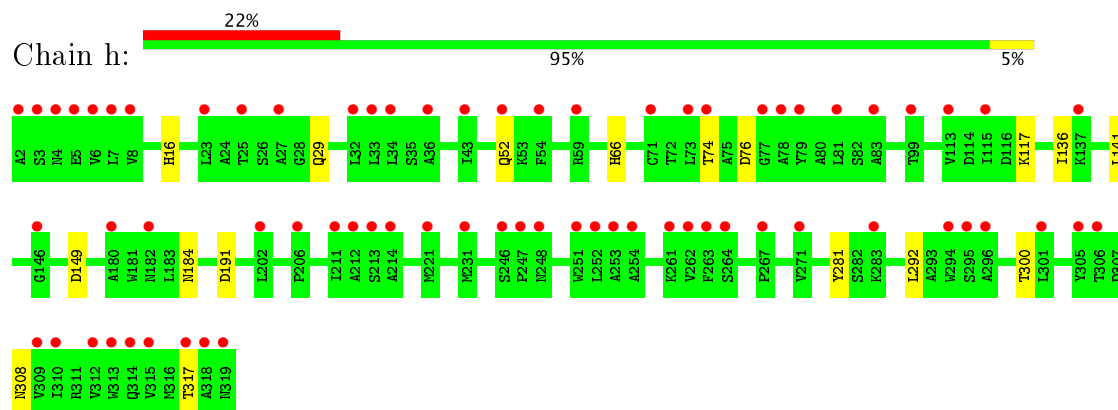
- Molecule 80: 40S ribosomal protein S30-A



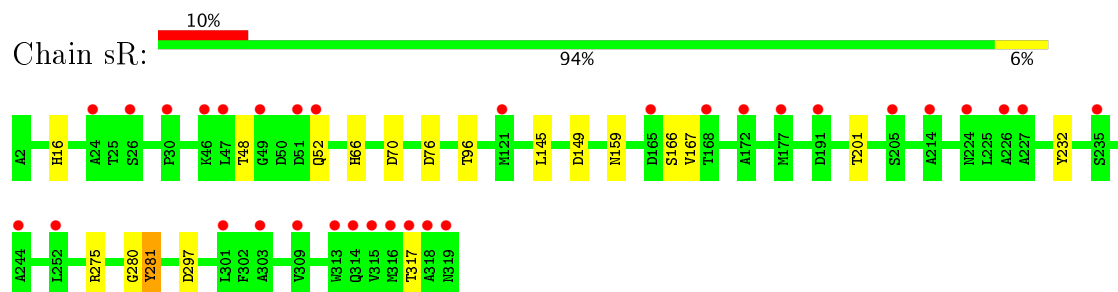
- Molecule 81: Ubiquitin-40S ribosomal protein S31



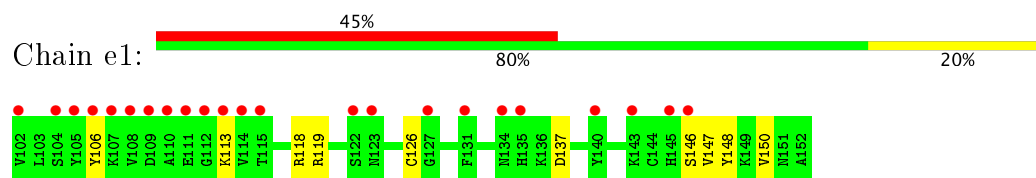
- Molecule 82: Guanine nucleotide-binding protein subunit beta-like protein



- Molecule 82: Guanine nucleotide-binding protein subunit beta-like protein



- 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, $\alpha$ , $\beta$ , $\gamma$	303.13Å 286.50Å 435.66Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	99.84 – 3.10 99.94 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (99.84-3.10) 99.5 (99.94-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 3.13Å)	Xtriage
Refinement program	PHENIX dev_2450	Depositor
R, $R_{free}$	0.222 , 0.252 0.228 , 0.257	Depositor DCC
$R_{free}$ test set	26196 reflections (2.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.3	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 69.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	410383	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, ZN, OHX, MG, HN8

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	0.60	1/75394 (0.0%)	1.02	117/117545 (0.1%)
1	AR	0.61	0/75394	1.03	127/117545 (0.1%)
2	3	0.51	0/2883	0.88	0/4491
2	AS	0.57	0/2883	0.97	1/4491 (0.0%)
3	4	0.57	0/3746	0.97	0/5832
3	AT	0.50	0/3746	0.90	2/5832 (0.0%)
4	CD	0.36	0/1948	0.55	0/2617
4	j	0.39	0/1948	0.60	0/2617
5	CE	0.44	1/3146 (0.0%)	0.61	0/4228
5	k	0.39	0/3146	0.58	0/4228
6	CF	0.40	1/2800 (0.0%)	0.62	2/3790 (0.1%)
6	l	0.41	0/2800	0.62	2/3790 (0.1%)
7	CG	0.40	0/2425	0.55	0/3271
7	m	0.34	0/2425	0.53	0/3271
8	CH	0.41	0/1260	0.56	0/1694
8	n	0.39	0/1260	0.53	0/1694
9	CI	0.44	0/1821	0.61	1/2451 (0.0%)
9	o	0.43	0/1821	0.60	1/2451 (0.0%)
10	CJ	0.32	0/1836	0.48	0/2481
10	p	0.32	0/1836	0.49	0/2481
11	CK	0.40	0/1539	0.57	0/2073
11	q	0.39	0/1539	0.56	0/2073
12	CL	0.42	0/1741	0.57	1/2335 (0.0%)
12	r	0.42	0/1741	0.57	1/2335 (0.0%)
13	CM	0.41	1/1374 (0.1%)	0.60	1/1842 (0.1%)
13	s	0.33	0/1374	0.56	0/1842
14	CN	0.39	1/1568 (0.1%)	0.58	1/2106 (0.0%)
14	t	0.42	1/1568 (0.1%)	0.57	0/2106
15	CO	0.40	0/1068	0.59	1/1438 (0.1%)
15	u	0.40	0/1068	0.55	0/1438
16	CP	0.35	0/1757	0.53	0/2354
16	v	0.39	0/1757	0.58	0/2354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	CQ	0.51	0/1585	0.61	2/2128 (0.1%)
17	w	0.46	0/1585	0.59	0/2128
18	CR	0.45	0/1443	0.61	0/1944
18	x	0.42	0/1443	0.61	1/1944 (0.1%)
19	CS	0.41	0/1465	0.58	0/1965
19	y	0.40	0/1465	0.60	1/1965 (0.1%)
20	CT	0.34	0/1538	0.49	0/2050
20	z	0.32	0/1538	0.47	0/2050
21	0	0.40	0/1481	0.58	0/1990
21	CU	0.44	0/1481	0.59	0/1990
22	2	0.40	0/1300	0.57	0/1743
22	CV	0.46	0/1300	0.58	0/1743
23	5	0.30	0/812	0.47	0/1099
23	CW	0.35	0/812	0.51	0/1099
24	CX	0.46	0/1018	0.59	0/1369
24	lR	0.41	0/1018	0.58	0/1369
25	6	0.43	0/42490	0.88	37/66207 (0.1%)
25	A	0.39	0/42443	0.87	34/66134 (0.1%)
26	7	0.35	0/712	0.50	0/958
26	CY	0.38	0/712	0.54	0/958
27	8	0.35	0/979	0.55	0/1321
27	CZ	0.35	0/979	0.52	0/1321
28	9	0.37	0/1004	0.58	0/1341
28	DA	0.38	0/1004	0.55	0/1341
29	AA	0.36	0/1118	0.50	0/1497
29	DB	0.47	1/1118 (0.1%)	0.48	0/1497
30	AB	0.43	0/1204	0.64	0/1612
30	DC	0.39	0/1204	0.62	0/1612
31	AC	0.34	0/473	0.54	0/629
31	DD	0.39	0/473	0.57	0/629
32	AD	0.30	0/751	0.48	0/1008
32	DE	0.30	0/751	0.47	0/1008
33	AE	0.39	0/890	0.54	0/1196
33	DF	0.37	0/890	0.55	0/1196
34	AF	0.42	0/1041	0.59	0/1394
34	DG	0.42	0/1041	0.57	0/1394
35	AG	0.47	0/868	0.57	0/1168
35	DH	0.46	0/868	0.62	0/1168
36	AH	0.36	0/890	0.57	1/1189 (0.1%)
36	DI	0.35	0/890	0.54	0/1189
37	AI	0.37	0/978	0.53	0/1301
37	DJ	0.35	0/978	0.52	1/1301 (0.1%)
38	AJ	0.33	0/778	0.52	0/1034

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DK	0.32	0/778	0.51	0/1034
39	AK	0.39	0/696	0.60	0/923
39	DL	0.39	0/696	0.58	0/923
40	AL	0.34	0/618	0.50	0/826
40	DM	0.32	0/618	0.49	0/826
41	AM	0.40	0/443	0.59	0/588
41	DN	0.36	0/443	0.59	0/588
42	AN	0.44	0/423	0.56	0/562
42	DO	0.43	0/423	0.60	0/562
43	AO	0.36	0/234	0.62	0/300
43	DP	0.39	0/234	0.51	0/300
44	AP	0.41	0/860	0.59	0/1136
44	DQ	0.41	0/860	0.59	0/1136
45	AQ	0.40	0/701	0.56	0/934
45	DR	0.39	0/701	0.58	0/934
46	i	0.31	0/1113	0.54	1/1502 (0.1%)
48	sM	0.34	0/480	0.58	0/642
49	p0	0.30	0/1091	0.53	2/1472 (0.1%)
50	B	0.29	0/1617	0.51	0/2215
50	s0	0.36	1/1623 (0.1%)	0.49	0/2222
51	C	0.27	0/1735	0.54	0/2335
51	s1	0.30	0/1748	0.55	1/2352 (0.0%)
52	D	0.30	0/1665	0.50	0/2263
52	s2	0.31	0/1665	0.52	0/2263
53	E	0.30	0/1759	0.51	0/2368
53	s3	0.28	0/1759	0.50	0/2368
54	F	0.31	0/2109	0.53	0/2839
54	s4	0.36	1/2109 (0.0%)	0.52	0/2839
55	G	0.27	0/1629	0.50	0/2202
55	s5	0.29	0/1629	0.47	0/2202
56	H	0.32	0/1823	0.51	1/2439 (0.0%)
56	s6	0.32	0/1779	0.53	0/2379
57	I	0.30	0/1506	0.52	0/2028
57	s7	0.30	0/1516	0.51	0/2043
58	J	0.31	0/1514	0.57	1/2021 (0.0%)
58	s8	0.33	0/1514	0.53	0/2021
59	K	0.29	0/1519	0.49	0/2035
59	s9	0.30	0/1519	0.49	0/2035
60	L	0.29	0/789	0.57	1/1067 (0.1%)
60	c0	0.27	0/775	0.62	3/1045 (0.3%)
61	M	0.33	0/1239	0.52	0/1673
61	c1	0.34	0/1194	0.52	0/1610
62	N	0.30	0/898	0.62	0/1220



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
62	c2	0.35	1/898 (0.1%)	0.62	1/1220 (0.1%)
63	O	0.31	0/1215	0.49	0/1638
63	c3	0.32	0/1215	0.53	0/1638
64	P	0.28	0/901	0.54	0/1217
64	c4	0.32	0/960	0.55	0/1290
65	Q	0.31	0/998	0.49	0/1341
65	c5	0.29	0/1060	0.60	0/1426
66	R	0.29	0/1125	0.55	0/1510
66	c6	0.29	0/1131	0.54	0/1518
67	S	0.29	0/935	0.52	0/1254
67	c7	0.28	0/914	0.48	0/1224
68	T	0.29	0/1211	0.50	0/1628
68	c8	0.29	0/1211	0.50	0/1628
69	U	0.29	0/1130	0.46	0/1517
69	c9	0.29	0/1130	0.46	0/1517
70	V	0.27	0/865	0.51	0/1169
70	d0	0.29	0/892	0.52	0/1205
71	W	0.31	0/693	0.50	0/935
71	d1	0.30	0/693	0.51	0/935
72	X	0.30	0/1038	0.55	0/1395
72	d2	0.31	0/1038	0.52	0/1395
73	Y	0.33	0/1139	0.55	0/1518
73	d3	0.35	0/1139	0.54	0/1518
74	Z	0.31	0/1087	0.49	0/1449
74	d4	0.32	0/1087	0.54	0/1449
75	a	0.29	0/571	0.53	0/768
75	d5	0.27	0/566	0.46	0/761
76	b	0.34	0/782	0.61	0/1047
76	d6	0.33	0/782	0.60	0/1047
77	c	0.27	0/620	0.54	0/838
77	d7	0.28	0/620	0.54	0/838
78	d	0.43	1/499 (0.2%)	0.53	0/670
78	d8	0.28	0/499	0.62	0/670
79	d9	0.33	0/452	0.51	0/600
79	e	0.30	0/452	0.50	0/600
80	e0	0.32	0/499	0.49	0/665
80	f	0.29	0/483	0.48	0/643
81	g	0.29	0/577	0.58	0/770
82	h	0.26	0/2494	0.49	0/3393
82	sR	0.27	0/2495	0.50	0/3395
83	e1	0.27	0/404	0.56	0/542
All	All	0.47	11/429967 (0.0%)	0.83	346/631328 (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
5	CE	0	3
5	k	0	2
6	l	0	2
7	CG	0	3
7	m	0	1
9	CI	0	2
9	o	0	2
10	CJ	0	2
10	p	0	1
11	CK	0	1
11	q	0	1
12	CL	0	1
13	CM	0	2
13	s	0	2
14	CN	0	1
14	t	0	2
15	CO	0	1
15	u	0	1
16	CP	0	1
17	CQ	0	1
17	w	0	1
18	x	0	1
19	CS	0	1
21	CU	0	2
26	CY	0	1
29	AA	0	2
30	DC	0	2
31	AC	0	1
31	DD	0	1
37	AI	0	1
37	DJ	0	1
50	B	0	1
51	s1	0	1
53	E	0	2
53	s3	0	2
55	G	0	3
55	s5	0	1
56	H	0	2
57	I	0	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
57	s7	0	2
58	J	0	2
58	s8	0	2
59	K	0	1
60	c0	0	1
61	M	0	1
62	N	0	1
62	c2	0	2
63	c3	0	2
64	P	0	1
64	c4	0	2
65	Q	0	1
65	c5	0	2
66	R	0	2
66	c6	0	4
67	S	0	1
67	c7	0	2
68	T	0	3
68	c8	0	1
70	d0	0	1
74	d4	0	1
75	a	0	2
76	b	0	2
80	e0	0	1
81	g	0	1
82	sR	0	1
83	e1	0	1
All	All	0	103

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	DB	36	HIS	C-N	11.46	1.56	1.34
54	s4	82	TYR	C-N	-8.48	1.18	1.34
14	t	132	ALA	C-N	8.06	1.49	1.34
50	s0	160	ILE	C-N	-7.98	1.19	1.34
78	d	5	THR	C-N	7.62	1.48	1.34
62	c2	81	ASP	C-N	6.82	1.47	1.34
5	CE	168	LYS	C-N	-6.50	1.19	1.34
13	CM	43	GLN	C-N	6.35	1.48	1.34
6	CF	94	CYS	CB-SG	-5.58	1.72	1.81
14	CN	49	ARG	C-N	5.20	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1308	A	N7-C5	-5.02	1.36	1.39

All (346) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3278	C	N1-C2-O2	10.14	124.98	118.90
1	1	2373	A	O5'-P-OP1	-9.82	96.86	105.70
1	1	1308	A	C8-N9-C4	-8.98	102.21	105.80
1	AR	2846	U	N3-C2-O2	-8.79	116.05	122.20
1	AR	2714	G	N3-C4-C5	8.71	132.95	128.60
1	AR	2870	C	C2-N1-C1'	-8.67	109.26	118.80
1	1	3278	C	N3-C2-O2	-8.64	115.86	121.90
1	1	2870	C	C2-N1-C1'	-8.61	109.33	118.80
1	AR	1307	G	P-O3'-C3'	8.57	129.98	119.70
1	AR	3217	C	N1-C2-O2	8.51	124.01	118.90
1	AR	3344	A	N7-C8-N9	8.48	118.04	113.80
1	AR	2726	C	C6-N1-C2	-8.34	116.96	120.30
1	1	3217	C	C2-N1-C1'	8.29	127.91	118.80
1	1	1308	A	N7-C8-N9	8.01	117.81	113.80
1	1	1192	C	N1-C2-O2	8.00	123.70	118.90
1	1	1495	U	C5-C6-N1	-7.96	118.72	122.70
25	6	453	U	N1-C2-O2	7.92	128.34	122.80
1	AR	2714	G	N3-C4-N9	-7.89	121.27	126.00
1	1	406	G	O4'-C1'-N9	7.88	114.51	108.20
1	AR	2846	U	C5-C4-O4	7.85	130.61	125.90
1	1	3217	C	N3-C2-O2	-7.85	116.41	121.90
1	1	1495	U	N1-C2-O2	-7.85	117.31	122.80
1	AR	2404	A	N1-C6-N6	7.82	123.29	118.60
1	AR	3344	A	C8-N9-C4	-7.77	102.69	105.80
1	1	2870	C	C6-N1-C1'	7.60	129.92	120.80
1	1	3217	C	N1-C2-O2	7.53	123.42	118.90
1	AR	1149	G	N1-C6-O6	7.53	124.42	119.90
1	AR	2871	G	O5'-P-OP2	-7.52	98.93	105.70
1	1	3278	C	C2-N1-C1'	7.51	127.06	118.80
1	1	3306	U	C5-C4-O4	7.47	130.38	125.90
1	AR	2870	C	C6-N1-C1'	7.43	129.71	120.80
1	AR	1495	U	C5-C6-N1	-7.36	119.02	122.70
25	6	453	U	C2-N1-C1'	7.32	126.48	117.70
1	AR	3217	C	C2-N1-C1'	7.27	126.79	118.80
1	AR	3306	U	N3-C2-O2	-7.22	117.14	122.20
25	6	163	G	N3-C4-N9	-7.20	121.68	126.00
25	6	453	U	N3-C2-O2	-7.19	117.17	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2846	U	N3-C2-O2	-7.18	117.17	122.20
1	1	1858	A	C2-N3-C4	7.11	114.15	110.60
51	s1	231	LEU	CA-CB-CG	6.98	131.35	115.30
60	c0	97	PRO	N-CA-CB	6.97	111.67	103.30
1	AR	3057	U	C5-C4-O4	6.95	130.07	125.90
25	A	553	G	N1-C6-O6	6.95	124.07	119.90
25	A	507	U	C2-N1-C1'	6.91	125.99	117.70
1	1	3306	U	N3-C2-O2	-6.91	117.37	122.20
1	AR	3217	C	N3-C2-O2	-6.87	117.09	121.90
1	1	937	G	C5-C6-O6	-6.86	124.48	128.60
1	1	1269	U	C2-N1-C1'	6.84	125.91	117.70
25	6	1274	C	N1-C2-O2	6.75	122.95	118.90
1	AR	2263	C	C4-C5-C6	-6.73	114.04	117.40
1	AR	3093	C	N1-C2-O2	-6.71	114.87	118.90
1	1	2726	C	C6-N1-C2	-6.69	117.62	120.30
1	1	1849	C	O5'-P-OP1	-6.68	99.69	105.70
60	c0	88	PRO	N-CA-CB	6.67	111.30	103.30
1	AR	2726	C	N3-C2-O2	-6.65	117.24	121.90
25	6	1274	C	C2-N1-C1'	6.65	126.11	118.80
1	AR	2819	A	O5'-P-OP2	-6.64	99.72	105.70
25	A	577	G	N1-C6-O6	6.62	123.87	119.90
1	AR	2808	A	C8-N9-C4	6.59	108.44	105.80
1	1	3217	C	C6-N1-C2	-6.58	117.67	120.30
1	1	1307	G	P-O3'-C3'	6.57	127.58	119.70
1	AR	2617	U	C4-C5-C6	6.57	123.64	119.70
1	1	407	A	N1-C6-N6	6.56	122.54	118.60
1	AR	2257	C	C2-N1-C1'	6.55	126.00	118.80
1	AR	2404	A	N7-C8-N9	6.55	117.07	113.80
6	1	327	LEU	CA-CB-CG	6.50	130.26	115.30
25	A	553	G	C5-C6-O6	-6.49	124.71	128.60
25	A	728	U	C2-N1-C1'	6.47	125.46	117.70
1	1	2726	C	C5-C4-N4	6.45	124.72	120.20
25	A	577	G	C5-C6-O6	-6.45	124.73	128.60
1	AR	1495	U	C5-C4-O4	6.43	129.76	125.90
1	AR	2272	G	O4'-C1'-N9	6.43	113.35	108.20
1	1	2620	G	N1-C6-O6	6.42	123.75	119.90
25	A	639	U	N3-C2-O2	-6.41	117.71	122.20
1	1	3306	U	N3-C4-O4	-6.40	114.92	119.40
25	6	813	U	N1-C2-O2	6.40	127.28	122.80
1	AR	3344	A	C5-N7-C8	-6.38	100.71	103.90
1	1	1192	C	C2-N1-C1'	6.38	125.81	118.80
1	AR	2870	C	N3-C4-C5	6.37	124.45	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1160	C	C6-N1-C2	6.37	122.85	120.30
1	1	2827	U	C5-C6-N1	-6.37	119.52	122.70
25	A	507	U	N1-C2-O2	6.34	127.24	122.80
49	p0	278	PRO	N-CA-CB	6.33	110.89	103.30
1	1	1556	C	N1-C2-O2	6.32	122.69	118.90
25	A	507	U	N3-C2-O2	-6.31	117.78	122.20
1	1	2870	C	N1-C2-O2	-6.31	115.12	118.90
1	1	65	A	P-O3'-C3'	6.29	127.25	119.70
60	L	88	PRO	N-CA-CB	6.26	110.81	103.30
25	6	813	U	C2-N1-C1'	6.25	125.21	117.70
1	1	1495	U	N1-C2-N3	6.25	118.65	114.90
1	1	3278	C	C6-N1-C2	-6.22	117.81	120.30
1	AR	1311	G	O5'-P-OP2	-6.21	100.11	105.70
56	H	69	LEU	CA-CB-CG	6.20	129.56	115.30
6	CF	182	LEU	CA-CB-CG	6.20	129.56	115.30
1	1	3181	C	N3-C2-O2	-6.17	117.58	121.90
1	1	1495	U	C2-N1-C1'	-6.16	110.31	117.70
1	1	353	G	C5-C6-O6	-6.15	124.91	128.60
1	AR	2257	C	C6-N1-C2	-6.14	117.84	120.30
25	A	959	U	C2-N1-C1'	6.14	125.07	117.70
1	AR	3309	G	N3-C4-N9	6.14	129.68	126.00
1	AR	3057	U	N3-C2-O2	-6.13	117.91	122.20
12	r	57	LEU	CA-CB-CG	6.12	129.37	115.30
1	1	2281	A	O4'-C1'-N9	6.09	113.07	108.20
1	AR	3309	G	C4-N9-C1'	6.09	134.41	126.50
1	AR	2899	C	C6-N1-C2	-6.08	117.87	120.30
46	i	254	PRO	N-CA-CB	6.07	110.58	103.30
1	AR	637	C	C6-N1-C2	-6.06	117.88	120.30
25	A	1389	C	C2-N1-C1'	6.06	125.46	118.80
1	AR	1495	U	C4-C5-C6	6.04	123.33	119.70
14	CN	46	ILE	C-N-CA	6.04	136.81	121.70
1	AR	3057	U	N3-C4-O4	-6.04	115.17	119.40
1	1	2257	C	C2-N1-C1'	6.03	125.43	118.80
1	AR	2950	G	O4'-C1'-N9	6.03	113.02	108.20
25	6	1389	C	C2-N1-C1'	6.02	125.42	118.80
1	AR	637	C	C2-N1-C1'	6.02	125.42	118.80
1	1	1329	U	C2-N1-C1'	6.01	124.91	117.70
1	1	3344	A	N7-C8-N9	5.99	116.79	113.80
1	AR	1103	A	O4'-C1'-N9	5.98	112.98	108.20
1	AR	2726	C	C5-C4-N4	5.96	124.37	120.20
1	1	2355	G	N1-C6-O6	5.95	123.47	119.90
1	1	1820	U	P-O3'-C3'	5.95	126.84	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AR	2343	C	C6-N1-C2	5.94	122.68	120.30
1	AR	437	G	N7-C8-N9	5.94	116.07	113.10
1	AR	2846	U	N3-C4-O4	-5.93	115.25	119.40
1	AR	2714	G	C2-N3-C4	-5.91	108.94	111.90
25	A	1274	C	C6-N1-C2	-5.91	117.94	120.30
1	AR	2404	A	C5-N7-C8	-5.90	100.95	103.90
1	1	1269	U	N1-C2-O2	5.90	126.93	122.80
25	A	1560	U	N3-C2-O2	-5.90	118.07	122.20
25	6	163	G	N3-C4-C5	5.89	131.54	128.60
1	AR	2996	U	N1-C2-O2	5.88	126.92	122.80
1	1	1858	A	C8-N9-C4	-5.87	103.45	105.80
49	p0	290	PRO	N-CA-CB	5.84	110.31	103.30
25	A	728	U	N1-C2-O2	5.82	126.88	122.80
1	1	835	G	O4'-C1'-N9	5.82	112.86	108.20
17	CQ	68	ARG	NE-CZ-NH1	-5.81	117.40	120.30
1	AR	3309	G	C6-C5-N7	-5.80	126.92	130.40
1	AR	637	C	P-O3'-C3'	5.79	126.65	119.70
1	AR	2899	C	N3-C2-O2	-5.79	117.85	121.90
1	1	3214	U	N3-C2-O2	-5.79	118.15	122.20
1	AR	2385	G	N3-C4-C5	5.79	131.49	128.60
1	1	1858	A	N3-C4-C5	-5.78	122.76	126.80
1	AR	2404	A	C6-C5-N7	-5.77	128.26	132.30
25	6	795	U	N3-C2-O2	-5.76	118.17	122.20
25	A	720	G	OP1-P-O3'	5.76	117.86	105.20
1	1	895	A	N1-C6-N6	5.75	122.05	118.60
1	1	2714	G	N3-C4-C5	5.75	131.47	128.60
1	AR	637	C	C5-C6-N1	5.74	123.87	121.00
25	A	959	U	N3-C2-O2	-5.72	118.19	122.20
1	1	1556	C	N3-C2-O2	-5.72	117.90	121.90
1	AR	407	A	N1-C6-N6	5.71	122.03	118.60
25	6	965	U	N1-C2-O2	5.70	126.79	122.80
1	AR	1556	C	C2-N1-C1'	5.70	125.07	118.80
1	AR	1149	G	C5-C6-O6	-5.70	125.18	128.60
1	1	1581	C	N1-C2-O2	5.69	122.32	118.90
1	AR	2662	G	N1-C6-O6	-5.69	116.49	119.90
1	1	895	A	C6-C5-N7	-5.68	128.32	132.30
1	1	2871	G	O5'-P-OP2	-5.68	100.58	105.70
25	A	453	U	C2-N1-C1'	5.68	124.52	117.70
25	A	959	U	N1-C2-O2	5.68	126.78	122.80
1	1	2169	G	N1-C6-O6	-5.67	116.50	119.90
1	AR	3344	A	O4'-C1'-N9	5.67	112.73	108.20
1	1	2808	A	N1-C6-N6	5.66	122.00	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1456	C	C2-N1-C1'	5.66	125.03	118.80
1	1	3344	A	O4'-C1'-N9	5.66	112.73	108.20
15	CO	72	LEU	CA-CB-CG	5.65	128.29	115.30
1	1	218	G	O5'-P-OP2	-5.64	100.62	105.70
25	A	639	U	N1-C2-O2	5.64	126.75	122.80
25	A	1698	G	P-O3'-C3'	5.62	126.44	119.70
1	AR	1103	A	P-O3'-C3'	5.62	126.44	119.70
1	AR	2617	U	C5-C6-N1	-5.62	119.89	122.70
1	1	2314	U	C5-C4-O4	-5.59	122.55	125.90
1	1	1149	G	N1-C6-O6	5.58	123.25	119.90
25	A	1039	A	O4'-C1'-N9	5.57	112.66	108.20
1	1	2899	C	C6-N1-C2	-5.57	118.07	120.30
25	A	75	U	N1-C2-O2	5.56	126.69	122.80
1	1	2726	C	N3-C2-O2	-5.55	118.01	121.90
1	1	770	G	O4'-C1'-N9	5.55	112.64	108.20
1	AR	2808	A	N9-C4-C5	-5.54	103.58	105.80
1	1	1377	G	C5-C6-O6	-5.53	125.28	128.60
1	AR	2714	G	C5-N7-C8	-5.53	101.53	104.30
1	AR	2334	U	N3-C2-O2	-5.53	118.33	122.20
1	AR	3309	G	C8-N9-C1'	-5.51	119.84	127.00
25	6	337	G	C4-N9-C1'	5.50	133.66	126.50
1	AR	2358	A	C8-N9-C4	5.50	108.00	105.80
1	1	2627	C	C6-N1-C2	5.49	122.50	120.30
1	AR	3212	C	N1-C2-O2	-5.49	115.61	118.90
1	AR	2870	C	N1-C2-O2	-5.48	115.61	118.90
1	1	979	U	P-O3'-C3'	5.48	126.27	119.70
25	6	1473	U	C2-N1-C1'	5.47	124.27	117.70
25	6	1473	U	N1-C2-O2	5.47	126.63	122.80
1	AR	3217	C	C6-N1-C1'	-5.46	114.24	120.80
1	AR	3181	C	N3-C2-O2	-5.46	118.08	121.90
1	AR	2281	A	O4'-C1'-N9	5.46	112.56	108.20
1	AR	1588	A	N1-C6-N6	-5.45	115.33	118.60
25	6	1097	U	P-O3'-C3'	5.45	126.24	119.70
60	c0	83	PRO	N-CA-CB	5.45	109.84	103.30
1	1	2550	U	N1-C2-O2	5.45	126.61	122.80
1	1	2944	U	C5-C4-O4	-5.45	122.63	125.90
1	AR	979	U	P-O3'-C3'	5.45	126.23	119.70
25	6	1473	U	N3-C2-O2	-5.44	118.39	122.20
1	AR	1605	A	O4'-C1'-N9	5.44	112.55	108.20
1	1	2286	U	O5'-P-OP2	-5.44	100.81	105.70
1	AR	2617	U	N3-C2-O2	-5.44	118.39	122.20
25	A	1761	U	P-O3'-C3'	5.44	126.22	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3057	U	N3-C2-O2	-5.43	118.40	122.20
1	AR	2263	C	N3-C4-C5	5.43	124.07	121.90
1	1	646	A	O5'-P-OP2	-5.43	100.82	105.70
25	6	610	G	C4-N9-C1'	5.42	133.55	126.50
25	6	1000	C	C2-N1-C1'	5.42	124.77	118.80
25	6	1389	C	N1-C2-O2	5.42	122.16	118.90
1	AR	2816	G	C8-N9-C4	5.42	108.57	106.40
17	CQ	84	LEU	CB-CG-CD1	-5.42	101.79	111.00
1	AR	881	C	N1-C2-O2	5.42	122.15	118.90
1	1	2374	C	N3-C2-O2	-5.41	118.11	121.90
25	A	1241	G	O4'-C1'-N9	5.41	112.53	108.20
25	A	1370	U	P-O3'-C3'	5.41	126.19	119.70
25	6	25	C	P-O3'-C3'	5.41	126.19	119.70
1	1	776	U	C4-C5-C6	5.40	122.94	119.70
1	1	1556	C	C2-N1-C1'	5.40	124.74	118.80
1	AR	895	A	C6-C5-N7	-5.40	128.52	132.30
1	1	937	G	N1-C6-O6	5.40	123.14	119.90
1	1	66	A	O5'-P-OP1	-5.39	100.85	105.70
1	1	1604	G	C4-N9-C1'	5.39	133.51	126.50
1	AR	65	A	P-O3'-C3'	5.39	126.17	119.70
1	AR	3057	U	N1-C2-N3	5.39	118.14	114.90
25	6	1560	U	C2-N1-C1'	5.39	124.16	117.70
1	AR	2541	U	P-O3'-C3'	5.38	126.16	119.70
1	AR	406	G	O4'-C1'-N9	5.38	112.50	108.20
1	AR	1097	G	P-O3'-C3'	5.38	126.16	119.70
25	A	610	G	C4-N9-C1'	5.38	133.49	126.50
1	1	3217	C	C6-N1-C1'	-5.37	114.35	120.80
1	AR	3344	A	C6-C5-N7	-5.37	128.54	132.30
1	1	1367	G	N1-C6-O6	5.36	123.12	119.90
9	o	179	LEU	CA-CB-CG	5.35	127.61	115.30
1	AR	1495	U	N1-C2-N3	5.35	118.11	114.90
25	A	158	U	P-O3'-C3'	5.35	126.12	119.70
25	6	158	U	P-O3'-C3'	5.35	126.12	119.70
36	AH	51	LEU	CA-CB-CG	5.35	127.60	115.30
1	AR	1192	C	N1-C2-O2	5.34	122.10	118.90
1	AR	1886	A	O5'-P-OP2	-5.34	100.89	105.70
1	1	1269	U	N3-C2-O2	-5.33	118.47	122.20
1	AR	2273	G	C8-N9-C4	5.33	108.53	106.40
1	1	353	G	N1-C6-O6	5.33	123.10	119.90
1	AR	437	G	C8-N9-C4	-5.33	104.27	106.40
1	1	1114	U	N1-C2-O2	5.32	126.52	122.80
25	6	1773	C	N3-C4-C5	-5.31	119.78	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	422	A	N1-C6-N6	-5.31	115.41	118.60
1	AR	2257	C	O4'-C1'-N1	5.30	112.44	108.20
1	1	1495	U	C4-C5-C6	5.30	122.88	119.70
25	A	1196	A	P-O3'-C3'	5.30	126.06	119.70
25	6	542	A	P-O3'-C3'	5.30	126.06	119.70
1	1	1196	C	C6-N1-C2	5.29	122.42	120.30
1	AR	1556	C	N1-C2-O2	5.29	122.07	118.90
25	6	1137	A	C8-N9-C4	5.27	107.91	105.80
1	1	497	C	N1-C2-O2	-5.27	115.74	118.90
1	AR	2679	A	C2-N3-C4	-5.27	107.97	110.60
1	1	3275	U	OP1-P-O3'	5.26	116.78	105.20
25	6	610	G	C8-N9-C1'	-5.26	120.16	127.00
13	CM	172	LEU	C-N-CA	5.26	134.85	121.70
1	AR	3309	G	N3-C4-C5	-5.26	125.97	128.60
1	1	3362	A	O4'-C1'-N9	5.25	112.40	108.20
1	1	651	G	N3-C4-N9	5.25	129.15	126.00
19	y	41	ASP	CB-CG-OD1	5.25	123.02	118.30
1	1	1897	G	C5-C6-O6	-5.25	125.45	128.60
1	AR	2899	C	N3-C4-C5	-5.24	119.80	121.90
1	1	922	U	N1-C2-O2	5.23	126.46	122.80
25	6	1058	U	OP1-P-O3'	5.23	116.70	105.20
1	AR	1149	G	C4-C5-C6	5.22	121.93	118.80
6	1	313	LEU	CA-CB-CG	5.22	127.31	115.30
1	AR	878	G	C8-N9-C4	-5.22	104.31	106.40
1	1	2550	U	N3-C2-O2	-5.22	118.55	122.20
1	1	936	A	P-O3'-C3'	5.22	125.96	119.70
1	AR	2943	G	N1-C6-O6	5.21	123.03	119.90
37	DJ	28	LEU	CA-CB-CG	5.21	127.29	115.30
25	6	1573	A	P-O3'-C3'	5.21	125.95	119.70
25	A	581	U	C2-N1-C1'	5.21	123.95	117.70
25	A	720	G	P-O3'-C3'	5.21	125.95	119.70
1	1	2358	A	N1-C6-N6	5.21	121.72	118.60
1	AR	1858	A	C4-N9-C1'	5.20	135.66	126.30
1	AR	3306	U	N3-C4-O4	-5.19	115.77	119.40
1	1	2827	U	C2-N3-C4	-5.18	123.89	127.00
1	AR	942	U	N3-C4-O4	5.18	123.03	119.40
58	J	29	LEU	CA-CB-CG	5.18	127.21	115.30
3	AT	82	U	C2-N1-C1'	5.18	123.91	117.70
1	1	2585	G	N3-C4-C5	-5.18	126.01	128.60
1	1	3344	A	C8-N9-C4	-5.17	103.73	105.80
1	AR	1521	G	N1-C6-O6	-5.17	116.80	119.90
1	1	1904	C	C6-N1-C2	-5.16	118.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AS	101	G	N1-C6-O6	5.16	122.99	119.90
1	AR	3214	U	C2-N1-C1'	5.16	123.89	117.70
62	c2	103	LEU	CA-CB-CG	5.16	127.16	115.30
1	AR	1496	C	C2-N1-C1'	5.15	124.47	118.80
1	AR	800	G	N3-C4-N9	5.15	129.09	126.00
1	1	2418	G	OP1-P-O3'	5.14	116.51	105.20
25	A	831	U	C5-C6-N1	5.14	125.27	122.70
25	6	1000	C	N3-C2-O2	-5.14	118.30	121.90
25	A	1060	U	N1-C2-O2	5.13	126.39	122.80
18	x	41	LEU	CA-CB-CG	5.13	127.10	115.30
1	1	1897	G	C6-C5-N7	-5.13	127.32	130.40
1	1	3277	U	N3-C2-O2	-5.13	118.61	122.20
1	AR	1151	U	N3-C2-O2	5.13	125.79	122.20
1	AR	2615	G	N9-C4-C5	-5.13	103.35	105.40
1	AR	1887	A	O5'-P-OP2	-5.12	101.09	105.70
3	AT	82	U	P-O3'-C3'	5.12	125.85	119.70
1	1	1002	A	N1-C6-N6	5.12	121.67	118.60
9	CI	179	LEU	CA-CB-CG	5.11	127.05	115.30
1	AR	2679	A	N1-C6-N6	5.11	121.67	118.60
1	1	2593	A	P-O3'-C3'	5.11	125.83	119.70
25	6	453	U	C6-N1-C1'	-5.11	114.05	121.20
25	6	1246	C	C2-N1-C1'	5.11	124.42	118.80
1	AR	1047	A	N1-C6-N6	5.11	121.66	118.60
1	1	2112	U	P-O3'-C3'	5.10	125.82	119.70
1	1	2400	G	N1-C6-O6	5.10	122.96	119.90
1	AR	895	A	C5-N7-C8	-5.10	101.35	103.90
1	AR	2869	U	C5-C4-O4	-5.09	122.84	125.90
25	6	795	U	C2-N1-C1'	5.08	123.80	117.70
1	AR	2679	A	O4'-C1'-N9	5.08	112.27	108.20
1	AR	3362	A	O4'-C1'-N9	5.08	112.26	108.20
1	AR	2808	A	N1-C6-N6	5.07	121.64	118.60
25	6	1274	C	N3-C2-O2	-5.07	118.35	121.90
1	1	2176	U	N3-C2-O2	-5.07	118.65	122.20
1	1	922	U	C2-N1-C1'	5.06	123.77	117.70
1	1	3209	A	N1-C6-N6	5.06	121.64	118.60
1	1	109	A	OP1-P-O3'	5.05	116.32	105.20
1	AR	2846	U	C6-N1-C2	-5.05	117.97	121.00
1	AR	3306	U	C5-C4-O4	5.05	128.93	125.90
25	A	1060	U	N3-C2-O2	-5.05	118.66	122.20
1	AR	2930	A	O4'-C1'-N9	5.05	112.24	108.20
25	6	1697	G	C4-N9-C1'	5.04	133.06	126.50
1	AR	1437	C	C2-N1-C1'	5.04	124.35	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AR	1483	G	O4'-C1'-N9	5.04	112.23	108.20
1	1	1495	U	C2-N3-C4	-5.04	123.98	127.00
6	CF	315	LYS	C-N-CA	-5.04	109.10	121.70
1	AR	2794	G	O4'-C1'-N9	5.04	112.23	108.20
1	AR	3278	C	C2-N1-C1'	5.04	124.34	118.80
12	CL	87	LEU	CA-CB-CG	5.04	126.88	115.30
1	AR	648	C	O5'-P-OP1	-5.03	101.17	105.70
1	1	2808	A	N9-C4-C5	-5.03	103.79	105.80
25	6	678	A	P-O3'-C3'	5.03	125.73	119.70
1	1	936	A	O4'-C1'-N9	5.02	112.21	108.20
1	1	2802	A	OP2-P-O3'	5.01	116.23	105.20
25	6	813	U	N3-C2-O2	-5.01	118.70	122.20
1	AR	2874	G	C5-C6-O6	5.00	131.60	128.60
1	1	2541	U	P-O3'-C3'	5.00	125.70	119.70
1	AR	3140	G	N1-C6-O6	5.00	122.90	119.90

There are no chirality outliers.

All (103) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	AA	102	GLU	Peptide
29	AA	124	ALA	Peptide
31	AC	19	ASN	Peptide
37	AI	83	LYS	Peptide
50	B	191	ARG	Peptide
5	CE	186	GLY	Peptide
5	CE	315	GLY	Peptide
5	CE	385	LYS	Peptide
7	CG	257	GLU	Peptide
7	CG	258	LYS	Peptide
7	CG	43	LYS	Peptide
9	CI	157	ASN	Peptide
9	CI	190	THR	Peptide
10	CJ	34	PHE	Peptide
10	CJ	35	GLY	Peptide
11	CK	21	LYS	Peptide
12	CL	218	ALA	Peptide
13	CM	172	LEU	Peptide
13	CM	73	GLY	Peptide
14	CN	4	SER	Peptide
15	CO	7	VAL	Peptide
16	CP	92	LEU	Peptide

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Mol	Chain	Res	Type	Group
17	CQ	110	PRO	Peptide
19	CS	98	LYS	Peptide
21	CU	133	ALA	Peptide
21	CU	22	PRO	Peptide
26	CY	80	ARG	Peptide
30	DC	115	LYS	Peptide
30	DC	45	MET	Peptide
31	DD	19	ASN	Peptide
37	DJ	118	ILE	Peptide
53	E	198	GLY	Peptide
53	E	216	PRO	Peptide
55	G	56	ALA	Peptide
55	G	58	LEU	Peptide
55	G	65	ARG	Peptide
56	H	148	SER	Peptide
56	H	67	VAL	Peptide
57	I	30	SER	Peptide
57	I	63	PRO	Peptide
58	J	146	ARG	Peptide
58	J	147	ALA	Peptide
59	K	163	PRO	Peptide
61	M	3	THR	Peptide
62	N	111	ASN	Peptide
64	P	41	ARG	Peptide
65	Q	124	THR	Peptide
66	R	14	LYS	Peptide
66	R	40	GLU	Peptide
67	S	84	TYR	Peptide
68	T	13	HIS	Peptide
68	T	144	ARG	Peptide
68	T	81	ILE	Peptide
75	a	87	GLY	Peptide
75	a	94	LYS	Peptide
76	b	10	ARG	Peptide
76	b	84	VAL	Peptide
60	c0	34	GLU	Peptide
62	c2	108	ARG	Peptide
62	c2	130	THR	Peptide
63	c3	22	ALA	Peptide
63	c3	65	VAL	Peptide
64	c4	11	SER	Peptide
64	c4	125	SER	Peptide

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Mol	Chain	Res	Type	Group
65	c5	134	THR	Peptide
65	c5	52	LYS	Peptide
66	c6	114	ARG	Peptide
66	c6	13	LYS	Peptide
66	c6	40	GLU	Peptide
66	c6	41	PRO	Peptide
67	c7	105	GLN	Peptide
67	c7	66	VAL	Peptide
68	c8	13	HIS	Peptide
70	d0	70	THR	Peptide
74	d4	29	HIS	Peptide
80	e0	46	ASN	Peptide
83	e1	146	SER	Peptide
81	g	102	VAL	Peptide
5	k	186	GLY	Peptide
5	k	349	LYS	Peptide
6	l	291	ASN	Peptide
6	l	338	LYS	Peptide
7	m	258	LYS	Peptide
9	o	157	ASN	Peptide
9	o	190	THR	Peptide
10	p	76	ALA	Peptide
11	q	21	LYS	Peptide
13	s	171	VAL	Peptide
13	s	94	ARG	Peptide
51	s1	146	GLN	Peptide
53	s3	144	ALA	Peptide
53	s3	216	PRO	Peptide
55	s5	44	ASN	Peptide
57	s7	130	VAL	Peptide
57	s7	63	PRO	Peptide
58	s8	100	ALA	Peptide
58	s8	148	ALA	Peptide
82	sR	280	GLY	Peptide
14	t	46	ILE	Peptide
14	t	47	ALA	Peptide
15	u	7	VAL	Peptide
17	w	110	PRO	Peptide
18	x	157	VAL	Peptide

## 5.2 Too-close contacts ⓘ

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	658	0
1	AR	67355	0	33845	844	0
2	3	2579	0	1304	20	0
2	AS	2579	0	1304	42	0
3	4	3353	0	1695	38	0
3	AT	3353	0	1695	45	0
4	CD	1914	0	1981	45	0
4	j	1914	0	1981	0	0
5	CE	3075	0	3141	105	0
5	k	3075	0	3142	0	0
6	CF	2748	0	2859	80	0
6	l	2748	0	2859	0	0
7	CG	2375	0	2325	73	0
7	m	2375	0	2325	0	0
8	CH	1239	0	1326	27	0
8	n	1239	0	1326	0	0
9	CI	1784	0	1862	45	0
9	o	1784	0	1862	0	0
10	CJ	1804	0	1877	45	0
10	p	1804	0	1877	0	0
11	CK	1518	0	1587	55	0
11	q	1518	0	1587	0	0
12	CL	1705	0	1736	54	0
12	r	1705	0	1736	0	0
13	CM	1353	0	1383	36	0
13	s	1353	0	1383	0	0
14	CN	1543	0	1608	57	0
14	t	1543	0	1608	0	0
15	CO	1053	0	1149	39	0
15	u	1053	0	1149	0	0
16	CP	1720	0	1779	41	0
16	v	1720	0	1779	0	0
17	CQ	1555	0	1659	49	0
17	w	1555	0	1659	0	0
18	CR	1420	0	1437	51	0
18	x	1420	0	1437	0	0
19	CS	1441	0	1543	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	y	1441	0	1543	0	0
20	CT	1521	0	1617	36	0
20	z	1521	0	1617	0	0
21	0	1445	0	1487	36	0
21	CU	1445	0	1487	37	0
22	2	1276	0	1323	32	0
22	CV	1276	0	1323	47	0
23	5	796	0	812	14	0
23	CW	796	0	812	17	0
24	CX	1003	0	1048	27	0
24	lR	1003	0	1048	0	0
25	6	37990	0	19115	356	0
25	A	37948	0	19094	563	0
26	7	699	0	640	10	0
26	CY	699	0	640	13	0
27	8	964	0	1025	23	0
27	CZ	964	0	1025	26	0
28	9	993	0	1081	25	0
28	DA	993	0	1081	30	0
29	AA	1092	0	1155	36	0
29	DB	1092	0	1155	35	0
30	AB	1173	0	1215	42	0
30	DC	1173	0	1215	46	0
31	AC	462	0	491	16	0
31	DD	462	0	491	13	0
32	AD	743	0	797	20	0
32	DE	743	0	797	15	0
33	AE	876	0	912	23	0
33	DF	876	0	912	23	0
34	AF	1020	0	1090	23	0
34	DG	1020	0	1090	24	0
35	AG	850	0	880	18	0
35	DH	850	0	880	23	0
36	AH	880	0	945	26	0
36	DI	880	0	945	26	0
37	AI	969	0	1078	23	0
37	DJ	969	0	1078	37	0
38	AJ	771	0	849	27	0
38	DK	771	0	849	13	0
39	AK	681	0	683	22	0
39	DL	681	0	683	27	0
40	AL	612	0	682	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DM	612	0	682	14	0
41	AM	436	0	475	18	0
41	DN	436	0	475	14	0
42	AN	417	0	455	11	0
42	DO	417	0	455	8	0
43	AO	233	0	284	9	0
43	DP	233	0	284	11	0
44	AP	847	0	914	14	0
44	DQ	847	0	915	16	0
45	AQ	694	0	734	21	0
45	DR	694	0	734	19	0
46	i	1104	0	1002	0	0
47	m2	750	0	172	0	0
48	sM	680	0	540	0	0
49	p0	1076	0	1076	0	0
50	B	1577	0	1567	58	0
50	s0	1583	0	1578	0	0
51	C	1709	0	1784	64	0
51	s1	1722	0	1793	0	0
52	D	1635	0	1723	62	0
52	s2	1635	0	1723	0	0
53	E	1734	0	1817	46	0
53	s3	1734	0	1817	0	0
54	F	2068	0	2154	69	0
54	s4	2068	0	2154	0	0
55	G	1609	0	1675	55	0
55	s5	1609	0	1675	0	0
56	H	1799	0	1878	56	0
56	s6	1755	0	1846	0	0
57	I	1481	0	1572	63	0
57	s7	1491	0	1578	0	0
58	J	1489	0	1525	48	0
58	s8	1489	0	1525	0	0
59	K	1494	0	1573	49	0
59	s9	1494	0	1573	0	0
60	L	772	0	727	27	0
60	c0	760	0	696	0	0
61	M	1213	0	1257	33	0
61	c1	1168	0	1233	0	0
62	N	890	0	887	25	0
62	c2	890	0	887	0	0
63	O	1192	0	1255	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	c3	1192	0	1255	0	0
64	P	891	0	883	33	0
64	c4	949	0	985	0	0
65	Q	977	0	1002	27	0
65	c5	1039	0	1050	0	0
66	R	1105	0	1166	40	0
66	c6	1111	0	1171	0	0
67	S	926	0	930	34	0
67	c7	906	0	909	0	0
68	T	1192	0	1222	30	0
68	c8	1192	0	1222	0	0
69	U	1112	0	1124	32	0
69	c9	1112	0	1124	0	0
70	V	855	0	917	40	0
70	d0	882	0	939	0	0
71	W	684	0	672	21	0
71	d1	684	0	672	0	0
72	X	1021	0	1060	36	0
72	d2	1021	0	1060	0	0
73	Y	1121	0	1196	37	0
73	d3	1121	0	1196	0	0
74	Z	1073	0	1132	39	0
74	d4	1073	0	1132	0	0
75	a	563	0	603	0	0
75	d5	558	0	598	0	0
76	b	769	0	814	0	0
76	d6	769	0	814	0	0
77	c	610	0	633	0	0
77	d7	610	0	633	0	0
78	d	497	0	535	0	0
78	d8	497	0	535	0	0
79	d9	442	0	429	0	0
79	e	442	0	428	0	0
80	e0	491	0	542	0	0
80	f	475	0	525	0	0
81	g	566	0	602	0	0
82	h	2441	0	2397	0	0
82	sR	2442	0	2392	0	0
83	e1	397	0	396	0	0
84	1	2262	0	0	17	0
84	2	7	0	0	0	0
84	3	63	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	4	112	0	0	0	0
84	6	1064	0	0	10	0
84	A	1001	0	0	10	0
84	AC	7	0	0	0	0
84	AG	7	0	0	0	0
84	AH	7	0	0	0	0
84	AK	7	0	0	0	0
84	AM	7	0	0	0	0
84	AP	7	0	0	0	0
84	AR	2415	0	0	36	0
84	AS	77	0	0	5	0
84	AT	119	0	0	2	0
84	CE	14	0	0	0	0
84	CF	14	0	0	0	0
84	CG	14	0	0	1	0
84	CK	7	0	0	0	0
84	CL	7	0	0	0	0
84	CM	7	0	0	0	0
84	CP	7	0	0	0	0
84	CV	7	0	0	0	0
84	CX	14	0	0	1	0
84	DD	7	0	0	0	0
84	DH	7	0	0	0	0
84	DQ	7	0	0	0	0
84	J	7	0	0	0	0
84	K	7	0	0	0	0
84	M	7	0	0	0	0
84	O	7	0	0	0	0
84	Q	7	0	0	0	0
84	T	7	0	0	0	0
84	c1	7	0	0	0	0
84	c3	7	0	0	0	0
84	c4	7	0	0	0	0
84	c5	7	0	0	0	0
84	c8	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	s8	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	sR	7	0	0	0	0
84	v	7	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	498	0	0	0	0
85	3	13	0	0	0	0
85	4	25	0	0	0	0
85	6	146	0	0	0	0
85	A	116	0	0	0	0
85	AB	7	0	0	0	0
85	AF	2	0	0	0	0
85	AG	1	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
85	AR	515	0	0	0	0
85	AS	20	0	0	0	0
85	AT	14	0	0	0	0
85	CD	2	0	0	0	0
85	CE	5	0	0	0	0
85	CF	1	0	0	0	0
85	CG	2	0	0	0	0
85	CI	1	0	0	0	0
85	CJ	1	0	0	0	0
85	CK	1	0	0	0	0
85	CL	1	0	0	0	0
85	CM	2	0	0	0	0
85	CO	1	0	0	0	0
85	CP	4	0	0	0	0
85	CQ	4	0	0	0	0
85	CR	5	0	0	0	0
85	CU	1	0	0	0	0
85	CX	2	0	0	0	0
85	D	1	0	0	0	0
85	DA	2	0	0	0	0
85	DC	4	0	0	0	0
85	DE	1	0	0	0	0
85	DH	2	0	0	0	0
85	DI	2	0	0	0	0
85	DL	1	0	0	0	0
85	DO	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	DQ	2	0	0	0	0
85	F	1	0	0	0	0
85	H	1	0	0	0	0
85	T	1	0	0	0	0
85	U	1	0	0	0	0
85	V	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	c8	1	0	0	0	0
85	c9	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	j	2	0	0	0	0
85	k	3	0	0	0	0
85	l	3	0	0	0	0
85	lR	1	0	0	0	0
85	n	1	0	0	0	0
85	o	2	0	0	0	0
85	r	1	0	0	0	0
85	s	1	0	0	0	0
85	s4	1	0	0	0	0
85	s6	1	0	0	0	0
85	s8	1	0	0	0	0
85	sM	2	0	0	0	0
85	t	3	0	0	0	0
85	v	3	0	0	0	0
85	w	2	0	0	0	0
85	x	7	0	0	0	0
85	z	1	0	0	0	0
86	1	22	0	0	0	0
86	AR	22	0	0	0	0
87	6	6	0	8	0	0
87	A	6	0	8	0	0
87	AR	12	0	14	3	0
87	v	6	0	8	0	0
88	AK	1	0	0	0	0
88	AN	1	0	0	0	0
88	AP	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	AQ	1	0	0	0	0
88	DL	1	0	0	0	0
88	DO	1	0	0	0	0
88	DQ	1	0	0	0	0
88	DR	1	0	0	0	0
88	b	1	0	0	0	0
88	c	1	0	0	0	0
88	d6	1	0	0	0	0
88	d7	1	0	0	0	0
88	d9	1	0	0	0	0
88	e	1	0	0	0	0
88	e1	1	0	0	0	0
88	g	1	0	0	0	0
All	All	410383	0	296944	4796	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 (4796) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1481:A:O2'	1:1:1858:A:N3	1.96	0.98
65:Q:68:PRO:HG2	65:Q:71:GLU:HB3	1.51	0.93
5:CE:296:THR:HG22	5:CE:298:PHE:H	1.35	0.91
1:AR:2108:C:H1'	1:AR:3344:A:H8	1.37	0.90
1:1:1230:G:H1	1:1:1279:C:H42	1.19	0.90
1:1:3343:G:H21	1:1:3362:A:H2	1.20	0.89
25:A:169:A:H5''	56:H:176:GLN:HG2	1.54	0.89
1:AR:3194:C:O2	1:AR:3197:G:N2	2.06	0.88
1:AR:2836:C:H5	1:AR:2852:C:H42	1.20	0.88
64:P:84:ARG:HE	64:P:84:ARG:H	7.20	0.88
1:AR:640:U:OP1	30:DC:21:ARG:NH2	2.07	0.87
5:CE:218:ILE:HG12	5:CE:276:THR:HG23	1.54	0.87
12:CL:174:THR:HG23	12:CL:176:LEU:H	1.36	0.87
1:AR:1639:C:OP2	36:DI:74:ARG:NH2	2.06	0.87
25:A:237:C:H5''	25:A:238:U:H5'	1.57	0.87
69:U:117:SER:HB2	69:U:123:ARG:HB2	1.55	0.87
1:1:1015:U:O2'	1:1:1017:C:OP2	1.93	0.87
14:CN:47:ALA:O	14:CN:49:ARG:N	2.07	0.87
25:A:885:G:H21	64:P:123:SER:HB2	1.39	0.87
59:K:109:LEU:HB2	59:K:146:PHE:HB3	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:AK:21:ARG:NH2	39:AK:41:ALA:O	2.08	0.86
57:I:11:GLN:HG3	57:I:13:PRO:HD2	1.57	0.86
5:CE:41:VAL:HA	5:CE:185:GLY:HA3	1.58	0.86
1:AR:2703:A:OP2	7:CG:23:ARG:NH1	2.09	0.85
25:6:1588:G:H1	25:6:1608:U:H3	1.22	0.85
27:CZ:57:LEU:HD12	27:CZ:61:LYS:HG2	1.59	0.85
2:AS:49:G:N7	7:CG:58:LYS:HG3	1.92	0.84
25:A:140:A:N6	25:A:281:G:OP1	2.10	0.84
6:CF:203:ARG:NH1	6:CF:226:GLU:OE2	2.11	0.84
1:1:3344:A:H2	1:1:3361:G:H21	1.22	0.83
1:1:1427:U:OP2	30:AB:4:ARG:NH2	2.11	0.83
52:D:38:VAL:HG13	52:D:39:THR:HG23	1.60	0.83
1:AR:1381:A:OP1	6:CF:197:ARG:NH1	2.12	0.83
25:6:895:G:H1	25:6:917:U:H3	1.26	0.82
37:DJ:78:LYS:HA	37:DJ:81:ARG:HD2	1.61	0.82
56:H:163:THR:HG22	56:H:168:THR:HG22	1.59	0.82
58:J:12:SER:HA	58:J:18:ARG:HH21	1.44	0.82
25:A:702:G:O6	25:A:736:C:N4	2.12	0.82
25:A:478:A:HO2'	59:K:124:HIS:HD1	1.28	0.82
74:Z:42:GLU:HG3	74:Z:52:LYS:HD3	1.61	0.81
1:1:640:U:OP1	30:AB:21:ARG:NH2	2.12	0.81
3:4:135:G:OP2	27:8:56:ARG:NH2	2.12	0.81
22:CV:39:ILE:HD12	22:CV:102:ARG:HD3	1.62	0.81
56:H:2:LYS:HB3	56:H:108:VAL:HG22	1.63	0.81
61:M:17:PRO:HG3	61:M:63:LEU:HD11	1.62	0.81
1:AR:3182:G:OP1	17:CQ:160:ARG:NH2	2.14	0.81
61:M:94:ILE:HG12	73:Y:16:ARG:HD2	1.61	0.81
58:J:57:ALA:HB2	58:J:177:GLY:HA2	1.62	0.81
1:AR:2268:U:H3'	1:AR:2269:U:H5''	1.63	0.81
1:AR:2356:A:OP1	18:CR:138:LYS:NZ	2.14	0.81
21:0:91:TYR:O	21:0:137:ARG:NH1	2.14	0.80
37:AI:101:THR:HG22	37:AI:104:GLN:H	1.46	0.80
26:7:39:LEU:HD12	26:7:44:LYS:HG3	1.62	0.80
25:A:895:G:H1	25:A:917:U:H3	1.29	0.80
1:AR:2108:C:H1'	1:AR:3344:A:C8	2.17	0.80
54:F:79:ASP:HB3	54:F:82:TYR:HB2	1.61	0.80
25:A:79:C:H1'	56:H:174:LYS:HD3	1.62	0.80
6:CF:20:LEU:HD11	6:CF:252:GLU:HG3	1.64	0.80
1:AR:2533:G:O6	1:AR:2546:C:N4	2.15	0.80
1:AR:1015:U:O2'	1:AR:1017:C:OP2	2.00	0.79
15:CO:55:ARG:NH2	15:CO:76:ALA:O	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:104:A:H61	25:6:308:C:H5'	1.46	0.79
25:A:1339:C:O2'	25:A:1341:A:N7	2.14	0.79
5:CE:169:THR:HG23	5:CE:171:LEU:H	1.48	0.79
33:DF:75:ILE:HG12	33:DF:93:VAL:HG13	1.63	0.79
1:1:1942:U:HO2'	1:1:3345:G:HO2'	1.29	0.78
1:AR:1565:G:N2	1:AR:1574:C:N3	2.32	0.78
55:G:94:THR:HG22	55:G:114:ILE:HG13	1.66	0.78
72:X:6:VAL:HG13	72:X:29:PRO:HD2	1.62	0.78
25:A:795:U:OP1	72:X:82:LYS:NZ	2.15	0.78
25:6:1595:U:H3	25:6:1600:A:H2	1.31	0.78
1:AR:283:G:OP2	44:DQ:45:ARG:NH2	2.16	0.78
6:CF:300:ARG:O	19:CS:39:ARG:NH1	2.17	0.78
1:1:1493:G:O6	41:AM:2:ALA:N	2.16	0.78
23:CW:19:VAL:HG12	23:CW:105:LEU:HD22	1.63	0.78
1:AR:2988:C:OP1	17:CQ:68:ARG:NH1	2.17	0.77
1:AR:2854:U:OP2	12:CL:3:ARG:NH2	2.17	0.77
25:A:753:A:H5'	54:F:221:ARG:HG3	1.66	0.77
14:CN:48:PRO:HA	14:CN:137:GLN:HB3	1.65	0.77
32:DE:13:LYS:HB3	32:DE:100:ILE:HG22	1.66	0.77
25:A:1473:U:O2'	55:G:103:ASN:ND2	2.17	0.77
25:A:487:G:H1	25:A:500:C:H42	1.32	0.77
7:CG:120:LYS:O	7:CG:248:ARG:NH2	2.16	0.77
1:1:2818:U:H6	1:1:2818:U:H5'	1.46	0.77
36:AH:41:ARG:HG2	36:AH:56:THR:HG21	1.66	0.77
51:C:129:THR:HA	51:C:177:GLN:HA	1.65	0.77
1:AR:31:C:OP2	16:CP:188:ARG:NH2	2.18	0.77
25:A:1595:U:H3	25:A:1600:A:H2	1.33	0.77
1:1:838:G:O6	45:AQ:4:ARG:NH2	2.18	0.76
56:H:120:GLU:HG3	56:H:125:THR:HB	1.67	0.76
1:AR:72:C:H5'	14:CN:63:VAL:HG22	1.65	0.76
52:D:137:ILE:HG12	52:D:138:PRO:HD2	1.68	0.76
15:CO:113:THR:HG23	15:CO:116:GLU:H	1.50	0.76
1:AR:1493:G:O6	41:DN:2:ALA:N	2.19	0.76
1:1:2736:A:OP1	22:2:92:ARG:NH1	2.19	0.76
25:A:818:C:N4	25:A:819:G:O6	2.19	0.76
16:CP:84:PRO:HA	16:CP:87:GLN:HG3	1.66	0.76
37:DJ:64:GLU:HA	37:DJ:67:ARG:HB2	1.68	0.76
25:A:1169:G:N1	25:A:1575:G:OP2	2.18	0.75
37:AI:78:LYS:HA	37:AI:81:ARG:HD2	1.66	0.75
1:1:3166:C:H42	1:1:3284:G:H1	1.33	0.75
58:J:5:ARG:NH1	58:J:29:LEU:O	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:978:G:O2'	1:1:979:U:O2	2.03	0.75
61:M:99:ARG:NH1	73:Y:7:ARG:O	2.19	0.75
25:6:67:A:O2'	25:6:69:G:OP1	2.05	0.75
25:6:868:G:H1	25:6:960:U:H3	1.33	0.75
4:CD:111:THR:HB	4:CD:136:ILE:HD13	1.68	0.75
1:AR:979:U:H1'	1:AR:980:A:C8	2.22	0.75
1:AR:744:A:OP1	19:CS:66:ARG:NH2	2.20	0.75
25:A:1500:C:OP1	69:U:122:ARG:NH2	2.20	0.75
1:1:1567:U:O2	1:1:1571:A:N6	2.19	0.74
25:A:1542:G:N2	25:A:1569:A:OP2	2.20	0.74
25:A:339:C:OP2	58:J:10:LYS:NZ	2.20	0.74
1:1:1833:G:OP1	41:AM:10:LYS:NZ	2.20	0.74
1:AR:1605:A:O2'	1:AR:1607:U:OP2	2.03	0.74
55:G:51:VAL:O	55:G:65:ARG:NH2	2.19	0.74
25:A:992:A:H2	25:A:1012:U:H3	1.34	0.74
29:AA:127:ASN:O	29:AA:129:TRP:N	2.21	0.74
25:A:7:G:O6	52:D:205:ARG:NH2	2.19	0.74
1:1:964:G:HO2'	30:AB:41:HIS:HE2	1.33	0.74
53:E:178:ARG:H	53:E:178:ARG:HE	1.34	0.74
25:A:158:U:O2'	25:A:160:C:OP2	2.05	0.74
25:A:475:A:OP2	59:K:126:ARG:NH1	2.21	0.74
1:AR:3349:C:H42	1:AR:3356:G:H1	1.35	0.74
29:DB:46:ILE:HD13	29:DB:68:ILE:HG23	1.69	0.74
1:1:2593:A:H4'	1:1:2594:C:O5'	1.88	0.74
34:AF:100:ILE:O	34:AF:105:ARG:NH1	2.21	0.74
11:CK:49:ASN:HD21	11:CK:51:GLN:HB2	1.52	0.74
25:A:1429:G:H1'	70:V:74:GLU:HG2	1.67	0.74
66:R:110:THR:HA	66:R:113:ASP:HB2	1.68	0.73
25:A:1535:U:O2'	25:A:1536:G:N3	2.20	0.73
25:A:1559:A:H5''	68:T:135:GLY:HA3	1.68	0.73
25:6:158:U:O2'	25:6:160:C:OP2	2.06	0.73
25:A:1521:G:O6	69:U:68:ARG:NH1	2.22	0.73
25:A:1681:A:H1'	56:H:66:GLY:HA3	1.69	0.73
8:CH:40:LEU:HD13	8:CH:84:VAL:HG11	1.70	0.73
1:AR:3230:G:H4'	15:CO:132:LYS:HD3	1.70	0.73
1:1:2836:C:H5	1:1:2852:C:H42	1.35	0.73
25:6:1696:G:O2'	25:6:1698:G:N7	2.21	0.73
1:AR:986:U:OP1	9:CI:98:LYS:NZ	2.21	0.73
22:CV:41:ASP:HB2	22:CV:97:LYS:HG3	1.70	0.73
1:AR:1740:U:H1'	1:AR:1741:A:H2	1.51	0.73
6:CF:204:GLY:O	6:CF:246:ARG:NH1	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:CH:31:ARG:NH1	35:DH:107:ILE:O	2.22	0.73
53:E:164:VAL:HG13	53:E:168:ILE:HD11	1.71	0.73
25:A:803:A:H1'	57:I:104:ARG:HH11	1.54	0.73
1:1:1639:C:OP2	36:AH:74:ARG:NH2	2.22	0.73
1:AR:20:A:OP2	37:DJ:90:ARG:NH1	2.21	0.73
51:C:173:THR:O	51:C:177:GLN:NE2	2.22	0.72
3:AT:95:G:OP2	39:DL:72:ARG:NH1	2.22	0.72
1:AR:66:A:OP2	14:CN:100:ARG:NH2	2.22	0.72
52:D:45:VAL:HG21	52:D:68:ILE:HG23	1.70	0.72
51:C:61:LEU:HG	51:C:64:ARG:HH21	1.55	0.72
59:K:110:GLN:HE22	59:K:126:ARG:HG2	1.54	0.72
69:U:28:LEU:HD13	69:U:30:VAL:HG22	1.71	0.72
11:CK:163:GLN:O	11:CK:166:ARG:NH1	2.18	0.72
12:CL:14:ASN:O	12:CL:128:ARG:NH2	2.22	0.72
73:Y:102:VAL:HG12	73:Y:127:VAL:HG12	1.71	0.72
11:CK:41:ILE:HD11	11:CK:67:ALA:HB1	1.71	0.72
25:A:732:G:O2'	25:A:733:A:O4'	2.07	0.72
25:A:856:A:N7	57:I:97:ARG:HB2	2.04	0.72
25:6:140:A:N6	25:6:281:G:OP1	2.23	0.72
2:AS:121:U:OP2	7:CG:265:TYR:OH	2.03	0.72
37:DJ:101:THR:HG22	37:DJ:104:GLN:HB2	1.70	0.72
35:AG:14:LEU:HD11	35:AG:31:LYS:HB2	1.72	0.71
9:CI:157:ASN:O	9:CI:159:GLN:HG2	1.90	0.71
1:AR:1028:U:O2	13:CM:94:ARG:NH1	2.23	0.71
9:CI:143:THR:HG22	9:CI:241:LYS:HG3	1.71	0.71
1:1:3375:A:O2'	1:1:3378:C:OP2	2.07	0.71
25:A:1034:C:HO2'	72:X:2:THR:N	1.86	0.71
7:CG:40:HIS:CD2	22:CV:69:LYS:HA	2.25	0.71
74:Z:83:LYS:HE2	74:Z:96:LEU:HB3	1.73	0.71
4:CD:79:ASN:ND2	4:CD:166:ILE:O	2.24	0.71
1:AR:3155:U:H3'	1:AR:3156:U:H4'	1.69	0.71
1:AR:440:A:OP1	1:AR:494:G:O2'	2.04	0.71
1:AR:1807:G:H5"	29:DB:135:ARG:HH22	1.55	0.71
14:CN:48:PRO:HB2	37:DJ:117:ALA:HB2	1.73	0.71
73:Y:69:ARG:NH1	73:Y:116:ASP:OD2	2.21	0.71
1:1:904:A:OP2	39:AK:30:GLN:NE2	2.23	0.71
69:U:37:VAL:HG11	69:U:100:ILE:HD11	1.71	0.71
1:1:1320:C:O2	21:O:115:ARG:NH2	2.24	0.71
1:AR:1630:U:OP1	29:DB:67:LYS:NZ	2.24	0.71
1:AR:837:A:OP2	45:DR:4:ARG:NH1	2.24	0.71
15:CO:19:ARG:HA	15:CO:69:THR:HG22	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:718:G:C2	1:AR:721:G:H1'	2.26	0.71
1:AR:289:A:O2'	16:CP:93:LYS:O	2.09	0.71
1:AR:1473:G:OP2	20:CT:8:LYS:NZ	2.23	0.71
72:X:30:SER:HB2	72:X:61:ILE:HG13	1.72	0.71
3:4:95:G:OP2	39:AK:72:ARG:NH1	2.23	0.70
27:CZ:86:VAL:HG11	27:CZ:95:ILE:HG12	1.70	0.70
52:D:56:ILE:HG23	52:D:61:LEU:HB2	1.72	0.70
1:1:676:G:HO2'	1:1:678:G:HO2'	1.35	0.70
25:6:1690:G:H1	25:6:1711:C:H42	1.37	0.70
29:DB:83:THR:HG23	29:DB:85:TYR:H	1.56	0.70
1:1:2112:U:H4'	1:1:2113:A:H5'	1.73	0.70
1:1:263:C:H2'	1:1:264:G:O4'	1.92	0.70
1:AR:3115:C:OP1	11:CK:62:ARG:NH2	2.24	0.70
16:CP:31:ARG:NH1	16:CP:124:ASP:OD2	2.24	0.70
58:J:39:GLY:HA2	58:J:61:GLU:HB3	1.72	0.70
1:1:801:A:OP1	30:AB:27:LYS:NZ	2.23	0.70
1:AR:2759:U:H5''	1:AR:2760:C:H5'	1.74	0.70
51:C:175:GLU:HG3	51:C:193:ILE:HD12	1.74	0.70
6:CF:299:ILE:HG23	19:CS:39:ARG:HB3	1.73	0.70
57:I:74:GLN:HE22	57:I:92:PHE:HB2	1.56	0.70
25:6:1542:G:N2	25:6:1569:A:OP2	2.24	0.70
32:AD:40:LYS:HB3	32:AD:101:LEU:HD11	1.74	0.70
1:AR:2818:U:H6	1:AR:2818:U:H5'	1.54	0.70
60:L:25:LYS:HD2	60:L:59:PHE:HZ	1.56	0.70
25:A:778:G:H3'	25:A:780:A:H2	1.56	0.69
1:AR:900:G:H1'	1:AR:1589:A:N6	2.06	0.69
11:CK:21:LYS:HA	15:CO:8:LYS:HD2	1.72	0.69
25:A:761:G:OP1	59:K:54:ARG:NH1	2.24	0.69
1:AR:276:U:O2	16:CP:93:LYS:NZ	2.24	0.69
15:CO:16:GLU:HB3	21:CU:149:LYS:HB3	1.74	0.69
25:A:123:G:H21	54:F:146:THR:HG21	1.56	0.69
25:A:320:U:H3'	25:A:321:C:H5''	1.75	0.69
72:X:15:ASN:HD21	72:X:71:LYS:HG3	1.58	0.69
1:1:1145:G:OP1	34:AF:44:ARG:NH1	2.25	0.69
35:AG:49:ILE:HG23	35:AG:100:ILE:HG13	1.73	0.69
37:AI:76:GLN:O	37:AI:81:ARG:NH1	2.25	0.69
1:AR:402:A:OP1	41:DN:36:ARG:NH2	2.25	0.69
3:AT:21:C:OP1	6:CF:193:LYS:NZ	2.25	0.69
21:CU:1:MET:HE1	21:CU:31:ALA:HA	1.74	0.69
25:6:486:G:H22	25:6:501:U:H3	1.40	0.69
51:C:88:VAL:HG11	51:C:96:LEU:HD12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:I:50:ASP:N	57:I:50:ASP:OD1	2.26	0.69
73:Y:79:ASN:HB3	73:Y:81:LYS:HG3	1.75	0.69
25:A:523:G:OP2	74:Z:37:LYS:NZ	2.26	0.69
25:A:542:A:H8	25:A:543:C:H5'	1.57	0.69
30:AB:46:ASP:N	30:AB:46:ASP:OD1	2.22	0.69
12:CL:66:GLU:OE1	12:CL:69:ARG:NH2	2.25	0.69
53:E:8:LYS:HE2	70:V:61:LYS:HD3	1.75	0.69
25:A:45:U:O2'	25:A:46:A:H2'	1.92	0.69
19:CS:185:LYS:HD3	19:CS:186:VAL:HG23	1.75	0.69
52:D:40:LYS:HB3	52:D:247:ALA:HB1	1.75	0.69
22:CV:12:ARG:HD3	22:CV:13:TYR:CZ	2.28	0.68
1:1:2108:C:H1'	1:1:3344:A:C8	2.27	0.68
22:2:48:ILE:HG13	22:2:94:GLU:HG2	1.74	0.68
1:AR:269:G:N2	1:AR:295:A:OP2	2.26	0.68
13:CM:92:ARG:HH21	13:CM:94:ARG:HH21	1.42	0.68
1:1:2960:C:H2'	1:1:2961:G:H8	1.59	0.68
1:1:1841:A:H1'	41:AM:45:ARG:HH22	1.58	0.68
1:1:283:G:OP1	44:AP:45:ARG:NH2	2.26	0.68
1:AR:2728:G:N7	22:CV:87:LYS:NZ	2.33	0.68
1:AR:2953:U:H2'	1:AR:2954:U:H2'	1.74	0.68
1:AR:3343:G:H21	1:AR:3362:A:H2	1.39	0.68
35:DH:59:VAL:O	35:DH:61:GLY:N	2.26	0.68
25:6:845:G:H2'	25:6:846:G:H8	1.59	0.68
25:A:1529:C:OP1	55:G:112:ARG:NH1	2.25	0.68
51:C:109:LYS:HG3	51:C:113:MET:HE3	1.75	0.68
6:CF:3:ARG:NE	6:CF:22:LEU:O	2.26	0.68
50:B:189:VAL:HG22	50:B:190:ASP:H	1.59	0.68
52:D:53:ILE:HB	55:G:57:SER:HB3	87.47	0.68
45:DR:49:ARG:HB2	45:DR:55:TRP:CZ3	2.28	0.68
25:A:1459:C:OP1	68:T:126:ARG:NH2	2.27	0.68
25:A:190:C:N4	25:A:196:G:O6	2.27	0.68
1:AR:2261:G:O2'	1:AR:2263:C:N4	2.27	0.68
5:CE:139:GLN:HB2	5:CE:141:GLY:H	1.59	0.68
6:CF:139:GLY:O	6:CF:141:ARG:NH1	2.27	0.68
58:J:61:GLU:HG3	58:J:62:THR:HG23	1.76	0.68
68:T:49:LYS:NZ	68:T:80:LYS:O	2.26	0.68
21:0:2:ALA:HB3	21:0:32:SER:HB3	1.76	0.67
25:6:1699:G:H22	25:6:1702:A:H5''	1.57	0.67
1:AR:2793:G:C5	87:AR:4262:GOL:H32	2.29	0.67
50:B:117:GLU:O	52:D:40:LYS:NZ	2.27	0.67
67:S:82:ASP:O	67:S:83:GLN:NE2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CF:321:LYS:HA	6:CF:324:LEU:HB3	1.76	0.67
1:AR:3214:U:OP2	15:CO:128:ARG:NH2	2.27	0.67
58:J:147:ALA:HA	58:J:149:SER:H	1.58	0.67
25:A:820:U:H2'	25:A:821:U:H4'	1.75	0.67
33:DF:6:ASP:HB3	33:DF:77:ARG:HH21	1.58	0.67
1:1:3166:C:N3	1:1:3284:G:N2	2.34	0.67
1:AR:3122:A:N1	11:CK:70:THR:HG21	2.10	0.67
15:CO:123:LEU:HD23	17:CQ:190:VAL:HG23	1.77	0.67
25:6:1542:G:H22	25:6:1568:C:H1'	1.59	0.67
40:AL:24:THR:HG23	40:AL:44:LYS:HB2	1.76	0.67
7:CG:76:ALA:HB3	7:CG:109:THR:HG22	1.77	0.67
53:E:166:ASP:O	53:E:190:ARG:NH1	2.27	0.67
3:AT:63:G:O2'	37:DJ:49:LYS:NZ	2.27	0.67
7:CG:22:ARG:NH2	7:CG:28:THR:OG1	2.27	0.67
28:9:112:ASP:HB2	28:9:115:ARG:HB2	1.75	0.67
50:B:150:ASP:OD2	50:B:165:ARG:NH2	2.28	0.67
72:X:47:ILE:HG22	72:X:65:LEU:HB3	1.75	0.67
25:6:691:C:OP1	25:6:696:C:N4	2.27	0.67
1:1:2722:U:OP1	31:AC:33:LYS:NZ	2.27	0.67
1:1:2207:A:H2'	1:1:2208:A:H8	1.60	0.66
1:1:2538:U:O2'	1:1:2541:U:O4	2.11	0.66
1:1:2897:A:H2'	1:1:2899:C:H5''	1.76	0.66
25:6:1280:C:H2'	25:6:1281:G:C8	2.30	0.66
25:6:716:C:H42	25:6:722:G:H1	1.42	0.66
25:A:656:G:O2'	25:A:657:U:O4'	2.13	0.66
1:AR:3157:U:H4'	1:AR:3158:G:H5'	1.76	0.66
6:CF:119:ARG:NH1	6:CF:271:LYS:HB3	2.10	0.66
25:A:741:C:O2	57:I:107:ARG:NH1	2.29	0.66
5:CE:187:SER:O	5:CE:190:GLU:N	2.28	0.66
10:CJ:84:ARG:H	10:CJ:84:ARG:HE	1.41	0.66
1:1:2960:C:H2'	1:1:2961:G:C8	2.30	0.66
1:AR:2356:A:H61	1:AR:2983:C:H5	1.43	0.66
1:AR:3112:G:O2'	11:CK:70:THR:HB	1.94	0.66
13:CM:109:HIS:HD2	13:CM:114:ILE:HD13	1.61	0.66
1:AR:3206:C:O2	21:CU:155:ARG:NH1	2.28	0.66
26:CY:39:LEU:HD12	26:CY:44:LYS:HG3	1.75	0.66
1:1:1407:A:O3'	34:AF:33:ARG:NH2	2.28	0.66
1:AR:2193:U:H5'	1:AR:2194:G:H5'	1.76	0.66
27:CZ:50:ALA:O	37:DJ:66:VAL:HG21	1.95	0.66
38:DK:70:ARG:HD3	38:DK:84:LYS:HG2	1.77	0.66
3:AT:45:C:OP1	41:DN:12:LYS:NZ	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:888:U:H1'	64:P:126:THR:HG21	1.76	0.66
1:1:1308:A:N1	1:1:2381:G:O2'	2.28	0.66
1:1:3348:G:H1	1:1:3357:U:H3	1.42	0.66
12:CL:47:PRO:O	12:CL:172:GLY:N	2.28	0.66
1:1:1243:G:N2	1:1:1244:A:N7	2.44	0.66
5:CE:53:MET:HG2	5:CE:77:THR:HG22	1.76	0.66
12:CL:33:ILE:HD11	12:CL:36:LEU:HG	1.76	0.66
2:AS:5:G:OP1	13:CM:143:ARG:NH2	2.28	0.66
20:CT:13:SER:OG	20:CT:38:ARG:NH2	2.29	0.66
40:DM:32:ASN:ND2	40:DM:36:LYS:O	2.29	0.66
12:CL:21:ARG:NH1	12:CL:22:TYR:OH	2.28	0.66
25:A:1232:U:H4'	60:L:2:LEU:HD21	1.76	0.66
25:6:75:U:O2'	25:6:76:A:O4'	2.13	0.66
1:AR:1724:U:H1'	1:AR:1725:C:C6	2.30	0.66
1:AR:1814:A:H4'	1:AR:1815:U:H5'	1.78	0.66
1:AR:2880:U:H1'	5:CE:250:ALA:HB3	1.78	0.66
14:CN:61:PRO:HB2	14:CN:62:THR:HG23	1.77	0.66
25:6:542:A:H1'	25:6:543:C:H5'	1.78	0.66
7:CG:52:VAL:HG21	7:CG:65:ILE:HD12	1.78	0.66
72:X:27:ILE:HG12	72:X:61:ILE:HB	1.77	0.66
32:AD:16:LEU:HB3	32:AD:98:SER:HB2	1.78	0.65
3:AT:82:U:O2'	3:AT:83:C:OP1	2.13	0.65
12:CL:68:ALA:HB2	12:CL:158:LYS:HB2	1.78	0.65
25:6:151:G:H1	25:6:163:G:H1	1.43	0.65
1:AR:2394:G:H5'	5:CE:252:ILE:HG22	1.77	0.65
45:DR:56:THR:HG22	45:DR:63:THR:HG23	1.78	0.65
25:A:1529:C:O2'	69:U:12:GLN:OE1	2.11	0.65
1:AR:2100:A:N7	1:AR:2101:C:N4	2.44	0.65
50:B:64:ILE:HG23	50:B:73:VAL:HG11	1.77	0.65
25:6:1280:C:H2'	25:6:1281:G:H8	1.62	0.65
1:AR:1863:G:N1	1:AR:1866:C:OP2	2.27	0.65
1:AR:2916:U:H5	1:AR:2935:U:HO2'	1.43	0.65
17:CQ:18:ARG:O	17:CQ:22:VAL:HG12	1.97	0.65
32:AD:13:LYS:HZ1	32:AD:103:THR:HG21	1.62	0.65
5:CE:92:TYR:HB2	5:CE:157:VAL:HG22	1.78	0.65
14:CN:123:ILE:HG22	37:DJ:118:ILE:HG12	1.79	0.65
39:DL:21:ARG:NH2	39:DL:41:ALA:O	2.24	0.65
25:A:811:A:N7	57:I:111:LYS:HB3	2.12	0.65
25:A:1267:G:HO2'	25:A:1448:G:HO2'	1.42	0.65
6:CF:122:THR:HG22	6:CF:235:LEU:HB2	1.79	0.65
6:CF:226:GLU:OE1	6:CF:237:GLN:NE2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:O:93:LYS:HG3	63:O:150:VAL:HG11	1.78	0.65
1:1:979:U:H1'	1:1:980:A:C8	2.31	0.65
25:A:823:G:H2'	25:A:824:G:C8	2.32	0.65
21:CU:12:ARG:HB3	21:CU:24:LEU:HD23	1.79	0.65
57:I:73:VAL:O	57:I:75:THR:N	2.30	0.65
61:M:80:MET:HB2	61:M:83:THR:HG23	1.79	0.65
25:A:74:U:O2'	25:A:75:U:H5''	1.97	0.65
45:AQ:84:ARG:NH1	45:AQ:88:GLU:OE1	2.30	0.65
6:CF:16:THR:HG22	6:CF:18:ASN:H	1.61	0.65
34:DG:40:SER:O	34:DG:44:ARG:HG3	1.97	0.65
54:F:73:ASP:OD2	54:F:122:LYS:NZ	2.27	0.65
55:G:206:SER:O	55:G:212:LYS:NZ	2.30	0.65
25:A:1564:U:H2'	25:A:1565:C:C6	2.32	0.65
25:A:52:U:H2'	25:A:53:G:C8	2.32	0.65
1:AR:3151:U:OP2	5:CE:132:LYS:NZ	2.26	0.65
21:0:167:ARG:HG3	21:0:168:PRO:HD2	1.78	0.64
25:A:67:A:O2'	25:A:69:G:OP1	2.12	0.64
1:AR:528:U:H2'	1:AR:529:A:H8	1.60	0.64
23:5:51:GLY:O	23:5:52:ASN:ND2	2.30	0.64
51:C:34:ALA:HB3	51:C:41:ARG:HA	1.79	0.64
11:CK:49:ASN:ND2	11:CK:51:GLN:OE1	2.31	0.64
57:I:30:SER:HB2	57:I:34:LEU:HB2	1.79	0.64
63:O:34:ILE:HG13	63:O:67:THR:HG21	1.79	0.64
1:1:269:G:N2	1:1:295:A:OP2	2.29	0.64
35:DH:14:LEU:HD11	35:DH:31:LYS:HB2	1.79	0.64
1:1:2108:C:H1'	1:1:3344:A:H8	1.63	0.64
1:AR:3272:C:OP2	8:CH:78:ARG:NH1	2.30	0.64
1:AR:912:G:OP2	4:CD:9:ARG:NH1	2.31	0.64
13:CM:82:ARG:HG2	13:CM:112:LEU:HB2	1.78	0.64
37:DJ:31:LEU:HD22	37:DJ:41:LEU:HD21	1.79	0.64
25:A:196:G:O6	58:J:141:ARG:NH2	2.30	0.64
25:A:337:G:H3'	61:M:133:LYS:HB2	1.78	0.64
1:1:1222:G:O2'	1:1:1285:G:N1	2.31	0.64
1:AR:1405:U:OP2	34:DG:59:SER:OG	2.16	0.64
21:CU:2:ALA:HB3	21:CU:32:SER:HB3	1.78	0.64
25:6:1058:U:H4'	25:6:1059:U:OP1	1.97	0.64
25:A:788:A:OP1	54:F:106:LYS:NZ	2.29	0.64
1:AR:1043:C:O3'	12:CL:90:ARG:NH1	2.30	0.64
51:C:181:LEU:HA	51:C:184:LEU:HB3	1.80	0.64
37:DJ:85:THR:HB	37:DJ:88:LEU:HB2	1.80	0.64
25:A:1291:G:N2	25:A:1324:G:H22	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:CO:72:LEU:HD22	15:CO:73:PRO:HD2	1.79	0.64
35:DH:75:HIS:HB2	35:DH:82:ARG:HG3	1.78	0.64
68:T:94:ASP:OD2	68:T:98:TYR:OH	2.14	0.64
1:AR:86:G:O2'	1:AR:98:G:O6	2.15	0.64
30:DC:3:SER:O	30:DC:6:THR:HG22	1.97	0.64
66:R:41:PRO:HG2	66:R:78:VAL:HG21	1.80	0.64
1:1:2683:U:H2'	1:1:2684:C:C6	2.32	0.63
25:6:1533:C:H4'	25:6:1539:G:N1	2.13	0.63
29:AA:25:ILE:HA	29:AA:43:VAL:HG12	1.80	0.63
53:E:137:VAL:HG22	53:E:151:LYS:HG3	1.80	0.63
27:8:38:LEU:HD11	27:8:40:LEU:HD13	1.79	0.63
1:AR:2943:G:OP2	5:CE:2:SER:OG	2.15	0.63
1:AR:1447:G:H3'	18:CR:67:ILE:HD11	1.79	0.63
54:F:100:ARG:NH2	54:F:121:TYR:O	2.31	0.63
70:V:72:ASN:HD22	70:V:74:GLU:H	1.45	0.63
1:1:1235:U:H4'	1:1:1236:G:H5'	1.80	0.63
25:6:518:A:O2'	25:6:534:A:N6	2.32	0.63
25:A:1588:G:H1	25:A:1608:U:H3	1.46	0.63
25:A:337:G:H1'	58:J:10:LYS:HZ1	1.64	0.63
55:G:117:THR:HG21	55:G:194:LEU:HD12	1.79	0.63
25:A:1228:G:N2	62:N:68:GLU:OE1	2.32	0.63
68:T:139:LYS:O	68:T:143:ARG:NH1	2.32	0.63
69:U:4:VAL:HG11	69:U:137:ALA:HB2	1.80	0.63
27:8:46:TYR:OH	37:AI:78:LYS:NZ	2.28	0.63
43:AO:7:LYS:NZ	25:A:1774:G:OP1	2.30	0.63
1:AR:1720:U:OP2	20:CT:110:ARG:NH1	2.32	0.63
29:DB:50:PRO:HD3	29:DB:68:ILE:HG12	1.79	0.63
25:A:149:C:O2'	56:H:132:ARG:NH1	2.32	0.63
33:AE:24:SER:HB2	33:AE:27:LYS:HE3	1.80	0.63
1:AR:1580:A:H4'	1:AR:1581:C:H5'	1.81	0.63
4:CD:143:GLU:O	4:CD:145:LYS:N	2.32	0.63
34:DG:100:ILE:O	34:DG:105:ARG:NH1	2.31	0.63
61:M:3:THR:OG1	61:M:82:ARG:NE	2.31	0.63
25:6:454:U:H5''	25:6:455:C:H5	1.64	0.63
25:6:58:U:O2'	25:6:451:A:N3	2.32	0.63
33:AE:13:THR:HG22	33:AE:72:ARG:HD3	1.80	0.63
41:AM:9:ILE:HG22	41:AM:13:MET:HE2	1.80	0.63
51:C:40:ASN:ND2	51:C:42:ASN:O	2.32	0.63
5:CE:347:SER:HB3	5:CE:350:ALA:H	1.63	0.63
27:CZ:139:ILE:HD11	27:CZ:141:TYR:HE2	1.64	0.63
1:AR:497:C:O3'	35:DH:86:ARG:NH2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:AC:16:ALA:O	31:AC:20:GLY:HA2	1.98	0.63
1:AR:1065:A:N1	31:DD:26:THR:OG1	2.32	0.63
1:AR:2207:A:H62	1:AR:2236:G:H1	1.47	0.63
1:AR:3317:U:H4'	1:AR:3318:G:O5'	1.99	0.63
7:CG:40:HIS:HD2	7:CG:42:ALA:H	1.46	0.63
56:H:148:SER:O	56:H:150:GLU:N	2.32	0.63
1:1:2138:A:HO2'	39:AK:2:GLY:N	1.97	0.63
7:CG:64:ILE:HD12	7:CG:109:THR:HG21	1.81	0.63
12:CL:192:ASP:HA	12:CL:197:VAL:HG23	1.81	0.63
58:J:106:ALA:HB2	58:J:165:LEU:HG	1.80	0.63
1:1:1807:G:H5''	29:AA:135:ARG:HH22	1.63	0.62
6:CF:26:PHE:HA	6:CF:127:ALA:HA	1.81	0.62
22:CV:51:GLY:HA3	22:CV:92:ARG:HG3	1.80	0.62
54:F:106:LYS:O	54:F:187:ARG:NH2	2.32	0.62
56:H:114:VAL:HG12	56:H:115:LYS:HD3	1.81	0.62
1:1:900:G:H1'	1:1:1589:A:N6	2.14	0.62
36:AH:46:ASP:OD1	36:AH:80:ARG:NH1	2.31	0.62
41:AM:23:LEU:HD22	41:AM:24:PRO:HD2	1.80	0.62
1:AR:836:A:O2'	45:DR:9:GLY:O	2.17	0.62
2:AS:107:C:H2'	2:AS:108:A:C8	2.35	0.62
33:DF:84:ASP:N	33:DF:84:ASP:OD1	2.32	0.62
71:W:40:ASP:OD1	71:W:44:ARG:NH1	2.32	0.62
1:AR:229:G:H5''	28:DA:4:GLN:HB2	1.81	0.62
1:AR:524:U:OP1	15:CO:77:ARG:NH2	2.30	0.62
1:1:1798:A:H2'	1:1:1799:A:C8	2.34	0.62
25:A:458:G:OP2	74:Z:105:ARG:NH2	2.32	0.62
9:CI:121:LYS:HB2	22:CV:133:ALA:HB3	1.80	0.62
1:AR:945:C:H2'	1:AR:946:U:C6	2.35	0.62
51:C:38:PHE:HA	51:C:74:GLN:HE22	1.65	0.62
11:CK:171:ASP:OD2	11:CK:173:ARG:NH1	2.33	0.62
1:1:1740:U:H1'	1:1:1741:A:H2	1.62	0.62
25:6:486:G:O6	25:6:488:G:N2	2.26	0.62
25:A:1600:A:H4'	25:A:1601:G:OP1	1.99	0.62
1:1:715:A:H8	30:AB:115:LYS:HG2	1.65	0.62
1:AR:1895:A:O2'	1:AR:3053:G:H4'	1.98	0.62
1:AR:528:U:H2'	1:AR:529:A:C8	2.34	0.62
52:D:102:VAL:HG11	52:D:129:ILE:HG12	1.82	0.62
21:0:138:GLN:HA	21:0:141:LYS:HB2	1.80	0.62
25:A:280:U:O2'	25:A:281:G:OP2	2.16	0.62
25:A:283:U:H5''	56:H:188:ARG:HD3	1.81	0.62
1:AR:1152:G:OP2	1:AR:1152:G:N2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:1949:G:OP2	20:CT:135:LYS:NZ	2.31	0.62
24:CX:89:ASP:OD1	24:CX:91:VAL:HG12	2.00	0.62
53:E:142:LEU:HD13	53:E:182:LEU:HD21	1.81	0.62
25:6:1370:U:H4'	25:6:1371:A:H4'	1.82	0.62
25:A:1280:C:H2'	25:A:1281:G:H8	1.65	0.62
25:A:1488:G:H3'	25:A:1515:A:H61	1.65	0.62
25:A:800:U:H2'	25:A:801:G:H8	1.63	0.62
45:AQ:32:GLN:HG2	45:AQ:70:THR:HB	1.82	0.62
1:AR:1407:A:O3'	34:DG:33:ARG:NH2	2.33	0.62
1:AR:805:G:H1'	6:CF:73:ARG:HH11	1.64	0.62
58:J:138:ASN:N	58:J:138:ASN:OD1	2.32	0.62
25:6:737:A:H2'	25:6:738:G:H8	1.65	0.62
1:AR:3255:U:H2'	1:AR:3256:G:C8	2.34	0.62
6:CF:45:ASN:HA	6:CF:110:ASN:HD22	1.65	0.62
8:CH:72:ASN:HB3	8:CH:160:SER:HA	1.82	0.62
15:CO:128:ARG:HD3	15:CO:132:LYS:HD2	1.81	0.62
1:AR:2433:U:H1'	16:CP:125:SER:HB3	1.80	0.62
1:AR:692:A:OP1	16:CP:201:ARG:NH2	2.33	0.62
54:F:88:ASP:OD1	54:F:122:LYS:NZ	2.32	0.62
64:P:85:ALA:H	64:P:119:THR:HG22	1.63	0.62
1:AR:1603:A:OP1	20:CT:38:ARG:NH1	2.33	0.62
25:A:1046:G:OP1	51:C:157:GLN:NE2	2.30	0.62
2:AS:17:A:OP1	7:CG:2:ALA:N	2.33	0.62
21:CU:92:LYS:NZ	21:CU:109:ASP:OD2	2.27	0.62
52:D:39:THR:O	52:D:42:GLY:N	2.26	0.62
25:6:1268:G:H1'	25:6:1448:G:H5''	1.80	0.61
45:AQ:56:THR:HG22	45:AQ:63:THR:HG23	1.82	0.61
84:AR:3443:OHX:N5	84:AR:3731:OHX:N3	2.48	0.61
6:CF:226:GLU:OE2	6:CF:246:ARG:NH2	2.33	0.61
8:CH:3:ALA:HB2	34:DG:77:ALA:HB2	1.81	0.61
1:AR:1507:G:N7	18:CR:129:THR:HG22	2.14	0.61
37:DJ:76:GLN:O	37:DJ:81:ARG:NH1	2.33	0.61
1:1:1805:C:H2'	1:1:1806:A:H8	1.65	0.61
28:9:73:VAL:HA	28:9:80:VAL:HG23	1.82	0.61
1:1:1634:G:N7	29:AA:17:ARG:NH2	2.48	0.61
34:AF:21:HIS:ND1	34:AF:24:ARG:HD2	2.16	0.61
10:CJ:161:GLU:OE1	16:CP:26:ARG:NH1	2.28	0.61
18:CR:60:PHE:HB3	18:CR:64:ASN:HB3	1.82	0.61
54:F:19:LEU:HD11	54:F:108:ARG:HD2	1.82	0.61
25:A:1382:A:H5''	70:V:60:THR:HG22	1.82	0.61
25:6:1600:A:H4'	25:6:1601:G:OP1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:737:A:H2'	25:6:738:G:C8	2.35	0.61
1:AR:1940:G:H21	1:AR:3362:A:H8	1.45	0.61
1:AR:2268:U:H3'	1:AR:2269:U:C5'	2.30	0.61
19:CS:34:THR:HG22	19:CS:49:LEU:HD21	1.81	0.61
52:D:113:LEU:HD21	52:D:211:LEU:HB3	1.82	0.61
1:1:1308:A:H8	1:1:1308:A:OP2	1.82	0.61
25:A:993:A:OP1	25:A:1777:G:N2	2.24	0.61
1:AR:1717:U:H2'	1:AR:1718:G:C8	2.36	0.61
50:B:124:THR:HG22	50:B:174:TRP:HE1	1.65	0.61
8:CH:51:ARG:NH1	15:CO:114:ASP:OD2	2.33	0.61
56:H:135:PRO:HB2	56:H:141:ILE:HG12	1.83	0.61
73:Y:68:ILE:O	73:Y:70:LYS:NZ	2.29	0.61
50:B:55:GLU:OE2	71:W:80:LYS:N	2.18	0.61
5:CE:152:LYS:HG2	5:CE:192:VAL:HG11	1.81	0.61
60:L:25:LYS:HD2	60:L:59:PHE:CZ	2.35	0.61
1:1:2768:U:H2'	1:1:2769:A:C8	2.35	0.61
2:3:19:C:H2'	2:3:20:A:H8	1.65	0.61
25:6:454:U:H5''	25:6:455:C:C5	2.35	0.61
28:9:56:VAL:HG11	28:9:104:LEU:HD13	1.82	0.61
25:A:1773:C:H2'	25:A:1774:G:H8	1.66	0.61
40:DM:24:THR:HG23	40:DM:44:LYS:HB2	1.81	0.61
25:A:1424:A:H1'	52:D:92:ALA:HB1	1.81	0.61
1:AR:2895:G:H2'	1:AR:2896:A:H5''	1.80	0.61
1:AR:3259:U:H5''	1:AR:3261:C:H5	1.66	0.61
1:AR:3151:U:H4'	1:AR:3294:A:H1'	1.83	0.61
84:AR:3443:OHX:N2	84:AR:3731:OHX:N4	2.48	0.61
7:CG:58:LYS:HD2	7:CG:93:THR:HG21	1.83	0.61
65:Q:22:LEU:HD21	65:Q:109:PRO:HB3	1.81	0.61
72:X:29:PRO:HB2	72:X:58:SER:HB2	1.81	0.61
9:CI:173:LEU:HB3	9:CI:178:ILE:HB	1.82	0.61
11:CK:48:VAL:HG13	11:CK:52:LEU:HB3	1.82	0.61
13:CM:47:GLN:HG2	13:CM:67:VAL:HG12	1.81	0.61
14:CN:28:GLN:OE1	16:CP:201:ARG:NH1	2.34	0.61
1:1:1688:U:H2'	1:1:1689:U:C6	2.36	0.61
1:1:2818:U:C6	1:1:2818:U:H5'	2.32	0.61
1:1:543:C:H42	1:1:548:G:H1	1.48	0.61
25:6:489:C:O2'	25:6:490:C:O4'	2.19	0.61
25:A:482:U:H2'	25:A:483:A:H8	1.66	0.61
29:AA:52:LYS:O	29:AA:65:ARG:NH1	2.32	0.61
1:AR:3228:C:O3'	15:CO:137:LYS:NZ	2.34	0.61
3:AT:135:G:OP2	27:CZ:56:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CR:108:ASP:N	18:CR:152:GLU:OE2	2.21	0.61
25:A:687:G:H5'	72:X:119:LYS:HD2	1.83	0.61
1:1:595:G:N1	1:1:609:G:H5''	2.15	0.61
25:6:1160:A:H2'	25:6:1161:C:C6	2.36	0.61
25:6:1350:U:H2'	25:6:1351:G:C8	2.36	0.61
19:CS:178:ARG:HE	30:DC:50:PRO:HG2	1.66	0.61
72:X:27:ILE:HD11	72:X:61:ILE:HD12	1.82	0.61
25:A:1280:C:H2'	25:A:1281:G:C8	2.37	0.60
25:A:1350:U:H2'	25:A:1351:G:C8	2.36	0.60
1:AR:847:A:H2'	1:AR:848:A:C8	2.36	0.60
25:6:853:G:N7	20:CT:173:ARG:NH2	2.49	0.60
52:D:218:ILE:O	52:D:221:THR:OG1	2.19	0.60
25:A:1542:G:N2	25:A:1568:C:H1'	2.16	0.60
1:AR:2700:G:OP1	22:CV:17:ARG:HB2	2.01	0.60
3:AT:85:G:O2'	3:AT:86:U:O5'	2.19	0.60
9:CI:163:LEU:O	9:CI:165:ASP:N	2.34	0.60
23:CW:14:THR:HG23	23:CW:66:VAL:HG22	1.84	0.60
25:6:407:A:H2'	25:6:408:C:C6	2.36	0.60
25:A:1533:C:H4'	25:A:1539:G:N1	2.15	0.60
51:C:81:PHE:HD1	51:C:82:ARG:HG3	1.66	0.60
5:CE:313:HIS:O	5:CE:333:LYS:HE3	2.02	0.60
14:CN:62:THR:O	14:CN:64:LYS:N	2.34	0.60
17:CQ:127:LEU:HD11	21:CU:168:PRO:HG3	1.84	0.60
67:S:66:VAL:HB	67:S:69:ILE:HD11	1.82	0.60
1:1:1245:A:H3'	1:1:1246:G:H5''	1.82	0.60
1:1:1895:A:O2'	1:1:3053:G:H4'	2.01	0.60
25:A:1701:A:H3'	25:A:1702:A:H5''	1.83	0.60
25:A:477:A:H2'	25:A:478:A:H8	1.66	0.60
1:AR:1239:C:H42	1:AR:1249:G:H1	1.49	0.60
1:AR:1249:G:H2'	1:AR:1250:G:H8	1.65	0.60
1:AR:824:C:H5''	4:CD:21:ARG:HD3	1.82	0.60
30:DC:112:ILE:HB	30:DC:130:VAL:HG12	1.83	0.60
54:F:159:THR:HB	54:F:227:VAL:HG23	1.82	0.60
56:H:57:ASP:HA	56:H:106:LEU:HA	1.82	0.60
1:1:1308:A:C8	1:1:1308:A:OP2	2.55	0.60
1:AR:1661:G:H2'	1:AR:1662:G:C8	2.36	0.60
6:CF:44:LYS:HB3	6:CF:47:ARG:HH11	1.66	0.60
11:CK:9:GLN:O	11:CK:72:LYS:NZ	2.32	0.60
67:S:32:LYS:HG3	67:S:47:ARG:HD3	1.82	0.60
66:R:33:GLY:HA3	69:U:7:ARG:HE	1.64	0.60
1:1:1243:G:HO2'	1:1:1271:A:HO2'	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2946:A:H5''	1:1:2947:G:H5'	1.83	0.60
25:A:591:A:H2'	25:A:592:A:C8	2.36	0.60
1:AR:1481:A:O2'	1:AR:1858:A:N3	2.21	0.60
5:CE:296:THR:HG22	5:CE:298:PHE:N	2.13	0.60
25:A:698:U:H1'	57:I:107:ARG:HH11	1.66	0.60
1:1:1390:A:N6	1:1:1418:A:O2'	2.34	0.60
1:1:1596:C:H2'	1:1:1597:C:C6	2.37	0.60
29:AA:41:ALA:HB2	29:AA:77:TYR:HE1	1.65	0.60
1:AR:2138:A:HO2'	39:DL:2:GLY:N	1.98	0.60
57:I:50:ASP:HA	57:I:56:LYS:HA	1.83	0.60
65:Q:128:HIS:O	65:Q:130:ARG:NH1	2.35	0.60
1:1:1064:A:H4'	1:1:1065:A:O5'	2.01	0.60
25:A:151:G:O6	74:Z:124:ARG:NH2	2.35	0.60
25:A:520:A:H2'	25:A:521:A:C8	2.37	0.60
51:C:190:PRO:HG2	51:C:192:VAL:HG23	1.84	0.60
84:AR:3502:OHX:N2	9:CI:217:PRO:HA	2.16	0.60
1:AR:1427:U:OP2	30:DC:4:ARG:NH2	2.34	0.60
56:H:68:LEU:HD22	56:H:68:LEU:H	1.66	0.60
25:6:898:A:N1	25:6:911:U:O2'	2.26	0.60
38:AJ:25:LYS:HB2	38:AJ:28:TYR:HD1	1.66	0.60
1:AR:2635:A:H4'	1:AR:2636:A:O5'	2.02	0.60
1:AR:2995:A:H2'	1:AR:2996:U:H5''	1.84	0.60
1:AR:2988:C:P	17:CQ:68:ARG:HH12	2.24	0.60
21:O:77:VAL:HG22	21:O:126:VAL:HG22	1.84	0.60
1:1:132:C:H2'	1:1:133:U:H5''	1.83	0.60
1:1:3107:U:OP1	42:AN:114:LYS:NZ	2.27	0.60
25:A:513:U:H2'	25:A:514:G:C8	2.37	0.60
63:O:132:VAL:HG23	63:O:134:VAL:HG13	1.83	0.60
66:R:22:VAL:HG22	66:R:65:ILE:HG23	1.84	0.60
66:R:71:GLY:O	66:R:77:GLN:NE2	2.35	0.60
70:V:106:ILE:HG23	70:V:107:THR:HG23	1.84	0.60
25:A:1114:G:O2'	25:A:1130:G:O6	2.19	0.59
25:A:134:U:OP1	25:A:136:C:N4	2.34	0.59
29:AA:83:THR:HG23	29:AA:85:TYR:H	1.65	0.59
1:1:1748:G:OP2	40:AL:42:LYS:NZ	2.35	0.59
30:DC:77:LYS:C	30:DC:79:TRP:H	2.05	0.59
1:1:2376:G:H2'	1:1:2377:G:C8	2.37	0.59
25:A:1194:A:OP2	70:V:75:GLY:N	2.32	0.59
5:CE:4:ARG:O	5:CE:5:LYS:HB3	2.00	0.59
14:CN:46:ILE:O	14:CN:47:ALA:O	2.20	0.59
25:A:535:A:OP1	59:K:168:ARG:NH1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:L:59:PHE:CZ	60:L:62:GLN:HA	2.37	0.59
1:1:2683:U:H2'	1:1:2684:C:H6	1.67	0.59
1:AR:22:G:H1'	3:AT:104:A:N3	2.16	0.59
22:CV:78:LYS:HE3	22:CV:87:LYS:HE3	1.85	0.59
54:F:230:GLU:HB2	54:F:233:LYS:HB2	1.83	0.59
55:G:222:LYS:HE3	55:G:225:ARG:HH12	1.66	0.59
66:R:32:ASN:HD21	66:R:69:VAL:H	1.50	0.59
70:V:20:ILE:HD13	70:V:22:ILE:HD13	1.84	0.59
1:AR:2960:C:H2'	1:AR:2961:G:C8	2.37	0.59
1:AR:3375:A:O2'	1:AR:3378:C:OP2	2.19	0.59
51:C:137:ILE:HD11	51:C:172:LEU:HB3	1.84	0.59
72:X:86:ILE:HD12	72:X:87:GLU:HG3	1.84	0.59
1:1:1488:G:H5''	1:1:1838:G:O6	2.02	0.59
1:1:3268:A:OP1	62:N:46:ARG:NH2	190.25	0.59
1:1:3353:G:H3'	58:J:162:ALA:HA	1.84	0.59
25:A:1585:U:H3	25:A:1611:A:H2	1.50	0.59
25:A:704:C:N4	25:A:735:C:N3	2.50	0.59
10:CJ:190:VAL:HG13	10:CJ:192:GLN:HG2	1.83	0.59
57:I:155:ASP:OD1	57:I:156:SER:N	2.31	0.59
68:T:88:ARG:NH1	68:T:112:ASP:OD1	2.34	0.59
1:1:345:G:OP1	1:1:1429:G:N2	2.33	0.59
25:6:1317:C:H2'	25:6:1318:G:O4'	2.03	0.59
25:6:800:U:H2'	25:6:801:G:H8	1.68	0.59
25:A:1606:C:H2'	25:A:1607:G:C8	2.37	0.59
25:A:780:A:N7	74:Z:8:ARG:NH2	2.49	0.59
1:AR:1662:G:N2	1:AR:1788:C:O2	2.35	0.59
1:AR:3090:U:OP1	5:CE:270:ARG:NH2	2.35	0.59
1:AR:980:A:H2'	1:AR:981:U:N1	2.18	0.59
11:CK:8:GLN:HG2	11:CK:68:LEU:HD13	1.84	0.59
54:F:34:GLY:HA3	54:F:83:PRO:HG2	1.85	0.59
28:9:45:ILE:HD12	28:9:119:ILE:HG23	1.85	0.59
32:AD:30:THR:HG22	32:AD:91:SER:HB2	1.84	0.59
1:AR:314:U:H2'	1:AR:315:C:C6	2.38	0.59
1:AR:3316:A:OP1	1:AR:3318:G:N2	2.36	0.59
68:T:83:ALA:HA	68:T:86:LEU:HD23	1.85	0.59
1:1:2768:U:H2'	1:1:2769:A:H8	1.68	0.59
25:A:7:G:N7	52:D:205:ARG:NH1	2.40	0.59
1:AR:1306:G:C6	17:CQ:62:THR:HA	2.37	0.59
1:AR:595:G:H1	1:AR:609:G:H5''	1.67	0.59
50:B:41:ARG:HD2	50:B:42:PRO:O	2.02	0.59
6:CF:30:ILE:HA	6:CF:124:SER:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:860:G:OP1	45:DR:17:ARG:NH1	2.36	0.59
56:H:71:THR:OG1	56:H:72:ARG:N	2.36	0.59
59:K:39:LYS:HB3	59:K:43:TYR:CZ	2.38	0.59
65:Q:81:ARG:HH12	65:Q:120:SER:HB3	1.68	0.59
1:1:1951:C:H42	1:1:2095:G:H1	1.47	0.59
1:1:2953:U:H2'	1:1:2954:U:H2'	1.84	0.59
25:6:477:A:H2'	25:6:478:A:H8	1.68	0.59
6:CF:237:GLN:O	6:CF:246:ARG:HG3	2.03	0.59
45:DR:73:THR:HG23	45:DR:76:ALA:H	1.68	0.59
10:CJ:100:GLU:OE2	10:CJ:108:ARG:NH1	2.36	0.59
56:H:7:TYR:HE2	56:H:125:THR:HG23	1.68	0.59
67:S:105:GLN:CD	67:S:105:GLN:H	2.06	0.59
73:Y:76:LEU:HD21	73:Y:104:LEU:HD12	1.84	0.59
2:3:4:U:H2'	2:3:5:G:C8	2.38	0.58
25:6:1783:C:H2'	25:6:1784:C:H6	1.68	0.58
1:AR:1039:U:H2'	1:AR:1040:A:C8	2.38	0.58
2:AS:91:G:H2'	2:AS:92:A:C8	2.38	0.58
23:CW:50:LEU:HB3	23:CW:54:VAL:HG23	1.84	0.58
1:1:655:C:H2'	1:1:656:A:C8	2.38	0.58
25:A:1102:G:OP1	72:X:76:SER:OG	2.19	0.58
25:A:142:G:H1	25:A:173:A:H2	1.51	0.58
33:AE:6:ASP:O	33:AE:8:VAL:HG22	2.02	0.58
1:1:2897:A:OP2	42:AN:124:LYS:NZ	2.36	0.58
1:AR:3089:C:H2'	1:AR:3090:U:O4'	2.03	0.58
6:CF:328:ASN:OD1	9:CI:48:ASN:ND2	2.36	0.58
19:CS:170:ARG:HD2	30:DC:56:VAL:HG23	1.85	0.58
1:1:837:A:OP1	45:AQ:5:THR:OG1	2.21	0.58
10:CJ:121:SER:O	10:CJ:123:GLN:N	2.34	0.58
58:J:8:ARG:HD3	58:J:21:PHE:HD1	1.68	0.58
66:R:40:GLU:HA	66:R:42:GLU:HB2	1.84	0.58
1:1:3192:U:H2'	1:1:3193:C:C6	2.38	0.58
25:A:1175:U:H2'	25:A:1176:G:C8	2.38	0.58
25:A:478:A:O2'	59:K:124:HIS:ND1	2.23	0.58
25:A:855:A:C2	25:A:857:U:H1'	2.39	0.58
1:AR:352:A:H61	1:AR:365:A:H5''	1.68	0.58
11:CK:28:VAL:HG22	11:CK:33:THR:HB	1.86	0.58
18:CR:32:THR:HG21	18:CR:87:SER:HB3	1.85	0.58
53:E:114:ALA:HB3	53:E:117:ARG:HB3	1.85	0.58
1:1:2303:A:P	43:AO:23:ARG:HH22	2.26	0.58
25:6:1773:C:H2'	25:6:1774:G:H8	1.69	0.58
25:A:720:G:H1'	25:A:721:U:H5''	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:2793:G:C4	87:AR:4262:GOL:H32	2.37	0.58
14:CN:91:ARG:NH2	14:CN:97:VAL:O	2.37	0.58
52:D:161:LYS:HB2	52:D:166:THR:HG22	1.85	0.58
28:DA:54:ASP:OD2	28:DA:115:ARG:NH2	2.30	0.58
1:1:2193:U:H5'	1:1:2194:G:H5'	1.86	0.58
25:6:1511:U:H2'	25:6:1512:G:C8	2.38	0.58
1:AR:1412:G:OP1	34:DG:105:ARG:NH2	2.36	0.58
1:AR:2389:C:H1'	18:CR:69:ARG:NH1	2.19	0.58
1:AR:1456:A:N7	33:DF:26:LYS:HE2	2.18	0.58
33:DF:6:ASP:O	33:DF:8:VAL:HG22	2.04	0.58
44:DQ:2:VAL:N	44:DQ:90:HIS:O	2.37	0.58
26:7:98:PRO:HG3	56:H:148:SER:HB3	1.83	0.58
38:AJ:66:GLU:OE1	38:AJ:70:ARG:NH2	2.37	0.58
1:AR:1833:G:OP1	41:DN:10:LYS:NZ	2.32	0.58
84:AR:3443:OHX:N1	84:AR:3731:OHX:N3	2.51	0.58
12:CL:171:TRP:CE3	12:CL:178:ARG:HD2	2.39	0.58
1:AR:799:G:HO2'	14:CN:18:TRP:HE1	1.50	0.58
36:DI:8:ARG:HH21	36:DI:31:ARG:HD2	1.68	0.58
1:AR:361:A:O3'	39:DL:45:ARG:NH2	2.36	0.58
56:H:51:LYS:HB3	56:H:112:VAL:HB	1.85	0.58
67:S:23:LYS:HB3	67:S:34:LEU:HD11	1.85	0.58
70:V:28:SER:OG	70:V:111:GLY:O	2.13	0.58
73:Y:23:ARG:O	73:Y:26:GLU:HB2	2.03	0.58
1:1:217:U:H4'	28:9:100:HIS:CD2	2.39	0.58
25:6:1458:G:H5''	25:6:1459:C:OP2	2.03	0.58
25:A:218:A:N6	25:A:844:A:H1'	2.17	0.58
30:AB:47:LYS:HE2	30:AB:48:TYR:CZ	2.39	0.58
1:AR:1555:U:O2'	1:AR:2169:G:N2	2.37	0.58
1:AR:2228:A:H2'	1:AR:2229:A:C8	2.38	0.58
1:AR:595:G:N1	1:AR:609:G:H5''	2.19	0.58
64:P:81:VAL:HG22	64:P:115:ILE:HB	1.86	0.58
14:CN:165:SER:O	14:CN:167:PHE:N	2.37	0.58
58:J:76:THR:HG22	58:J:108:PRO:HG2	1.84	0.58
25:6:820:U:O2'	25:6:821:U:H5''	2.04	0.58
32:AD:17:VAL:HG11	32:AD:92:ILE:HD12	1.84	0.58
1:AR:715:A:H4'	1:AR:716:A:OP1	2.04	0.58
5:CE:185:GLY:O	5:CE:191:LYS:NZ	2.37	0.58
7:CG:156:GLY:HA2	7:CG:181:PRO:HD3	1.84	0.58
20:CT:160:GLU:HA	20:CT:163:ARG:HB3	1.86	0.58
1:AR:3051:U:H1'	24:CX:92:PHE:CE2	2.39	0.58
63:O:91:LEU:HB3	63:O:122:ILE:HG12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2572:C:O2'	1:1:2573:G:O4'	2.20	0.57
25:6:950:C:H2'	25:6:951:A:C8	2.39	0.57
25:A:93:A:O2'	54:F:4:GLY:HA3	2.03	0.57
28:DA:32:SER:HA	28:DA:49:PRO:HA	1.86	0.57
28:DA:45:ILE:HD12	28:DA:119:ILE:HG23	1.86	0.57
33:DF:79:ARG:NE	33:DF:79:ARG:H	2.01	0.57
64:P:17:ALA:HB3	64:P:81:VAL:HA	1.85	0.57
71:W:74:GLN:HA	71:W:79:LEU:HB2	1.86	0.57
1:1:1233:G:H22	1:1:1255:C:H42	1.51	0.57
1:1:1620:U:H2'	1:1:1621:A:C8	2.39	0.57
25:A:730:G:H21	25:A:731:C:H5'	1.69	0.57
29:AA:26:VAL:HG21	29:AA:96:VAL:HB	1.86	0.57
50:B:31:VAL:HG12	50:B:33:GLN:H	1.68	0.57
5:CE:41:VAL:HA	5:CE:185:GLY:CA	2.33	0.57
1:1:1278:A:O2'	1:1:1279:C:O5'	2.22	0.57
25:6:1537:C:O2'	25:6:1540:G:O6	2.22	0.57
25:6:180:A:H2'	25:6:181:A:O4'	2.04	0.57
4:CD:27:ALA:O	4:CD:128:ARG:NH2	2.38	0.57
15:CO:21:VAL:HB	15:CO:63:VAL:HG13	1.86	0.57
1:AR:13:A:H4'	27:CZ:39:LYS:HG3	1.86	0.57
39:DL:31:LYS:O	39:DL:33:THR:HG22	2.05	0.57
40:DM:46:ARG:NH1	40:DM:47:GLY:O	2.36	0.57
53:E:70:THR:O	53:E:74:GLN:N	2.36	0.57
1:1:650:C:H2'	1:1:651:G:C8	2.40	0.57
25:A:325:G:H4'	61:M:83:THR:HG21	1.87	0.57
40:AL:8:ILE:H	40:AL:8:ILE:HD12	1.69	0.57
41:AM:21:ARG:CZ	41:AM:24:PRO:HG3	2.35	0.57
29:DB:24:VAL:HG11	29:DB:87:LEU:HB3	1.87	0.57
60:L:50:THR:HA	60:L:55:VAL:HG13	1.85	0.57
68:T:35:ILE:HG23	68:T:102:ALA:HB2	1.85	0.57
1:1:1072:G:H21	31:AC:50:THR:HB	1.68	0.57
1:1:3255:U:H2'	1:1:3256:G:H8	1.70	0.57
1:1:3346:U:H3	1:1:3359:A:N6	2.02	0.57
1:1:627:U:H2'	1:1:628:A:C8	2.39	0.57
25:6:686:C:H2'	25:6:687:G:C8	2.40	0.57
25:A:514:G:O2'	25:A:515:A:H5'	2.03	0.57
6:CF:180:LYS:NZ	6:CF:203:ARG:O	2.37	0.57
7:CG:226:TYR:HE2	7:CG:236:LEU:HD11	1.68	0.57
14:CN:47:ALA:HB1	14:CN:48:PRO:HD2	1.87	0.57
17:CQ:110:PRO:O	17:CQ:112:TYR:N	2.38	0.57
23:CW:38:ILE:HD12	23:CW:56:VAL:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:3228:C:H4'	1:1:3229:G:O5'	2.04	0.57
25:A:1711:C:H2'	25:A:1712:A:H5''	1.86	0.57
84:A:1909:OHX:N6	84:A:2024:OHX:N2	2.51	0.57
29:AA:83:THR:HG23	29:AA:85:TYR:N	2.20	0.57
38:AJ:34:SER:OG	38:AJ:34:SER:O	2.22	0.57
51:C:181:LEU:O	51:C:185:THR:N	2.30	0.57
1:AR:3215:A:N7	15:CO:125:LYS:NZ	2.53	0.57
14:CN:28:GLN:HB3	16:CP:201:ARG:HH11	1.70	0.57
54:F:122:LYS:HD2	54:F:164:LEU:HD21	1.86	0.57
25:A:66:U:C5	56:H:173:PRO:HG3	2.39	0.57
1:1:1634:G:OP1	29:AA:107:ARG:NH1	2.38	0.57
1:1:837:A:OP2	45:AQ:4:ARG:NH1	2.37	0.57
1:1:873:C:H5''	1:1:874:U:O5'	2.05	0.57
25:6:808:U:H2'	25:6:809:A:C8	2.39	0.57
1:AR:138:U:H2'	1:AR:139:G:H8	1.68	0.57
5:CE:41:VAL:CA	5:CE:185:GLY:HA3	2.33	0.57
5:CE:25:ILE:H	5:CE:25:ILE:HD13	1.70	0.57
25:A:142:G:H22	25:A:173:A:H2	1.52	0.57
84:AR:3443:OHX:N1	84:AR:3731:OHX:N4	2.53	0.57
7:CG:8:LYS:HG2	7:CG:12:TYR:CE1	2.40	0.57
23:CW:33:TYR:HE1	23:CW:80:THR:HG22	1.69	0.57
25:A:197:A:H61	58:J:138:ASN:ND2	2.03	0.57
70:V:55:PRO:HA	70:V:91:ILE:HG12	1.86	0.57
1:1:1117:G:OP1	31:AC:4:SER:HB2	2.04	0.57
1:1:118:U:O2	1:1:121:A:H5'	2.03	0.57
1:1:1621:A:H2'	1:1:1622:U:C6	2.40	0.57
84:1:3473:OHX:N5	84:1:3720:OHX:N6	2.52	0.57
22:2:57:TYR:CG	22:2:89:LEU:HD21	2.40	0.57
25:6:482:U:H3	25:6:505:A:H61	1.50	0.57
29:AA:53:VAL:HA	29:AA:57:HIS:HD2	1.69	0.57
41:AM:21:ARG:HD3	41:AM:22:PRO:O	2.05	0.57
5:CE:77:THR:HG23	5:CE:326:GLY:O	2.05	0.57
52:D:144:TRP:CE2	52:D:173:PRO:HG3	2.40	0.57
52:D:87:GLN:HG2	52:D:96:THR:HB	1.86	0.57
36:DI:41:ARG:HG2	36:DI:56:THR:HG21	1.86	0.57
1:1:1317:A:O2'	1:1:1318:A:H3'	2.05	0.57
1:1:2356:A:H61	1:1:2983:C:H5	1.48	0.57
1:1:3316:A:OP1	1:1:3318:G:N2	2.38	0.57
1:1:595:G:H1	1:1:609:G:H5''	1.69	0.57
25:6:1350:U:H2'	25:6:1351:G:H8	1.70	0.57
25:6:1799:U:H4'	25:6:1800:A:H2'	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:3279:A:H2'	1:AR:3280:U:H5'	1.86	0.57
1:AR:3295:A:OP2	5:CE:126:LYS:N	2.37	0.57
1:AR:789:A:H2'	1:AR:790:U:C6	2.40	0.57
84:AS:203:OHX:N4	84:AS:210:OHX:N2	2.53	0.57
50:B:200:ASP:OD1	50:B:200:ASP:N	2.38	0.57
33:DF:88:PRO:HG2	33:DF:89:LEU:HD12	1.87	0.57
25:A:1555:A:OP2	65:Q:47:ARG:NH2	2.37	0.57
66:R:50:GLU:OE1	66:R:112:TYR:OH	2.17	0.57
1:1:2207:A:H2'	1:1:2208:A:C8	2.40	0.56
1:1:792:G:H2'	1:1:793:C:C6	2.40	0.56
1:AR:1063:G:N3	1:AR:1066:G:O2'	2.35	0.56
12:CL:84:ALA:O	12:CL:140:THR:HG22	2.04	0.56
14:CN:105:ASN:OD1	14:CN:107:GLU:HG2	2.05	0.56
53:E:70:THR:HG22	53:E:86:LEU:HD13	1.86	0.56
57:I:84:LYS:NZ	66:R:143:ARG:HH22	140.64	0.56
43:AO:8:LYS:HD3	43:AO:12:ARG:HH21	1.69	0.56
1:AR:673:U:OP1	19:CS:21:SER:OG	2.16	0.56
2:3:106:U:H2'	2:3:107:C:C6	2.41	0.56
50:B:168:HIS:HB3	50:B:203:PHE:CZ	2.40	0.56
51:C:61:LEU:O	51:C:63:GLY:N	2.39	0.56
52:D:80:VAL:HA	52:D:102:VAL:HG22	1.87	0.56
25:A:144:U:H5	56:H:137:ARG:HH12	1.53	0.56
25:A:1228:G:H5'	62:N:45:LEU:HB2	1.86	0.56
25:A:802:G:H21	72:X:107:SER:HB3	1.70	0.56
1:1:542:G:H1	1:1:549:U:H3	1.54	0.56
1:1:70:A:N1	1:1:313:A:O2'	2.32	0.56
22:2:7:TYR:OH	22:2:54:HIS:HB2	2.05	0.56
25:A:1600:A:O2'	25:A:1602:C:N4	2.38	0.56
25:A:647:G:N2	25:A:687:G:H22	2.03	0.56
30:AB:46:ASP:O	30:AB:47:LYS:HB3	2.05	0.56
1:AR:1366:A:C2	1:AR:1367:G:C4	2.94	0.56
1:AR:849:C:H2'	1:AR:850:U:C6	2.40	0.56
51:C:168:ILE:HG12	51:C:197:ILE:HD12	1.86	0.56
1:AR:3294:A:H5'	5:CE:128:LYS:HG3	1.87	0.56
1:AR:3330:A:H4'	5:CE:366:GLY:HA3	1.87	0.56
8:CH:97:ASN:O	8:CH:99:GLU:N	2.38	0.56
20:CT:154:ALA:O	20:CT:158:GLU:HB3	2.06	0.56
25:6:1112:G:OP1	43:DP:6:ARG:NH2	2.39	0.56
54:F:240:LYS:H	54:F:240:LYS:HE2	1.70	0.56
56:H:69:LEU:HB3	56:H:71:THR:HG23	1.88	0.56
25:6:1767:G:OP1	25:6:1770:U:H4'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:542:A:C8	25:6:543:C:H2'	2.39	0.56
25:A:138:A:N6	25:A:266:A:H61	2.02	0.56
25:A:1542:G:H22	25:A:1568:C:H1'	1.71	0.56
1:AR:308:A:H5'	1:AR:2223:A:O2'	2.05	0.56
1:AR:3267:A:H2'	8:CH:69:PHE:CZ	2.41	0.56
50:B:50:VAL:HG22	67:S:109:LEU:HD21	1.87	0.56
16:CP:10:LEU:HD22	16:CP:19:LEU:HD11	1.87	0.56
1:AR:266:A:H2'	38:DK:30:LYS:HE2	1.88	0.56
54:F:37:LYS:HB2	54:F:40:GLU:HG2	1.88	0.56
56:H:69:LEU:O	56:H:71:THR:N	2.37	0.56
57:I:141:ARG:HH12	57:I:143:LEU:HD11	1.71	0.56
50:B:62:ARG:HH21	71:W:39:VAL:HG22	1.70	0.56
73:Y:62:LYS:HD2	73:Y:118:PRO:HB3	1.88	0.56
1:1:1307:G:H1'	1:1:1308:A:C8	2.40	0.56
25:A:735:C:O2'	25:A:736:C:H5''	2.05	0.56
32:AD:43:ILE:HG22	32:AD:70:PHE:HB2	1.86	0.56
45:AQ:79:VAL:HA	45:AQ:82:THR:HG22	1.88	0.56
1:AR:291:C:H5''	16:CP:68:ARG:NH1	2.20	0.56
1:1:2218:G:H2'	1:1:2219:A:H8	1.68	0.56
1:1:3027:A:H2'	1:1:3028:G:O4'	2.05	0.56
1:AR:2355:G:H4'	18:CR:139:TYR:CE1	2.40	0.56
1:AR:271:C:O2	38:DK:82:ARG:NH2	2.36	0.56
1:AR:2960:C:H2'	1:AR:2961:G:H8	1.70	0.56
1:AR:3159:C:H2'	1:AR:3160:U:C6	2.40	0.56
6:CF:44:LYS:HB3	6:CF:47:ARG:NH1	2.21	0.56
8:CH:56:LYS:HB2	8:CH:98:VAL:HG11	1.86	0.56
9:CI:24:GLU:CD	9:CI:25:GLN:H	2.09	0.56
61:M:57:LYS:HD3	61:M:131:ILE:HG23	1.88	0.56
1:1:156:G:OP2	38:AJ:25:LYS:HB3	2.06	0.56
25:6:1655:A:N1	1:AR:2291:A:O2'	2.31	0.56
25:A:1555:A:H5''	65:Q:44:ARG:HD3	1.87	0.56
25:A:321:C:N4	25:A:1667:A:OP1	2.39	0.56
25:A:973:A:H2'	25:A:974:A:H8	1.70	0.56
29:AA:24:VAL:HG21	29:AA:87:LEU:HD23	1.87	0.56
1:AR:2818:U:C6	1:AR:2818:U:H5'	2.38	0.56
12:CL:43:VAL:HG21	12:CL:197:VAL:HB	1.88	0.56
18:CR:29:THR:HA	18:CR:32:THR:HG23	1.88	0.56
25:A:144:U:H5	56:H:137:ARG:NH1	2.04	0.56
68:T:123:ARG:HG3	68:T:133:VAL:HG21	1.87	0.56
74:Z:35:VAL:HG13	74:Z:36:SER:H	1.70	0.56
25:A:1022:C:O2'	25:A:1125:A:N1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1290:U:H2'	25:A:1291:G:C8	2.40	0.56
25:A:52:U:H2'	25:A:53:G:H8	1.69	0.56
30:AB:75:LEU:HA	30:AB:78:LEU:HB2	1.87	0.56
71:W:60:ARG:HA	71:W:65:SER:HB2	1.87	0.56
1:1:1445:U:H5''	1:1:1446:A:OP2	2.06	0.56
25:A:319:U:H1'	25:A:323:A:C4	2.41	0.56
1:AR:59:G:H4'	1:AR:60:A:H4'	1.88	0.56
6:CF:295:ILE:O	6:CF:299:ILE:HG12	2.05	0.56
22:CV:124:VAL:HG12	22:CV:125:ALA:H	1.70	0.56
29:DB:25:ILE:HG23	29:DB:41:ALA:HB1	1.88	0.56
74:Z:51:GLU:O	74:Z:53:ASP:N	2.39	0.56
32:AD:34:LEU:HD23	32:AD:59:TYR:HB3	1.88	0.56
1:AR:715:A:H8	30:DC:115:LYS:HG2	1.71	0.56
1:AR:805:G:H1'	6:CF:73:ARG:NH1	2.21	0.56
1:AR:2153:U:OP1	4:CD:246:LEU:HB2	2.06	0.56
5:CE:188:ILE:HD12	5:CE:189:SER:H	1.70	0.56
10:CJ:84:ARG:N	10:CJ:84:ARG:HE	2.04	0.56
1:AR:1307:G:H5''	17:CQ:60:LYS:HZ2	1.70	0.56
57:I:73:VAL:C	57:I:75:THR:H	2.09	0.56
1:1:2747:A:H2'	1:1:2748:A:C8	2.41	0.55
25:6:1081:A:H1'	25:6:1082:C:H5	1.71	0.55
1:AR:2213:A:H2'	1:AR:2214:A:C8	2.40	0.55
5:CE:303:LYS:HD2	5:CE:361:THR:HG21	1.88	0.55
17:CQ:22:VAL:HG11	17:CQ:120:VAL:HG11	1.87	0.55
1:AR:904:A:OP2	39:DL:30:GLN:NE2	2.39	0.55
42:DO:94:SER:OG	42:DO:104:PRO:O	2.24	0.55
66:R:67:VAL:HG11	66:R:81:ILE:HG22	1.88	0.55
1:1:59:G:H2'	3:4:33:A:O2'	2.06	0.55
25:6:654:C:H2'	25:6:655:G:H8	1.71	0.55
25:A:1773:C:H2'	25:A:1774:G:C8	2.41	0.55
39:AK:52:LYS:HA	39:AK:55:ARG:HD2	1.88	0.55
84:AR:3443:OHX:N5	84:AR:3731:OHX:N6	2.54	0.55
7:CG:163:LEU:HD11	7:CG:175:HIS:CG	2.42	0.55
12:CL:77:THR:HG22	12:CL:82:ARG:HA	1.88	0.55
25:6:848:C:H2'	25:6:849:C:C6	2.41	0.55
25:A:1244:A:O2'	25:A:1245:G:OP1	2.21	0.55
25:A:740:A:H2'	25:A:741:C:H5''	1.89	0.55
25:A:830:U:HO2'	25:A:831:U:H6	1.52	0.55
1:AR:3045:G:OP1	5:CE:19:ARG:NH2	2.39	0.55
84:AR:3443:OHX:N2	84:AR:3731:OHX:N6	2.54	0.55
2:AS:28:C:OP1	13:CM:137:ARG:NH1	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CE:293:ASN:HB2	5:CE:304:THR:HA	1.87	0.55
57:I:13:PRO:HB3	57:I:14:THR:HB	1.88	0.55
25:6:647:G:H22	25:6:687:G:H1	1.53	0.55
25:A:1291:G:O5'	25:A:1291:G:H8	1.90	0.55
25:A:734:A:H5''	25:A:735:C:OP1	2.05	0.55
45:AQ:8:VAL:HB	45:AQ:11:THR:HG22	1.88	0.55
1:AR:1064:A:H4'	1:AR:1065:A:O5'	2.06	0.55
1:AR:1190:A:C8	1:AR:1193:A:H1'	2.42	0.55
4:CD:83:HIS:CE1	4:CD:86:GLN:HB2	2.41	0.55
6:CF:188:ARG:HB3	6:CF:193:LYS:HB2	1.89	0.55
12:CL:153:ARG:HG2	12:CL:156:ARG:NH2	2.22	0.55
52:D:140:ARG:HH22	52:D:228:ASN:HD21	1.54	0.55
28:DA:5:SER:HB3	28:DA:8:VAL:HG12	1.87	0.55
32:DE:43:ILE:HG22	32:DE:70:PHE:HB2	1.88	0.55
58:J:39:GLY:O	58:J:59:ARG:HB3	2.07	0.55
60:L:27:PHE:CD1	60:L:40:LEU:HD23	2.42	0.55
58:J:10:LYS:HG2	61:M:133:LYS:HE3	1.89	0.55
1:1:1581:C:H2'	1:1:1582:C:H5'	1.87	0.55
22:2:79:MET:HA	22:2:84:TYR:HA	1.87	0.55
25:A:1490:C:H4'	25:A:1491:U:OP1	2.07	0.55
30:AB:3:SER:O	30:AB:6:THR:HG22	2.07	0.55
33:AE:19:ARG:HD3	33:AE:35:GLU:HG2	1.89	0.55
1:AR:2339:C:P	24:CX:48:ARG:HG2	2.47	0.55
2:AS:48:U:O4	7:CG:58:LYS:HE2	2.06	0.55
24:CX:15:LEU:HD13	24:CX:51:ALA:HB3	1.89	0.55
29:DB:104:PRO:HA	29:DB:107:ARG:HD2	1.89	0.55
68:T:83:ALA:HA	68:T:117:LYS:HE3	27.17	0.55
1:1:1362:G:H2'	1:1:1363:A:C8	2.42	0.55
1:1:2218:G:H2'	1:1:2219:A:C8	2.41	0.55
25:A:568:G:H4'	73:Y:90:ASP:HB2	1.87	0.55
1:AR:291:C:H5''	16:CP:68:ARG:HH12	1.70	0.55
21:CU:24:LEU:HD13	22:CV:148:PRO:HG3	1.89	0.55
38:DK:45:ARG:NH2	38:DK:54:GLU:OE1	2.40	0.55
25:6:1584:G:H22	25:6:1611:A:P	2.29	0.55
2:AS:26:C:H5'	7:CG:56:THR:HB	1.88	0.55
7:CG:64:ILE:HG13	7:CG:105:ILE:HD12	1.89	0.55
1:AR:412:G:OP1	18:CR:62:ARG:NH1	2.40	0.55
33:DF:19:ARG:HD3	33:DF:35:GLU:HG3	1.88	0.55
21:O:155:ARG:NH2	21:O:172:TYR:HA	2.22	0.55
1:1:174:C:H2'	1:1:175:C:H6	1.72	0.55
1:1:601:U:H2'	1:1:602:A:O4'	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:1698:G:O2'	25:6:1699:G:O5'	2.20	0.55
84:A:1909:OHX:N6	84:A:2024:OHX:N5	2.54	0.55
39:AK:65:ARG:HG3	39:AK:65:ARG:HH11	1.72	0.55
1:AR:2298:U:O4	1:AR:2923:U:H5	1.89	0.55
51:C:131:ASP:O	51:C:133:TYR:N	2.34	0.55
4:CD:70:ARG:NH1	4:CD:72:ARG:HD3	2.22	0.55
19:CS:96:PHE:CD1	19:CS:97:PRO:HD2	2.42	0.55
30:DC:126:LYS:HG2	30:DC:146:GLU:HB2	1.88	0.55
73:Y:44:GLY:H	73:Y:78:LYS:NZ	2.05	0.55
74:Z:113:ASN:HA	74:Z:116:LYS:HD3	1.89	0.55
1:1:1204:A:H2	1:1:2834:G:N3	2.05	0.55
25:A:1584:G:N2	25:A:1611:A:OP2	2.31	0.55
25:A:868:G:H1	25:A:960:U:H3	1.53	0.55
11:CK:162:GLN:HG3	11:CK:163:GLN:N	2.22	0.55
56:H:98:ARG:NH2	56:H:101:ILE:O	2.36	0.55
25:A:996:U:H3	25:A:1008:G:H1	1.55	0.55
29:AA:102:GLU:O	29:AA:103:GLN:HB2	2.07	0.55
29:AA:46:ILE:HD11	29:AA:49:TYR:HA	1.89	0.55
4:CD:116:VAL:HG22	4:CD:126:LEU:HB2	1.89	0.55
9:CI:151:ARG:NH1	9:CI:244:ASN:O	2.40	0.55
11:CK:126:VAL:HG21	11:CK:161:LEU:HA	1.89	0.55
18:CR:116:HIS:HB3	18:CR:149:VAL:HB	1.89	0.55
20:CT:28:GLU:HG3	20:CT:49:THR:HG22	1.89	0.55
22:CV:12:ARG:HD3	22:CV:13:TYR:CE1	2.42	0.55
25:A:448:C:OP1	54:F:29:PRO:HD3	2.07	0.55
59:K:53:ARG:NH2	59:K:97:LEU:O	2.39	0.55
68:T:41:ARG:NH1	69:U:38:LYS:HG3	2.22	0.55
1:1:1015:U:O2	1:1:1017:C:O2'	2.17	0.54
1:1:1805:C:H2'	1:1:1806:A:C8	2.42	0.54
1:1:849:C:H2'	1:1:850:U:H6	1.70	0.54
25:6:218:A:H2'	25:6:219:A:H5''	1.89	0.54
84:A:1909:OHX:N4	84:A:2024:OHX:N1	2.55	0.54
25:A:641:G:H2'	25:A:642:G:H8	1.72	0.54
1:AR:2659:G:H4'	1:AR:2751:G:O2'	2.08	0.54
1:AR:2989:U:O2'	5:CE:232:ARG:NH2	2.40	0.54
50:B:123:VAL:HG11	50:B:133:ILE:HD11	1.88	0.54
5:CE:375:GLU:OE1	26:CY:14:TYR:OH	2.19	0.54
17:CQ:73:PHE:CD2	17:CQ:78:ARG:HG2	2.42	0.54
29:DB:9:LYS:HD2	29:DB:83:THR:O	2.06	0.54
64:P:30:VAL:HG13	64:P:39:ILE:HG13	1.87	0.54
69:U:52:GLY:C	69:U:54:PHE:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2179:C:H4'	1:1:2180:G:OP2	2.08	0.54
1:1:3121:U:H1'	1:1:3122:A:H5''	1.89	0.54
25:A:1315:U:OP1	25:A:1328:G:N2	2.39	0.54
12:CL:169:LYS:NZ	22:CV:159:PHE:H	2.04	0.54
1:AR:2854:U:P	12:CL:3:ARG:HH22	2.29	0.54
13:CM:9:MET:O	13:CM:9:MET:HG3	2.06	0.54
52:D:106:ASP:OD1	52:D:107:SER:N	2.41	0.54
22:CV:88:ARG:HH21	31:DD:33:LYS:HB3	1.73	0.54
39:DL:28:HIS:CD2	39:DL:31:LYS:HE2	2.42	0.54
70:V:68:ARG:NH2	70:V:77:LYS:HA	2.22	0.54
1:1:3164:C:H1'	1:1:3165:A:H5'	1.89	0.54
27:8:135:ILE:O	27:8:139:ILE:HG22	2.06	0.54
25:A:1487:A:OP2	53:E:8:LYS:NZ	2.40	0.54
36:AH:47:CYS:HB3	36:AH:84:CYS:SG	2.48	0.54
1:AR:138:U:H2'	1:AR:139:G:C8	2.42	0.54
15:CO:17:VAL:HG11	15:CO:74:ARG:HA	1.88	0.54
28:DA:45:ILE:HD11	28:DA:122:LYS:HB2	1.89	0.54
34:DG:85:LEU:HB2	34:DG:117:ILE:HD13	1.89	0.54
1:AR:3120:C:H3'	42:DO:111:ARG:HH21	1.73	0.54
65:Q:81:ARG:NH1	65:Q:97:TYR:O	2.34	0.54
1:1:1724:U:H1'	1:1:1725:C:C6	2.41	0.54
25:6:219:A:C6	25:6:843:U:H1'	2.43	0.54
25:A:808:U:H2'	25:A:809:A:C8	2.43	0.54
1:1:18:G:OP1	37:AI:81:ARG:NH2	2.40	0.54
1:AR:3165:A:H61	1:AR:3285:C:H42	1.56	0.54
33:DF:55:LEU:HB2	33:DF:95:PRO:HD3	1.88	0.54
36:DI:8:ARG:NH2	36:DI:31:ARG:HD2	2.22	0.54
51:C:77:GLU:OE1	64:P:114:ARG:NH2	2.37	0.54
69:U:34:VAL:HG23	69:U:53:TRP:CZ2	2.42	0.54
1:1:1194:G:H2'	1:1:1195:A:C8	2.43	0.54
1:1:155:G:H5''	1:1:156:G:C8	2.43	0.54
25:6:1573:A:H4'	25:6:1574:G:H5'	1.88	0.54
25:A:1254:U:OP2	62:N:46:ARG:NH1	2.41	0.54
84:A:1909:OHX:N4	84:A:2024:OHX:N2	2.56	0.54
1:AR:501:A:H2'	1:AR:502:U:C6	2.42	0.54
1:AR:3268:A:OP1	8:CH:46:ARG:NH2	2.40	0.54
15:CO:22:LEU:HB3	15:CO:64:VAL:HG13	1.88	0.54
18:CR:67:ILE:HG13	18:CR:82:ARG:CZ	2.37	0.54
1:AR:2992:U:H1'	18:CR:69:ARG:HH21	1.73	0.54
55:G:23:VAL:O	55:G:34:GLN:NE2	2.39	0.54
25:A:127:G:N7	56:H:202:ARG:NH2	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:H:68:LEU:O	56:H:69:LEU:HB2	2.07	0.54
65:Q:61:ARG:NH2	65:Q:88:GLU:OE1	2.40	0.54
68:T:30:TYR:HE2	68:T:40:ARG:HH11	1.56	0.54
1:1:2213:A:H2'	1:1:2214:A:C8	2.42	0.54
1:1:299:G:H22	38:AJ:30:LYS:HD3	1.72	0.54
27:8:137:ASN:HB3	27:8:142:ILE:HG12	1.88	0.54
25:A:1586:A:H1'	25:A:1611:A:N6	2.23	0.54
25:A:927:C:H1'	64:P:125:SER:HB2	1.88	0.54
84:AS:203:OHX:N5	84:AS:210:OHX:N3	2.56	0.54
4:CD:20:THR:O	4:CD:20:THR:OG1	2.25	0.54
8:CH:175:LYS:O	15:CO:117:ARG:NH2	2.41	0.54
11:CK:12:VAL:HG13	11:CK:16:VAL:HG22	1.89	0.54
18:CR:33:ALA:HB1	18:CR:117:ILE:HG12	1.89	0.54
24:CX:80:ARG:NH1	24:CX:116:GLY:HA3	2.22	0.54
30:DC:77:LYS:O	30:DC:79:TRP:N	2.40	0.54
45:DR:8:VAL:HB	45:DR:11:THR:HG22	1.89	0.54
55:G:162:VAL:HG23	55:G:166:ARG:HB3	1.88	0.54
59:K:110:GLN:NE2	59:K:126:ARG:HG2	2.22	0.54
60:L:23:ALA:O	60:L:64:TYR:HB2	2.08	0.54
60:L:76:LEU:HD13	60:L:76:LEU:H	1.73	0.54
1:1:1062:A:N3	22:2:130:ARG:NH2	2.55	0.54
1:1:1230:G:N2	1:1:1279:C:N3	2.51	0.54
1:1:1940:G:H21	1:1:3362:A:H8	1.53	0.54
25:A:166:C:H4'	56:H:131:LYS:HE3	1.89	0.54
31:AC:14:ARG:CZ	31:AC:18:ARG:HD2	2.37	0.54
1:AR:2217:U:H2'	1:AR:2218:G:H8	1.73	0.54
1:AR:2801:A:O2'	1:AR:2802:A:H2'	2.07	0.54
1:AR:600:G:N2	1:AR:603:A:OP2	2.41	0.54
5:CE:46:PHE:CD2	5:CE:205:VAL:HG13	2.43	0.54
9:CI:88:ARG:NH1	9:CI:91:GLY:O	2.40	0.54
19:CS:165:ILE:HD11	19:CS:172:PHE:HB3	1.90	0.54
25:A:885:G:N2	64:P:123:SER:HB2	2.17	0.54
68:T:100:THR:HG21	68:T:108:LYS:HG3	1.90	0.54
1:1:2927:C:H2'	1:1:2928:C:C6	2.43	0.54
1:1:409:A:H61	3:4:15:G:H1'	1.73	0.54
25:6:1657:U:O2'	25:6:1658:G:OP2	2.22	0.54
25:6:1773:C:H2'	25:6:1774:G:C8	2.42	0.54
25:6:500:C:O2'	25:6:501:U:O4'	2.26	0.54
30:AB:91:LEU:HD13	30:AB:121:VAL:HG21	1.89	0.54
33:AE:13:THR:HG23	33:AE:72:ARG:HH11	1.73	0.54
1:AR:3159:C:H2'	1:AR:3160:U:H6	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AT:84:C:H5'	3:AT:85:G:C5	2.42	0.54
51:C:180:THR:O	51:C:182:ALA:N	2.40	0.54
51:C:87:ARG:NH2	51:C:220:GLN:OE1	2.41	0.54
1:AR:911:C:N4	4:CD:3:ARG:HD3	2.22	0.54
52:D:170:ILE:HB	52:D:197:TYR:HB2	1.89	0.54
28:DA:51:ARG:HG2	28:DA:115:ARG:NH2	2.23	0.54
30:DC:46:ASP:OD1	30:DC:46:ASP:N	2.40	0.54
55:G:53:VAL:HB	55:G:59:VAL:HG22	1.90	0.54
58:J:36:THR:HB	58:J:57:ALA:O	2.07	0.54
73:Y:42:PRO:O	73:Y:79:ASN:ND2	2.41	0.54
1:1:1593:A:H4'	36:AH:60:ARG:HG2	1.90	0.54
2:3:62:U:O4	2:3:63:A:N6	2.41	0.54
25:6:578:U:H4'	25:6:579:A:H5'	1.88	0.54
25:6:639:U:H5	25:6:695:U:C5	2.25	0.54
28:9:47:ALA:O	28:9:122:LYS:NZ	2.41	0.54
25:A:144:U:HO2'	25:A:145:A:H8	1.54	0.54
25:A:607:G:H5'	25:A:613:G:N2	2.23	0.54
1:AR:764:U:H3'	1:AR:765:C:H5''	1.89	0.54
10:CJ:247:ASP:O	10:CJ:251:LYS:HB2	2.08	0.54
17:CQ:42:ASN:OD1	17:CQ:125:ARG:HD3	2.08	0.54
22:CV:68:THR:HG22	22:CV:71:SER:O	2.08	0.54
24:CX:35:TYR:CD2	24:CX:63:LYS:HE2	2.43	0.54
28:DA:71:SER:N	28:DA:81:GLN:O	2.39	0.54
25:6:1257:U:O2'	25:6:1258:U:O4'	2.26	0.54
25:6:138:A:N6	25:6:266:A:H61	2.05	0.54
25:6:484:C:H42	25:6:503:G:H22	1.55	0.54
25:6:647:G:N2	25:6:687:G:H22	2.06	0.54
25:6:830:U:H2'	25:6:831:U:H5'	1.89	0.54
25:A:480:G:N2	25:A:509:G:H1'	2.23	0.54
1:AR:1637:A:OP2	29:DB:73:LYS:NZ	2.40	0.54
1:AR:2572:C:O2'	1:AR:2573:G:O4'	2.26	0.54
1:AR:3316:A:O2'	1:AR:3317:U:OP2	2.25	0.54
1:AR:637:C:H4'	1:AR:638:C:OP1	2.07	0.54
1:AR:990:U:H4'	22:CV:100:LYS:HB3	1.88	0.54
28:DA:100:HIS:CE1	28:DA:102:SER:HG	2.19	0.54
62:N:43:ARG:HD3	62:N:43:ARG:H	1.72	0.54
1:1:872:U:H2'	1:1:873:C:C6	2.43	0.53
1:AR:1591:G:OP1	36:DI:37:LYS:NZ	2.34	0.53
3:AT:37:A:H5''	3:AT:39:G:O4'	2.08	0.53
50:B:23:HIS:HA	50:B:48:ILE:HB	1.90	0.53
6:CF:330:TYR:CZ	9:CI:49:ALA:HA	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:CP:190:THR:O	16:CP:194:GLN:HG2	2.08	0.53
7:CG:34:LYS:HD3	22:CV:30:TYR:CE1	2.44	0.53
52:D:58:LEU:O	71:W:15:ARG:NE	2.40	0.53
59:K:27:GLU:OE1	59:K:39:LYS:NZ	2.40	0.53
1:1:1294:A:O2'	1:1:1295:G:H5''	2.07	0.53
1:1:2407:C:H1'	1:1:2818:U:O2	2.09	0.53
1:1:696:C:HO2'	1:1:697:A:H8	1.55	0.53
25:6:1126:G:OP1	43:DP:15:ARG:NH1	2.37	0.53
25:6:1273:G:H4'	25:6:1274:C:H5''	1.90	0.53
25:6:1535:U:O2'	25:6:1536:G:O5'	2.24	0.53
25:6:1776:A:H2'	25:6:1777:G:C8	2.43	0.53
25:A:1297:G:N2	25:A:1300:A:OP2	2.40	0.53
25:A:1449:U:H2'	25:A:1450:U:C6	2.44	0.53
25:A:71:A:H2'	25:A:72:A:O4'	2.09	0.53
25:A:800:U:H2'	25:A:801:G:C8	2.43	0.53
1:1:662:U:OP1	30:AB:8:THR:HG21	2.08	0.53
1:AR:637:C:H1'	1:AR:638:C:C6	2.44	0.53
1:AR:786:A:H4'	1:AR:787:G:H5'	1.89	0.53
11:CK:100:ASN:HB3	11:CK:115:ARG:HB2	1.90	0.53
1:AR:799:G:O2'	14:CN:18:TRP:NE1	2.37	0.53
22:CV:48:ILE:HG13	22:CV:94:GLU:HG2	1.90	0.53
19:CS:175:ALA:O	30:DC:51:GLY:HA2	2.08	0.53
37:DJ:85:THR:HG22	37:DJ:87:ALA:N	2.23	0.53
54:F:139:VAL:HG13	54:F:150:PRO:HG3	1.90	0.53
25:A:197:A:H61	58:J:138:ASN:HD22	1.56	0.53
59:K:162:SER:O	59:K:162:SER:OG	2.25	0.53
63:O:115:LEU:HD22	63:O:119:GLU:HG3	1.90	0.53
25:6:654:C:H2'	25:6:655:G:C8	2.43	0.53
33:AE:23:VAL:O	33:AE:28:ARG:NH1	2.41	0.53
44:AP:71:ARG:HE	44:AP:80:ARG:CZ	2.20	0.53
13:CM:34:SER:HB2	13:CM:67:VAL:HG11	1.89	0.53
12:CL:169:LYS:HZ1	22:CV:159:PHE:H	1.55	0.53
40:DM:26:LYS:NZ	40:DM:28:ASN:OD1	2.28	0.53
40:DM:44:LYS:HG2	40:DM:53:THR:HB	1.89	0.53
62:N:136:ILE:HA	62:N:139:HIS:HB3	1.89	0.53
25:A:1552:U:OP2	65:Q:43:ARG:NH2	2.40	0.53
69:U:28:LEU:HD12	69:U:29:GLU:H	1.73	0.53
1:1:3094:A:H2'	1:1:3095:U:C6	2.44	0.53
1:1:565:U:H2'	1:1:566:G:H8	1.74	0.53
25:6:837:G:H2'	25:6:838:G:C8	2.44	0.53
32:AD:13:LYS:NZ	32:AD:99:ASP:OD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:2859:U:H4'	1:AR:2860:U:OP1	2.09	0.53
51:C:144:ARG:HB3	51:C:208:GLN:HB3	1.90	0.53
6:CF:181:VAL:O	6:CF:182:LEU:HB2	2.07	0.53
19:CS:30:VAL:O	19:CS:34:THR:HG23	2.08	0.53
29:DB:10:VAL:O	29:DB:83:THR:HG22	2.07	0.53
41:DN:50:ASN:O	41:DN:51:ILE:HB	2.08	0.53
44:DQ:47:GLN:NE2	44:DQ:53:GLN:OE1	2.41	0.53
55:G:73:THR:OG1	66:R:114:ARG:NH2	2.41	0.53
25:A:68:A:H5'	56:H:160:ARG:HH12	1.73	0.53
57:I:50:ASP:HB3	57:I:56:LYS:HG2	1.90	0.53
58:J:66:SER:HA	58:J:73:SER:HA	1.90	0.53
64:P:26:THR:HG23	64:P:55:SER:HA	1.91	0.53
25:A:1410:A:H5''	66:R:118:ILE:HD11	1.90	0.53
53:E:40:ARG:HG2	70:V:110:PRO:HB3	1.90	0.53
1:1:1688:U:H2'	1:1:1689:U:H6	1.72	0.53
25:A:872:G:H2'	25:A:873:U:O4'	2.09	0.53
1:AR:1307:G:H5''	17:CQ:60:LYS:NZ	2.24	0.53
1:AR:2267:C:H2'	1:AR:2268:U:C6	2.42	0.53
84:AR:3521:OHX:N3	84:AR:3715:OHX:N1	2.56	0.53
7:CG:276:LYS:HG2	7:CG:277:LEU:H	1.72	0.53
12:CL:169:LYS:HD3	22:CV:159:PHE:HA	1.90	0.53
13:CM:21:ILE:HG21	13:CM:33:ALA:HB1	1.90	0.53
14:CN:165:SER:C	14:CN:167:PHE:H	2.11	0.53
21:CU:77:VAL:HG11	21:CU:106:LEU:HD22	1.90	0.53
45:DR:84:ARG:O	45:DR:88:GLU:HG2	2.08	0.53
62:N:131:ASP:OD1	62:N:132:GLU:N	2.38	0.53
1:1:1097:G:O2'	22:2:108:ARG:NH2	2.40	0.53
1:1:1159:A:O2'	1:1:1160:C:H5''	2.08	0.53
1:1:2676:A:H4'	1:1:2677:G:O5'	2.08	0.53
1:1:3084:C:H2'	1:1:3085:G:O4'	2.09	0.53
25:6:1097:U:H4'	25:6:1098:U:O5'	2.08	0.53
25:6:513:U:H2'	25:6:514:G:C8	2.43	0.53
25:6:626:U:H2'	25:6:627:C:H6	1.74	0.53
25:6:729:G:O2'	25:6:730:G:O5'	2.25	0.53
25:A:413:U:H2'	25:A:414:C:C6	2.43	0.53
1:AR:656:A:H2'	1:AR:657:A:C8	2.44	0.53
6:CF:10:SER:OG	6:CF:14:GLU:HB2	2.07	0.53
6:CF:283:THR:HG22	6:CF:285:ASP:H	1.73	0.53
1:AR:3043:C:P	24:CX:48:ARG:HH22	2.32	0.53
27:CZ:82:LEU:HD11	27:CZ:135:ILE:HG21	1.90	0.53
28:DA:54:ASP:OD1	28:DA:110:HIS:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:1631:C:OP2	29:DB:48:ARG:NH2	2.42	0.53
53:E:176:LEU:HD12	53:E:176:LEU:H	1.73	0.53
63:O:42:ARG:HH21	63:O:80:LEU:HD21	1.74	0.53
1:1:1222:G:HO2'	1:1:1285:G:H1	1.48	0.53
1:1:1675:G:H2'	1:1:1676:A:C8	2.44	0.53
1:1:2787:G:O3'	30:AB:57:GLY:HA2	2.08	0.53
3:4:124:G:H1	3:4:129:C:H42	1.57	0.53
25:6:190:C:O2'	25:6:191:C:O5'	2.27	0.53
25:A:1550:A:P	65:Q:42:ARG:HH21	2.31	0.53
25:A:1657:U:H4'	25:A:1658:G:O5'	2.08	0.53
30:AB:90:TYR:CG	30:AB:100:PRO:HG3	2.44	0.53
33:AE:78:LYS:HB3	33:AE:79:ARG:HH21	1.72	0.53
1:AR:2373:A:N3	1:AR:2824:G:O2'	2.35	0.53
1:AR:59:G:H2'	3:AT:33:A:O2'	2.08	0.53
51:C:91:VAL:HG23	51:C:96:LEU:HB3	1.90	0.53
5:CE:113:GLU:HB3	5:CE:176:ALA:HB2	1.91	0.53
5:CE:236:LYS:HG3	5:CE:237:LYS:N	2.23	0.53
6:CF:317:PRO:C	6:CF:319:LYS:H	2.12	0.53
28:DA:47:ALA:O	28:DA:122:LYS:NZ	2.41	0.53
29:DB:41:ALA:HB2	29:DB:77:TYR:HE1	1.74	0.53
45:DR:84:ARG:NH1	45:DR:88:GLU:OE2	2.39	0.53
53:E:208:ILE:HD12	67:S:16:LEU:HD21	1.89	0.53
21:0:82:ASP:OD1	21:0:87:THR:HB	2.08	0.53
1:1:109:A:H4'	1:1:110:G:OP1	2.09	0.53
1:1:3278:C:H2'	1:1:3278:C:O2	2.07	0.53
1:1:439:C:H5	1:1:440:A:C6	2.27	0.53
3:4:136:G:OP1	27:8:48:SER:OG	2.24	0.53
25:A:1350:U:H2'	25:A:1351:G:H8	1.74	0.53
1:AR:1232:C:C5	1:AR:1261:G:H2'	2.43	0.53
1:AR:73:C:C2	14:CN:59:ARG:HD3	2.43	0.53
18:CR:105:LYS:HB3	18:CR:107:LEU:HD13	1.91	0.53
19:CS:64:VAL:HG13	19:CS:93:ILE:HD11	1.90	0.53
29:DB:48:ARG:NH2	29:DB:69:LYS:HD2	2.23	0.53
53:E:108:LYS:HB3	53:E:113:LEU:HD12	1.91	0.53
65:Q:29:SER:O	65:Q:31:GLU:N	2.42	0.53
25:A:778:G:H3'	25:A:780:A:C2	2.40	0.53
1:1:1178:G:O6	35:AG:20:LYS:HE2	2.09	0.53
37:AI:85:THR:HB	37:AI:88:LEU:HB2	1.91	0.53
1:AR:1944:U:H2'	1:AR:1945:A:C8	2.43	0.53
2:AS:91:G:H2'	2:AS:92:A:H8	1.73	0.53
10:CJ:143:ILE:HG23	10:CJ:175:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CT:106:LEU:HB3	20:CT:120:TYR:CE1	2.44	0.53
1:AR:838:G:O6	45:DR:4:ARG:NH2	2.42	0.53
55:G:116:HIS:O	55:G:120:ILE:HG13	2.09	0.53
25:A:866:G:OP1	63:O:2:GLY:HA3	2.09	0.53
66:R:123:ARG:HG3	66:R:124:PRO:HD2	1.90	0.53
25:6:1620:C:H2'	25:6:1621:U:H6	1.74	0.53
28:9:63:LYS:HE3	28:9:97:ILE:HD12	1.91	0.53
25:A:1338:C:H1'	25:A:1410:A:C4	2.43	0.53
25:A:968:U:H5''	25:A:1033:C:O2'	2.07	0.53
30:AB:116:GLY:HA2	30:AB:137:LYS:HE3	1.90	0.53
34:AF:121:ASN:N	34:AF:121:ASN:OD1	2.42	0.53
1:AR:955:U:H2'	1:AR:956:U:C6	2.44	0.53
1:AR:980:A:H2'	1:AR:981:U:C6	2.44	0.53
6:CF:23:PRO:HD2	6:CF:26:PHE:CD2	2.43	0.53
18:CR:125:GLN:HB2	18:CR:141:SER:HB2	1.91	0.53
1:AR:498:A:P	35:DH:86:ARG:HH21	2.32	0.53
41:DN:42:ARG:HG2	41:DN:43:ASN:H	1.74	0.53
21:0:106:LEU:HD23	21:0:110:MET:HG2	1.90	0.52
1:1:1724:U:H4'	1:1:1725:C:OP1	2.08	0.52
1:1:2444:C:H42	1:1:2503:G:H21	1.57	0.52
25:6:1405:G:H2'	25:6:1406:A:C8	2.43	0.52
31:AC:17:HIS:HA	31:AC:20:GLY:HA3	1.91	0.52
36:AH:84:CYS:O	36:AH:88:ARG:HG2	2.09	0.52
1:AR:1369:A:OP1	30:DC:21:ARG:NH1	2.42	0.52
1:AR:2181:C:H5''	4:CD:193:ARG:NH2	2.24	0.52
3:AT:16:G:O2'	3:AT:17:A:OP2	2.25	0.52
3:AT:38:U:C4	37:DJ:89:ARG:HD2	2.44	0.52
1:AR:2177:G:OP2	4:CD:128:ARG:NH1	2.42	0.52
5:CE:188:ILE:HA	5:CE:191:LYS:HD2	1.90	0.52
14:CN:42:ARG:HB3	14:CN:51:LEU:HD21	1.91	0.52
18:CR:27:LYS:HD3	18:CR:63:PHE:HB3	1.89	0.52
28:DA:56:VAL:HG11	28:DA:104:LEU:HD13	1.91	0.52
32:DE:26:GLY:O	32:DE:30:THR:HG23	2.09	0.52
55:G:73:THR:HG23	66:R:114:ARG:HG3	1.90	0.52
25:A:154:G:H5'	56:H:108:VAL:HG21	1.91	0.52
58:J:188:GLU:OE2	61:M:15:LYS:NZ	2.40	0.52
61:M:2:SER:HB2	61:M:81:HIS:CD2	2.44	0.52
22:2:79:MET:HB3	22:2:84:TYR:CD2	2.44	0.52
25:6:1524:A:H2'	25:6:1525:A:C8	2.44	0.52
25:6:25:C:OP2	25:6:25:C:H4'	2.08	0.52
25:A:851:U:H2'	25:A:852:C:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:AA:17:ARG:HG3	36:AH:73:SER:HB3	1.91	0.52
1:AR:1701:C:H2'	1:AR:1702:U:O4'	2.09	0.52
1:AR:2726:C:O2'	1:AR:2727:A:H2'	2.08	0.52
1:AR:2767:U:H2'	1:AR:2768:U:C6	2.44	0.52
1:AR:655:C:H2'	1:AR:656:A:C8	2.45	0.52
3:AT:103:G:OP2	3:AT:105:A:O2'	2.27	0.52
1:1:2303:A:OP1	43:AO:23:ARG:NH2	2.42	0.52
1:1:230:U:H2'	1:1:231:G:O4'	2.09	0.52
1:1:645:A:N6	1:1:2869:U:OP1	2.42	0.52
1:1:619:A:H5''	1:1:620:U:OP1	2.09	0.52
1:1:735:A:H2'	1:1:736:A:C8	2.43	0.52
25:6:152:U:C2	25:6:163:G:N2	2.76	0.52
25:A:1173:C:H3'	68:T:141:THR:HG21	1.92	0.52
25:A:1344:A:H2'	25:A:1345:A:C8	2.44	0.52
25:A:836:U:H2'	25:A:837:G:C8	2.44	0.52
1:AR:2875:U:H6	1:AR:2875:U:H5''	1.74	0.52
1:AR:495:G:H2'	1:AR:496:C:O4'	2.10	0.52
1:AR:850:U:H2'	1:AR:851:C:C6	2.43	0.52
3:AT:136:G:OP1	27:CZ:48:SER:OG	2.26	0.52
51:C:61:LEU:HD23	51:C:62:LYS:H	1.72	0.52
6:CF:354:VAL:HG11	22:CV:143:THR:HG21	1.91	0.52
39:DL:5:THR:HA	39:DL:8:PHE:CD2	2.45	0.52
69:U:52:GLY:HA2	69:U:55:TYR:CD1	2.44	0.52
1:1:1675:G:H2'	1:1:1676:A:H8	1.73	0.52
22:2:50:LYS:HB3	22:2:92:ARG:NH1	2.24	0.52
25:6:1783:C:OP2	43:DP:1:MET:HB2	2.09	0.52
25:A:568:G:O5'	73:Y:90:ASP:HA	2.10	0.52
25:A:778:G:H22	74:Z:10:ARG:NH1	2.07	0.52
31:AC:28:LYS:HD3	31:AC:29:TYR:H	1.73	0.52
1:AR:558:U:H4'	1:AR:559:A:OP2	2.10	0.52
4:CD:45:VAL:HG12	4:CD:88:ILE:HD13	1.91	0.52
5:CE:316:GLU:O	5:CE:318:LYS:HG3	2.09	0.52
7:CG:184:ASP:OD1	7:CG:187:THR:N	2.38	0.52
52:D:81:MET:HB2	52:D:101:VAL:HG12	1.90	0.52
32:DE:9:SER:HB3	32:DE:12:GLN:HB3	1.92	0.52
37:DJ:31:LEU:HD12	37:DJ:47:VAL:HG11	1.91	0.52
56:H:63:MET:HE1	56:H:106:LEU:HD13	1.90	0.52
62:N:63:VAL:HA	62:N:91:VAL:O	2.10	0.52
52:D:230:TRP:CD2	72:X:68:ARG:HD3	2.44	0.52
1:1:1838:G:H4'	1:1:1839:A:N3	2.24	0.52
25:6:1255:G:H4'	25:6:1256:A:OP1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:1699:G:O2'	25:6:1702:A:N6	2.43	0.52
25:6:1783:C:H2'	25:6:1784:C:C6	2.45	0.52
25:A:912:U:H4'	25:A:913:G:O5'	2.09	0.52
1:AR:1764:U:H3'	1:AR:1765:U:H4'	1.91	0.52
1:AR:2413:A:H2'	1:AR:2414:G:H8	1.74	0.52
7:CG:219:PHE:CE2	7:CG:227:LEU:HD11	2.45	0.52
13:CM:40:LEU:HD22	13:CM:79:ILE:HD13	1.92	0.52
1:AR:3006:A:OP2	17:CQ:148:LYS:NZ	2.43	0.52
20:CT:21:LYS:O	20:CT:53:LYS:HB2	2.09	0.52
52:D:250:GLN:H	52:D:250:GLN:CD	2.12	0.52
33:DF:72:ARG:HD3	33:DF:104:LEU:HD13	1.90	0.52
64:P:87:GLY:HA3	64:P:120:PRO:HG2	1.91	0.52
84:1:3473:OHX:N4	84:1:3720:OHX:N1	2.57	0.52
25:6:1542:G:N2	25:6:1568:C:H1'	2.22	0.52
25:A:1585:U:N3	25:A:1611:A:H2	2.08	0.52
25:A:1738:U:H2'	25:A:1739:C:C6	2.44	0.52
25:A:605:A:OP2	25:A:606:A:O2'	2.26	0.52
31:AC:59:LYS:H	31:AC:59:LYS:HD3	1.73	0.52
1:AR:2138:A:C4	39:DL:3:LYS:HB3	2.45	0.52
1:AR:3043:C:OP2	24:CX:48:ARG:NH2	2.40	0.52
1:AR:339:C:OP1	1:AR:1380:G:O2'	2.25	0.52
1:AR:517:G:P	9:CI:60:ARG:HH22	2.33	0.52
7:CG:208:MET:HB2	7:CG:233:ALA:HB2	1.92	0.52
13:CM:91:LEU:O	13:CM:172:LEU:HB2	2.09	0.52
16:CP:178:HIS:CE1	16:CP:179:LYS:HG3	2.45	0.52
27:CZ:95:ILE:HD13	27:CZ:122:ALA:HB2	1.92	0.52
1:AR:3107:U:OP1	42:DO:112:LYS:HG2	2.09	0.52
53:E:135:GLU:HB3	53:E:187:LYS:HB3	1.91	0.52
57:I:35:LYS:HG2	57:I:36:ALA:H	1.74	0.52
73:Y:43:PHE:CE1	73:Y:49:ALA:HB3	2.45	0.52
1:1:1611:G:H2'	1:1:1612:A:C8	2.45	0.52
1:1:2974:U:H2'	1:1:2975:U:C6	2.45	0.52
25:6:30:G:H2'	25:6:31:C:C6	2.45	0.52
25:A:1300:A:OP1	52:D:99:LYS:NZ	2.36	0.52
84:A:1909:OHX:N3	84:A:2024:OHX:N1	2.58	0.52
29:AA:4:PHE:CZ	32:AD:35:ARG:HA	2.44	0.52
1:AR:2418:G:H2'	1:AR:2418:G:N3	2.24	0.52
1:AR:3013:U:H2'	1:AR:3014:U:C6	2.44	0.52
1:AR:3304:U:O3'	5:CE:334:ARG:NH2	2.43	0.52
7:CG:111:GLN:HA	7:CG:116:ASP:HB2	1.92	0.52
11:CK:86:TYR:CE1	11:CK:151:VAL:HG22	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DJ:10:ARG:NH1	37:DJ:60:GLU:OE1	2.43	0.52
41:DN:23:LEU:HD22	41:DN:24:PRO:HD2	1.91	0.52
61:M:75:VAL:HG12	61:M:119:VAL:HA	1.91	0.52
25:A:959:U:C6	63:O:61:THR:HB	2.45	0.52
25:A:1195:C:N4	66:R:143:ARG:HA	2.25	0.52
1:1:1580:A:H5'	1:1:2522:G:C5	2.45	0.52
1:1:2592:G:H4'	1:1:2594:C:C2	2.44	0.52
1:1:497:C:H2'	1:1:498:A:O4'	2.09	0.52
1:1:661:G:OP1	30:AB:12:ARG:NH2	2.41	0.52
25:6:1213:G:O2'	25:6:1244:A:N6	2.42	0.52
5:CE:286:GLY:HA3	5:CE:321:PHE:CE2	2.45	0.52
11:CK:9:GLN:HB3	11:CK:52:LEU:HD21	1.90	0.52
19:CS:67:ILE:HG23	19:CS:81:VAL:HG11	1.91	0.52
1:AR:2741:C:H4'	44:DQ:19:LYS:HA	1.92	0.52
1:1:339:C:OP1	1:1:1380:G:O2'	2.24	0.52
25:6:1475:A:N6	25:6:1531:G:O6	2.43	0.52
25:6:978:A:H2'	25:6:979:A:O4'	2.10	0.52
25:A:1645:G:H22	25:A:1756:A:H2	1.57	0.52
32:AD:16:LEU:HD22	32:AD:19:LYS:HE2	1.92	0.52
40:AL:22:THR:HG22	40:AL:74:LYS:HD2	1.92	0.52
1:AR:2180:G:H2'	1:AR:2181:C:C6	2.45	0.52
1:AR:271:C:H2'	1:AR:272:G:O4'	2.10	0.52
1:AR:2767:U:H2'	1:AR:2768:U:H6	1.75	0.52
2:AS:3:U:H2'	2:AS:4:U:C6	2.45	0.52
13:CM:108:GLU:HA	13:CM:122:ILE:HG23	1.92	0.52
17:CQ:143:THR:HG21	17:CQ:150:GLU:OE2	2.10	0.52
36:DI:91:ARG:HG3	36:DI:95:ILE:HD13	1.91	0.52
37:DJ:44:ILE:O	37:DJ:48:ARG:HB2	2.10	0.52
58:J:54:LYS:HG2	58:J:175:GLN:O	2.10	0.52
59:K:118:LEU:HG	59:K:158:PHE:CE2	2.45	0.52
62:N:62:LEU:HB3	62:N:75:VAL:HG11	1.92	0.52
1:1:22:G:H1'	3:4:104:A:N3	2.25	0.52
22:2:44:ALA:HB2	22:2:53:PRO:HG2	1.92	0.52
25:A:1171:A:H2'	25:A:1172:G:C8	2.45	0.52
25:A:1600:A:HO2'	25:A:1602:C:N4	2.07	0.52
29:AA:103:GLN:HB3	29:AA:106:GLN:HG3	1.92	0.52
1:AR:2217:U:H2'	1:AR:2218:G:C8	2.45	0.52
16:CP:73:ARG:HG2	16:CP:75:VAL:HG13	1.90	0.52
17:CQ:79:ILE:HG21	17:CQ:138:LEU:HD11	1.91	0.52
9:CI:77:VAL:HG13	22:CV:139:ARG:HG2	1.92	0.52
28:DA:28:ARG:HB2	28:DA:75:ARG:NH2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DD:14:ARG:NH2	31:DD:18:ARG:HH11	2.08	0.52
37:DJ:119:LYS:HE2	37:DJ:119:LYS:HA	1.91	0.52
1:1:2424:A:H2'	1:1:2425:G:O4'	2.09	0.51
1:1:3218:A:H4'	1:1:3219:G:O5'	2.10	0.51
1:1:1831:U:O2'	3:4:114:G:OP1	2.17	0.51
30:AB:77:LYS:C	30:AB:79:TRP:H	2.14	0.51
34:AF:9:ILE:HG12	34:AF:63:THR:HB	1.91	0.51
1:AR:1063:G:OP2	1:AR:1097:G:H3'	2.10	0.51
50:B:164:ASN:HA	50:B:170:ILE:HD11	1.92	0.51
50:B:200:ASP:HB2	67:S:85:VAL:HG11	1.92	0.51
5:CE:232:ARG:NH1	5:CE:269:GLN:O	2.42	0.51
5:CE:292:ALA:HA	5:CE:303:LYS:O	2.10	0.51
7:CG:232:ASP:OD1	7:CG:232:ASP:N	2.42	0.51
17:CQ:85:ARG:HD3	17:CQ:90:HIS:ND1	2.25	0.51
18:CR:129:THR:HG23	18:CR:139:TYR:HB2	1.93	0.51
29:DB:102:GLU:O	29:DB:103:GLN:HB2	2.11	0.51
54:F:199:GLU:HB2	54:F:207:LEU:HB2	1.91	0.51
58:J:48:THR:HG21	58:J:54:LYS:HB2	1.92	0.51
25:A:246:G:H1'	61:M:40:LEU:HD13	1.91	0.51
1:1:849:C:H2'	1:1:850:U:C6	2.44	0.51
1:1:936:A:H5''	1:1:937:G:OP1	2.10	0.51
25:A:1615:C:O2'	25:A:1616:G:OP2	2.24	0.51
25:A:823:G:O2'	25:A:824:G:O4'	2.16	0.51
25:A:947:U:H2'	25:A:948:G:C8	2.45	0.51
39:AK:69:HIS:O	39:AK:73:ARG:HG3	2.10	0.51
1:AR:996:A:H2'	1:AR:997:A:O4'	2.10	0.51
1:AR:1618:G:H4'	3:AT:129:C:H1'	1.91	0.51
3:AT:52:A:H62	41:DN:27:ILE:HD13	1.75	0.51
6:CF:317:PRO:HB3	6:CF:324:LEU:HA	1.93	0.51
7:CG:126:GLU:HG3	7:CG:196:ARG:HD2	1.93	0.51
21:CU:7:TYR:CE1	21:CU:34:GLU:HG2	2.45	0.51
52:D:227:PRO:HA	52:D:230:TRP:CD1	2.45	0.51
29:DB:59:ALA:O	29:DB:61:LYS:N	2.43	0.51
53:E:17:PHE:O	53:E:21:LEU:HB2	2.10	0.51
54:F:131:LEU:HD22	54:F:137:PRO:HB3	1.90	0.51
1:1:3006:A:C2	1:1:3141:A:C4	2.98	0.51
23:5:14:THR:HG23	23:5:66:VAL:HG13	1.92	0.51
25:6:151:G:N2	25:6:163:G:N2	2.57	0.51
25:6:1595:U:N3	25:6:1600:A:H2	2.04	0.51
26:7:5:ILE:HD12	26:7:10:GLY:HA2	1.91	0.51
25:A:1390:U:OP2	67:S:49:LYS:NZ	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1437:U:H5'	53:E:176:LEU:HD23	1.91	0.51
1:1:2422:C:O5'	44:AP:52:GLY:HA2	2.10	0.51
1:AR:1521:G:H21	1:AR:1835:A:H1'	1.75	0.51
1:AR:3022:G:O2'	1:AR:3031:G:O6	2.17	0.51
10:CJ:130:TYR:HD2	10:CJ:204:ARG:HG3	1.76	0.51
10:CJ:139:VAL:O	10:CJ:143:ILE:HG13	2.10	0.51
16:CP:38:ARG:CZ	16:CP:60:VAL:HG13	2.41	0.51
28:DA:59:VAL:HG12	28:DA:103:LYS:O	2.10	0.51
39:DL:53:ALA:HA	39:DL:56:ARG:HH11	1.75	0.51
1:AR:353:G:O6	39:DL:55:ARG:NH1	2.43	0.51
57:I:94:ALA:HB3	57:I:96:ARG:NH1	2.26	0.51
71:W:1:MET:SD	71:W:10:GLU:HB3	2.51	0.51
72:X:6:VAL:HG12	72:X:34:ILE:HD11	1.92	0.51
74:Z:10:ARG:HD2	74:Z:26:ASP:HB2	1.92	0.51
1:1:439:C:H5'	1:1:440:A:C8	2.46	0.51
1:1:507:U:H2'	1:1:508:U:C6	2.43	0.51
25:6:250:C:H2'	25:6:251:A:H8	1.74	0.51
25:6:918:U:H2'	25:6:919:A:H8	1.74	0.51
32:AD:78:GLY:HA2	32:AD:87:VAL:HG13	1.92	0.51
1:AR:1794:G:H4'	4:CD:191:LEU:HD13	1.93	0.51
1:AR:879:U:O2	1:AR:2357:A:H1'	2.10	0.51
1:AR:2537:U:O2'	1:AR:2538:U:O5'	2.26	0.51
1:AR:2860:U:N3	1:AR:2938:G:O5'	2.43	0.51
1:AR:894:G:N2	1:AR:1660:C:OP1	2.43	0.51
12:CL:161:GLY:O	12:CL:163:GLN:NE2	2.43	0.51
1:AR:1010:G:H1'	12:CL:195:ALA:HB2	1.92	0.51
11:CK:4:ILE:N	21:CU:142:GLN:OE1	2.41	0.51
24:CX:83:LYS:HE2	24:CX:84:SER:H	1.75	0.51
26:CY:63:ILE:O	26:CY:65:GLU:N	2.44	0.51
29:DB:23:VAL:HG12	29:DB:45:GLY:HA3	1.93	0.51
70:V:57:ARG:HG3	70:V:89:ARG:CZ	2.40	0.51
74:Z:36:SER:HB3	74:Z:39:GLU:HB3	1.92	0.51
21:0:8:GLN:HB2	21:0:64:ILE:HD11	1.92	0.51
1:1:209:A:H4'	1:1:211:A:C8	2.46	0.51
25:6:1398:U:H3'	25:6:1399:C:H4'	1.92	0.51
25:6:1699:G:HO2'	25:6:1702:A:N6	2.07	0.51
25:6:1696:G:N2	25:6:1704:U:H3	2.08	0.51
25:6:492:A:H1'	25:6:496:G:H1	1.76	0.51
25:A:393:C:H4'	25:A:1673:G:O2'	2.11	0.51
43:AO:2:ARG:NH1	25:A:1773:C:OP2	2.43	0.51
84:A:1909:OHX:N3	84:A:2024:OHX:N5	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:632:U:OP1	61:M:102:LYS:HG3	2.11	0.51
25:A:804:A:N3	72:X:105:THR:HG22	2.26	0.51
25:A:844:A:H2'	25:A:845:G:H8	1.76	0.51
33:AE:62:ARG:HB2	33:AE:66:GLY:O	2.10	0.51
1:AR:1019:G:H1	1:AR:1033:U:H3	1.58	0.51
1:AR:1596:C:H2'	1:AR:1597:C:C6	2.46	0.51
1:AR:1786:G:H2'	1:AR:1787:A:C8	2.45	0.51
1:AR:2303:A:OP1	43:DP:23:ARG:NH2	2.42	0.51
8:CH:89:THR:HG21	15:CO:115:PHE:HB2	1.93	0.51
17:CQ:65:ASN:HB3	17:CQ:68:ARG:HD2	1.92	0.51
40:DM:43:PHE:CE2	40:DM:66:ILE:HG12	2.46	0.51
54:F:105:VAL:HG13	54:F:243:GLY:HA2	1.91	0.51
1:1:1687:U:H5''	1:1:1688:U:H5'	1.92	0.51
25:A:568:G:N7	73:Y:69:ARG:NH2	2.59	0.51
25:A:637:C:OP1	72:X:32:LYS:N	2.36	0.51
29:AA:46:ILE:HD13	29:AA:68:ILE:HG23	1.93	0.51
1:1:1488:G:O2'	36:AH:10:ARG:O	2.29	0.51
1:AR:1064:A:H62	1:AR:1096:U:H3	1.59	0.51
1:AR:1785:U:H2'	1:AR:1786:G:C8	2.46	0.51
1:AR:789:A:H2'	1:AR:790:U:H6	1.76	0.51
51:C:89:ASP:OD1	51:C:89:ASP:N	2.43	0.51
12:CL:3:ARG:CZ	12:CL:63:GLU:HG3	2.40	0.51
15:CO:25:LYS:HE3	15:CO:62:GLN:HG2	1.93	0.51
52:D:101:VAL:HG22	52:D:115:ILE:HG12	1.93	0.51
55:G:29:ILE:HG22	55:G:34:GLN:HG3	1.92	0.51
59:K:129:ILE:HG12	59:K:134:ILE:HD11	1.91	0.51
25:A:767:U:C6	59:K:143:ILE:HD11	2.44	0.51
63:O:3:ARG:HG2	63:O:6:SER:OG	2.10	0.51
71:W:20:THR:HB	71:W:22:ARG:HD3	1.92	0.51
73:Y:70:LYS:HB3	73:Y:93:LEU:HD22	1.93	0.51
73:Y:93:LEU:HD12	73:Y:96:VAL:HG21	1.92	0.51
1:1:2309:A:H4'	84:1:3666:OHX:N1	2.25	0.51
25:6:1564:U:H2'	25:6:1565:C:C6	2.45	0.51
25:6:607:G:H5'	25:6:613:G:N2	2.26	0.51
25:A:1201:G:N2	25:A:1600:A:H5'	2.25	0.51
43:AO:13:LEU:O	43:AO:17:ARG:HG3	2.10	0.51
1:AR:1495:U:H5	1:AR:1835:A:C2	2.28	0.51
1:AR:2185:G:O2'	1:AR:2314:U:OP2	2.28	0.51
1:AR:2897:A:H2'	1:AR:2899:C:H5''	1.91	0.51
1:AR:662:U:OP1	30:DC:8:THR:HG21	2.11	0.51
1:AR:723:U:HO2'	31:DD:29:TYR:HH	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:C:137:ILE:HD12	51:C:172:LEU:HD22	1.93	0.51
51:C:70:LEU:O	51:C:74:GLN:N	2.43	0.51
11:CK:57:VAL:HG23	11:CK:68:LEU:HG	1.91	0.51
14:CN:89:TYR:CE1	14:CN:93:ILE:HD11	2.46	0.51
2:AS:77:G:H5'	21:CU:46:GLN:O	2.10	0.51
3:AT:71:A:O2'	28:DA:52:ARG:NH2	2.43	0.51
1:AR:353:G:N7	39:DL:55:ARG:HD3	2.25	0.51
39:DL:52:LYS:HG2	39:DL:56:ARG:NH1	2.26	0.51
45:DR:49:ARG:HB2	45:DR:55:TRP:CH2	2.44	0.51
62:N:63:VAL:HG11	62:N:94:ALA:HA	1.92	0.51
70:V:22:ILE:HG22	70:V:93:LEU:HB2	1.93	0.51
25:6:496:G:O6	25:6:497:G:N2	2.44	0.51
25:A:1041:G:H2'	25:A:1042:G:C8	2.45	0.51
25:A:240:U:H4'	25:A:241:U:OP2	2.10	0.51
30:AB:77:LYS:O	30:AB:79:TRP:N	2.42	0.51
33:AE:60:TRP:CZ3	33:AE:64:VAL:HG12	2.45	0.51
44:AP:71:ARG:HE	44:AP:80:ARG:NE	2.08	0.51
1:AR:1587:A:O2'	1:AR:1590:G:O6	2.21	0.51
1:AR:805:G:H2'	1:AR:936:A:H61	1.76	0.51
2:AS:28:C:H1'	2:AS:55:A:H61	1.75	0.51
52:D:59:HIS:CD2	52:D:238:SER:HA	2.46	0.51
58:J:117:TYR:CD1	58:J:150:ALA:HB2	2.46	0.51
64:P:19:ILE:HB	64:P:83:ILE:HD12	1.91	0.51
1:1:1170:A:H2'	1:1:1171:G:O4'	2.11	0.51
1:1:2970:C:HO2'	1:1:2971:A:H2	1.55	0.51
25:A:926:A:OP1	25:A:1016:C:O2'	2.16	0.51
41:AM:44:TRP:CH2	41:AM:45:ARG:HG2	2.46	0.51
42:AN:98:LYS:HD3	42:AN:118:THR:HG21	1.92	0.51
1:AR:567:G:H2'	1:AR:568:G:C8	2.46	0.51
6:CF:234:ASN:OD1	6:CF:236:LEU:N	2.44	0.51
15:CO:32:LEU:HD11	15:CO:94:TRP:CG	2.46	0.51
35:DH:45:LEU:HA	35:DH:71:VAL:HG12	1.91	0.51
37:DJ:83:LYS:O	37:DJ:89:ARG:NE	2.37	0.51
58:J:121:LEU:H	58:J:121:LEU:HD22	1.76	0.51
1:1:1238:C:N4	1:1:1245:A:OP2	2.44	0.51
1:1:1554:U:H4'	1:1:1555:U:H5'	1.92	0.51
1:1:1915:A:H2'	1:1:1916:U:C6	2.46	0.51
25:6:1248:C:H2'	25:6:1249:U:C6	2.46	0.51
25:A:579:A:C2	53:E:143:ARG:HG3	2.46	0.51
1:1:361:A:O3'	39:AK:45:ARG:NH2	2.42	0.51
1:AR:1367:G:HO2'	1:AR:1368:U:H6	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:2585:G:N3	1:AR:2585:G:H2'	2.25	0.51
1:AR:549:U:H2'	1:AR:550:A:C8	2.46	0.51
25:A:799:A:H5''	54:F:201:HIS:CD2	2.45	0.51
70:V:99:ILE:O	70:V:103:ILE:N	2.38	0.51
73:Y:41:SER:O	73:Y:41:SER:OG	2.28	0.51
1:1:3281:U:H2'	1:1:3282:U:C6	2.46	0.50
2:3:71:G:H2'	2:3:72:A:C8	2.45	0.50
25:6:1733:C:H2'	25:6:1734:U:H6	1.75	0.50
25:6:195:G:H2'	25:6:196:G:H5''	1.93	0.50
34:AF:12:LYS:HD3	34:AF:57:TYR:HA	1.93	0.50
1:AR:1486:G:N7	84:AR:3534:OHX:N4	2.60	0.50
1:AR:293:C:H2'	1:AR:294:U:O4'	2.12	0.50
50:B:109:ASN:O	50:B:112:THR:HG22	2.11	0.50
1:AR:2179:C:HO2'	4:CD:130:SER:HG	1.53	0.50
10:CJ:81:THR:OG1	10:CJ:181:LYS:HB2	2.11	0.50
24:CX:54:LEU:HD21	24:CX:119:GLY:HA3	1.93	0.50
56:H:121:LEU:HD12	56:H:124:LEU:HD23	1.92	0.50
1:1:1108:U:H2'	1:1:1109:U:C6	2.46	0.50
25:6:822:U:H2'	25:6:823:G:H5''	1.92	0.50
25:A:1017:U:H2'	25:A:1018:U:C6	2.46	0.50
25:A:1358:G:H2'	25:A:1359:C:C6	2.46	0.50
33:AE:60:TRP:HZ3	33:AE:64:VAL:HG12	1.75	0.50
1:AR:1157:G:H2'	1:AR:1158:A:O4'	2.11	0.50
1:AR:1913:A:N3	1:AR:2120:A:H2'	2.26	0.50
2:AS:44:C:H4'	7:CG:152:ARG:HG3	1.93	0.50
1:AR:779:G:OP1	19:CS:185:LYS:NZ	2.44	0.50
2:AS:99:G:OP1	21:CU:53:LYS:HD3	2.11	0.50
24:CX:87:ARG:HH22	24:CX:137:VAL:HG22	1.76	0.50
30:DC:122:PRO:HB3	30:DC:142:GLY:O	2.11	0.50
4:CD:180:LEU:HG	45:DR:26:VAL:HG21	1.92	0.50
54:F:160:VAL:HG13	54:F:169:ILE:HG23	1.94	0.50
73:Y:57:LEU:HD11	73:Y:73:ARG:HG3	1.91	0.50
1:1:2771:U:O2'	1:1:2772:C:O4'	2.29	0.50
1:1:662:U:H2'	1:1:663:C:C6	2.46	0.50
25:6:16:G:H2'	25:6:17:C:C6	2.46	0.50
25:6:93:A:C6	25:6:398:G:C6	3.00	0.50
25:A:12:U:H2'	25:A:13:C:C6	2.46	0.50
25:A:1434:U:O2'	25:A:1436:A:OP1	2.21	0.50
1:AR:2263:C:O2'	1:AR:2264:U:P	2.69	0.50
1:AR:2842:U:OP1	1:AR:2844:C:N4	2.45	0.50
1:AR:3121:U:H1'	1:AR:3122:A:H5''	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:408:A:H61	3:AT:15:G:H1'	1.77	0.50
1:AR:428:A:H2'	1:AR:429:U:C6	2.46	0.50
1:AR:507:U:H2'	1:AR:508:U:C6	2.47	0.50
1:AR:850:U:H2'	1:AR:851:C:H6	1.76	0.50
3:AT:9:A:H2'	3:AT:10:A:C8	2.46	0.50
51:C:193:ILE:O	51:C:197:ILE:HG12	2.12	0.50
41:DN:44:TRP:CZ3	41:DN:45:ARG:HG3	2.47	0.50
63:O:87:ASP:OD1	63:O:88:LEU:N	2.43	0.50
64:P:16:VAL:O	64:P:30:VAL:HA	2.10	0.50
1:1:3294:A:H2'	1:1:3295:A:O4'	2.12	0.50
28:9:60:ARG:HB2	28:9:103:LYS:HB3	1.93	0.50
33:AE:13:THR:HG23	33:AE:72:ARG:NH1	2.26	0.50
84:AR:3743:OHX:N1	30:DC:22:ILE:HD11	2.27	0.50
51:C:105:PHE:CD1	51:C:213:ARG:HA	2.47	0.50
51:C:128:LYS:HG3	51:C:134:VAL:HG22	1.94	0.50
6:CF:192:GLY:HA2	6:CF:195:ARG:HG3	1.92	0.50
11:CK:22:SER:OG	11:CK:23:ARG:N	2.42	0.50
12:CL:86:HIS:HB3	12:CL:139:ARG:CG	2.41	0.50
15:CO:136:ALA:O	15:CO:137:LYS:HD2	2.11	0.50
16:CP:79:ALA:HB1	16:CP:81:TYR:CZ	2.47	0.50
23:CW:93:ILE:HA	23:CW:106:ALA:O	2.12	0.50
29:DB:24:VAL:HG21	29:DB:87:LEU:HD23	1.92	0.50
36:DI:84:CYS:O	36:DI:88:ARG:HG2	2.12	0.50
72:X:103:ILE:HA	72:X:112:ASP:HA	1.94	0.50
1:1:1110:U:H2'	1:1:1111:U:C6	2.47	0.50
1:1:2131:A:N6	45:AQ:18:TYR:HA	2.27	0.50
1:1:3255:U:H2'	1:1:3256:G:C8	2.47	0.50
1:1:3275:U:H5'	35:AG:68:TRP:HZ2	1.77	0.50
1:1:655:C:H2'	1:1:656:A:H8	1.75	0.50
3:4:35:C:H5"	39:AK:70:VAL:HG11	1.94	0.50
25:6:1688:U:H2'	25:6:1689:A:C8	2.47	0.50
25:A:1699:G:H2'	25:A:1700:C:H5"	1.94	0.50
25:A:641:G:H2'	25:A:642:G:C8	2.46	0.50
1:AR:1256:G:O6	1:AR:1261:G:N2	2.45	0.50
1:AR:2103:U:H2'	1:AR:2104:A:C8	2.46	0.50
1:AR:359:U:H4'	1:AR:817:A:N6	2.26	0.50
64:P:26:THR:HG21	64:P:97:GLY:HA3	1.93	0.50
1:1:1233:G:H22	1:1:1255:C:N4	2.09	0.50
1:1:2916:U:H5	1:1:2935:U:HO2'	1.59	0.50
1:1:908:G:H4'	1:1:909:G:O5'	2.12	0.50
25:6:986:G:H2'	25:6:987:G:O4'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1317:C:H2'	25:A:1318:G:O4'	2.11	0.50
25:A:1776:A:H2'	25:A:1777:G:C8	2.47	0.50
25:A:28:A:H2'	25:A:29:U:C6	2.46	0.50
25:A:581:U:OP2	53:E:143:ARG:NH1	2.45	0.50
1:AR:2514:U:OP2	1:AR:2586:G:N2	2.44	0.50
7:CG:57:ASN:HA	7:CG:58:LYS:HZ2	1.77	0.50
8:CH:65:ILE:HD12	8:CH:79:VAL:HB	1.94	0.50
24:CX:6:ALA:HB2	24:CX:126:TRP:CH2	2.47	0.50
52:D:41:LEU:HD12	52:D:68:ILE:HD13	1.93	0.50
54:F:45:ILE:HA	54:F:61:VAL:HG11	1.93	0.50
1:1:1014:U:H3	1:1:1036:A:H61	1.59	0.50
1:1:2848:G:OP1	42:AN:100:TYR:OH	2.14	0.50
1:1:94:G:H2'	1:1:95:A:C8	2.47	0.50
3:4:152:G:H2'	3:4:153:U:O4'	2.12	0.50
25:6:217:A:C8	25:6:218:A:C8	3.00	0.50
25:A:1018:U:OP1	63:O:107:LYS:NZ	2.44	0.50
25:A:145:A:O2'	25:A:146:U:O5'	2.26	0.50
25:A:582:U:H3'	25:A:583:C:C6	2.47	0.50
1:AR:1596:C:O2'	1:AR:1696:A:N3	2.33	0.50
1:AR:173:G:N1	1:AR:246:U:O2	2.45	0.50
1:AR:709:A:H1'	30:DC:57:GLY:HA3	1.92	0.50
50:B:101:ARG:NH2	50:B:104:PRO:HD2	2.26	0.50
5:CE:256:HIS:HA	5:CE:257:PRO:C	2.32	0.50
6:CF:209:TYR:O	6:CF:230:VAL:HG22	2.11	0.50
1:AR:2587:U:H4'	10:CJ:49:TYR:HD1	1.76	0.50
1:AR:617:G:H4'	18:CR:171:ARG:HH21	1.77	0.50
2:AS:10:C:OP2	22:CV:26:HIS:ND1	2.44	0.50
27:CZ:34:LEU:HD22	27:CZ:35:PRO:HD2	1.94	0.50
14:CN:165:SER:H	30:DC:139:ARG:HH21	1.58	0.50
43:DP:16:LYS:O	43:DP:20:VAL:HG23	2.12	0.50
56:H:64:LYS:O	56:H:67:VAL:HG22	2.11	0.50
1:1:174:C:H2'	1:1:175:C:C6	2.46	0.50
1:1:1886:A:O4'	1:1:3307:A:H5'	2.11	0.50
1:1:1952:G:H3'	1:1:1953:G:H5''	1.93	0.50
1:1:2558:U:O2'	1:1:2559:U:H5'	2.12	0.50
25:6:12:U:H2'	25:6:13:C:C6	2.47	0.50
25:6:538:A:C8	25:6:543:C:N4	2.77	0.50
25:A:130:C:O2'	25:A:131:C:OP1	2.22	0.50
25:A:602:U:H2'	25:A:603:U:C6	2.47	0.50
1:AR:3376:A:H5'	1:AR:3377:G:H5''	1.93	0.50
50:B:25:GLY:HA3	50:B:149:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:CK:156:GLN:NE2	11:CK:159:ALA:HB3	2.27	0.50
19:CS:60:PRO:HB2	19:CS:142:GLY:HA3	1.92	0.50
34:DG:32:TRP:CZ2	34:DG:53:PRO:HD2	2.47	0.50
55:G:64:VAL:HG22	55:G:89:ILE:HD11	1.92	0.50
62:N:126:TRP:O	62:N:128:ALA:N	2.44	0.50
62:N:63:VAL:HG21	62:N:94:ALA:HB2	1.94	0.50
1:1:3155:U:H3'	1:1:3156:U:H4'	1.94	0.50
25:6:417:A:H4'	25:6:418:G:O5'	2.11	0.50
25:6:830:U:C2'	25:6:831:U:H5'	2.42	0.50
26:7:4:GLU:HG2	26:7:30:ARG:HD3	1.93	0.50
27:8:105:VAL:HG11	27:8:126:LEU:HD22	1.94	0.50
25:A:1625:C:OP1	52:D:91:ARG:NH2	2.44	0.50
25:A:375:U:H2'	25:A:376:C:H6	1.77	0.50
32:AD:95:ALA:HB2	32:AD:101:LEU:HD23	1.94	0.50
44:AP:43:TYR:CZ	44:AP:47:GLN:NE2	2.80	0.50
1:AR:1816:A:O2'	1:AR:1817:G:OP1	2.26	0.50
1:AR:2404:A:H8	1:AR:2404:A:C5'	2.25	0.50
50:B:139:VAL:HG13	50:B:141:ILE:HG13	1.94	0.50
7:CG:211:LEU:HB3	7:CG:219:PHE:HB2	1.93	0.50
11:CK:29:GLY:HA3	11:CK:82:VAL:HG13	1.92	0.50
23:CW:33:TYR:CE1	23:CW:80:THR:HG22	2.46	0.50
54:F:151:ASP:HB3	54:F:154:ILE:HG13	1.94	0.50
58:J:89:GLU:OE1	58:J:92:ARG:NH2	2.33	0.50
59:K:169:PRO:HB2	59:K:174:ARG:HG2	1.93	0.50
61:M:72:THR:HG22	61:M:124:THR:HA	1.94	0.50
21:0:66:GLU:OE1	21:0:99:ARG:N	2.42	0.49
1:1:2947:G:H4'	1:1:2947:G:OP2	2.12	0.49
25:6:74:U:H5''	25:6:75:U:OP2	2.11	0.49
25:6:872:G:H2'	25:6:873:U:O4'	2.12	0.49
27:8:127:THR:OG1	27:8:129:ASP:OD2	2.27	0.49
27:8:92:LYS:HD2	27:8:112:THR:HG23	1.93	0.49
35:AG:52:VAL:HG13	35:AG:66:VAL:HG22	1.94	0.49
3:AT:83:C:H1'	3:AT:85:G:N2	2.27	0.49
5:CE:166:ILE:HD13	5:CE:173:GLN:HG2	1.94	0.49
7:CG:234:ASP:N	7:CG:234:ASP:OD1	2.46	0.49
1:AR:3198:U:H1'	11:CK:21:LYS:HB2	1.94	0.49
17:CQ:8:VAL:HG13	17:CQ:34:VAL:HG13	1.93	0.49
25:A:1514:U:O2'	53:E:5:ILE:O	2.27	0.49
63:O:76:LYS:HA	63:O:81:ALA:HB2	1.93	0.49
64:P:29:HIS:HB3	64:P:41:ARG:HG3	1.93	0.49
21:0:33:ASN:OD1	21:0:35:VAL:HB	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1170:A:OP2	84:1:3493:OHX:N3	2.45	0.49
1:1:1913:A:N3	1:1:2120:A:H2'	2.27	0.49
1:1:944:C:H4'	34:AF:33:ARG:NH1	2.27	0.49
1:1:979:U:C2	1:1:980:A:C4	3.01	0.49
22:2:79:MET:HB3	22:2:84:TYR:CE2	2.48	0.49
25:A:582:U:H3'	25:A:583:C:H6	1.77	0.49
25:A:649:U:O2'	25:A:650:U:O5'	2.30	0.49
1:1:1391:C:C2	34:AF:103:LYS:HD3	2.47	0.49
1:AR:2666:C:OP2	1:AR:2687:G:N1	2.42	0.49
1:AR:2952:G:H2'	1:AR:2953:U:C6	2.47	0.49
1:AR:743:C:O2	19:CS:141:ARG:HD3	2.12	0.49
20:CT:69:SER:HA	20:CT:72:GLU:HB2	1.94	0.49
21:CU:46:GLN:HG2	21:CU:51:VAL:O	2.11	0.49
14:CN:64:LYS:HG3	30:DC:69:TRP:CG	2.48	0.49
73:Y:79:ASN:HB3	73:Y:81:LYS:H	1.76	0.49
2:3:9:C:OP1	22:2:28:SER:HB3	2.12	0.49
25:6:340:U:H2'	25:6:341:A:C8	2.48	0.49
25:6:404:G:H2'	25:6:405:C:C6	2.48	0.49
25:A:1487:A:H2'	25:A:1488:G:H8	1.77	0.49
29:AA:53:VAL:HA	29:AA:57:HIS:CD2	2.47	0.49
1:AR:1481:A:H2'	1:AR:1481:A:N3	2.27	0.49
1:AR:794:U:H2'	1:AR:795:G:H8	1.76	0.49
51:C:36:SER:HB3	51:C:231:LEU:HB3	1.94	0.49
2:AS:62:U:O3'	7:CG:285:ARG:NH1	2.46	0.49
14:CN:46:ILE:HG23	14:CN:49:ARG:CZ	2.43	0.49
52:D:175:GLY:HA3	59:K:53:ARG:HH22	1.77	0.49
58:J:84:HIS:CE1	58:J:86:SER:HB2	2.47	0.49
66:R:12:LYS:HA	66:R:16:ALA:O	2.12	0.49
57:I:139:ARG:HD3	72:X:53:ILE:HA	1.94	0.49
1:1:2282:U:O2	1:1:2310:U:H4'	2.12	0.49
1:1:2807:U:O3'	1:1:2808:A:H3'	2.12	0.49
1:1:2881:C:H2'	1:1:2882:U:C6	2.47	0.49
1:1:816:A:H5''	1:1:920:A:H62	1.77	0.49
25:6:1133:A:H2'	25:6:1134:C:O4'	2.12	0.49
25:6:191:C:O2'	25:6:192:U:O5'	2.28	0.49
25:A:1220:C:OP1	60:L:48:SER:OG	2.25	0.49
30:AB:19:LYS:HD2	30:AB:25:HIS:HB2	1.93	0.49
1:AR:1906:G:N2	1:AR:1909:A:N1	2.56	0.49
1:AR:3349:C:N3	1:AR:3356:G:N2	2.60	0.49
1:AR:981:U:H2'	1:AR:982:C:O4'	2.12	0.49
50:B:74:VAL:HG22	50:B:96:THR:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CF:193:LYS:HA	6:CF:198:ARG:HA	1.94	0.49
14:CN:50:PRO:O	14:CN:52:ASP:N	2.45	0.49
26:CY:13:ILE:HG12	26:CY:32:GLN:HB2	1.93	0.49
3:AT:131:A:H5''	27:CZ:93:TYR:CE2	2.47	0.49
55:G:146:THR:HG23	55:G:221:ALA:HA	1.93	0.49
57:I:133:THR:HG21	57:I:162:ILE:HD11	1.93	0.49
57:I:93:LEU:HD21	57:I:129:LEU:HD23	1.94	0.49
63:O:55:ARG:HD2	63:O:56:ASP:OD1	2.13	0.49
65:Q:126:VAL:HG13	65:Q:127:ARG:H	1.78	0.49
70:V:48:HIS:CE1	70:V:50:LEU:HD11	2.47	0.49
2:3:19:C:H2'	2:3:20:A:C8	2.45	0.49
27:8:86:VAL:HG11	27:8:95:ILE:HD11	1.95	0.49
25:A:1226:A:O2'	25:A:1227:A:OP1	2.29	0.49
25:A:591:A:H2'	25:A:592:A:H8	1.76	0.49
25:A:830:U:O2'	25:A:831:U:H6	1.95	0.49
1:AR:1135:A:H5'	31:DD:7:HIS:O	2.12	0.49
1:AR:1723:A:OP1	20:CT:128:LYS:NZ	2.37	0.49
1:AR:2676:A:H4'	1:AR:2677:G:O5'	2.12	0.49
1:AR:2896:A:O2'	42:DO:122:ARG:NH2	2.44	0.49
1:AR:3215:A:H5'	15:CO:121:MET:HE1	1.94	0.49
4:CD:64:ARG:HH22	10:CJ:38:GLN:HA	1.77	0.49
5:CE:257:PRO:HG2	5:CE:261:MET:HE1	1.93	0.49
7:CG:204:VAL:O	7:CG:208:MET:HG3	2.11	0.49
12:CL:211:ARG:O	12:CL:214:PRO:HG3	2.12	0.49
18:CR:23:ARG:O	18:CR:86:LYS:HE2	2.12	0.49
52:D:237:VAL:HB	52:D:242:ILE:HD11	1.94	0.49
30:DC:104:THR:HG21	30:DC:112:ILE:HD11	1.94	0.49
55:G:89:ILE:HD12	55:G:90:ILE:H	1.77	0.49
57:I:150:GLN:HB3	57:I:181:ILE:HD12	1.95	0.49
59:K:83:VAL:HA	59:K:149:ARG:HA	1.93	0.49
61:M:14:GLN:HB3	61:M:54:ILE:HG12	1.95	0.49
61:M:53:TYR:HD1	61:M:55:ASP:H	1.60	0.49
67:S:34:LEU:O	67:S:38:ILE:HG22	2.13	0.49
67:S:71:PHE:CD1	67:S:73:LEU:HB3	2.47	0.49
1:1:1027:A:H2'	1:1:1029:G:H5''	1.95	0.49
1:1:1709:C:H2'	1:1:1710:C:H6	1.77	0.49
1:1:2093:A:H2'	1:1:2094:C:O4'	2.13	0.49
3:4:142:C:H2'	3:4:143:U:C6	2.47	0.49
25:6:1339:C:O2'	25:6:1341:A:N7	2.41	0.49
25:6:603:U:H2'	25:6:604:A:H8	1.77	0.49
25:6:73:U:H2'	25:6:74:U:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:13:A:H4'	27:8:39:LYS:HG2	1.94	0.49
25:A:1469:A:H4'	25:A:1541:G:H4'	1.93	0.49
38:AJ:74:LYS:HD2	38:AJ:80:PHE:HD1	1.78	0.49
41:AM:20:ASN:ND2	41:AM:20:ASN:O	2.45	0.49
42:AN:110:CYS:SG	42:AN:112:LYS:HB2	2.53	0.49
1:AR:3033:A:H2'	1:AR:3034:C:C6	2.47	0.49
1:AR:361:A:H5'	39:DL:35:SER:OG	2.12	0.49
50:B:83:GLN:HG2	50:B:99:ALA:HB1	1.93	0.49
5:CE:49:TYR:CZ	5:CE:166:ILE:HD12	2.47	0.49
9:CI:138:TYR:CE2	9:CI:233:GLU:HB3	2.48	0.49
55:G:133:VAL:HG22	55:G:198:LEU:HD13	1.94	0.49
1:1:1029:G:H2'	1:1:1030:A:C8	2.48	0.49
1:1:3115:C:O2'	1:1:3117:C:N4	2.42	0.49
1:1:3152:U:O2'	1:1:3153:U:H5'	2.13	0.49
25:A:116:U:H2'	25:A:117:U:C6	2.47	0.49
25:A:1248:C:H2'	25:A:1249:U:C6	2.48	0.49
25:A:337:G:H1'	58:J:10:LYS:NZ	2.27	0.49
36:AH:16:ARG:NH1	36:AH:37:LYS:HD2	2.27	0.49
27:8:46:TYR:HD2	37:AI:75:TYR:HB3	1.77	0.49
27:8:114:VAL:HB	41:AM:10:LYS:HZ3	1.77	0.49
1:AR:3349:C:N4	1:AR:3356:G:H1	2.08	0.49
3:AT:82:U:HO2'	3:AT:83:C:P	2.35	0.49
4:CD:44:ILE:HD12	4:CD:62:VAL:HG13	1.94	0.49
5:CE:323:MET:HE1	5:CE:356:LEU:HD11	1.94	0.49
7:CG:8:LYS:HD2	7:CG:8:LYS:H	1.77	0.49
12:CL:89:VAL:HG22	12:CL:136:PHE:CE1	2.48	0.49
52:D:99:LYS:HA	52:D:117:THR:HA	1.94	0.49
53:E:7:LYS:NZ	70:V:115:GLU:OE2	2.45	0.49
25:A:331:A:H5'	58:J:33:PRO:HA	1.94	0.49
59:K:13:SER:O	59:K:43:TYR:HB3	2.12	0.49
1:1:1482:A:H4'	1:1:1483:G:OP2	2.13	0.49
1:1:1495:U:H5	1:1:1835:A:C2	2.30	0.49
1:1:2890:A:N1	1:1:2913:C:N3	2.61	0.49
25:6:1584:G:N2	25:6:1611:A:OP2	2.35	0.49
25:6:609:U:H4'	25:6:610:G:O5'	2.12	0.49
25:A:312:A:C2	25:A:314:C:H2'	2.48	0.49
25:A:749:U:H3	25:A:800:U:H3	1.59	0.49
1:AR:1307:G:H1'	1:AR:1308:A:C8	2.48	0.49
1:AR:990:U:H1'	22:CV:101:CYS:HB3	1.94	0.49
51:C:29:TRP:CD1	51:C:47:LEU:HG	2.47	0.49
51:C:61:LEU:HD22	51:C:61:LEU:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:CU:6:GLU:OE1	21:CU:99:ARG:NH2	2.30	0.49
26:CY:27:LYS:HD3	26:CY:29:PHE:CZ	2.48	0.49
27:CZ:38:LEU:HD13	27:CZ:40:LEU:HD21	1.94	0.49
54:F:104:ASP:N	54:F:108:ARG:O	2.43	0.49
63:O:30:SER:HB3	63:O:67:THR:HG22	1.95	0.49
1:1:1352:A:H4'	1:1:1353:U:OP1	2.12	0.49
1:1:3057:U:H5'	1:1:3086:A:H61	1.78	0.49
1:1:3358:U:H2'	1:1:3359:A:O4'	2.13	0.49
1:1:92:G:H5'	1:1:93:C:H5''	1.95	0.49
25:6:700:C:H2'	25:6:701:U:C6	2.47	0.49
25:A:1409:G:N2	25:A:1411:A:H3'	2.28	0.49
25:A:1503:A:H2'	25:A:1504:G:O4'	2.12	0.49
25:A:705:U:H2'	25:A:706:A:C8	2.48	0.49
41:AM:9:ILE:HG22	41:AM:13:MET:CE	2.43	0.49
1:AR:3164:C:N4	1:AR:3287:U:O4	2.45	0.49
1:AR:364:G:OP1	6:CF:60:THR:HG23	2.13	0.49
2:AS:47:C:H2'	2:AS:48:U:H6	1.77	0.49
50:B:179:ARG:HH11	50:B:183:ARG:NH1	2.11	0.49
51:C:35:PRO:HD3	51:C:98:THR:HG23	1.94	0.49
1:AR:1758:G:H5''	23:CW:104:ARG:HH21	1.77	0.49
33:DF:28:ARG:HB3	33:DF:65:LYS:HA	1.94	0.49
1:1:1796:G:H5''	1:1:1797:A:OP1	2.13	0.49
1:1:180:C:H2'	1:1:181:U:C6	2.47	0.49
1:1:718:G:C2	1:1:721:G:H1'	2.48	0.49
25:6:139:C:H4'	25:6:140:A:O5'	2.12	0.49
25:6:1749:A:O3'	43:DP:16:LYS:NZ	2.45	0.49
25:A:1165:G:C6	25:A:1166:A:C6	3.01	0.49
25:A:1:U:O4	59:K:54:ARG:HD3	2.12	0.49
1:1:1807:G:C5'	29:AA:135:ARG:HH22	2.24	0.49
30:AB:85:ASP:OD1	30:AB:86:LYS:N	2.44	0.49
1:AR:1807:G:C6	1:AR:1808:G:N1	2.81	0.49
1:AR:3357:U:H2'	1:AR:3358:U:C6	2.47	0.49
1:AR:400:G:H4'	1:AR:401:U:O5'	2.13	0.49
1:AR:59:G:C4'	1:AR:60:A:H4'	2.43	0.49
4:CD:130:SER:HG	4:CD:174:ARG:HH21	1.60	0.49
5:CE:361:THR:HG23	5:CE:371:GLN:O	2.13	0.49
12:CL:30:LYS:H	12:CL:62:SER:HB2	1.78	0.49
16:CP:135:VAL:HG13	16:CP:142:ILE:HG12	1.95	0.49
29:DB:46:ILE:HD11	29:DB:49:TYR:HA	1.95	0.49
41:DN:3:ALA:H	41:DN:5:LYS:HZ1	1.60	0.49
55:G:89:ILE:HD12	55:G:90:ILE:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:V:57:ARG:HD2	70:V:89:ARG:HD3	1.95	0.49
1:1:1608:C:H2'	1:1:1609:C:H6	1.78	0.48
1:1:2712:U:H2'	1:1:2713:U:C6	2.48	0.48
1:1:786:A:H4'	1:1:787:G:H5'	1.95	0.48
3:4:104:A:C8	3:4:105:A:C8	3.01	0.48
25:6:1381:U:H1'	25:6:1516:A:N6	2.27	0.48
28:9:11:ASP:HB3	28:9:14:LYS:HB2	1.95	0.48
3:4:111:A:N3	39:AK:17:THR:HG21	2.28	0.48
1:AR:2697:A:H2'	1:AR:2698:G:C8	2.48	0.48
3:AT:95:G:H1'	39:DL:81:GLY:O	2.13	0.48
54:F:160:VAL:HG12	54:F:162:ILE:HG12	1.95	0.48
57:I:74:GLN:HG2	57:I:131:PHE:CD2	2.48	0.48
66:R:82:ARG:HH22	66:R:114:ARG:HB2	1.77	0.48
21:0:155:ARG:NH2	21:0:171:PHE:O	2.45	0.48
1:1:1299:U:H2'	1:1:1300:G:O4'	2.12	0.48
1:1:171:G:H2'	1:1:172:G:O4'	2.13	0.48
1:1:2097:U:H2'	1:1:2098:C:C6	2.47	0.48
1:1:2535:A:H61	1:1:2544:U:H3	1.60	0.48
1:1:2726:C:O2'	1:1:2727:A:H2'	2.13	0.48
1:1:618:C:H2'	1:1:619:A:O4'	2.14	0.48
2:3:71:G:H2'	2:3:72:A:H8	1.78	0.48
25:6:1515:A:O2'	25:6:1517:U:OP2	2.24	0.48
84:6:1975:OHX:N1	84:6:2025:OHX:N4	2.62	0.48
25:A:1277:G:H2'	25:A:1278:G:O4'	2.13	0.48
1:1:716:A:N6	30:AB:117:ARG:HG3	2.28	0.48
1:AR:212:G:OP2	28:DA:2:ALA:N	2.46	0.48
1:AR:3174:A:H2'	1:AR:3175:U:H5'	1.95	0.48
51:C:41:ARG:HH21	51:C:97:LEU:HD11	1.78	0.48
1:AR:2242:A:H5'	4:CD:244:GLY:HA3	1.95	0.48
1:AR:2163:C:H4'	4:CD:7:ASN:O	2.13	0.48
11:CK:86:TYR:CD2	11:CK:151:VAL:HG13	2.48	0.48
11:CK:163:GLN:O	11:CK:166:ARG:HD3	2.13	0.48
12:CL:19:LYS:HD2	12:CL:26:VAL:HG22	1.96	0.48
17:CQ:73:PHE:HB3	17:CQ:78:ARG:HB3	1.94	0.48
19:CS:151:ARG:O	19:CS:162:ALA:HB3	2.13	0.48
65:Q:123:TYR:OH	68:T:122:HIS:NE2	2.37	0.48
1:1:2984:C:H2'	1:1:2985:C:H6	1.79	0.48
2:3:79:A:C2	2:3:102:A:C4	3.01	0.48
25:6:1258:U:H5	25:6:1259:U:C4	2.31	0.48
25:6:831:U:O2'	25:6:832:U:H5'	2.13	0.48
25:A:1151:A:H2'	25:A:1152:A:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:93:A:C6	25:A:398:G:C6	3.02	0.48
39:AK:53:ALA:HA	39:AK:56:ARG:NH1	2.28	0.48
1:AR:1273:A:H3'	1:AR:1274:A:H8	1.78	0.48
1:AR:123:A:C6	1:AR:150:A:C5	3.01	0.48
1:AR:1615:C:H2'	1:AR:1616:U:H6	1.79	0.48
1:AR:3132:C:H2'	1:AR:3133:C:C6	2.48	0.48
5:CE:292:ALA:HA	5:CE:303:LYS:H	1.78	0.48
15:CO:60:LEU:HD13	21:CU:152:LEU:HD11	1.94	0.48
31:DD:23:LYS:HD2	31:DD:23:LYS:HA	1.69	0.48
34:DG:60:ASN:OD1	34:DG:62:LYS:HB2	2.13	0.48
55:G:58:LEU:HD13	55:G:138:THR:HG22	1.95	0.48
61:M:72:THR:O	61:M:88:ARG:HD2	2.13	0.48
67:S:21:TYR:C	67:S:23:LYS:H	2.16	0.48
1:1:1363:A:H2'	1:1:1364:C:H6	1.78	0.48
1:1:1662:G:N2	1:1:1788:C:O2	2.47	0.48
1:1:3049:A:H5'	1:1:3049:A:H8	1.78	0.48
1:1:3233:C:H2'	1:1:3234:A:C8	2.48	0.48
1:1:394:G:N2	1:1:396:A:H3'	2.29	0.48
25:6:708:C:H2'	25:6:709:C:O4'	2.13	0.48
25:A:1511:U:H2'	25:A:1512:G:C8	2.48	0.48
25:A:912:U:H4'	25:A:913:G:H2'	1.95	0.48
1:AR:1480:G:H4'	1:AR:1481:A:OP1	2.14	0.48
1:AR:2413:A:H2'	1:AR:2414:G:C8	2.49	0.48
1:AR:2656:A:P	44:DQ:97:LYS:HB3	2.53	0.48
1:AR:2881:C:H2'	1:AR:2882:U:H6	1.79	0.48
1:AR:304:G:H5'	1:AR:304:G:N3	2.27	0.48
1:AR:945:C:H2'	1:AR:946:U:H6	1.79	0.48
3:AT:102:U:H2'	3:AT:103:G:C8	2.49	0.48
51:C:201:THR:HG21	51:C:207:LEU:HD22	1.94	0.48
11:CK:7:GLU:OE1	11:CK:54:LYS:HD3	2.13	0.48
1:AR:3180:A:C6	17:CQ:114:LYS:HG2	2.49	0.48
9:CI:110:ARG:NH1	19:CS:3:ILE:HD11	2.28	0.48
20:CT:171:ASP:HA	20:CT:174:ALA:HB3	1.95	0.48
52:D:116:LYS:HG2	52:D:127:ALA:HB3	1.94	0.48
52:D:38:VAL:HG22	52:D:39:THR:H	1.78	0.48
29:DB:83:THR:HG23	29:DB:85:TYR:N	2.25	0.48
60:L:1:MET:HG2	60:L:2:LEU:N	2.28	0.48
65:Q:24:LYS:O	65:Q:28:MET:HB2	2.12	0.48
66:R:50:GLU:OE2	66:R:82:ARG:NH2	2.45	0.48
69:U:23:GLN:HG2	69:U:55:TYR:CD2	2.48	0.48
70:V:118:VAL:HG22	70:V:119:ALA:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1363:A:H2'	1:1:1364:C:C6	2.48	0.48
1:1:138:U:H2'	1:1:139:G:H8	1.79	0.48
1:1:1481:A:N3	1:1:1481:A:H2'	2.28	0.48
1:1:2630:C:H1'	1:1:2758:A:N3	2.29	0.48
25:6:1087:A:H2	25:6:1142:A:H4'	1.78	0.48
25:6:1533:C:H4'	25:6:1539:G:H1	1.78	0.48
25:A:582:U:H5'	25:A:583:C:H5	1.79	0.48
1:AR:65:A:C4	1:AR:110:G:N7	2.81	0.48
1:AR:1564:U:H2'	1:AR:1565:G:C8	2.48	0.48
1:AR:1614:C:H2'	1:AR:1615:C:H6	1.79	0.48
1:AR:314:U:H2'	1:AR:315:C:H6	1.76	0.48
1:AR:80:G:H2'	1:AR:81:C:C6	2.48	0.48
1:AR:939:U:H2'	1:AR:940:G:H8	1.79	0.48
5:CE:221:THR:O	5:CE:272:TYR:HA	2.13	0.48
9:CI:138:TYR:N	9:CI:233:GLU:O	2.44	0.48
1:AR:116:A:OP2	16:CP:2:GLY:HA3	2.13	0.48
27:CZ:132:ALA:O	27:CZ:136:ALA:N	2.45	0.48
30:DC:47:LYS:HE2	30:DC:48:TYR:CZ	2.48	0.48
1:AR:1145:G:H5'	34:DG:46:PHE:CE1	2.48	0.48
1:AR:1639:C:H5'	36:DI:52:GLN:HG2	1.96	0.48
41:DN:5:LYS:HD3	41:DN:13:MET:HE1	1.94	0.48
60:L:59:PHE:CE2	60:L:62:GLN:HA	2.48	0.48
1:1:138:U:H2'	1:1:139:G:C8	2.47	0.48
1:1:550:A:N6	1:1:551:A:H62	2.12	0.48
3:4:113:U:H5''	41:AM:7:PHE:HB3	1.96	0.48
25:6:906:A:H2'	25:6:907:A:C8	2.48	0.48
1:1:12:A:H1'	27:8:37:THR:HG21	1.96	0.48
25:A:1407:U:H2'	25:A:1408:G:O4'	2.12	0.48
25:A:321:C:H41	25:A:1667:A:P	2.36	0.48
25:A:16:G:H2'	25:A:17:C:C6	2.49	0.48
25:A:276:C:O2'	25:A:277:U:H5''	2.14	0.48
25:A:68:A:OP1	56:H:160:ARG:NH2	2.27	0.48
1:AR:1507:G:C8	18:CR:129:THR:HG22	2.48	0.48
1:AR:911:C:H5''	4:CD:15:ILE:HD13	1.95	0.48
13:CM:95:ASN:HB3	13:CM:103:GLY:O	2.12	0.48
17:CQ:121:PRO:HA	17:CQ:124:LEU:HD22	1.95	0.48
1:AR:2111:G:H1'	26:CY:44:LYS:HD2	1.94	0.48
28:DA:55:GLU:HB2	28:DA:108:LYS:HB2	1.95	0.48
19:CS:94:PHE:CZ	30:DC:119:PRO:HD3	2.48	0.48
25:A:1366:U:H4'	69:U:7:ARG:HD3	1.95	0.48
74:Z:104:SER:HB3	74:Z:107:GLN:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2659:G:H4'	1:1:2751:G:O2'	2.13	0.48
1:1:2881:C:H2'	1:1:2882:U:H6	1.78	0.48
1:1:3269:U:H4'	1:1:3270:U:O5'	2.12	0.48
1:1:73:C:C4	38:AJ:15:LYS:HD3	2.49	0.48
3:4:10:A:H2'	3:4:11:C:C6	2.49	0.48
25:6:1591:C:H2'	25:6:1592:A:C8	2.48	0.48
25:A:1332:C:O2'	53:E:162:GLN:HB3	2.14	0.48
25:A:1400:A:H4'	67:S:60:ARG:HH22	1.79	0.48
25:A:1682:U:O2'	25:A:1683:C:H5'	2.12	0.48
33:AE:19:ARG:HD3	33:AE:35:GLU:CG	2.44	0.48
84:AS:203:OHX:N1	84:AS:210:OHX:N2	2.61	0.48
50:B:120:LEU:HD13	50:B:142:PRO:HB2	1.95	0.48
5:CE:92:TYR:CE2	5:CE:159:ARG:HD2	2.49	0.48
7:CG:259:LYS:O	7:CG:260:PHE:HB2	2.12	0.48
7:CG:34:LYS:O	7:CG:38:THR:HG23	2.14	0.48
7:CG:8:LYS:HB3	7:CG:12:TYR:CD1	2.49	0.48
18:CR:59:PRO:HG3	18:CR:76:PHE:CD2	2.48	0.48
19:CS:86:THR:HB	19:CS:105:ARG:HB2	1.94	0.48
52:D:140:ARG:HB3	52:D:221:THR:HB	1.96	0.48
32:DE:22:LYS:HB2	32:DE:94:GLU:HB2	1.95	0.48
55:G:144:GLU:OE1	55:G:225:ARG:NH2	2.46	0.48
62:N:24:ILE:O	62:N:25:GLU:HG2	2.14	0.48
64:P:20:TYR:HB3	64:P:27:PHE:HB2	1.96	0.48
68:T:28:ILE:HA	68:T:31:ALA:HB3	1.96	0.48
25:6:250:C:H2'	25:6:251:A:C8	2.49	0.48
25:6:450:U:H2'	25:6:451:A:C8	2.49	0.48
25:6:819:G:O2'	25:6:821:U:OP2	2.31	0.48
25:6:829:A:H1'	25:6:830:U:C5	2.48	0.48
28:9:86:THR:HG22	28:9:96:PRO:HA	1.94	0.48
25:A:1133:A:H2'	25:A:1134:C:O4'	2.14	0.48
25:A:1450:U:H2'	25:A:1451:C:C6	2.49	0.48
25:A:1533:C:H4'	25:A:1539:G:C6	2.49	0.48
25:A:452:A:H3'	25:A:453:U:C5	2.48	0.48
25:A:480:G:H22	25:A:509:G:H1'	1.77	0.48
36:AH:58:ARG:HG3	36:AH:59:PRO:HD2	1.95	0.48
1:AR:1659:U:H2'	1:AR:1660:C:C6	2.48	0.48
1:AR:655:C:H2'	1:AR:656:A:H8	1.76	0.48
12:CL:191:LYS:HE2	12:CL:212:GLU:HB3	1.96	0.48
28:DA:39:LEU:HD22	28:DA:43:TYR:CE2	2.48	0.48
25:A:927:C:H1'	64:P:125:SER:CB	2.43	0.48
72:X:86:ILE:HD12	72:X:87:GLU:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1004:U:C4	1:1:1005:G:N7	2.82	0.48
1:1:1802:C:H2'	1:1:1803:C:C6	2.49	0.48
1:1:2611:U:H2'	1:1:2612:U:C6	2.48	0.48
1:1:345:G:OP1	1:1:1429:G:N1	2.46	0.48
1:1:829:U:H3	1:1:895:A:H62	1.61	0.48
23:5:32:SER:HA	23:5:35:LYS:HB3	1.96	0.48
25:6:755:A:HO2'	25:6:756:A:H8	1.62	0.48
25:A:1621:U:H2'	25:A:1622:G:C8	2.49	0.48
25:A:1689:A:H2'	25:A:1690:G:H8	1.79	0.48
25:A:40:A:OP1	59:K:3:ARG:NH1	2.45	0.48
25:A:78:A:H1'	56:H:175:ILE:HG12	1.96	0.48
25:A:836:U:H2'	25:A:837:G:H8	1.79	0.48
25:A:992:A:O2'	25:A:1785:U:O2	2.32	0.48
38:AJ:33:ALA:O	38:AJ:37:THR:OG1	2.32	0.48
41:AM:23:LEU:O	41:AM:25:GLN:NE2	2.46	0.48
44:AP:25:VAL:HG22	44:AP:72:LEU:HD22	1.95	0.48
1:AR:1714:A:H2	1:AR:1727:G:N3	2.12	0.48
5:CE:49:TYR:O	5:CE:80:ASP:N	2.41	0.48
11:CK:122:LYS:HE3	11:CK:123:ILE:O	2.14	0.48
1:AR:2899:C:C5	11:CK:171:ASP:HA	2.49	0.48
17:CQ:16:VAL:HG23	17:CQ:42:ASN:O	2.13	0.48
3:AT:84:C:H1'	28:DA:113:LYS:HG3	1.96	0.48
33:DF:16:LEU:HA	33:DF:16:LEU:HD12	1.75	0.48
1:AR:256:G:H4'	37:DJ:111:PHE:HZ	1.79	0.48
25:A:788:A:C4	54:F:19:LEU:HD13	2.48	0.48
55:G:56:ALA:O	55:G:57:SER:O	2.31	0.48
62:N:50:LYS:O	62:N:54:ARG:HG2	2.14	0.48
1:1:269:G:O6	70:V:15:GLN:NE2	193.85	0.48
1:1:1340:G:H2'	1:1:1341:U:C6	2.49	0.48
1:1:1657:C:C5	1:1:1797:A:H5''	2.49	0.48
1:1:193:C:H2'	1:1:194:U:H6	1.78	0.48
1:1:2971:A:N3	1:1:2971:A:H3'	2.29	0.48
1:1:952:A:OP1	31:AC:14:ARG:NH2	2.47	0.48
25:6:84:A:H2'	25:6:85:A:O4'	2.14	0.48
25:A:1591:C:H2'	25:A:1592:A:C8	2.49	0.48
25:A:635:A:H2'	25:A:636:A:C8	2.49	0.48
30:AB:74:ASN:HB3	30:AB:76:ASP:HB2	1.96	0.48
30:AB:96:LYS:C	30:AB:98:THR:H	2.16	0.48
45:AQ:73:THR:HG23	45:AQ:76:ALA:H	1.79	0.48
1:AR:3045:G:H2'	1:AR:3046:A:O4'	2.14	0.48
1:AR:3308:C:O2	18:CR:69:ARG:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:601:U:H2'	1:AR:602:A:O4'	2.14	0.48
1:AR:90:C:H2'	1:AR:91:G:H5'	1.94	0.48
51:C:28:GLU:HB2	51:C:49:ASN:O	2.14	0.48
11:CK:13:PRO:HG2	11:CK:16:VAL:HG13	1.95	0.48
19:CS:176:ARG:HA	19:CS:182:LYS:O	2.14	0.48
20:CT:6:THR:HG22	20:CT:10:LEU:HD22	1.95	0.48
21:CU:1:MET:SD	21:CU:32:SER:OG	2.71	0.48
35:DH:41:ALA:HB3	35:DH:74:THR:HG22	1.96	0.48
45:DR:7:LYS:O	45:DR:27:LYS:NZ	2.38	0.48
59:K:108:ARG:HH21	59:K:145:SER:HB2	1.78	0.48
60:L:14:TYR:CE1	60:L:18:GLU:HG3	2.49	0.48
62:N:43:ARG:HA	62:N:121:VAL:HG12	1.96	0.48
65:Q:85:ILE:HA	65:Q:89:MET:SD	2.54	0.48
67:S:19:ARG:HG3	67:S:20:TYR:CD1	2.49	0.48
72:X:10:ALA:HB2	72:X:34:ILE:HD13	1.96	0.48
21:0:1:MET:HE3	21:0:32:SER:HB3	1.96	0.47
1:1:1245:A:N6	1:1:1272:C:O2'	2.47	0.47
1:1:1724:U:OP2	74:Z:128:LYS:NZ	99.27	0.47
1:1:29:C:H4'	1:1:62:A:H4'	1.96	0.47
25:6:1488:G:O2'	25:6:1494:C:O2	2.23	0.47
25:6:1347:U:O2	25:6:1516:A:H5'	2.14	0.47
25:A:1561:U:H2'	25:A:1562:G:H8	1.79	0.47
30:AB:73:LEU:HB2	30:AB:109:TYR:CD1	2.49	0.47
1:AR:2656:A:OP2	44:DQ:97:LYS:HB3	2.14	0.47
1:AR:2993:G:H2'	1:AR:3142:A:N6	2.28	0.47
1:AR:3171:U:H3	1:AR:3279:A:H61	1.62	0.47
1:AR:3350:C:O2'	1:AR:3351:U:OP1	2.26	0.47
6:CF:119:ARG:HH12	6:CF:271:LYS:HB3	1.76	0.47
15:CO:92:GLU:H	15:CO:92:GLU:CD	2.16	0.47
17:CQ:78:ARG:HG3	17:CQ:78:ARG:NH1	2.28	0.47
53:E:31:GLU:O	53:E:54:ARG:NH1	2.47	0.47
64:P:29:HIS:HB3	64:P:41:ARG:HA	1.95	0.47
74:Z:21:LYS:HE3	74:Z:55:VAL:HA	11.67	0.47
1:1:1667:A:H2'	1:1:1668:G:C8	2.49	0.47
1:1:2438:A:H2'	1:1:2439:A:C8	2.49	0.47
1:1:2723:U:H2'	1:1:2724:U:C6	2.48	0.47
84:1:3539:OHX:N6	84:1:3697:OHX:N1	2.62	0.47
1:1:92:G:OP2	1:1:93:C:H5''	2.14	0.47
22:2:84:TYR:O	22:2:85:LEU:HD23	2.14	0.47
25:6:835:U:H2'	25:6:836:U:C6	2.49	0.47
25:A:1091:A:H5''	25:A:1091:A:N3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:512:A:H2'	25:A:513:U:C6	2.48	0.47
25:A:950:C:H2'	25:A:951:A:C8	2.49	0.47
43:AO:3:ALA:HB3	25:A:1773:C:OP1	2.13	0.47
1:AR:1429:G:C5	6:CF:99:MET:HE1	2.49	0.47
1:AR:1925:U:O2	45:DR:19:GLY:HA2	2.13	0.47
1:AR:2268:U:C3'	1:AR:2269:U:H5''	2.40	0.47
1:AR:80:G:H2'	1:AR:81:C:H6	1.77	0.47
3:AT:121:U:H2'	3:AT:122:U:C6	2.49	0.47
14:CN:64:LYS:HA	30:DC:69:TRP:CE3	2.50	0.47
26:CY:63:ILE:HG23	26:CY:64:THR:H	1.78	0.47
27:CZ:135:ILE:HD13	27:CZ:138:ARG:HE	1.79	0.47
1:AR:655:C:OP1	34:DG:27:ARG:HB3	2.14	0.47
36:DI:74:ARG:HG2	36:DI:75:ALA:N	2.29	0.47
44:DQ:10:THR:OG1	44:DQ:11:TYR:N	2.47	0.47
54:F:193:GLY:HA3	54:F:210:ILE:HG22	1.97	0.47
58:J:36:THR:HG23	58:J:96:LEU:O	2.14	0.47
67:S:101:ASN:HA	67:S:120:SER:CB	2.45	0.47
68:T:40:ARG:HB3	69:U:45:MET:SD	2.53	0.47
74:Z:57:VAL:HG13	74:Z:60:PHE:HE2	1.78	0.47
1:1:1564:U:H2'	1:1:1565:G:C8	2.49	0.47
1:1:3160:U:H2'	1:1:3161:C:C6	2.49	0.47
21:O:27:MET:HG2	22:2:151:LEU:O	2.13	0.47
25:6:197:A:H2'	25:6:198:A:H8	1.80	0.47
25:A:1354:G:H5'	25:A:1355:C:OP2	2.14	0.47
25:A:1450:U:H2'	25:A:1451:C:H6	1.79	0.47
25:A:387:A:H5''	25:A:389:G:OP2	2.14	0.47
1:AR:1064:A:H5''	1:AR:1066:G:O4'	2.14	0.47
1:AR:1495:U:H5	1:AR:1835:A:N1	2.12	0.47
1:AR:3348:G:H1	1:AR:3357:U:H3	1.61	0.47
84:AS:203:OHX:N3	84:AS:210:OHX:N6	2.62	0.47
51:C:62:LYS:HD2	51:C:91:VAL:HB	1.97	0.47
12:CL:87:LEU:HD22	12:CL:88:ARG:N	2.30	0.47
11:CK:59:ASN:HB2	15:CO:41:GLN:NE2	2.29	0.47
17:CQ:23:VAL:CG1	17:CQ:84:LEU:HD11	2.44	0.47
18:CR:136:ILE:O	18:CR:137:ASN:ND2	2.47	0.47
1:AR:2737:C:H4'	22:CV:68:THR:OG1	2.13	0.47
34:DG:24:ARG:HD3	34:DG:25:TYR:CZ	2.50	0.47
1:AR:1485:G:N2	36:DI:4:ARG:HD2	2.29	0.47
1:AR:1821:U:N3	36:DI:67:LYS:HD3	2.29	0.47
54:F:163:ASP:HB3	54:F:166:SER:O	2.14	0.47
70:V:106:ILE:HG13	70:V:107:THR:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2111:G:H5''	26:7:48:ARG:CZ	2.43	0.47
1:1:2115:G:H22	1:1:2120:A:H1'	1.79	0.47
23:5:82:LYS:O	23:5:86:LYS:N	2.45	0.47
25:6:1018:U:H2'	25:6:1019:A:C8	2.49	0.47
25:6:1405:G:H2'	25:6:1406:A:H8	1.78	0.47
25:6:29:U:H2'	25:6:30:G:C8	2.49	0.47
25:6:846:G:H2'	25:6:847:A:C8	2.49	0.47
25:A:407:A:H2'	25:A:408:C:C6	2.50	0.47
25:A:955:A:H4'	25:A:1073:G:O2'	2.14	0.47
33:AE:31:ARG:HH11	33:AE:31:ARG:HB3	1.78	0.47
1:AR:2612:U:H2'	1:AR:2613:U:O4'	2.14	0.47
2:AS:19:C:H2'	2:AS:20:A:C8	2.49	0.47
50:B:175:TYR:HE1	50:B:197:ILE:HG22	1.78	0.47
4:CD:204:MET:HE3	4:CD:209:HIS:HB2	1.96	0.47
4:CD:65:ASP:HB3	4:CD:68:LYS:O	2.15	0.47
5:CE:123:TYR:CZ	5:CE:124:LYS:HG3	2.50	0.47
5:CE:187:SER:HB3	5:CE:190:GLU:HB2	1.95	0.47
11:CK:67:ALA:HA	11:CK:70:THR:HG23	1.97	0.47
12:CL:12:GLN:NE2	12:CL:128:ARG:HB3	2.29	0.47
12:CL:142:ASP:OD2	12:CL:178:ARG:NH2	2.47	0.47
21:CU:79:VAL:HG21	21:CU:106:LEU:HD11	1.95	0.47
52:D:97:ARG:HG2	52:D:97:ARG:H	1.45	0.47
22:CV:79:MET:SD	31:DD:21:ILE:HG21	2.54	0.47
56:H:142:ARG:HA	56:H:147:LEU:HB2	1.97	0.47
53:E:27:ARG:HD2	60:L:60:SER:HB2	1.96	0.47
61:M:14:GLN:HB3	61:M:54:ILE:HG21	1.96	0.47
63:O:29:SER:N	63:O:32:SER:OG	2.46	0.47
64:P:88:GLY:H	64:P:120:PRO:HG2	1.79	0.47
70:V:17:GLN:HE22	70:V:98:GLN:HB3	1.79	0.47
73:Y:23:ARG:HD2	73:Y:26:GLU:OE1	2.14	0.47
21:O:79:VAL:HG21	21:O:106:LEU:HD21	1.96	0.47
1:1:2660:G:O3'	1:1:2749:G:N2	2.48	0.47
3:4:79:A:H5''	37:AI:43:LYS:NZ	2.30	0.47
25:6:1429:G:H2'	25:6:1430:U:C6	2.49	0.47
25:6:188:A:H2'	25:6:189:C:O4'	2.15	0.47
25:A:505:A:H2'	25:A:505:A:N3	2.30	0.47
25:A:685:A:H2'	25:A:686:C:C6	2.49	0.47
25:A:75:U:H2'	25:A:76:A:O4'	2.14	0.47
33:AE:24:SER:O	33:AE:28:ARG:HG3	2.15	0.47
33:AE:46:THR:HG21	33:AE:91:SER:OG	2.14	0.47
1:AR:1471:U:H2'	1:AR:1472:U:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:1547:G:H2'	1:AR:1548:C:C6	2.50	0.47
1:AR:1590:G:OP2	87:AR:4261:GOL:O3	2.13	0.47
1:AR:1954:G:H2'	1:AR:1955:U:C6	2.50	0.47
51:C:128:LYS:HE3	51:C:132:ASP:HB3	1.97	0.47
6:CF:82:THR:HG23	6:CF:84:ARG:H	1.79	0.47
20:CT:23:TRP:HB3	20:CT:51:VAL:HG22	1.96	0.47
52:D:38:VAL:O	52:D:39:THR:OG1	2.27	0.47
30:DC:111:LYS:HA	30:DC:129:PHE:O	2.14	0.47
54:F:125:LYS:HE3	54:F:157:ASN:HA	1.96	0.47
68:T:60:GLU:O	68:T:61:LEU:HB2	2.15	0.47
25:A:1132:A:OP1	73:Y:30:LYS:HE3	2.14	0.47
1:1:1192:C:O2	1:1:1192:C:H2'	2.15	0.47
1:1:1618:G:H4'	3:4:129:C:H1'	1.96	0.47
1:1:3393:U:H2'	1:1:3394:U:C6	2.49	0.47
1:1:824:C:H2'	1:1:825:U:C6	2.49	0.47
25:6:1410:A:H2'	25:6:1411:A:O4'	2.14	0.47
25:6:1388:A:C5	25:6:1411:A:C6	3.03	0.47
25:6:234:G:H2'	25:6:235:G:O4'	2.14	0.47
25:A:1609:U:OP2	66:R:14:LYS:NZ	2.46	0.47
25:A:1689:A:H2'	25:A:1690:G:C8	2.49	0.47
25:A:694:U:H5"	25:A:695:U:H5	1.79	0.47
1:1:256:G:H4'	37:AI:111:PHE:HZ	1.78	0.47
1:AR:627:U:H4'	1:AR:1399:A:O2'	2.14	0.47
25:6:1758:U:H1'	1:AR:2255:A:N3	2.30	0.47
9:CI:92:ILE:HD12	9:CI:92:ILE:HA	1.59	0.47
13:CM:14:ILE:HD11	13:CM:80:LEU:HD12	1.95	0.47
1:AR:2629:U:O4	22:CV:2:GLY:N	2.47	0.47
22:CV:82:ASN:O	31:DD:21:ILE:HA	2.15	0.47
57:I:111:LYS:HG3	57:I:112:ARG:N	2.29	0.47
63:O:64:ARG:HD3	63:O:64:ARG:O	2.13	0.47
73:Y:130:VAL:HG21	73:Y:142:LYS:HA	1.96	0.47
74:Z:47:VAL:HG23	74:Z:48:TYR:CD2	2.50	0.47
1:1:1160:C:OP1	73:Y:2:GLY:N	159.70	0.47
1:1:2532:U:H3	1:1:2547:A:H61	1.62	0.47
1:1:789:A:H2'	1:1:790:U:C6	2.50	0.47
25:6:1120:U:H2'	25:6:1121:C:C6	2.50	0.47
25:6:603:U:H2'	25:6:604:A:C8	2.50	0.47
25:A:404:G:H2'	25:A:405:C:C6	2.49	0.47
1:1:2552:C:N4	32:AD:54:SER:OG	2.48	0.47
1:1:1927:G:P	45:AQ:6:LYS:H	2.37	0.47
1:AR:1508:C:OP1	18:CR:127:ARG:NH2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:1614:C:H2'	1:AR:1615:C:C6	2.50	0.47
1:AR:999:G:C6	1:AR:1000:C:N4	2.83	0.47
2:AS:64:A:H5'	2:AS:65:G:H5"	1.95	0.47
7:CG:132:THR:HG21	7:CG:170:GLY:HA2	1.97	0.47
2:AS:49:G:C5	7:CG:58:LYS:HG3	2.48	0.47
10:CJ:203:VAL:HG13	10:CJ:204:ARG:O	2.14	0.47
15:CO:48:GLY:HA3	15:CO:53:VAL:HG13	1.96	0.47
18:CR:13:LYS:HE2	18:CR:152:GLU:HB2	1.95	0.47
24:CX:5:GLY:HA3	24:CX:106:LYS:O	2.14	0.47
63:O:89:TYR:CE1	63:O:150:VAL:HG22	2.50	0.47
67:S:105:GLN:H	67:S:105:GLN:NE2	2.13	0.47
1:1:1507:G:N3	1:1:1507:G:H5'	2.30	0.47
1:1:2406:C:H2'	1:1:2407:C:C6	2.49	0.47
1:1:2635:A:H2	22:2:10:ARG:HH21	1.61	0.47
1:1:3252:G:H2'	1:1:3253:G:C8	2.49	0.47
1:1:440:A:OP2	1:1:440:A:H8	1.97	0.47
1:1:594:U:H2'	1:1:609:G:O6	2.14	0.47
25:6:1087:A:C2	25:6:1142:A:H4'	2.49	0.47
25:6:300:A:H2'	25:6:301:A:C8	2.49	0.47
25:A:1410:A:H2'	25:A:1411:A:O4'	2.15	0.47
25:A:196:G:O2'	25:A:197:A:OP2	2.28	0.47
25:A:269:G:N7	56:H:186:ARG:NH2	2.62	0.47
25:A:778:G:H5'	25:A:780:A:N1	2.30	0.47
37:AI:96:GLU:H	37:AI:96:GLU:HG2	1.42	0.47
1:AR:1235:U:H4'	1:AR:1236:G:H5'	1.96	0.47
1:AR:3180:A:C5	17:CQ:114:LYS:HG2	2.50	0.47
1:AR:3228:C:H4'	1:AR:3229:G:O5'	2.14	0.47
1:AR:3231:U:H2'	1:AR:3232:G:H8	1.80	0.47
50:B:193:GLN:O	50:B:195:TRP:N	2.48	0.47
5:CE:305:ILE:HG12	5:CE:321:PHE:CZ	2.50	0.47
10:CJ:144:GLU:OE1	38:DK:36:ARG:NH2	2.46	0.47
12:CL:48:LEU:HB2	12:CL:142:ASP:OD1	2.14	0.47
12:CL:48:LEU:HD22	12:CL:49:CYS:H	1.80	0.47
52:D:139:ILE:HD11	52:D:218:ILE:HD13	1.95	0.47
41:DN:42:ARG:HG2	41:DN:43:ASN:N	2.29	0.47
54:F:36:HIS:NE2	54:F:88:ASP:OD2	2.46	0.47
54:F:54:TYR:OH	54:F:97:GLU:OE2	2.26	0.47
55:G:62:VAL:HG13	55:G:89:ILE:HG12	1.95	0.47
57:I:58:LEU:HG	57:I:88:ARG:HD2	1.96	0.47
61:M:53:TYR:CG	61:M:113:PRO:HG2	2.50	0.47
21:0:5:LYS:HD3	21:0:63:GLN:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:437:G:O2'	1:1:438:A:H5'	2.15	0.47
25:6:1081:A:H1'	25:6:1082:C:C5	2.48	0.47
25:6:1672:G:H2'	25:6:1673:G:C8	2.50	0.47
25:6:488:G:N2	25:6:499:U:H3	2.12	0.47
25:6:686:C:H2'	25:6:687:G:H8	1.80	0.47
25:A:1404:C:H2'	25:A:1405:G:H8	1.80	0.47
25:A:304:U:H2'	25:A:305:C:H6	1.79	0.47
25:A:380:U:C4	59:K:5:PRO:HB3	2.49	0.47
25:A:523:G:H5''	74:Z:59:GLY:O	2.15	0.47
1:AR:3047:U:O2'	1:AR:3048:A:H5'	2.14	0.47
1:AR:3086:A:OP1	84:AR:3671:OHX:N2	2.48	0.47
50:B:71:GLU:HA	50:B:94:GLY:O	2.15	0.47
4:CD:206:PRO:HG3	4:CD:213:GLY:HA3	1.96	0.47
1:AR:2969:A:N7	4:CD:215:ASN:ND2	2.62	0.47
7:CG:126:GLU:HA	7:CG:196:ARG:HD2	1.97	0.47
7:CG:153:THR:HG23	7:CG:160:PHE:HZ	1.80	0.47
7:CG:83:LEU:HB3	7:CG:88:ILE:HB	1.97	0.47
1:AR:129:U:OP1	27:CZ:45:LYS:NZ	2.48	0.47
52:D:130:ILE:O	52:D:134:LEU:HD22	2.14	0.47
14:CN:166:ALA:HB1	30:DC:147:LEU:HD21	1.97	0.47
34:DG:102:ALA:HB2	34:DG:125:ARG:HG2	1.96	0.47
37:DJ:38:ARG:HG2	37:DJ:39:PRO:HD2	1.95	0.47
54:F:11:ARG:NH1	54:F:20:LEU:HB3	2.30	0.47
62:N:43:ARG:NH1	62:N:102:GLY:HA3	2.29	0.47
72:X:15:ASN:ND2	72:X:71:LYS:HG3	2.28	0.47
1:1:1547:G:H2'	1:1:1548:C:C6	2.50	0.47
1:1:1805:C:OP1	36:AH:67:LYS:NZ	2.43	0.47
1:1:2767:U:H2'	1:1:2768:U:C6	2.50	0.47
1:1:3251:U:H2'	1:1:3252:G:C8	2.50	0.47
23:5:59:ASP:N	23:5:62:VAL:O	2.40	0.47
28:9:39:LEU:HD22	28:9:43:TYR:HE2	1.80	0.47
25:A:1073:G:H2'	25:A:1074:G:H5''	1.96	0.47
25:A:1268:G:C2	25:A:1270:G:N7	2.83	0.47
25:A:17:C:H2'	25:A:18:C:C6	2.50	0.47
25:A:844:A:H2'	25:A:845:G:C8	2.50	0.47
25:A:919:A:H2'	25:A:920:U:C6	2.50	0.47
36:AH:44:CYS:HB2	36:AH:81:CYS:HB3	1.97	0.47
1:AR:1221:A:H3'	1:AR:1222:G:H5'	1.96	0.47
1:AR:2437:G:N2	1:AR:2511:A:H1'	2.29	0.47
1:AR:3157:U:H4'	1:AR:3158:G:C5'	2.44	0.47
84:AR:3511:OHX:N6	84:AR:3698:OHX:N5	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CE:166:ILE:O	5:CE:169:THR:HG22	2.15	0.47
7:CG:200:PHE:HB3	7:CG:237:GLU:HG3	1.97	0.47
11:CK:129:ARG:O	11:CK:132:VAL:HG13	2.15	0.47
11:CK:162:GLN:HB2	11:CK:179:ILE:O	2.15	0.47
21:CU:155:ARG:HD3	21:CU:172:TYR:CG	2.50	0.47
52:D:166:THR:OG1	52:D:201:ASN:HB3	2.14	0.47
30:DC:73:LEU:HD13	30:DC:109:TYR:CZ	2.49	0.47
37:DJ:5:LYS:O	37:DJ:9:LEU:HG	2.15	0.47
16:CP:143:ARG:NH2	37:DJ:92:LEU:HD23	2.30	0.47
54:F:253:ASP:O	54:F:257:ALA:N	2.47	0.47
56:H:10:ASN:N	56:H:10:ASN:OD1	2.47	0.47
60:L:50:THR:HG22	60:L:55:VAL:HG22	1.97	0.47
72:X:11:LEU:HD12	72:X:74:VAL:HB	1.97	0.47
1:1:1101:G:C2'	1:1:1102:A:H5'	2.45	0.47
1:1:1695:U:O2'	1:1:1749:A:N1	2.40	0.47
1:1:2801:A:O2'	1:1:2802:A:H2'	2.15	0.47
1:1:3006:A:H2'	1:1:3007:U:O4'	2.15	0.47
1:1:22:G:O4'	3:4:104:A:H1'	2.15	0.47
25:6:187:G:H1'	25:6:198:A:H61	1.79	0.47
26:7:17:ARG:HA	26:7:17:ARG:HD3	1.69	0.47
25:A:887:A:H1'	64:P:122:PRO:HB3	1.97	0.47
31:AC:46:ALA:O	31:AC:50:THR:HG22	2.14	0.47
1:1:3275:U:O4'	35:AG:66:VAL:HG21	2.15	0.47
1:AR:2438:A:H2'	1:AR:2439:A:H8	1.80	0.47
1:AR:629:U:H2'	1:AR:630:A:C8	2.50	0.47
1:AR:638:C:H2'	1:AR:639:G:C8	2.50	0.47
2:AS:85:G:O3'	9:CI:218:ARG:NH2	2.48	0.47
10:CJ:163:VAL:HG22	10:CJ:166:LEU:HD12	1.97	0.47
30:DC:93:SER:OG	30:DC:93:SER:O	2.34	0.47
56:H:10:ASN:HB3	56:H:128:THR:HA	1.97	0.47
59:K:122:VAL:HG23	59:K:123:HIS:CD2	2.50	0.47
59:K:134:ILE:HG22	59:K:158:PHE:CD1	2.50	0.47
1:1:1083:G:H2'	1:1:1084:A:C8	2.50	0.46
1:1:2677:G:H2'	1:1:2679:A:C2	2.50	0.46
25:6:876:G:H1'	25:6:944:A:O4'	2.15	0.46
25:A:1175:U:H2'	25:A:1176:G:H8	1.77	0.46
25:A:306:U:H2'	25:A:307:G:C8	2.49	0.46
25:A:325:G:H2'	25:A:326:G:H8	1.81	0.46
25:A:858:G:OP1	57:I:116:ARG:NH2	2.48	0.46
25:A:885:G:O6	25:A:926:A:N6	2.48	0.46
25:A:986:G:H2'	25:A:987:G:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:AJ:66:GLU:HB3	38:AJ:70:ARG:HH21	1.80	0.46
44:AP:69:VAL:HG22	44:AP:84:THR:HB	1.97	0.46
1:AR:1018:G:H2'	1:AR:1019:G:O4'	2.15	0.46
1:AR:1340:G:H2'	1:AR:1341:U:H6	1.80	0.46
1:AR:1750:A:H4'	1:AR:1751:G:H5'	1.96	0.46
1:AR:182:U:H2'	1:AR:183:G:C8	2.50	0.46
1:AR:2213:A:N1	1:AR:2429:G:H1'	2.30	0.46
1:AR:651:G:C6	1:AR:652:G:C6	3.02	0.46
7:CG:182:GLY:HA2	7:CG:194:LEU:HD13	1.97	0.46
17:CQ:171:LYS:O	17:CQ:175:THR:HG23	2.15	0.46
1:AR:1809:A:P	29:DB:65:ARG:HH12	2.37	0.46
14:CN:159:VAL:HG13	30:DC:144:VAL:HG13	1.96	0.46
33:DF:29:ALA:N	33:DF:64:VAL:O	2.45	0.46
54:F:59:ARG:NH1	74:Z:87:PRO:HG3	2.30	0.46
56:H:185:GLN:HA	56:H:188:ARG:NH1	2.30	0.46
57:I:44:LYS:NZ	57:I:95:GLU:HG2	2.30	0.46
58:J:26:LYS:O	58:J:29:LEU:HB3	2.15	0.46
60:L:46:LEU:O	60:L:50:THR:HG23	2.15	0.46
66:R:16:ALA:HB2	66:R:72:GLY:HA3	1.96	0.46
66:R:46:PHE:O	66:R:50:GLU:HG3	2.15	0.46
68:T:120:ARG:HD3	68:T:120:ARG:HA	1.80	0.46
74:Z:133:ASN:OD1	74:Z:133:ASN:N	2.48	0.46
1:1:890:C:O2'	1:1:2324:A:N3	2.41	0.46
1:1:2400:G:H5''	1:1:2401:A:OP2	2.16	0.46
1:1:559:A:O2'	69:U:84:LYS:NZ	170.91	0.46
1:1:698:U:H2'	1:1:699:A:O4'	2.14	0.46
25:6:162:A:H2'	25:6:163:G:C8	2.50	0.46
25:6:260:U:H5'	25:6:261:U:H5''	1.97	0.46
84:A:1968:OHX:N5	84:A:2009:OHX:N2	2.63	0.46
25:A:446:A:H2'	25:A:447:U:H6	1.80	0.46
32:AD:9:SER:OG	32:AD:10:ILE:N	2.47	0.46
33:AE:55:LEU:HB2	33:AE:95:PRO:HD3	1.97	0.46
38:AJ:21:THR:OG1	38:AJ:21:THR:O	2.32	0.46
1:AR:1128:U:H2'	1:AR:1129:A:O4'	2.15	0.46
1:AR:114:A:H2'	1:AR:115:A:O4'	2.15	0.46
1:AR:1375:G:O6	30:DC:10:LYS:HE2	2.15	0.46
1:AR:1801:U:H2'	1:AR:1802:C:C6	2.51	0.46
1:AR:1816:A:HO2'	1:AR:1817:G:P	2.39	0.46
1:AR:830:A:O2'	1:AR:1866:C:H2'	2.16	0.46
1:AR:2282:U:O2	1:AR:2310:U:H4'	2.15	0.46
1:AR:2696:A:H2'	1:AR:2697:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CE:86:VAL:HG22	5:CE:162:VAL:HG12	1.98	0.46
6:CF:23:PRO:HD2	6:CF:26:PHE:CE2	2.50	0.46
9:CI:73:GLY:O	22:CV:143:THR:HB	2.15	0.46
10:CJ:61:GLN:HA	10:CJ:64:ILE:HD12	1.97	0.46
1:AR:687:U:OP2	14:CN:36:ARG:NH2	2.47	0.46
14:CN:46:ILE:HG23	14:CN:49:ARG:NH1	2.29	0.46
52:D:157:LYS:HD3	52:D:168:ARG:HH21	1.81	0.46
35:DH:48:ARG:HG3	35:DH:104:PRO:HD3	1.96	0.46
37:DJ:96:GLU:HA	37:DJ:99:GLN:HG2	1.96	0.46
44:DQ:28:TYR:HB3	44:DQ:69:VAL:HB	1.97	0.46
62:N:33:ARG:HA	62:N:36:LEU:HB2	1.97	0.46
69:U:38:LYS:NZ	69:U:43:ASN:O	2.34	0.46
1:1:1214:U:OP2	21:0:137:ARG:NH2	2.37	0.46
1:1:2770:G:O2'	1:1:2771:U:H5'	2.15	0.46
1:1:298:U:OP2	38:AJ:33:ALA:HB2	2.16	0.46
25:6:151:G:H22	25:6:163:G:N2	2.12	0.46
25:6:1691:A:H2'	25:6:1692:G:C8	2.50	0.46
25:6:647:G:N2	25:6:687:G:H1	2.13	0.46
25:6:800:U:H2'	25:6:801:G:C8	2.50	0.46
25:A:103:A:O3'	25:A:308:C:N4	2.49	0.46
38:AJ:58:ILE:HG22	38:AJ:90:MET:HG3	1.97	0.46
1:1:361:A:H5'	39:AK:35:SER:OG	2.16	0.46
1:AR:1108:U:H2'	1:AR:1109:U:C6	2.51	0.46
1:AR:1724:U:O4	20:CT:125:LYS:NZ	2.38	0.46
1:AR:1838:G:H4'	1:AR:1839:A:N3	2.30	0.46
1:AR:1888:U:OP1	5:CE:247:ARG:NH1	2.38	0.46
1:AR:2689:A:H2'	1:AR:2689:A:N3	2.30	0.46
1:AR:436:A:N7	1:AR:621:A:N6	2.64	0.46
1:AR:856:G:OP1	1:AR:1722:U:O2'	2.23	0.46
3:AT:67:U:H2'	3:AT:68:G:H8	1.81	0.46
25:A:1067:C:H5''	51:C:150:VAL:HG23	1.97	0.46
51:C:176:VAL:C	51:C:178:GLY:H	2.19	0.46
4:CD:249:SER:OG	4:CD:251:LYS:NZ	2.27	0.46
12:CL:99:ILE:HG22	12:CL:123:HIS:HB2	1.98	0.46
12:CL:48:LEU:HD22	12:CL:49:CYS:N	2.30	0.46
12:CL:74:LYS:O	12:CL:78:THR:HG23	2.15	0.46
53:E:134:CYS:SG	53:E:135:GLU:N	2.88	0.46
57:I:104:ARG:H	57:I:104:ARG:HG2	1.38	0.46
58:J:41:LYS:HA	58:J:59:ARG:O	2.15	0.46
65:Q:13:LYS:HD2	65:Q:13:LYS:HA	1.64	0.46
74:Z:36:SER:OG	74:Z:37:LYS:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1863:G:N1	1:1:1866:C:OP2	2.47	0.46
1:1:2606:G:H2'	1:1:2606:G:N3	2.30	0.46
1:1:3066:U:H2'	1:1:3067:C:C6	2.50	0.46
1:1:999:G:C6	1:1:1000:C:N4	2.84	0.46
25:6:1125:A:C5	25:6:1126:G:H1'	2.50	0.46
25:6:1511:U:H2'	25:6:1512:G:H8	1.79	0.46
84:6:1915:OHX:N1	84:6:2001:OHX:N3	2.64	0.46
25:6:704:C:H2'	25:6:705:U:O4'	2.15	0.46
25:6:720:G:N2	25:6:720:G:OP2	2.49	0.46
25:A:1244:A:HO2'	25:A:1245:G:P	2.39	0.46
25:A:513:U:OP1	59:K:133:HIS:NE2	2.44	0.46
25:A:778:G:H22	74:Z:10:ARG:NH2	2.14	0.46
30:AB:92:LYS:H	30:AB:92:LYS:HG2	1.45	0.46
1:1:1845:G:O2'	39:AK:5:THR:HG22	2.16	0.46
44:AP:77:CYS:O	44:AP:78:LYS:HD3	2.14	0.46
1:AR:155:G:O2'	38:DK:27:SER:HB3	2.15	0.46
1:AR:2898:G:O6	42:DO:125:LYS:NZ	2.48	0.46
1:AR:3244:A:C2	5:CE:97:ARG:NH1	2.84	0.46
50:B:9:LEU:HD11	50:B:14:ALA:HB2	1.97	0.46
8:CH:52:VAL:HG11	8:CH:65:ILE:HG13	1.98	0.46
12:CL:54:SER:OG	12:CL:130:ASP:O	2.33	0.46
1:AR:1723:A:OP2	20:CT:103:ARG:NH2	2.49	0.46
33:DF:6:ASP:HB3	33:DF:77:ARG:NH2	2.29	0.46
1:AR:634:C:O3'	34:DG:47:ARG:NH1	2.48	0.46
55:G:166:ARG:NH1	55:G:170:GLN:OE1	2.48	0.46
57:I:51:VAL:HG11	57:I:168:SER:HB3	1.97	0.46
58:J:70:GLU:HG3	58:J:112:TRP:CH2	2.50	0.46
25:A:1401:A:OP1	67:S:60:ARG:NH1	2.48	0.46
74:Z:62:THR:HA	74:Z:69:SER:HA	1.97	0.46
1:1:1350:A:H2'	1:1:1351:U:C6	2.51	0.46
1:1:1908:A:H2'	1:1:1909:A:O4'	2.16	0.46
84:1:3473:OHX:N1	84:1:3720:OHX:N1	2.64	0.46
84:1:3473:OHX:N5	84:1:3720:OHX:N2	2.64	0.46
25:6:1381:U:O4	25:6:1382:A:N6	2.49	0.46
25:A:1696:G:N2	25:A:1705:C:H41	2.14	0.46
25:A:1785:U:OP2	64:P:133:ARG:NH2	2.48	0.46
25:A:224:C:H2'	25:A:225:A:C8	2.50	0.46
25:A:301:A:H2'	25:A:302:U:O4'	2.16	0.46
25:A:693:U:H5'	25:A:694:U:H5'	1.98	0.46
33:AE:54:GLU:N	33:AE:54:GLU:OE2	2.45	0.46
34:AF:24:ARG:HD3	34:AF:25:TYR:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:AH:71:THR:HG22	36:AH:77:GLY:HA3	1.97	0.46
1:AR:1764:U:H3'	1:AR:1765:U:C4'	2.46	0.46
1:AR:2163:C:H4'	4:CD:8:GLN:HA	1.98	0.46
50:B:85:ALA:HA	50:B:202:TYR:HD2	1.80	0.46
9:CI:89:ILE:HA	9:CI:89:ILE:HD12	1.76	0.46
12:CL:78:THR:OG1	12:CL:79:VAL:N	2.49	0.46
15:CO:113:THR:HG22	15:CO:116:GLU:OE1	2.15	0.46
20:CT:76:SER:O	20:CT:81:ARG:NH1	2.48	0.46
24:CX:83:LYS:HE2	24:CX:84:SER:N	2.31	0.46
3:AT:25:G:N7	28:DA:13:ARG:NH2	2.63	0.46
54:F:181:VAL:HG21	54:F:195:ILE:HG13	1.98	0.46
55:G:156:ARG:HH11	55:G:156:ARG:HB2	1.80	0.46
25:A:1471:A:OP1	55:G:185:ARG:NH2	2.49	0.46
65:Q:43:ARG:O	65:Q:47:ARG:HG3	2.16	0.46
50:B:32:HIS:HE1	71:W:87:ARG:HH12	1.64	0.46
1:1:1460:A:H2'	1:1:1461:A:C8	2.51	0.46
1:1:2261:G:H21	1:1:2262:A:N6	2.13	0.46
1:1:2689:A:H2'	1:1:2689:A:N3	2.30	0.46
1:1:563:U:OP1	21:O:71:LYS:NZ	2.47	0.46
1:1:663:C:H2'	1:1:664:U:C6	2.50	0.46
1:1:677:A:H4'	1:1:678:G:O5'	2.15	0.46
1:1:839:C:H4'	1:1:1724:U:H2'	1.98	0.46
25:6:329:G:H2'	25:6:330:G:C8	2.50	0.46
1:1:392:G:O2'	28:9:90:VAL:HG11	2.16	0.46
25:A:138:A:OP2	25:A:1706:C:O2'	2.33	0.46
25:A:1517:U:OP2	25:A:1518:C:N4	2.47	0.46
25:A:1573:A:H4'	25:A:1574:G:OP2	2.15	0.46
25:A:698:U:H1'	57:I:107:ARG:HD3	1.97	0.46
1:1:1433:A:N3	34:AF:27:ARG:NH1	2.63	0.46
40:AL:43:PHE:O	40:AL:53:THR:HA	2.15	0.46
1:AR:103:G:OP1	14:CN:70:ARG:NH2	2.41	0.46
1:AR:420:G:N2	1:AR:2385:G:OP2	2.36	0.46
1:AR:3283:U:H2'	1:AR:3284:G:C8	2.51	0.46
1:AR:670:C:OP1	19:CS:147:ARG:NH2	2.36	0.46
3:AT:141:C:H2'	3:AT:142:C:C6	2.51	0.46
5:CE:92:TYR:O	5:CE:155:ALA:HA	2.16	0.46
11:CK:3:TYR:HA	21:CU:142:GLN:OE1	2.15	0.46
18:CR:47:TYR:OH	18:CR:58:ILE:HD13	2.16	0.46
21:CU:5:LYS:HD3	21:CU:63:GLN:NE2	2.30	0.46
1:AR:1746:U:O2'	40:DM:4:GLU:OE1	2.31	0.46
67:S:85:VAL:O	67:S:85:VAL:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:Z:23:PHE:HE1	74:Z:75:VAL:HG12	1.79	0.46
1:1:180:C:H2'	1:1:181:U:H6	1.81	0.46
1:1:26:A:C4	1:1:330:G:C8	3.04	0.46
1:1:370:U:H4'	1:1:404:G:H5'	1.98	0.46
1:1:748:U:H2'	1:1:749:C:C6	2.50	0.46
1:1:1097:G:C8	22:2:128:LEU:HD13	2.50	0.46
2:3:36:C:O2	2:3:45:A:H1'	2.16	0.46
25:6:1371:A:H5'	25:6:1372:U:OP2	2.16	0.46
25:6:1413:U:H4'	25:6:1414:U:OP2	2.15	0.46
25:6:1545:A:H2'	25:6:1546:G:H8	1.80	0.46
27:8:58:ASP:OD1	27:8:61:LYS:N	2.47	0.46
25:A:147:A:H2'	25:A:148:A:O4'	2.16	0.46
25:A:1558:U:OP2	25:A:1559:A:H1'	2.16	0.46
25:A:1688:U:H3	25:A:1713:G:H22	1.63	0.46
25:A:185:U:O2	25:A:201:G:N2	2.49	0.46
25:A:703:G:H2'	25:A:704:C:H5'	1.98	0.46
33:AE:44:MET:HB2	33:AE:46:THR:HG22	1.97	0.46
33:AE:79:ARG:H	33:AE:79:ARG:NE	2.13	0.46
38:AJ:51:SER:HB2	70:V:15:GLN:HB3	192.86	0.46
1:1:817:A:H8	39:AK:15:SER:HG	1.64	0.46
1:AR:2144:A:H1'	1:AR:2281:A:N6	2.31	0.46
1:AR:2271:A:N7	1:AR:2272:G:C6	2.83	0.46
1:AR:2528:G:O3'	10:CJ:248:LYS:NZ	2.48	0.46
11:CK:19:SER:HA	15:CO:6:ILE:O	2.16	0.46
14:CN:46:ILE:O	14:CN:46:ILE:HG22	2.15	0.46
21:CU:101:ALA:O	21:CU:104:GLU:HB3	2.15	0.46
21:CU:24:LEU:O	22:CV:148:PRO:HA	2.16	0.46
27:CZ:46:TYR:HD2	37:DJ:75:TYR:HB3	1.81	0.46
52:D:168:ARG:HD3	52:D:170:ILE:HD11	1.98	0.46
30:DC:46:ASP:O	30:DC:47:LYS:HB3	2.15	0.46
32:DE:24:THR:HG22	32:DE:91:SER:HB3	1.97	0.46
33:DF:26:LYS:HA	33:DF:26:LYS:HD2	1.60	0.46
1:1:116:A:P	38:AJ:36:ARG:HH12	2.38	0.46
1:1:2344:U:H2'	1:1:2345:A:H8	1.81	0.46
1:1:283:G:O6	1:1:304:G:H1'	2.16	0.46
25:6:823:G:H2'	25:6:824:G:O4'	2.15	0.46
25:A:1316:G:OP1	67:S:7:LYS:NZ	2.28	0.46
25:A:278:U:OP1	25:A:279:G:N2	2.49	0.46
29:AA:81:LEU:HD22	29:AA:81:LEU:HA	1.77	0.46
1:AR:2593:A:H4'	1:AR:2594:C:O5'	2.14	0.46
1:AR:3006:A:H2'	1:AR:3007:U:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:1192:C:H5''	84:AR:3591:OHX:N2	2.30	0.46
1:AR:408:A:N6	3:AT:15:G:H1'	2.31	0.46
1:AR:596:C:OP1	9:CI:33:ARG:NH1	2.49	0.46
1:AR:1889:G:OP1	5:CE:247:ARG:HG3	2.16	0.46
7:CG:210:GLU:O	7:CG:214:ASP:HB2	2.16	0.46
13:CM:18:VAL:HG22	13:CM:70:THR:HB	1.98	0.46
13:CM:81:GLU:OE2	13:CM:89:TYR:OH	2.16	0.46
15:CO:24:LYS:HE2	15:CO:61:GLY:O	2.16	0.46
20:CT:105:LEU:HD13	20:CT:138:LEU:HD12	1.97	0.46
30:DC:74:ASN:CG	30:DC:115:LYS:HB2	2.36	0.46
38:DK:4:LYS:HD3	38:DK:14:GLY:HA3	1.97	0.46
55:G:45:LYS:HA	55:G:45:LYS:HE3	1.97	0.46
57:I:46:ILE:HD13	57:I:60:ILE:HA	1.97	0.46
1:1:999:G:O2'	1:1:1000:C:H5'	2.16	0.46
1:1:1584:U:H2'	1:1:1585:C:C6	2.51	0.46
1:1:1699:A:H2'	1:1:1700:G:C8	2.51	0.46
1:1:1481:A:H2'	1:1:1858:A:H1'	1.97	0.46
1:1:2137:U:OP2	1:1:2142:A:N6	2.42	0.46
1:1:669:U:H1'	1:1:1110:U:H4'	1.97	0.46
1:1:7:C:H2'	1:1:8:C:C6	2.51	0.46
1:1:993:G:N3	1:1:2637:A:H2'	2.31	0.46
25:6:709:C:O2	25:6:730:G:N2	2.48	0.46
25:6:939:A:H2'	25:6:940:A:C8	2.50	0.46
25:A:1147:A:H2'	25:A:1148:C:C6	2.51	0.46
25:A:485:A:H2'	25:A:486:G:H8	1.81	0.46
25:A:540:G:H2'	25:A:540:G:OP2	2.16	0.46
25:A:826:U:H2'	25:A:827:C:C6	2.51	0.46
1:AR:1734:G:H2'	1:AR:1735:G:O4'	2.16	0.46
1:AR:595:G:C8	1:AR:609:G:C6	3.04	0.46
1:AR:847:A:H2'	1:AR:848:A:H8	1.81	0.46
51:C:121:ILE:HG12	51:C:161:ILE:HG23	1.97	0.46
5:CE:286:GLY:HA3	5:CE:321:PHE:CZ	2.51	0.46
5:CE:346:THR:HG23	5:CE:351:LEU:HD11	1.96	0.46
12:CL:52:LEU:HD23	12:CL:165:ILE:HG22	1.98	0.46
16:CP:56:LYS:NZ	16:CP:145:ASP:OD2	2.36	0.46
18:CR:94:LEU:CD2	18:CR:146:ILE:HB	2.46	0.46
25:6:852:C:OP1	20:CT:172:ARG:NH1	2.49	0.46
22:CV:128:LEU:H	22:CV:128:LEU:HD12	1.80	0.46
22:CV:57:TYR:CG	22:CV:89:LEU:HD21	2.51	0.46
24:CX:134:GLY:HA2	84:CX:202:OHX:N5	2.31	0.46
28:DA:36:SER:HB2	28:DA:37:LYS:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:DA:39:LEU:HD22	28:DA:43:TYR:HE2	1.79	0.46
34:DG:41:VAL:HG12	34:DG:46:PHE:CD2	2.51	0.46
40:DM:43:PHE:HE2	40:DM:66:ILE:HG12	1.80	0.46
40:DM:72:THR:O	40:DM:72:THR:OG1	2.30	0.46
55:G:48:PHE:CG	55:G:67:PRO:HB3	2.50	0.46
1:1:120:G:N1	64:P:124:ASP:OD1	125.14	0.46
66:R:60:PHE:HA	66:R:63:ILE:HG12	1.97	0.46
74:Z:14:SER:HA	74:Z:21:LYS:HG3	1.98	0.46
54:F:95:THR:HG22	74:Z:16:PRO:HD2	1.97	0.46
21:O:154:HIS:CE1	21:O:170:THR:HG21	2.51	0.46
1:1:1121:U:C4	1:1:1122:U:C4	3.03	0.46
1:1:112:U:O2'	1:1:113:C:OP2	2.25	0.46
1:1:565:U:H2'	1:1:566:G:C8	2.50	0.46
1:1:975:C:H2'	1:1:976:U:C6	2.51	0.46
22:2:7:TYR:CZ	22:2:54:HIS:HB2	2.50	0.46
2:3:3:U:H2'	2:3:4:U:C6	2.51	0.46
25:A:1487:A:H2'	25:A:1488:G:C8	2.51	0.46
25:A:1600:A:HO2'	25:A:1602:C:H41	1.61	0.46
30:AB:71:PRO:HB2	30:AB:109:TYR:HA	1.98	0.46
37:AI:85:THR:HG22	37:AI:87:ALA:H	1.80	0.46
1:AR:1591:G:OP1	36:DI:16:ARG:NH1	2.49	0.46
1:AR:2815:G:N2	1:AR:2818:U:O2	2.42	0.46
2:AS:47:C:H2'	2:AS:48:U:C6	2.50	0.46
50:B:73:VAL:O	50:B:95:ALA:HB1	2.15	0.46
51:C:59:ASP:HA	51:C:62:LYS:NZ	2.31	0.46
51:C:70:LEU:HA	51:C:73:LEU:HB3	1.97	0.46
22:CV:7:TYR:OH	22:CV:54:HIS:HB2	2.15	0.46
29:DB:46:ILE:HD11	29:DB:48:ARG:C	2.35	0.46
30:DC:94:ALA:HB2	30:DC:121:VAL:HG22	1.98	0.46
56:H:178:LEU:O	56:H:180:THR:HG23	2.16	0.46
58:J:114:GLU:HG2	58:J:120:THR:HA	1.98	0.46
67:S:60:ARG:HG3	67:S:66:VAL:HG21	1.98	0.46
68:T:18:LEU:HD21	68:T:70:VAL:HG13	1.97	0.46
1:1:1811:G:H2'	1:1:1812:G:O4'	2.15	0.45
1:1:2534:G:H2'	1:1:2535:A:H8	1.80	0.45
1:1:3275:U:H5'	35:AG:68:TRP:CZ2	2.51	0.45
1:1:2698:G:O2'	22:2:12:ARG:HG2	2.16	0.45
3:4:25:G:N7	28:9:13:ARG:NH2	2.58	0.45
25:6:1650:U:H2'	25:6:1651:A:C8	2.51	0.45
25:A:1087:A:H2'	25:A:1088:A:C8	2.52	0.45
25:A:144:U:O2'	25:A:145:A:H8	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:61:A:H8	25:A:269:G:HO2'	1.63	0.45
25:A:755:A:HO2'	25:A:756:A:P	2.39	0.45
34:AF:94:ALA:O	34:AF:119:VAL:HA	2.16	0.45
40:AL:30:LYS:HB2	40:AL:38:PHE:CE1	2.51	0.45
1:AR:1942:U:OP2	20:CT:74:ARG:NH1	2.49	0.45
1:AR:2503:G:H1'	1:AR:2504:U:H5	1.80	0.45
1:AR:265:A:H5''	1:AR:266:A:OP2	2.16	0.45
5:CE:238:LEU:HB3	5:CE:242:THR:HG21	1.97	0.45
5:CE:347:SER:O	5:CE:348:ARG:HB3	2.16	0.45
1:AR:3049:A:C2	5:CE:75:ALA:HB2	2.51	0.45
6:CF:138:ARG:HH21	6:CF:240:PRO:HB2	1.81	0.45
7:CG:44:TYR:H	7:CG:44:TYR:HD1	1.64	0.45
1:AR:612:U:OP1	8:CH:21:THR:HB	2.16	0.45
10:CJ:41:GLN:HG3	10:CJ:42:PRO:HD2	1.98	0.45
16:CP:16:SER:O	16:CP:20:ARG:HG3	2.16	0.45
27:CZ:105:VAL:HG12	27:CZ:106:ASP:H	1.80	0.45
14:CN:2:ALA:N	30:DC:31:GLY:O	2.49	0.45
33:DF:28:ARG:HB3	33:DF:64:VAL:O	2.16	0.45
45:DR:74:ALA:O	45:DR:78:THR:HG23	2.16	0.45
55:G:64:VAL:HG12	55:G:65:ARG:HD3	1.98	0.45
55:G:71:ALA:HB1	55:G:91:GLU:HA	1.98	0.45
56:H:186:ARG:O	56:H:190:GLN:HG2	2.16	0.45
60:L:69:THR:O	60:L:73:VAL:HG23	2.16	0.45
67:S:96:SER:HA	67:S:97:ASN:HA	1.61	0.45
71:W:41:GLU:H	71:W:41:GLU:CD	2.20	0.45
21:O:166:LYS:HB3	21:O:167:ARG:H	1.44	0.45
21:O:155:ARG:HD3	21:O:172:TYR:CG	2.51	0.45
1:1:1633:C:H2'	1:1:1634:G:H8	1.81	0.45
1:1:2249:G:H5''	1:1:2272:G:O2'	2.16	0.45
1:1:2707:C:H2'	1:1:2708:C:H6	1.80	0.45
1:1:49:A:C2	1:1:279:U:H4'	2.52	0.45
1:1:578:A:H5''	1:1:579:G:O5'	2.17	0.45
25:6:837:G:H2'	25:6:838:G:H8	1.81	0.45
25:A:1186:U:OP2	25:A:1456:C:H1'	2.16	0.45
25:A:1646:C:H2'	25:A:1647:U:C6	2.51	0.45
25:A:289:U:H2'	25:A:290:G:O4'	2.16	0.45
25:A:390:G:H5''	58:J:23:LYS:NZ	2.31	0.45
25:A:69:G:H1	25:A:82:U:H3	1.64	0.45
25:A:947:U:H2'	25:A:948:G:H8	1.80	0.45
36:AH:42:PRO:HB2	36:AH:51:LEU:HD21	1.96	0.45
36:AH:8:ARG:HH21	36:AH:31:ARG:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:AO:22:ALA:C	43:AO:24:SER:H	2.19	0.45
1:AR:2144:A:C4	1:AR:2281:A:C6	3.04	0.45
1:AR:2192:C:O2'	1:AR:2312:A:N1	2.39	0.45
1:AR:2340:U:OP1	5:CE:236:LYS:HE2	2.16	0.45
1:AR:3255:U:H2'	1:AR:3256:G:H8	1.76	0.45
1:AR:517:G:H5'	9:CI:67:ARG:NH2	2.31	0.45
1:AR:92:G:H5''	1:AR:94:G:N7	2.32	0.45
51:C:70:LEU:HD21	51:C:79:HIS:CD2	2.51	0.45
1:AR:3215:A:C5'	15:CO:121:MET:HE1	2.46	0.45
1:AR:1543:G:OP1	16:CP:35:VAL:HG23	2.16	0.45
1:AR:2736:A:O2'	22:CV:68:THR:HG21	2.16	0.45
55:G:89:ILE:HG13	55:G:89:ILE:H	1.51	0.45
55:G:98:MET:HB2	55:G:105:GLY:O	2.16	0.45
56:H:2:LYS:HE3	56:H:2:LYS:HB2	1.72	0.45
57:I:96:ARG:CZ	57:I:124:LYS:HB3	2.46	0.45
62:N:75:VAL:HG21	62:N:120:VAL:HG21	1.98	0.45
63:O:5:HIS:CE1	63:O:121:ARG:HG3	2.51	0.45
65:Q:121:ILE:HG23	65:Q:123:TYR:H	1.80	0.45
65:Q:28:MET:HE3	65:Q:33:PHE:HA	1.98	0.45
1:1:999:G:N3	1:1:1002:A:N6	2.65	0.45
1:1:1033:U:H2'	1:1:1034:U:C6	2.51	0.45
1:1:1480:G:H4'	1:1:1481:A:OP1	2.16	0.45
1:1:1449:A:C2	1:1:2356:A:C4	3.04	0.45
1:1:342:A:N1	1:1:349:A:O2'	2.42	0.45
2:3:60:G:H2'	2:3:61:G:C8	2.51	0.45
25:6:1623:C:H2'	25:6:1624:C:H6	1.81	0.45
25:6:727:U:H2'	25:6:728:U:C6	2.51	0.45
25:6:955:A:H2'	25:6:956:C:O4'	2.17	0.45
25:A:1061:A:H2'	25:A:1062:A:H5'	1.98	0.45
25:A:603:U:H2'	25:A:604:A:H8	1.81	0.45
45:AQ:56:THR:HA	45:AQ:63:THR:HA	1.97	0.45
1:AR:1500:G:H2'	1:AR:1501:U:O4'	2.17	0.45
1:AR:1481:A:O2'	1:AR:1858:A:C2	2.66	0.45
1:AR:654:C:OP1	34:DG:27:ARG:NH2	2.50	0.45
51:C:202:LYS:NZ	51:C:202:LYS:HB2	2.31	0.45
5:CE:261:MET:HE2	17:CQ:63:ALA:C	2.37	0.45
9:CI:116:PHE:HB2	9:CI:199:ASN:OD1	2.15	0.45
11:CK:171:ASP:OD1	11:CK:173:ARG:HB2	2.16	0.45
11:CK:1:MET:SD	21:CU:138:GLN:NE2	2.77	0.45
13:CM:133:ARG:HD2	13:CM:152:HIS:O	2.16	0.45
1:AR:75:G:H5'	14:CN:59:ARG:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:3243:A:C8	17:CQ:156:LEU:HD13	2.51	0.45
19:CS:58:ASN:C	19:CS:60:PRO:HD3	2.37	0.45
22:CV:126:VAL:HG12	22:CV:128:LEU:HG	1.97	0.45
27:CZ:67:ILE:HD12	27:CZ:121:LYS:HG3	1.98	0.45
36:DI:46:ASP:CG	36:DI:88:ARG:HH21	2.20	0.45
54:F:121:TYR:CD2	54:F:161:LYS:HE3	2.50	0.45
1:1:1170:A:OP2	84:1:3493:OHX:N5	2.49	0.45
1:1:1636:U:H5''	29:AA:73:LYS:HZ2	1.81	0.45
1:1:1656:A:H4'	1:1:1657:C:O5'	2.15	0.45
84:1:3473:OHX:N3	84:1:3720:OHX:N4	2.64	0.45
22:2:39:ILE:HG22	22:2:99:SER:HB3	1.98	0.45
25:6:1079:U:H2'	25:6:1080:U:C6	2.50	0.45
25:6:1639:C:H2'	25:6:1640:C:O4'	2.17	0.45
25:6:961:U:H2'	25:6:962:C:C6	2.52	0.45
25:A:1081:A:H2'	25:A:1083:G:N7	2.31	0.45
25:A:1141:G:H2'	25:A:1142:A:C8	2.51	0.45
25:A:1367:G:H2'	25:A:1368:G:H8	1.81	0.45
84:A:1968:OHX:N1	84:A:2009:OHX:N1	2.63	0.45
25:A:30:G:H2'	25:A:31:C:C6	2.52	0.45
25:A:312:A:H4'	25:A:313:U:H5''	1.98	0.45
25:A:538:A:H8	25:A:543:C:N4	2.14	0.45
25:A:603:U:H2'	25:A:604:A:C8	2.51	0.45
25:A:729:G:C5	25:A:730:G:H8	2.35	0.45
25:A:995:A:H2'	25:A:996:U:O4'	2.17	0.45
32:AD:13:LYS:HB3	32:AD:100:ILE:CG2	2.47	0.45
32:AD:73:GLY:O	32:AD:76:GLU:HG2	2.17	0.45
1:1:654:C:OP1	34:AF:27:ARG:NH2	2.49	0.45
1:AR:155:G:H5''	1:AR:156:G:C8	2.52	0.45
1:AR:3132:C:H2'	1:AR:3133:C:H6	1.80	0.45
1:AR:624:G:H2'	1:AR:625:G:C8	2.51	0.45
1:AR:823:C:H5''	4:CD:19:HIS:CD2	2.52	0.45
51:C:70:LEU:HD11	51:C:79:HIS:HB3	1.98	0.45
51:C:70:LEU:HD12	51:C:82:ARG:O	2.16	0.45
9:CI:126:LEU:O	9:CI:130:ILE:HG12	2.16	0.45
9:CI:188:ILE:HA	9:CI:188:ILE:HD13	1.82	0.45
13:CM:33:ALA:HB2	13:CM:123:PHE:CE1	2.51	0.45
16:CP:94:TYR:CZ	16:CP:96:ARG:HB2	2.51	0.45
52:D:67:GLN:HA	52:D:70:ASP:HB2	1.98	0.45
36:DI:74:ARG:HG2	36:DI:75:ALA:H	1.80	0.45
1:AR:2785:A:O2'	44:DQ:41:ARG:NH2	2.50	0.45
54:F:35:PRO:HB3	54:F:143:ASP:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:G:25:LEU:H	55:G:25:LEU:HD22	1.81	0.45
59:K:133:HIS:CD2	59:K:162:SER:HB2	2.52	0.45
69:U:86:ARG:NH1	69:U:90:PRO:O	2.49	0.45
1:1:889:U:H2'	1:1:890:C:O4'	2.17	0.45
25:6:1623:C:H2'	25:6:1624:C:C6	2.52	0.45
25:6:246:G:C6	25:6:247:A:C6	3.05	0.45
25:6:291:G:H2'	25:6:292:U:C6	2.52	0.45
25:6:649:U:H2'	25:6:650:U:C5	2.51	0.45
25:6:696:C:H4'	25:6:697:C:C6	2.51	0.45
25:6:829:A:H1'	25:6:830:U:H5	1.80	0.45
25:6:886:U:H2'	25:6:887:A:H8	1.82	0.45
25:A:654:C:H3'	25:A:655:G:H5''	1.98	0.45
33:AE:98:VAL:HG21	33:AE:104:LEU:HD11	1.99	0.45
38:AJ:93:ILE:O	38:AJ:97:SER:HB3	2.17	0.45
40:AL:31:LEU:HA	40:AL:37:PRO:HA	1.98	0.45
1:AR:1108:U:H2'	1:AR:1109:U:H6	1.81	0.45
1:AR:230:U:H2'	1:AR:231:G:O4'	2.17	0.45
1:AR:1580:A:H5'	1:AR:2522:G:N7	2.31	0.45
1:AR:2794:G:H1'	1:AR:2795:U:C6	2.51	0.45
84:AR:3627:OHX:N6	84:AR:3645:OHX:N2	2.64	0.45
1:AR:716:A:C6	30:DC:117:ARG:HG3	2.52	0.45
1:AR:916:G:H5'	1:AR:917:A:OP1	2.17	0.45
51:C:61:LEU:HG	51:C:64:ARG:NH2	2.28	0.45
5:CE:106:TRP:HB2	5:CE:133:TYR:CE1	2.52	0.45
7:CG:55:PHE:CZ	7:CG:158:ARG:HG3	2.52	0.45
10:CJ:33:ASN:O	10:CJ:39:ALA:HB3	2.17	0.45
13:CM:164:LYS:HE2	13:CM:171:VAL:HB	1.97	0.45
27:CZ:105:VAL:HG13	27:CZ:130:TYR:CD1	2.52	0.45
42:DO:96:CYS:HB2	42:DO:103:LEU:HD11	1.99	0.45
57:I:74:GLN:HG3	57:I:74:GLN:O	2.16	0.45
58:J:46:VAL:HG13	58:J:54:LYS:O	2.16	0.45
73:Y:74:VAL:HG21	73:Y:104:LEU:HD21	1.98	0.45
74:Z:36:SER:O	74:Z:40:LEU:HG	2.17	0.45
1:1:1785:U:H2'	1:1:1786:G:C8	2.51	0.45
1:1:2273:G:N2	1:1:2311:G:H2'	2.32	0.45
1:1:2585:G:N3	1:1:2585:G:H2'	2.31	0.45
25:A:1202:A:H1'	25:A:1207:C:N4	2.31	0.45
25:A:1248:C:H2'	25:A:1249:U:H6	1.82	0.45
25:A:1592:A:H2'	25:A:1593:A:C8	2.52	0.45
25:A:323:A:OP2	58:J:10:LYS:HA	2.17	0.45
25:A:778:G:H22	74:Z:10:ARG:CZ	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AB:74:ASN:HB3	30:AB:115:LYS:HB2	1.97	0.45
30:AB:7:LYS:O	30:AB:10:LYS:N	2.46	0.45
1:AR:1184:A:H2'	1:AR:1185:C:C6	2.52	0.45
1:AR:1802:C:H2'	1:AR:1803:C:C6	2.52	0.45
1:AR:1944:U:H2'	1:AR:1945:A:H8	1.82	0.45
1:AR:2810:C:OP2	1:AR:2955:U:O2'	2.34	0.45
1:AR:685:G:OP2	14:CN:35:ARG:NH1	2.50	0.45
50:B:154:GLU:HA	71:W:63:GLY:HA2	1.98	0.45
5:CE:187:SER:HB3	5:CE:190:GLU:OE1	2.17	0.45
6:CF:98:ARG:HB3	6:CF:98:ARG:CZ	2.46	0.45
13:CM:107:ASP:OD1	13:CM:107:ASP:N	2.49	0.45
19:CS:158:HIS:H	19:CS:186:VAL:CG1	2.29	0.45
36:DI:42:PRO:HB2	36:DI:51:LEU:HD21	1.97	0.45
53:E:46:THR:HB	53:E:84:ILE:HG12	1.98	0.45
57:I:131:PHE:HB3	57:I:132:PRO:HD3	1.98	0.45
65:Q:98:ASN:ND2	65:Q:121:ILE:O	2.50	0.45
74:Z:44:LEU:HA	74:Z:47:VAL:HG22	1.98	0.45
1:1:1340:G:H2'	1:1:1341:U:H6	1.80	0.45
1:1:1750:A:H4'	1:1:1751:G:H5'	1.97	0.45
3:4:9:A:H2'	3:4:10:A:C8	2.51	0.45
25:A:1440:C:H2'	25:A:1441:C:C6	2.52	0.45
25:A:996:U:O2	25:A:1008:G:N2	2.36	0.45
1:1:1389:G:H5''	34:AF:101:SER:HB3	1.97	0.45
36:AH:20:ILE:HA	36:AH:20:ILE:HD13	1.68	0.45
38:AJ:34:SER:O	38:AJ:37:THR:N	2.50	0.45
1:AR:1304:A:N6	1:AR:2860:U:OP1	2.48	0.45
1:AR:1481:A:H2'	1:AR:1858:A:H1'	1.97	0.45
1:AR:1675:G:H2'	1:AR:1676:A:C8	2.52	0.45
1:AR:2938:G:C2	1:AR:2939:G:C8	3.05	0.45
1:AR:638:C:H2'	1:AR:639:G:H8	1.82	0.45
51:C:61:LEU:CD2	51:C:62:LYS:H	2.30	0.45
6:CF:59:GLN:OE1	39:DL:55:ARG:NH2	2.48	0.45
13:CM:60:ARG:O	13:CM:63:GLU:HB2	2.17	0.45
18:CR:22:LEU:HD13	18:CR:90:PHE:HD2	1.81	0.45
54:F:11:ARG:C	54:F:13:ALA:H	2.20	0.45
25:A:1389:C:O2'	67:S:52:GLY:HA3	2.17	0.45
25:A:522:U:OP1	74:Z:37:LYS:HB2	2.17	0.45
1:1:65:A:H3'	1:1:111:C:N4	2.31	0.45
1:1:1636:U:H5''	29:AA:73:LYS:NZ	2.32	0.45
1:1:386:A:C5	1:1:387:A:H1'	2.52	0.45
1:1:709:A:H2'	1:1:710:A:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:29:U:H2'	25:6:30:G:H8	1.81	0.45
25:6:901:G:C6	25:6:902:G:C6	3.04	0.45
26:7:47:ARG:O	26:7:55:PHE:HD2	2.00	0.45
25:A:1368:G:C6	25:A:1369:U:C4	3.05	0.45
29:AA:54:THR:H	29:AA:57:HIS:CD2	2.34	0.45
36:AH:47:CYS:SG	36:AH:48:GLY:N	2.90	0.45
1:AR:112:U:O2'	1:AR:113:C:OP2	2.27	0.45
1:AR:2677:G:H2'	1:AR:2679:A:H2	1.82	0.45
1:AR:2822:U:C2	1:AR:2823:G:C8	3.05	0.45
1:AR:2881:C:H2'	1:AR:2882:U:C6	2.52	0.45
1:AR:2896:A:OP1	42:DO:102:ARG:NE	2.32	0.45
1:AR:336:A:O2'	1:AR:337:G:H5'	2.17	0.45
1:AR:944:C:H4'	34:DG:33:ARG:NH1	2.31	0.45
6:CF:131:VAL:O	6:CF:135:VAL:HG23	2.17	0.45
6:CF:207:VAL:HB	6:CF:227:THR:HG22	1.97	0.45
6:CF:36:HIS:O	6:CF:40:THR:HG23	2.16	0.45
17:CQ:34:VAL:HG11	17:CQ:112:TYR:CE1	2.52	0.45
52:D:95:ARG:HB3	52:D:97:ARG:HD3	1.98	0.45
35:DH:49:ILE:HG12	35:DH:100:ILE:HG13	1.99	0.45
53:E:167:PHE:HA	53:E:190:ARG:HH11	1.81	0.45
57:I:174:ASN:O	57:I:178:GLY:N	2.50	0.45
67:S:99:VAL:CB	67:S:118:PRO:HB2	2.47	0.45
70:V:106:ILE:HD12	70:V:106:ILE:HA	1.86	0.45
70:V:50:LEU:HD23	70:V:94:GLU:O	2.17	0.45
73:Y:50:LYS:HD3	73:Y:101:GLU:HG2	1.97	0.45
1:1:1228:C:H2'	1:1:1229:G:H8	1.82	0.45
1:1:1327:C:O2'	35:AG:76:GLY:HA2	2.16	0.45
1:1:1355:A:H4'	1:1:1356:U:O5'	2.16	0.45
1:1:2107:A:H2	1:1:3344:A:C8	2.34	0.45
1:1:3347:A:OP2	1:1:3347:A:H8	2.00	0.45
1:1:995:U:C2	1:1:2637:A:C8	3.04	0.45
1:1:996:A:H2'	1:1:997:A:O4'	2.17	0.45
25:6:1488:G:H3'	25:6:1515:A:H61	1.81	0.45
25:6:845:G:H2'	25:6:846:G:C8	2.45	0.45
27:8:58:ASP:O	27:8:62:VAL:HG23	2.17	0.45
25:A:811:A:C2	25:A:858:G:H1'	2.52	0.45
35:AG:54:ARG:NH1	35:AG:64:ILE:HD11	2.32	0.45
1:AR:1729:A:H4'	1:AR:1730:G:OP2	2.17	0.45
1:AR:2146:C:H2'	1:AR:2147:A:H8	1.80	0.45
1:AR:2528:G:H1	1:AR:2582:C:H42	1.65	0.45
1:AR:3350:C:HO2'	1:AR:3351:U:P	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:661:G:OP1	30:DC:12:ARG:NH2	2.48	0.45
1:AR:734:C:H2'	1:AR:735:A:O4'	2.16	0.45
50:B:168:HIS:HB3	50:B:203:PHE:CE2	2.52	0.45
7:CG:110:LEU:HA	7:CG:110:LEU:HD12	1.69	0.45
24:CX:127:PRO:O	24:CX:131:SER:N	2.49	0.45
30:DC:91:LEU:HA	30:DC:121:VAL:HG21	1.99	0.45
37:DJ:21:LEU:HD21	37:DJ:51:ILE:HG23	1.98	0.45
39:DL:2:GLY:O	39:DL:6:PRO:HG2	2.17	0.45
56:H:67:VAL:O	56:H:68:LEU:O	2.35	0.45
73:Y:19:ARG:O	73:Y:23:ARG:HG2	2.16	0.45
1:1:1734:G:H2'	1:1:1735:G:O4'	2.17	0.45
1:1:3174:A:H2'	1:1:3175:U:H5'	1.99	0.45
84:1:3506:OHX:N2	84:1:3683:OHX:N6	2.64	0.45
1:1:2736:A:O2'	22:2:68:THR:HG21	2.16	0.45
25:6:1584:G:O2'	25:6:1610:G:O6	2.20	0.45
25:6:486:G:N2	25:6:501:U:H3	2.11	0.45
25:6:886:U:H2'	25:6:887:A:C8	2.52	0.45
25:A:1585:U:N3	25:A:1611:A:C2	2.85	0.45
25:A:495:C:H3'	25:A:496:G:C4'	2.47	0.45
38:AJ:71:LYS:HE2	38:AJ:71:LYS:HB3	1.81	0.45
1:AR:662:U:H2'	1:AR:663:C:C6	2.52	0.45
1:AR:715:A:H2'	1:AR:782:U:O2'	2.16	0.45
2:AS:3:U:H2'	2:AS:4:U:H6	1.81	0.45
3:AT:88:A:H2'	3:AT:89:A:O4'	2.17	0.45
5:CE:56:ILE:HA	5:CE:56:ILE:HD12	1.73	0.45
6:CF:141:ARG:CZ	6:CF:180:LYS:HD3	2.47	0.45
6:CF:361:HIS:O	21:CU:28:ARG:NH2	2.49	0.45
8:CH:19:LYS:O	8:CH:21:THR:N	2.50	0.45
8:CH:97:ASN:CG	8:CH:97:ASN:O	2.55	0.45
11:CK:156:GLN:NE2	11:CK:156:GLN:HA	2.32	0.45
12:CL:156:ARG:HD3	12:CL:163:GLN:O	2.16	0.45
27:CZ:137:ASN:HB3	27:CZ:142:ILE:HD11	1.99	0.45
1:AR:1488:G:O2'	36:DI:10:ARG:O	2.34	0.45
36:DI:94:LEU:HD23	36:DI:94:LEU:HA	1.80	0.45
44:DQ:76:LYS:HD3	44:DQ:76:LYS:HA	1.79	0.45
25:A:790:U:OP1	54:F:187:ARG:NH1	2.50	0.45
64:P:13:VAL:HG13	64:P:77:THR:H	1.82	0.45
1:1:1743:G:H2'	1:1:1744:G:H8	1.82	0.44
1:1:1809:A:H2'	1:1:1810:A:O4'	2.17	0.44
1:1:2610:G:H2'	1:1:2611:U:O4'	2.17	0.44
1:1:2735:U:H2'	1:1:2736:A:C8	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:6:1915:OHX:N5	84:6:2001:OHX:N3	2.65	0.44
25:A:108:A:H2'	25:A:109:G:C8	2.52	0.44
25:A:1346:A:H8	25:A:1370:U:O2	1.99	0.44
29:AA:14:VAL:HG13	36:AH:86:LYS:HG2	1.99	0.44
1:AR:1110:U:H2'	1:AR:1111:U:C6	2.52	0.44
1:AR:1445:U:H5''	1:AR:1446:A:OP2	2.17	0.44
1:AR:1727:G:OP1	45:DR:44:LYS:NZ	2.49	0.44
1:AR:1827:C:H2'	1:AR:1828:A:C8	2.52	0.44
1:AR:2167:A:OP1	16:CP:72:LYS:NZ	2.46	0.44
1:AR:2309:A:N3	1:AR:2961:G:O2'	2.49	0.44
1:AR:2943:G:N7	1:AR:2944:U:C4	2.85	0.44
1:AR:508:U:H2'	1:AR:509:U:C6	2.52	0.44
1:AR:436:A:H61	1:AR:623:U:H3	1.66	0.44
1:AR:824:C:H2'	1:AR:825:U:H6	1.81	0.44
84:AT:203:OHX:N6	84:AT:212:OHX:N4	2.64	0.44
4:CD:137:ILE:HG12	4:CD:147:ARG:HB2	1.98	0.44
13:CM:155:THR:OG1	13:CM:158:ASP:HB2	2.16	0.44
18:CR:119:VAL:HA	18:CR:145:HIS:O	2.18	0.44
24:CX:62:VAL:CG2	24:CX:74:MET:HE1	2.48	0.44
28:DA:3:LYS:HG3	28:DA:8:VAL:HG13	1.99	0.44
43:DP:8:LYS:NZ	43:DP:12:ARG:HH21	2.14	0.44
44:DQ:72:LEU:HD11	44:DQ:83:LEU:HD12	1.98	0.44
54:F:176:ASP:HB2	54:F:179:LYS:NZ	2.31	0.44
54:F:187:ARG:HD3	54:F:187:ARG:O	2.16	0.44
61:M:3:THR:HG21	61:M:82:ARG:HH21	1.81	0.44
62:N:61:VAL:HG13	62:N:121:VAL:HG23	1.98	0.44
1:1:345:G:P	1:1:1429:G:H22	2.39	0.44
1:1:776:U:H5	1:1:2719:U:O2	1.99	0.44
1:1:663:C:H2'	1:1:664:U:H6	1.82	0.44
1:1:716:A:C6	30:AB:117:ARG:HG3	2.52	0.44
1:1:718:G:N2	1:1:721:G:H1'	2.32	0.44
25:6:652:G:N2	25:6:682:C:O2	2.50	0.44
25:A:121:U:H1'	54:F:33:ALA:HB3	1.98	0.44
25:A:1649:G:H2'	25:A:1650:U:C6	2.51	0.44
27:8:60:TYR:OH	37:AI:26:LYS:HG3	2.17	0.44
27:8:114:VAL:HB	41:AM:10:LYS:NZ	2.32	0.44
1:AR:1222:G:H8	1:AR:1222:G:OP2	1.99	0.44
1:AR:644:G:H2'	1:AR:2372:A:N7	2.32	0.44
1:AR:2400:G:H5''	1:AR:2401:A:OP2	2.17	0.44
2:AS:107:C:H2'	2:AS:108:A:H8	1.81	0.44
51:C:143:THR:HB	51:C:205:PHE:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:C:61:LEU:C	51:C:63:GLY:H	2.21	0.44
7:CG:21:ARG:O	7:CG:25:GLU:HG3	2.17	0.44
10:CJ:134:TYR:CG	10:CJ:190:VAL:HG21	2.52	0.44
11:CK:49:ASN:ND2	11:CK:51:GLN:HB2	2.25	0.44
13:CM:59:ILE:HD12	13:CM:65:ILE:HD11	1.98	0.44
17:CQ:119:VAL:HG23	21:CU:164:SER:HB3	1.99	0.44
19:CS:24:VAL:HA	19:CS:27:LYS:HD2	1.99	0.44
22:CV:101:CYS:O	22:CV:104:GLU:HG3	2.18	0.44
23:CW:54:VAL:HG12	23:CW:67:SER:HB2	2.00	0.44
27:CZ:46:TYR:HB3	37:DJ:75:TYR:O	2.18	0.44
28:DA:37:LYS:H	28:DA:37:LYS:CD	2.29	0.44
25:A:799:A:O3'	54:F:201:HIS:NE2	2.49	0.44
63:O:5:HIS:ND1	63:O:121:ARG:HG3	2.32	0.44
53:E:11:LEU:HD12	70:V:86:ILE:HG12	2.00	0.44
61:M:101:GLU:OE2	73:Y:16:ARG:NH2	2.49	0.44
21:O:74:ASN:HD21	21:O:144:LEU:HD21	1.82	0.44
1:1:2221:G:N2	1:1:2224:A:OP2	2.44	0.44
1:1:2861:U:H2'	1:1:2862:U:O4'	2.18	0.44
1:1:2925:C:H2'	1:1:2926:A:O4'	2.18	0.44
1:1:3317:U:H1'	84:1:3559:OHX:N6	2.32	0.44
23:5:54:VAL:HG12	23:5:67:SER:HA	2.00	0.44
23:5:53:ALA:HB1	23:5:68:THR:HG22	1.98	0.44
25:6:1489:U:H5'	25:6:1494:C:H1'	1.99	0.44
25:A:1573:A:H4'	25:A:1574:G:H5'	1.99	0.44
25:A:399:A:H4'	54:F:3:ARG:HG2	1.99	0.44
25:A:848:C:H2'	25:A:849:C:C6	2.52	0.44
33:AE:29:ALA:HB3	33:AE:30:PRO:HD3	1.99	0.44
34:AF:20:HIS:CG	34:AF:42:VAL:HG21	2.52	0.44
35:AG:73:ARG:HG3	35:AG:82:ARG:HD2	1.98	0.44
1:AR:1064:A:N6	1:AR:1096:U:H3	2.15	0.44
1:AR:1362:G:H2'	1:AR:1363:A:C8	2.52	0.44
1:AR:1621:A:H2'	1:AR:1622:U:C6	2.52	0.44
1:AR:3203:U:H2'	1:AR:3204:C:C6	2.52	0.44
1:AR:3242:G:N2	1:AR:3245:A:H5''	2.33	0.44
84:AR:3521:OHX:N5	84:AR:3715:OHX:N1	2.65	0.44
1:AR:551:A:HO2'	1:AR:552:G:H8	1.65	0.44
1:AR:959:C:N4	1:AR:2801:A:C8	2.86	0.44
1:AR:979:U:C2	1:AR:980:A:C4	3.05	0.44
1:AR:22:G:O4'	3:AT:104:A:H1'	2.17	0.44
6:CF:125:ALA:HB1	6:CF:238:LEU:HB3	1.98	0.44
7:CG:224:LYS:HB2	7:CG:224:LYS:HE3	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:CL:53:VAL:O	12:CL:164:LYS:N	2.50	0.44
21:CU:91:TYR:O	21:CU:137:ARG:NH1	2.49	0.44
52:D:185:LYS:O	52:D:189:GLN:HB2	2.17	0.44
35:DH:20:LYS:HZ3	35:DH:20:LYS:HB2	1.82	0.44
40:DM:62:ALA:O	40:DM:66:ILE:HG13	2.16	0.44
54:F:122:LYS:HB2	54:F:122:LYS:HE3	1.83	0.44
54:F:128:LYS:HE2	54:F:128:LYS:HB3	1.84	0.44
57:I:134:GLU:HG2	63:O:21:ASN:HD21	1.82	0.44
66:R:73:GLY:H	66:R:76:SER:HB3	1.82	0.44
68:T:26:ILE:HD11	68:T:31:ALA:HA	2.00	0.44
21:O:132:THR:C	21:O:134:ASP:H	2.19	0.44
21:O:45:LEU:HA	21:O:45:LEU:HD22	1.72	0.44
1:1:1257:C:H42	1:1:1261:G:H22	1.64	0.44
1:1:198:A:C6	1:1:219:A:C6	3.06	0.44
1:1:2281:A:N3	1:1:2974:U:O2'	2.48	0.44
1:1:2358:A:H2'	1:1:2359:C:O4'	2.17	0.44
1:1:372:A:H2'	1:1:373:A:C8	2.53	0.44
22:2:68:THR:OG1	22:2:69:LYS:N	2.50	0.44
23:5:56:VAL:HG22	23:5:65:VAL:HG22	1.98	0.44
25:6:1166:A:H2'	25:6:1167:G:O4'	2.18	0.44
25:6:17:C:H2'	25:6:18:C:C6	2.52	0.44
25:6:841:U:H2'	25:6:842:C:O4'	2.18	0.44
28:9:112:ASP:HB2	28:9:115:ARG:H	1.82	0.44
25:A:1150:G:HO2'	25:A:1151:A:P	2.40	0.44
25:A:1664:C:H42	25:A:1737:G:H1	1.65	0.44
25:A:40:A:H2'	25:A:41:A:O4'	2.17	0.44
25:A:631:G:H2'	25:A:632:U:C6	2.53	0.44
31:AC:17:HIS:HA	31:AC:20:GLY:CA	2.47	0.44
1:AR:1155:C:H2'	1:AR:1156:C:H6	1.83	0.44
1:AR:199:A:C4	1:AR:201:A:C8	3.05	0.44
1:AR:3296:A:H2'	1:AR:3297:U:C6	2.52	0.44
84:AR:3521:OHX:N2	84:AR:3715:OHX:N6	2.64	0.44
2:AS:19:C:H2'	2:AS:20:A:H8	1.81	0.44
51:C:34:ALA:HA	51:C:98:THR:HG22	2.00	0.44
5:CE:117:ARG:CZ	5:CE:175:LYS:HD3	2.47	0.44
19:CS:100:THR:HG23	19:CS:120:GLU:HB3	1.99	0.44
26:CY:4:GLU:HG2	26:CY:30:ARG:CZ	2.47	0.44
39:DL:25:ARG:HE	41:DN:51:ILE:HD12	1.81	0.44
58:J:152:ILE:H	58:J:152:ILE:HD12	1.82	0.44
25:A:767:U:C5	59:K:143:ILE:HD11	2.52	0.44
74:Z:84:LYS:HD2	74:Z:85:PHE:CE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1709:C:H2'	1:1:1710:C:C6	2.51	0.44
1:1:1716:U:O2'	1:1:1717:U:H4'	2.18	0.44
1:1:2225:U:H2'	1:1:2226:U:C6	2.53	0.44
1:1:2927:C:H2'	1:1:2928:C:H6	1.83	0.44
1:1:3121:U:C1'	1:1:3122:A:H5''	2.46	0.44
22:2:12:ARG:HD2	22:2:13:TYR:CE1	2.52	0.44
3:4:126:A:O2'	3:4:128:U:OP1	2.36	0.44
25:6:1209:C:H42	25:6:1454:G:H1	1.64	0.44
25:6:1469:A:H4'	25:6:1541:G:H4'	1.99	0.44
25:6:991:G:OP2	84:6:2025:OHX:N2	2.50	0.44
84:6:1975:OHX:N6	84:6:2025:OHX:N5	2.66	0.44
25:6:705:U:HO2'	25:6:706:A:H8	1.64	0.44
25:A:1039:A:O2'	25:A:1040:G:OP2	2.33	0.44
25:A:1261:G:H2'	25:A:1262:U:C6	2.53	0.44
25:A:1672:G:H2'	25:A:1673:G:C8	2.53	0.44
84:A:1968:OHX:N3	84:A:2009:OHX:N6	2.64	0.44
25:A:263:C:H4'	25:A:292:U:H5'	2.00	0.44
25:A:912:U:H5'	25:A:913:G:H8	1.83	0.44
1:AR:1001:G:O2'	1:AR:1041:U:OP2	2.35	0.44
1:AR:2658:G:C6	1:AR:2659:G:N7	2.86	0.44
14:CN:83:ALA:HA	14:CN:117:LYS:HE3	1.98	0.44
22:CV:27:LEU:HD22	22:CV:27:LEU:HA	1.77	0.44
1:AR:2765:C:O3'	44:DQ:39:GLY:HA3	2.16	0.44
58:J:96:LEU:HD13	58:J:179:CYS:SG	2.58	0.44
61:M:57:LYS:HB2	61:M:110:HIS:CE1	2.52	0.44
1:1:291:C:H5''	70:V:68:ARG:HH12	120.06	0.44
71:W:17:CYS:O	71:W:21:ASN:N	2.50	0.44
1:1:1120:A:H2'	1:1:1121:U:C6	2.53	0.44
1:1:1234:G:H2'	1:1:1235:U:C5	2.53	0.44
1:1:1471:U:H2'	1:1:1472:U:C6	2.53	0.44
84:1:3473:OHX:N4	84:1:3720:OHX:N4	2.66	0.44
1:1:3:U:H2'	1:1:4:U:O4'	2.18	0.44
1:1:438:A:H8	1:1:438:A:OP2	2.00	0.44
1:1:651:G:C6	1:1:652:G:C6	3.05	0.44
1:1:656:A:H2'	1:1:657:A:C8	2.52	0.44
22:2:9:SER:O	22:2:11:THR:HG23	2.17	0.44
28:9:43:TYR:CD1	28:9:126:LEU:HA	2.53	0.44
25:A:1646:C:H2'	25:A:1647:U:H6	1.82	0.44
25:A:25:C:OP2	25:A:26:A:H2'	2.17	0.44
35:AG:13:HIS:ND1	35:AG:93:THR:OG1	2.48	0.44
40:AL:7:ASP:HB3	40:AL:10:GLN:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AQ:7:LYS:HB3	45:AQ:7:LYS:HE2	1.62	0.44
1:AR:1101:G:H1'	9:CI:105:LEU:HD23	2.00	0.44
1:AR:269:G:H5''	16:CP:14:LYS:HE2	2.00	0.44
2:AS:43:U:C4	2:AS:44:C:C4	3.05	0.44
50:B:69:ASN:HB3	50:B:71:GLU:CD	2.38	0.44
5:CE:124:LYS:HE3	5:CE:124:LYS:HB2	1.89	0.44
5:CE:57:VAL:HG11	26:CY:1:MET:HG3	2.00	0.44
6:CF:216:VAL:O	6:CF:220:ARG:N	2.51	0.44
10:CJ:248:LYS:HD2	10:CJ:248:LYS:N	2.33	0.44
15:CO:72:LEU:HD23	15:CO:84:LYS:HG3	2.00	0.44
28:DA:80:VAL:HG12	28:DA:99:LEU:O	2.17	0.44
14:CN:106:GLN:HB3	38:DK:18:THR:OG1	2.18	0.44
1:AR:309:U:OP1	38:DK:84:LYS:HE2	2.17	0.44
39:DL:76:ASN:O	39:DL:79:GLN:HG3	2.18	0.44
54:F:129:VAL:HB	54:F:139:VAL:HG12	2.00	0.44
55:G:102:ARG:HG3	55:G:103:ASN:ND2	2.32	0.44
25:A:143:G:N7	56:H:177:ARG:NH2	2.65	0.44
59:K:81:VAL:O	59:K:150:LEU:HD22	2.17	0.44
25:A:1368:G:H5''	69:U:69:LYS:HG2	2.00	0.44
70:V:108:ILE:H	70:V:108:ILE:HG13	1.57	0.44
1:1:1047:A:C6	1:1:1048:A:C6	3.05	0.44
1:1:1127:G:N2	1:1:1129:A:H3'	2.33	0.44
1:1:1135:A:OP1	31:AC:6:ASN:HB2	2.17	0.44
1:1:795:G:O2'	1:1:796:U:H5'	2.18	0.44
23:5:36:TYR:OH	23:5:82:LYS:HG2	2.18	0.44
25:6:156:A:H2'	25:6:157:A:O4'	2.18	0.44
25:6:168:A:C6	25:6:169:A:N6	2.86	0.44
25:6:1011:G:N7	84:6:1975:OHX:N1	2.66	0.44
1:1:224:C:O2	28:9:103:LYS:NZ	2.51	0.44
25:A:1511:U:H2'	25:A:1512:G:H8	1.82	0.44
1:1:39:A:H5''	30:AB:35:ALA:HB2	2.00	0.44
1:AR:953:G:O2'	1:AR:1116:G:H5'	2.18	0.44
1:AR:1352:A:H4'	1:AR:1353:U:OP1	2.17	0.44
1:AR:1482:A:N7	1:AR:1866:C:O2'	2.41	0.44
1:AR:2746:A:H2'	1:AR:2747:A:O4'	2.18	0.44
1:AR:3390:G:C2	1:AR:3391:A:C8	3.05	0.44
1:AR:794:U:H2'	1:AR:795:G:C8	2.52	0.44
1:AR:824:C:H2'	1:AR:825:U:C6	2.53	0.44
1:AR:900:G:H1'	1:AR:1589:A:H61	1.78	0.44
50:B:52:LYS:HD2	71:W:82:VAL:HG22	2.00	0.44
50:B:74:VAL:HG12	50:B:76:ILE:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:CH:92:SER:HB3	8:CH:148:GLU:HG2	2.00	0.44
18:CR:141:SER:O	18:CR:143:PRO:HD3	2.18	0.44
23:CW:59:ASP:HB3	23:CW:62:VAL:HB	2.00	0.44
27:CZ:96:LYS:O	27:CZ:100:LYS:HB2	2.17	0.44
52:D:245:ASP:N	52:D:245:ASP:OD1	2.51	0.44
37:AI:71:LYS:HD2	28:DA:125:LYS:HB3	2.00	0.44
33:DF:62:ARG:HB2	33:DF:66:GLY:O	2.17	0.44
3:AT:35:C:H5'	39:DL:70:VAL:HG11	2.00	0.44
53:E:167:PHE:O	53:E:190:ARG:HG2	2.16	0.44
55:G:125:THR:O	55:G:126:ASP:O	2.36	0.44
55:G:222:LYS:HE3	55:G:225:ARG:NH1	2.33	0.44
56:H:63:MET:HA	56:H:98:ARG:O	2.18	0.44
59:K:153:GLU:HA	59:K:156:ILE:HD11	2.00	0.44
1:1:1100:U:H2'	1:1:1101:G:O4'	2.18	0.44
1:1:1608:C:H2'	1:1:1609:C:C6	2.53	0.44
1:1:1742:U:H2'	1:1:1743:G:H8	1.82	0.44
1:1:2203:U:H2'	1:1:2204:C:C6	2.53	0.44
1:1:242:C:HO2'	1:1:243:G:H8	1.64	0.44
1:1:856:G:C6	1:1:857:G:N1	2.86	0.44
23:5:33:TYR:CE2	23:5:63:VAL:HG21	2.53	0.44
25:6:1186:U:H2'	25:6:1187:U:O4'	2.17	0.44
25:6:358:U:O2'	25:6:360:A:H5''	2.18	0.44
25:6:591:A:H2'	25:6:592:A:C8	2.53	0.44
28:9:53:ASP:HB2	28:9:110:HIS:ND1	2.33	0.44
25:A:140:A:H61	25:A:281:G:H5''	1.83	0.44
25:A:1486:G:C8	25:A:1487:A:C8	3.06	0.44
25:A:1613:U:H2'	25:A:1614:A:H5''	2.00	0.44
25:A:1789:G:OP2	64:P:132:ARG:NH2	2.23	0.44
25:A:190:C:O2'	25:A:191:C:H5'	2.18	0.44
25:A:386:G:O2'	25:A:387:A:H5'	2.17	0.44
34:AF:104:ASN:O	34:AF:108:ILE:HG13	2.18	0.44
45:AQ:84:ARG:HG2	45:AQ:87:ARG:HH22	1.83	0.44
1:AR:1785:U:H2'	1:AR:1786:G:H8	1.83	0.44
1:AR:1798:A:H2'	1:AR:1799:A:C8	2.52	0.44
1:AR:3067:C:OP2	20:CT:62:ARG:NH1	2.51	0.44
1:AR:3162:C:H2'	1:AR:3163:A:C8	2.53	0.44
1:AR:887:G:H2'	1:AR:888:A:C8	2.53	0.44
4:CD:117:GLU:HG2	4:CD:124:GLY:H	1.82	0.44
1:AR:2947:G:C2	5:CE:250:ALA:HB1	2.53	0.44
10:CJ:67:ILE:O	10:CJ:236:GLY:N	2.51	0.44
2:AS:39:C:N3	13:CM:70:THR:HG23	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CT:15:VAL:HG11	20:CT:52:LYS:HG3	1.99	0.44
1:AR:3275:U:H5'	35:DH:68:TRP:HZ2	1.82	0.44
25:A:400:A:N6	58:J:29:LEU:HD12	2.33	0.44
1:1:1877:U:H5''	1:1:1878:G:O4'	2.18	0.44
1:1:2735:U:H2'	1:1:2736:A:H8	1.82	0.44
84:1:3539:OHX:N6	84:1:3697:OHX:N5	2.65	0.44
1:1:729:C:H2'	1:1:730:C:H6	1.83	0.44
1:1:981:U:HO2'	1:1:982:C:P	2.40	0.44
25:6:1695:G:H21	25:6:1706:C:H41	1.66	0.44
25:6:263:C:H4'	25:6:292:U:H5'	2.00	0.44
25:6:329:G:H2'	25:6:330:G:H8	1.82	0.44
25:6:523:G:O2'	25:6:529:A:N6	2.46	0.44
25:A:1230:A:H2'	25:A:1258:U:C5	2.53	0.44
25:A:783:G:HO2'	25:A:784:C:H6	1.64	0.44
25:A:856:A:C4	57:I:64:VAL:HG21	2.53	0.44
35:AG:59:VAL:HG23	35:AG:60:ARG:H	1.82	0.44
1:AR:1135:A:C2	1:AR:1136:A:C8	3.06	0.44
1:AR:241:G:C6	1:AR:242:C:N4	2.86	0.44
1:AR:2971:A:N3	1:AR:2971:A:H3'	2.32	0.44
1:AR:978:G:O2'	1:AR:979:U:O2	2.36	0.44
3:AT:94:C:H3'	39:DL:72:ARG:HH11	1.83	0.44
50:B:26:ALA:H	50:B:149:LEU:HB2	1.82	0.44
51:C:181:LEU:HD13	51:C:182:ALA:H	1.83	0.44
6:CF:258:LEU:HD12	6:CF:258:LEU:HA	1.85	0.44
6:CF:3:ARG:HH11	6:CF:22:LEU:HB3	1.83	0.44
9:CI:137:GLY:HA3	9:CI:236:ILE:HB	2.00	0.44
14:CN:119:TYR:HD1	14:CN:145:PHE:CE2	2.36	0.44
14:CN:76:THR:HG23	14:CN:79:GLU:OE1	2.17	0.44
1:AR:3214:U:C4	15:CO:121:MET:HG3	2.53	0.44
1:AR:781:G:OP1	19:CS:151:ARG:HD2	2.17	0.44
22:CV:14:MET:CE	22:CV:55:LYS:HB2	2.48	0.44
27:CZ:139:ILE:HD11	27:CZ:141:TYR:CE2	2.48	0.44
29:DB:16:GLY:C	29:DB:18:TYR:H	2.20	0.44
33:DF:7:VAL:HG21	33:DF:79:ARG:HG3	1.99	0.44
35:DH:20:LYS:HG2	35:DH:21:ARG:HG3	1.99	0.44
25:A:1515:A:OP2	53:E:7:LYS:HB2	2.17	0.44
54:F:193:GLY:HA2	54:F:212:ASP:HA	2.00	0.44
60:L:74:GLU:O	60:L:77:ARG:HB3	2.17	0.44
70:V:18:GLN:OE1	70:V:18:GLN:N	2.42	0.44
53:E:40:ARG:NH2	70:V:71:PRO:O	38.32	0.44
1:1:1479:U:O2'	1:1:1484:U:H2'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2344:U:H2'	1:1:2345:A:C8	2.52	0.43
1:1:829:U:H3	1:1:895:A:N6	2.16	0.43
25:6:1042:G:N2	25:6:1077:C:O2	2.51	0.43
25:6:1572:G:H2'	25:6:1572:G:N3	2.32	0.43
25:6:990:C:H2'	25:6:991:G:O4'	2.18	0.43
25:A:1165:G:O6	25:A:1166:A:N6	2.51	0.43
25:A:1603:U:H2'	25:A:1604:U:C6	2.53	0.43
25:A:372:G:H1'	25:A:612:U:O2	2.16	0.43
29:AA:23:VAL:HG12	29:AA:45:GLY:HA3	2.00	0.43
32:AD:54:SER:HB3	36:AH:94:LEU:HD13	1.99	0.43
35:AG:72:THR:HG23	35:AG:83:ALA:HA	2.00	0.43
37:AI:73:LYS:HE2	37:AI:73:LYS:HB3	1.86	0.43
45:AQ:45:LYS:HB2	45:AQ:45:LYS:HE3	1.81	0.43
1:AR:129:U:H2'	1:AR:130:A:C8	2.53	0.43
1:AR:1313:G:O3'	17:CQ:17:GLY:HA3	2.18	0.43
1:AR:1348:U:O2	1:AR:1349:G:N2	2.51	0.43
1:AR:3193:C:H2'	1:AR:3194:C:H6	1.83	0.43
1:AR:3374:U:H2'	1:AR:3378:C:N4	2.33	0.43
1:AR:3379:C:H2'	1:AR:3380:U:H6	1.83	0.43
1:AR:763:G:O2'	1:AR:764:U:OP1	2.32	0.43
50:B:202:TYR:O	50:B:203:PHE:HB2	2.18	0.43
7:CG:259:LYS:HB2	7:CG:259:LYS:HE2	1.74	0.43
7:CG:65:ILE:HG12	7:CG:74:VAL:HG22	2.00	0.43
14:CN:56:PRO:HG3	14:CN:74:GLY:C	2.39	0.43
18:CR:72:GLN:OE1	18:CR:83:TRP:NE1	2.49	0.43
18:CR:69:ARG:HA	18:CR:79:THR:O	2.18	0.43
20:CT:165:LYS:C	20:CT:167:ARG:H	2.21	0.43
17:CQ:116:LYS:HE2	21:CU:165:TYR:HB3	1.99	0.43
52:D:140:ARG:HD3	52:D:222:TYR:CE1	2.53	0.43
52:D:82:ASN:HB2	52:D:207:LEU:HD13	1.99	0.43
30:DC:48:TYR:O	30:DC:49:HIS:CG	2.71	0.43
54:F:246:LEU:HD11	54:F:254:ARG:NH1	2.33	0.43
64:P:85:ALA:H	64:P:119:THR:CG2	2.29	0.43
72:X:17:ALA:HB2	72:X:25:VAL:HG11	2.00	0.43
72:X:77:PRO:O	72:X:79:PHE:N	2.50	0.43
73:Y:35:GLY:O	73:Y:39:LYS:HG2	2.18	0.43
25:A:159:U:H5'	74:Z:117:LYS:HB3	2.01	0.43
1:1:534:U:O2	21:O:146:LYS:HA	2.18	0.43
1:1:1742:U:H2'	1:1:1743:G:C8	2.53	0.43
25:6:139:C:C2	25:6:176:C:C2	3.06	0.43
25:6:1590:G:H2'	25:6:1591:C:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:200:A:H2'	25:6:201:G:C8	2.53	0.43
25:6:939:A:N1	25:6:975:C:H1'	2.33	0.43
25:A:1067:C:H2'	25:A:1068:C:C6	2.52	0.43
25:A:25:C:H4'	25:A:26:A:O5'	2.18	0.43
25:A:737:A:HO2'	25:A:738:G:H8	1.66	0.43
25:A:823:G:O2'	25:A:824:G:O5'	2.35	0.43
38:AJ:4:LYS:HD2	38:AJ:13:LYS:O	2.18	0.43
1:AR:209:A:H4'	1:AR:211:A:C8	2.53	0.43
1:AR:274:G:H2'	1:AR:275:U:O4'	2.18	0.43
1:AR:352:A:N6	1:AR:365:A:H5''	2.32	0.43
6:CF:35:VAL:HG21	6:CF:244:LEU:HD21	2.00	0.43
10:CJ:160:ILE:O	10:CJ:164:VAL:HG13	2.18	0.43
11:CK:90:MET:HB2	11:CK:144:ILE:HG22	1.99	0.43
14:CN:178:LYS:HD3	14:CN:179:PHE:CZ	2.53	0.43
16:CP:36:ILE:HG12	16:CP:64:VAL:HG23	1.99	0.43
16:CP:8:GLU:HG3	16:CP:50:ARG:HH12	1.83	0.43
17:CQ:56:ASP:O	17:CQ:59:ARG:HG2	2.17	0.43
18:CR:4:TYR:CE2	18:CR:16:SER:HB2	2.54	0.43
20:CT:10:LEU:HA	20:CT:10:LEU:HD12	1.87	0.43
22:CV:75:ILE:HA	22:CV:87:LYS:O	2.19	0.43
27:CZ:53:HIS:CE1	27:CZ:56:ARG:HG3	2.52	0.43
52:D:53:ILE:HB	55:G:57:SER:CB	87.73	0.43
1:AR:1433:A:P	34:DG:19:ARG:HH22	2.41	0.43
54:F:191:ARG:C	54:F:192:ILE:HG12	2.38	0.43
61:M:5:LEU:O	61:M:6:THR:OG1	2.28	0.43
67:S:51:ALA:O	67:S:55:THR:OG1	2.30	0.43
68:T:17:LEU:HD12	68:T:18:LEU:HD23	2.00	0.43
25:A:1498:G:OP1	69:U:75:LYS:HD3	2.18	0.43
53:E:40:ARG:HB2	70:V:67:THR:HG21	31.49	0.43
70:V:23:ARG:HD3	70:V:92:ASP:OD1	2.18	0.43
71:W:25:LYS:HG3	71:W:28:ASP:HB2	2.00	0.43
21:O:40:ARG:HD2	21:O:40:ARG:HA	1.86	0.43
1:1:1813:A:OP1	1:1:1817:G:O2'	2.36	0.43
1:1:2180:G:H2'	1:1:2181:C:C6	2.53	0.43
1:1:2373:A:N3	1:1:2824:G:O2'	2.35	0.43
1:1:2986:U:H2'	1:1:2987:A:C8	2.54	0.43
1:1:888:A:H2'	1:1:889:U:O4'	2.18	0.43
25:6:1182:U:H2'	25:6:1184:A:OP2	2.18	0.43
25:6:215:A:H5''	25:6:216:U:OP2	2.18	0.43
25:6:333:A:C6	25:6:334:G:C6	3.07	0.43
25:6:631:G:C6	25:6:632:U:C4	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:675:U:O2'	25:6:676:G:H5'	2.19	0.43
25:A:1211:A:N3	65:Q:97:TYR:OH	2.49	0.43
25:A:1638:G:H2'	25:A:1639:C:O4'	2.19	0.43
31:AC:32:LEU:HB2	31:AC:40:ARG:NH1	2.33	0.43
32:AD:99:ASP:N	32:AD:99:ASP:OD1	2.47	0.43
1:AR:1103:A:N3	1:AR:1103:A:H2'	2.33	0.43
1:AR:1174:G:H1'	1:AR:1181:U:N3	2.34	0.43
1:AR:1340:G:H2'	1:AR:1341:U:C6	2.53	0.43
1:AR:651:G:O2'	1:AR:1435:A:OP1	2.35	0.43
1:AR:2533:G:C2	1:AR:2534:G:H1'	2.53	0.43
1:AR:3279:A:N6	1:AR:3280:U:C4	2.87	0.43
50:B:71:GLU:O	50:B:96:THR:HG22	2.18	0.43
1:AR:3307:A:OP1	5:CE:226:PHE:HB2	2.18	0.43
1:AR:3045:G:O3'	5:CE:275:ARG:NH1	2.52	0.43
17:CQ:173:ALA:O	17:CQ:176:LYS:HB3	2.18	0.43
52:D:157:LYS:HD3	52:D:168:ARG:NH2	2.33	0.43
29:DB:34:LYS:O	29:DB:37:PRO:HG3	2.18	0.43
55:G:90:ILE:O	55:G:94:THR:HG23	2.18	0.43
60:L:77:ARG:HG3	60:L:82:LEU:HD12	2.00	0.43
62:N:32:LEU:O	62:N:36:LEU:N	2.52	0.43
64:P:16:VAL:HG23	64:P:31:THR:HG23	2.00	0.43
68:T:84:TRP:HA	68:T:89:GLN:OE1	2.18	0.43
69:U:26:GLY:O	69:U:28:LEU:HG	2.18	0.43
1:1:241:G:C6	1:1:242:C:C4	3.07	0.43
1:1:2536:A:H2'	1:1:2537:U:C5	2.53	0.43
1:1:2843:U:H5''	1:1:2844:C:OP2	2.17	0.43
2:3:112:G:H2'	2:3:113:C:C6	2.53	0.43
2:3:58:C:H2'	2:3:59:U:H6	1.84	0.43
25:6:1586:A:H2'	25:6:1587:A:O4'	2.18	0.43
25:A:320:U:H3'	25:A:321:C:C5'	2.46	0.43
25:A:992:A:H2	25:A:1012:U:N3	2.09	0.43
29:AA:124:ALA:O	29:AA:126:LYS:N	2.52	0.43
29:AA:36:HIS:HB3	29:AA:38:PHE:CZ	2.54	0.43
37:AI:18:ALA:O	37:AI:22:VAL:HG23	2.19	0.43
45:AQ:21:SER:HA	45:AQ:24:ARG:NH1	2.32	0.43
1:AR:1355:A:H4'	1:AR:1356:U:O5'	2.17	0.43
1:AR:1389:G:N2	1:AR:1390:A:N1	2.67	0.43
1:AR:1567:U:H5	1:AR:1568:U:C2	2.36	0.43
1:AR:1861:G:N7	84:AR:3554:OHX:N1	2.66	0.43
1:AR:1910:A:H2'	1:AR:1911:A:C8	2.53	0.43
1:AR:1936:A:H2'	1:AR:1937:U:O4'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:2339:C:OP2	24:CX:48:ARG:HG2	2.19	0.43
1:AR:3158:G:H22	1:AR:3292:A:H2	1.66	0.43
51:C:48:VAL:HG13	51:C:61:LEU:HD11	2.00	0.43
4:CD:43:GLY:O	4:CD:88:ILE:N	2.38	0.43
5:CE:188:ILE:O	5:CE:192:VAL:HG12	2.19	0.43
5:CE:79:VAL:HG22	5:CE:81:THR:HG23	2.00	0.43
9:CI:139:PRO:HA	9:CI:237:ASN:OD1	2.18	0.43
9:CI:140:SER:O	9:CI:144:ILE:HG13	2.17	0.43
10:CJ:78:PHE:C	10:CJ:80:TYR:H	2.22	0.43
14:CN:190:LYS:HD3	14:CN:190:LYS:HA	1.84	0.43
17:CQ:124:LEU:HA	17:CQ:124:LEU:HD12	1.82	0.43
17:CQ:181:ALA:O	17:CQ:184:THR:HB	2.18	0.43
18:CR:175:ARG:O	18:CR:179:GLN:HB2	2.18	0.43
21:CU:43:TYR:OH	21:CU:47:LYS:HE2	2.18	0.43
52:D:106:ASP:OD1	52:D:108:ASN:N	2.34	0.43
30:DC:96:LYS:C	30:DC:98:THR:H	2.21	0.43
54:F:105:VAL:HG11	54:F:245:LYS:H	1.83	0.43
60:L:60:SER:O	60:L:61:TRP:HB2	2.18	0.43
68:T:136:GLN:HB3	68:T:136:GLN:HE21	1.58	0.43
72:X:86:ILE:HD12	72:X:87:GLU:N	2.33	0.43
1:1:900:G:H1'	1:1:1589:A:H61	1.82	0.43
1:1:3206:C:O2	21:0:155:ARG:NH1	2.52	0.43
3:4:91:C:H2'	3:4:92:A:C8	2.54	0.43
25:6:1397:U:C4	25:6:1399:C:H1'	2.53	0.43
25:6:1773:C:OP2	43:DP:2:ARG:NH1	2.51	0.43
25:6:309:C:H2'	25:6:310:C:H6	1.83	0.43
25:6:696:C:H4'	25:6:697:C:H6	1.84	0.43
25:6:894:U:H2'	25:6:895:G:C8	2.54	0.43
25:A:1100:G:O2'	72:X:76:SER:N	2.51	0.43
29:AA:68:ILE:O	29:AA:115:LYS:HE2	2.18	0.43
1:1:715:A:C8	30:AB:115:LYS:HG2	2.49	0.43
30:AB:116:GLY:HA2	30:AB:137:LYS:CE	2.48	0.43
1:AR:1940:G:H2'	1:AR:1941:C:O4'	2.18	0.43
1:AR:2985:C:H2'	1:AR:2986:U:C6	2.53	0.43
1:AR:71:A:C2	1:AR:313:A:H1'	2.53	0.43
1:AR:1464:G:H4'	84:AR:3413:OHX:N1	2.34	0.43
1:AR:70:A:N1	1:AR:313:A:O2'	2.45	0.43
50:B:172:LEU:O	50:B:176:LEU:HG	2.18	0.43
50:B:24:LEU:O	50:B:163:ASN:ND2	2.51	0.43
1:AR:200:C:OP1	28:DA:60:ARG:NH1	2.51	0.43
1:AR:1076:C:O3'	31:DD:38:LYS:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:DF:31:ARG:O	33:DF:35:GLU:HB2	2.18	0.43
38:DK:26:ILE:C	38:DK:28:TYR:H	2.22	0.43
40:DM:8:ILE:H	40:DM:8:ILE:HD12	1.83	0.43
57:I:74:GLN:NE2	57:I:92:PHE:HB2	2.29	0.43
61:M:64:VAL:HG11	61:M:131:ILE:HD11	2.01	0.43
69:U:135:ILE:H	69:U:135:ILE:HG13	1.61	0.43
1:1:1195:A:H2'	1:1:1309:U:O2	2.18	0.43
1:1:1613:A:OP1	40:AL:2:ALA:N	2.52	0.43
1:1:1727:G:OP1	45:AQ:44:LYS:NZ	2.43	0.43
1:1:3302:U:C2	1:1:3313:U:C2	3.07	0.43
1:1:613:G:C6	1:1:614:C:C4	3.07	0.43
25:6:489:C:O2'	25:6:490:C:O5'	2.33	0.43
25:6:595:G:H2'	25:6:596:C:C6	2.53	0.43
25:A:97:C:H2'	25:A:98:U:C6	2.54	0.43
44:AP:14:GLY:C	44:AP:16:THR:H	2.21	0.43
44:AP:77:CYS:SG	44:AP:79:THR:OG1	2.72	0.43
1:AR:54:C:O2'	1:AR:1547:G:H1'	2.18	0.43
1:AR:1688:U:H2'	1:AR:1689:U:C6	2.53	0.43
1:AR:1765:U:H5''	20:CT:43:LYS:HD3	2.00	0.43
1:AR:3346:U:H3	1:AR:3359:A:H61	1.67	0.43
5:CE:173:GLN:O	5:CE:174:LYS:HB2	2.18	0.43
8:CH:56:LYS:HE3	8:CH:98:VAL:HG12	2.01	0.43
14:CN:122:LYS:HB3	14:CN:122:LYS:HE3	1.71	0.43
1:AR:398:A:C5	18:CR:3:ARG:NH2	2.87	0.43
1:AR:1722:U:H5''	20:CT:99:LEU:HD12	2.00	0.43
21:CU:73:LYS:NZ	21:CU:97:VAL:O	2.32	0.43
1:AR:3056:U:O2	33:DF:28:ARG:NH1	2.51	0.43
34:DG:55:ILE:HD12	34:DG:55:ILE:HA	1.81	0.43
53:E:175:VAL:HG13	53:E:182:LEU:HB2	2.00	0.43
62:N:84:ASN:O	62:N:85:LYS:HB3	2.18	0.43
25:A:859:A:C6	63:O:73:ARG:HD3	2.54	0.43
68:T:136:GLN:H	68:T:136:GLN:HG2	1.56	0.43
69:U:52:GLY:HA2	69:U:55:TYR:HD1	1.82	0.43
53:E:7:LYS:HE3	70:V:27:THR:HG21	2.01	0.43
70:V:46:GLU:HB2	70:V:52:LYS:NZ	2.34	0.43
21:0:13:ARG:O	21:0:22:PRO:HG2	2.19	0.43
1:1:523:A:O2'	21:0:69:PRO:HD2	2.19	0.43
1:1:1222:G:H1'	1:1:1286:A:N6	2.34	0.43
1:1:1477:A:OP1	1:1:3075:G:O2'	2.30	0.43
1:1:167:U:H2'	1:1:168:U:H6	1.82	0.43
1:1:3259:U:H6	1:1:3259:U:H5'	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:5:59:ASP:O	23:5:61:THR:N	2.48	0.43
25:6:17:C:O2'	25:6:1137:A:N1	2.45	0.43
25:6:1263:G:H2'	25:6:1264:G:O4'	2.18	0.43
25:6:130:C:O2'	25:6:137:U:N3	2.50	0.43
25:6:307:G:H2'	25:6:308:C:H5''	2.01	0.43
27:8:142:ILE:HD13	27:8:142:ILE:HA	1.75	0.43
27:8:34:LEU:HD22	27:8:35:PRO:HD2	2.00	0.43
25:A:1182:U:O2	25:A:1184:A:H8	2.02	0.43
25:A:1521:G:O2'	25:A:1523:G:OP2	2.23	0.43
25:A:1642:G:H2'	25:A:1643:U:H6	1.84	0.43
25:A:487:G:H3'	25:A:488:G:H5''	2.00	0.43
25:A:702:G:O6	25:A:737:A:N6	2.51	0.43
36:AH:20:ILE:HD11	36:AH:34:HIS:CE1	2.54	0.43
37:AI:49:LYS:HA	37:AI:49:LYS:HD3	1.84	0.43
1:1:155:G:H1'	38:AJ:26:ILE:HD13	2.00	0.43
1:AR:1349:G:H5'	6:CF:291:ASN:HD21	1.84	0.43
1:AR:1766:G:C8	20:CT:46:LYS:NZ	2.84	0.43
1:AR:2356:A:H5'	18:CR:138:LYS:HZ1	1.83	0.43
1:AR:3057:U:H5'	1:AR:3086:A:H61	1.82	0.43
1:AR:659:G:H2'	1:AR:1432:C:H42	1.83	0.43
4:CD:62:VAL:HA	4:CD:73:GLU:HA	2.00	0.43
1:AR:3314:A:OP1	5:CE:173:GLN:O	2.36	0.43
1:AR:2939:G:C8	5:CE:2:SER:O	2.72	0.43
8:CH:148:GLU:OE1	8:CH:151:LYS:HE2	2.19	0.43
15:CO:108:ARG:NH1	15:CO:112:LEU:HD23	2.34	0.43
19:CS:23:ASN:HB3	19:CS:26:LEU:HB2	2.00	0.43
30:DC:14:HIS:ND1	30:DC:14:HIS:N	2.66	0.43
1:AR:1369:A:H4'	30:DC:21:ARG:HG3	2.01	0.43
44:DQ:11:TYR:HE2	44:DQ:13:LYS:HB3	1.83	0.43
54:F:181:VAL:O	54:F:192:ILE:HA	2.18	0.43
55:G:51:VAL:HG21	55:G:130:ILE:HG23	2.00	0.43
55:G:214:LYS:HD3	55:G:215:ASP:OD1	2.18	0.43
59:K:133:HIS:HD2	59:K:162:SER:HB2	1.83	0.43
60:L:3:MET:SD	60:L:8:ARG:NH1	2.91	0.43
63:O:46:THR:O	63:O:50:ILE:HG13	2.18	0.43
64:P:20:TYR:CE1	64:P:22:SER:HB3	2.53	0.43
66:R:32:ASN:ND2	66:R:69:VAL:H	2.14	0.43
67:S:24:LEU:HG	67:S:34:LEU:HD13	1.99	0.43
71:W:71:ARG:HB2	71:W:83:TRP:CE2	2.54	0.43
1:1:1495:U:H5	1:1:1835:A:N1	2.16	0.43
1:1:1870:C:H4'	1:1:3076:C:O2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1925:U:H1'	45:AQ:20:SER:HB3	2.00	0.43
3:4:78:G:H2'	3:4:79:A:C8	2.54	0.43
25:6:542:A:H1'	25:6:543:C:P	2.58	0.43
25:6:895:G:H2'	25:6:896:U:C6	2.53	0.43
25:A:142:G:N1	25:A:173:A:H2	2.17	0.43
25:A:784:C:H2'	25:A:785:U:O4'	2.19	0.43
25:A:870:C:H2'	25:A:871:G:C8	2.54	0.43
34:AF:126:LEU:HD23	34:AF:126:LEU:HA	1.86	0.43
1:AR:1447:G:H3'	18:CR:67:ILE:CD1	2.48	0.43
1:AR:2586:G:C5	10:CJ:241:LYS:HB2	2.54	0.43
84:AR:3511:OHX:N3	84:AR:3698:OHX:N5	2.66	0.43
1:AR:435:C:N4	1:AR:621:A:N7	2.67	0.43
2:AS:38:U:HO2'	2:AS:40:C:H5	1.65	0.43
3:AT:27:U:H2'	3:AT:28:C:H6	1.84	0.43
50:B:169:SER:O	50:B:173:ILE:HG12	2.18	0.43
5:CE:173:GLN:HG3	5:CE:175:LYS:H	1.83	0.43
6:CF:138:ARG:NH2	6:CF:240:PRO:HB2	2.34	0.43
19:CS:22:ASP:HA	19:CS:27:LYS:HE3	2.00	0.43
23:CW:49:ASN:O	23:CW:49:ASN:ND2	2.46	0.43
32:DE:74:ASN:OD1	32:DE:74:ASN:N	2.52	0.43
53:E:116:ARG:O	53:E:120:TYR:HB2	2.19	0.43
56:H:52:ILE:HD13	56:H:102:VAL:HG21	2.01	0.43
1:1:2926:A:C2'	1:1:2927:C:H5'	2.48	0.43
2:3:73:C:H5''	2:3:74:C:OP1	2.19	0.43
25:6:1244:A:H3'	25:6:1244:A:N3	2.34	0.43
25:6:138:A:H5''	25:6:138:A:N3	2.34	0.43
25:6:1451:C:H2'	25:6:1452:U:C6	2.54	0.43
25:6:1473:U:O2	25:6:1473:U:H2'	2.19	0.43
25:6:1686:C:N3	25:6:1716:C:N4	2.67	0.43
25:6:1726:G:N7	84:6:2001:OHX:N2	2.67	0.43
28:9:51:ARG:HG2	28:9:115:ARG:NH2	2.33	0.43
28:9:5:SER:OG	28:9:6:LEU:N	2.51	0.43
25:A:1551:U:H3'	65:Q:43:ARG:HH21	1.84	0.43
25:A:320:U:H2'	25:A:321:C:C6	2.54	0.43
25:A:432:G:H2'	25:A:433:C:O4'	2.19	0.43
25:A:823:G:H2'	25:A:824:G:H8	1.82	0.43
25:A:973:A:H2'	25:A:974:A:C8	2.52	0.43
34:AF:32:TRP:CG	34:AF:33:ARG:N	2.87	0.43
1:AR:1003:A:H1'	7:CG:15:ARG:NH1	2.34	0.43
1:1:246:U:OP1	1:AR:176:G:O2'	2.36	0.43
1:AR:2303:A:P	43:DP:23:ARG:HH22	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:2232:A:O2'	1:AR:2429:G:H5'	2.19	0.43
1:AR:2516:U:O2	1:AR:2594:C:N4	2.52	0.43
1:AR:2533:G:H2'	1:AR:2534:G:O4'	2.19	0.43
1:AR:2799:A:H5''	1:AR:2800:G:O5'	2.18	0.43
1:AR:3344:A:H2	1:AR:3361:G:H21	1.64	0.43
1:AR:618:C:O2'	1:AR:620:U:H1'	2.18	0.43
1:AR:982:C:H42	1:AR:1101:G:H1	1.66	0.43
84:AT:203:OHX:N3	84:AT:212:OHX:N3	2.66	0.43
7:CG:25:GLU:O	7:CG:27:LYS:HG3	2.19	0.43
9:CI:151:ARG:HD2	9:CI:244:ASN:OD1	2.18	0.43
9:CI:163:LEU:O	9:CI:168:ILE:HD12	2.19	0.43
11:CK:168:ARG:HE	11:CK:168:ARG:HB3	1.70	0.43
15:CO:14:LEU:H	15:CO:19:ARG:NH1	2.17	0.43
9:CI:110:ARG:CZ	19:CS:3:ILE:HD11	2.48	0.43
20:CT:106:LEU:HB3	20:CT:120:TYR:HE1	1.84	0.43
20:CT:176:ARG:HD3	20:CT:176:ARG:HA	1.81	0.43
24:CX:23:MET:SD	24:CX:78:VAL:HG22	2.59	0.43
29:DB:81:LEU:HA	29:DB:81:LEU:HD22	1.72	0.43
31:DD:22:LYS:HE3	31:DD:22:LYS:HB3	1.81	0.43
35:DH:57:LYS:HE3	35:DH:57:LYS:HB3	1.73	0.43
56:H:67:VAL:HG23	56:H:99:GLY:HA2	2.00	0.43
66:R:18:ALA:HB2	66:R:69:VAL:HG13	2.01	0.43
74:Z:60:PHE:H	74:Z:71:GLY:HA2	1.82	0.43
1:1:1569:U:H5'	1:1:1570:U:H5''	2.01	0.43
1:1:1497:C:O2'	1:1:1602:A:N3	2.42	0.43
1:1:1719:G:H2'	1:1:1720:U:O4'	2.19	0.43
1:1:2437:G:N2	1:1:2511:A:H1'	2.33	0.43
1:1:3033:A:H2'	1:1:3034:C:C6	2.54	0.43
1:1:3087:A:OP1	84:1:3704:OHX:N2	2.52	0.43
23:5:99:LYS:HB2	23:5:102:GLU:HB2	1.99	0.43
25:6:1208:A:H5''	25:6:1209:C:OP2	2.19	0.43
25:6:1561:U:H4'	25:6:1599:C:H4'	2.01	0.43
25:6:23:G:O2'	25:6:368:U:OP1	2.36	0.43
25:6:694:U:H3'	25:6:695:U:O2	2.19	0.43
25:A:1151:A:H2'	25:A:1152:A:C8	2.54	0.43
25:A:1178:G:H2'	25:A:1179:G:O4'	2.19	0.43
25:A:1207:C:H42	25:A:1456:C:H5	1.67	0.43
25:A:142:G:N2	25:A:173:A:H2	2.15	0.43
25:A:693:U:C5'	25:A:694:U:H5'	2.49	0.43
1:1:2552:C:C5	32:AD:53:LYS:HE3	2.54	0.43
1:1:2895:G:O2'	42:AN:100:TYR:O	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AQ:14:TYR:HA	45:AQ:17:ARG:HH12	1.84	0.43
45:AQ:38:ASP:HA	45:AQ:45:LYS:HA	2.01	0.43
1:AR:1014:U:H2'	1:AR:1015:U:O4'	2.19	0.43
1:AR:206:G:H1	1:AR:223:U:H3	1.67	0.43
1:AR:2103:U:H2'	1:AR:2104:A:H8	1.83	0.43
1:AR:2732:G:H2'	1:AR:2733:A:O4'	2.19	0.43
1:AR:3047:U:O2'	5:CE:53:MET:HE1	2.19	0.43
1:AR:3152:U:OP2	1:AR:3395:G:N1	2.30	0.43
1:AR:3266:G:C6	1:AR:3267:A:C6	3.07	0.43
84:AR:3501:OHX:N4	84:AR:3590:OHX:N2	2.67	0.43
1:AR:819:U:OP1	39:DL:10:LYS:NZ	2.45	0.43
1:AR:2178:A:H5''	4:CD:129:ALA:HB3	2.00	0.43
7:CG:155:THR:HA	7:CG:179:ARG:HA	2.00	0.43
7:CG:281:GLU:O	7:CG:285:ARG:HG3	2.19	0.43
10:CJ:196:ALA:O	10:CJ:197:VAL:HG13	2.18	0.43
10:CJ:60:ARG:O	10:CJ:64:ILE:HG13	2.19	0.43
13:CM:34:SER:HA	13:CM:67:VAL:HG21	2.00	0.43
14:CN:47:ALA:CB	14:CN:48:PRO:HD2	2.49	0.43
15:CO:38:ILE:HD12	21:CU:150:PHE:HE1	1.84	0.43
17:CQ:128:ARG:HA	17:CQ:128:ARG:HD2	1.36	0.43
17:CQ:42:ASN:HA	17:CQ:136:THR:O	2.18	0.43
17:CQ:54:TYR:CD1	17:CQ:58:LEU:HD22	2.53	0.43
35:DH:89:LEU:HA	35:DH:90:PRO:HD3	1.86	0.43
53:E:182:LEU:HD12	53:E:182:LEU:H	1.84	0.43
54:F:199:GLU:OE1	54:F:201:HIS:HE1	2.01	0.43
25:A:1406:A:OP2	55:G:80:LYS:HE2	2.18	0.43
58:J:39:GLY:CA	58:J:61:GLU:HB3	2.46	0.43
59:K:138:LYS:NZ	59:K:138:LYS:HB2	2.33	0.43
59:K:17:ARG:O	59:K:23:ARG:NH2	2.51	0.43
67:S:71:PHE:HD1	67:S:73:LEU:HB3	1.81	0.43
73:Y:126:LYS:HG2	73:Y:131:SER:HA	2.00	0.43
74:Z:12:VAL:HG13	74:Z:23:PHE:HB3	2.01	0.43
1:1:1659:U:H2'	1:1:1660:C:C6	2.53	0.42
1:1:2341:A:O3'	1:1:3090:U:H4'	2.19	0.42
1:1:2413:A:H2'	1:1:2414:G:C8	2.54	0.42
1:1:2945:G:O2'	1:1:2948:C:OP2	2.28	0.42
1:1:543:C:N4	1:1:548:G:H1	2.16	0.42
1:1:54:C:O2'	1:1:1547:G:H1'	2.19	0.42
25:6:1771:U:H2'	25:6:1772:C:C6	2.54	0.42
25:6:21:U:H2'	25:6:22:A:H8	1.83	0.42
25:6:282:C:H2'	25:6:283:U:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:218:A:H61	25:6:829:A:H2	1.66	0.42
28:9:39:LEU:HD22	28:9:43:TYR:CE2	2.54	0.42
25:A:1535:U:O2'	25:A:1536:G:H5''	2.19	0.42
25:A:1586:A:H2'	25:A:1587:A:O4'	2.19	0.42
25:A:180:A:H2'	25:A:181:A:O4'	2.19	0.42
25:A:625:C:H2'	25:A:626:U:C6	2.54	0.42
1:AR:1349:G:N3	1:AR:1349:G:H3'	2.33	0.42
1:AR:1886:A:O4'	1:AR:3307:A:H5'	2.18	0.42
1:AR:2537:U:H3	1:AR:2542:U:H3	1.67	0.42
1:AR:2996:U:O2	1:AR:2996:U:H2'	2.18	0.42
1:AR:3057:U:O2'	1:AR:3059:G:OP1	2.36	0.42
1:AR:3133:C:H2'	1:AR:3134:A:O4'	2.18	0.42
1:AR:2993:G:H2'	1:AR:3142:A:H61	1.84	0.42
1:AR:3181:C:H2'	1:AR:3182:G:C8	2.54	0.42
1:AR:3166:C:H42	1:AR:3284:G:H1	1.66	0.42
1:AR:423:A:C6	1:AR:424:G:C6	3.07	0.42
1:AR:90:C:C2'	1:AR:91:G:H5'	2.49	0.42
50:B:81:PHE:HA	50:B:204:TYR:CB	2.49	0.42
4:CD:227:ARG:HG2	4:CD:239:ALA:HB2	2.00	0.42
1:AR:2880:U:O2	5:CE:250:ALA:HB3	2.19	0.42
10:CJ:109:LEU:HA	10:CJ:109:LEU:HD23	1.89	0.42
14:CN:47:ALA:HB1	14:CN:48:PRO:CD	2.48	0.42
15:CO:115:PHE:O	15:CO:119:GLN:HG3	2.17	0.42
16:CP:138:GLN:HA	16:CP:143:ARG:HH11	1.83	0.42
10:CJ:140:VAL:HG21	16:CP:3:ALA:HB2	2.00	0.42
21:CU:1:MET:HE1	21:CU:31:ALA:CA	2.45	0.42
21:CU:26:ARG:O	22:CV:150:THR:HA	2.19	0.42
1:AR:1682:U:O4	23:CW:90:ARG:NH1	2.52	0.42
24:CX:102:ILE:HG13	24:CX:110:LYS:HB2	2.01	0.42
24:CX:19:VAL:HG13	24:CX:37:ILE:HA	2.01	0.42
24:CX:17:LEU:HD21	24:CX:98:ASN:CG	2.40	0.42
28:DA:87:LYS:HB2	28:DA:97:ILE:HD11	2.01	0.42
30:DC:79:TRP:CE3	30:DC:82:ILE:HD12	2.53	0.42
1:AR:1431:G:N7	30:DC:9:ARG:NH2	2.67	0.42
36:DI:58:ARG:HH11	36:DI:58:ARG:HG3	1.83	0.42
43:DP:23:ARG:HB3	43:DP:23:ARG:NH2	2.34	0.42
54:F:148:ARG:HG2	54:F:148:ARG:H	1.64	0.42
66:R:59:LYS:HB2	66:R:59:LYS:HE2	1.73	0.42
70:V:27:THR:HG23	70:V:113:ASP:HB3	2.02	0.42
72:X:104:LEU:HB2	72:X:124:LYS:O	2.19	0.42
1:1:1093:A:OP1	1:1:1093:A:H4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1350:A:H2'	1:1:1351:U:H6	1.83	0.42
1:1:2544:U:H2'	1:1:2545:C:C6	2.55	0.42
1:1:2986:U:H2'	1:1:2987:A:H8	1.84	0.42
1:1:839:C:H2'	1:1:840:C:C6	2.53	0.42
1:1:956:U:H2'	1:1:957:C:C6	2.55	0.42
25:6:570:A:H5''	25:6:571:G:OP2	2.18	0.42
25:6:647:G:H8	25:6:647:G:O5'	2.01	0.42
25:A:976:G:C6	25:A:1023:A:C4	3.07	0.42
25:A:1244:A:N3	25:A:1244:A:H3'	2.34	0.42
25:A:1767:G:OP2	25:A:1770:U:O2'	2.28	0.42
25:A:278:U:H4'	25:A:279:G:O5'	2.19	0.42
25:A:702:G:N2	25:A:703:G:H1'	2.34	0.42
30:AB:48:TYR:O	30:AB:49:HIS:CG	2.72	0.42
30:AB:6:THR:HG23	30:AB:8:THR:HG23	2.01	0.42
35:AG:35:VAL:HG13	35:AG:40:ASP:HB3	2.01	0.42
35:AG:89:LEU:HD23	35:AG:89:LEU:HA	1.84	0.42
38:AJ:60:LEU:HD13	38:AJ:60:LEU:HA	1.78	0.42
1:AR:1657:C:O2'	1:AR:1797:A:OP2	2.25	0.42
1:AR:1932:A:H5'	1:AR:1933:A:OP2	2.20	0.42
1:AR:2761:G:H1'	1:AR:2800:G:H21	1.84	0.42
1:AR:3275:U:OP1	1:AR:3276:G:N2	2.52	0.42
1:AR:2273:G:O6	84:AR:3696:OHX:N5	2.52	0.42
1:AR:499:G:H2'	1:AR:500:C:C6	2.54	0.42
1:AR:897:U:H2'	1:AR:898:U:H6	1.84	0.42
50:B:87:LEU:HA	50:B:87:LEU:HD12	1.83	0.42
6:CF:23:PRO:O	6:CF:25:VAL:N	2.50	0.42
23:CW:27:VAL:HG21	23:CW:107:PHE:HE1	1.83	0.42
52:D:118:ALA:HB3	52:D:124:ALA:HB2	1.99	0.42
35:DH:80:VAL:HG12	35:DH:81:VAL:N	2.33	0.42
1:AR:1591:G:H5''	36:DI:16:ARG:HH12	1.83	0.42
37:DJ:6:ALA:O	37:DJ:10:ARG:HG3	2.19	0.42
53:E:101:GLN:HG3	53:E:126:VAL:CG2	2.49	0.42
55:G:205:SER:C	55:G:207:THR:H	2.22	0.42
69:U:52:GLY:O	69:U:54:PHE:N	2.52	0.42
59:K:61:THR:HA	72:X:97:ARG:HH12	1.84	0.42
1:1:1116:G:H4'	1:1:1116:G:OP2	2.17	0.42
1:1:1932:A:H5'	1:1:1933:A:OP2	2.19	0.42
1:1:2635:A:H2	22:2:10:ARG:NH2	2.18	0.42
1:1:729:C:H2'	1:1:730:C:C6	2.54	0.42
2:3:119:U:H2'	2:3:120:C:C6	2.54	0.42
25:6:140:A:H4'	25:6:140:A:OP2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:1595:U:H5	25:6:1596:C:C5	2.36	0.42
25:6:540:G:O2'	25:6:542:A:H5'	2.18	0.42
25:6:813:U:O2	25:6:813:U:H2'	2.20	0.42
25:A:1461:C:H2'	25:A:1462:G:H8	1.84	0.42
25:A:1475:A:H2'	25:A:1476:C:O4'	2.19	0.42
25:A:87:C:O2'	25:A:169:A:N1	2.44	0.42
25:A:476:U:H5''	25:A:477:A:O4'	2.19	0.42
35:AG:49:ILE:HG13	35:AG:70:LYS:HA	2.02	0.42
1:1:1486:G:H21	36:AH:6:THR:HG22	1.83	0.42
1:1:817:A:C4	39:AK:13:ASN:O	2.72	0.42
1:AR:1214:U:H2'	1:AR:1215:U:C6	2.55	0.42
1:AR:1420:C:OP2	6:CF:193:LYS:NZ	2.52	0.42
1:AR:1493:G:N2	1:AR:1493:G:OP2	2.44	0.42
1:AR:290:G:H1'	16:CP:93:LYS:HD2	2.02	0.42
1:AR:592:A:H5'	8:CH:17:ALA:O	2.20	0.42
1:AR:620:U:O2'	1:AR:622:A:OP1	2.34	0.42
1:AR:897:U:H2'	1:AR:898:U:C6	2.53	0.42
2:AS:2:G:O2'	2:AS:23:A:N1	2.39	0.42
50:B:74:VAL:HG23	50:B:118:PRO:HB3	2.02	0.42
5:CE:66:LYS:HE2	24:CX:124:ASP:OD2	2.19	0.42
6:CF:120:TYR:CE2	6:CF:277:PRO:HB3	2.55	0.42
1:AR:658:G:N2	6:CF:93:MET:HB2	2.33	0.42
7:CG:3:PHE:O	7:CG:6:ASP:HB2	2.20	0.42
8:CH:11:PRO:HD2	34:DG:91:THR:HG21	2.01	0.42
2:AS:64:A:C6	12:CL:202:LYS:HA	2.53	0.42
14:CN:168:ARG:O	14:CN:172:LEU:HG	2.19	0.42
22:CV:105:PHE:O	22:CV:109:VAL:HG23	2.18	0.42
23:CW:33:TYR:CE2	23:CW:63:VAL:HG21	2.54	0.42
26:CY:8:PHE:CD2	26:CY:46:PRO:HG3	2.54	0.42
31:DD:58:LYS:HA	31:DD:58:LYS:HD2	1.72	0.42
33:DF:19:ARG:HB3	33:DF:35:GLU:HG2	2.01	0.42
53:E:119:ALA:O	53:E:123:VAL:HG23	2.19	0.42
53:E:216:PRO:HB2	53:E:217:ILE:H	1.68	0.42
25:A:757:A:H4'	54:F:22:LYS:HD2	2.01	0.42
55:G:110:ALA:HA	55:G:113:ILE:HD12	2.01	0.42
55:G:34:GLN:HG2	66:R:57:LEU:HD22	2.01	0.42
57:I:30:SER:O	57:I:34:LEU:HB2	2.19	0.42
59:K:34:PHE:HD2	59:K:111:THR:HG21	1.83	0.42
65:Q:98:ASN:HB2	65:Q:122:THR:HG22	2.00	0.42
73:Y:27:ASN:O	73:Y:31:LYS:HG2	2.19	0.42
1:1:1699:A:H2'	1:1:1700:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2267:C:H2'	1:1:2268:U:O4'	2.20	0.42
1:1:2970:C:H4'	1:1:2971:A:N1	2.34	0.42
1:1:654:C:H2'	1:1:655:C:C6	2.55	0.42
1:1:669:U:H2'	1:1:670:C:O4'	2.19	0.42
1:1:945:C:H2'	1:1:946:U:C6	2.54	0.42
25:6:138:A:H62	25:6:266:A:H61	1.68	0.42
26:7:4:GLU:HG2	26:7:30:ARG:CD	2.49	0.42
25:A:1207:C:H4'	25:A:1208:A:O5'	2.20	0.42
25:A:150:U:OP1	74:Z:123:LYS:NZ	2.46	0.42
25:A:93:A:H4'	25:A:94:U:OP2	2.19	0.42
30:AB:73:LEU:HD23	30:AB:112:ILE:HD12	2.01	0.42
37:AI:67:ARG:HA	37:AI:80:LEU:HD13	2.01	0.42
40:AL:78:LEU:HD13	40:AL:78:LEU:HA	1.82	0.42
42:AN:91:CYS:O	42:AN:126:LYS:NZ	2.42	0.42
1:AR:1506:A:H1'	1:AR:1848:G:O6	2.20	0.42
1:AR:2257:C:H2'	1:AR:2258:U:O4'	2.19	0.42
1:AR:2514:U:OP1	10:CJ:68:ARG:NH1	2.48	0.42
1:AR:2771:U:O2'	1:AR:2772:C:O4'	2.25	0.42
1:AR:2995:A:C2'	1:AR:2996:U:H5''	2.48	0.42
1:AR:3078:U:H1'	84:AR:3693:OHX:N1	2.33	0.42
2:AS:64:A:H3'	12:CL:204:GLY:O	2.20	0.42
3:AT:73:U:H2'	3:AT:74:U:O4'	2.19	0.42
50:B:10:THR:OG1	50:B:12:GLU:OE1	2.24	0.42
12:CL:30:LYS:HB2	12:CL:62:SER:OG	2.19	0.42
13:CM:18:VAL:HG13	13:CM:70:THR:HG22	2.02	0.42
23:CW:16:THR:HG22	23:CW:64:THR:OG1	2.19	0.42
27:CZ:103:TYR:CE2	27:CZ:139:ILE:HG21	2.54	0.42
27:CZ:47:ALA:HB3	37:DJ:77:PRO:HG3	2.01	0.42
32:DE:23:TYR:OH	32:DE:83:LYS:HE3	2.19	0.42
35:DH:35:VAL:HG13	35:DH:40:ASP:HB3	2.02	0.42
56:H:63:MET:HE1	56:H:106:LEU:CD1	2.48	0.42
56:H:98:ARG:HD3	56:H:99:GLY:N	2.35	0.42
57:I:164:TYR:CE2	57:I:165:LYS:HG3	2.54	0.42
59:K:83:VAL:HG23	59:K:85:VAL:HG23	1.99	0.42
59:K:99:LEU:HD12	59:K:99:LEU:HA	1.87	0.42
63:O:40:TYR:HB3	63:O:45:LEU:HD12	2.01	0.42
64:P:28:VAL:O	64:P:41:ARG:O	2.37	0.42
67:S:7:LYS:O	67:S:11:ARG:HB2	2.20	0.42
73:Y:56:LYS:HE3	73:Y:96:VAL:HG23	2.01	0.42
1:1:2394:G:H2'	1:1:2395:G:O4'	2.19	0.42
1:1:3078:U:H4'	1:1:3079:U:OP2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:113:C:H2'	2:3:114:U:O4'	2.19	0.42
25:6:1063:U:H2'	25:6:1064:G:H8	1.85	0.42
25:6:1161:C:H1'	25:6:1619:C:H42	1.83	0.42
25:6:521:A:H2'	25:6:522:U:O4'	2.19	0.42
25:A:1174:C:H2'	25:A:1175:U:O4'	2.19	0.42
25:A:350:U:H5''	25:A:352:A:H5'	2.01	0.42
25:A:487:G:H1	25:A:500:C:N4	2.10	0.42
25:A:542:A:C8	25:A:543:C:H5'	2.46	0.42
39:AK:25:ARG:NH2	41:AM:50:ASN:HD22	2.17	0.42
40:AL:58:ASP:OD1	40:AL:61:LYS:N	2.36	0.42
41:AM:5:LYS:HD3	41:AM:13:MET:HE3	2.00	0.42
1:AR:1706:C:H2'	1:AR:1707:A:O4'	2.20	0.42
1:AR:2404:A:C8	1:AR:2404:A:H5''	2.55	0.42
1:AR:2426:U:H2'	1:AR:2427:U:C6	2.54	0.42
1:AR:2537:U:H1'	1:AR:2538:U:O4'	2.19	0.42
1:AR:2714:G:H4'	1:AR:2715:A:O5'	2.19	0.42
1:AR:2774:C:H2'	1:AR:2775:U:C6	2.55	0.42
84:AR:3566:OHX:N4	84:AR:3642:OHX:N1	2.68	0.42
1:AR:624:G:H2'	1:AR:625:G:H8	1.84	0.42
1:AR:643:U:H5''	84:AR:3743:OHX:N3	2.33	0.42
1:AR:665:A:H1'	14:CN:14:PHE:CE2	2.53	0.42
4:CD:149:ARG:NH2	4:CD:155:LYS:HE2	2.33	0.42
5:CE:347:SER:C	5:CE:349:LYS:H	2.23	0.42
1:AR:505:G:H5''	6:CF:315:LYS:HG2	2.00	0.42
7:CG:86:TYR:CE1	7:CG:247:ILE:HA	2.54	0.42
1:AR:3272:C:O2	8:CH:80:ASN:HB2	2.20	0.42
11:CK:38:LEU:HD23	11:CK:38:LEU:HA	1.85	0.42
12:CL:77:THR:HG23	12:CL:85:PHE:HZ	1.85	0.42
29:DB:14:VAL:HG22	36:DI:86:LYS:HG2	2.01	0.42
37:DJ:86:ARG:HG3	37:DJ:90:ARG:NH2	2.35	0.42
45:DR:6:LYS:HD3	45:DR:7:LYS:HZ2	1.85	0.42
56:H:27:PHE:HD1	56:H:52:ILE:HD11	1.84	0.42
57:I:140:VAL:HB	72:X:52:TYR:HB3	2.01	0.42
59:K:55:ALA:O	59:K:59:LEU:HG	2.19	0.42
62:N:43:ARG:HH12	62:N:102:GLY:HA3	1.85	0.42
66:R:55:VAL:HG22	66:R:59:LYS:HE3	2.01	0.42
71:W:36:VAL:HG11	71:W:78:LEU:HD13	2.01	0.42
1:1:2305:G:N2	1:1:2305:G:OP2	2.47	0.42
1:1:816:A:H1'	1:1:819:U:O4	2.19	0.42
22:2:86:GLU:OE1	22:2:88:ARG:NH1	2.53	0.42
3:4:90:U:H5'	3:4:90:U:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:1174:C:C4	25:6:1175:U:C4	3.08	0.42
28:9:112:ASP:HB3	28:9:114:ASP:H	1.82	0.42
25:A:712:G:N2	25:A:726:C:O2'	2.53	0.42
25:A:876:G:H1'	25:A:944:A:O4'	2.20	0.42
30:AB:7:LYS:HD2	30:AB:7:LYS:HA	1.81	0.42
1:AR:1029:G:H2'	1:AR:1030:A:C8	2.54	0.42
1:AR:109:A:H4'	1:AR:110:G:OP1	2.19	0.42
1:AR:2258:U:H2'	1:AR:2259:A:O4'	2.20	0.42
1:AR:283:G:O6	1:AR:304:G:H1'	2.20	0.42
1:AR:2885:C:O2'	1:AR:2886:U:H5'	2.19	0.42
1:AR:2922:G:N1	1:AR:2923:U:O2	2.52	0.42
84:AR:3477:OHX:N4	84:AR:3696:OHX:N3	2.68	0.42
50:B:17:LEU:HD13	50:B:50:VAL:HB	2.00	0.42
5:CE:147:GLU:HA	5:CE:150:ARG:HB3	2.01	0.42
5:CE:218:ILE:HD11	5:CE:339:ARG:HD3	2.02	0.42
7:CG:146:LEU:HD13	7:CG:148:ILE:HG13	2.00	0.42
7:CG:297:GLN:HA	84:CG:302:OHX:N1	2.35	0.42
2:AS:7:G:OP1	7:CG:33:ARG:HD2	2.19	0.42
8:CH:65:ILE:HD13	8:CH:77:ARG:O	2.18	0.42
12:CL:45:GLU:O	12:CL:141:LYS:HE3	2.19	0.42
17:CQ:58:LEU:HA	17:CQ:72:HIS:CD2	2.55	0.42
1:AR:744:A:P	19:CS:66:ARG:HH21	2.43	0.42
19:CS:93:ILE:HG13	19:CS:93:ILE:H	1.50	0.42
24:CX:87:ARG:HH12	24:CX:137:VAL:HG11	1.84	0.42
41:DN:48:LYS:HD2	41:DN:48:LYS:HA	1.80	0.42
69:U:93:HIS:O	69:U:94:ILE:HD12	2.19	0.42
71:W:1:MET:O	71:W:9:VAL:HG12	2.20	0.42
73:Y:24:TRP:HE3	73:Y:30:LYS:HD2	1.85	0.42
25:A:150:U:P	74:Z:123:LYS:HZ1	2.41	0.42
1:1:2796:G:H4'	1:1:2798:C:C6	2.55	0.42
1:1:2910:A:O2'	1:1:3130:A:N1	2.38	0.42
1:1:718:G:O6	1:1:751:A:H1'	2.19	0.42
3:4:19:C:H2'	3:4:20:U:O4'	2.19	0.42
25:6:1483:A:C6	25:6:1484:G:C6	3.08	0.42
27:8:96:LYS:O	27:8:100:LYS:HG3	2.18	0.42
25:A:811:A:H5'	25:A:816:G:O2'	2.20	0.42
25:A:892:A:H2'	25:A:893:U:C6	2.55	0.42
44:AP:61:LYS:HB3	44:AP:61:LYS:NZ	2.34	0.42
1:AR:1171:G:O6	84:AR:3502:OHX:N1	2.52	0.42
1:AR:1783:U:H2'	1:AR:1784:G:C8	2.55	0.42
1:AR:1783:U:H2'	1:AR:1784:G:H8	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:1908:A:H2'	1:AR:1909:A:O4'	2.19	0.42
1:AR:2404:A:C8	1:AR:2404:A:C5'	3.02	0.42
1:AR:2689:A:C8	1:AR:2702:A:C6	3.07	0.42
1:AR:501:A:H2'	1:AR:502:U:H6	1.85	0.42
1:AR:895:A:C6	1:AR:897:U:C4	3.07	0.42
2:AS:112:G:H2'	2:AS:113:C:C6	2.55	0.42
50:B:52:LYS:HG2	50:B:52:LYS:H	1.40	0.42
11:CK:48:VAL:HG11	11:CK:52:LEU:HD13	2.02	0.42
14:CN:158:ALA:O	30:DC:124:ILE:HD11	2.20	0.42
14:CN:28:GLN:HB3	16:CP:201:ARG:NH1	2.34	0.42
32:DE:99:ASP:OD1	32:DE:99:ASP:N	2.53	0.42
39:DL:28:HIS:CE1	39:DL:31:LYS:HG3	2.55	0.42
53:E:74:GLN:HG3	53:E:79:TYR:HB2	2.02	0.42
57:I:67:LEU:HD23	57:I:67:LEU:HA	1.81	0.42
59:K:93:LEU:HA	59:K:96:VAL:HG13	2.02	0.42
62:N:62:LEU:H	62:N:62:LEU:HD23	1.85	0.42
63:O:99:ARG:O	63:O:103:GLU:HG2	2.19	0.42
66:R:52:LEU:HA	66:R:52:LEU:HD23	2.55	0.42
67:S:10:LYS:HG2	67:S:53:TYR:CE2	2.55	0.42
1:1:1019:G:H2'	1:1:1020:G:O4'	2.20	0.42
1:1:1054:A:H5''	1:1:2637:A:H61	1.84	0.42
1:1:1681:U:H2'	1:1:1682:U:O4'	2.20	0.42
1:1:2427:U:H2'	1:1:2428:U:C6	2.53	0.42
1:1:2830:G:H1'	1:1:2861:U:C2	2.54	0.42
1:1:2984:C:H2'	1:1:2985:C:C6	2.54	0.42
1:1:1940:G:N2	1:1:3362:A:H8	2.17	0.42
1:1:818:C:H2'	1:1:819:U:O4'	2.20	0.42
25:6:1451:C:H2'	25:6:1452:U:H6	1.84	0.42
25:6:869:A:H2'	25:6:870:C:O4'	2.20	0.42
25:A:117:U:H2'	25:A:118:U:O4'	2.20	0.42
25:A:1291:G:N2	25:A:1324:G:N2	2.66	0.42
25:A:1619:C:H2'	25:A:1620:C:H6	1.85	0.42
25:A:102:U:O4	25:A:360:A:H2'	2.19	0.42
29:AA:127:ASN:C	29:AA:129:TRP:H	2.15	0.42
34:AF:82:LEU:HD11	34:AF:112:ALA:HA	2.02	0.42
36:AH:8:ARG:NH2	36:AH:31:ARG:HD2	2.34	0.42
39:AK:53:ALA:HA	39:AK:56:ARG:HH11	1.84	0.42
40:AL:26:LYS:HD2	40:AL:26:LYS:HA	1.94	0.42
1:AR:118:U:O2	1:AR:121:A:H5'	2.20	0.42
1:AR:1307:G:C2	1:AR:1308:A:C2	3.08	0.42
1:AR:1334:U:H5''	9:CI:206:LYS:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:1827:C:H2'	1:AR:1828:A:H8	1.84	0.42
1:AR:2927:C:H2'	1:AR:2928:C:C6	2.55	0.42
84:AR:3511:OHX:N6	84:AR:3698:OHX:N2	2.67	0.42
84:AR:3687:OHX:N1	84:AR:3689:OHX:N2	2.68	0.42
1:AR:374:A:N3	1:AR:376:G:H5'	2.35	0.42
84:AS:203:OHX:N5	84:AS:210:OHX:N5	2.68	0.42
5:CE:3:HIS:O	5:CE:5:LYS:N	2.53	0.42
9:CI:88:ARG:HD2	9:CI:90:LYS:O	2.19	0.42
12:CL:72:ALA:HB2	12:CL:155:ALA:HB2	2.02	0.42
17:CQ:78:ARG:HG3	17:CQ:78:ARG:HH11	1.83	0.42
19:CS:8:LYS:HB2	19:CS:8:LYS:HE3	1.80	0.42
7:CG:69:ILE:HD13	22:CV:28:SER:HB2	2.01	0.42
39:DL:21:ARG:HD2	39:DL:37:CYS:SG	2.60	0.42
53:E:211:PRO:HG3	67:S:20:TYR:CZ	2.55	0.42
56:H:55:GLY:O	56:H:63:MET:HG3	2.20	0.42
57:I:12:ALA:HB3	57:I:13:PRO:HD3	2.02	0.42
60:L:12:HIS:CE1	60:L:49:LEU:HD21	2.54	0.42
1:1:3095:U:H2'	1:1:3096:C:C6	2.54	0.42
1:1:309:U:OP1	38:AJ:84:LYS:NZ	2.44	0.42
1:1:3269:U:O2	1:1:3269:U:H5'	2.20	0.42
1:1:716:A:O2'	1:1:718:G:OP2	2.36	0.42
25:6:485:A:N6	25:6:486:G:N3	2.68	0.42
25:A:715:U:H3	25:A:723:G:H1	1.68	0.42
30:AB:19:LYS:HD2	30:AB:25:HIS:CD2	2.55	0.42
37:AI:89:ARG:HH11	37:AI:89:ARG:HG2	1.84	0.42
1:AR:1397:C:O2'	1:AR:1398:U:H5'	2.19	0.42
1:AR:1486:G:N2	36:DI:6:THR:HG22	2.35	0.42
1:AR:1498:A:H2'	1:AR:1499:C:C6	2.55	0.42
1:AR:1915:A:H2'	1:AR:1916:U:C6	2.54	0.42
1:AR:2623:G:C4	1:AR:2624:G:C8	3.07	0.42
1:AR:627:U:H2'	1:AR:628:A:C8	2.55	0.42
51:C:123:ALA:HB2	51:C:165:ARG:HG2	2.02	0.42
6:CF:184:SER:HB2	6:CF:202:ARG:HG2	2.02	0.42
6:CF:325:LEU:HA	6:CF:325:LEU:HD23	1.85	0.42
1:AR:1139:G:OP1	9:CI:97:PRO:HG3	2.20	0.42
11:CK:13:PRO:HG2	11:CK:16:VAL:CG1	2.50	0.42
14:CN:32:LYS:HA	14:CN:35:ARG:NH1	2.34	0.42
17:CQ:43:ILE:HD11	17:CQ:138:LEU:HD13	2.02	0.42
26:CY:60:LYS:HB2	26:CY:60:LYS:HE2	1.93	0.42
30:DC:77:LYS:C	30:DC:79:TRP:N	2.73	0.42
34:DG:19:ARG:HD2	34:DG:28:VAL:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DJ:93:THR:OG1	37:DJ:96:GLU:HG2	2.20	0.42
38:DK:57:LEU:HA	38:DK:57:LEU:HD23	1.92	0.42
53:E:127:MET:HE1	53:E:133:GLY:HA2	2.02	0.42
53:E:45:LYS:HE2	53:E:45:LYS:HB2	1.88	0.42
54:F:179:LYS:O	54:F:194:THR:HA	2.20	0.42
54:F:246:LEU:HD21	54:F:254:ARG:CZ	2.50	0.42
57:I:111:LYS:HG3	57:I:112:ARG:H	1.85	0.42
57:I:60:ILE:HD11	57:I:90:VAL:HG13	2.00	0.42
59:K:163:PRO:HG3	59:K:169:PRO:O	2.19	0.42
60:L:55:VAL:HA	60:L:69:THR:HG23	2.02	0.42
60:L:81:ASN:O	60:L:81:ASN:ND2	2.53	0.42
25:A:1340:U:O4	66:R:9:THR:HA	2.19	0.42
67:S:61:ILE:C	67:S:63:LYS:H	2.21	0.42
1:1:2423:U:H2'	1:1:2424:A:C8	2.54	0.42
1:1:2700:G:O2'	1:1:2705:A:N1	2.42	0.42
1:1:274:G:H2'	1:1:275:U:O4'	2.20	0.42
25:6:1325:A:H2'	25:6:1326:A:H8	1.85	0.42
25:6:1641:C:H2'	25:6:1642:G:C8	2.55	0.42
25:6:1711:C:H2'	25:6:1712:A:H5''	2.01	0.42
25:A:1003:A:H4'	25:A:1004:U:O5'	2.20	0.42
25:A:131:C:O2'	25:A:132:U:OP1	2.36	0.42
25:A:1544:U:H5''	68:T:132:ARG:HD2	2.01	0.42
25:A:330:G:C6	25:A:331:A:C6	3.08	0.42
36:AH:20:ILE:HD13	36:AH:34:HIS:HA	2.02	0.42
36:AH:3:GLN:HB3	36:AH:30:LEU:HD12	2.02	0.42
1:1:116:A:OP1	38:AJ:36:ARG:NH1	2.53	0.42
1:AR:1141:C:O2'	1:AR:1153:A:N3	2.40	0.42
1:AR:1474:A:O2'	33:DF:57:GLN:NE2	2.53	0.42
1:AR:160:G:H2'	1:AR:161:G:O4'	2.20	0.42
1:AR:1767:C:H2'	1:AR:1768:U:O4'	2.20	0.42
1:AR:209:A:O2'	1:AR:211:A:OP2	2.29	0.42
84:AR:3511:OHX:N3	84:AR:3698:OHX:N1	2.68	0.42
1:AR:432:G:OP1	35:DH:57:LYS:HB2	2.20	0.42
1:AR:867:G:C6	1:AR:868:C:C4	3.08	0.42
1:AR:926:A:H2'	1:AR:927:C:C6	2.55	0.42
51:C:180:THR:O	51:C:183:GLN:N	2.50	0.42
6:CF:193:LYS:HE3	6:CF:193:LYS:HB3	1.73	0.42
1:AR:364:G:O3'	6:CF:84:ARG:HG2	2.19	0.42
10:CJ:158:ASP:HB3	10:CJ:159:PRO:HD3	2.02	0.42
12:CL:74:LYS:HE3	12:CL:74:LYS:HB2	1.63	0.42
18:CR:95:LEU:HA	18:CR:95:LEU:HD23	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:D:35:TRP:CZ2	52:D:67:GLN:HB2	2.55	0.42
31:DD:28:LYS:HD3	31:DD:29:TYR:H	1.85	0.42
55:G:216:GLU:HA	55:G:219:ARG:HB3	2.02	0.42
57:I:98:ILE:HG21	57:I:118:LEU:HD23	2.02	0.42
59:K:84:GLY:O	59:K:107:ARG:HD3	2.20	0.42
67:S:41:ILE:HD13	67:S:47:ARG:HA	2.02	0.42
69:U:10:ALA:HB3	69:U:13:ASP:OD1	2.20	0.42
69:U:61:VAL:O	69:U:65:ILE:HG13	2.20	0.42
69:U:9:VAL:HG22	69:U:140:LEU:HD11	2.01	0.42
1:1:398:A:N7	72:X:3:ARG:NH2	171.94	0.42
1:1:1018:G:H8	1:1:1018:G:OP2	2.03	0.41
1:1:2144:A:C4	1:1:2281:A:C6	3.08	0.41
1:1:2313:A:O5'	1:1:2315:G:H1'	2.20	0.41
1:1:2367:A:H2'	1:1:2368:A:O4'	2.20	0.41
2:3:90:U:C4	2:3:91:G:C5	3.08	0.41
3:4:85:G:H4'	3:4:86:U:OP1	2.20	0.41
23:5:21:SER:HA	23:5:24:GLU:OE2	2.20	0.41
25:6:1398:U:H4'	25:6:1399:C:OP2	2.19	0.41
25:6:1699:G:H2'	25:6:1700:C:H5'	2.02	0.41
25:6:82:U:H2'	25:6:83:G:O4'	2.19	0.41
26:7:52:THR:O	26:7:56:ARG:HG3	2.20	0.41
28:9:60:ARG:HA	28:9:60:ARG:HD3	1.79	0.41
25:A:1756:A:O5'	25:A:1756:A:H8	2.03	0.41
25:A:856:A:N9	57:I:64:VAL:HG21	2.34	0.41
1:AR:1317:A:C4	1:AR:1319:G:N7	2.87	0.41
1:AR:1677:G:OP2	23:CW:103:TYR:OH	2.16	0.41
1:AR:1943:C:OP1	1:AR:3346:U:H1'	2.20	0.41
1:AR:3165:A:H2'	1:AR:3166:C:C6	2.55	0.41
1:AR:391:A:H2'	1:AR:392:G:O4'	2.20	0.41
1:AR:585:A:H2'	1:AR:586:C:C6	2.55	0.41
1:AR:955:U:H2'	1:AR:956:U:H6	1.84	0.41
2:AS:33:U:H2'	2:AS:34:C:O4'	2.20	0.41
51:C:35:PRO:HG3	51:C:98:THR:O	2.20	0.41
6:CF:346:LYS:H	6:CF:346:LYS:HG2	1.48	0.41
6:CF:72:ALA:O	6:CF:76:ARG:NH1	2.53	0.41
9:CI:149:TYR:CE1	9:CI:181:ILE:HD13	2.54	0.41
11:CK:92:TYR:CD1	11:CK:92:TYR:N	2.87	0.41
12:CL:30:LYS:HA	12:CL:30:LYS:HD2	1.89	0.41
14:CN:50:PRO:HB3	14:CN:138:VAL:O	2.20	0.41
21:CU:1:MET:HE1	21:CU:32:SER:N	2.34	0.41
1:AR:2787:G:O3'	30:DC:57:GLY:HA2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:DE:14:LEU:HA	32:DE:14:LEU:HD23	1.82	0.41
57:I:147:ASN:N	57:I:147:ASN:OD1	2.29	0.41
57:I:43:PHE:HB2	57:I:61:PHE:O	2.20	0.41
57:I:44:LYS:HZ3	57:I:95:GLU:HG2	1.85	0.41
60:L:24:LYS:HB2	60:L:63:TYR:CE1	2.55	0.41
25:A:895:G:H21	64:P:38:THR:HG21	1.85	0.41
72:X:90:THR:HB	72:X:94:LEU:HD12	2.00	0.41
1:1:1792:C:H2'	1:1:1795:U:C5	2.55	0.41
1:1:2713:U:O2'	44:AP:8:ARG:HD2	2.20	0.41
1:1:2882:U:H2'	1:1:2883:U:C6	2.55	0.41
1:1:3326:G:H2'	1:1:3327:G:H8	1.84	0.41
1:1:34:A:H2'	1:1:35:A:C8	2.56	0.41
1:1:507:U:H2'	1:1:508:U:H6	1.85	0.41
22:2:75:ILE:HA	22:2:87:LYS:O	2.20	0.41
3:4:154:C:H2'	3:4:155:A:O4'	2.20	0.41
25:6:1147:A:H2'	25:6:1148:C:C6	2.55	0.41
25:6:320:U:H2'	25:6:321:C:C6	2.54	0.41
28:9:118:LEU:O	28:9:122:LYS:HG3	2.19	0.41
25:A:1202:A:H1'	25:A:1207:C:H42	1.85	0.41
25:A:1504:G:C6	25:A:1505:A:C6	3.08	0.41
25:A:1586:A:OP1	66:R:136:SER:N	2.48	0.41
25:A:1609:U:OP1	66:R:76:SER:N	2.46	0.41
25:A:894:U:H2'	25:A:895:G:C8	2.55	0.41
33:AE:13:THR:CG2	33:AE:72:ARG:HD3	2.46	0.41
34:AF:21:HIS:CE1	34:AF:24:ARG:HD2	2.56	0.41
37:AI:90:ARG:H	37:AI:90:ARG:HG2	1.39	0.41
40:AL:31:LEU:HD23	40:AL:31:LEU:H	1.84	0.41
42:AN:113:ARG:HA	42:AN:117:HIS:CE1	2.55	0.41
1:AR:1334:U:H5'	9:CI:207:LEU:O	2.21	0.41
1:AR:132:C:H2'	1:AR:133:U:H5''	2.02	0.41
1:AR:1662:G:H2'	1:AR:1663:C:C6	2.56	0.41
1:AR:1495:U:C5	1:AR:1835:A:N1	2.89	0.41
1:AR:1133:A:H1'	1:AR:2618:G:O6	2.20	0.41
1:AR:3028:G:H2'	1:AR:3029:A:C8	2.55	0.41
84:AR:3477:OHX:N2	84:AR:3696:OHX:N5	2.68	0.41
1:AR:434:U:H2'	1:AR:435:C:C6	2.55	0.41
1:AR:92:G:H5'	1:AR:93:C:H5''	2.02	0.41
2:AS:106:U:H2'	2:AS:107:C:C6	2.55	0.41
1:AR:406:G:H1'	3:AT:16:G:N2	2.35	0.41
50:B:117:GLU:OE1	52:D:40:LYS:HG3	2.20	0.41
51:C:119:THR:HB	51:C:143:THR:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:C:157:GLN:C	51:C:159:SER:H	2.22	0.41
51:C:97:LEU:HG	51:C:232:HIS:CE1	2.55	0.41
7:CG:219:PHE:O	7:CG:219:PHE:CG	2.73	0.41
9:CI:159:GLN:O	9:CI:161:VAL:HG23	2.20	0.41
10:CJ:161:GLU:HA	10:CJ:164:VAL:HG22	2.02	0.41
13:CM:106:ILE:HD13	13:CM:125:MET:HB3	2.01	0.41
14:CN:128:ARG:HD3	37:DJ:114:ARG:CZ	2.49	0.41
14:CN:8:PRO:HD3	19:CS:164:ARG:HB3	2.01	0.41
21:CU:139:TYR:CD1	21:CU:140:VAL:HG23	2.55	0.41
52:D:53:ILE:O	52:D:56:ILE:N	2.53	0.41
29:DB:25:ILE:HA	29:DB:43:VAL:HG12	2.01	0.41
37:DJ:14:LYS:HG2	37:DJ:14:LYS:H	1.62	0.41
54:F:31:PRO:HB2	54:F:38:LEU:HD22	2.02	0.41
61:M:80:MET:HB3	61:M:80:MET:HE2	1.75	0.41
25:A:1584:G:C8	66:R:122:ARG:HB3	2.55	0.41
73:Y:92:CYS:HA	73:Y:95:PHE:CD2	2.55	0.41
21:O:1:MET:HB2	21:O:118:PHE:CD2	2.56	0.41
1:1:1211:U:H2'	1:1:1212:A:C8	2.54	0.41
1:1:1767:C:H2'	1:1:1768:U:C6	2.55	0.41
1:1:1922:A:H2'	1:1:1923:C:O4'	2.19	0.41
1:1:2222:A:H2'	1:1:2223:A:C8	2.55	0.41
1:1:2376:G:C6	1:1:2377:G:C6	3.08	0.41
1:1:246:U:H2'	1:1:247:C:C6	2.55	0.41
1:1:90:C:H4'	1:1:282:G:H5''	2.03	0.41
1:1:3089:C:H2'	1:1:3090:U:O4'	2.20	0.41
1:1:315:C:OP2	38:AJ:28:TYR:OH	2.30	0.41
84:1:3510:OHX:N5	84:1:3682:OHX:N6	2.68	0.41
1:1:40:A:C2	30:AB:40:HIS:CE1	3.08	0.41
1:1:938:C:OP1	1:1:963:G:H5'	2.19	0.41
3:4:79:A:O3'	3:4:80:A:H4'	2.19	0.41
25:6:1117:U:H2'	25:6:1118:G:C8	2.56	0.41
25:6:982:U:H4'	45:DR:24:ARG:NH1	2.35	0.41
25:6:988:A:C2	25:6:989:U:H1'	2.55	0.41
25:A:1146:G:C6	25:A:1147:A:C6	3.08	0.41
25:A:1785:U:OP1	64:P:136:ARG:NH1	2.53	0.41
25:A:488:G:OP1	25:A:488:G:H4'	2.21	0.41
32:AD:13:LYS:O	32:AD:17:VAL:HG23	2.20	0.41
1:AR:2550:U:O4	4:CD:40:TYR:N	2.48	0.41
1:AR:2880:U:H1'	5:CE:250:ALA:CB	2.47	0.41
1:AR:594:U:H2'	1:AR:609:G:O6	2.21	0.41
1:AR:718:G:N1	1:AR:721:G:H1'	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:B:177:LEU:HA	50:B:177:LEU:HD23	1.90	0.41
51:C:181:LEU:HA	51:C:184:LEU:CB	2.48	0.41
5:CE:148:LEU:HD12	5:CE:148:LEU:HA	1.86	0.41
5:CE:361:THR:HG22	5:CE:371:GLN:OE1	2.20	0.41
8:CH:35:VAL:HG12	8:CH:36:PRO:HD2	2.03	0.41
11:CK:106:LYS:HG2	11:CK:107:ASP:OD1	2.19	0.41
11:CK:81:GLY:HA3	11:CK:149:ASN:O	2.21	0.41
18:CR:137:ASN:HD22	18:CR:137:ASN:HA	1.68	0.41
24:CX:66:LYS:HB2	24:CX:69:LEU:HD22	2.03	0.41
26:CY:52:THR:O	26:CY:56:ARG:HG3	2.20	0.41
32:DE:34:LEU:HD12	32:DE:34:LEU:HA	1.79	0.41
38:DK:68:ARG:HD2	38:DK:68:ARG:O	2.20	0.41
56:H:27:PHE:O	56:H:102:VAL:HB	2.20	0.41
57:I:125:ILE:O	57:I:129:LEU:N	2.48	0.41
65:Q:86:VAL:O	65:Q:89:MET:HG3	2.20	0.41
25:A:1390:U:OP1	67:S:5:ARG:HD2	2.20	0.41
1:1:1246:G:H8	1:1:1246:G:OP1	2.03	0.41
22:2:8:ARG:O	22:2:11:THR:OG1	2.29	0.41
25:6:1274:C:O2	25:6:1274:C:H2'	2.20	0.41
25:6:1417:A:H2'	25:6:1418:G:O4'	2.20	0.41
25:6:1638:G:C2	25:6:1639:C:H1'	2.55	0.41
25:6:1660:A:H2'	25:6:1661:U:C6	2.56	0.41
25:6:542:A:OP1	25:6:544:A:C5	2.73	0.41
26:7:9:SER:HA	26:7:52:THR:HG22	2.02	0.41
25:A:517:U:H2'	25:A:518:A:O4'	2.21	0.41
1:AR:2209:U:H1'	1:AR:2210:G:P	2.60	0.41
1:AR:2310:U:OP1	84:AR:3696:OHX:N2	2.53	0.41
1:AR:2617:U:C5	1:AR:2621:G:OP2	2.73	0.41
1:AR:2840:C:H2'	1:AR:2841:G:O4'	2.20	0.41
1:AR:3307:A:C5	1:AR:3308:C:C5	3.08	0.41
1:AR:3351:U:H3'	1:AR:3352:U:H5''	2.03	0.41
1:AR:1839:A:OP1	84:AR:3534:OHX:N3	2.54	0.41
1:AR:976:U:H2'	1:AR:977:C:O4'	2.19	0.41
2:AS:8:G:C6	2:AS:9:C:C4	3.09	0.41
3:AT:145:U:H2'	3:AT:146:U:O4'	2.20	0.41
50:B:155:PHE:HA	50:B:155:PHE:HD1	1.74	0.41
6:CF:222:VAL:HA	6:CF:223:PRO:HD3	1.91	0.41
10:CJ:140:VAL:O	10:CJ:144:GLU:HG3	2.20	0.41
20:CT:134:HIS:CE1	20:CT:137:ALA:HB2	2.55	0.41
20:CT:78:TYR:HA	20:CT:81:ARG:HD3	2.01	0.41
22:CV:63:VAL:HB	22:CV:75:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:CX:87:ARG:HH22	24:CX:137:VAL:CG2	2.34	0.41
28:DA:57:LEU:HD22	28:DA:58:VAL:N	2.34	0.41
55:G:42:LEU:HB2	55:G:46:TRP:O	2.19	0.41
55:G:92:ARG:HA	55:G:95:ASN:HD22	1.85	0.41
56:H:58:LYS:HG2	56:H:105:ASP:O	2.21	0.41
63:O:113:PHE:CE2	63:O:117:LEU:HD11	2.56	0.41
68:T:41:ARG:NE	69:U:46:PRO:HD3	2.35	0.41
70:V:43:LYS:HD2	70:V:43:LYS:HA	1.72	0.41
71:W:16:LYS:HB2	71:W:16:LYS:HE3	1.86	0.41
1:1:2097:U:H2'	1:1:2098:C:H6	1.83	0.41
1:1:2361:A:N6	1:1:2376:G:O6	2.54	0.41
1:1:3222:U:H1'	1:1:3264:G:N2	2.35	0.41
1:1:3258:U:O2'	1:1:3260:G:OP1	2.21	0.41
1:1:2997:G:C6	1:1:3396:U:C4	3.09	0.41
1:1:623:U:P	84:1:3661:OHX:N3	2.94	0.41
1:1:871:U:H2'	1:1:872:U:C6	2.55	0.41
25:6:1258:U:H5	25:6:1259:U:N3	2.18	0.41
84:6:1915:OHX:N5	84:6:2001:OHX:N6	2.68	0.41
25:6:74:U:H3'	25:6:75:U:H3'	2.01	0.41
25:6:97:C:O2'	25:6:426:G:H5'	2.20	0.41
1:1:1603:A:H61	27:8:71:THR:HG21	1.85	0.41
25:A:275:C:O2	25:A:276:C:N4	2.54	0.41
25:A:778:G:H22	74:Z:10:ARG:HH12	1.68	0.41
25:A:843:U:H2'	25:A:844:A:C8	2.55	0.41
35:AG:17:GLN:OE1	35:AG:24:ASN:ND2	2.45	0.41
1:1:1485:G:N2	36:AH:4:ARG:HD2	2.35	0.41
37:AI:62:GLN:O	37:AI:66:VAL:HG23	2.20	0.41
37:AI:70:TYR:CD1	37:AI:76:GLN:HA	2.56	0.41
42:AN:113:ARG:O	42:AN:113:ARG:HG3	2.20	0.41
1:AR:1674:G:H2'	1:AR:1675:G:O4'	2.21	0.41
1:AR:2611:U:H2'	1:AR:2612:U:C6	2.55	0.41
1:AR:2736:A:OP1	22:CV:92:ARG:NH1	2.54	0.41
1:AR:2944:U:H1'	5:CE:251:CYS:SG	2.60	0.41
1:AR:578:A:H5''	1:AR:579:G:O5'	2.20	0.41
2:AS:8:G:C5	2:AS:9:C:C4	3.09	0.41
50:B:203:PHE:N	50:B:203:PHE:CD1	2.88	0.41
7:CG:143:LYS:HG3	7:CG:172:TYR:HD2	1.85	0.41
9:CI:40:LYS:HE2	9:CI:170:GLU:OE1	2.20	0.41
13:CM:37:LEU:HA	13:CM:37:LEU:HD23	1.83	0.41
18:CR:126:ARG:HD3	18:CR:140:GLU:HG3	2.02	0.41
18:CR:48:LEU:HB3	18:CR:88:VAL:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DJ:85:THR:O	37:DJ:89:ARG:HB2	2.20	0.41
40:DM:54:LEU:HD21	40:DM:56:ILE:HD11	2.03	0.41
55:G:109:LYS:O	55:G:113:ILE:HG13	2.20	0.41
57:I:69:GLY:HA2	57:I:72:LYS:HD2	2.01	0.41
58:J:36:THR:HG21	58:J:173:PRO:HB2	2.02	0.41
59:K:38:ASN:HB2	59:K:41:GLU:H	1.85	0.41
61:M:127:GLN:HB2	61:M:137:PHE:CE2	2.55	0.41
65:Q:110:GLU:HG3	68:T:119:ILE:HD11	2.02	0.41
66:R:93:HIS:HA	66:R:97:VAL:HG23	2.02	0.41
68:T:28:ILE:O	68:T:32:LEU:HG	2.20	0.41
68:T:7:GLU:H	68:T:7:GLU:HG3	1.63	0.41
69:U:27:LYS:HB3	69:U:111:ILE:HD11	2.02	0.41
73:Y:110:LYS:O	73:Y:112:LYS:HG2	2.20	0.41
74:Z:44:LEU:HA	74:Z:44:LEU:HD13	4.32	0.41
1:1:1066:G:C6	1:1:1067:U:C4	3.09	0.41
1:1:1618:G:H2'	1:1:1619:A:O4'	2.21	0.41
1:1:1804:A:H2'	1:1:1805:C:C6	2.55	0.41
1:1:2207:A:O2'	1:1:2208:A:H5'	2.20	0.41
1:1:317:A:C2	1:1:318:A:C4	3.09	0.41
22:2:56:PHE:CE2	22:2:78:LYS:HE2	2.55	0.41
22:2:96:ILE:HA	22:2:96:ILE:HD12	1.73	0.41
25:6:1058:U:H1'	25:6:1059:U:H5''	2.01	0.41
25:6:1255:G:O2'	25:6:1256:A:O5'	2.32	0.41
25:6:1557:U:O2'	25:6:1558:U:H2'	2.20	0.41
25:6:727:U:H2'	25:6:728:U:H6	1.84	0.41
25:A:1489:U:H5'	25:A:1494:C:H1'	2.03	0.41
29:AA:9:LYS:HD2	29:AA:83:THR:O	2.21	0.41
34:AF:75:LEU:HA	34:AF:75:LEU:HD23	1.83	0.41
39:AK:31:LYS:O	39:AK:33:THR:HG22	2.21	0.41
3:4:57:C:OP2	39:AK:68:LYS:HE3	2.21	0.41
42:AN:95:VAL:HA	42:AN:101:ALA:O	2.20	0.41
43:AO:8:LYS:HD3	43:AO:12:ARG:NH2	2.34	0.41
1:AR:1080:A:OP1	7:CG:140:ARG:HD3	2.20	0.41
1:AR:1263:A:H2'	1:AR:1263:A:N3	2.36	0.41
1:AR:1262:G:H5''	1:AR:1263:A:OP2	2.20	0.41
1:AR:1266:G:C2	1:AR:1276:U:H1'	2.55	0.41
1:AR:2112:U:H4'	1:AR:2113:A:O5'	2.20	0.41
1:AR:2406:C:H2'	1:AR:2407:C:C6	2.56	0.41
1:AR:2546:C:H2'	1:AR:2547:A:O4'	2.21	0.41
1:AR:3017:A:H2'	1:AR:3018:C:H6	1.86	0.41
84:AR:3521:OHX:N2	84:AR:3715:OHX:N2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:589:A:H1'	1:AR:1337:A:H5''	2.02	0.41
2:AS:110:G:C6	2:AS:111:U:C4	3.09	0.41
3:AT:67:U:H2'	3:AT:68:G:C8	2.54	0.41
6:CF:188:ARG:NH2	6:CF:197:ARG:HB3	2.35	0.41
1:AR:1385:C:HO2'	8:CH:2:SER:N	2.19	0.41
10:CJ:190:VAL:HG22	10:CJ:190:VAL:O	2.20	0.41
12:CL:80:SER:HB3	12:CL:147:VAL:HG11	2.01	0.41
13:CM:15:GLU:HB3	13:CM:130:VAL:HG22	2.02	0.41
1:AR:618:C:OP1	18:CR:169:THR:HA	2.21	0.41
26:CY:9:SER:O	26:CY:53:VAL:HG23	2.20	0.41
52:D:49:LYS:HE3	52:D:246:GLU:OE1	2.20	0.41
29:DB:5:LEU:HD13	29:DB:77:TYR:CE1	2.55	0.41
32:DE:13:LYS:O	32:DE:17:VAL:HG23	2.20	0.41
36:DI:103:LYS:HD3	36:DI:103:LYS:HA	1.89	0.41
25:6:1772:C:OP1	43:DP:2:ARG:HD3	2.21	0.41
55:G:121:ILE:HB	55:G:129:PRO:HB3	2.03	0.41
25:A:581:U:P	57:I:108:GLN:HE21	92.77	0.41
57:I:39:ARG:N	57:I:40:PRO:HD2	2.35	0.41
57:I:42:GLN:HG2	57:I:43:PHE:N	2.36	0.41
1:1:1594:A:H1'	1:1:1615:C:H1'	2.03	0.41
1:1:1131:G:O2'	1:1:2373:A:N1	2.45	0.41
1:1:3087:A:H2'	1:1:3088:G:O4'	2.21	0.41
1:1:3099:C:O2'	1:1:3100:U:H5'	2.21	0.41
1:1:3375:A:H5''	1:1:3378:C:H5	1.85	0.41
84:1:3575:OHX:N6	84:1:3604:OHX:N5	2.69	0.41
3:4:26:U:H2'	3:4:27:U:C6	2.55	0.41
25:6:1579:U:H2'	25:6:1580:C:C6	2.56	0.41
25:6:482:U:H3	25:6:505:A:N6	2.17	0.41
25:6:74:U:C2	25:6:76:A:H5''	2.55	0.41
25:6:803:A:O2'	25:6:804:A:OP2	2.38	0.41
28:9:40:ARG:HG2	28:9:45:ILE:O	2.21	0.41
25:A:1458:G:H5''	25:A:1459:C:OP2	2.20	0.41
25:A:397:A:C6	25:A:398:G:C2	3.09	0.41
25:A:438:A:H1'	25:A:466:U:O2	2.21	0.41
25:A:539:G:H8	25:A:539:G:OP2	2.03	0.41
25:A:850:A:C2	25:A:851:U:C2	3.09	0.41
25:A:990:C:H2'	25:A:991:G:O4'	2.20	0.41
40:AL:5:ILE:HG22	40:AL:54:LEU:HB2	2.01	0.41
41:AM:44:TRP:CZ3	41:AM:45:ARG:HG2	2.55	0.41
45:AQ:38:ASP:OD1	45:AQ:45:LYS:HB3	2.20	0.41
1:AR:1345:G:C2	1:AR:1360:C:C2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:1382:G:OP2	6:CF:188:ARG:NH1	2.52	0.41
1:AR:1641:U:O2'	1:AR:1642:A:H3'	2.21	0.41
1:AR:2404:A:H8	1:AR:2404:A:H5''	1.83	0.41
1:AR:2703:A:N3	13:CM:142:LYS:HE2	2.36	0.41
1:AR:2713:U:H3'	44:DQ:9:LYS:O	2.21	0.41
3:AT:2:A:H2'	3:AT:3:A:O4'	2.21	0.41
50:B:203:PHE:N	50:B:203:PHE:HD1	2.19	0.41
5:CE:10:ARG:NH2	5:CE:263:SER:O	2.54	0.41
5:CE:21:ARG:HG2	5:CE:269:GLN:HG2	2.03	0.41
7:CG:39:GLN:HA	7:CG:48:LYS:HD2	2.01	0.41
7:CG:58:LYS:HA	7:CG:93:THR:HB	2.03	0.41
9:CI:166:ASN:OD1	9:CI:181:ILE:N	2.50	0.41
15:CO:8:LYS:HB2	15:CO:8:LYS:HE3	1.86	0.41
16:CP:27:VAL:HB	16:CP:122:ASN:ND2	2.35	0.41
17:CQ:15:LEU:HD21	17:CQ:125:ARG:HG3	2.01	0.41
29:DB:5:LEU:HD11	32:DE:35:ARG:HD2	2.02	0.41
36:DI:19:LYS:NZ	36:DI:38:LEU:HD23	2.35	0.41
39:DL:75:LYS:HE3	39:DL:75:LYS:HB3	1.87	0.41
54:F:32:SER:O	54:F:83:PRO:HG3	2.21	0.41
55:G:32:GLU:OE2	55:G:33:VAL:HG23	2.19	0.41
57:I:141:ARG:NH2	72:X:49:GLU:OE2	2.53	0.41
60:L:8:ARG:HG2	60:L:79:TYR:OH	2.21	0.41
67:S:115:LEU:HD23	67:S:115:LEU:HA	1.92	0.41
70:V:45:ALA:HB1	70:V:50:LEU:HD13	2.02	0.41
1:1:1419:A:H5'	3:4:20:U:O3'	2.21	0.41
1:1:2765:C:O3'	44:AP:39:GLY:HA3	2.20	0.41
1:1:3060:C:H1'	1:1:3332:U:H1'	2.03	0.41
1:1:3295:A:H2'	1:1:3296:A:C8	2.56	0.41
1:1:546:C:H5'	1:1:547:G:O4'	2.21	0.41
3:4:108:C:H2'	3:4:109:A:O4'	2.20	0.41
25:6:1733:C:H2'	25:6:1734:U:C6	2.55	0.41
28:9:42:GLN:OE1	28:9:127:GLU:HB2	2.21	0.41
25:A:1483:A:H2'	25:A:1484:G:C8	2.56	0.41
25:A:1553:G:O6	65:Q:40:ARG:NH2	2.51	0.41
25:A:1575:G:H2'	25:A:1576:A:C8	2.56	0.41
25:A:1760:G:H2'	25:A:1761:U:H5'	2.03	0.41
25:A:187:G:OP2	58:J:142:LYS:NZ	2.54	0.41
25:A:207:U:O2	58:J:178:ARG:NH1	2.54	0.41
25:A:330:G:OP2	58:J:172:ARG:NH1	2.52	0.41
25:A:463:U:H2'	25:A:464:A:C8	2.56	0.41
25:A:472:U:H5''	59:K:11:THR:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:704:C:O2	25:A:705:U:H1'	2.20	0.41
25:A:819:G:O6	25:A:853:G:C6	2.74	0.41
29:AA:51:LEU:HB2	29:AA:65:ARG:HD2	2.02	0.41
1:AR:1438:U:H2'	1:AR:1439:U:H6	1.85	0.41
1:AR:1728:G:H5''	1:AR:1730:G:O4'	2.20	0.41
1:AR:1874:A:OP2	20:CT:20:ARG:HD3	2.21	0.41
1:AR:2370:G:H2'	1:AR:2371:G:O4'	2.20	0.41
1:AR:269:G:P	16:CP:44:ARG:HH22	2.43	0.41
1:AR:2774:C:H2'	1:AR:2775:U:H6	1.86	0.41
1:AR:407:A:C2	3:AT:17:A:H1'	2.55	0.41
1:AR:815:G:C6	1:AR:906:A:C4	3.09	0.41
1:AR:825:U:OP1	4:CD:21:ARG:NH1	2.51	0.41
2:AS:55:A:H2'	2:AS:56:A:O4'	2.20	0.41
3:AT:84:C:H4'	3:AT:85:G:C8	2.56	0.41
51:C:33:LYS:O	51:C:98:THR:HG22	2.20	0.41
4:CD:116:VAL:HA	4:CD:163:ARG:O	2.21	0.41
1:AR:2175:U:C4	4:CD:20:THR:OG1	2.74	0.41
5:CE:53:MET:CE	5:CE:327:CYS:HB3	2.51	0.41
8:CH:55:LEU:HD21	8:CH:145:LEU:HD11	2.03	0.41
9:CI:102:VAL:HG13	9:CI:126:LEU:HD22	2.01	0.41
9:CI:149:TYR:CD1	9:CI:181:ILE:HD13	2.56	0.41
10:CJ:41:GLN:HG3	10:CJ:44:ARG:NH1	2.36	0.41
11:CK:74:LEU:O	11:CK:78:MET:HG3	2.20	0.41
13:CM:20:ASN:HB3	13:CM:126:ASP:HB2	2.02	0.41
17:CQ:65:ASN:HB3	17:CQ:68:ARG:CD	2.51	0.41
1:AR:2730:G:H4'	19:CS:184:PHE:CG	2.56	0.41
22:CV:9:SER:OG	22:CV:10:ARG:HG3	2.20	0.41
28:DA:43:TYR:CE2	28:DA:109:LEU:HD12	2.55	0.41
29:DB:5:LEU:CD1	32:DE:35:ARG:HD2	2.51	0.41
37:DJ:70:TYR:CE2	37:DJ:77:PRO:HD3	2.56	0.41
53:E:55:THR:HG23	53:E:90:ARG:HG2	2.02	0.41
25:A:800:U:P	54:F:201:HIS:HE2	2.43	0.41
54:F:24:SER:OG	54:F:24:SER:O	2.35	0.41
57:I:10:SER:HB2	57:I:42:GLN:CD	2.41	0.41
59:K:159:ALA:HB3	59:K:162:SER:OG	2.20	0.41
60:L:88:PRO:C	60:L:90:THR:H	2.24	0.41
62:N:40:GLY:HA3	62:N:124:LYS:O	2.21	0.41
63:O:94:LYS:HG2	63:O:118:ILE:HD13	2.03	0.41
69:U:72:GLY:H	69:U:75:LYS:HB2	1.86	0.41
1:1:1658:G:O4'	1:1:1796:G:H2'	2.21	0.41
1:1:1711:C:H2'	1:1:1712:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2314:U:H2'	1:1:2314:U:H6	1.43	0.41
1:1:2403:G:C2	1:1:2405:C:C4	3.08	0.41
1:1:2413:A:H2'	1:1:2414:G:H8	1.86	0.41
1:1:2443:A:H2	38:AJ:63:ASN:ND2	2.18	0.41
1:1:3045:G:H2'	1:1:3046:A:O4'	2.20	0.41
1:1:423:A:N1	1:1:424:G:C2	2.89	0.41
1:1:439:C:C5	1:1:440:A:C6	3.09	0.41
1:1:725:G:C6	1:1:746:A:C6	3.08	0.41
3:4:41:A:O2'	39:AK:59:THR:HG22	2.21	0.41
25:6:1175:U:H2'	25:6:1176:G:C8	2.55	0.41
25:6:1235:C:OP2	25:6:1245:G:H8	2.04	0.41
25:6:1164:G:H1	25:6:1581:C:H42	1.68	0.41
25:6:542:A:H1'	25:6:543:C:C5'	2.47	0.41
25:6:922:G:H2'	25:6:923:A:C8	2.56	0.41
25:A:1193:A:H8	25:A:1193:A:OP1	2.04	0.41
25:A:1250:U:O2'	25:A:1251:U:OP1	2.36	0.41
25:A:328:A:H2'	25:A:329:G:O4'	2.21	0.41
25:A:720:G:H2'	25:A:720:G:N3	2.35	0.41
35:AG:38:PRO:HD3	35:AG:77:ASN:O	2.20	0.41
1:AR:1155:C:H2'	1:AR:1156:C:C6	2.56	0.41
1:AR:119:U:H4'	1:AR:120:G:H3'	2.03	0.41
1:AR:2203:U:H4'	4:CD:241:ARG:HA	2.02	0.41
1:AR:2683:U:H2'	1:AR:2684:C:C6	2.56	0.41
1:AR:2856:G:H2'	1:AR:2857:C:H6	1.85	0.41
1:AR:3094:A:H2'	1:AR:3095:U:C6	2.55	0.41
1:AR:3265:C:H2'	1:AR:3266:G:O4'	2.21	0.41
1:AR:378:A:N7	1:AR:391:A:H2	2.19	0.41
1:AR:654:C:H2'	1:AR:655:C:C6	2.56	0.41
1:AR:361:A:N3	1:AR:814:U:H1'	2.36	0.41
3:AT:141:C:H2'	3:AT:142:C:H6	1.85	0.41
5:CE:257:PRO:HG2	5:CE:261:MET:CE	2.51	0.41
5:CE:296:THR:HG21	5:CE:357:LYS:C	2.40	0.41
5:CE:311:PHE:N	5:CE:315:GLY:O	2.54	0.41
6:CF:290:ILE:HG23	19:CS:35:PHE:CE2	2.56	0.41
7:CG:41:LYS:HA	7:CG:41:LYS:HE2	2.01	0.41
7:CG:68:THR:HG22	7:CG:70:THR:H	1.84	0.41
10:CJ:64:ILE:O	10:CJ:68:ARG:HG2	2.21	0.41
10:CJ:71:VAL:HG12	10:CJ:235:GLY:HA3	2.02	0.41
12:CL:51:HIS:O	12:CL:165:ILE:HA	2.21	0.41
12:CL:76:MET:HE2	12:CL:148:VAL:HG22	2.03	0.41
16:CP:143:ARG:HH21	37:DJ:92:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:CQ:138:LEU:HD12	17:CQ:138:LEU:HA	1.79	0.41
1:AR:2555:G:N2	29:DB:135:ARG:O	2.43	0.41
53:E:135:GLU:HG3	53:E:153:ALA:HB2	2.02	0.41
55:G:128:ASN:HB3	55:G:130:ILE:HG22	2.03	0.41
55:G:49:GLU:O	55:G:51:VAL:HG23	2.21	0.41
56:H:3:LEU:N	56:H:16:PHE:O	2.40	0.41
57:I:97:ARG:O	57:I:98:ILE:C	2.59	0.41
66:R:46:PHE:HA	66:R:49:TYR:HB2	2.02	0.41
66:R:22:VAL:HG13	66:R:65:ILE:HD13	2.03	0.41
50:B:198:MET:SD	67:S:88:VAL:HB	2.61	0.41
1:1:1017:C:OP2	1:1:1017:C:H2'	2.21	0.41
1:1:1825:G:OP2	40:AL:49:SER:OG	2.37	0.41
1:1:2158:A:O4'	1:1:2160:G:C8	2.74	0.41
1:1:237:G:H2'	1:1:238:A:O4'	2.20	0.41
1:1:2623:G:H2'	1:1:2624:G:H8	1.86	0.41
1:1:2677:G:H2'	1:1:2679:A:H2	1.86	0.41
1:1:885:U:H2'	1:1:886:C:H6	1.86	0.41
25:6:1013:A:H2'	25:6:1014:G:O4'	2.21	0.41
25:A:1147:A:H2'	25:A:1148:C:H6	1.85	0.41
25:A:304:U:H2'	25:A:305:C:C6	2.55	0.41
25:A:609:U:H4'	25:A:610:G:O5'	2.20	0.41
25:A:627:C:H2'	25:A:628:G:O4'	2.21	0.41
29:AA:95:VAL:HG21	29:AA:113:VAL:HG11	2.03	0.41
30:AB:78:LEU:O	30:AB:78:LEU:HD22	2.21	0.41
30:AB:94:ALA:HB1	30:AB:121:VAL:HA	2.03	0.41
31:AC:14:ARG:NH2	31:AC:18:ARG:HD2	2.36	0.41
31:AC:21:ILE:HG12	31:AC:21:ILE:H	1.52	0.41
34:AF:32:TRP:CZ2	34:AF:53:PRO:HD2	2.56	0.41
34:AF:8:LYS:HE3	34:AF:8:LYS:HB2	1.91	0.41
38:AJ:89:GLU:O	38:AJ:93:ILE:HG12	2.20	0.41
39:AK:30:GLN:HE21	39:AK:30:GLN:HB3	1.72	0.41
1:AR:1258:U:O2	1:AR:1260:A:H8	2.04	0.41
1:AR:2430:A:H2'	1:AR:2431:C:C6	2.55	0.41
1:AR:2984:C:H2'	1:AR:2985:C:H6	1.86	0.41
1:AR:299:G:N7	84:AR:3687:OHX:N1	2.69	0.41
1:AR:3353:G:H1'	1:AR:3356:G:O4'	2.21	0.41
1:AR:664:U:H2'	1:AR:665:A:C8	2.55	0.41
2:AS:27:A:H2'	2:AS:28:C:C6	2.56	0.41
6:CF:262:TRP:CZ3	6:CF:271:LYS:HE3	2.56	0.41
11:CK:147:SER:HB2	11:CK:187:ILE:HD11	2.03	0.41
13:CM:49:LYS:HB3	13:CM:62:ASN:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:CN:46:ILE:HD12	14:CN:49:ARG:HH12	1.86	0.41
1:AR:3243:A:C5	17:CQ:156:LEU:HB3	2.56	0.41
18:CR:112:LEU:HA	18:CR:151:THR:O	2.21	0.41
20:CT:77:GLY:O	20:CT:81:ARG:HD2	2.21	0.41
52:D:179:VAL:O	52:D:198:THR:OG1	2.35	0.41
1:AR:1178:G:O6	35:DH:20:LYS:NZ	2.54	0.41
1:AR:3215:A:H5''	35:DH:2:ALA:HB2	2.03	0.41
40:DM:46:ARG:HA	40:DM:51:LEU:HD12	2.02	0.41
42:DO:127:LEU:O	42:DO:128:LYS:HG2	2.21	0.41
61:M:93:TYR:HB2	61:M:100:TYR:CE2	2.56	0.41
66:R:35:PRO:HG2	66:R:38:LEU:HG	2.02	0.41
72:X:30:SER:HB2	72:X:61:ILE:CG1	2.46	0.41
21:O:117:ARG:HG2	21:O:117:ARG:H	1.61	0.41
1:1:1240:A:H3'	1:1:1241:U:H5'	2.02	0.41
1:1:3366:G:H2'	1:1:3367:C:C6	2.56	0.41
1:1:727:G:H2'	1:1:728:G:O4'	2.20	0.41
22:2:131:GLN:HA	22:2:132:PRO:HD3	1.95	0.41
22:2:17:ARG:HG3	22:2:22:HIS:HA	2.03	0.41
2:3:103:A:H2'	2:3:104:A:O4'	2.21	0.41
3:4:30:C:H2'	3:4:31:G:H8	1.86	0.41
23:5:93:ILE:HA	23:5:106:ALA:O	2.21	0.41
25:6:1299:G:C6	25:6:1300:A:N6	2.89	0.41
25:6:1620:C:H2'	25:6:1621:U:C6	2.56	0.41
25:6:760:A:H2'	25:6:761:G:O4'	2.21	0.41
25:A:1059:U:O2'	25:A:1060:U:N3	2.54	0.41
25:A:1226:A:HO2'	25:A:1227:A:P	2.43	0.41
25:A:566:C:H2'	25:A:567:A:O4'	2.21	0.41
25:A:67:A:C2	25:A:69:G:H1'	2.56	0.41
25:A:705:U:H2'	25:A:706:A:N7	2.35	0.41
25:A:763:G:C6	25:A:764:U:C4	3.09	0.41
30:AB:94:ALA:HB1	30:AB:122:PRO:HD3	2.03	0.41
1:AR:1804:A:H2'	1:AR:1805:C:C6	2.55	0.41
1:AR:2674:A:H5''	13:CM:105:GLY:HA3	2.03	0.41
1:AR:2923:U:H2'	1:AR:2924:U:C6	2.54	0.41
1:AR:113:C:C2	1:AR:319:A:C2	3.09	0.41
1:AR:3378:C:H2'	1:AR:3379:C:C6	2.56	0.41
84:AR:3501:OHX:N3	84:AR:3590:OHX:N1	2.69	0.41
1:AR:655:C:P	34:DG:27:ARG:HB3	2.61	0.41
1:AR:873:C:H5''	1:AR:874:U:O5'	2.20	0.41
1:AR:916:G:H4'	1:AR:917:A:O5'	2.21	0.41
3:AT:126:A:O2'	3:AT:129:C:N4	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:B:137:SER:O	71:W:30:ALA:HA	2.21	0.41
6:CF:180:LYS:HE3	6:CF:180:LYS:HB3	1.86	0.41
9:CI:191:VAL:HG22	9:CI:195:PHE:CE2	2.56	0.41
11:CK:41:ILE:HG21	11:CK:71:VAL:HG21	2.03	0.41
17:CQ:156:LEU:HA	17:CQ:156:LEU:HD23	1.85	0.41
18:CR:88:VAL:O	18:CR:92:GLN:HG2	2.21	0.41
1:AR:2093:A:P	20:CT:143:ILE:HG23	2.61	0.41
24:CX:13:ILE:HD13	24:CX:54:LEU:HB3	2.03	0.41
52:D:218:ILE:H	52:D:218:ILE:HG13	1.52	0.41
29:DB:51:LEU:HB2	29:DB:65:ARG:HB3	2.02	0.41
35:DH:53:TYR:CZ	35:DH:65:ARG:HB2	2.55	0.41
29:DB:136:PHE:CD2	36:DI:89:ILE:HG12	2.55	0.41
37:DJ:71:LYS:HE3	37:DJ:72:GLY:H	1.85	0.41
40:DM:20:VAL:HG12	40:DM:73:LEU:HD11	2.02	0.41
45:DR:8:VAL:O	45:DR:27:LYS:HD2	2.21	0.41
25:A:788:A:P	54:F:106:LYS:HZ2	2.40	0.41
54:F:143:ASP:OD1	54:F:143:ASP:N	2.49	0.41
56:H:148:SER:O	56:H:148:SER:OG	2.34	0.41
57:I:86:GLN:HG2	57:I:87:ASP:H	1.86	0.41
59:K:38:ASN:HB2	59:K:41:GLU:HG3	2.03	0.41
60:L:1:MET:HG2	60:L:2:LEU:H	1.86	0.41
21:O:155:ARG:HH21	21:O:172:TYR:HA	1.86	0.40
1:1:1069:C:H2'	1:1:1070:U:C6	2.56	0.40
1:1:1571:A:H2'	1:1:1572:U:O4'	2.20	0.40
1:1:1602:A:C6	1:1:1603:A:C6	3.09	0.40
1:1:1611:G:H2'	1:1:1612:A:H8	1.85	0.40
1:1:3139:A:N6	1:1:3140:G:C2	2.89	0.40
1:1:3350:C:O2'	1:1:3351:U:O5'	2.32	0.40
1:1:350:C:N3	1:1:367:A:H2'	2.36	0.40
1:1:653:A:C2	1:1:1443:G:C4	3.09	0.40
1:1:65:A:H3'	1:1:111:C:H41	1.86	0.40
2:3:22:A:C6	2:3:23:A:C6	3.09	0.40
25:6:209:U:H2'	25:6:210:A:C8	2.57	0.40
25:6:272:U:H4'	25:6:273:G:O5'	2.20	0.40
25:A:617:U:O4'	25:A:1031:U:C2	2.74	0.40
25:A:1079:U:H2'	25:A:1080:U:C6	2.57	0.40
25:A:1323:C:H2'	25:A:1324:G:O4'	2.21	0.40
25:A:1381:U:H4'	70:V:59:PRO:HG3	2.03	0.40
25:A:327:U:O2'	61:M:10:GLU:HG2	2.20	0.40
25:A:641:G:H1	25:A:693:U:H3	1.69	0.40
25:A:919:A:H5'	64:P:18:ARG:HH12	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:AK:14:LYS:HZ1	41:AM:51:ILE:HG13	1.85	0.40
1:AR:1284:C:O2'	1:AR:1285:G:OP1	2.36	0.40
1:AR:1374:G:O6	30:DC:10:LYS:NZ	2.48	0.40
1:AR:2537:U:H6	1:AR:2537:U:H2'	1.64	0.40
1:AR:3218:A:H4'	1:AR:3219:G:O5'	2.20	0.40
1:AR:3317:U:H5'	1:AR:3318:G:C2	2.56	0.40
1:AR:537:A:H2'	1:AR:538:G:O4'	2.21	0.40
1:AR:65:A:H4'	1:AR:66:A:O5'	2.21	0.40
50:B:62:ARG:HE	71:W:39:VAL:HG13	1.85	0.40
5:CE:308:MET:HB3	5:CE:308:MET:HE3	1.72	0.40
10:CJ:107:GLU:HG2	10:CJ:111:LYS:HE3	2.03	0.40
14:CN:126:PHE:HZ	14:CN:135:ALA:HB2	1.86	0.40
1:AR:267:G:H4'	16:CP:50:ARG:HH11	1.85	0.40
18:CR:101:ASN:O	18:CR:105:LYS:HB2	2.21	0.40
18:CR:56:ARG:NH1	18:CR:75:GLU:OE2	2.54	0.40
1:AR:563:U:OP1	21:CU:71:LYS:NZ	2.54	0.40
1:AR:1062:A:H4'	22:CV:105:PHE:CE1	2.55	0.40
32:DE:13:LYS:HA	32:DE:13:LYS:HD3	1.88	0.40
34:DG:61:LYS:HE2	34:DG:61:LYS:HB2	1.86	0.40
37:DJ:85:THR:HG22	37:DJ:88:LEU:H	1.85	0.40
54:F:90:ILE:HB	54:F:99:PHE:HB2	2.02	0.40
58:J:26:LYS:HD2	58:J:29:LEU:HD13	2.02	0.40
59:K:128:LEU:O	59:K:133:HIS:HB2	2.21	0.40
25:A:461:G:OP1	59:K:2:PRO:HG2	2.21	0.40
61:M:4:GLU:O	61:M:5:LEU:HB2	2.21	0.40
25:A:886:U:O2'	64:P:121:VAL:O	2.38	0.40
66:R:25:GLY:H	66:R:63:ILE:HA	1.87	0.40
25:A:611:U:OP1	73:Y:19:ARG:NH2	2.54	0.40
73:Y:30:LYS:O	73:Y:34:LEU:HG	2.21	0.40
21:O:16:THR:HG23	21:O:19:VAL:HB	2.04	0.40
1:1:1083:G:C2	1:1:1084:A:C4	3.09	0.40
1:1:1129:A:OP1	66:R:13:LYS:NZ	133.29	0.40
1:1:1230:G:O6	1:1:1231:A:N6	2.54	0.40
1:1:1581:C:H2'	1:1:1582:C:C5'	2.51	0.40
1:1:2314:U:O2'	1:1:2315:G:OP1	2.32	0.40
1:1:2877:G:H2'	1:1:2878:G:O4'	2.21	0.40
1:1:291:C:H5''	70:V:68:ARG:NH1	120.58	0.40
1:1:397:A:H5'	1:1:399:A:OP1	2.22	0.40
1:1:3:U:C2	3:4:157:U:C2	3.09	0.40
1:1:532:A:C8	1:1:555:U:C4	3.10	0.40
1:1:2585:G:N3	3:4:151:C:H5	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:1532:U:H2'	25:6:1533:C:O4'	2.21	0.40
25:6:1203:A:C6	25:6:1555:A:C6	3.10	0.40
25:6:542:A:C8	25:6:543:C:H5'	2.57	0.40
25:6:69:G:H2'	25:6:70:C:O4'	2.21	0.40
27:8:47:ALA:HB3	37:AI:77:PRO:HG3	2.02	0.40
25:A:1157:A:H2'	25:A:1160:A:N7	2.35	0.40
25:A:632:U:OP2	61:M:102:LYS:NZ	2.52	0.40
25:A:992:A:C2	25:A:1012:U:N3	2.74	0.40
1:1:750:G:P	31:AC:40:ARG:HH21	2.42	0.40
37:AI:70:TYR:CE1	37:AI:77:PRO:HD3	2.57	0.40
40:AL:46:ARG:NH1	40:AL:47:GLY:O	2.53	0.40
1:AR:1615:C:H2'	1:AR:1616:U:C6	2.55	0.40
1:AR:1711:C:H2'	1:AR:1712:G:O4'	2.21	0.40
1:AR:53:G:P	39:DL:48:ASN:HD22	2.44	0.40
1:AR:634:C:H5'	35:DH:21:ARG:O	2.20	0.40
1:AR:610:G:C8	6:CF:312:VAL:HG21	2.56	0.40
6:CF:351:PRO:HA	9:CI:71:ALA:HA	2.02	0.40
6:CF:47:ARG:NH1	6:CF:109:TRP:O	2.54	0.40
7:CG:211:LEU:HD23	7:CG:211:LEU:HA	1.88	0.40
12:CL:76:MET:HE2	12:CL:138:VAL:HG11	2.03	0.40
16:CP:48:ALA:C	16:CP:53:TYR:HB3	2.41	0.40
18:CR:22:LEU:HD12	18:CR:146:ILE:HG13	2.02	0.40
19:CS:96:PHE:CE2	19:CS:114:ILE:HA	2.57	0.40
52:D:143:TYR:CE2	52:D:151:PRO:HG3	2.56	0.40
52:D:57:PHE:CZ	52:D:138:PRO:HD3	2.57	0.40
29:DB:110:ALA:O	29:DB:114:VAL:HG23	2.22	0.40
34:DG:82:LEU:HD11	34:DG:112:ALA:HB2	2.03	0.40
36:DI:102:LYS:HB3	36:DI:103:LYS:HE3	2.02	0.40
54:F:43:PRO:HA	54:F:82:TYR:O	2.21	0.40
56:H:87:ARG:HA	56:H:87:ARG:HD3	1.93	0.40
57:I:9:LEU:HD21	57:I:17:GLU:OE1	2.21	0.40
59:K:117:GLY:O	59:K:119:ALA:N	2.53	0.40
25:A:1199:G:N7	70:V:67:THR:HG23	2.36	0.40
1:1:1064:A:H5''	1:1:1066:G:O4'	2.22	0.40
1:1:1245:A:C3'	1:1:1246:G:H5''	2.51	0.40
1:1:1498:A:H2'	1:1:1499:C:C6	2.56	0.40
1:1:1583:A:H5''	1:1:1584:U:OP2	2.21	0.40
1:1:2623:G:H2'	1:1:2624:G:O4'	2.22	0.40
1:1:3056:U:O2	33:AE:28:ARG:NH1	2.55	0.40
1:1:531:G:N2	1:1:532:A:N3	2.70	0.40
21:0:26:ARG:N	22:2:149:GLN:O	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:6:U:H2'	3:4:7:U:C6	2.56	0.40
25:6:1031:U:H4'	25:6:1032:G:OP2	2.20	0.40
25:6:1354:G:H5'	25:6:1355:C:OP2	2.21	0.40
25:6:21:U:H2'	25:6:22:A:C8	2.56	0.40
25:6:922:G:H2'	25:6:923:A:H8	1.87	0.40
25:A:179:A:H2'	25:A:180:A:O4'	2.21	0.40
25:A:327:U:H2'	25:A:328:A:C8	2.56	0.40
25:A:489:C:H2'	25:A:490:C:C6	2.56	0.40
1:1:1638:A:OP2	29:AA:16:GLY:HA2	2.22	0.40
1:AR:65:A:H3'	1:AR:111:C:N4	2.36	0.40
1:AR:2249:G:C8	1:AR:2272:G:C8	3.09	0.40
1:AR:2279:A:O5'	1:AR:2280:A:H5'	2.20	0.40
1:AR:2694:A:N6	1:AR:2695:A:C6	2.90	0.40
1:AR:2743:A:H2'	1:AR:2744:U:O4'	2.22	0.40
1:AR:3041:U:H2'	1:AR:3042:U:C6	2.56	0.40
1:AR:3275:U:H5	1:AR:3276:G:H21	1.70	0.40
1:AR:3353:G:H1'	1:AR:3356:G:H5'	2.04	0.40
1:AR:550:A:N1	1:AR:551:A:N6	2.70	0.40
2:AS:28:C:H5''	13:CM:137:ARG:HG2	2.04	0.40
4:CD:49:VAL:HG22	4:CD:50:HIS:H	1.86	0.40
5:CE:252:ILE:HA	5:CE:252:ILE:HD12	1.65	0.40
5:CE:227:GLU:HG2	5:CE:270:ARG:HD3	2.04	0.40
5:CE:35:ASP:OD2	5:CE:37:ARG:HD2	2.22	0.40
7:CG:61:ILE:HG12	7:CG:79:TYR:CD2	2.56	0.40
10:CJ:148:ALA:HA	10:CJ:201:THR:HG22	2.02	0.40
10:CJ:166:LEU:HD23	10:CJ:166:LEU:HA	1.93	0.40
12:CL:170:LYS:HE2	12:CL:177:ASP:OD1	2.21	0.40
13:CM:35:LYS:HE3	13:CM:35:LYS:HB2	1.87	0.40
31:DD:21:ILE:H	31:DD:21:ILE:HG12	1.50	0.40
36:DI:42:PRO:HG2	36:DI:54:ILE:HG21	2.03	0.40
38:DK:66:GLU:O	38:DK:70:ARG:HB2	2.22	0.40
57:I:14:THR:OG1	57:I:15:GLU:N	2.54	0.40
57:I:38:LEU:HD23	57:I:41:LEU:HD12	2.04	0.40
65:Q:87:PRO:HA	65:Q:90:ILE:HG13	2.02	0.40
1:1:2539:C:H5'	1:1:2541:U:O4	2.21	0.40
1:1:2946:A:C5'	1:1:2947:G:H5'	2.51	0.40
1:1:2995:A:H2'	1:1:2996:U:H5''	2.04	0.40
1:1:3166:C:N4	1:1:3284:G:H1	2.10	0.40
1:1:380:U:H2'	1:1:381:U:C6	2.57	0.40
1:1:573:C:H2'	1:1:574:U:C6	2.57	0.40
1:1:824:C:H2'	1:1:825:U:H6	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:1081:A:O2'	25:6:1082:C:O5'	2.39	0.40
25:6:1402:G:H2'	25:6:1403:C:C6	2.57	0.40
25:6:1461:C:H2'	25:6:1462:G:C8	2.56	0.40
25:6:577:G:C6	84:6:2013:OHX:N6	2.89	0.40
25:6:235:G:H2'	25:6:236:A:C8	2.56	0.40
25:6:892:A:H2'	25:6:893:U:O4'	2.22	0.40
25:A:195:G:H2'	25:A:196:G:H5'	2.03	0.40
25:A:355:G:OP2	84:A:1914:OHX:N4	2.55	0.40
25:A:460:A:H5'	25:A:461:G:OP2	2.21	0.40
25:A:704:C:N4	25:A:735:C:C2	2.90	0.40
25:A:955:A:H2'	25:A:956:C:O4'	2.21	0.40
29:AA:46:ILE:HD11	29:AA:48:ARG:C	2.41	0.40
29:AA:5:LEU:HA	29:AA:5:LEU:HD23	1.75	0.40
30:AB:97:GLU:O	30:AB:98:THR:HG23	2.22	0.40
1:1:157:A:C8	38:AJ:26:ILE:HG12	2.57	0.40
44:AP:9:LYS:HE3	44:AP:9:LYS:HB2	1.72	0.40
1:AR:1768:U:H2'	1:AR:1769:G:O4'	2.22	0.40
1:AR:2780:A:H2'	1:AR:2781:U:C6	2.57	0.40
1:AR:3051:U:C2	1:AR:3052:G:C8	3.10	0.40
1:AR:3194:C:O2'	1:AR:3195:U:H2'	2.21	0.40
84:AR:3566:OHX:N5	84:AR:3642:OHX:N6	2.70	0.40
1:AR:68:C:O3'	16:CP:177:GLY:HA2	2.22	0.40
1:AR:873:C:H4'	1:AR:874:U:OP2	2.20	0.40
1:AR:908:G:H4'	1:AR:909:G:O5'	2.22	0.40
1:AR:956:U:H2'	1:AR:957:C:C6	2.57	0.40
50:B:101:ARG:HG2	50:B:103:THR:H	1.86	0.40
6:CF:233:LEU:HD23	6:CF:233:LEU:HA	1.77	0.40
1:AR:121:A:C6	10:CJ:129:PRO:HG3	2.56	0.40
11:CK:41:ILE:HG23	11:CK:43:VAL:HG13	2.02	0.40
15:CO:135:LEU:HD22	15:CO:135:LEU:HA	1.90	0.40
16:CP:183:THR:O	16:CP:183:THR:OG1	2.38	0.40
18:CR:112:LEU:HD12	18:CR:112:LEU:HA	1.85	0.40
1:AR:3276:G:O6	18:CR:171:ARG:HD2	2.22	0.40
21:CU:42:TRP:O	21:CU:46:GLN:HG3	2.21	0.40
23:CW:29:ASP:OD2	23:CW:31:ALA:HB3	2.21	0.40
29:DB:133:LYS:HE3	29:DB:135:ARG:HG2	2.03	0.40
39:DL:65:ARG:HG3	39:DL:65:ARG:HH11	1.87	0.40
53:E:172:THR:HA	53:E:184:ILE:O	2.21	0.40
55:G:156:ARG:H	55:G:156:ARG:HG3	1.59	0.40
56:H:64:LYS:O	56:H:100:ALA:HB2	2.22	0.40
58:J:113:PHE:HB3	58:J:121:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:J:136:SER:HB3	58:J:139:ALA:HB3	2.02	0.40
59:K:34:PHE:CD1	59:K:105:LEU:HD23	2.57	0.40
66:R:47:LYS:HD2	66:R:47:LYS:HA	1.84	0.40
21:O:8:GLN:HG3	21:O:26:ARG:HE	1.87	0.40
1:1:1115:G:H5'	1:1:1116:G:C5'	2.51	0.40
1:1:1668:G:H2'	1:1:1669:C:O4'	2.21	0.40
1:1:2373:A:H3'	1:1:2373:A:OP2	2.21	0.40
1:1:2710:C:H2'	1:1:2711:C:C6	2.57	0.40
1:1:2896:A:H4'	42:AN:95:VAL:HG11	2.03	0.40
1:1:3013:U:H2'	1:1:3014:U:C6	2.57	0.40
1:1:385:A:C6	1:1:386:A:C6	3.09	0.40
1:1:595:G:C8	1:1:609:G:C6	3.10	0.40
3:4:45:C:H2'	3:4:46:G:O4'	2.22	0.40
25:6:1045:C:C2	25:6:1074:G:C2	3.09	0.40
25:6:1244:A:H4'	25:6:1245:G:OP1	2.21	0.40
25:6:1780:G:H3'	25:6:1781:A:H8	1.86	0.40
84:6:1975:OHX:N6	84:6:2025:OHX:N3	2.69	0.40
25:6:389:G:C6	25:6:390:G:C5	3.10	0.40
25:6:811:A:C4	25:6:858:G:H1'	2.57	0.40
25:6:946:U:H2'	25:6:947:U:C6	2.56	0.40
25:A:1481:C:O2'	25:A:1482:C:O5'	2.32	0.40
25:A:552:G:C6	25:A:553:G:C6	3.09	0.40
25:A:577:G:C8	25:A:577:G:H3'	2.57	0.40
25:A:701:U:H3	25:A:737:A:H61	1.68	0.40
36:AH:86:LYS:O	36:AH:90:ILE:HG13	2.21	0.40
38:AJ:45:ARG:NH2	38:AJ:54:GLU:OE1	2.54	0.40
1:AR:172:G:H3'	1:AR:173:G:H5'	2.02	0.40
1:AR:1952:G:H8	1:AR:1952:G:OP2	2.04	0.40
1:AR:2663:G:H2'	1:AR:2664:C:O4'	2.21	0.40
1:AR:2746:A:H2	7:CG:146:LEU:HB3	1.86	0.40
1:AR:306:A:C2	1:AR:2784:G:H1'	2.57	0.40
1:AR:92:G:OP1	44:DQ:46:LYS:NZ	2.44	0.40
50:B:13:ASP:HA	50:B:16:LEU:HD12	2.03	0.40
51:C:157:GLN:O	51:C:159:SER:N	2.54	0.40
4:CD:19:HIS:N	4:CD:19:HIS:ND1	2.70	0.40
5:CE:232:ARG:HG2	5:CE:233:TRP:CD1	2.57	0.40
5:CE:53:MET:CG	5:CE:77:THR:HG22	2.47	0.40
7:CG:148:ILE:HG12	7:CG:159:VAL:HG21	2.03	0.40
10:CJ:34:PHE:CD1	10:CJ:42:PRO:HD3	2.57	0.40
10:CJ:47:SER:O	10:CJ:50:VAL:HG12	2.21	0.40
10:CJ:48:ARG:HH21	10:CJ:49:TYR:HE1	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:1212:A:OP1	11:CK:1:MET:HB3	2.22	0.40
11:CK:9:GLN:HG2	11:CK:52:LEU:HD11	2.02	0.40
14:CN:116:LEU:HA	14:CN:116:LEU:HD23	1.95	0.40
14:CN:67:ARG:HG3	14:CN:67:ARG:H	1.40	0.40
16:CP:10:LEU:HA	16:CP:10:LEU:HD23	1.90	0.40
17:CQ:85:ARG:HD3	17:CQ:90:HIS:CG	2.56	0.40
18:CR:13:LYS:HE2	18:CR:13:LYS:HB3	1.89	0.40
22:CV:100:LYS:HD2	22:CV:103:GLN:OE1	2.22	0.40
33:DF:19:ARG:HD3	33:DF:35:GLU:CG	2.50	0.40
35:DH:6:ARG:HG3	35:DH:8:TYR:CD2	2.57	0.40
44:DQ:46:LYS:O	44:DQ:54:THR:HG21	2.21	0.40
55:G:62:VAL:HG13	55:G:89:ILE:HG21	2.04	0.40
61:M:34:TRP:HH2	61:M:36:LYS:HD3	1.87	0.40
61:M:84:ILE:HG13	61:M:109:VAL:HG13	2.04	0.40
62:N:108:ARG:O	62:N:110:GLY:N	2.55	0.40
70:V:18:GLN:O	70:V:96:PRO:HA	2.22	0.40
71:W:35:ASN:HB3	71:W:50:TYR:CD1	2.57	0.40
72:X:36:LYS:O	72:X:40:VAL:HG23	2.21	0.40
72:X:26:LEU:HD21	72:X:60:LYS:HD3	2.02	0.40
54:F:53:LYS:O	74:Z:22:GLN:NE2	2.53	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%)	226 (90%)	23 (9%)	1 (0%)	38	75
4	j	250/252 (99%)	230 (92%)	19 (8%)	1 (0%)	38	75
5	CE	384/386 (100%)	349 (91%)	31 (8%)	4 (1%)	18	57
5	k	384/386 (100%)	348 (91%)	33 (9%)	3 (1%)	22	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	CF	359/361 (99%)	326 (91%)	33 (9%)	0	100	100
6	l	359/361 (99%)	320 (89%)	37 (10%)	2 (1%)	28	67
7	CG	294/296 (99%)	254 (86%)	38 (13%)	2 (1%)	25	64
7	m	294/296 (99%)	263 (90%)	30 (10%)	1 (0%)	44	79
8	CH	152/175 (87%)	139 (91%)	12 (8%)	1 (1%)	25	64
8	n	152/175 (87%)	145 (95%)	6 (4%)	1 (1%)	25	64
9	CI	220/222 (99%)	199 (90%)	16 (7%)	5 (2%)	7	33
9	o	220/222 (99%)	204 (93%)	13 (6%)	3 (1%)	13	47
10	CJ	231/233 (99%)	201 (87%)	28 (12%)	2 (1%)	20	60
10	p	231/233 (99%)	207 (90%)	24 (10%)	0	100	100
11	CK	189/191 (99%)	176 (93%)	13 (7%)	0	100	100
11	q	189/191 (99%)	168 (89%)	21 (11%)	0	100	100
12	CL	207/220 (94%)	188 (91%)	19 (9%)	0	100	100
12	r	207/220 (94%)	189 (91%)	17 (8%)	1 (0%)	32	71
13	CM	167/169 (99%)	145 (87%)	19 (11%)	3 (2%)	10	40
13	s	167/169 (99%)	137 (82%)	23 (14%)	7 (4%)	3	19
14	CN	191/193 (99%)	168 (88%)	17 (9%)	6 (3%)	5	26
14	t	191/193 (99%)	171 (90%)	13 (7%)	7 (4%)	4	22
15	CO	134/136 (98%)	122 (91%)	11 (8%)	1 (1%)	25	64
15	u	134/136 (98%)	120 (90%)	13 (10%)	1 (1%)	25	64
16	CP	201/203 (99%)	188 (94%)	13 (6%)	0	100	100
16	v	201/203 (99%)	177 (88%)	23 (11%)	1 (0%)	32	71
17	CQ	195/197 (99%)	185 (95%)	8 (4%)	2 (1%)	18	57
17	w	195/197 (99%)	187 (96%)	6 (3%)	2 (1%)	18	57
18	CR	181/183 (99%)	161 (89%)	17 (9%)	3 (2%)	11	42
18	x	181/183 (99%)	164 (91%)	17 (9%)	0	100	100
19	CS	183/185 (99%)	166 (91%)	16 (9%)	1 (0%)	32	71
19	y	183/185 (99%)	167 (91%)	16 (9%)	0	100	100
20	CT	186/188 (99%)	171 (92%)	15 (8%)	0	100	100
20	z	186/188 (99%)	175 (94%)	11 (6%)	0	100	100
21	0	170/172 (99%)	158 (93%)	11 (6%)	1 (1%)	28	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	CU	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
22	2	157/159 (99%)	142 (90%)	13 (8%)	2 (1%)	14	48
22	CV	157/159 (99%)	146 (93%)	10 (6%)	1 (1%)	28	67
23	5	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
23	CW	98/100 (98%)	81 (83%)	16 (16%)	1 (1%)	18	57
24	CX	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
24	IR	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
26	7	96/98 (98%)	83 (86%)	13 (14%)	0	100	100
26	CY	96/98 (98%)	79 (82%)	15 (16%)	2 (2%)	8	36
27	8	119/121 (98%)	108 (91%)	11 (9%)	0	100	100
27	CZ	119/121 (98%)	111 (93%)	8 (7%)	0	100	100
28	9	124/126 (98%)	113 (91%)	11 (9%)	0	100	100
28	DA	124/126 (98%)	119 (96%)	5 (4%)	0	100	100
29	AA	133/135 (98%)	115 (86%)	15 (11%)	3 (2%)	7	33
29	DB	133/135 (98%)	119 (90%)	10 (8%)	4 (3%)	5	27
30	AB	146/148 (99%)	125 (86%)	19 (13%)	2 (1%)	13	47
30	DC	146/148 (99%)	123 (84%)	21 (14%)	2 (1%)	13	47
31	AC	56/58 (97%)	48 (86%)	8 (14%)	0	100	100
31	DD	56/58 (97%)	50 (89%)	5 (9%)	1 (2%)	10	40
32	AD	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
32	DE	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
33	AE	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	20	60
33	DF	107/109 (98%)	99 (92%)	7 (6%)	1 (1%)	20	60
34	AF	125/127 (98%)	116 (93%)	9 (7%)	0	100	100
34	DG	125/127 (98%)	119 (95%)	6 (5%)	0	100	100
35	AG	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
35	DH	104/106 (98%)	99 (95%)	4 (4%)	1 (1%)	18	57
36	AH	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
36	DI	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
37	AI	117/119 (98%)	104 (89%)	12 (10%)	1 (1%)	20	60
37	DJ	117/119 (98%)	109 (93%)	7 (6%)	1 (1%)	20	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	AJ	97/99 (98%)	83 (86%)	11 (11%)	3 (3%)	5	26
38	DK	97/99 (98%)	84 (87%)	13 (13%)	0	100	100
39	AK	85/87 (98%)	77 (91%)	8 (9%)	0	100	100
39	DL	85/87 (98%)	79 (93%)	6 (7%)	0	100	100
40	AL	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
40	DM	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
41	AM	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
41	DN	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
42	AN	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
42	DO	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
43	AO	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
43	DP	23/25 (92%)	23 (100%)	0	0	100	100
44	AP	103/105 (98%)	84 (82%)	19 (18%)	0	100	100
44	DQ	103/105 (98%)	88 (85%)	15 (15%)	0	100	100
45	AQ	89/91 (98%)	79 (89%)	10 (11%)	0	100	100
45	DR	89/91 (98%)	82 (92%)	7 (8%)	0	100	100
46	i	155/272 (57%)	121 (78%)	30 (19%)	4 (3%)	6	31
48	sM	61/104 (59%)	45 (74%)	14 (23%)	2 (3%)	4	25
49	p0	139/311 (45%)	131 (94%)	8 (6%)	0	100	100
50	B	204/206 (99%)	157 (77%)	40 (20%)	7 (3%)	4	24
50	s0	204/206 (99%)	172 (84%)	30 (15%)	2 (1%)	18	57
51	C	212/216 (98%)	167 (79%)	43 (20%)	2 (1%)	20	60
51	s1	214/216 (99%)	190 (89%)	23 (11%)	1 (0%)	32	71
52	D	215/217 (99%)	189 (88%)	25 (12%)	1 (0%)	32	71
52	s2	215/217 (99%)	190 (88%)	23 (11%)	2 (1%)	20	60
53	E	221/223 (99%)	200 (90%)	19 (9%)	2 (1%)	20	60
53	s3	221/223 (99%)	195 (88%)	22 (10%)	4 (2%)	10	40
54	F	258/260 (99%)	233 (90%)	25 (10%)	0	100	100
54	s4	258/260 (99%)	229 (89%)	28 (11%)	1 (0%)	38	75
55	G	204/206 (99%)	166 (81%)	36 (18%)	2 (1%)	18	57
55	s5	204/206 (99%)	168 (82%)	36 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	H	224/226 (99%)	202 (90%)	19 (8%)	3 (1%)	14	48
56	s6	216/226 (96%)	199 (92%)	15 (7%)	2 (1%)	20	60
57	I	182/186 (98%)	154 (85%)	25 (14%)	3 (2%)	11	43
57	s7	184/186 (99%)	158 (86%)	21 (11%)	5 (3%)	6	30
58	J	184/199 (92%)	159 (86%)	21 (11%)	4 (2%)	8	35
58	s8	184/199 (92%)	159 (86%)	23 (12%)	2 (1%)	17	54
59	K	183/185 (99%)	160 (87%)	21 (12%)	2 (1%)	17	54
59	s9	183/185 (99%)	161 (88%)	22 (12%)	0	100	100
60	L	94/105 (90%)	70 (74%)	23 (24%)	1 (1%)	17	54
60	c0	92/105 (88%)	61 (66%)	25 (27%)	6 (6%)	1	9
61	M	153/155 (99%)	137 (90%)	14 (9%)	2 (1%)	14	48
61	c1	144/155 (93%)	128 (89%)	15 (10%)	1 (1%)	25	64
62	N	122/124 (98%)	81 (66%)	33 (27%)	8 (7%)	1	9
62	c2	122/124 (98%)	81 (66%)	37 (30%)	4 (3%)	4	25
63	O	148/150 (99%)	137 (93%)	9 (6%)	2 (1%)	13	47
63	c3	148/150 (99%)	128 (86%)	14 (10%)	6 (4%)	3	19
64	P	125/128 (98%)	103 (82%)	21 (17%)	1 (1%)	22	62
64	c4	126/128 (98%)	110 (87%)	16 (13%)	0	100	100
65	Q	122/141 (86%)	100 (82%)	19 (16%)	3 (2%)	6	31
65	c5	133/141 (94%)	99 (74%)	27 (20%)	7 (5%)	2	14
66	R	139/142 (98%)	122 (88%)	16 (12%)	1 (1%)	25	64
66	c6	140/142 (99%)	124 (89%)	15 (11%)	1 (1%)	25	64
67	S	116/125 (93%)	93 (80%)	22 (19%)	1 (1%)	20	60
67	c7	113/125 (90%)	91 (80%)	21 (19%)	1 (1%)	20	60
68	T	143/145 (99%)	126 (88%)	16 (11%)	1 (1%)	25	64
68	c8	143/145 (99%)	121 (85%)	19 (13%)	3 (2%)	8	36
69	U	141/143 (99%)	127 (90%)	14 (10%)	0	100	100
69	c9	141/143 (99%)	130 (92%)	11 (8%)	0	100	100
70	V	105/110 (96%)	89 (85%)	15 (14%)	1 (1%)	18	57
70	d0	108/110 (98%)	92 (85%)	14 (13%)	2 (2%)	9	39
71	W	85/87 (98%)	62 (73%)	22 (26%)	1 (1%)	15	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	d1	85/87 (98%)	77 (91%)	7 (8%)	1 (1%)	15	51
72	X	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	22	62
72	d2	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
73	Y	142/144 (99%)	115 (81%)	24 (17%)	3 (2%)	8	36
73	d3	142/144 (99%)	130 (92%)	12 (8%)	0	100	100
74	Z	132/134 (98%)	120 (91%)	10 (8%)	2 (2%)	12	45
74	d4	132/134 (98%)	114 (86%)	16 (12%)	2 (2%)	12	45
75	a	68/70 (97%)	51 (75%)	14 (21%)	3 (4%)	3	18
75	d5	67/70 (96%)	56 (84%)	11 (16%)	0	100	100
76	b	95/97 (98%)	66 (70%)	24 (25%)	5 (5%)	2	14
76	d6	95/97 (98%)	73 (77%)	20 (21%)	2 (2%)	8	36
77	c	79/81 (98%)	65 (82%)	14 (18%)	0	100	100
77	d7	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
78	d	61/63 (97%)	51 (84%)	10 (16%)	0	100	100
78	d8	61/63 (97%)	47 (77%)	14 (23%)	0	100	100
79	d9	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
79	e	51/53 (96%)	46 (90%)	5 (10%)	0	100	100
80	e0	60/62 (97%)	52 (87%)	8 (13%)	0	100	100
80	f	58/62 (94%)	47 (81%)	10 (17%)	1 (2%)	11	42
81	g	69/71 (97%)	38 (55%)	31 (45%)	0	100	100
82	h	316/318 (99%)	277 (88%)	39 (12%)	0	100	100
82	sR	316/318 (99%)	285 (90%)	30 (10%)	1 (0%)	44	79
83	e1	49/51 (96%)	30 (61%)	18 (37%)	1 (2%)	9	37
All	All	22260/23067 (96%)	19629 (88%)	2417 (11%)	214 (1%)	18	57

All (214) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	l	339	LEU
13	s	74	PRO
13	s	95	ASN
13	s	172	LEU
14	t	47	ALA
14	t	63	VAL

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Mol	Chain	Res	Type
15	u	8	LYS
29	AA	128	GLN
46	i	176	VAL
46	i	254	PRO
13	CM	173	ASP
14	CN	5	LYS
14	CN	47	ALA
14	CN	48	PRO
14	CN	63	VAL
51	C	62	LYS
51	C	181	LEU
55	G	57	SER
55	G	126	ASP
56	H	68	LEU
56	H	149	LYS
57	I	63	PRO
57	I	74	GLN
58	J	147	ALA
60	L	88	PRO
62	N	106	ILE
63	O	28	LEU
74	Z	52	LYS
53	s3	220	PRO
56	s6	68	LEU
57	s7	63	PRO
57	s7	67	LEU
60	c0	88	PRO
60	c0	97	PRO
62	c2	130	THR
63	c3	66	ILE
65	c5	51	SER
65	c5	128	HIS
74	d4	52	LYS
5	k	347	SER
6	l	292	SER
9	o	158	LYS
14	t	77	LEU
17	w	111	PRO
30	AB	57	GLY
30	AB	78	LEU
37	AI	92	LEU
38	AJ	35	ASN

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Mol	Chain	Res	Type
4	CD	144	ASN
5	CE	386	ASP
7	CG	20	PHE
9	CI	158	LYS
10	CJ	36	ILE
15	CO	8	LYS
19	CS	99	THR
29	DB	60	LYS
30	DC	78	LEU
35	DH	60	ARG
50	B	4	PRO
50	B	191	ARG
50	B	196	SER
61	M	4	GLU
62	N	109	GLU
62	N	112	ALA
63	O	27	LYS
64	P	42	VAL
65	Q	30	THR
73	Y	137	LYS
75	a	39	ALA
51	s1	107	THR
52	s2	106	ASP
53	s3	216	PRO
53	s3	217	ILE
57	s7	74	GLN
58	s8	100	ALA
58	s8	101	ILE
60	c0	32	HIS
60	c0	35	ILE
62	c2	106	ILE
62	c2	131	ASP
76	d6	46	GLU
82	sR	281	TYR
7	m	259	LYS
9	o	191	VAL
13	s	94	ARG
14	t	48	PRO
14	t	166	ALA
38	AJ	77	LEU
46	i	86	ASN
7	CG	259	LYS

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Mol	Chain	Res	Type
8	CH	98	VAL
9	CI	164	SER
9	CI	191	VAL
17	CQ	110	PRO
17	CQ	111	PRO
18	CR	159	LYS
30	DC	57	GLY
37	DJ	85	THR
48	sM	42	ALA
50	B	190	ASP
52	D	40	LYS
53	E	216	PRO
58	J	11	ARG
58	J	146	ARG
61	M	6	THR
62	N	85	LYS
62	N	108	ARG
62	N	126	TRP
62	N	130	THR
65	Q	125	PRO
71	W	11	LEU
76	b	63	ALA
60	c0	34	GLU
63	c3	23	PRO
63	c3	65	VAL
65	c5	68	PRO
67	c7	67	ARG
68	c8	9	GLY
71	d1	11	LEU
4	j	250	GLN
9	o	164	SER
13	s	8	PRO
13	s	73	GLY
14	t	76	THR
17	w	110	PRO
5	CE	385	LYS
13	CM	172	LEU
18	CR	158	ALA
50	B	167	LYS
50	B	202	TYR
57	I	64	VAL
58	J	23	LYS

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Mol	Chain	Res	Type
70	V	119	ALA
73	Y	98	GLU
75	a	38	HIS
76	b	61	GLU
76	b	85	ARG
57	s7	64	VAL
57	s7	66	SER
62	c2	109	GLU
63	c3	22	ALA
63	c3	140	LYS
65	c5	125	PRO
70	d0	73	GLY
76	d6	34	LYS
5	k	142	ALA
13	s	173	ASP
14	t	6	ASN
21	0	167	ARG
22	2	125	ALA
29	AA	102	GLU
29	AA	103	GLN
38	AJ	78	GLY
9	CI	25	GLN
9	CI	159	GLN
14	CN	166	ALA
18	CR	160	ALA
26	CY	25	ASP
29	DB	59	ALA
29	DB	102	GLU
29	DB	103	GLN
48	sM	43	ASP
53	E	217	ILE
68	T	60	GLU
50	s0	31	VAL
50	s0	168	HIS
65	c5	135	THR
68	c8	8	GLN
33	AE	7	VAL
46	i	87	THR
10	CJ	122	LYS
13	CM	8	PRO
23	CW	52	ASN
26	CY	81	PRO

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Mol	Chain	Res	Type
62	N	84	ASN
66	R	33	GLY
75	a	44	GLN
53	s3	221	SER
63	c3	139	TRP
65	c5	52	LYS
70	d0	52	LYS
83	e1	118	ARG
5	k	188	ILE
8	n	98	VAL
31	DD	21	ILE
33	DF	7	VAL
50	B	194	PRO
56	H	69	LEU
59	K	134	ILE
59	K	163	PRO
65	Q	126	VAL
76	b	9	GLY
52	s2	239	PRO
22	2	124	VAL
5	CE	188	ILE
14	CN	50	PRO
67	S	65	PRO
72	X	67	GLY
76	b	60	PRO
80	f	60	PRO
61	c1	129	ARG
16	v	75	VAL
22	CV	124	VAL
73	Y	41	SER
74	Z	35	VAL
68	c8	14	ILE
74	d4	30	PRO
12	r	188	GLY
5	CE	317	ILE
54	s4	90	ILE
56	s6	70	PRO
66	c6	5	PRO
60	c0	92	ILE
65	c5	126	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%)	169 (88%)	24 (12%)	5	23
4	j	193/194 (100%)	166 (86%)	27 (14%)	4	18
5	CE	319/322 (99%)	272 (85%)	47 (15%)	3	16
5	k	321/322 (100%)	274 (85%)	47 (15%)	3	16
6	CF	288/288 (100%)	256 (89%)	32 (11%)	7	29
6	l	288/288 (100%)	249 (86%)	39 (14%)	4	19
7	CG	244/244 (100%)	207 (85%)	37 (15%)	3	14
7	m	244/244 (100%)	216 (88%)	28 (12%)	6	27
8	CH	134/152 (88%)	116 (87%)	18 (13%)	4	19
8	n	134/152 (88%)	120 (90%)	14 (10%)	8	31
9	CI	186/186 (100%)	167 (90%)	19 (10%)	8	32
9	o	186/186 (100%)	165 (89%)	21 (11%)	7	28
10	CJ	187/191 (98%)	172 (92%)	15 (8%)	14	47
10	p	187/191 (98%)	167 (89%)	20 (11%)	8	30
11	CK	171/171 (100%)	143 (84%)	28 (16%)	2	12
11	q	171/171 (100%)	148 (86%)	23 (14%)	4	19
12	CL	177/186 (95%)	151 (85%)	26 (15%)	3	16
12	r	177/186 (95%)	149 (84%)	28 (16%)	3	13
13	CM	147/147 (100%)	125 (85%)	22 (15%)	3	15
13	s	147/147 (100%)	127 (86%)	20 (14%)	4	19
14	CN	154/154 (100%)	128 (83%)	26 (17%)	2	11
14	t	154/154 (100%)	136 (88%)	18 (12%)	6	26
15	CO	107/107 (100%)	93 (87%)	14 (13%)	5	20
15	u	107/107 (100%)	89 (83%)	18 (17%)	2	11
16	CP	175/175 (100%)	160 (91%)	15 (9%)	12	44
16	v	175/175 (100%)	155 (89%)	20 (11%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	CQ	160/160 (100%)	144 (90%)	16 (10%)	9	33
17	w	160/160 (100%)	139 (87%)	21 (13%)	5	20
18	CR	140/145 (97%)	120 (86%)	20 (14%)	4	17
18	x	140/145 (97%)	118 (84%)	22 (16%)	3	13
19	CS	150/150 (100%)	128 (85%)	22 (15%)	3	16
19	y	150/150 (100%)	130 (87%)	20 (13%)	4	20
20	CT	153/153 (100%)	132 (86%)	21 (14%)	4	19
20	z	153/153 (100%)	140 (92%)	13 (8%)	12	44
21	0	156/156 (100%)	131 (84%)	25 (16%)	3	12
21	CU	156/156 (100%)	133 (85%)	23 (15%)	3	16
22	2	136/136 (100%)	116 (85%)	20 (15%)	3	16
22	CV	136/136 (100%)	112 (82%)	24 (18%)	2	10
23	5	87/87 (100%)	80 (92%)	7 (8%)	14	47
23	CW	87/87 (100%)	77 (88%)	10 (12%)	6	27
24	CX	104/104 (100%)	93 (89%)	11 (11%)	8	30
24	IR	104/104 (100%)	89 (86%)	15 (14%)	4	16
26	7	57/86 (66%)	52 (91%)	5 (9%)	12	42
26	CY	57/86 (66%)	47 (82%)	10 (18%)	2	10
27	8	104/105 (99%)	91 (88%)	13 (12%)	5	22
27	CZ	104/105 (99%)	90 (86%)	14 (14%)	4	19
28	9	109/109 (100%)	95 (87%)	14 (13%)	5	21
28	DA	109/109 (100%)	95 (87%)	14 (13%)	5	21
29	AA	115/115 (100%)	104 (90%)	11 (10%)	10	36
29	DB	115/115 (100%)	104 (90%)	11 (10%)	10	36
30	AB	118/118 (100%)	106 (90%)	12 (10%)	8	32
30	DC	118/118 (100%)	103 (87%)	15 (13%)	5	21
31	AC	46/46 (100%)	40 (87%)	6 (13%)	5	21
31	DD	46/46 (100%)	39 (85%)	7 (15%)	3	14
32	AD	81/81 (100%)	70 (86%)	11 (14%)	4	19
32	DE	81/81 (100%)	76 (94%)	5 (6%)	21	57
33	AE	92/96 (96%)	80 (87%)	12 (13%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	DF	92/96 (96%)	75 (82%)	17 (18%)	2	8
34	AF	109/109 (100%)	94 (86%)	15 (14%)	4	19
34	DG	109/109 (100%)	96 (88%)	13 (12%)	6	25
35	AG	90/90 (100%)	81 (90%)	9 (10%)	9	33
35	DH	90/90 (100%)	83 (92%)	7 (8%)	15	48
36	AH	95/95 (100%)	84 (88%)	11 (12%)	6	26
36	DI	95/95 (100%)	85 (90%)	10 (10%)	8	31
37	AI	104/104 (100%)	92 (88%)	12 (12%)	6	27
37	DJ	104/104 (100%)	86 (83%)	18 (17%)	2	10
38	AJ	81/81 (100%)	69 (85%)	12 (15%)	3	15
38	DK	81/81 (100%)	71 (88%)	10 (12%)	5	23
39	AK	70/70 (100%)	63 (90%)	7 (10%)	9	33
39	DL	70/70 (100%)	59 (84%)	11 (16%)	3	13
40	AL	68/68 (100%)	58 (85%)	10 (15%)	3	16
40	DM	68/68 (100%)	61 (90%)	7 (10%)	8	32
41	AM	45/45 (100%)	38 (84%)	7 (16%)	3	13
41	DN	45/45 (100%)	41 (91%)	4 (9%)	11	41
42	AN	47/47 (100%)	39 (83%)	8 (17%)	2	11
42	DO	47/47 (100%)	42 (89%)	5 (11%)	8	30
43	AO	23/23 (100%)	20 (87%)	3 (13%)	5	21
43	DP	23/23 (100%)	19 (83%)	4 (17%)	2	10
44	AP	90/90 (100%)	82 (91%)	8 (9%)	11	41
44	DQ	90/90 (100%)	81 (90%)	9 (10%)	9	33
45	AQ	71/71 (100%)	59 (83%)	12 (17%)	2	11
45	DR	71/71 (100%)	63 (89%)	8 (11%)	7	28
46	i	97/227 (43%)	82 (84%)	15 (16%)	3	14
48	sM	54/54 (100%)	47 (87%)	7 (13%)	5	21
49	p0	105/253 (42%)	91 (87%)	14 (13%)	4	20
50	B	164/173 (95%)	146 (89%)	18 (11%)	7	30
50	s0	165/173 (95%)	140 (85%)	25 (15%)	3	14
51	C	191/192 (100%)	167 (87%)	24 (13%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	s1	192/192 (100%)	164 (85%)	28 (15%)	3	16
52	D	176/176 (100%)	151 (86%)	25 (14%)	4	17
52	s2	176/176 (100%)	144 (82%)	32 (18%)	2	9
53	E	182/182 (100%)	159 (87%)	23 (13%)	5	22
53	s3	182/182 (100%)	164 (90%)	18 (10%)	9	34
54	F	221/221 (100%)	196 (89%)	25 (11%)	7	28
54	s4	221/221 (100%)	200 (90%)	21 (10%)	10	37
55	G	173/173 (100%)	153 (88%)	20 (12%)	6	26
55	s5	173/173 (100%)	155 (90%)	18 (10%)	8	31
56	H	188/193 (97%)	163 (87%)	25 (13%)	4	20
56	s6	187/193 (97%)	163 (87%)	24 (13%)	5	21
57	I	165/166 (99%)	146 (88%)	19 (12%)	6	27
57	s7	165/166 (99%)	145 (88%)	20 (12%)	6	24
58	J	150/160 (94%)	139 (93%)	11 (7%)	16	50
58	s8	150/160 (94%)	140 (93%)	10 (7%)	19	54
59	K	158/158 (100%)	134 (85%)	24 (15%)	3	14
59	s9	158/158 (100%)	129 (82%)	29 (18%)	2	9
60	L	77/98 (79%)	68 (88%)	9 (12%)	6	26
60	c0	73/98 (74%)	65 (89%)	8 (11%)	7	30
61	M	129/136 (95%)	120 (93%)	9 (7%)	18	52
61	c1	129/136 (95%)	113 (88%)	16 (12%)	5	23
62	N	88/100 (88%)	73 (83%)	15 (17%)	2	11
62	c2	88/100 (88%)	73 (83%)	15 (17%)	2	11
63	O	127/127 (100%)	110 (87%)	17 (13%)	4	19
63	c3	127/127 (100%)	111 (87%)	16 (13%)	5	22
64	P	81/97 (84%)	70 (86%)	11 (14%)	4	19
64	c4	97/97 (100%)	85 (88%)	12 (12%)	5	23
65	Q	101/117 (86%)	92 (91%)	9 (9%)	11	41
65	c5	103/117 (88%)	91 (88%)	12 (12%)	6	26
66	R	117/118 (99%)	101 (86%)	16 (14%)	4	19
66	c6	118/118 (100%)	98 (83%)	20 (17%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	S	94/113 (83%)	80 (85%)	14 (15%)	3	15
67	c7	92/113 (81%)	81 (88%)	11 (12%)	6	24
68	T	128/128 (100%)	108 (84%)	20 (16%)	3	13
68	c8	128/128 (100%)	109 (85%)	19 (15%)	3	15
69	U	115/115 (100%)	95 (83%)	20 (17%)	2	10
69	c9	115/115 (100%)	99 (86%)	16 (14%)	4	18
70	V	100/103 (97%)	86 (86%)	14 (14%)	4	18
70	d0	103/103 (100%)	90 (87%)	13 (13%)	5	22
71	W	74/74 (100%)	62 (84%)	12 (16%)	3	12
71	d1	74/74 (100%)	63 (85%)	11 (15%)	3	15
72	X	110/110 (100%)	95 (86%)	15 (14%)	4	19
72	d2	110/110 (100%)	103 (94%)	7 (6%)	20	56
73	Y	119/119 (100%)	102 (86%)	17 (14%)	4	17
73	d3	119/119 (100%)	104 (87%)	15 (13%)	5	22
74	Z	112/112 (100%)	101 (90%)	11 (10%)	9	35
74	d4	112/112 (100%)	105 (94%)	7 (6%)	21	56
75	a	61/61 (100%)	49 (80%)	12 (20%)	1	6
75	d5	61/61 (100%)	58 (95%)	3 (5%)	29	66
76	b	83/83 (100%)	76 (92%)	7 (8%)	13	44
76	d6	83/83 (100%)	71 (86%)	12 (14%)	4	16
77	c	70/70 (100%)	67 (96%)	3 (4%)	33	70
77	d7	70/70 (100%)	65 (93%)	5 (7%)	17	52
78	d	56/56 (100%)	48 (86%)	8 (14%)	4	17
78	d8	56/56 (100%)	47 (84%)	9 (16%)	3	12
79	d9	47/47 (100%)	43 (92%)	4 (8%)	12	44
79	e	47/47 (100%)	42 (89%)	5 (11%)	8	30
80	e0	53/53 (100%)	45 (85%)	8 (15%)	3	15
80	f	51/53 (96%)	47 (92%)	4 (8%)	15	48
81	g	62/62 (100%)	50 (81%)	12 (19%)	1	7
82	h	260/261 (100%)	243 (94%)	17 (6%)	20	55
82	sR	260/261 (100%)	242 (93%)	18 (7%)	18	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
83	e1	43/43 (100%)	35 (81%)	8 (19%)	2	8
All	All	18684/19337 (97%)	16334 (87%)	2350 (13%)	5	22

All (2350) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	j	20	THR
4	j	23	ARG
4	j	32	LEU
4	j	44	ILE
4	j	45	VAL
4	j	48	ILE
4	j	49	VAL
4	j	62	VAL
4	j	72	ARG
4	j	74	GLU
4	j	84	THR
4	j	96	LEU
4	j	101	VAL
4	j	104	LEU
4	j	119	LYS
4	j	157	VAL
4	j	165	VAL
4	j	179	LEU
4	j	180	LEU
4	j	202	VAL
4	j	204	MET
4	j	207	VAL
4	j	226	SER
4	j	227	ARG
4	j	230	VAL
4	j	231	SER
4	j	247	ARG
5	k	4	ARG
5	k	7	GLU
5	k	10	ARG
5	k	17	LEU
5	k	19	ARG
5	k	25	ILE
5	k	37	ARG
5	k	47	LEU
5	k	69	LYS

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Mol	Chain	Res	Type
5	k	73	VAL
5	k	79	VAL
5	k	84	VAL
5	k	85	VAL
5	k	103	THR
5	k	114	VAL
5	k	139	GLN
5	k	148	LEU
5	k	150	ARG
5	k	156	SER
5	k	169	THR
5	k	183	LEU
5	k	188	ILE
5	k	192	VAL
5	k	196	ARG
5	k	202	THR
5	k	210	GLU
5	k	212	ASN
5	k	229	VAL
5	k	235	THR
5	k	238	LEU
5	k	241	LYS
5	k	244	ARG
5	k	252	ILE
5	k	261	MET
5	k	264	VAL
5	k	284	ARG
5	k	291	GLU
5	k	296	THR
5	k	300	ARG
5	k	305	ILE
5	k	320	ASP
5	k	324	VAL
5	k	325	LYS
5	k	332	ARG
5	k	338	LEU
5	k	352	GLU
5	k	361	THR
6	l	22	LEU
6	l	71	VAL
6	l	73	ARG
6	l	74	ILE

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Mol	Chain	Res	Type
6	l	93	MET
6	l	98	ARG
6	l	103	THR
6	l	112	LYS
6	l	120	TYR
6	l	133	SER
6	l	138	ARG
6	l	150	LEU
6	l	156	LEU
6	l	161	LYS
6	l	163	LYS
6	l	172	VAL
6	l	177	ASP
6	l	179	LEU
6	l	187	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	246	ARG
6	l	258	LEU
6	l	267	VAL
6	l	287	THR
6	l	308	LYS
6	l	313	LEU
6	l	323	VAL
6	l	327	LEU
6	l	333	VAL
6	l	338	LYS
6	l	339	LEU
6	l	349	THR
7	m	5	LYS
7	m	8	LYS
7	m	23	ARG
7	m	35	ARG
7	m	41	LYS
7	m	67	SER
7	m	75	LEU

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Mol	Chain	Res	Type
7	m	93	THR
7	m	105	ILE
7	m	113	LEU
7	m	115	LEU
7	m	118	THR
7	m	131	LEU
7	m	137	ASP
7	m	140	ARG
7	m	144	VAL
7	m	146	LEU
7	m	148	ILE
7	m	152	ARG
7	m	155	THR
7	m	163	LEU
7	m	177	GLU
7	m	185	PHE
7	m	216	GLU
7	m	217	GLU
7	m	222	LEU
7	m	231	ILE
7	m	234	ASP
8	n	2	SER
8	n	5	LYS
8	n	21	THR
8	n	35	VAL
8	n	52	VAL
8	n	64	LEU
8	n	78	ARG
8	n	79	VAL
8	n	84	VAL
8	n	88	SER
8	n	98	VAL
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	45	LEU
9	o	60	ARG
9	o	80	GLN
9	o	82	LYS

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Mol	Chain	Res	Type
9	o	83	LEU
9	o	88	ARG
9	o	93	ASN
9	o	101	LYS
9	o	110	ARG
9	o	121	LYS
9	o	124	LEU
9	o	157	ASN
9	o	158	LYS
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	50	VAL
10	p	57	ARG
10	p	71	VAL
10	p	74	THR
10	p	79	GLN
10	p	81	THR
10	p	84	ARG
10	p	106	LYS
10	p	110	THR
10	p	136	LEU
10	p	145	ASN
10	p	156	ASP
10	p	163	VAL
10	p	169	LEU
10	p	185	ARG
10	p	194	THR
10	p	206	GLU
10	p	248	LYS
11	q	5	GLN
11	q	6	THR
11	q	18	VAL
11	q	19	SER
11	q	41	ILE
11	q	42	ASP
11	q	44	THR
11	q	48	VAL

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Mol	Chain	Res	Type
11	q	52	LEU
11	q	55	VAL
11	q	68	LEU
11	q	69	ARG
11	q	70	THR
11	q	129	ARG
11	q	132	VAL
11	q	133	THR
11	q	139	ASN
11	q	151	VAL
11	q	157	ASN
11	q	161	LEU
11	q	162	GLN
11	q	172	ILE
11	q	173	ARG
12	r	3	ARG
12	r	21	ARG
12	r	24	ARG
12	r	26	VAL
12	r	30	LYS
12	r	32	ARG
12	r	35	ASP
12	r	39	LYS
12	r	40	LYS
12	r	42	THR
12	r	52	LEU
12	r	63	GLU
12	r	87	LEU
12	r	91	VAL
12	r	130	ASP
12	r	138	VAL
12	r	139	ARG
12	r	140	THR
12	r	142	ASP
12	r	148	VAL
12	r	163	GLN
12	r	165	ILE
12	r	169	LYS
12	r	174	THR
12	r	176	LEU
12	r	177	ASP
12	r	190	VAL

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Mol	Chain	Res	Type
12	r	203	LYS
13	s	9	MET
13	s	10	ARG
13	s	11	ASP
13	s	12	LEU
13	s	31	THR
13	s	46	VAL
13	s	47	GLN
13	s	63	GLU
13	s	70	THR
13	s	80	LEU
13	s	82	ARG
13	s	94	ARG
13	s	95	ASN
13	s	106	ILE
13	s	107	ASP
13	s	112	LEU
13	s	115	LYS
13	s	138	VAL
13	s	140	ARG
13	s	158	ASP
14	t	13	HIS
14	t	23	LYS
14	t	24	VAL
14	t	34	SER
14	t	54	LEU
14	t	55	ARG
14	t	59	ARG
14	t	64	LYS
14	t	67	ARG
14	t	69	VAL
14	t	85	LEU
14	t	104	ARG
14	t	114	GLN
14	t	122	LYS
14	t	131	LYS
14	t	164	GLU
14	t	168	ARG
14	t	171	ARG
15	u	3	THR
15	u	5	SER
15	u	10	SER

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Mol	Chain	Res	Type
15	u	15	VAL
15	u	27	GLN
15	u	38	ILE
15	u	50	LYS
15	u	53	VAL
15	u	58	ILE
15	u	63	VAL
15	u	66	THR
15	u	69	THR
15	u	90	VAL
15	u	91	CYS
15	u	102	LYS
15	u	107	GLU
15	u	135	LEU
15	u	137	LYS
16	v	10	LEU
16	v	15	GLN
16	v	19	LEU
16	v	22	LEU
16	v	38	ARG
16	v	49	ARG
16	v	50	ARG
16	v	80	THR
16	v	85	THR
16	v	96	ARG
16	v	106	VAL
16	v	109	ARG
16	v	117	ASN
16	v	132	VAL
16	v	133	ILE
16	v	151	ILE
16	v	182	ASN
16	v	183	THR
16	v	187	ARG
16	v	201	ARG
17	w	22	VAL
17	w	34	VAL
17	w	68	ARG
17	w	78	ARG
17	w	84	LEU
17	w	85	ARG
17	w	106	GLU

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Mol	Chain	Res	Type
17	w	116	LYS
17	w	117	ARG
17	w	122	GLN
17	w	124	LEU
17	w	126	VAL
17	w	128	ARG
17	w	129	LEU
17	w	143	THR
17	w	160	ARG
17	w	161	LYS
17	w	180	SER
17	w	184	THR
17	w	188	SER
17	w	190	VAL
18	x	13	LYS
18	x	16	SER
18	x	20	SER
18	x	23	ARG
18	x	24	VAL
18	x	29	THR
18	x	32	THR
18	x	36	ILE
18	x	41	LEU
18	x	49	GLU
18	x	52	LEU
18	x	53	ASP
18	x	69	ARG
18	x	94	LEU
18	x	103	GLU
18	x	112	LEU
18	x	119	VAL
18	x	127	ARG
18	x	142	SER
18	x	168	LEU
18	x	180	LYS
18	x	181	ARG
19	y	3	ILE
19	y	7	SER
19	y	17	THR
19	y	22	ASP
19	y	24	VAL
19	y	26	LEU

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Mol	Chain	Res	Type
19	y	32	LEU
19	y	39	ARG
19	y	41	ASP
19	y	49	LEU
19	y	57	ILE
19	y	66	ARG
19	y	69	ARG
19	y	74	GLU
19	y	81	VAL
19	y	115	VAL
19	y	135	GLN
19	y	138	LEU
19	y	150	VAL
19	y	170	ARG
20	z	29	THR
20	z	44	LEU
20	z	51	VAL
20	z	57	VAL
20	z	60	LYS
20	z	74	ARG
20	z	91	SER
20	z	103	ARG
20	z	104	ARG
20	z	115	ILE
20	z	171	ASP
20	z	175	GLN
20	z	177	VAL
21	0	1	MET
21	0	16	THR
21	0	45	LEU
21	0	49	HIS
21	0	50	LYS
21	0	61	ILE
21	0	71	LYS
21	0	73	LYS
21	0	80	ARG
21	0	85	SER
21	0	87	THR
21	0	105	THR
21	0	115	ARG
21	0	117	ARG
21	0	122	HIS

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Mol	Chain	Res	Type
21	0	131	LYS
21	0	132	THR
21	0	136	LYS
21	0	137	ARG
21	0	155	ARG
21	0	157	GLN
21	0	160	THR
21	0	162	THR
21	0	167	ARG
21	0	172	TYR
22	2	12	ARG
22	2	18	ASP
22	2	25	VAL
22	2	27	LEU
22	2	32	LYS
22	2	52	MET
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	96	ILE
22	2	103	GLN
22	2	122	GLN
22	2	126	VAL
22	2	128	LEU
22	2	139	ARG
22	2	143	THR
22	2	160	ILE
23	5	10	LYS
23	5	35	LYS
23	5	52	ASN
23	5	66	VAL
23	5	93	ILE
23	5	100	THR
23	5	104	ARG
24	lR	12	ARG
24	lR	13	ILE
24	lR	14	SER
24	lR	32	ARG
24	lR	45	ARG

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Mol	Chain	Res	Type
24	lR	48	ARG
24	lR	63	LYS
24	lR	64	LYS
24	lR	69	LEU
24	lR	72	LYS
24	lR	83	LYS
24	lR	102	ILE
24	lR	106	LYS
24	lR	115	THR
24	lR	120	LYS
26	7	4	GLU
26	7	5	ILE
26	7	19	THR
26	7	39	LEU
26	7	64	THR
27	8	27	ARG
27	8	28	THR
27	8	36	LYS
27	8	63	ILE
27	8	92	LYS
27	8	104	GLU
27	8	108	LEU
27	8	115	ARG
27	8	125	ARG
27	8	129	ASP
27	8	135	ILE
27	8	139	ILE
27	8	142	ILE
28	9	5	SER
28	9	13	ARG
28	9	37	LYS
28	9	38	GLU
28	9	40	ARG
28	9	45	ILE
28	9	56	VAL
28	9	60	ARG
28	9	64	LYS
28	9	67	GLU
28	9	74	TYR
28	9	105	VAL
28	9	113	LYS
28	9	115	ARG

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Mol	Chain	Res	Type
29	AA	14	VAL
29	AA	24	VAL
29	AA	46	ILE
29	AA	52	LYS
29	AA	81	LEU
29	AA	83	THR
29	AA	90	GLU
29	AA	102	GLU
29	AA	103	GLN
29	AA	107	ARG
29	AA	109	GLU
30	AB	4	ARG
30	AB	8	THR
30	AB	42	ARG
30	AB	46	ASP
30	AB	60	TYR
30	AB	76	ASP
30	AB	78	LEU
30	AB	88	ASP
30	AB	92	LYS
30	AB	115	LYS
30	AB	120	ASN
30	AB	135	GLU
31	AC	13	THR
31	AC	14	ARG
31	AC	25	LYS
31	AC	31	SER
31	AC	50	THR
31	AC	59	LYS
32	AD	14	LEU
32	AD	16	LEU
32	AD	18	ILE
32	AD	34	LEU
32	AD	54	SER
32	AD	61	MET
32	AD	76	GLU
32	AD	99	ASP
32	AD	101	LEU
32	AD	103	THR
32	AD	104	LEU
33	AE	8	VAL
33	AE	16	LEU

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Mol	Chain	Res	Type
33	AE	26	LYS
33	AE	31	ARG
33	AE	55	LEU
33	AE	79	ARG
33	AE	86	LYS
33	AE	96	VAL
33	AE	100	SER
33	AE	106	THR
33	AE	107	VAL
33	AE	110	GLU
34	AF	14	THR
34	AF	16	LYS
34	AF	19	ARG
34	AF	27	ARG
34	AF	33	ARG
34	AF	44	ARG
34	AF	51	SER
34	AF	61	LYS
34	AF	62	LYS
34	AF	73	THR
34	AF	89	THR
34	AF	106	VAL
34	AF	109	LEU
34	AF	111	ARG
34	AF	128	LEU
35	AG	15	SER
35	AG	20	LYS
35	AG	22	VAL
35	AG	49	ILE
35	AG	59	VAL
35	AG	70	LYS
35	AG	81	VAL
35	AG	98	VAL
35	AG	105	SER
36	AH	8	ARG
36	AH	20	ILE
36	AH	24	LYS
36	AH	29	ILE
36	AH	31	ARG
36	AH	51	LEU
36	AH	58	ARG
36	AH	65	VAL

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Mol	Chain	Res	Type
36	AH	71	THR
36	AH	102	LYS
36	AH	104	VAL
37	AI	15	GLU
37	AI	20	GLN
37	AI	21	LEU
37	AI	30	GLU
37	AI	31	LEU
37	AI	46	THR
37	AI	84	LYS
37	AI	89	ARG
37	AI	90	ARG
37	AI	92	LEU
37	AI	96	GLU
37	AI	101	THR
38	AJ	11	LEU
38	AJ	18	THR
38	AJ	25	LYS
38	AJ	26	ILE
38	AJ	34	SER
38	AJ	45	ARG
38	AJ	57	LEU
38	AJ	60	LEU
38	AJ	62	ARG
38	AJ	68	ARG
38	AJ	88	GLU
38	AJ	90	MET
39	AK	24	ARG
39	AK	25	ARG
39	AK	33	THR
39	AK	58	THR
39	AK	59	THR
39	AK	67	LEU
39	AK	82	SER
40	AL	5	ILE
40	AL	24	THR
40	AL	32	ASN
40	AL	46	ARG
40	AL	53	THR
40	AL	65	LEU
40	AL	67	GLN
40	AL	69	LEU

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Mol	Chain	Res	Type
40	AL	77	ARG
40	AL	78	LEU
41	AM	4	GLN
41	AM	10	LYS
41	AM	21	ARG
41	AM	34	THR
41	AM	36	ARG
41	AM	45	ARG
41	AM	51	ILE
42	AN	77	ILE
42	AN	83	LYS
42	AN	85	LEU
42	AN	112	LYS
42	AN	113	ARG
42	AN	114	LYS
42	AN	126	LYS
42	AN	127	LEU
43	AO	2	ARG
43	AO	11	ARG
43	AO	13	LEU
44	AP	2	VAL
44	AP	8	ARG
44	AP	26	THR
44	AP	35	LEU
44	AP	78	LYS
44	AP	83	LEU
44	AP	84	THR
44	AP	104	LEU
45	AQ	11	THR
45	AQ	16	VAL
45	AQ	25	GLN
45	AQ	45	LYS
45	AQ	46	THR
45	AQ	49	ARG
45	AQ	56	THR
45	AQ	59	CYS
45	AQ	60	CYS
45	AQ	84	ARG
45	AQ	90	VAL
45	AQ	91	GLU
46	i	34	LYS
46	i	46	LYS

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Mol	Chain	Res	Type
46	i	68	ARG
46	i	75	ASP
46	i	77	THR
46	i	84	LYS
46	i	91	THR
46	i	96	ARG
46	i	97	THR
46	i	100	THR
46	i	102	THR
46	i	116	GLU
46	i	130	GLU
46	i	131	ILE
46	i	134	ASP
4	CD	10	LYS
4	CD	19	HIS
4	CD	20	THR
4	CD	32	LEU
4	CD	44	ILE
4	CD	45	VAL
4	CD	48	ILE
4	CD	62	VAL
4	CD	64	ARG
4	CD	70	ARG
4	CD	82	VAL
4	CD	96	LEU
4	CD	101	VAL
4	CD	137	ILE
4	CD	142	ASP
4	CD	149	ARG
4	CD	179	LEU
4	CD	180	LEU
4	CD	204	MET
4	CD	207	VAL
4	CD	227	ARG
4	CD	230	VAL
4	CD	250	GLN
4	CD	252	THR
5	CE	2	SER
5	CE	7	GLU
5	CE	17	LEU
5	CE	25	ILE
5	CE	30	LYS

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Mol	Chain	Res	Type
5	CE	37	ARG
5	CE	47	LEU
5	CE	55	THR
5	CE	56	ILE
5	CE	73	VAL
5	CE	79	VAL
5	CE	84	VAL
5	CE	100	ARG
5	CE	103	THR
5	CE	111	SER
5	CE	114	VAL
5	CE	146	ARG
5	CE	156	SER
5	CE	167	ARG
5	CE	169	THR
5	CE	173	GLN
5	CE	183	LEU
5	CE	188	ILE
5	CE	192	VAL
5	CE	196	ARG
5	CE	202	THR
5	CE	205	VAL
5	CE	212	ASN
5	CE	222	LYS
5	CE	232	ARG
5	CE	235	THR
5	CE	284	ARG
5	CE	296	THR
5	CE	305	ILE
5	CE	308	MET
5	CE	316	GLU
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	349	LYS
5	CE	364	LYS
5	CE	382	THR
5	CE	386	ASP
5	CE	387	LEU

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Mol	Chain	Res	Type
6	CF	53	SER
6	CF	73	ARG
6	CF	74	ILE
6	CF	85	SER
6	CF	93	MET
6	CF	99	MET
6	CF	118	LYS
6	CF	120	TYR
6	CF	138	ARG
6	CF	150	LEU
6	CF	156	LEU
6	CF	170	LYS
6	CF	177	ASP
6	CF	179	LEU
6	CF	187	LEU
6	CF	201	GLN
6	CF	203	ARG
6	CF	206	LEU
6	CF	220	ARG
6	CF	222	VAL
6	CF	230	VAL
6	CF	246	ARG
6	CF	307	GLN
6	CF	313	LEU
6	CF	316	ASN
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	346	LYS
7	CG	5	LYS
7	CG	23	ARG
7	CG	35	ARG
7	CG	41	LYS
7	CG	63	GLN
7	CG	69	ILE
7	CG	70	THR
7	CG	75	LEU
7	CG	89	THR
7	CG	92	LEU

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Mol	Chain	Res	Type
7	CG	95	TRP
7	CG	105	ILE
7	CG	107	ARG
7	CG	110	LEU
7	CG	113	LEU
7	CG	115	LEU
7	CG	118	THR
7	CG	126	GLU
7	CG	131	LEU
7	CG	140	ARG
7	CG	144	VAL
7	CG	146	LEU
7	CG	148	ILE
7	CG	151	GLN
7	CG	152	ARG
7	CG	155	THR
7	CG	173	VAL
7	CG	185	PHE
7	CG	188	GLU
7	CG	189	GLU
7	CG	190	ILE
7	CG	194	LEU
7	CG	211	LEU
7	CG	222	LEU
7	CG	234	ASP
7	CG	261	THR
7	CG	293	LEU
8	CH	8	LYS
8	CH	14	ASP
8	CH	15	VAL
8	CH	21	THR
8	CH	35	VAL
8	CH	48	ARG
8	CH	52	VAL
8	CH	64	LEU
8	CH	65	ILE
8	CH	79	VAL
8	CH	88	SER
8	CH	89	THR
8	CH	93	VAL
8	CH	129	GLU
8	CH	134	ARG

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Mol	Chain	Res	Type
8	CH	140	VAL
8	CH	152	THR
8	CH	155	LEU
9	CI	24	GLU
9	CI	25	GLN
9	CI	45	LEU
9	CI	57	THR
9	CI	60	ARG
9	CI	77	VAL
9	CI	82	LYS
9	CI	83	LEU
9	CI	89	ILE
9	CI	92	ILE
9	CI	98	LYS
9	CI	111	ILE
9	CI	121	LYS
9	CI	124	LEU
9	CI	179	LEU
9	CI	180	SER
9	CI	181	ILE
9	CI	184	LEU
9	CI	239	LEU
10	CJ	50	VAL
10	CJ	71	VAL
10	CJ	74	THR
10	CJ	79	GLN
10	CJ	81	THR
10	CJ	84	ARG
10	CJ	85	ASN
10	CJ	136	LEU
10	CJ	160	ILE
10	CJ	163	VAL
10	CJ	169	LEU
10	CJ	185	ARG
10	CJ	197	VAL
10	CJ	203	VAL
10	CJ	248	LYS
11	CK	5	GLN
11	CK	16	VAL
11	CK	18	VAL
11	CK	33	THR
11	CK	41	ILE

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Mol	Chain	Res	Type
11	CK	48	VAL
11	CK	52	LEU
11	CK	62	ARG
11	CK	68	LEU
11	CK	69	ARG
11	CK	70	THR
11	CK	82	VAL
11	CK	92	TYR
11	CK	102	ASN
11	CK	121	LYS
11	CK	122	LYS
11	CK	129	ARG
11	CK	132	VAL
11	CK	133	THR
11	CK	151	VAL
11	CK	157	ASN
11	CK	161	LEU
11	CK	162	GLN
11	CK	164	ILE
11	CK	166	ARG
11	CK	172	ILE
11	CK	173	ARG
11	CK	190	ASP
12	CL	3	ARG
12	CL	24	ARG
12	CL	28	ASP
12	CL	30	LYS
12	CL	32	ARG
12	CL	33	ILE
12	CL	40	LYS
12	CL	42	THR
12	CL	52	LEU
12	CL	57	LEU
12	CL	58	GLU
12	CL	63	GLU
12	CL	71	CYS
12	CL	74	LYS
12	CL	77	THR
12	CL	87	LEU
12	CL	91	VAL
12	CL	139	ARG
12	CL	153	ARG

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Mol	Chain	Res	Type
12	CL	165	ILE
12	CL	169	LYS
12	CL	185	ARG
12	CL	197	VAL
12	CL	206	LEU
12	CL	208	ASN
12	CL	212	GLU
13	CM	9	MET
13	CM	10	ARG
13	CM	12	LEU
13	CM	29	ARG
13	CM	40	LEU
13	CM	44	THR
13	CM	56	THR
13	CM	80	LEU
13	CM	82	ARG
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	142	LYS
13	CM	145	LYS
13	CM	147	THR
13	CM	168	ASP
13	CM	171	VAL
13	CM	172	LEU
14	CN	4	SER
14	CN	5	LYS
14	CN	23	LYS
14	CN	42	ARG
14	CN	52	ASP
14	CN	53	LEU
14	CN	54	LEU
14	CN	55	ARG
14	CN	57	VAL
14	CN	58	VAL
14	CN	59	ARG
14	CN	63	VAL
14	CN	67	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	CN	69	VAL
14	CN	85	LEU
14	CN	107	GLU
14	CN	118	GLU
14	CN	124	ILE
14	CN	128	ARG
14	CN	131	LYS
14	CN	153	ASP
14	CN	154	VAL
14	CN	164	GLU
14	CN	165	SER
14	CN	168	ARG
14	CN	171	ARG
15	CO	4	ASP
15	CO	5	SER
15	CO	8	LYS
15	CO	15	VAL
15	CO	38	ILE
15	CO	45	LEU
15	CO	53	VAL
15	CO	63	VAL
15	CO	66	THR
15	CO	90	VAL
15	CO	121	MET
15	CO	123	LEU
15	CO	124	ARG
15	CO	130	THR
16	CP	10	LEU
16	CP	17	ASP
16	CP	20	ARG
16	CP	22	LEU
16	CP	68	ARG
16	CP	80	THR
16	CP	85	THR
16	CP	133	ILE
16	CP	138	GLN
16	CP	151	ILE
16	CP	153	ASP
16	CP	182	ASN
16	CP	183	THR
16	CP	190	THR
16	CP	198	SER

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Mol	Chain	Res	Type
17	CQ	41	LEU
17	CQ	58	LEU
17	CQ	67	THR
17	CQ	74	ARG
17	CQ	78	ARG
17	CQ	85	ARG
17	CQ	106	GLU
17	CQ	110	PRO
17	CQ	115	LYS
17	CQ	117	ARG
17	CQ	124	LEU
17	CQ	126	VAL
17	CQ	128	ARG
17	CQ	129	LEU
17	CQ	134	LYS
17	CQ	180	SER
18	CR	7	THR
18	CR	9	THR
18	CR	24	VAL
18	CR	32	THR
18	CR	42	THR
18	CR	49	GLU
18	CR	52	LEU
18	CR	56	ARG
18	CR	70	THR
18	CR	78	VAL
18	CR	111	LYS
18	CR	112	LEU
18	CR	114	VAL
18	CR	119	VAL
18	CR	128	ARG
18	CR	144	SER
18	CR	166	VAL
18	CR	168	LEU
18	CR	171	ARG
18	CR	175	ARG
19	CS	3	ILE
19	CS	7	SER
19	CS	11	LYS
19	CS	17	THR
19	CS	24	VAL
19	CS	26	LEU

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Mol	Chain	Res	Type
19	CS	32	LEU
19	CS	41	ASP
19	CS	49	LEU
19	CS	69	ARG
19	CS	80	THR
19	CS	81	VAL
19	CS	82	VAL
19	CS	86	THR
19	CS	93	ILE
19	CS	113	LYS
19	CS	135	GLN
19	CS	138	LEU
19	CS	150	VAL
19	CS	170	ARG
19	CS	180	ARG
19	CS	181	SER
20	CT	5	ARG
20	CT	10	LEU
20	CT	17	VAL
20	CT	22	VAL
20	CT	30	SER
20	CT	43	LYS
20	CT	57	VAL
20	CT	74	ARG
20	CT	81	ARG
20	CT	98	ARG
20	CT	99	LEU
20	CT	103	ARG
20	CT	104	ARG
20	CT	126	GLU
20	CT	130	ASN
20	CT	134	HIS
20	CT	144	GLN
20	CT	148	ASP
20	CT	165	LYS
20	CT	166	ASN
20	CT	180	LYS
21	CU	1	MET
21	CU	24	LEU
21	CU	45	LEU
21	CU	58	ILE
21	CU	61	ILE

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Mol	Chain	Res	Type
21	CU	71	LYS
21	CU	80	ARG
21	CU	81	TYR
21	CU	82	ASP
21	CU	97	VAL
21	CU	100	VAL
21	CU	104	GLU
21	CU	117	ARG
21	CU	132	THR
21	CU	137	ARG
21	CU	145	THR
21	CU	149	LYS
21	CU	155	ARG
21	CU	156	VAL
21	CU	160	THR
21	CU	162	THR
21	CU	167	ARG
21	CU	172	TYR
22	CV	9	SER
22	CV	16	GLN
22	CV	25	VAL
22	CV	26	HIS
22	CV	27	LEU
22	CV	32	LYS
22	CV	75	ILE
22	CV	78	LYS
22	CV	79	MET
22	CV	80	VAL
22	CV	88	ARG
22	CV	92	ARG
22	CV	96	ILE
22	CV	97	LYS
22	CV	100	LYS
22	CV	101	CYS
22	CV	102	ARG
22	CV	103	GLN
22	CV	106	LEU
22	CV	126	VAL
22	CV	127	GLN
22	CV	128	LEU
22	CV	139	ARG
22	CV	143	THR

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Mol	Chain	Res	Type
23	CW	10	LYS
23	CW	38	ILE
23	CW	43	VAL
23	CW	49	ASN
23	CW	55	THR
23	CW	58	GLU
23	CW	59	ASP
23	CW	100	THR
23	CW	104	ARG
23	CW	105	LEU
24	CX	13	ILE
24	CX	32	ARG
24	CX	45	ARG
24	CX	69	LEU
24	CX	73	VAL
24	CX	83	LYS
24	CX	88	ARG
24	CX	93	LEU
24	CX	102	ILE
24	CX	120	LYS
24	CX	128	ARG
26	CY	1	MET
26	CY	4	GLU
26	CY	5	ILE
26	CY	19	THR
26	CY	25	ASP
26	CY	34	SER
26	CY	39	LEU
26	CY	43	ARG
26	CY	54	LEU
26	CY	63	ILE
27	CZ	26	VAL
27	CZ	27	ARG
27	CZ	37	THR
27	CZ	38	LEU
27	CZ	39	LYS
27	CZ	63	ILE
27	CZ	71	THR
27	CZ	92	LYS
27	CZ	108	LEU
27	CZ	115	ARG
27	CZ	117	ASN

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Mol	Chain	Res	Type
27	CZ	125	ARG
27	CZ	133	LEU
27	CZ	135	ILE
28	DA	8	VAL
28	DA	9	SER
28	DA	13	ARG
28	DA	17	LYS
28	DA	37	LYS
28	DA	45	ILE
28	DA	50	ILE
28	DA	56	VAL
28	DA	57	LEU
28	DA	59	VAL
28	DA	67	GLU
28	DA	74	TYR
28	DA	76	LEU
28	DA	105	VAL
29	DB	14	VAL
29	DB	17	ARG
29	DB	24	VAL
29	DB	26	VAL
29	DB	30	ASP
29	DB	46	ILE
29	DB	66	THR
29	DB	81	LEU
29	DB	86	THR
29	DB	92	PHE
29	DB	103	GLN
30	DC	4	ARG
30	DC	8	THR
30	DC	10	LYS
30	DC	14	HIS
30	DC	42	ARG
30	DC	46	ASP
30	DC	56	VAL
30	DC	60	TYR
30	DC	76	ASP
30	DC	77	LYS
30	DC	85	ASP
30	DC	88	ASP
30	DC	91	LEU
30	DC	115	LYS

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Mol	Chain	Res	Type
30	DC	139	ARG
31	DD	13	THR
31	DD	14	ARG
31	DD	21	ILE
31	DD	22	LYS
31	DD	23	LYS
31	DD	26	THR
31	DD	59	LYS
32	DE	40	LYS
32	DE	61	MET
32	DE	83	LYS
32	DE	102	THR
32	DE	103	THR
33	DF	8	VAL
33	DF	13	THR
33	DF	16	LEU
33	DF	26	LYS
33	DF	31	ARG
33	DF	46	THR
33	DF	64	VAL
33	DF	68	GLU
33	DF	76	SER
33	DF	79	ARG
33	DF	86	LYS
33	DF	93	VAL
33	DF	96	VAL
33	DF	100	SER
33	DF	104	LEU
33	DF	106	THR
33	DF	110	GLU
34	DG	4	LEU
34	DG	19	ARG
34	DG	31	ASN
34	DG	33	ARG
34	DG	34	LYS
34	DG	40	SER
34	DG	73	THR
34	DG	75	LEU
34	DG	82	LEU
34	DG	91	THR
34	DG	109	LEU
34	DG	125	ARG

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Mol	Chain	Res	Type
34	DG	128	LEU
35	DH	20	LYS
35	DH	31	LYS
35	DH	60	ARG
35	DH	70	LYS
35	DH	81	VAL
35	DH	92	LYS
35	DH	98	VAL
36	DI	5	VAL
36	DI	20	ILE
36	DI	23	VAL
36	DI	29	ILE
36	DI	31	ARG
36	DI	36	LYS
36	DI	58	ARG
36	DI	64	THR
36	DI	65	VAL
36	DI	71	THR
37	DJ	11	THR
37	DJ	20	GLN
37	DJ	21	LEU
37	DJ	27	GLU
37	DJ	28	LEU
37	DJ	36	LEU
37	DJ	46	THR
37	DJ	48	ARG
37	DJ	49	LYS
37	DJ	59	ASN
37	DJ	64	GLU
37	DJ	68	GLN
37	DJ	69	LEU
37	DJ	71	LYS
37	DJ	89	ARG
37	DJ	101	THR
37	DJ	107	LYS
37	DJ	119	LYS
38	DK	2	THR
38	DK	17	VAL
38	DK	21	THR
38	DK	26	ILE
38	DK	43	LEU
38	DK	45	ARG

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Mol	Chain	Res	Type
38	DK	68	ARG
38	DK	76	ARG
38	DK	81	THR
38	DK	99	ARG
39	DL	17	THR
39	DL	24	ARG
39	DL	25	ARG
39	DL	33	THR
39	DL	36	SER
39	DL	44	THR
39	DL	45	ARG
39	DL	55	ARG
39	DL	59	THR
39	DL	67	LEU
39	DL	80	THR
40	DM	24	THR
40	DM	41	THR
40	DM	53	THR
40	DM	65	LEU
40	DM	69	LEU
40	DM	72	THR
40	DM	77	ARG
41	DN	4	GLN
41	DN	21	ARG
41	DN	45	ARG
41	DN	48	LYS
42	DO	85	LEU
42	DO	112	LYS
42	DO	113	ARG
42	DO	114	LYS
42	DO	127	LEU
43	DP	6	ARG
43	DP	9	ARG
43	DP	11	ARG
43	DP	13	LEU
44	DQ	7	THR
44	DQ	35	LEU
44	DQ	78	LYS
44	DQ	79	THR
44	DQ	83	LEU
44	DQ	84	THR
44	DQ	85	LEU

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Mol	Chain	Res	Type
44	DQ	100	LYS
44	DQ	105	GLN
45	DR	7	LYS
45	DR	10	ILE
45	DR	11	THR
45	DR	25	GLN
45	DR	49	ARG
45	DR	56	THR
45	DR	60	CYS
45	DR	70	THR
48	sM	33	LYS
48	sM	43	ASP
48	sM	50	ASN
48	sM	68	ARG
48	sM	71	ASN
48	sM	74	LYS
48	sM	77	THR
49	p0	4	ILE
49	p0	5	ARG
49	p0	30	VAL
49	p0	42	ARG
49	p0	44	GLU
49	p0	48	ARG
49	p0	51	VAL
49	p0	70	LEU
49	p0	72	ASP
49	p0	76	LEU
49	p0	93	LEU
49	p0	97	LYS
49	p0	104	ARG
49	p0	192	ASP
50	B	6	THR
50	B	10	THR
50	B	37	VAL
50	B	59	LEU
50	B	62	ARG
50	B	84	ARG
50	B	87	LEU
50	B	88	LYS
50	B	96	THR
50	B	111	ILE
50	B	155	PHE

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Mol	Chain	Res	Type
50	B	168	HIS
50	B	172	LEU
50	B	188	LEU
50	B	197	ILE
50	B	198	MET
50	B	200	ASP
50	B	203	PHE
51	C	21	VAL
51	C	25	THR
51	C	29	TRP
51	C	46	THR
51	C	61	LEU
51	C	70	LEU
51	C	74	GLN
51	C	77	GLU
51	C	78	ASP
51	C	89	ASP
51	C	95	ASN
51	C	97	LEU
51	C	105	PHE
51	C	111	ARG
51	C	117	TRP
51	C	129	THR
51	C	177	GLN
51	C	181	LEU
51	C	198	GLU
51	C	202	LYS
51	C	218	LEU
51	C	220	GLN
51	C	222	LYS
51	C	223	PHE
52	D	53	ILE
52	D	69	ILE
52	D	72	LEU
52	D	73	LEU
52	D	76	LEU
52	D	91	ARG
52	D	95	ARG
52	D	96	THR
52	D	97	ARG
52	D	99	LYS
52	D	111	VAL

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Mol	Chain	Res	Type
52	D	113	LEU
52	D	117	THR
52	D	134	LEU
52	D	137	ILE
52	D	141	ARG
52	D	147	ASN
52	D	148	LEU
52	D	207	LEU
52	D	221	THR
52	D	225	LEU
52	D	226	THR
52	D	235	LEU
52	D	244	SER
52	D	245	ASP
53	E	4	LEU
53	E	21	LEU
53	E	23	GLU
53	E	76	ARG
53	E	84	ILE
53	E	92	GLN
53	E	105	MET
53	E	117	ARG
53	E	151	LYS
53	E	158	ILE
53	E	172	THR
53	E	174	HIS
53	E	175	VAL
53	E	176	LEU
53	E	178	ARG
53	E	181	VAL
53	E	182	LEU
53	E	195	SER
53	E	196	ARG
53	E	215	GLU
53	E	217	ILE
53	E	222	VAL
53	E	224	ASP
54	F	6	LYS
54	F	7	LYS
54	F	9	LEU
54	F	38	LEU
54	F	39	ARG

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Mol	Chain	Res	Type
54	F	48	LEU
54	F	68	ARG
54	F	70	VAL
54	F	71	LYS
54	F	77	ARG
54	F	102	VAL
54	F	105	VAL
54	F	115	THR
54	F	116	ASP
54	F	126	VAL
54	F	131	LEU
54	F	142	HIS
54	F	180	LEU
54	F	182	TYR
54	F	187	ARG
54	F	192	ILE
54	F	227	VAL
54	F	240	LYS
54	F	242	LYS
54	F	258	GLN
55	G	25	LEU
55	G	32	GLU
55	G	38	THR
55	G	40	ILE
55	G	41	LYS
55	G	43	PHE
55	G	45	LYS
55	G	48	PHE
55	G	58	LEU
55	G	65	ARG
55	G	76	ARG
55	G	79	ASN
55	G	93	LEU
55	G	146	THR
55	G	149	VAL
55	G	156	ARG
55	G	162	VAL
55	G	186	ASN
55	G	194	LEU
55	G	216	GLU
56	H	7	TYR
56	H	10	ASN

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Mol	Chain	Res	Type
56	H	15	THR
56	H	25	ARG
56	H	39	GLU
56	H	45	PHE
56	H	71	THR
56	H	81	VAL
56	H	82	SER
56	H	109	LEU
56	H	120	GLU
56	H	126	ASP
56	H	127	THR
56	H	128	THR
56	H	129	VAL
56	H	133	LEU
56	H	137	ARG
56	H	154	ARG
56	H	155	ASP
56	H	158	ILE
56	H	169	TYR
56	H	170	THR
56	H	174	LYS
56	H	193	LEU
56	H	211	LEU
57	I	15	GLU
57	I	16	LEU
57	I	31	SER
57	I	50	ASP
57	I	67	LEU
57	I	80	GLU
57	I	85	PHE
57	I	87	ASP
57	I	97	ARG
57	I	99	LEU
57	I	104	ARG
57	I	110	GLN
57	I	114	ARG
57	I	116	ARG
57	I	126	LEU
57	I	133	THR
57	I	147	ASN
57	I	166	LEU
57	I	185	ILE

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Mol	Chain	Res	Type
58	J	21	PHE
58	J	22	ARG
58	J	29	LEU
58	J	36	THR
58	J	58	LEU
58	J	107	THR
58	J	138	ASN
58	J	151	LYS
58	J	152	ILE
58	J	184	LEU
58	J	196	LEU
59	K	3	ARG
59	K	6	ARG
59	K	7	THR
59	K	14	THR
59	K	28	LEU
59	K	39	LYS
59	K	40	LYS
59	K	78	ARG
59	K	89	ASP
59	K	92	LYS
59	K	93	LEU
59	K	97	LEU
59	K	99	LEU
59	K	101	VAL
59	K	109	LEU
59	K	110	GLN
59	K	134	ILE
59	K	138	LYS
59	K	149	ARG
59	K	161	THR
59	K	171	ARG
59	K	172	VAL
59	K	174	ARG
59	K	182	GLU
60	L	5	LYS
60	L	8	ARG
60	L	20	VAL
60	L	27	PHE
60	L	28	ASN
60	L	55	VAL
60	L	62	GLN

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Mol	Chain	Res	Type
60	L	76	LEU
60	L	82	LEU
61	M	21	ASN
61	M	29	LYS
61	M	44	THR
61	M	67	ARG
61	M	69	LYS
61	M	74	THR
61	M	80	MET
61	M	99	ARG
61	M	123	VAL
62	N	28	LEU
62	N	36	LEU
62	N	37	VAL
62	N	43	ARG
62	N	45	LEU
62	N	50	LYS
62	N	61	VAL
62	N	74	LEU
62	N	89	ILE
62	N	103	LEU
62	N	125	ASN
62	N	126	TRP
62	N	129	GLU
62	N	132	GLU
62	N	140	PHE
63	O	3	ARG
63	O	6	SER
63	O	9	LYS
63	O	27	LYS
63	O	28	LEU
63	O	32	SER
63	O	39	LYS
63	O	64	ARG
63	O	66	ILE
63	O	76	LYS
63	O	83	GLU
63	O	88	LEU
63	O	102	LEU
63	O	115	LEU
63	O	125	LEU
63	O	134	VAL

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Mol	Chain	Res	Type
63	O	149	LEU
64	P	29	HIS
64	P	31	THR
64	P	42	VAL
64	P	81	VAL
64	P	83	ILE
64	P	92	LYS
64	P	103	ARG
64	P	115	ILE
64	P	123	SER
64	P	132	ARG
64	P	137	LEU
65	Q	22	LEU
65	Q	26	LEU
65	Q	34	VAL
65	Q	36	LEU
65	Q	44	ARG
65	Q	52	LYS
65	Q	110	GLU
65	Q	121	ILE
65	Q	124	THR
66	R	29	ILE
66	R	31	VAL
66	R	40	GLU
66	R	42	GLU
66	R	43	ILE
66	R	58	ASP
66	R	65	ILE
66	R	66	ARG
66	R	69	VAL
66	R	98	ASP
66	R	106	LYS
66	R	109	PHE
66	R	114	ARG
66	R	123	ARG
66	R	128	LYS
66	R	137	ARG
67	S	18	GLU
67	S	29	GLN
67	S	34	LEU
67	S	38	ILE
67	S	40	THR

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Mol	Chain	Res	Type
67	S	43	SER
67	S	46	LEU
67	S	62	GLN
67	S	69	ILE
67	S	72	LYS
67	S	84	TYR
67	S	105	GLN
67	S	113	LEU
67	S	115	LEU
68	T	3	LEU
68	T	5	VAL
68	T	6	GLN
68	T	7	GLU
68	T	8	GLN
68	T	11	PHE
68	T	12	GLN
68	T	13	HIS
68	T	15	LEU
68	T	26	ILE
68	T	28	ILE
68	T	40	ARG
68	T	71	GLN
68	T	77	THR
68	T	80	LYS
68	T	136	GLN
68	T	138	THR
68	T	140	THR
68	T	143	ARG
68	T	145	ARG
69	U	4	VAL
69	U	6	VAL
69	U	18	TYR
69	U	22	LEU
69	U	28	LEU
69	U	33	TYR
69	U	35	ASP
69	U	36	ILE
69	U	57	ARG
69	U	67	MET
69	U	70	GLN
69	U	71	VAL
69	U	94	ILE

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Mol	Chain	Res	Type
69	U	126	GLU
69	U	127	ASN
69	U	130	ARG
69	U	131	ASP
69	U	139	THR
69	U	143	ASP
69	U	144	GLU
70	V	15	GLN
70	V	23	ARG
70	V	27	THR
70	V	30	LYS
70	V	31	VAL
70	V	57	ARG
70	V	60	THR
70	V	61	LYS
70	V	62	VAL
70	V	74	GLU
70	V	76	SER
70	V	89	ARG
70	V	103	ILE
70	V	117	VAL
71	W	5	LYS
71	W	9	VAL
71	W	10	GLU
71	W	11	LEU
71	W	25	LYS
71	W	32	VAL
71	W	41	GLU
71	W	68	SER
71	W	69	LEU
71	W	76	ASP
71	W	78	LEU
71	W	80	LYS
72	X	4	SER
72	X	7	LEU
72	X	24	GLN
72	X	25	VAL
72	X	26	LEU
72	X	53	ILE
72	X	65	LEU
72	X	76	SER
72	X	81	VAL

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Mol	Chain	Res	Type
72	X	87	GLU
72	X	98	GLN
72	X	103	ILE
72	X	119	LYS
72	X	121	VAL
72	X	126	LEU
73	Y	7	ARG
73	Y	9	LEU
73	Y	18	HIS
73	Y	19	ARG
73	Y	32	ARG
73	Y	69	ARG
73	Y	73	ARG
73	Y	75	GLN
73	Y	84	THR
73	Y	96	VAL
73	Y	107	PHE
73	Y	110	LYS
73	Y	114	LYS
73	Y	117	ILE
73	Y	132	LEU
73	Y	140	LYS
73	Y	144	ARG
74	Z	21	LYS
74	Z	32	ARG
74	Z	57	VAL
74	Z	81	GLU
74	Z	84	LYS
74	Z	99	LYS
74	Z	102	LYS
74	Z	104	SER
74	Z	124	ARG
74	Z	127	LYS
74	Z	133	ASN
75	a	40	VAL
75	a	42	LEU
75	a	43	ASP
75	a	58	ARG
75	a	60	VAL
75	a	69	LEU
75	a	71	ILE
75	a	75	LEU

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Mol	Chain	Res	Type
75	a	78	ILE
75	a	85	LYS
75	a	92	ILE
75	a	96	SER
76	b	41	ILE
76	b	44	ILE
76	b	62	TYR
76	b	64	LEU
76	b	76	SER
76	b	85	ARG
76	b	90	GLU
77	c	33	LEU
77	c	65	THR
77	c	77	THR
78	d	15	VAL
78	d	19	THR
78	d	31	GLU
78	d	32	PHE
78	d	35	ASP
78	d	48	VAL
78	d	49	ARG
78	d	58	GLU
79	e	9	SER
79	e	12	ARG
79	e	30	LEU
79	e	32	ARG
79	e	49	ASP
80	f	3	LYS
80	f	21	VAL
80	f	22	GLU
80	f	28	LYS
81	g	83	LYS
81	g	97	LYS
81	g	102	VAL
81	g	106	TYR
81	g	114	VAL
81	g	120	GLU
81	g	130	VAL
81	g	135	HIS
81	g	137	ASP
81	g	138	ARG
81	g	147	VAL

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Mol	Chain	Res	Type
81	g	151	ASN
82	h	16	HIS
82	h	29	GLN
82	h	52	GLN
82	h	66	HIS
82	h	74	THR
82	h	76	ASP
82	h	117	LYS
82	h	136	ILE
82	h	141	LEU
82	h	149	ASP
82	h	184	ASN
82	h	191	ASP
82	h	281	TYR
82	h	292	LEU
82	h	300	THR
82	h	308	ASN
82	h	317	THR
50	s0	12	GLU
50	s0	29	VAL
50	s0	30	GLN
50	s0	41	ARG
50	s0	45	VAL
50	s0	50	VAL
50	s0	55	GLU
50	s0	59	LEU
50	s0	87	LEU
50	s0	96	THR
50	s0	101	ARG
50	s0	119	ARG
50	s0	146	LEU
50	s0	154	GLU
50	s0	156	VAL
50	s0	158	VAL
50	s0	164	ASN
50	s0	165	ARG
50	s0	172	LEU
50	s0	179	ARG
50	s0	185	ARG
50	s0	188	LEU
50	s0	189	VAL
50	s0	191	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	s0	198	MET
51	s1	21	VAL
51	s1	25	THR
51	s1	37	THR
51	s1	47	LEU
51	s1	48	VAL
51	s1	68	VAL
51	s1	70	LEU
51	s1	73	LEU
51	s1	81	PHE
51	s1	91	VAL
51	s1	105	PHE
51	s1	110	LEU
51	s1	126	THR
51	s1	127	VAL
51	s1	135	LEU
51	s1	153	HIS
51	s1	159	SER
51	s1	173	THR
51	s1	175	GLU
51	s1	181	LEU
51	s1	183	GLN
51	s1	185	THR
51	s1	194	ASN
51	s1	205	PHE
51	s1	222	LYS
51	s1	223	PHE
51	s1	231	LEU
51	s1	234	GLU
52	s2	41	LEU
52	s2	51	THR
52	s2	53	ILE
52	s2	55	GLU
52	s2	69	ILE
52	s2	72	LEU
52	s2	73	LEU
52	s2	84	LYS
52	s2	90	THR
52	s2	91	ARG
52	s2	95	ARG
52	s2	97	ARG
52	s2	111	VAL

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Mol	Chain	Res	Type
52	s2	113	LEU
52	s2	117	THR
52	s2	134	LEU
52	s2	137	ILE
52	s2	139	ILE
52	s2	140	ARG
52	s2	141	ARG
52	s2	148	LEU
52	s2	150	GLN
52	s2	153	SER
52	s2	166	THR
52	s2	206	THR
52	s2	225	LEU
52	s2	228	ASN
52	s2	237	VAL
52	s2	238	SER
52	s2	245	ASP
52	s2	246	GLU
52	s2	250	GLN
53	s3	4	LEU
53	s3	21	LEU
53	s3	45	LYS
53	s3	66	ILE
53	s3	69	LEU
53	s3	84	ILE
53	s3	90	ARG
53	s3	115	ILE
53	s3	142	LEU
53	s3	158	ILE
53	s3	164	VAL
53	s3	168	ILE
53	s3	178	ARG
53	s3	196	ARG
53	s3	215	GLU
53	s3	217	ILE
53	s3	223	LYS
53	s3	224	ASP
54	s4	9	LEU
54	s4	38	LEU
54	s4	42	LEU
54	s4	49	ARG
54	s4	51	ARG

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Mol	Chain	Res	Type
54	s4	67	GLN
54	s4	70	VAL
54	s4	78	THR
54	s4	89	VAL
54	s4	95	THR
54	s4	104	ASP
54	s4	131	LEU
54	s4	156	VAL
54	s4	176	ASP
54	s4	180	LEU
54	s4	181	VAL
54	s4	182	TYR
54	s4	221	ARG
54	s4	222	LEU
54	s4	227	VAL
54	s4	245	LYS
55	s5	24	VAL
55	s5	25	LEU
55	s5	27	THR
55	s5	43	PHE
55	s5	45	LYS
55	s5	59	VAL
55	s5	66	GLN
55	s5	68	ILE
55	s5	76	ARG
55	s5	100	ASN
55	s5	104	ASN
55	s5	125	THR
55	s5	146	THR
55	s5	149	VAL
55	s5	157	ARG
55	s5	194	LEU
55	s5	208	SER
55	s5	216	GLU
56	s6	9	VAL
56	s6	65	GLN
56	s6	67	VAL
56	s6	68	LEU
56	s6	71	THR
56	s6	76	LEU
56	s6	78	THR
56	s6	97	VAL

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Mol	Chain	Res	Type
56	s6	98	ARG
56	s6	108	VAL
56	s6	120	GLU
56	s6	121	LEU
56	s6	126	ASP
56	s6	128	THR
56	s6	129	VAL
56	s6	133	LEU
56	s6	143	LYS
56	s6	151	ASP
56	s6	177	ARG
56	s6	179	VAL
56	s6	182	GLN
56	s6	193	LEU
56	s6	215	ARG
56	s6	216	LEU
57	s7	10	SER
57	s7	17	GLU
57	s7	30	SER
57	s7	33	GLU
57	s7	49	ILE
57	s7	50	ASP
57	s7	67	LEU
57	s7	79	ARG
57	s7	80	GLU
57	s7	101	LYS
57	s7	105	THR
57	s7	110	GLN
57	s7	111	LYS
57	s7	114	ARG
57	s7	116	ARG
57	s7	117	THR
57	s7	129	LEU
57	s7	143	LEU
57	s7	144	VAL
57	s7	185	ILE
58	s8	20	GLN
58	s8	22	ARG
58	s8	29	LEU
58	s8	36	THR
58	s8	46	VAL
58	s8	89	GLU

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Mol	Chain	Res	Type
58	s8	138	ASN
58	s8	151	LYS
58	s8	183	ILE
58	s8	184	LEU
59	s9	3	ARG
59	s9	6	ARG
59	s9	7	THR
59	s9	16	LYS
59	s9	20	GLU
59	s9	21	SER
59	s9	28	LEU
59	s9	37	LYS
59	s9	39	LYS
59	s9	49	LEU
59	s9	54	ARG
59	s9	78	ARG
59	s9	89	ASP
59	s9	93	LEU
59	s9	96	VAL
59	s9	99	LEU
59	s9	103	ASP
59	s9	109	LEU
59	s9	111	THR
59	s9	116	LEU
59	s9	118	LEU
59	s9	130	THR
59	s9	132	ARG
59	s9	134	ILE
59	s9	145	SER
59	s9	151	ASP
59	s9	172	VAL
59	s9	180	LYS
59	s9	182	GLU
60	c0	3	MET
60	c0	15	LEU
60	c0	20	VAL
60	c0	28	ASN
60	c0	33	GLU
60	c0	35	ILE
60	c0	55	VAL
60	c0	71	GLU
61	c1	5	LEU

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Mol	Chain	Res	Type
61	c1	10	GLU
61	c1	26	LYS
61	c1	27	THR
61	c1	31	THR
61	c1	32	LYS
61	c1	40	LEU
61	c1	44	THR
61	c1	47	THR
61	c1	60	PHE
61	c1	67	ARG
61	c1	74	THR
61	c1	76	VAL
61	c1	83	THR
61	c1	109	VAL
61	c1	129	ARG
62	c2	28	LEU
62	c2	43	ARG
62	c2	52	LEU
62	c2	58	LEU
62	c2	61	VAL
62	c2	62	LEU
62	c2	71	ILE
62	c2	86	VAL
62	c2	89	ILE
62	c2	90	LYS
62	c2	103	LEU
62	c2	129	GLU
62	c2	132	GLU
62	c2	137	MET
62	c2	140	PHE
63	c3	6	SER
63	c3	12	SER
63	c3	14	SER
63	c3	16	ILE
63	c3	19	SER
63	c3	28	LEU
63	c3	39	LYS
63	c3	60	VAL
63	c3	66	ILE
63	c3	76	LYS
63	c3	97	SER
63	c3	102	LEU

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Mol	Chain	Res	Type
63	c3	115	LEU
63	c3	125	LEU
63	c3	127	ARG
63	c3	138	ASN
64	c4	18	ARG
64	c4	49	LYS
64	c4	51	ASP
64	c4	52	ARG
64	c4	81	VAL
64	c4	91	THR
64	c4	107	ARG
64	c4	114	ARG
64	c4	119	THR
64	c4	124	ASP
64	c4	133	ARG
64	c4	136	ARG
65	c5	12	PHE
65	c5	28	MET
65	c5	36	LEU
65	c5	60	LEU
65	c5	65	LEU
65	c5	69	GLU
65	c5	72	LYS
65	c5	84	ILE
65	c5	110	GLU
65	c5	122	THR
65	c5	127	ARG
65	c5	128	HIS
66	c6	15	SER
66	c6	17	THR
66	c6	23	LYS
66	c6	26	LYS
66	c6	28	LEU
66	c6	37	THR
66	c6	42	GLU
66	c6	43	ILE
66	c6	48	VAL
66	c6	53	LEU
66	c6	57	LEU
66	c6	63	ILE
66	c6	68	ARG
66	c6	69	VAL

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Mol	Chain	Res	Type
66	c6	82	ARG
66	c6	94	GLN
66	c6	127	LYS
66	c6	128	LYS
66	c6	137	ARG
66	c6	143	ARG
67	c7	3	ARG
67	c7	8	THR
67	c7	29	GLN
67	c7	34	LEU
67	c7	46	LEU
67	c7	69	ILE
67	c7	72	LYS
67	c7	82	ASP
67	c7	85	VAL
67	c7	106	THR
67	c7	110	VAL
68	c8	3	LEU
68	c8	4	VAL
68	c8	5	VAL
68	c8	6	GLN
68	c8	12	GLN
68	c8	14	ILE
68	c8	25	ASN
68	c8	40	ARG
68	c8	61	LEU
68	c8	77	THR
68	c8	85	PHE
68	c8	92	ILE
68	c8	111	ASP
68	c8	112	ASP
68	c8	116	LEU
68	c8	133	VAL
68	c8	136	GLN
68	c8	138	THR
68	c8	143	ARG
69	c9	6	VAL
69	c9	13	ASP
69	c9	28	LEU
69	c9	29	GLU
69	c9	34	VAL
69	c9	37	VAL

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Mol	Chain	Res	Type
69	c9	68	ARG
69	c9	70	GLN
69	c9	115	GLU
69	c9	122	ARG
69	c9	126	GLU
69	c9	131	ASP
69	c9	135	ILE
69	c9	140	LEU
69	c9	142	GLU
69	c9	143	ASP
70	d0	21	LYS
70	d0	23	ARG
70	d0	27	THR
70	d0	30	LYS
70	d0	51	VAL
70	d0	57	ARG
70	d0	60	THR
70	d0	70	THR
70	d0	72	ASN
70	d0	74	GLU
70	d0	103	ILE
70	d0	107	THR
70	d0	108	ILE
71	d1	2	GLU
71	d1	4	ASP
71	d1	5	LYS
71	d1	12	TYR
71	d1	17	CYS
71	d1	32	VAL
71	d1	44	ARG
71	d1	50	TYR
71	d1	52	THR
71	d1	78	LEU
71	d1	80	LYS
72	d2	7	LEU
72	d2	15	ASN
72	d2	23	ARG
72	d2	25	VAL
72	d2	26	LEU
72	d2	31	SER
72	d2	103	ILE
73	d3	9	LEU

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Mol	Chain	Res	Type
73	d3	16	ARG
73	d3	19	ARG
73	d3	27	ASN
73	d3	28	ASN
73	d3	33	LEU
73	d3	52	ILE
73	d3	55	GLU
73	d3	73	ARG
73	d3	84	THR
73	d3	96	VAL
73	d3	100	ASP
73	d3	103	LEU
73	d3	107	PHE
73	d3	132	LEU
74	d4	5	VAL
74	d4	34	ASN
74	d4	43	LYS
74	d4	47	VAL
74	d4	49	LYS
74	d4	62	THR
74	d4	105	ARG
75	d5	46	LYS
75	d5	51	LEU
75	d5	57	TYR
76	d6	8	ASN
76	d6	10	ARG
76	d6	11	ASN
76	d6	12	LYS
76	d6	18	VAL
76	d6	45	VAL
76	d6	46	GLU
76	d6	51	ARG
76	d6	55	GLU
76	d6	82	ARG
76	d6	85	ARG
76	d6	90	GLU
77	d7	3	LEU
77	d7	4	VAL
77	d7	43	ILE
77	d7	59	CYS
77	d7	77	THR
78	d8	8	THR

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Mol	Chain	Res	Type
78	d8	16	LEU
78	d8	22	ARG
78	d8	39	THR
78	d8	52	ASP
78	d8	58	GLU
78	d8	64	ARG
78	d8	65	ARG
78	d8	66	LEU
79	d9	12	ARG
79	d9	21	CYS
79	d9	30	LEU
79	d9	54	LYS
80	e0	22	GLU
80	e0	25	GLU
80	e0	26	LYS
80	e0	29	LYS
80	e0	46	ASN
80	e0	48	THR
80	e0	55	ARG
80	e0	61	SER
83	e1	106	TYR
83	e1	113	LYS
83	e1	119	ARG
83	e1	126	CYS
83	e1	137	ASP
83	e1	147	VAL
83	e1	148	TYR
83	e1	150	VAL
82	sR	16	HIS
82	sR	48	THR
82	sR	52	GLN
82	sR	66	HIS
82	sR	70	ASP
82	sR	76	ASP
82	sR	96	THR
82	sR	145	LEU
82	sR	149	ASP
82	sR	159	ASN
82	sR	166	SER
82	sR	167	VAL
82	sR	201	THR
82	sR	232	TYR

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Mol	Chain	Res	Type
82	sR	275	ARG
82	sR	281	TYR
82	sR	297	ASP
82	sR	317	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
4	j	132	ASN
6	l	307	GLN
7	m	40	HIS
12	r	144	ASN
12	r	163	GLN
29	AA	29	HIS
29	AA	57	HIS
6	CF	110	ASN
7	CG	40	HIS
11	CK	49	ASN
11	CK	51	GLN
18	CR	137	ASN
40	DM	32	ASN
51	C	177	GLN
55	G	103	ASN
57	I	74	GLN
59	K	110	GLN
62	N	125	ASN
67	S	105	GLN
68	T	136	GLN
69	U	16	ASN
74	Z	107	GLN
82	h	159	ASN
56	s6	34	GLN
57	s7	71	HIS
64	c4	10	ASN
65	c5	103	ASN

### 5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3145/3396 (92%)	559 (17%)	46 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AR	3145/3396 (92%)	562 (17%)	58 (1%)
2	3	120/121 (99%)	13 (10%)	0
2	AS	120/121 (99%)	14 (11%)	1 (0%)
25	6	1780/1800 (98%)	376 (21%)	32 (1%)
25	A	1778/1800 (98%)	419 (23%)	45 (2%)
3	4	157/158 (99%)	34 (21%)	2 (1%)
3	AT	157/158 (99%)	29 (18%)	2 (1%)
All	All	10402/10950 (94%)	2006 (19%)	186 (1%)

All (2006) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	26	A
1	1	40	A
1	1	43	A
1	1	45	A
1	1	49	A
1	1	57	A
1	1	59	G
1	1	60	A
1	1	65	A
1	1	66	A
1	1	72	C
1	1	73	C
1	1	76	G
1	1	83	U
1	1	92	G
1	1	93	C
1	1	99	A
1	1	109	A
1	1	110	G
1	1	113	C
1	1	117	U
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	170	G

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Mol	Chain	Res	Type
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	240	U
1	1	243	G
1	1	247	C
1	1	249	U
1	1	250	U
1	1	251	G
1	1	252	U
1	1	269	G
1	1	282	G
1	1	283	G
1	1	284	A
1	1	286	U
1	1	295	A
1	1	298	U
1	1	315	C
1	1	323	A
1	1	329	U
1	1	337	G
1	1	338	A
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	401	U
1	1	402	A
1	1	403	C
1	1	414	U
1	1	421	G
1	1	422	A
1	1	438	A
1	1	439	C

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Mol	Chain	Res	Type
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	552	G
1	1	555	U
1	1	557	A
1	1	559	A
1	1	578	A
1	1	579	G
1	1	592	A
1	1	604	G
1	1	609	G
1	1	611	A
1	1	619	A
1	1	620	U
1	1	621	A
1	1	636	C
1	1	649	A
1	1	651	G
1	1	658	G
1	1	660	A
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	727	G
1	1	764	U
1	1	766	U
1	1	767	U
1	1	776	U
1	1	777	U

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Mol	Chain	Res	Type
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	861	C
1	1	869	G
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	921	A
1	1	923	C
1	1	924	G
1	1	925	A
1	1	937	G
1	1	938	C
1	1	943	U
1	1	944	C
1	1	959	C
1	1	960	U
1	1	979	U
1	1	980	A
1	1	981	U
1	1	982	C
1	1	994	G
1	1	1001	G
1	1	1002	A
1	1	1010	G
1	1	1017	C
1	1	1018	G
1	1	1020	G
1	1	1024	G
1	1	1025	A
1	1	1029	G

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Mol	Chain	Res	Type
1	1	1036	A
1	1	1037	C
1	1	1047	A
1	1	1049	C
1	1	1052	U
1	1	1064	A
1	1	1065	A
1	1	1072	G
1	1	1081	U
1	1	1082	U
1	1	1083	G
1	1	1087	G
1	1	1093	A
1	1	1094	U
1	1	1095	U
1	1	1097	G
1	1	1098	A
1	1	1102	A
1	1	1103	A
1	1	1104	G
1	1	1116	G
1	1	1117	G
1	1	1131	G
1	1	1153	A
1	1	1159	A
1	1	1160	C
1	1	1168	U
1	1	1180	A
1	1	1181	U
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	1217	A
1	1	1222	G
1	1	1227	C
1	1	1232	C
1	1	1235	U
1	1	1236	G
1	1	1237	G

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Mol	Chain	Res	Type
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	1265	U
1	1	1267	U
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
1	1	1308	A
1	1	1309	U
1	1	1313	G
1	1	1330	A
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	1386	A
1	1	1399	A
1	1	1400	G
1	1	1418	A
1	1	1419	A
1	1	1421	G
1	1	1429	G
1	1	1433	A
1	1	1434	G

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Mol	Chain	Res	Type
1	1	1437	C
1	1	1443	G
1	1	1446	A
1	1	1450	G
1	1	1481	A
1	1	1482	A
1	1	1485	G
1	1	1491	A
1	1	1508	C
1	1	1527	C
1	1	1533	U
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	1567	U
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	1605	A
1	1	1620	U
1	1	1629	U
1	1	1639	C
1	1	1643	A
1	1	1655	G
1	1	1656	A
1	1	1657	C
1	1	1658	G
1	1	1683	A
1	1	1716	U
1	1	1717	U
1	1	1724	U
1	1	1729	A

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Mol	Chain	Res	Type
1	1	1736	G
1	1	1741	A
1	1	1750	A
1	1	1751	G
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
1	1	1821	U
1	1	1835	A
1	1	1839	A
1	1	1842	A
1	1	1846	C
1	1	1849	C
1	1	1850	A
1	1	1858	A
1	1	1866	C
1	1	1879	A
1	1	1880	U
1	1	1895	A
1	1	1901	A
1	1	1906	G
1	1	1951	C
1	1	1952	G
1	1	1953	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

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Mol	Chain	Res	Type
1	1	2121	G
1	1	2122	G
1	1	2131	A
1	1	2134	G
1	1	2140	U
1	1	2145	A
1	1	2158	A
1	1	2169	G
1	1	2170	U
1	1	2177	G
1	1	2205	U
1	1	2210	G
1	1	2228	A
1	1	2244	A
1	1	2246	G
1	1	2249	G
1	1	2250	G
1	1	2255	A
1	1	2256	A
1	1	2262	A
1	1	2272	G
1	1	2273	G
1	1	2281	A
1	1	2282	U
1	1	2288	G
1	1	2298	U
1	1	2301	U
1	1	2303	A
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	2361	A
1	1	2362	C
1	1	2372	A
1	1	2373	A
1	1	2374	C
1	1	2375	G
1	1	2382	G

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Mol	Chain	Res	Type
1	1	2385	G
1	1	2393	G
1	1	2397	A
1	1	2398	A
1	1	2402	A
1	1	2403	G
1	1	2404	A
1	1	2405	C
1	1	2411	U
1	1	2418	G
1	1	2419	A
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
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	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	2582	C

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Mol	Chain	Res	Type
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	2626	A
1	1	2637	A
1	1	2652	U
1	1	2656	A
1	1	2674	A
1	1	2677	G
1	1	2689	A
1	1	2690	G
1	1	2691	A
1	1	2694	A
1	1	2696	A
1	1	2714	G
1	1	2728	G
1	1	2729	U
1	1	2737	C
1	1	2752	U
1	1	2753	G
1	1	2755	C
1	1	2771	U
1	1	2772	C
1	1	2773	C
1	1	2777	G
1	1	2778	G
1	1	2780	A
1	1	2796	G
1	1	2797	C
1	1	2799	A
1	1	2800	G
1	1	2801	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

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Mol	Chain	Res	Type
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	2899	C
1	1	2910	A
1	1	2914	G
1	1	2923	U
1	1	2927	C
1	1	2935	U
1	1	2936	A
1	1	2942	C
1	1	2945	G
1	1	2947	G
1	1	2954	U
1	1	2955	U
1	1	2971	A
1	1	2980	U
1	1	2983	C
1	1	2990	G
1	1	2992	U
1	1	2997	G
1	1	3012	A
1	1	3056	U
1	1	3059	G
1	1	3078	U
1	1	3079	U
1	1	3080	G
1	1	3086	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

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Mol	Chain	Res	Type
1	1	3150	A
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	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
1	1	3245	A
1	1	3246	G
1	1	3247	G
1	1	3259	U
1	1	3270	U
1	1	3271	G
1	1	3272	C
1	1	3273	A
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

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Mol	Chain	Res	Type
1	1	3295	A
1	1	3304	U
1	1	3309	G
1	1	3313	U
1	1	3316	A
1	1	3318	G
1	1	3319	U
1	1	3341	U
1	1	3342	A
1	1	3345	G
1	1	3347	A
1	1	3351	U
1	1	3352	U
1	1	3353	G
1	1	3354	U
1	1	3355	U
1	1	3369	G
1	1	3375	A
1	1	3376	A
1	1	3378	C
1	1	3381	U
1	1	3382	U
1	1	3389	U
1	1	3390	G
1	1	3396	U
2	3	7	G
2	3	11	A
2	3	13	A
2	3	22	A
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	23	U
3	4	34	U
3	4	35	C

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Mol	Chain	Res	Type
3	4	48	A
3	4	53	A
3	4	57	C
3	4	58	G
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	85	G
3	4	86	U
3	4	87	G
3	4	90	U
3	4	95	G
3	4	96	A
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	152	G
3	4	155	A
3	4	157	U
3	4	158	U
25	6	2	A
25	6	4	C
25	6	17	C
25	6	25	C
25	6	26	A
25	6	27	U
25	6	34	G
25	6	47	A
25	6	57	G
25	6	60	U
25	6	61	A
25	6	67	A

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Mol	Chain	Res	Type
25	6	68	A
25	6	69	G
25	6	72	A
25	6	73	U
25	6	75	U
25	6	76	A
25	6	77	U
25	6	104	A
25	6	114	C
25	6	126	A
25	6	132	U
25	6	137	U
25	6	138	A
25	6	140	A
25	6	141	U
25	6	144	U
25	6	145	A
25	6	146	U
25	6	153	G
25	6	159	U
25	6	166	C
25	6	178	U
25	6	181	A
25	6	185	U
25	6	188	A
25	6	191	C
25	6	192	U
25	6	193	U
25	6	194	U
25	6	195	G
25	6	200	A
25	6	215	A
25	6	216	U
25	6	217	A
25	6	218	A
25	6	219	A
25	6	220	A
25	6	227	U
25	6	228	G
25	6	232	U
25	6	233	C
25	6	240	U

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Mol	Chain	Res	Type
25	6	241	U
25	6	249	U
25	6	250	C
25	6	261	U
25	6	265	A
25	6	271	A
25	6	272	U
25	6	273	G
25	6	275	C
25	6	278	U
25	6	280	U
25	6	285	G
25	6	299	A
25	6	302	U
25	6	308	C
25	6	314	C
25	6	316	A
25	6	319	U
25	6	320	U
25	6	321	C
25	6	322	G
25	6	337	G
25	6	338	C
25	6	352	A
25	6	359	A
25	6	360	A
25	6	361	C
25	6	400	A
25	6	401	A
25	6	402	C
25	6	404	G
25	6	416	A
25	6	418	G
25	6	424	C
25	6	425	A
25	6	426	G
25	6	434	G
25	6	439	U
25	6	444	C
25	6	445	A
25	6	448	C
25	6	454	U

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Mol	Chain	Res	Type
25	6	468	A
25	6	477	A
25	6	480	G
25	6	486	G
25	6	488	G
25	6	489	C
25	6	490	C
25	6	492	A
25	6	493	U
25	6	494	U
25	6	496	G
25	6	497	G
25	6	500	C
25	6	501	U
25	6	504	U
25	6	505	A
25	6	506	A
25	6	507	U
25	6	510	G
25	6	511	A
25	6	512	A
25	6	513	U
25	6	514	G
25	6	515	A
25	6	516	G
25	6	519	C
25	6	527	A
25	6	538	A
25	6	539	G
25	6	540	G
25	6	541	A
25	6	542	A
25	6	543	C
25	6	544	A
25	6	548	G
25	6	557	G
25	6	558	U
25	6	559	C
25	6	565	C
25	6	568	G
25	6	570	A
25	6	574	G

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Mol	Chain	Res	Type
25	6	579	A
25	6	580	A
25	6	582	U
25	6	594	A
25	6	595	G
25	6	611	U
25	6	619	A
25	6	620	A
25	6	621	A
25	6	622	A
25	6	623	A
25	6	624	G
25	6	639	U
25	6	640	U
25	6	650	U
25	6	652	G
25	6	653	C
25	6	658	C
25	6	676	G
25	6	679	U
25	6	680	U
25	6	681	U
25	6	682	C
25	6	683	C
25	6	684	A
25	6	685	A
25	6	691	C
25	6	696	C
25	6	709	C
25	6	711	U
25	6	714	G
25	6	715	U
25	6	718	U
25	6	719	U
25	6	720	G
25	6	721	U
25	6	722	G
25	6	723	G
25	6	730	G
25	6	742	U
25	6	745	U
25	6	753	A

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Mol	Chain	Res	Type
25	6	754	A
25	6	755	A
25	6	756	A
25	6	765	G
25	6	766	U
25	6	774	A
25	6	775	G
25	6	780	A
25	6	781	U
25	6	782	U
25	6	783	G
25	6	789	A
25	6	793	A
25	6	794	U
25	6	803	A
25	6	811	A
25	6	812	A
25	6	815	G
25	6	821	U
25	6	823	G
25	6	825	U
25	6	826	U
25	6	829	A
25	6	830	U
25	6	831	U
25	6	832	U
25	6	834	G
25	6	835	U
25	6	863	A
25	6	876	G
25	6	898	A
25	6	906	A
25	6	912	U
25	6	913	G
25	6	914	G
25	6	916	U
25	6	933	A
25	6	935	U
25	6	942	G
25	6	959	U
25	6	960	U
25	6	966	A

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Mol	Chain	Res	Type
25	6	970	A
25	6	971	A
25	6	983	A
25	6	992	A
25	6	1003	A
25	6	1004	U
25	6	1005	A
25	6	1021	C
25	6	1026	A
25	6	1028	C
25	6	1039	A
25	6	1040	G
25	6	1052	U
25	6	1053	G
25	6	1057	U
25	6	1058	U
25	6	1059	U
25	6	1060	U
25	6	1072	C
25	6	1073	G
25	6	1076	A
25	6	1082	C
25	6	1092	A
25	6	1096	C
25	6	1097	U
25	6	1098	U
25	6	1099	U
25	6	1100	G
25	6	1109	G
25	6	1137	A
25	6	1138	A
25	6	1151	A
25	6	1155	G
25	6	1158	C
25	6	1159	C
25	6	1160	A
25	6	1167	G
25	6	1185	U
25	6	1194	A
25	6	1196	A
25	6	1199	G
25	6	1200	G

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Mol	Chain	Res	Type
25	6	1202	A
25	6	1208	A
25	6	1217	A
25	6	1218	G
25	6	1225	U
25	6	1228	G
25	6	1229	G
25	6	1230	A
25	6	1231	U
25	6	1241	G
25	6	1243	G
25	6	1244	A
25	6	1245	G
25	6	1246	C
25	6	1255	G
25	6	1256	A
25	6	1257	U
25	6	1258	U
25	6	1286	U
25	6	1291	G
25	6	1314	U
25	6	1315	U
25	6	1316	G
25	6	1321	A
25	6	1344	A
25	6	1345	A
25	6	1346	A
25	6	1354	G
25	6	1361	U
25	6	1363	U
25	6	1364	G
25	6	1371	A
25	6	1372	U
25	6	1388	A
25	6	1390	U
25	6	1398	U
25	6	1399	C
25	6	1400	A
25	6	1402	G
25	6	1413	U
25	6	1414	U
25	6	1415	U

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Mol	Chain	Res	Type
25	6	1427	A
25	6	1428	G
25	6	1433	G
25	6	1445	G
25	6	1446	A
25	6	1448	G
25	6	1458	G
25	6	1459	C
25	6	1461	C
25	6	1471	A
25	6	1481	C
25	6	1482	C
25	6	1490	C
25	6	1491	U
25	6	1492	A
25	6	1493	A
25	6	1506	G
25	6	1514	U
25	6	1515	A
25	6	1516	A
25	6	1521	G
25	6	1523	G
25	6	1524	A
25	6	1535	U
25	6	1536	G
25	6	1537	C
25	6	1538	U
25	6	1540	G
25	6	1554	U
25	6	1557	U
25	6	1559	A
25	6	1569	A
25	6	1573	A
25	6	1574	G
25	6	1584	G
25	6	1590	G
25	6	1601	G
25	6	1616	G
25	6	1621	U
25	6	1657	U
25	6	1658	G
25	6	1682	U

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Mol	Chain	Res	Type
25	6	1683	C
25	6	1696	G
25	6	1697	G
25	6	1698	G
25	6	1699	G
25	6	1700	C
25	6	1701	A
25	6	1702	A
25	6	1703	C
25	6	1712	A
25	6	1716	C
25	6	1717	G
25	6	1731	A
25	6	1760	G
25	6	1762	A
25	6	1766	A
25	6	1767	G
25	6	1769	U
25	6	1780	G
25	6	1782	A
25	6	1783	C
25	6	1792	G
25	6	1793	G
25	6	1794	A
25	6	1795	U
25	6	1796	C
25	6	1799	U
25	6	1800	A
1	AR	16	A
1	AR	24	G
1	AR	26	A
1	AR	40	A
1	AR	43	A
1	AR	49	A
1	AR	57	A
1	AR	59	G
1	AR	60	A
1	AR	65	A
1	AR	66	A
1	AR	76	G
1	AR	92	G
1	AR	93	C

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Mol	Chain	Res	Type
1	AR	99	A
1	AR	109	A
1	AR	110	G
1	AR	111	C
1	AR	113	C
1	AR	116	A
1	AR	120	G
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	187	A
1	AR	190	U
1	AR	191	U
1	AR	192	C
1	AR	200	C
1	AR	210	U
1	AR	211	A
1	AR	213	A
1	AR	218	G
1	AR	219	A
1	AR	231	G
1	AR	240	U
1	AR	241	G
1	AR	243	G
1	AR	245	U
1	AR	249	U
1	AR	250	U
1	AR	251	G
1	AR	252	U
1	AR	269	G
1	AR	270	U
1	AR	286	U
1	AR	295	A

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Mol	Chain	Res	Type
1	AR	298	U
1	AR	323	A
1	AR	329	U
1	AR	334	A
1	AR	338	A
1	AR	339	C
1	AR	350	C
1	AR	351	A
1	AR	370	U
1	AR	376	G
1	AR	399	A
1	AR	401	U
1	AR	402	A
1	AR	403	C
1	AR	404	G
1	AR	409	A
1	AR	421	G
1	AR	422	A
1	AR	439	C
1	AR	440	A
1	AR	495	G
1	AR	516	A
1	AR	521	A
1	AR	535	G
1	AR	544	C
1	AR	546	C
1	AR	548	G
1	AR	551	A
1	AR	552	G
1	AR	555	U
1	AR	557	A
1	AR	558	U
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	607	A
1	AR	609	G
1	AR	611	A
1	AR	621	A

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Mol	Chain	Res	Type
1	AR	622	A
1	AR	636	C
1	AR	638	C
1	AR	649	A
1	AR	651	G
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	758	C
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	780	A
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	874	U
1	AR	879	U
1	AR	896	A
1	AR	907	G
1	AR	908	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

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Mol	Chain	Res	Type
1	AR	944	C
1	AR	959	C
1	AR	960	U
1	AR	964	G
1	AR	979	U
1	AR	980	A
1	AR	981	U
1	AR	982	C
1	AR	984	G
1	AR	994	G
1	AR	1001	G
1	AR	1002	A
1	AR	1006	A
1	AR	1010	G
1	AR	1015	U
1	AR	1016	C
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	1064	A
1	AR	1065	A
1	AR	1072	G
1	AR	1081	U
1	AR	1082	U
1	AR	1093	A
1	AR	1094	U
1	AR	1095	U
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	1143	A

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Mol	Chain	Res	Type
1	AR	1153	A
1	AR	1159	A
1	AR	1180	A
1	AR	1181	U
1	AR	1190	A
1	AR	1192	C
1	AR	1196	C
1	AR	1201	C
1	AR	1202	A
1	AR	1209	G
1	AR	1214	U
1	AR	1216	C
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	1244	A
1	AR	1245	A
1	AR	1246	G
1	AR	1252	A
1	AR	1258	U
1	AR	1262	G
1	AR	1263	A
1	AR	1285	G
1	AR	1292	C
1	AR	1295	G
1	AR	1307	G
1	AR	1308	A
1	AR	1309	U
1	AR	1313	G
1	AR	1330	A
1	AR	1348	U
1	AR	1349	G
1	AR	1351	U
1	AR	1352	A
1	AR	1353	U
1	AR	1355	A
1	AR	1356	U

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Mol	Chain	Res	Type
1	AR	1357	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	1453	A
1	AR	1481	A
1	AR	1482	A
1	AR	1488	G
1	AR	1508	C
1	AR	1536	G
1	AR	1555	U
1	AR	1556	C
1	AR	1560	G
1	AR	1562	C
1	AR	1563	C
1	AR	1566	A
1	AR	1567	U
1	AR	1568	U
1	AR	1569	U
1	AR	1570	U
1	AR	1572	U
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	1589	A
1	AR	1593	A
1	AR	1605	A
1	AR	1607	U
1	AR	1620	U

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Mol	Chain	Res	Type
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	1736	G
1	AR	1741	A
1	AR	1742	U
1	AR	1750	A
1	AR	1751	G
1	AR	1762	C
1	AR	1765	U
1	AR	1766	G
1	AR	1769	G
1	AR	1770	G
1	AR	1780	G
1	AR	1797	A
1	AR	1809	A
1	AR	1810	A
1	AR	1814	A
1	AR	1815	U
1	AR	1816	A
1	AR	1817	G
1	AR	1820	U
1	AR	1821	U
1	AR	1835	A
1	AR	1839	A
1	AR	1841	A
1	AR	1842	A
1	AR	1846	C
1	AR	1849	C
1	AR	1878	G
1	AR	1879	A
1	AR	1893	A
1	AR	1906	G
1	AR	1952	G

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Mol	Chain	Res	Type
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	2134	G
1	AR	2140	U
1	AR	2144	A
1	AR	2158	A
1	AR	2169	G
1	AR	2187	G
1	AR	2198	A
1	AR	2201	G
1	AR	2205	U
1	AR	2209	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
1	AR	2269	U
1	AR	2270	A
1	AR	2271	A
1	AR	2272	G
1	AR	2273	G
1	AR	2279	A
1	AR	2280	A
1	AR	2281	A

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Mol	Chain	Res	Type
1	AR	2282	U
1	AR	2288	G
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	2336	U
1	AR	2372	A
1	AR	2373	A
1	AR	2374	C
1	AR	2375	G
1	AR	2385	G
1	AR	2393	G
1	AR	2397	A
1	AR	2401	A
1	AR	2402	A
1	AR	2403	G
1	AR	2404	A
1	AR	2411	U
1	AR	2418	G
1	AR	2419	A
1	AR	2435	G
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	2507	C
1	AR	2508	U
1	AR	2514	U
1	AR	2515	A
1	AR	2522	G
1	AR	2523	A
1	AR	2524	A
1	AR	2530	G
1	AR	2533	G
1	AR	2536	A
1	AR	2538	U
1	AR	2539	C

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Mol	Chain	Res	Type
1	AR	2540	A
1	AR	2541	U
1	AR	2542	U
1	AR	2543	U
1	AR	2547	A
1	AR	2549	G
1	AR	2552	C
1	AR	2555	G
1	AR	2561	A
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	2586	G
1	AR	2589	G
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	2634	U
1	AR	2638	C
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	2691	A
1	AR	2694	A
1	AR	2696	A
1	AR	2705	A
1	AR	2714	G
1	AR	2719	U
1	AR	2727	A
1	AR	2728	G
1	AR	2729	U
1	AR	2752	U

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Mol	Chain	Res	Type
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	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	2819	A
1	AR	2842	U
1	AR	2843	U
1	AR	2845	A
1	AR	2847	A
1	AR	2860	U
1	AR	2867	C
1	AR	2871	G
1	AR	2872	A
1	AR	2873	U
1	AR	2875	U
1	AR	2887	A
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	2945	G
1	AR	2947	G
1	AR	2951	G
1	AR	2952	G
1	AR	2971	A
1	AR	2983	C
1	AR	2990	G
1	AR	2996	U

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Mol	Chain	Res	Type
1	AR	2997	G
1	AR	3012	A
1	AR	3049	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	3092	C
1	AR	3104	U
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	3155	U
1	AR	3156	U
1	AR	3157	U
1	AR	3164	C
1	AR	3165	A
1	AR	3167	A
1	AR	3168	A
1	AR	3170	A
1	AR	3171	U
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	3197	G
1	AR	3207	U
1	AR	3217	C
1	AR	3218	A
1	AR	3219	G
1	AR	3222	U
1	AR	3224	G
1	AR	3229	G

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Mol	Chain	Res	Type
1	AR	3243	A
1	AR	3244	A
1	AR	3245	A
1	AR	3246	G
1	AR	3247	G
1	AR	3253	G
1	AR	3259	U
1	AR	3266	G
1	AR	3269	U
1	AR	3270	U
1	AR	3273	A
1	AR	3276	G
1	AR	3277	U
1	AR	3281	U
1	AR	3287	U
1	AR	3289	G
1	AR	3294	A
1	AR	3295	A
1	AR	3303	G
1	AR	3304	U
1	AR	3307	A
1	AR	3313	U
1	AR	3316	A
1	AR	3317	U
1	AR	3318	G
1	AR	3319	U
1	AR	3320	A
1	AR	3330	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	3369	G
1	AR	3375	A
1	AR	3378	C

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Mol	Chain	Res	Type
1	AR	3383	G
1	AR	3389	U
2	AS	7	G
2	AS	22	A
2	AS	52	G
2	AS	53	U
2	AS	54	U
2	AS	60	G
2	AS	65	G
2	AS	73	C
2	AS	74	C
2	AS	99	G
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	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	85	G
3	AT	86	U
3	AT	87	G
3	AT	90	U
3	AT	95	G
3	AT	97	A
3	AT	104	A
3	AT	106	C
3	AT	111	A
3	AT	113	U
3	AT	125	U
3	AT	126	A
3	AT	148	G
3	AT	151	C

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Mol	Chain	Res	Type
3	AT	152	G
3	AT	155	A
3	AT	158	U
25	A	2	A
25	A	4	C
25	A	17	C
25	A	25	C
25	A	26	A
25	A	27	U
25	A	34	G
25	A	42	G
25	A	45	U
25	A	46	A
25	A	47	A
25	A	50	C
25	A	57	G
25	A	60	U
25	A	67	A
25	A	68	A
25	A	69	G
25	A	72	A
25	A	73	U
25	A	74	U
25	A	104	A
25	A	114	C
25	A	116	U
25	A	128	U
25	A	130	C
25	A	131	C
25	A	132	U
25	A	133	U
25	A	134	U
25	A	135	A
25	A	136	C
25	A	137	U
25	A	140	A
25	A	141	U
25	A	144	U
25	A	145	A
25	A	146	U
25	A	153	G
25	A	158	U

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Mol	Chain	Res	Type
25	A	159	U
25	A	161	U
25	A	176	C
25	A	178	U
25	A	179	A
25	A	185	U
25	A	186	C
25	A	187	G
25	A	188	A
25	A	190	C
25	A	191	C
25	A	192	U
25	A	193	U
25	A	194	U
25	A	195	G
25	A	196	G
25	A	197	A
25	A	200	A
25	A	215	A
25	A	217	A
25	A	218	A
25	A	219	A
25	A	226	A
25	A	227	U
25	A	228	G
25	A	229	U
25	A	233	C
25	A	234	G
25	A	235	G
25	A	238	U
25	A	240	U
25	A	241	U
25	A	250	C
25	A	260	U
25	A	261	U
25	A	265	A
25	A	271	A
25	A	272	U
25	A	274	G
25	A	275	C
25	A	276	C
25	A	277	U

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Mol	Chain	Res	Type
25	A	278	U
25	A	279	G
25	A	280	U
25	A	281	G
25	A	284	G
25	A	288	A
25	A	290	G
25	A	299	A
25	A	308	C
25	A	309	C
25	A	314	C
25	A	316	A
25	A	319	U
25	A	321	C
25	A	322	G
25	A	337	G
25	A	338	C
25	A	352	A
25	A	359	A
25	A	360	A
25	A	361	C
25	A	387	A
25	A	390	G
25	A	400	A
25	A	402	C
25	A	403	G
25	A	404	G
25	A	416	A
25	A	418	G
25	A	424	C
25	A	425	A
25	A	426	G
25	A	428	A
25	A	434	G
25	A	439	U
25	A	444	C
25	A	445	A
25	A	448	C
25	A	454	U
25	A	468	A
25	A	480	G
25	A	484	C

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Mol	Chain	Res	Type
25	A	485	A
25	A	488	G
25	A	493	U
25	A	494	U
25	A	495	C
25	A	496	G
25	A	497	G
25	A	498	G
25	A	499	U
25	A	500	C
25	A	502	U
25	A	503	G
25	A	504	U
25	A	505	A
25	A	506	A
25	A	507	U
25	A	510	G
25	A	511	A
25	A	512	A
25	A	513	U
25	A	515	A
25	A	516	G
25	A	527	A
25	A	532	U
25	A	538	A
25	A	539	G
25	A	540	G
25	A	541	A
25	A	542	A
25	A	543	C
25	A	544	A
25	A	555	A
25	A	556	A
25	A	557	G
25	A	558	U
25	A	559	C
25	A	565	C
25	A	579	A
25	A	580	A
25	A	583	C
25	A	594	A
25	A	595	G

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Mol	Chain	Res	Type
25	A	606	A
25	A	611	U
25	A	619	A
25	A	620	A
25	A	621	A
25	A	622	A
25	A	623	A
25	A	624	G
25	A	639	U
25	A	640	U
25	A	650	U
25	A	653	C
25	A	654	C
25	A	655	G
25	A	656	G
25	A	658	C
25	A	677	G
25	A	679	U
25	A	684	A
25	A	685	A
25	A	686	C
25	A	692	C
25	A	694	U
25	A	696	C
25	A	697	C
25	A	700	C
25	A	702	G
25	A	703	G
25	A	704	C
25	A	705	U
25	A	707	A
25	A	708	C
25	A	709	C
25	A	710	U
25	A	711	U
25	A	712	G
25	A	714	G
25	A	717	C
25	A	718	U
25	A	719	U
25	A	721	U
25	A	722	G

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Mol	Chain	Res	Type
25	A	723	G
25	A	725	U
25	A	727	U
25	A	728	U
25	A	731	C
25	A	732	G
25	A	733	A
25	A	734	A
25	A	735	C
25	A	736	C
25	A	737	A
25	A	738	G
25	A	742	U
25	A	743	U
25	A	745	U
25	A	754	A
25	A	755	A
25	A	756	A
25	A	765	G
25	A	766	U
25	A	774	A
25	A	775	G
25	A	778	G
25	A	780	A
25	A	781	U
25	A	783	G
25	A	784	C
25	A	789	A
25	A	794	U
25	A	812	A
25	A	814	A
25	A	815	G
25	A	816	G
25	A	818	C
25	A	819	G
25	A	820	U
25	A	821	U
25	A	822	U
25	A	824	G
25	A	830	U
25	A	831	U
25	A	833	U

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Mol	Chain	Res	Type
25	A	862	A
25	A	863	A
25	A	864	U
25	A	886	U
25	A	898	A
25	A	912	U
25	A	913	G
25	A	914	G
25	A	915	A
25	A	916	U
25	A	928	U
25	A	933	A
25	A	935	U
25	A	942	G
25	A	951	A
25	A	960	U
25	A	966	A
25	A	988	A
25	A	991	G
25	A	992	A
25	A	993	A
25	A	1003	A
25	A	1004	U
25	A	1005	A
25	A	1020	A
25	A	1026	A
25	A	1028	C
25	A	1039	A
25	A	1040	G
25	A	1052	U
25	A	1053	G
25	A	1058	U
25	A	1061	A
25	A	1074	G
25	A	1076	A
25	A	1080	U
25	A	1082	C
25	A	1091	A
25	A	1092	A
25	A	1093	A
25	A	1096	C
25	A	1097	U

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Mol	Chain	Res	Type
25	A	1100	G
25	A	1109	G
25	A	1111	G
25	A	1138	A
25	A	1146	G
25	A	1150	G
25	A	1151	A
25	A	1157	A
25	A	1158	C
25	A	1160	A
25	A	1164	G
25	A	1167	G
25	A	1185	U
25	A	1194	A
25	A	1196	A
25	A	1197	C
25	A	1199	G
25	A	1200	G
25	A	1202	A
25	A	1207	C
25	A	1208	A
25	A	1217	A
25	A	1218	G
25	A	1227	A
25	A	1229	G
25	A	1243	G
25	A	1244	A
25	A	1245	G
25	A	1251	U
25	A	1256	A
25	A	1257	U
25	A	1258	U
25	A	1286	U
25	A	1314	U
25	A	1315	U
25	A	1321	A
25	A	1339	C
25	A	1340	U
25	A	1341	A
25	A	1344	A
25	A	1345	A
25	A	1349	G

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Mol	Chain	Res	Type
25	A	1354	G
25	A	1361	U
25	A	1362	U
25	A	1363	U
25	A	1364	G
25	A	1370	U
25	A	1371	A
25	A	1372	U
25	A	1390	U
25	A	1398	U
25	A	1399	C
25	A	1400	A
25	A	1412	G
25	A	1413	U
25	A	1415	U
25	A	1427	A
25	A	1428	G
25	A	1446	A
25	A	1458	G
25	A	1459	C
25	A	1461	C
25	A	1471	A
25	A	1473	U
25	A	1474	G
25	A	1475	A
25	A	1482	C
25	A	1486	G
25	A	1490	C
25	A	1491	U
25	A	1492	A
25	A	1493	A
25	A	1506	G
25	A	1515	A
25	A	1516	A
25	A	1517	U
25	A	1521	G
25	A	1523	G
25	A	1524	A
25	A	1526	A
25	A	1535	U
25	A	1536	G
25	A	1537	C

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Mol	Chain	Res	Type
25	A	1538	U
25	A	1542	G
25	A	1557	U
25	A	1559	A
25	A	1569	A
25	A	1574	G
25	A	1584	G
25	A	1590	G
25	A	1601	G
25	A	1614	A
25	A	1616	G
25	A	1619	C
25	A	1624	C
25	A	1626	U
25	A	1631	A
25	A	1657	U
25	A	1658	G
25	A	1680	G
25	A	1683	C
25	A	1684	U
25	A	1686	C
25	A	1698	G
25	A	1699	G
25	A	1700	C
25	A	1701	A
25	A	1702	A
25	A	1703	C
25	A	1711	C
25	A	1712	A
25	A	1713	G
25	A	1731	A
25	A	1750	A
25	A	1760	G
25	A	1762	A
25	A	1766	A
25	A	1769	U
25	A	1780	G
25	A	1782	A
25	A	1783	C
25	A	1792	G
25	A	1793	G
25	A	1794	A

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Mol	Chain	Res	Type
25	A	1795	U
25	A	1796	C

All (186) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	65	A
1	1	210	U
1	1	239	G
1	1	282	G
1	1	547	G
1	1	647	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	1273	A
1	1	1307	G
1	1	1329	U
1	1	1352	A
1	1	1355	A
1	1	1562	C
1	1	1568	U
1	1	1716	U
1	1	1820	U
1	1	2101	C
1	1	2112	U
1	1	2209	U
1	1	2249	G
1	1	2372	A
1	1	2418	G
1	1	2537	U
1	1	2541	U
1	1	2593	A
1	1	2772	C
1	1	2801	A
1	1	2818	U

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Mol	Chain	Res	Type
1	1	3056	U
1	1	3078	U
1	1	3121	U
1	1	3218	A
1	1	3228	C
1	1	3269	U
1	1	3350	C
1	1	3351	U
1	1	3353	G
1	1	3375	A
3	4	85	G
3	4	125	U
25	6	25	C
25	6	139	C
25	6	145	A
25	6	158	U
25	6	187	G
25	6	192	U
25	6	217	A
25	6	272	U
25	6	417	A
25	6	512	A
25	6	542	A
25	6	558	U
25	6	678	A
25	6	755	A
25	6	829	A
25	6	834	G
25	6	1051	G
25	6	1058	U
25	6	1081	A
25	6	1097	U
25	6	1207	C
25	6	1244	A
25	6	1255	G
25	6	1344	A
25	6	1481	C
25	6	1489	U
25	6	1491	U
25	6	1535	U
25	6	1568	C
25	6	1573	A

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Mol	Chain	Res	Type
25	6	1620	C
25	6	1657	U
1	AR	40	A
1	AR	65	A
1	AR	588	G
1	AR	637	C
1	AR	715	A
1	AR	763	G
1	AR	873	C
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
1	AR	1307	G
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	2252	A
1	AR	2255	A
1	AR	2260	U
1	AR	2269	U
1	AR	2373	A
1	AR	2374	C
1	AR	2404	A

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Mol	Chain	Res	Type
1	AR	2418	G
1	AR	2537	U
1	AR	2541	U
1	AR	2593	A
1	AR	2728	G
1	AR	2801	A
1	AR	2818	U
1	AR	2872	A
1	AR	3078	U
1	AR	3121	U
1	AR	3218	A
1	AR	3228	C
1	AR	3269	U
1	AR	3276	G
1	AR	3316	A
1	AR	3317	U
1	AR	3350	C
1	AR	3375	A
2	AS	52	G
3	AT	82	U
3	AT	85	G
25	A	25	C
25	A	45	U
25	A	73	U
25	A	130	C
25	A	131	C
25	A	139	C
25	A	158	U
25	A	187	G
25	A	218	A
25	A	240	U
25	A	278	U
25	A	280	U
25	A	417	A
25	A	497	G
25	A	499	U
25	A	501	U
25	A	503	G
25	A	512	A
25	A	555	A
25	A	685	A
25	A	704	C

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Mol	Chain	Res	Type
25	A	720	G
25	A	721	U
25	A	755	A
25	A	829	A
25	A	1051	G
25	A	1081	A
25	A	1150	G
25	A	1157	A
25	A	1196	A
25	A	1207	C
25	A	1226	A
25	A	1244	A
25	A	1250	U
25	A	1344	A
25	A	1370	U
25	A	1481	C
25	A	1489	U
25	A	1568	C
25	A	1573	A
25	A	1600	A
25	A	1615	C
25	A	1657	U
25	A	1698	G
25	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 2548 ligands modelled in this entry, 1 is modelled with single atom and 1477 are monoatomic - leaving 1070 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	1	3401	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3402	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3403	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3404	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3405	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3406	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3407	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3408	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3409	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3410	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3411	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3412	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3413	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3414	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3415	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3416	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3417	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3418	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3419	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3420	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3421	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3422	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3423	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3424	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3426	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3427	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3428	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3429	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3430	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3431	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3432	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3433	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3434	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3435	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3437	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3438	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3439	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3440	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3441	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3442	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3443	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3444	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3445	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3446	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3447	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3448	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3449	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3450	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3451	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3452	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3453	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3454	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3455	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3456	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3457	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3458	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3459	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3460	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3461	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3462	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3463	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3464	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3465	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3466	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3467	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3468	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3469	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3470	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3471	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3472	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3473	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3474	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3475	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3476	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3477	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3478	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3479	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3480	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3481	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3482	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3483	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3485	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3486	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3487	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3488	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3489	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3491	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3492	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3493	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3494	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3495	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3496	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3497	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3498	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3499	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3500	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3501	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3502	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3503	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3504	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3505	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3506	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3507	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3508	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3509	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3510	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3511	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3512	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3513	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3514	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3515	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3516	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3517	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3518	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3519	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3520	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3521	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3522	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3523	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3524	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3525	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3526	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3527	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3528	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3529	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3530	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3531	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3532	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3533	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3534	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3535	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3536	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3537	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3538	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3539	84	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3540	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3541	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3542	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3543	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3544	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3545	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3546	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3547	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3548	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3549	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3550	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3551	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3552	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3553	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3554	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3555	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3556	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3557	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3558	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3559	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3560	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3561	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3562	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3563	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3564	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3565	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3566	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3567	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3568	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3569	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3570	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3571	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3572	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3573	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3574	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3575	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3576	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3577	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3578	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3579	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3580	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3581	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3582	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3583	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3584	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3585	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3586	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3587	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3588	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3589	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3590	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3591	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3592	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3593	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3594	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3595	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3596	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3597	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3598	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3599	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3600	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3601	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3602	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3603	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3604	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3605	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3606	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3607	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3608	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3609	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3610	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3611	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3612	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3613	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3614	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3615	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3616	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3617	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3618	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3619	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3620	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3621	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3622	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3623	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3624	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3625	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3626	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3627	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3628	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3629	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3630	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3631	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3632	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3633	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3634	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3635	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3636	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3637	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3638	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3639	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3640	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3641	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3642	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3643	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3644	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3645	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3646	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3647	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3648	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3649	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3650	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3651	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3652	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3653	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3654	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3655	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3656	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3657	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3658	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3659	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3660	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3661	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3662	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3663	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3664	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3665	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3666	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3667	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3668	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3669	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3670	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3671	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3672	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3673	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3674	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3675	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3676	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3677	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3678	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3679	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3680	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3681	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3682	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3683	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3684	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3685	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3686	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3687	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3688	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3689	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3690	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3691	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3692	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3693	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3694	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3695	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3696	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3697	84	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3698	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3699	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3700	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3701	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3702	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3703	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3704	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3705	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3706	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3707	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3708	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3709	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3710	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3711	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3712	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3713	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3714	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3715	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3716	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3717	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3718	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3719	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3720	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3721	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3723	1	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	1	3724	-	0,6,6	0.00	-	0,15,15	0.00	-
86	HN8	1	4223	-	26,26,26	0.27	0	36,41,41	1.04	2 (5%)
84	OHX	2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	3	204	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	3	205	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	3	206	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	3	207	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	3	208	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	3	209	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	203	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	204	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	205	-	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	4	206	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	207	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	208	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	209	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	210	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	211	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	212	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	213	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	214	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	215	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	4	216	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1901	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1902	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1903	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1904	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1905	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1906	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1907	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1908	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1909	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1910	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1911	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1912	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1913	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1914	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1915	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1916	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1917	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1918	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1919	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1920	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1921	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1922	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1923	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1924	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1925	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1926	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1927	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1928	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1929	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1930	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1931	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1932	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	6	1933	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1934	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1935	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1936	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1937	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1938	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1939	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1940	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1941	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1942	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1943	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1944	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1945	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1946	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1947	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1948	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1949	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1950	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1951	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1952	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1953	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1954	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1955	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1956	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1957	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1958	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1959	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1960	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1961	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1962	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1963	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1964	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1965	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1966	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1967	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1968	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1969	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1970	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1971	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1972	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1973	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1974	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1975	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	6	1976	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1977	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1978	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1979	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1980	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1981	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1982	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1983	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1984	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1985	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1986	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1987	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1988	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1989	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1990	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1991	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1992	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1993	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1994	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1995	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1996	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1997	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1998	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	1999	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2000	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2001	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2002	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2003	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2004	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2005	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2006	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2007	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2008	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2009	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2010	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2011	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2012	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2013	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2014	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2015	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2016	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2017	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2018	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	6	2019	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2020	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2021	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	6	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	GOL	6	2199	-	5,5,5	0.09	0	5,5,5	0.36	0
84	OHX	A	1901	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1902	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1903	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1904	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1905	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1906	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1907	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1908	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	A	1909	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1910	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1911	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1912	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1913	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1914	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1915	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1916	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1917	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1918	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1919	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1920	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1921	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1922	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1923	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1924	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1925	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1926	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1927	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1928	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1929	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1930	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1931	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1932	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1933	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1934	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1935	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1936	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1937	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1938	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1939	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1940	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1941	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1942	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1943	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1944	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1945	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1946	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1947	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1948	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1949	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1950	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1951	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	A	1952	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1953	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1954	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1955	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1956	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1957	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1958	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1959	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1960	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1961	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1962	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1963	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1964	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1965	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1966	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1967	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1968	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1969	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1970	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1971	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1972	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1973	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1974	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1975	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1976	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1977	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1978	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1979	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1980	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1981	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1982	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1983	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1984	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1985	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1986	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1987	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1988	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1989	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1990	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1991	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1992	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1993	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1994	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	A	1995	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1996	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1997	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1998	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	1999	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2000	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2001	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2002	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2003	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2004	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2005	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2006	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2007	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2008	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2009	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2010	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2011	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2012	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2013	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2014	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2015	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2016	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2017	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2018	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2019	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2020	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2021	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2037	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	A	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	A	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	GOL	A	2160	-	5,5,5	0.11	0	5,5,5	0.32	0
84	OHX	AC	101	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AG	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AH	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AK	102	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AM	101	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AP	502	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3401	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3402	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3403	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3404	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3405	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3406	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3407	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3408	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3409	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3410	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3411	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3412	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3413	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3414	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3415	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3416	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3417	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3418	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3419	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3420	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3421	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3422	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3423	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3424	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3426	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3427	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3428	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3429	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3430	-	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3431	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3432	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3433	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3434	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3435	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3437	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3438	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3439	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3440	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3441	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3442	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3443	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3444	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3445	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3446	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3447	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3448	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3449	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3450	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3451	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3452	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3453	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3454	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3455	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3456	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3457	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3458	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3459	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3460	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3461	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3462	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3463	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3464	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3465	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3466	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3467	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3468	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3469	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3470	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3471	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3472	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3473	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3474	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3475	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3476	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3477	84	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3478	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3479	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3480	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3481	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3482	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3483	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3485	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3486	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3487	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3488	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3489	87	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3491	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3492	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3493	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3494	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3495	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3496	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3497	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3498	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3499	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3500	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3501	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3502	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3503	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3504	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3505	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3506	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3507	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3508	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3509	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3510	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3511	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3512	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3513	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3514	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3515	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3516	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3517	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3518	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3519	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3520	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3521	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3522	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3523	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3524	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3525	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3526	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3527	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3528	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3529	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3530	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3531	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3532	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3533	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3534	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3535	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3536	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3537	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3538	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3539	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3540	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3541	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3542	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3543	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3544	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3545	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3546	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3547	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3548	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3549	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3550	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3551	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3552	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3553	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3554	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3555	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3556	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3557	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3558	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3559	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3560	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3561	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3562	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3563	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3564	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3565	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3566	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3567	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3568	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3569	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3570	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3571	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3572	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3573	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3574	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3575	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3576	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3577	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3578	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3579	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3580	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3581	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3582	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3583	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3584	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3585	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3586	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3587	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3588	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3589	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3590	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3591	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3592	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3593	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3594	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3595	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3596	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3597	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3598	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3599	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3600	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3601	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3602	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3603	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3604	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3605	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3606	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3607	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3608	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3609	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3610	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3611	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3612	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3613	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3614	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3615	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3616	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3617	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3618	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3619	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3620	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3621	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3622	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3623	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3624	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3625	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3626	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3627	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3628	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3629	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3630	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3631	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3632	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3633	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3634	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3635	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3636	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3637	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3638	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3639	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3640	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3641	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3642	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3643	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3644	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3645	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3646	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3647	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3648	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3649	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3650	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3651	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3652	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3653	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3654	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3655	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3656	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3657	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3658	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3659	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3660	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3661	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3662	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3663	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3664	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3665	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3666	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3667	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3668	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3669	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3670	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3671	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3672	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3673	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3674	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3675	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3676	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3677	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3678	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3679	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3680	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3681	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3682	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3683	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3684	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3685	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3686	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3687	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3688	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3689	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3690	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3691	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3692	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3693	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3694	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3695	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3696	84	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3697	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3698	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3699	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3700	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3701	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3702	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3703	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3704	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3705	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3706	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3707	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3708	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3709	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3710	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3711	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3712	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3713	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3714	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3715	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3716	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3717	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3718	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3719	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3720	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3721	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3722	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3723	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3724	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3725	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3726	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3727	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3728	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3729	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3730	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3731	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3732	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3733	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3734	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3735	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3736	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3737	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3738	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3739	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3740	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3741	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3742	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3743	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3744	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AR	3745	-	0,6,6	0.00	-	0,15,15	0.00	-
87	GOL	AR	4261	1	5,5,5	0.16	0	5,5,5	0.31	0
87	GOL	AR	4262	84	5,5,5	0.28	0	5,5,5	0.54	0
86	HN8	AR	4263	-	26,26,26	0.28	0	36,41,41	1.69	4 (11%)
84	OHX	AS	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AS	202	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AS	203	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AS	204	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AS	205	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AS	206	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AS	207	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AS	208	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AS	209	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AS	210	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AS	211	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	202	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	203	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	204	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	205	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	206	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	207	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	208	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	209	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	210	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	211	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	212	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	213	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	214	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	215	-	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AT	216	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	AT	217	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CE	401	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CE	402	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CF	401	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CF	402	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CG	301	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CG	302	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CK	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CL	301	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CM	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CP	501	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CV	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CX	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	CX	202	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	DD	101	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	DH	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	DQ	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	J	301	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	K	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	M	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	O	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	Q	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	T	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	c1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	c4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	c8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	d9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	e	101	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	h	401	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	k	401	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	l	401	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	r	301	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	s8	301	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	sR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	v	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	GOL	v	305	-	5,5,5	0.14	0	5,5,5	0.55	0
84	OHX	x	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	x	202	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	y	201	-	0,6,6	0.00	-	0,15,15	0.00	-
84	OHX	z	201	-	0,6,6	0.00	-	0,15,15	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
84	OHX	1	3401	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3402	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3403	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3404	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3405	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3406	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3407	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3408	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3409	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3410	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3411	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3412	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3413	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3414	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3415	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3416	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3417	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3418	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3419	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3420	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3421	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3422	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3423	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3424	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3425	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3426	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3427	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3428	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3429	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3430	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3431	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3432	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3433	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3434	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3435	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3436	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3437	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3438	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3439	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	1	3440	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3441	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3442	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3443	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3444	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3445	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3446	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3447	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3448	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3449	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3450	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3451	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3452	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3453	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3454	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3455	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3456	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3457	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3458	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3459	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3460	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3461	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3462	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3463	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3464	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3465	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3466	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3467	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3468	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3469	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3470	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3471	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3472	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3473	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3474	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3475	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3476	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3477	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3478	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3479	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3480	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3481	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	1	3482	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3483	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3484	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3485	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3486	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3487	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3488	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3489	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3490	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3491	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3492	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3493	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3494	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3495	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3496	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3497	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3498	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3499	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3500	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3501	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3502	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3503	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3504	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3505	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3506	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3507	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3508	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3509	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3510	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3511	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3512	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3513	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3514	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3515	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3516	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3517	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3518	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3519	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3520	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3521	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3522	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3523	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	1	3524	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3525	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3526	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3527	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3528	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3529	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3530	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3531	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3532	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3533	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3534	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3535	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3536	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3537	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3538	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3539	84	-	0/0/0/0	0/0/0/0
84	OHX	1	3540	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3541	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3542	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3543	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3544	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3545	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3546	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3547	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3548	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3549	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3550	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3551	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3552	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3553	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3554	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3555	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3556	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3557	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3558	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3559	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3560	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3561	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3562	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3563	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3564	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3565	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	1	3566	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3567	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3568	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3569	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3570	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3571	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3572	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3573	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3574	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3575	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3576	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3577	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3578	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3579	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3580	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3581	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3582	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3583	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3584	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3585	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3586	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3587	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3588	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3589	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3590	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3591	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3592	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3593	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3594	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3595	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3596	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3597	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3598	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3599	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3600	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3601	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3602	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3603	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3604	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3605	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3606	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3607	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	1	3608	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3609	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3610	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3611	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3612	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3613	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3614	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3615	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3616	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3617	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3618	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3619	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3620	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3621	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3622	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3623	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3624	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3625	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3626	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3627	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3628	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3629	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3630	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3631	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3632	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3633	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3634	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3635	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3636	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3637	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3638	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3639	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3640	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3641	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3642	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3643	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3644	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3645	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3646	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3647	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3648	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3649	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	1	3650	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3651	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3652	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3653	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3654	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3655	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3656	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3657	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3658	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3659	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3660	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3661	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3662	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3663	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3664	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3665	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3666	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3667	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3668	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3669	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3670	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3671	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3672	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3673	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3674	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3675	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3676	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3677	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3678	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3679	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3680	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3681	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3682	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3683	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3684	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3685	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3686	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3687	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3688	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3689	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3690	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3691	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	1	3692	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3693	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3694	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3695	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3696	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3697	84	-	0/0/0/0	0/0/0/0
84	OHX	1	3698	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3699	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3700	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3701	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3702	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3703	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3704	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3705	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3706	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3707	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3708	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3709	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3710	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3711	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3712	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3713	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3714	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3715	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3716	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3717	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3718	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3719	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3720	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3721	-	-	0/0/0/0	0/0/0/0
84	OHX	1	3723	1	-	0/0/0/0	0/0/0/0
84	OHX	1	3724	-	-	0/0/0/0	0/0/0/0
86	HN8	1	4223	-	-	0/2/48/48	0/3/5/5
84	OHX	2	201	-	-	0/0/0/0	0/0/0/0
84	OHX	3	201	-	-	0/0/0/0	0/0/0/0
84	OHX	3	202	-	-	0/0/0/0	0/0/0/0
84	OHX	3	203	-	-	0/0/0/0	0/0/0/0
84	OHX	3	204	-	-	0/0/0/0	0/0/0/0
84	OHX	3	205	-	-	0/0/0/0	0/0/0/0
84	OHX	3	206	-	-	0/0/0/0	0/0/0/0
84	OHX	3	207	-	-	0/0/0/0	0/0/0/0
84	OHX	3	208	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	3	209	-	-	0/0/0/0	0/0/0/0
84	OHX	4	201	-	-	0/0/0/0	0/0/0/0
84	OHX	4	202	-	-	0/0/0/0	0/0/0/0
84	OHX	4	203	-	-	0/0/0/0	0/0/0/0
84	OHX	4	204	-	-	0/0/0/0	0/0/0/0
84	OHX	4	205	-	-	0/0/0/0	0/0/0/0
84	OHX	4	206	-	-	0/0/0/0	0/0/0/0
84	OHX	4	207	-	-	0/0/0/0	0/0/0/0
84	OHX	4	208	-	-	0/0/0/0	0/0/0/0
84	OHX	4	209	-	-	0/0/0/0	0/0/0/0
84	OHX	4	210	-	-	0/0/0/0	0/0/0/0
84	OHX	4	211	-	-	0/0/0/0	0/0/0/0
84	OHX	4	212	-	-	0/0/0/0	0/0/0/0
84	OHX	4	213	-	-	0/0/0/0	0/0/0/0
84	OHX	4	214	-	-	0/0/0/0	0/0/0/0
84	OHX	4	215	-	-	0/0/0/0	0/0/0/0
84	OHX	4	216	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1901	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1902	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1903	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1904	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1905	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1906	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1907	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1908	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1909	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1910	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1911	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1912	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1913	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1914	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1915	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1916	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1917	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1918	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1919	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1920	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1921	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1922	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1923	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1924	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1925	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	6	1926	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1927	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1928	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1929	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1930	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1931	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1932	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1933	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1934	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1935	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1936	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1937	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1938	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1939	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1940	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1941	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1942	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1943	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1944	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1945	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1946	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1947	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1948	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1949	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1950	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1951	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1952	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1953	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1954	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1955	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1956	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1957	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1958	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1959	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1960	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1961	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1962	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1963	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1964	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1965	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1966	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1967	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	6	1968	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1969	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1970	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1971	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1972	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1973	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1974	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1975	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1976	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1977	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1978	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1979	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1980	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1981	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1982	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1983	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1984	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1985	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1986	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1987	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1988	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1989	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1990	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1991	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1992	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1993	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1994	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1995	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1996	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1997	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1998	-	-	0/0/0/0	0/0/0/0
84	OHX	6	1999	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2000	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2001	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2002	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2003	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2004	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2005	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2006	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2007	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2008	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2009	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	6	2010	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2011	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2012	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2013	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2014	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2015	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2016	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2017	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2018	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2019	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2020	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2021	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2022	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2023	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2024	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2025	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2026	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2027	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2028	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2029	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2030	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2031	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2032	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2033	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2034	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2035	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2036	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2037	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2038	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2039	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2040	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2041	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2042	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2043	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2044	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2045	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2046	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
84	OHX	6	2051	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
87	GOL	6	2199	-	-	0/4/4/4	0/0/0/0
84	OHX	A	1901	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1902	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1903	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1904	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1905	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1906	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1907	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1908	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1909	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1910	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1911	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1912	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1913	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1914	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1915	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1916	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1917	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1918	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1919	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1920	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1921	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1922	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1923	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1924	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1925	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1926	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1927	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1928	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1929	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1930	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1931	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1932	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1933	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1934	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1935	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1936	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1937	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1938	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1939	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1940	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	A	1941	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1942	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1943	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1944	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1945	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1946	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1947	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1948	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1949	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1950	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1951	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1952	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1953	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1954	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1955	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1956	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1957	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1958	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1959	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1960	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1961	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1962	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1963	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1964	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1965	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1966	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1967	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1968	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1969	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1970	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1971	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1972	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1973	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1974	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1975	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1976	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1977	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1978	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1979	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1980	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1981	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1982	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	A	1983	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1984	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1985	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1986	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1987	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1988	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1989	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1990	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1991	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1992	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1993	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1994	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1995	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1996	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1997	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1998	-	-	0/0/0/0	0/0/0/0
84	OHX	A	1999	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2000	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2001	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2002	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2003	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2004	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2005	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2006	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2007	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2008	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2009	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2010	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2011	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2012	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2013	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2014	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2015	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2016	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2017	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2018	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2019	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2020	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2021	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2022	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2023	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2024	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	A	2025	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2026	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2027	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2028	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2029	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2030	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2031	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2032	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2033	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2034	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2035	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2036	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2037	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2038	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2039	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2040	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2041	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2042	-	-	0/0/0/0	0/0/0/0
84	OHX	A	2043	-	-	0/0/0/0	0/0/0/0
87	GOL	A	2160	-	-	0/4/4/4	0/0/0/0
84	OHX	AC	101	-	-	0/0/0/0	0/0/0/0
84	OHX	AG	201	-	-	0/0/0/0	0/0/0/0
84	OHX	AH	201	-	-	0/0/0/0	0/0/0/0
84	OHX	AK	102	-	-	0/0/0/0	0/0/0/0
84	OHX	AM	101	-	-	0/0/0/0	0/0/0/0
84	OHX	AP	502	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3401	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3402	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3403	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3404	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3405	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3406	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3407	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3408	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3409	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3410	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3411	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3412	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3413	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3414	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3415	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3416	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	AR	3417	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3418	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3419	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3420	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3421	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3422	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3423	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3424	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3425	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3426	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3427	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3428	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3429	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3430	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3431	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3432	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3433	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3434	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3435	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3436	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3437	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3438	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3439	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3440	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3441	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3442	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3443	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3444	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3445	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3446	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3447	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3448	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3449	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3450	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3451	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3452	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3453	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3454	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3455	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3456	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3457	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3458	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	AR	3459	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3460	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3461	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3462	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3463	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3464	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3465	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3466	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3467	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3468	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3469	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3470	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3471	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3472	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3473	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3474	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3475	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3476	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3477	84	-	0/0/0/0	0/0/0/0
84	OHX	AR	3478	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3479	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3480	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3481	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3482	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3483	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3484	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3485	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3486	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3487	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3488	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3489	87	-	0/0/0/0	0/0/0/0
84	OHX	AR	3490	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3491	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3492	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3493	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3494	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3495	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3496	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3497	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3498	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3499	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3500	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	AR	3501	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3502	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3503	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3504	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3505	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3506	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3507	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3508	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3509	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3510	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3511	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3512	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3513	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3514	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3515	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3516	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3517	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3518	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3519	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3520	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3521	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3522	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3523	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3524	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3525	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3526	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3527	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3528	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3529	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3530	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3531	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3532	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3533	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3534	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3535	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3536	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3537	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3538	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3539	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3540	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3541	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3542	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	AR	3543	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3544	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3545	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3546	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3547	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3548	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3549	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3550	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3551	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3552	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3553	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3554	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3555	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3556	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3557	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3558	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3559	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3560	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3561	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3562	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3563	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3564	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3565	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3566	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3567	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3568	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3569	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3570	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3571	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3572	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3573	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3574	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3575	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3576	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3577	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3578	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3579	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3580	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3581	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3582	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3583	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3584	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	AR	3585	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3586	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3587	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3588	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3589	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3590	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3591	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3592	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3593	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3594	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3595	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3596	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3597	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3598	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3599	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3600	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3601	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3602	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3603	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3604	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3605	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3606	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3607	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3608	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3609	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3610	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3611	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3612	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3613	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3614	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3615	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3616	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3617	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3618	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3619	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3620	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3621	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3622	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3623	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3624	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3625	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3626	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	AR	3627	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3628	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3629	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3630	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3631	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3632	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3633	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3634	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3635	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3636	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3637	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3638	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3639	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3640	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3641	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3642	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3643	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3644	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3645	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3646	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3647	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3648	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3649	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3650	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3651	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3652	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3653	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3654	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3655	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3656	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3657	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3658	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3659	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3660	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3661	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3662	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3663	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3664	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3665	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3666	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3667	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3668	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	AR	3669	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3670	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3671	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3672	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3673	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3674	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3675	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3676	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3677	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3678	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3679	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3680	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3681	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3682	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3683	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3684	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3685	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3686	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3687	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3688	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3689	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3690	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3691	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3692	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3693	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3694	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3695	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3696	84	-	0/0/0/0	0/0/0/0
84	OHX	AR	3697	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3698	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3699	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3700	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3701	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3702	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3703	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3704	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3705	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3706	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3707	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3708	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3709	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3710	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	AR	3711	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3712	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3713	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3714	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3715	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3716	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3717	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3718	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3719	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3720	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3721	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3722	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3723	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3724	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3725	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3726	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3727	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3728	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3729	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3730	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3731	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3732	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3733	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3734	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3735	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3736	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3737	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3738	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3739	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3740	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3741	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3742	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3743	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3744	-	-	0/0/0/0	0/0/0/0
84	OHX	AR	3745	-	-	0/0/0/0	0/0/0/0
87	GOL	AR	4261	1	-	0/4/4/4	0/0/0/0
87	GOL	AR	4262	84	-	0/4/4/4	0/0/0/0
86	HN8	AR	4263	-	-	0/2/48/48	0/3/5/5
84	OHX	AS	201	-	-	0/0/0/0	0/0/0/0
84	OHX	AS	202	-	-	0/0/0/0	0/0/0/0
84	OHX	AS	203	-	-	0/0/0/0	0/0/0/0
84	OHX	AS	204	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	AS	205	-	-	0/0/0/0	0/0/0/0
84	OHX	AS	206	-	-	0/0/0/0	0/0/0/0
84	OHX	AS	207	-	-	0/0/0/0	0/0/0/0
84	OHX	AS	208	-	-	0/0/0/0	0/0/0/0
84	OHX	AS	209	-	-	0/0/0/0	0/0/0/0
84	OHX	AS	210	-	-	0/0/0/0	0/0/0/0
84	OHX	AS	211	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	201	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	202	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	203	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	204	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	205	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	206	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	207	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	208	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	209	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	210	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	211	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	212	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	213	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	214	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	215	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	216	-	-	0/0/0/0	0/0/0/0
84	OHX	AT	217	-	-	0/0/0/0	0/0/0/0
84	OHX	CE	401	-	-	0/0/0/0	0/0/0/0
84	OHX	CE	402	-	-	0/0/0/0	0/0/0/0
84	OHX	CF	401	-	-	0/0/0/0	0/0/0/0
84	OHX	CF	402	-	-	0/0/0/0	0/0/0/0
84	OHX	CG	301	-	-	0/0/0/0	0/0/0/0
84	OHX	CG	302	-	-	0/0/0/0	0/0/0/0
84	OHX	CK	201	-	-	0/0/0/0	0/0/0/0
84	OHX	CL	301	-	-	0/0/0/0	0/0/0/0
84	OHX	CM	201	-	-	0/0/0/0	0/0/0/0
84	OHX	CP	501	-	-	0/0/0/0	0/0/0/0
84	OHX	CV	201	-	-	0/0/0/0	0/0/0/0
84	OHX	CX	201	-	-	0/0/0/0	0/0/0/0
84	OHX	CX	202	-	-	0/0/0/0	0/0/0/0
84	OHX	DD	101	-	-	0/0/0/0	0/0/0/0
84	OHX	DH	201	-	-	0/0/0/0	0/0/0/0
84	OHX	DQ	201	-	-	0/0/0/0	0/0/0/0
84	OHX	J	301	-	-	0/0/0/0	0/0/0/0
84	OHX	K	201	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OHX	M	201	-	-	0/0/0/0	0/0/0/0
84	OHX	O	201	-	-	0/0/0/0	0/0/0/0
84	OHX	Q	201	-	-	0/0/0/0	0/0/0/0
84	OHX	T	201	-	-	0/0/0/0	0/0/0/0
84	OHX	c1	201	-	-	0/0/0/0	0/0/0/0
84	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
84	OHX	c4	201	-	-	0/0/0/0	0/0/0/0
84	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
84	OHX	c8	201	-	-	0/0/0/0	0/0/0/0
84	OHX	d9	101	-	-	0/0/0/0	0/0/0/0
84	OHX	e	101	-	-	0/0/0/0	0/0/0/0
84	OHX	h	401	-	-	0/0/0/0	0/0/0/0
84	OHX	k	401	-	-	0/0/0/0	0/0/0/0
84	OHX	l	401	-	-	0/0/0/0	0/0/0/0
84	OHX	r	301	-	-	0/0/0/0	0/0/0/0
84	OHX	s8	301	-	-	0/0/0/0	0/0/0/0
84	OHX	sR	401	-	-	0/0/0/0	0/0/0/0
84	OHX	v	301	-	-	0/0/0/0	0/0/0/0
87	GOL	v	305	-	-	0/4/4/4	0/0/0/0
84	OHX	x	201	-	-	0/0/0/0	0/0/0/0
84	OHX	x	202	-	-	0/0/0/0	0/0/0/0
84	OHX	y	201	-	-	0/0/0/0	0/0/0/0
84	OHX	z	201	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	AR	4263	HN8	C5-C1-C2	-5.98	102.67	106.80
86	AR	4263	HN8	C5-C1-C3	-5.14	100.15	105.94
86	1	4223	HN8	O1-C9-C17	-2.42	102.25	109.31
86	AR	4263	HN8	C3-C1-C2	2.84	107.05	102.25
86	1	4223	HN8	C5-C1-C7	3.85	116.17	114.47
86	AR	4263	HN8	C5-C1-C7	4.14	116.29	114.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

57 monomers are involved in 85 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	1	3473	OHX	6	0
84	1	3493	OHX	2	0
84	1	3506	OHX	1	0
84	1	3510	OHX	1	0
84	1	3539	OHX	2	0
84	1	3559	OHX	1	0
84	1	3575	OHX	1	0
84	1	3604	OHX	1	0
84	1	3661	OHX	1	0
84	1	3666	OHX	1	0
84	1	3682	OHX	1	0
84	1	3683	OHX	1	0
84	1	3697	OHX	2	0
84	1	3704	OHX	1	0
84	1	3720	OHX	6	0
84	6	1915	OHX	3	0
84	6	1975	OHX	4	0
84	6	2001	OHX	4	0
84	6	2013	OHX	1	0
84	6	2025	OHX	4	0
84	A	1909	OHX	6	0
84	A	1914	OHX	1	0
84	A	1968	OHX	3	0
84	A	2009	OHX	3	0
84	A	2024	OHX	6	0
84	AR	3413	OHX	1	0
84	AR	3443	OHX	6	0
84	AR	3477	OHX	2	0
84	AR	3501	OHX	2	0
84	AR	3502	OHX	2	0
84	AR	3511	OHX	4	0
84	AR	3521	OHX	4	0
84	AR	3534	OHX	2	0
84	AR	3554	OHX	1	0
84	AR	3566	OHX	2	0
84	AR	3590	OHX	2	0
84	AR	3591	OHX	1	0
84	AR	3627	OHX	1	0
84	AR	3642	OHX	2	0
84	AR	3645	OHX	1	0
84	AR	3671	OHX	1	0
84	AR	3687	OHX	2	0
84	AR	3689	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AR	3693	OHX	1	0
84	AR	3696	OHX	4	0
84	AR	3698	OHX	4	0
84	AR	3715	OHX	4	0
84	AR	3731	OHX	6	0
84	AR	3743	OHX	2	0
87	AR	4261	GOL	1	0
87	AR	4262	GOL	2	0
84	AS	203	OHX	5	0
84	AS	210	OHX	5	0
84	AT	203	OHX	2	0
84	AT	212	OHX	2	0
84	CG	302	OHX	1	0
84	CX	202	OHX	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	sM	2
50	s0	1
47	m2	1
25	A	1
54	s4	1
5	CE	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	44.14
1	sM	139:UNK	C	155:UNK	N	37.59
1	A	1716:C	O3'	1717:G	P	4.52
1	m2	23:UNK	C	28:UNK	N	3.62
1	CE	168:LYS	C	169:THR	N	1.19
1	s0	160:ILE	C	161:PRO	N	1.19
1	s4	82:TYR	C	83:PRO	N	1.18

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1	3149/3396 (92%)	0.21	98 (3%)	49	26	26, 47, 129, 223	0
1	AR	3149/3396 (92%)	0.30	103 (3%)	47	24	27, 49, 123, 225	0
2	3	121/121 (100%)	-0.11	0	100	100	35, 63, 75, 82	0
2	AS	121/121 (100%)	-0.04	1 (0%)	86	71	34, 52, 66, 73	0
3	4	158/158 (100%)	0.21	5 (3%)	48	25	34, 51, 91, 138	0
3	AT	158/158 (100%)	0.24	6 (3%)	41	20	34, 60, 99, 128	0
4	CD	252/252 (100%)	0.04	3 (1%)	79	61	33, 52, 74, 82	0
4	j	252/252 (100%)	0.04	1 (0%)	92	84	31, 46, 64, 77	0
5	CE	386/386 (100%)	-0.18	1 (0%)	93	86	25, 41, 55, 95	0
5	k	386/386 (100%)	-0.02	3 (0%)	86	71	25, 48, 62, 80	0
6	CF	361/361 (100%)	-0.11	1 (0%)	93	86	31, 47, 65, 88	0
6	l	361/361 (100%)	-0.12	1 (0%)	93	86	27, 44, 62, 71	0
7	CG	296/296 (100%)	0.15	13 (4%)	35	17	39, 57, 83, 104	0
7	m	296/296 (100%)	0.48	17 (5%)	24	11	46, 69, 89, 115	0
8	CH	156/175 (89%)	0.07	3 (1%)	67	46	37, 46, 68, 84	0
8	n	156/175 (89%)	0.04	1 (0%)	89	77	36, 43, 66, 86	0
9	CI	222/222 (100%)	-0.13	3 (1%)	75	57	27, 35, 78, 133	0
9	o	222/222 (100%)	-0.16	4 (1%)	69	47	29, 38, 73, 123	0
10	CJ	233/233 (100%)	0.79	32 (13%)	3	1	70, 82, 123, 144	0
10	p	233/233 (100%)	0.49	13 (5%)	25	11	56, 70, 105, 116	0
11	CK	191/191 (100%)	-0.16	3 (1%)	72	51	35, 45, 66, 82	0
11	q	191/191 (100%)	-0.24	0	100	100	42, 53, 66, 86	0
12	CL	211/220 (95%)	0.45	12 (5%)	24	11	39, 59, 80, 93	0
12	r	211/220 (95%)	-0.04	2 (0%)	84	69	33, 46, 81, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	CM	169/169 (100%)	-0.18	1 (0%) 89 77	40, 61, 75, 83	0
13	s	169/169 (100%)	0.09	4 (2%) 59 37	55, 77, 90, 96	0
14	CN	193/193 (100%)	0.54	15 (7%) 14 5	41, 62, 101, 119	0
14	t	193/193 (100%)	-0.05	0 100 100	33, 53, 95, 125	0
15	CO	136/136 (100%)	-0.35	1 (0%) 87 75	34, 40, 63, 71	0
15	u	136/136 (100%)	-0.29	3 (2%) 62 41	37, 43, 60, 68	0
16	CP	203/203 (100%)	-0.12	0 100 100	38, 55, 67, 71	0
16	v	203/203 (100%)	-0.17	0 100 100	33, 44, 57, 64	0
17	CQ	197/197 (100%)	-0.20	3 (1%) 74 54	25, 30, 60, 66	0
17	w	197/197 (100%)	-0.27	0 100 100	28, 34, 55, 60	0
18	CR	183/183 (100%)	1.33	29 (15%) 2 1	31, 39, 137, 167	0
18	x	183/183 (100%)	0.53	21 (11%) 5 2	32, 40, 105, 140	0
19	CS	185/185 (100%)	-0.16	0 100 100	32, 45, 56, 60	0
19	y	185/185 (100%)	-0.14	0 100 100	33, 43, 63, 87	0
20	CT	188/188 (100%)	0.12	9 (4%) 31 14	48, 63, 158, 169	0
20	z	188/188 (100%)	0.16	7 (3%) 42 21	48, 64, 150, 167	0
21	0	172/172 (100%)	-0.19	1 (0%) 89 77	35, 41, 55, 65	0
21	CU	172/172 (100%)	-0.35	0 100 100	30, 37, 50, 57	0
22	2	159/159 (100%)	-0.07	2 (1%) 77 59	34, 45, 87, 97	0
22	CV	159/159 (100%)	-0.21	0 100 100	31, 41, 74, 84	0
23	5	100/100 (100%)	0.81	13 (13%) 4 2	79, 93, 105, 123	0
23	CW	100/100 (100%)	1.12	20 (20%) 1 0	77, 87, 98, 119	0
24	CX	136/136 (100%)	0.14	1 (0%) 87 75	29, 38, 57, 59	0
24	IR	136/136 (100%)	0.04	4 (2%) 52 28	31, 43, 56, 62	0
25	6	1783/1800 (99%)	0.43	114 (6%) 20 7	41, 78, 169, 233	0
25	A	1781/1800 (98%)	0.51	125 (7%) 17 7	49, 87, 186, 250	0
26	7	98/98 (100%)	1.75	29 (29%) 1 0	43, 59, 150, 157	0
26	CY	98/98 (100%)	0.41	11 (11%) 6 2	38, 53, 145, 177	0
27	8	121/121 (100%)	-0.03	1 (0%) 86 71	44, 57, 77, 117	0
27	CZ	121/121 (100%)	0.05	4 (3%) 47 24	48, 64, 85, 100	0
28	9	126/126 (100%)	0.67	6 (4%) 31 14	40, 55, 64, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DA	126/126 (100%)	0.69	7 (5%) 25 11	40, 57, 73, 82	0
29	AA	135/135 (100%)	1.73	47 (34%) 0 0	69, 83, 94, 104	0
29	DB	135/135 (100%)	0.89	17 (12%) 4 2	81, 95, 110, 120	0
30	AB	148/148 (100%)	-0.08	0 100 100	27, 46, 73, 86	0
30	DC	148/148 (100%)	0.02	1 (0%) 87 75	30, 51, 71, 77	0
31	AC	58/58 (100%)	-0.07	0 100 100	32, 52, 102, 122	0
31	DD	58/58 (100%)	-0.06	0 100 100	38, 51, 80, 89	0
32	AD	97/97 (100%)	0.38	6 (6%) 21 8	67, 77, 99, 110	0
32	DE	97/97 (100%)	-0.29	0 100 100	71, 83, 105, 109	0
33	AE	109/109 (100%)	0.20	2 (1%) 69 47	42, 56, 95, 106	0
33	DF	109/109 (100%)	0.19	3 (2%) 53 29	41, 52, 92, 111	0
34	AF	127/127 (100%)	0.01	3 (2%) 59 37	25, 40, 52, 69	0
34	DG	127/127 (100%)	0.06	2 (1%) 72 51	24, 43, 55, 77	0
35	AG	106/106 (100%)	-0.15	1 (0%) 84 69	31, 36, 61, 72	0
35	DH	106/106 (100%)	-0.13	1 (0%) 84 69	28, 35, 64, 87	0
36	AH	112/112 (100%)	0.26	6 (5%) 26 12	43, 63, 104, 114	0
36	DI	112/112 (100%)	0.29	1 (0%) 84 69	46, 68, 113, 125	0
37	AI	119/119 (100%)	0.28	6 (5%) 30 13	46, 61, 70, 77	0
37	DJ	119/119 (100%)	0.27	6 (5%) 30 13	51, 67, 81, 88	0
38	AJ	99/99 (100%)	0.24	3 (3%) 51 27	52, 61, 93, 113	0
38	DK	99/99 (100%)	0.26	4 (4%) 39 19	59, 70, 92, 110	0
39	AK	87/87 (100%)	0.10	3 (3%) 46 23	32, 36, 63, 86	0
39	DL	87/87 (100%)	0.24	3 (3%) 46 23	36, 42, 77, 113	0
40	AL	77/77 (100%)	0.19	2 (2%) 56 33	67, 79, 101, 108	0
40	DM	77/77 (100%)	1.93	30 (38%) 0 0	76, 88, 107, 115	0
41	AM	50/50 (100%)	-0.07	0 100 100	42, 45, 52, 62	0
41	DN	50/50 (100%)	-0.04	0 100 100	45, 49, 59, 70	0
42	AN	52/52 (100%)	0.61	4 (7%) 14 5	37, 43, 61, 69	0
42	DO	52/52 (100%)	0.02	1 (1%) 67 46	32, 35, 48, 62	0
43	AO	25/25 (100%)	-0.14	0 100 100	52, 54, 59, 59	0
43	DP	25/25 (100%)	-0.20	0 100 100	43, 46, 59, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	AP	105/105 (100%)	0.66	9 (8%) 11 4	34, 50, 74, 103	0
44	DQ	105/105 (100%)	0.25	0 100 100	37, 50, 65, 97	0
45	AQ	91/91 (100%)	-0.22	0 100 100	40, 50, 67, 80	0
45	DR	91/91 (100%)	-0.24	0 100 100	39, 53, 69, 79	0
46	i	159/272 (58%)	0.57	19 (11%) 5 2	70, 90, 143, 148	0
47	m2	0/150	-	-	-	-
48	sM	63/104 (60%)	0.77	6 (9%) 9 3	62, 91, 108, 114	0
49	p0	143/311 (45%)	1.60	53 (37%) 0 0	89, 108, 172, 179	0
50	B	206/206 (100%)	0.86	28 (13%) 3 1	93, 110, 125, 146	0
50	s0	206/206 (100%)	0.32	8 (3%) 40 19	77, 97, 115, 120	0
51	C	214/216 (99%)	1.63	77 (35%) 0 0	93, 121, 142, 150	0
51	s1	216/216 (100%)	0.53	13 (6%) 23 9	68, 83, 110, 129	0
52	D	217/217 (100%)	0.03	2 (0%) 84 69	68, 87, 108, 125	0
52	s2	217/217 (100%)	0.07	2 (0%) 84 69	57, 76, 92, 106	0
53	E	223/223 (100%)	0.64	19 (8%) 11 4	74, 91, 118, 137	0
53	s3	223/223 (100%)	0.70	27 (12%) 5 2	75, 103, 134, 148	0
54	F	260/260 (100%)	0.62	22 (8%) 11 4	63, 87, 97, 121	0
54	s4	260/260 (100%)	0.16	7 (2%) 55 30	53, 84, 98, 128	0
55	G	206/206 (100%)	0.77	22 (10%) 7 2	92, 112, 131, 141	0
55	s5	206/206 (100%)	0.95	34 (16%) 2 1	74, 95, 114, 122	0
56	H	226/226 (100%)	0.87	40 (17%) 2 1	61, 94, 116, 143	0
56	s6	218/226 (96%)	0.63	26 (11%) 5 2	52, 83, 111, 124	0
57	I	184/186 (98%)	1.03	30 (16%) 2 1	87, 119, 148, 156	0
57	s7	186/186 (100%)	0.99	31 (16%) 2 1	77, 112, 147, 152	0
58	J	188/199 (94%)	0.29	9 (4%) 31 14	53, 70, 111, 126	0
58	s8	188/199 (94%)	0.57	14 (7%) 15 5	49, 73, 124, 140	0
59	K	185/185 (100%)	1.07	34 (18%) 1 1	77, 95, 129, 158	0
59	s9	185/185 (100%)	0.68	14 (7%) 15 5	67, 85, 116, 151	0
60	L	96/105 (91%)	1.12	16 (16%) 2 1	81, 102, 129, 139	0
60	c0	96/105 (91%)	2.34	56 (58%) 0 0	96, 126, 139, 147	0
61	M	155/155 (100%)	0.83	16 (10%) 7 2	56, 70, 126, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
61	c1	146/155 (94%)	0.46	8 (5%) 26 11	55, 70, 104, 131	0
62	N	124/124 (100%)	1.99	63 (50%) 0 0	133, 140, 152, 160	0
62	c2	124/124 (100%)	3.01	87 (70%) 0 0	161, 169, 184, 190	0
63	O	150/150 (100%)	0.41	9 (6%) 23 9	64, 85, 100, 104	0
63	c3	150/150 (100%)	0.16	4 (2%) 55 30	59, 78, 96, 111	0
64	P	127/128 (99%)	1.41	36 (28%) 1 0	66, 119, 135, 138	0
64	c4	128/128 (100%)	0.64	11 (8%) 11 4	57, 81, 91, 94	0
65	Q	124/141 (87%)	0.49	7 (5%) 25 11	75, 89, 126, 146	0
65	c5	135/141 (95%)	0.80	16 (11%) 5 2	82, 97, 119, 131	0
66	R	141/142 (99%)	1.05	26 (18%) 1 1	81, 107, 115, 120	0
66	c6	142/142 (100%)	0.70	15 (10%) 7 2	67, 91, 106, 127	0
67	S	120/125 (96%)	0.56	13 (10%) 6 2	90, 109, 134, 138	0
67	c7	117/125 (93%)	0.13	6 (5%) 29 13	78, 97, 122, 130	0
68	T	145/145 (100%)	0.79	17 (11%) 5 2	71, 99, 129, 140	0
68	c8	145/145 (100%)	0.70	16 (11%) 6 2	79, 91, 116, 127	0
69	U	143/143 (100%)	0.99	22 (15%) 2 1	84, 102, 119, 133	0
69	c9	143/143 (100%)	1.11	30 (20%) 1 0	71, 86, 106, 119	0
70	V	107/110 (97%)	0.14	2 (1%) 67 46	73, 109, 141, 145	0
70	d0	110/110 (100%)	0.46	12 (10%) 6 2	70, 111, 154, 172	0
71	W	87/87 (100%)	0.61	8 (9%) 10 3	90, 96, 115, 124	0
71	d1	87/87 (100%)	0.14	4 (4%) 33 15	75, 83, 110, 121	0
72	X	129/129 (100%)	0.15	2 (1%) 72 51	68, 81, 88, 101	0
72	d2	129/129 (100%)	0.06	1 (0%) 86 71	57, 70, 81, 97	0
73	Y	144/144 (100%)	0.22	3 (2%) 64 43	57, 62, 73, 88	0
73	d3	144/144 (100%)	-0.07	0 100 100	46, 52, 66, 78	0
74	Z	134/134 (100%)	0.47	15 (11%) 6 2	69, 97, 114, 125	0
74	d4	134/134 (100%)	0.23	11 (8%) 12 5	62, 88, 103, 122	0
75	a	70/70 (100%)	2.04	28 (40%) 0 0	111, 123, 138, 139	0
75	d5	69/70 (98%)	1.43	22 (31%) 0 0	93, 113, 124, 127	0
76	b	97/97 (100%)	0.43	5 (5%) 28 12	67, 83, 135, 138	0
76	d6	97/97 (100%)	0.13	1 (1%) 82 67	51, 63, 95, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
77	c	81/81 (100%)	1.04	15 (18%) 1 1	82, 95, 127, 134	0
77	d7	81/81 (100%)	1.14	15 (18%) 1 1	72, 87, 126, 132	0
78	d	63/63 (100%)	0.97	7 (11%) 6 2	104, 121, 132, 134	0
78	d8	63/63 (100%)	1.96	34 (53%) 0 0	91, 107, 121, 125	0
79	d9	53/53 (100%)	1.19	10 (18%) 1 1	71, 82, 120, 128	0
79	e	53/53 (100%)	0.68	4 (7%) 15 5	75, 80, 96, 104	0
80	e0	62/62 (100%)	0.97	9 (14%) 3 1	59, 83, 113, 125	0
80	f	60/62 (96%)	1.14	11 (18%) 1 1	63, 92, 131, 134	0
81	g	71/71 (100%)	1.74	29 (40%) 0 0	105, 124, 144, 150	0
82	h	318/318 (100%)	1.11	70 (22%) 1 0	97, 115, 135, 147	0
82	sR	318/318 (100%)	0.61	32 (10%) 8 2	99, 121, 140, 157	0
83	e1	51/51 (100%)	2.31	23 (45%) 0 0	145, 157, 165, 167	0
All	All	33004/34167 (96%)	0.38	2302 (6%) 17 7	24, 66, 132, 250	0

All (2302) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	CR	161	ALA	24.0
18	CR	162	GLU	20.3
26	7	76	VAL	17.9
18	CR	160	ALA	16.2
26	7	75	THR	15.8
18	CR	159	LYS	15.4
18	CR	179	GLN	14.3
18	x	162	GLU	13.1
18	CR	178	ALA	12.4
18	CR	158	ALA	12.0
55	G	152	GLY	11.8
75	a	36	ALA	11.2
28	DA	127	GLU	10.9
25	A	1702	A	10.7
26	7	84	GLY	10.4
1	AR	1569	U	10.1
18	x	161	ALA	10.0
61	M	147	GLY	9.9
25	A	1709	C	9.7
61	c1	3	THR	9.6
25	A	1708	U	9.6

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Mol	Chain	Res	Type	RSRZ
62	c2	105	LYS	9.3
18	CR	165	VAL	9.3
51	C	100	PHE	8.8
26	7	88	ASP	8.7
25	A	913	G	8.7
61	M	145	ALA	8.6
61	M	146	ALA	8.6
25	A	1694	A	8.5
1	AR	2445	A	8.4
18	x	163	LYS	8.4
18	CR	168	LEU	8.3
18	x	184	ALA	8.3
26	7	81	PRO	8.2
18	CR	167	ARG	8.1
18	CR	176	ILE	8.0
80	e0	62	VAL	7.9
62	c2	63	VAL	7.7
49	p0	192	ASP	7.7
77	c	38	PRO	7.7
18	CR	174	GLY	7.7
25	A	1703	C	7.7
26	7	86	SER	7.6
55	G	151	GLY	7.6
10	CJ	254	ASP	7.5
18	CR	163	LYS	7.5
61	M	2	SER	7.5
18	CR	175	ARG	7.5
25	A	1698	G	7.5
44	AP	106	PHE	7.5
23	CW	9	GLN	7.4
25	A	1699	G	7.4
74	d4	134	ALA	7.4
1	1	1569	U	7.4
20	CT	182	ASP	7.4
25	A	1704	U	7.4
61	M	152	GLN	7.4
25	A	194	U	7.3
25	A	1711	C	7.3
59	K	181	ALA	7.3
25	A	1696	G	7.2
61	M	150	ASN	7.2
18	CR	180	LYS	7.1

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Mol	Chain	Res	Type	RSRZ
26	CY	81	PRO	7.1
60	c0	79	TYR	7.1
18	x	160	ALA	7.1
25	A	1693	A	7.0
65	c5	4	ALA	7.0
1	1	1568	U	7.0
18	CR	170	SER	7.0
74	d4	135	ASP	7.0
1	AR	2502	A	7.0
18	CR	164	LYS	6.9
1	1	1570	U	6.9
82	h	4	ASN	6.9
83	e1	102	VAL	6.8
1	AR	252	U	6.8
25	A	134	U	6.8
26	CY	95	SER	6.7
1	AR	2535	A	6.7
1	1	2539	C	6.7
61	M	153	PHE	6.7
64	P	16	VAL	6.6
66	R	92	TYR	6.6
26	7	85	ALA	6.6
25	A	1697	G	6.6
62	c2	64	SER	6.6
62	N	62	LEU	6.6
25	A	1059	U	6.6
55	G	153	GLY	6.6
18	x	159	LYS	6.5
82	h	52	GLN	6.5
46	i	85	SER	6.5
18	x	164	LYS	6.5
25	A	135	A	6.5
25	A	1700	C	6.5
46	i	16	ASP	6.4
82	h	3	SER	6.4
26	7	82	ILE	6.4
18	CR	184	ALA	6.4
64	P	15	GLY	6.4
25	A	1705	C	6.4
18	CR	157	VAL	6.4
79	d9	4	GLU	6.3
46	i	88	ARG	6.3

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Mol	Chain	Res	Type	RSRZ
77	d7	59	CYS	6.3
25	6	1694	A	6.3
25	6	718	U	6.3
62	c2	47	GLU	6.2
26	7	74	LYS	6.2
26	7	77	LYS	6.2
66	R	66	ARG	6.2
82	h	212	ALA	6.2
1	AR	1567	U	6.1
1	1	1955	U	6.1
25	A	238	U	6.1
83	e1	113	LYS	6.0
10	CJ	253	SER	6.0
1	AR	2504	U	6.0
51	C	98	THR	6.0
79	d9	5	ASN	6.0
62	c2	43	ARG	6.0
51	C	230	ALA	6.0
62	c2	121	VAL	6.0
1	AR	2539	C	5.9
60	c0	67	THR	5.9
62	c2	123	VAL	5.9
3	AT	81	U	5.9
66	R	21	HIS	5.9
1	1	1952	G	5.9
25	A	1692	G	5.9
61	M	155	LYS	5.9
18	CR	183	ALA	5.8
40	DM	34	ALA	5.8
28	9	127	GLU	5.8
26	7	87	LEU	5.8
25	6	658	C	5.8
82	h	2	ALA	5.8
26	7	90	ILE	5.8
66	R	20	ALA	5.8
61	c1	2	SER	5.8
62	c2	28	LEU	5.7
80	f	60	PRO	5.7
25	6	225	A	5.7
51	C	20	VAL	5.7
25	6	194	U	5.7
55	s5	152	GLY	5.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
39	DL	88	ALA	5.7
26	CY	96	LEU	5.6
1	AR	1570	U	5.6
25	6	1228	G	5.6
1	AR	2503	G	5.5
25	A	656	G	5.5
7	CG	295	GLY	5.5
62	c2	65	SER	5.5
83	e1	112	GLY	5.5
51	C	96	LEU	5.5
55	s5	37	GLN	5.5
61	M	3	THR	5.5
62	c2	75	VAL	5.4
25	6	239	C	5.4
80	e0	63	GLN	5.4
55	G	154	ALA	5.4
25	6	1256	A	5.4
25	A	1707	A	5.4
64	P	75	GLY	5.4
1	1	1349	G	5.4
1	AR	2506	U	5.4
60	c0	48	SER	5.3
1	AR	1571	A	5.3
1	1	2205	U	5.3
66	R	5	PRO	5.3
82	h	79	TYR	5.3
53	s3	145	ALA	5.3
25	A	719	U	5.3
62	c2	74	LEU	5.3
62	c2	92	ALA	5.3
25	6	656	G	5.3
82	h	7	LEU	5.3
25	6	1695	G	5.3
39	DL	87	SER	5.3
60	c0	64	TYR	5.2
1	AR	1581	C	5.2
1	AR	3154	C	5.2
10	CJ	121	SER	5.2
56	s6	169	TYR	5.2
1	AR	3275	U	5.2
10	CJ	118	GLU	5.2
75	a	67	ASP	5.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	AR	2537	U	5.2
26	7	69	LYS	5.2
65	c5	50	THR	5.2
61	M	149	ALA	5.1
1	AR	2505	U	5.1
1	AR	1351	U	5.1
80	f	53	LYS	5.1
44	AP	104	LEU	5.1
1	AR	1572	U	5.1
74	Z	2	SER	5.1
75	a	97	LYS	5.1
25	6	506	A	5.1
51	C	95	ASN	5.1
53	s3	176	LEU	5.0
60	c0	76	LEU	5.0
23	CW	11	ILE	5.0
50	B	28	ASN	5.0
83	e1	146	SER	5.0
1	AR	1566	A	5.0
25	A	132	U	5.0
62	c2	103	LEU	5.0
55	G	222	LYS	5.0
25	A	1695	G	5.0
25	6	229	U	5.0
57	I	74	GLN	5.0
18	CR	169	THR	5.0
25	A	261	U	5.0
18	x	158	ALA	5.0
51	C	231	LEU	5.0
25	A	914	G	4.9
81	g	146	SER	4.9
65	Q	51	SER	4.9
62	c2	30	VAL	4.9
25	A	1686	C	4.9
75	d5	37	GLN	4.9
25	6	676	G	4.9
82	sR	319	ASN	4.9
34	AF	128	LEU	4.9
26	CY	97	LYS	4.9
10	CJ	107	GLU	4.9
1	AR	1025	A	4.9
25	6	1227	A	4.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
65	c5	5	VAL	4.9
51	C	86	LEU	4.9
26	7	68	ALA	4.9
18	CR	177	ALA	4.9
1	1	1571	A	4.9
26	7	80	ARG	4.9
82	h	6	VAL	4.8
62	c2	45	LEU	4.8
62	c2	59	LEU	4.8
1	AR	1574	C	4.8
7	CG	290	ILE	4.8
7	CG	296	GLN	4.8
26	7	95	SER	4.8
55	G	155	ALA	4.8
62	c2	104	GLY	4.8
55	s5	151	GLY	4.8
40	DM	32	ASN	4.8
1	1	1243	G	4.8
1	AR	3156	U	4.8
26	CY	67	VAL	4.7
60	c0	98	THR	4.7
25	6	678	A	4.7
25	6	1707	A	4.7
75	a	69	LEU	4.7
40	DM	31	LEU	4.7
25	6	1229	G	4.7
77	c	33	LEU	4.7
1	AR	2444	C	4.7
1	AR	2507	C	4.7
82	sR	121	MET	4.7
51	C	101	HIS	4.7
62	c2	60	VAL	4.7
69	c9	4	VAL	4.7
75	a	48	ASP	4.7
46	i	89	ARG	4.6
80	e0	49	LEU	4.6
57	I	87	ASP	4.6
65	c5	10	ARG	4.6
62	c2	34	THR	4.6
61	M	4	GLU	4.6
57	I	32	PRO	4.6
69	c9	2	PRO	4.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
64	P	40	ALA	4.6
62	c2	80	ASN	4.6
1	1	1236	G	4.6
1	1	1268	G	4.6
62	c2	107	ASP	4.6
25	A	133	U	4.6
25	A	1701	A	4.6
78	d8	65	ARG	4.6
62	c2	112	ALA	4.6
18	x	174	GLY	4.6
62	N	67	THR	4.6
83	e1	115	THR	4.6
25	6	721	U	4.6
1	1	1350	A	4.6
60	c0	50	THR	4.6
65	Q	50	THR	4.6
83	e1	104	SER	4.5
59	K	138	LYS	4.5
18	x	179	GLN	4.5
25	A	718	U	4.5
39	AK	87	SER	4.5
56	s6	217	SER	4.5
1	1	1242	G	4.5
3	AT	80	A	4.5
25	A	1687	U	4.5
55	s5	156	ARG	4.5
25	A	658	C	4.5
1	1	1266	G	4.5
40	DM	11	PHE	4.5
26	7	83	THR	4.5
55	s5	155	ALA	4.5
61	M	154	ALA	4.5
62	N	49	THR	4.5
60	c0	57	THR	4.5
60	c0	65	TYR	4.5
29	AA	95	VAL	4.5
68	T	2	SER	4.5
26	7	96	LEU	4.5
64	P	29	HIS	4.5
1	1	1762	C	4.5
69	U	71	VAL	4.4
25	A	241	U	4.4

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Mol	Chain	Res	Type	RSRZ
1	1	1352	A	4.4
51	C	47	LEU	4.4
25	A	715	U	4.4
25	A	239	C	4.4
62	N	64	SER	4.4
29	AA	5	LEU	4.4
1	AR	2536	A	4.4
7	CG	297	GLN	4.4
26	7	70	LYS	4.4
37	DJ	120	ALA	4.4
75	a	65	LEU	4.4
40	DM	71	PRO	4.4
18	CR	172	GLN	4.4
62	c2	115	VAL	4.4
62	N	50	LYS	4.4
46	i	87	THR	4.4
26	CY	68	ALA	4.4
23	5	89	LEU	4.4
10	CJ	115	ALA	4.4
25	A	1710	U	4.3
57	I	38	LEU	4.3
1	AR	1579	C	4.3
29	AA	99	GLU	4.3
60	c0	69	THR	4.3
65	c5	52	LYS	4.3
18	CR	166	VAL	4.3
62	c2	71	ILE	4.3
58	s8	67	TRP	4.3
51	C	226	GLY	4.3
79	e	4	GLU	4.3
51	C	84	ILE	4.3
51	C	99	ASN	4.3
62	N	111	ASN	4.3
29	AA	72	ILE	4.3
10	CJ	106	LYS	4.3
61	M	148	LYS	4.3
62	c2	114	LYS	4.3
62	c2	116	VAL	4.3
1	AR	2501	U	4.3
25	A	1706	C	4.3
83	e1	145	HIS	4.3
33	DF	82	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
22	2	121	ALA	4.3
62	c2	56	GLU	4.3
54	F	167	GLY	4.3
62	c2	76	GLU	4.3
40	DM	30	LYS	4.3
68	T	13	HIS	4.3
1	1	1567	U	4.2
56	s6	166	GLU	4.2
61	M	151	LYS	4.2
61	M	156	PHE	4.2
59	K	186	GLU	4.2
25	6	240	U	4.2
1	1	1265	U	4.2
53	E	217	ILE	4.2
25	A	136	C	4.2
51	C	55	LYS	4.2
53	s3	174	HIS	4.2
60	c0	68	LEU	4.2
82	h	253	ALA	4.2
62	c2	91	VAL	4.2
78	d8	43	ASN	4.2
1	AR	3276	G	4.2
10	CJ	252	ASN	4.2
78	d8	13	ILE	4.2
25	6	226	A	4.2
25	A	183	U	4.2
55	G	41	LYS	4.2
70	d0	121	ASN	4.2
62	c2	113	ARG	4.2
81	g	104	SER	4.2
63	O	151	ASN	4.2
77	d7	33	LEU	4.2
82	sR	46	LYS	4.2
60	c0	70	GLU	4.2
28	9	120	GLN	4.1
62	c2	119	SER	4.2
75	a	73	GLY	4.1
33	AE	82	GLU	4.1
51	C	41	ARG	4.1
29	AA	107	ARG	4.1
62	c2	61	VAL	4.1
83	e1	114	VAL	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
62	N	41	LEU	4.1
1	1	1351	U	4.1
1	AR	1815	U	4.1
26	7	89	LEU	4.1
49	p0	197	PHE	4.1
83	e1	107	LYS	4.1
9	CI	26	VAL	4.1
77	c	41	LEU	4.1
25	A	820	U	4.1
82	sR	51	ASP	4.1
60	c0	9	ASN	4.1
25	6	679	U	4.1
49	p0	25	LEU	4.1
7	CG	287	ALA	4.1
60	c0	3	MET	4.1
10	CJ	117	ALA	4.1
60	c0	37	THR	4.0
65	c5	6	ASN	4.0
62	c2	93	ASP	4.0
26	7	72	SER	4.0
10	CJ	111	LYS	4.0
38	AJ	99	ARG	4.0
46	i	18	VAL	4.0
67	S	126	ALA	4.0
68	T	8	GLN	4.0
1	1	2207	A	4.0
75	a	71	ILE	4.0
64	P	27	PHE	4.0
48	sM	84	LYS	4.0
62	c2	46	ARG	4.0
25	A	1690	G	4.0
51	C	91	VAL	4.0
62	c2	29	LYS	4.0
82	h	115	ILE	4.0
26	7	79	GLN	4.0
1	1	1267	U	4.0
62	c2	125	ASN	4.0
77	d7	62	ILE	4.0
12	CL	112	GLN	4.0
25	6	214	G	4.0
25	A	131	C	4.0
1	1	1278	A	4.0

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Mol	Chain	Res	Type	RSRZ
60	c0	55	VAL	3.9
55	s5	153	GLY	3.9
57	s7	93	LEU	3.9
75	a	60	VAL	3.9
40	DM	33	LYS	3.9
60	c0	95	ARG	3.9
62	c2	111	ASN	3.9
23	CW	10	LYS	3.9
39	AK	84	SER	3.9
82	h	262	VAL	3.9
25	A	506	A	3.9
51	C	25	THR	3.9
62	N	110	GLY	3.9
60	c0	42	VAL	3.9
69	c9	19	ALA	3.9
51	C	38	PHE	3.9
40	DM	72	THR	3.9
55	G	150	GLY	3.9
21	0	1	MET	3.9
49	p0	292	GLU	3.9
1	AR	1580	A	3.9
1	AR	2441	A	3.9
25	6	1255	G	3.9
46	i	17	VAL	3.9
62	N	28	LEU	3.9
70	d0	18	GLN	3.9
25	6	487	G	3.9
25	6	712	G	3.9
70	d0	17	GLN	3.9
60	c0	49	LEU	3.9
25	6	1700	C	3.8
29	AA	106	GLN	3.8
54	s4	261	LEU	3.8
64	P	41	ARG	3.8
62	N	63	VAL	3.8
82	h	263	PHE	3.8
10	CJ	250	ALA	3.8
71	d1	43	GLY	3.8
18	x	181	ARG	3.8
55	G	181	GLU	3.8
1	1	1271	A	3.8
65	c5	134	THR	3.8

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Mol	Chain	Res	Type	RSRZ
82	h	315	VAL	3.8
25	A	195	G	3.8
54	F	143	ASP	3.8
67	S	86	PRO	3.8
59	K	182	GLU	3.8
20	CT	183	ALA	3.8
25	6	1710	U	3.8
10	CJ	122	LYS	3.8
62	N	78	LEU	3.8
68	c8	18	LEU	3.8
55	s5	154	ALA	3.8
62	N	20	ALA	3.8
20	CT	175	GLN	3.8
56	s6	164	LYS	3.8
1	1	3154	C	3.8
83	e1	106	TYR	3.8
66	c6	4	VAL	3.8
7	m	124	GLU	3.8
25	A	899	G	3.8
69	U	5	SER	3.8
25	6	75	U	3.7
62	N	32	LEU	3.7
62	c2	62	LEU	3.7
46	i	273	THR	3.7
23	5	108	TYR	3.7
62	c2	72	ILE	3.7
68	c8	17	LEU	3.7
60	L	12	HIS	3.7
62	c2	102	GLY	3.7
25	A	228	G	3.7
55	G	210	ALA	3.7
51	C	59	ASP	3.7
1	AR	2538	U	3.7
55	s5	61	TYR	3.7
26	7	67	VAL	3.7
48	sM	85	SER	3.7
49	p0	284	ALA	3.7
53	s3	44	THR	3.7
62	c2	23	THR	3.7
23	CW	97	SER	3.7
56	H	217	SER	3.7
51	C	29	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
60	c0	73	VAL	3.7
1	1	1576	G	3.7
7	m	131	LEU	3.7
10	CJ	249	ARG	3.7
62	N	91	VAL	3.7
1	AR	1352	A	3.7
1	AR	1568	U	3.7
25	6	1693	A	3.7
1	AR	546	C	3.7
75	a	38	HIS	3.7
25	6	1692	G	3.7
25	6	1699	G	3.7
62	c2	122	VAL	3.7
63	O	61	THR	3.7
57	s7	3	ALA	3.7
68	T	44	ASN	3.7
53	E	179	GLN	3.7
62	c2	124	LYS	3.7
10	p	121	SER	3.7
81	g	87	THR	3.7
61	c1	145	ALA	3.7
62	N	85	LYS	3.7
7	m	297	GLN	3.7
25	6	675	U	3.7
55	G	37	GLN	3.7
51	C	130	SER	3.7
57	s7	90	VAL	3.7
51	C	94	LYS	3.7
46	i	15	ALA	3.7
20	z	187	GLU	3.7
68	T	6	GLN	3.7
25	6	727	U	3.6
77	c	32	PHE	3.6
82	sR	191	ASP	3.6
1	1	1259	A	3.6
68	T	22	VAL	3.6
81	g	105	TYR	3.6
78	d8	31	GLU	3.6
14	CN	131	LYS	3.6
25	6	1059	U	3.6
60	c0	54	TYR	3.6
1	1	1566	A	3.6

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Mol	Chain	Res	Type	RSRZ
51	C	207	LEU	3.6
62	c2	120	VAL	3.6
18	x	180	LYS	3.6
7	m	295	GLY	3.6
56	H	147	LEU	3.6
29	AA	109	GLU	3.6
25	A	232	U	3.6
1	AR	2442	G	3.6
53	E	88	ALA	3.6
1	AR	1016	C	3.6
49	p0	293	GLU	3.6
25	6	1257	U	3.6
62	N	52	LEU	3.6
10	p	115	ALA	3.6
26	7	78	ALA	3.6
62	c2	94	ALA	3.6
1	AR	1562	C	3.6
1	AR	2546	C	3.6
59	K	184	SER	3.6
67	S	125	SER	3.6
11	CK	189	GLU	3.6
39	AK	86	ALA	3.6
14	CN	129	ASN	3.6
1	1	1577	G	3.6
18	x	176	ILE	3.6
25	A	488	G	3.6
25	A	1060	U	3.6
53	s3	175	VAL	3.6
29	AA	94	SER	3.6
57	s7	2	SER	3.6
29	AA	2	ALA	3.6
1	AR	1349	G	3.6
67	c7	104	ASN	3.6
62	N	66	VAL	3.6
62	N	112	ALA	3.6
56	s6	165	GLY	3.6
1	AR	2545	C	3.6
81	g	93	HIS	3.6
77	d7	57	GLU	3.5
25	A	182	A	3.5
49	p0	50	VAL	3.5
80	e0	50	VAL	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
53	s3	71	LEU	3.5
80	f	49	LEU	3.5
25	A	196	G	3.5
25	A	201	G	3.5
50	B	196	SER	3.5
14	CN	93	ILE	3.5
25	6	710	U	3.5
50	B	198	MET	3.5
62	c2	117	GLY	3.5
1	AR	2440	G	3.5
62	N	109	GLU	3.5
83	e1	111	GLU	3.5
25	6	493	U	3.5
61	M	144	ALA	3.5
66	R	3	ALA	3.5
75	a	42	LEU	3.5
50	B	39	ASN	3.5
51	C	31	ASP	3.5
51	s1	89	ASP	3.5
14	CN	95	ILE	3.5
7	m	117	GLU	3.5
79	d9	23	VAL	3.5
23	CW	14	THR	3.5
29	AA	100	THR	3.5
82	h	261	LYS	3.5
81	g	129	GLY	3.5
82	h	296	ALA	3.5
82	h	314	GLN	3.5
49	p0	191	TYR	3.5
56	s6	215	ARG	3.5
10	p	116	VAL	3.5
64	P	79	VAL	3.5
64	P	80	HIS	3.5
50	B	97	PRO	3.5
59	K	178	ALA	3.5
53	E	218	LEU	3.5
64	P	33	LEU	3.5
58	s8	123	LYS	3.5
23	5	27	VAL	3.5
1	AR	2443	A	3.5
1	1	2570	U	3.5
29	AA	92	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
68	T	5	VAL	3.5
76	d6	45	VAL	3.5
1	1	1764	U	3.5
75	a	44	GLN	3.5
77	d7	58	SER	3.5
56	H	41	VAL	3.5
54	F	261	LEU	3.5
62	c2	85	LYS	3.5
64	P	14	PHE	3.5
69	U	50	ALA	3.5
81	g	109	ASP	3.4
1	1	1572	U	3.4
10	CJ	255	SER	3.4
18	x	166	VAL	3.4
77	c	45	THR	3.4
51	C	32	ILE	3.4
40	DM	74	LYS	3.4
78	d	44	VAL	3.4
56	H	12	SER	3.4
60	c0	46	LEU	3.4
68	c8	14	ILE	3.4
1	AR	544	C	3.4
53	s3	42	THR	3.4
57	I	78	THR	3.4
65	c5	136	SER	3.4
60	c0	78	GLU	3.4
62	N	68	GLU	3.4
58	s8	200	LYS	3.4
59	s9	93	LEU	3.4
55	s5	92	ARG	3.4
77	d7	82	LYS	3.4
60	L	66	TYR	3.4
66	c6	142	TYR	3.4
50	B	166	GLY	3.4
74	Z	34	ASN	3.4
46	i	274	LYS	3.4
1	1	1248	C	3.4
20	z	188	ASP	3.4
32	AD	35	ARG	3.4
50	B	199	PRO	3.4
29	AA	105	SER	3.4
62	c2	27	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
62	c2	79	ALA	3.4
18	CR	181	ARG	3.4
23	5	10	LYS	3.4
56	H	50	PHE	3.4
75	d5	86	GLU	3.4
51	C	97	LEU	3.4
51	C	217	LEU	3.4
83	e1	109	ASP	3.4
65	c5	51	SER	3.4
23	CW	44	GLU	3.4
82	h	252	LEU	3.4
25	6	228	G	3.4
74	d4	2	SER	3.4
25	A	240	U	3.4
60	c0	1	MET	3.4
82	h	221	MET	3.4
83	e1	143	LYS	3.4
62	c2	86	VAL	3.4
3	4	82	U	3.3
25	A	192	U	3.3
25	A	1691	A	3.3
29	AA	70	PRO	3.3
82	h	313	TRP	3.3
58	s8	199	LYS	3.3
51	s1	54	LEU	3.3
52	s2	92	ALA	3.3
1	1	1269	U	3.3
25	A	1058	U	3.3
62	N	71	ILE	3.3
62	c2	89	ILE	3.3
53	E	183	GLY	3.3
82	sR	314	GLN	3.3
28	DA	126	LEU	3.3
71	d1	39	VAL	3.3
18	x	177	ALA	3.3
37	DJ	2	ALA	3.3
77	d7	38	PRO	3.3
55	s5	35	GLN	3.3
51	s1	97	LEU	3.3
69	U	108	LEU	3.3
64	P	11	SER	3.3
12	CL	186	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
26	7	71	ARG	3.3
62	N	94	ALA	3.3
25	A	231	U	3.3
49	p0	280	ALA	3.3
74	Z	67	GLY	3.3
1	AR	1350	A	3.3
18	x	165	VAL	3.3
25	6	484	C	3.3
25	6	719	U	3.3
29	AA	108	GLU	3.3
51	C	42	ASN	3.3
81	g	85	TYR	3.3
82	h	248	ASN	3.3
59	K	180	LYS	3.3
25	6	1221	A	3.3
25	A	1712	A	3.3
83	e1	108	VAL	3.3
55	s5	145	ASP	3.3
82	h	254	ALA	3.3
25	6	495	C	3.3
25	A	912	U	3.3
51	C	40	ASN	3.3
37	AI	13	SER	3.3
81	g	124	PRO	3.3
1	1	1270	A	3.3
25	6	483	A	3.3
58	s8	148	ALA	3.3
62	N	40	GLY	3.3
68	c8	15	LEU	3.3
78	d8	66	LEU	3.3
1	AR	250	U	3.3
62	c2	126	TRP	3.3
60	c0	41	TYR	3.3
69	c9	55	TYR	3.3
57	I	89	HIS	3.3
66	c6	19	VAL	3.3
27	CZ	22	LYS	3.3
81	g	143	LYS	3.3
7	m	126	GLU	3.3
25	6	224	C	3.3
55	G	161	ASP	3.3
57	I	52	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
65	c5	133	ALA	3.3
75	d5	89	ILE	3.3
20	z	177	VAL	3.3
32	AD	83	LYS	3.3
60	c0	44	LYS	3.3
62	N	73	LYS	3.3
25	A	713	A	3.2
74	Z	133	ASN	3.2
9	o	27	ALA	3.2
25	6	655	G	3.2
62	N	74	LEU	3.2
82	h	71	CYS	3.2
66	R	26	LYS	3.2
51	C	26	ARG	3.2
67	S	123	ASN	3.2
1	AR	3157	U	3.2
51	C	45	LYS	3.2
18	x	157	VAL	3.2
60	c0	74	GLU	3.2
62	c2	96	GLN	3.2
71	W	34	ILE	3.2
64	P	78	ALA	3.2
25	6	1226	A	3.2
25	A	730	G	3.2
51	C	233	GLY	3.2
68	T	17	LEU	3.2
82	sR	303	ALA	3.2
29	AA	18	TYR	3.2
58	J	136	SER	3.2
64	P	20	TYR	3.2
59	K	141	VAL	3.2
77	d7	77	THR	3.2
1	AR	2571	U	3.2
25	6	1708	U	3.2
67	c7	87	GLU	3.2
26	7	91	LYS	3.2
66	R	57	LEU	3.2
25	6	241	U	3.2
25	6	1231	U	3.2
81	g	107	LYS	3.2
25	A	1681	A	3.2
57	I	108	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
71	W	69	LEU	3.2
75	a	98	GLN	3.2
82	h	81	LEU	3.2
49	p0	296	ALA	3.2
55	s5	30	PRO	3.2
17	CQ	182	ASN	3.2
78	d	7	VAL	3.2
29	DB	56	LYS	3.2
1	AR	245	U	3.2
11	CK	190	ASP	3.2
62	c2	143	GLN	3.2
64	P	13	VAL	3.2
56	H	156	PHE	3.2
81	g	102	VAL	3.2
1	1	1237	G	3.2
56	s6	218	GLU	3.2
8	CH	130	ILE	3.2
59	s9	128	LEU	3.2
4	CD	252	THR	3.2
25	6	490	C	3.2
10	CJ	114	ALA	3.2
65	Q	12	PHE	3.2
50	B	50	VAL	3.2
64	P	42	VAL	3.2
7	m	123	GLU	3.2
23	CW	52	ASN	3.2
25	6	1696	G	3.2
53	s3	177	MET	3.2
61	c1	147	GLY	3.2
66	c6	46	PHE	3.2
10	CJ	116	VAL	3.2
50	B	175	TYR	3.2
62	c2	38	HIS	3.2
50	s0	24	LEU	3.2
18	CR	173	ARG	3.2
80	e0	61	SER	3.2
51	C	37	THR	3.2
10	CJ	256	ALA	3.1
49	p0	285	SER	3.1
69	c9	5	SER	3.1
57	s7	58	LEU	3.1
25	6	1712	A	3.1

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Mol	Chain	Res	Type	RSRZ
1	AR	2572	C	3.1
49	p0	288	ALA	3.1
60	c0	20	VAL	3.1
51	C	85	LYS	3.1
65	Q	10	ARG	3.1
68	T	23	ASP	3.1
53	s3	217	ILE	3.1
62	c2	44	GLY	3.1
25	A	193	U	3.1
25	A	1370	U	3.1
9	CI	25	GLN	3.1
55	s5	36	ALA	3.1
56	H	221	ALA	3.1
60	c0	94	GLU	3.1
62	c2	73	LYS	3.1
67	c7	88	VAL	3.1
69	c9	66	TYR	3.1
66	R	29	ILE	3.1
81	g	145	HIS	3.1
8	CH	129	GLU	3.1
39	DL	86	ALA	3.1
1	AR	246	U	3.1
5	k	387	LEU	3.1
25	6	238	U	3.1
25	A	230	C	3.1
1	AR	251	G	3.1
77	c	44	THR	3.1
51	C	28	GLU	3.1
51	C	227	ALA	3.1
56	s6	212	LEU	3.1
40	DM	29	LYS	3.1
81	g	151	ASN	3.1
1	1	439	C	3.1
51	C	56	SER	3.1
26	CY	98	PRO	3.1
62	c2	132	GLU	3.1
82	h	74	THR	3.1
54	F	168	LYS	3.1
82	sR	52	GLN	3.1
62	N	89	ILE	3.1
64	P	83	ILE	3.1
74	d4	133	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	AR	1563	C	3.1
9	o	25	GLN	3.1
69	c9	112	GLY	3.1
74	d4	67	GLY	3.1
75	a	41	ILE	3.1
62	N	48	SER	3.1
10	p	152	LEU	3.1
25	A	188	A	3.1
66	c6	36	ILE	3.1
53	s3	148	LYS	3.1
62	c2	90	LYS	3.1
82	h	33	LEU	3.1
54	F	252	ARG	3.1
54	F	255	ARG	3.1
64	P	43	THR	3.1
82	h	294	TRP	3.1
60	c0	47	GLN	3.1
1	1	1574	C	3.1
1	1	1761	C	3.1
7	CG	5	LYS	3.1
10	p	202	GLU	3.1
62	N	119	SER	3.1
68	c8	53	ASP	3.1
82	h	36	ALA	3.1
83	e1	134	ASN	3.1
25	A	845	G	3.1
56	s6	168	THR	3.1
69	U	21	PHE	3.1
29	AA	114	VAL	3.1
56	s6	162	VAL	3.1
57	s7	72	LYS	3.1
20	CT	176	ARG	3.1
58	s8	141	ARG	3.1
64	P	102	LEU	3.1
59	K	87	SER	3.0
59	s9	184	SER	3.0
29	AA	96	VAL	3.0
29	AA	91	ALA	3.0
51	C	221	PRO	3.0
50	B	54	TRP	3.0
57	s7	60	ILE	3.0
42	AN	108	THR	3.0

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Mol	Chain	Res	Type	RSRZ
68	c8	32	LEU	3.0
7	CG	291	ALA	3.0
51	C	223	PHE	3.0
59	K	164	PHE	3.0
83	e1	110	ALA	3.0
25	A	729	G	3.0
28	DA	120	GLN	3.0
29	DB	75	VAL	3.0
62	c2	39	ASP	3.0
40	DM	73	LEU	3.0
50	B	24	LEU	3.0
27	CZ	23	ALA	3.0
1	1	1272	C	3.0
23	CW	68	THR	3.0
25	6	489	C	3.0
25	6	1491	U	3.0
62	c2	128	ALA	3.0
71	W	53	TYR	3.0
29	DB	74	VAL	3.0
23	CW	53	ALA	3.0
55	s5	68	ILE	3.0
57	s7	162	ILE	3.0
82	h	283	LYS	3.0
4	CD	253	GLN	3.0
69	c9	131	ASP	3.0
23	5	80	THR	3.0
54	F	138	TYR	3.0
63	O	15	ALA	3.0
69	U	6	VAL	3.0
82	sR	252	LEU	3.0
25	A	1229	G	3.0
56	H	27	PHE	3.0
29	AA	93	LYS	3.0
64	c4	45	GLY	3.0
64	P	93	THR	3.0
56	s6	216	LEU	3.0
61	c1	5	LEU	3.0
1	1	1277	C	3.0
1	1	2538	U	3.0
3	4	158	U	3.0
25	6	227	U	3.0
1	1	1580	A	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	AR	1816	A	3.0
54	F	133	LYS	3.0
1	1	547	G	3.0
1	AR	1354	G	3.0
25	A	1713	G	3.0
55	G	36	ALA	3.0
40	DM	45	VAL	3.0
66	R	96	TYR	3.0
51	C	74	GLN	3.0
25	A	191	C	3.0
51	C	39	GLU	3.0
7	m	119	TYR	3.0
9	CI	27	ALA	3.0
68	c8	5	VAL	3.0
1	1	1261	G	3.0
66	R	56	GLY	3.0
55	s5	78	ALA	3.0
55	s5	148	ARG	3.0
25	A	189	C	3.0
49	p0	190	VAL	3.0
66	c6	64	ASP	3.0
25	6	1223	A	3.0
36	AH	73	SER	3.0
56	H	80	ASN	3.0
82	h	295	SER	3.0
64	P	99	GLN	3.0
75	d5	44	GLN	3.0
78	d	26	THR	3.0
58	s8	139	ALA	2.9
1	1	1815	U	2.9
29	AA	26	VAL	2.9
68	c8	22	VAL	2.9
12	r	209	ASN	2.9
78	d	43	ASN	2.9
1	1	1240	A	2.9
1	1	1260	A	2.9
80	f	54	ARG	2.9
10	CJ	245	LYS	2.9
46	i	19	VAL	2.9
71	W	54	ALA	2.9
1	AR	545	U	2.9
12	CL	213	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
12	CL	209	ASN	2.9
3	AT	83	C	2.9
69	U	72	GLY	2.9
75	a	82	HIS	2.9
34	AF	2	ALA	2.9
62	N	88	LEU	2.9
69	c9	18	TYR	2.9
25	6	1285	U	2.9
51	C	44	GLY	2.9
75	d5	52	LYS	2.9
25	6	726	C	2.9
25	A	696	C	2.9
57	s7	52	ALA	2.9
62	c2	133	LEU	2.9
82	h	32	LEU	2.9
29	AA	42	LEU	2.9
62	c2	77	GLY	2.9
25	6	1217	A	2.9
1	AR	249	U	2.9
78	d8	9	LEU	2.9
38	DK	27	SER	2.9
50	B	41	ARG	2.9
51	C	36	SER	2.9
65	c5	128	HIS	2.9
66	R	143	ARG	2.9
83	e1	135	HIS	2.9
53	s3	151	LYS	2.9
60	c0	56	LYS	2.9
25	6	677	G	2.9
25	6	1220	C	2.9
23	CW	105	LEU	2.9
56	H	153	VAL	2.9
62	N	86	VAL	2.9
74	Z	129	VAL	2.9
78	d8	64	ARG	2.9
81	g	100	LEU	2.9
53	s3	107	PHE	2.9
82	h	78	ALA	2.9
64	P	34	SER	2.9
51	s1	53	GLY	2.9
42	DO	77	ILE	2.9
49	p0	64	ARG	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
82	sR	301	LEU	2.9
1	1	1759	C	2.9
54	s4	134	LYS	2.9
77	d7	37	CYS	2.9
1	1	1763	U	2.9
25	A	137	U	2.9
60	c0	51	SER	2.9
62	N	47	GLU	2.9
32	AD	24	THR	2.9
66	c6	114	ARG	2.9
75	d5	87	GLY	2.9
59	K	116	LEU	2.9
75	d5	50	ILE	2.9
1	AR	543	C	2.9
49	p0	290	PRO	2.9
1	1	1256	G	2.9
1	AR	547	G	2.9
54	F	134	LYS	2.9
14	CN	182	ILE	2.9
20	CT	185	LEU	2.9
29	AA	80	LEU	2.9
50	B	9	LEU	2.9
66	R	63	ILE	2.9
78	d8	8	THR	2.9
58	J	148	ALA	2.9
60	c0	45	ALA	2.9
65	Q	101	ALA	2.9
25	A	184	C	2.9
56	H	212	LEU	2.9
57	I	77	LEU	2.9
81	g	134	ASN	2.9
1	AR	1028	U	2.9
62	c2	101	ALA	2.9
40	DM	69	LEU	2.9
51	C	66	VAL	2.8
53	s3	184	ILE	2.8
12	r	217	PHE	2.8
25	6	192	U	2.8
53	s3	150	MET	2.8
60	c0	22	VAL	2.8
18	CR	156	ALA	2.8
68	T	58	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	AR	3153	U	2.8
70	d0	14	GLN	2.8
77	c	37	CYS	2.8
7	m	236	LEU	2.8
51	C	89	ASP	2.8
54	s4	131	LEU	2.8
82	h	34	LEU	2.8
82	sR	49	GLY	2.8
67	S	85	VAL	2.8
53	s3	152	PHE	2.8
7	CG	294	ALA	2.8
25	6	722	G	2.8
53	E	148	LYS	2.8
66	R	22	VAL	2.8
23	CW	106	ALA	2.8
29	AA	35	SER	2.8
62	c2	57	ALA	2.8
69	c9	127	ASN	2.8
83	e1	105	TYR	2.8
1	AR	3155	U	2.8
49	p0	287	ASP	2.8
55	s5	20	PHE	2.8
68	T	11	PHE	2.8
51	C	35	PRO	2.8
54	F	123	LEU	2.8
1	AR	1814	A	2.8
24	CX	4	ASN	2.8
29	AA	69	LYS	2.8
50	B	18	LEU	2.8
25	6	829	A	2.8
23	5	11	ILE	2.8
40	AL	5	ILE	2.8
67	S	110	VAL	2.8
80	f	56	MET	2.8
25	A	491	C	2.8
34	DG	2	ALA	2.8
57	I	165	LYS	2.8
62	N	43	ARG	2.8
82	h	305	TYR	2.8
59	s9	185	GLY	2.8
78	d8	24	GLY	2.8
18	x	182	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
49	p0	196	VAL	2.8
69	c9	113	ILE	2.8
82	h	211	ILE	2.8
1	1	2569	A	2.8
57	I	80	GLU	2.8
25	6	1058	U	2.8
38	DK	100	HIS	2.8
34	DG	128	LEU	2.8
53	s3	182	LEU	2.8
57	I	86	GLN	2.8
46	i	84	LYS	2.8
25	6	1701	A	2.8
3	AT	158	U	2.8
25	A	657	U	2.8
25	A	921	U	2.8
75	d5	51	LEU	2.8
69	U	25	GLN	2.8
75	d5	60	VAL	2.8
1	1	1234	G	2.8
24	lR	4	ASN	2.8
51	C	67	GLU	2.8
69	c9	130	ARG	2.8
81	g	83	LYS	2.8
37	DJ	24	LEU	2.8
60	c0	23	ALA	2.8
62	N	36	LEU	2.8
81	g	137	ASP	2.8
82	sR	244	ALA	2.8
75	a	40	VAL	2.8
60	c0	35	ILE	2.8
29	AA	102	GLU	2.8
62	N	113	ARG	2.8
64	P	18	ARG	2.8
1	1	2095	G	2.8
1	AR	2573	G	2.8
59	s9	148	VAL	2.8
83	e1	131	PHE	2.8
1	AR	1564	U	2.8
10	p	89	GLU	2.8
26	CY	66	GLU	2.8
60	L	49	LEU	2.8
59	K	185	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
82	sR	24	ALA	2.8
33	DF	112	ASP	2.8
54	F	129	VAL	2.8
54	F	256	ARG	2.8
75	d5	88	ILE	2.7
1	1	1765	U	2.7
3	4	81	U	2.7
25	6	1052	U	2.7
56	H	1	MET	2.7
66	c6	38	LEU	2.7
1	AR	2540	A	2.7
25	A	197	A	2.7
28	9	71	SER	2.7
29	AA	11	ALA	2.7
68	T	10	SER	2.7
32	AD	23	TYR	2.7
32	AD	95	ALA	2.7
49	p0	26	PHE	2.7
79	d9	6	VAL	2.7
81	g	130	VAL	2.7
82	h	319	ASN	2.7
44	AP	105	GLN	2.7
23	CW	13	LYS	2.7
33	AE	79	ARG	2.7
58	J	8	ARG	2.7
28	9	85	VAL	2.7
59	K	104	PHE	2.7
62	N	117	GLY	2.7
79	d9	17	GLY	2.7
62	c2	37	VAL	2.7
56	H	152	ASP	2.7
73	Y	57	LEU	2.7
63	O	59	GLY	2.7
53	E	139	SER	2.7
1	AR	1954	G	2.7
53	E	143	ARG	2.7
54	F	163	ASP	2.7
59	K	118	LEU	2.7
49	p0	28	VAL	2.7
57	s7	92	PHE	2.7
78	d8	32	PHE	2.7
3	AT	84	C	2.7

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Mol	Chain	Res	Type	RSRZ
25	A	716	C	2.7
40	DM	5	ILE	2.7
57	s7	31	SER	2.7
51	C	220	GLN	2.7
62	N	108	ARG	2.7
62	c2	52	LEU	2.7
3	AT	79	A	2.7
29	AA	71	PHE	2.7
37	AI	2	ALA	2.7
50	B	189	VAL	2.7
60	L	41	TYR	2.7
60	c0	66	TYR	2.7
10	CJ	251	LYS	2.7
48	sM	83	LYS	2.7
58	J	72	ILE	2.7
1	AR	3277	U	2.7
25	6	320	U	2.7
53	s3	221	SER	2.7
82	sR	235	SER	2.7
52	s2	105	GLY	2.7
49	p0	295	ALA	2.7
1	1	1244	A	2.7
7	m	293	LEU	2.7
25	6	837	G	2.7
67	S	74	GLN	2.7
75	a	37	GLN	2.7
78	d8	6	PRO	2.7
78	d8	54	LEU	2.7
25	6	657	U	2.7
25	A	794	U	2.7
25	A	911	U	2.7
49	p0	88	PHE	2.7
50	s0	46	HIS	2.7
58	J	143	TRP	2.7
64	c4	47	LYS	2.7
82	h	310	ILE	2.7
51	s1	56	SER	2.7
68	c8	10	SER	2.7
25	6	496	G	2.7
25	A	1255	G	2.7
77	d7	46	VAL	2.7
12	CL	218	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
37	DJ	119	LYS	2.7
38	DK	98	ARG	2.7
40	DM	43	PHE	2.7
42	AN	106	ARG	2.7
25	A	200	A	2.7
77	d7	35	VAL	2.7
51	C	60	ALA	2.7
59	K	183	ALA	2.7
1	1	1238	C	2.7
1	AR	1576	G	2.7
25	6	1703	C	2.7
25	A	714	G	2.7
40	DM	54	LEU	2.7
40	DM	16	ARG	2.7
55	G	24	VAL	2.7
14	CN	132	ALA	2.7
51	C	182	ALA	2.7
66	c6	29	ILE	2.7
69	c9	125	SER	2.7
75	a	53	GLU	2.7
59	s9	183	ALA	2.7
82	sR	172	ALA	2.7
59	K	142	ASN	2.7
74	d4	26	ASP	2.7
53	E	54	ARG	2.7
59	K	54	ARG	2.7
57	s7	24	PHE	2.7
1	AR	1577	G	2.7
7	m	127	GLY	2.7
37	AI	8	GLU	2.7
82	sR	309	VAL	2.7
23	CW	108	TYR	2.6
56	H	175	ILE	2.7
64	P	110	LEU	2.6
66	c6	141	SER	2.6
1	AR	601	U	2.6
25	A	917	U	2.6
10	CJ	119	GLY	2.6
49	p0	47	GLY	2.6
1	1	1228	C	2.6
1	1	1275	C	2.6
29	AA	46	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
29	DB	116	LYS	2.6
57	I	55	LYS	2.6
48	sM	66	ALA	2.6
68	T	102	ALA	2.6
1	AR	1565	G	2.6
49	p0	24	SER	2.6
78	d8	56	LEU	2.6
49	p0	86	PHE	2.6
79	e	5	ASN	2.6
62	c2	40	GLY	2.6
17	CQ	187	GLU	2.6
25	A	178	U	2.6
29	DB	102	GLU	2.6
51	C	46	THR	2.6
68	c8	6	GLN	2.6
78	d8	44	VAL	2.6
35	AG	2	ALA	2.6
38	DK	58	ILE	2.6
59	K	76	LEU	2.6
60	L	23	ALA	2.6
63	c3	22	ALA	2.6
82	h	23	LEU	2.6
1	1	1581	C	2.6
54	F	24	SER	2.6
1	AR	1573	G	2.6
25	6	1698	G	2.6
49	p0	80	VAL	2.6
51	C	92	GLN	2.6
51	C	133	TYR	2.6
60	c0	11	ILE	2.6
64	c4	60	ALA	2.6
75	a	80	LEU	2.6
50	B	32	HIS	2.6
52	D	144	TRP	2.6
1	1	2772	C	2.6
1	AR	247	C	2.6
57	I	31	SER	2.6
82	h	251	TRP	2.6
49	p0	60	ARG	2.6
49	p0	188	VAL	2.6
60	c0	71	GLU	2.6
62	N	127	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
75	a	68	ARG	2.6
1	1	2522	G	2.6
25	6	488	G	2.6
25	6	1232	U	2.6
60	c0	14	TYR	2.6
62	c2	97	LEU	2.6
75	a	51	LEU	2.6
78	d	54	LEU	2.6
50	B	203	PHE	2.6
26	7	73	ARG	2.6
1	AR	621	A	2.6
25	6	1230	A	2.6
29	AA	45	GLY	2.6
1	AR	439	C	2.6
59	s9	139	GLN	2.6
60	c0	93	GLN	2.6
26	CY	82	ILE	2.6
74	d4	34	ASN	2.6
53	s3	223	LYS	2.6
1	1	3319	U	2.6
1	AR	2543	U	2.6
29	AA	47	GLU	2.6
83	e1	127	GLY	2.6
57	s7	49	ILE	2.6
63	c3	66	ILE	2.6
72	X	55	ASP	2.6
1	AR	1582	C	2.6
10	p	97	TYR	2.6
82	sR	226	ALA	2.6
23	CW	15	PHE	2.6
25	A	918	U	2.6
26	7	92	GLU	2.6
49	p0	29	GLY	2.6
10	CJ	109	LEU	2.6
75	a	88	ILE	2.6
1	1	1954	G	2.6
1	1	2206	G	2.6
18	x	183	ALA	2.6
25	A	142	G	2.6
77	c	79	PHE	2.6
10	CJ	161	GLU	2.6
23	CW	56	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
57	I	63	PRO	2.6
75	d5	105	THR	2.6
57	I	76	LYS	2.6
18	x	168	LEU	2.6
25	6	725	U	2.6
29	AA	111	LYS	2.6
40	DM	36	LYS	2.6
51	C	229	MET	2.6
79	d9	20	GLN	2.6
15	CO	138	ALA	2.6
37	AI	120	ALA	2.6
64	c4	125	SER	2.6
25	6	729	G	2.6
36	AH	71	THR	2.6
62	N	53	THR	2.6
62	c2	127	GLY	2.6
25	A	541	A	2.6
10	CJ	26	LEU	2.6
25	6	1254	U	2.6
25	6	1687	U	2.6
25	6	1704	U	2.6
63	O	16	ILE	2.6
29	AA	101	PHE	2.6
70	d0	15	GLN	2.6
55	G	70	VAL	2.6
57	s7	7	LYS	2.6
58	J	181	GLY	2.6
62	N	75	VAL	2.6
64	P	28	VAL	2.6
28	9	126	LEU	2.6
60	L	67	THR	2.6
29	DB	36	HIS	2.6
60	L	68	LEU	2.6
1	AR	1765	U	2.6
1	AR	3319	U	2.6
34	AF	127	ALA	2.6
57	s7	57	ALA	2.6
49	p0	286	GLY	2.6
55	s5	55	ASP	2.6
82	h	213	SER	2.6
14	CN	112	ASN	2.6
55	s5	129	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
76	b	60	PRO	2.6
66	c6	115	THR	2.6
70	d0	78	THR	2.6
80	f	48	THR	2.6
58	s8	137	LYS	2.5
58	s8	162	ALA	2.5
65	c5	7	ALA	2.5
1	1	2208	A	2.5
1	1	1239	C	2.5
25	6	1690	G	2.5
25	A	235	G	2.5
29	AA	113	VAL	2.5
35	DH	60	ARG	2.5
58	J	71	GLY	2.5
55	G	223	SER	2.5
62	N	121	VAL	2.5
69	c9	114	VAL	2.5
75	a	93	SER	2.5
82	h	264	SER	2.5
62	c2	136	ILE	2.5
82	sR	316	MET	2.5
51	C	232	HIS	2.5
77	d7	36	LYS	2.5
81	g	115	THR	2.5
50	B	139	VAL	2.5
51	C	43	VAL	2.5
62	N	120	VAL	2.5
1	1	252	U	2.5
53	s3	142	LEU	2.5
57	s7	123	ASP	2.5
56	s6	173	PRO	2.5
57	s7	157	LYS	2.5
65	c5	9	LYS	2.5
27	CZ	33	ARG	2.5
40	DM	6	THR	2.5
74	Z	29	HIS	2.5
50	s0	20	ALA	2.5
62	N	116	VAL	2.5
71	W	32	VAL	2.5
29	DB	72	ILE	2.5
25	A	181	A	2.5
56	H	173	PRO	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
60	c0	97	PRO	2.5
25	A	910	C	2.5
59	K	95	TYR	2.5
25	6	1265	G	2.5
53	s3	222	VAL	2.5
66	R	90	VAL	2.5
70	d0	98	GLN	2.5
13	CM	174	LYS	2.5
57	I	81	LEU	2.5
50	B	194	PRO	2.5
55	G	96	SER	2.5
64	P	101	ALA	2.5
10	CJ	120	LYS	2.5
62	N	124	LYS	2.5
82	sR	168	THR	2.5
25	6	1697	G	2.5
27	CZ	142	ILE	2.5
55	s5	130	ILE	2.5
82	sR	177	MET	2.5
64	P	94	PRO	2.5
75	a	61	SER	2.5
25	6	494	U	2.5
44	AP	11	TYR	2.5
60	c0	13	GLN	2.5
62	c2	42	ALA	2.5
64	c4	97	GLY	2.5
69	U	103	LYS	2.5
82	h	309	VAL	2.5
82	h	318	ALA	2.5
55	s5	79	ASN	2.5
57	I	29	ASN	2.5
10	CJ	110	THR	2.5
49	p0	89	THR	2.5
59	K	3	ARG	2.5
62	N	100	TRP	2.5
1	1	1103	A	2.5
25	6	1219	A	2.5
46	i	137	GLU	2.5
51	C	23	PRO	2.5
77	c	28	PRO	2.5
81	g	88	PRO	2.5
44	AP	102	GLN	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
50	B	201	LEU	2.5
42	AN	119	ASN	2.5
1	AR	2569	A	2.5
51	s1	90	GLU	2.5
26	CY	94	ARG	2.5
51	C	190	PRO	2.5
23	5	9	GLN	2.5
25	A	499	U	2.5
61	c1	20	PHE	2.5
66	R	60	PHE	2.5
62	c2	106	ILE	2.5
82	sR	313	TRP	2.5
65	c5	89	MET	2.5
74	Z	6	THR	2.5
7	m	122	VAL	2.5
38	AJ	98	ARG	2.5
18	x	178	ALA	2.5
26	CY	85	ALA	2.5
53	E	142	LEU	2.5
57	I	90	VAL	2.5
66	R	55	VAL	2.5
69	U	132	LEU	2.5
46	i	105	LYS	2.5
49	p0	81	LYS	2.5
56	H	45	PHE	2.5
78	d8	59	SER	2.5
62	c2	100	TRP	2.5
55	s5	224	ASN	2.5
56	H	218	GLU	2.5
66	R	114	ARG	2.5
70	d0	72	ASN	2.5
74	Z	61	ARG	2.5
10	CJ	113	ALA	2.5
25	6	142	G	2.5
25	6	720	G	2.5
55	G	182	ALA	2.5
56	H	66	GLY	2.5
64	P	114	ARG	2.5
25	A	507	U	2.5
49	p0	87	VAL	2.5
74	Z	35	VAL	2.5
61	c1	146	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
51	C	183	GLN	2.5
69	U	35	ASP	2.5
75	a	89	ILE	2.5
80	f	55	ARG	2.5
2	AS	73	C	2.4
3	4	79	A	2.4
12	CL	188	GLY	2.4
62	N	122	VAL	2.4
63	O	60	VAL	2.4
78	d8	41	VAL	2.4
9	o	23	ALA	2.4
82	sR	227	ALA	2.4
76	b	65	PRO	2.4
5	CE	386	ASP	2.4
51	C	131	ASP	2.4
60	c0	34	GLU	2.4
56	H	148	SER	2.4
60	L	48	SER	2.4
49	p0	76	LEU	2.4
51	C	225	VAL	2.4
67	S	124	VAL	2.4
1	1	1232	C	2.4
49	p0	79	PHE	2.4
25	6	1361	U	2.4
80	e0	48	THR	2.4
29	AA	103	GLN	2.4
63	O	17	PRO	2.4
64	P	12	GLN	2.4
82	h	5	GLU	2.4
36	AH	72	VAL	2.4
59	K	162	SER	2.4
67	S	107	SER	2.4
69	c9	9	VAL	2.4
69	c9	128	GLY	2.4
56	s6	213	ALA	2.4
56	H	226	ILE	2.4
1	1	1025	A	2.4
1	AR	1353	U	2.4
25	6	711	U	2.4
25	6	714	G	2.4
25	A	227	U	2.4
40	DM	10	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
20	z	185	LEU	2.4
78	d8	57	MET	2.4
82	h	271	VAL	2.4
68	c8	144	ARG	2.4
78	d8	63	ALA	2.4
37	AI	64	GLU	2.4
50	s0	173	ILE	2.4
68	T	14	ILE	2.4
78	d8	45	LYS	2.4
58	s8	111	GLN	2.4
78	d8	5	THR	2.4
1	AR	2544	U	2.4
25	A	920	U	2.4
37	AI	3	GLY	2.4
51	C	215	VAL	2.4
55	s5	157	ARG	2.4
60	L	3	MET	2.4
75	d5	42	LEU	2.4
78	d	35	ASP	2.4
12	CL	217	PHE	2.4
10	p	122	LYS	2.4
49	p0	283	ALA	2.4
62	c2	69	ALA	2.4
69	U	107	ALA	2.4
77	d7	53	ALA	2.4
80	f	2	ALA	2.4
40	DM	27	ILE	2.4
11	CK	191	LEU	2.4
49	p0	104	ARG	2.4
51	C	73	LEU	2.4
56	H	177	ARG	2.4
75	d5	68	ARG	2.4
14	CN	94	GLY	2.4
66	R	11	GLY	2.4
77	c	39	GLY	2.4
78	d8	48	VAL	2.4
25	A	894	U	2.4
50	B	23	HIS	2.4
57	s7	158	ASP	2.4
59	s9	146	PHE	2.4
44	AP	99	GLN	2.4
55	s5	165	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
67	c7	105	GLN	2.4
7	m	201	GLY	2.4
28	DA	90	VAL	2.4
1	AR	1628	C	2.4
25	6	1709	C	2.4
50	s0	185	ARG	2.4
55	s5	225	ARG	2.4
51	C	93	GLY	2.4
54	F	76	VAL	2.4
78	d8	27	GLN	2.4
23	CW	98	THR	2.4
40	DM	37	PRO	2.4
70	d0	36	ASN	2.4
60	c0	75	TYR	2.4
60	c0	26	ASP	2.4
1	1	3155	U	2.4
25	6	1706	C	2.4
59	K	148	VAL	2.4
62	N	105	LYS	2.4
68	T	43	SER	2.4
62	N	51	ALA	2.4
82	sR	317	THR	2.4
51	C	132	ASP	2.4
60	c0	43	ILE	2.4
29	AA	38	PHE	2.4
55	s5	150	GLY	2.4
56	H	190	GLN	2.4
57	s7	73	VAL	2.4
25	A	233	C	2.4
53	E	213	GLU	2.4
1	1	440	A	2.4
58	s8	115	ALA	2.4
62	N	128	ALA	2.4
62	c2	84	ASN	2.4
18	CR	182	ILE	2.4
65	c5	135	THR	2.4
68	c8	19	ASN	2.4
69	c9	136	ALA	2.4
51	C	224	ASP	2.4
62	c2	41	LEU	2.4
29	AA	74	VAL	2.4
29	DB	95	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	1	1229	G	2.4
1	AR	1024	G	2.4
36	AH	77	GLY	2.4
26	7	93	ARG	2.4
53	s3	25	PHE	2.4
53	s3	65	ARG	2.4
55	s5	43	PHE	2.4
57	s7	69	GLY	2.4
51	C	50	LYS	2.4
69	U	51	GLU	2.4
53	E	184	ILE	2.4
62	c2	32	LEU	2.4
78	d8	39	THR	2.4
81	g	117	LEU	2.4
10	CJ	182	GLY	2.3
25	A	793	A	2.3
29	DB	58	GLY	2.3
10	p	129	PRO	2.3
54	F	162	ILE	2.3
63	c3	15	ALA	2.3
69	c9	111	ILE	2.3
1	AR	1762	C	2.3
10	CJ	35	GLY	2.3
56	H	36	VAL	2.3
78	d8	67	ARG	2.3
50	B	43	ASP	2.3
72	X	73	GLY	2.3
57	I	56	LYS	2.3
57	I	150	GLN	2.3
25	6	794	U	2.3
49	p0	18	TYR	2.3
59	s9	177	ALA	2.3
62	c2	48	SER	2.3
82	h	246	SER	2.3
74	Z	125	LEU	2.3
76	b	44	ILE	2.3
82	h	301	LEU	2.3
7	m	125	VAL	2.3
50	B	29	VAL	2.3
57	I	101	LYS	2.3
10	p	109	LEU	2.3
20	CT	170	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
54	s4	149	TYR	2.3
56	H	169	TYR	2.3
59	K	156	ILE	2.3
69	U	28	LEU	2.3
78	d8	42	ARG	2.3
60	L	4	PRO	2.3
28	DA	113	LYS	2.3
55	s5	168	VAL	2.3
66	R	7	VAL	2.3
68	T	56	LYS	2.3
82	h	54	PHE	2.3
14	CN	136	GLU	2.3
40	DM	7	ASP	2.3
17	CQ	183	ALA	2.3
7	m	192	PRO	2.3
29	DB	10	VAL	2.3
49	p0	27	VAL	2.3
49	p0	282	SER	2.3
60	L	5	LYS	2.3
1	AR	1103	A	2.3
24	lR	5	GLY	2.3
56	H	16	PHE	2.3
56	s6	156	PHE	2.3
64	P	74	VAL	2.3
25	6	705	U	2.3
25	A	919	A	2.3
46	i	98	GLY	2.3
12	CL	185	ARG	2.3
23	5	52	ASN	2.3
29	AA	90	GLU	2.3
53	E	178	ARG	2.3
53	s3	40	ARG	2.3
62	N	80	ASN	2.3
64	P	38	THR	2.3
78	d8	29	ARG	2.3
82	h	99	THR	2.3
29	AA	25	ILE	2.3
29	AA	61	LYS	2.3
29	DB	21	LYS	2.3
56	s6	171	LYS	2.3
1	AR	3278	C	2.3
12	CL	194	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
49	p0	73	PHE	2.3
56	s6	148	SER	2.3
67	c7	86	PRO	2.3
71	W	18	SER	2.3
38	AJ	29	LYS	2.3
10	p	130	TYR	2.3
13	s	11	ASP	2.3
59	K	105	LEU	2.3
59	K	111	THR	2.3
62	N	59	LEU	2.3
64	P	31	THR	2.3
69	c9	22	LEU	2.3
75	d5	46	LYS	2.3
75	d5	70	LYS	2.3
82	h	25	THR	2.3
62	N	42	ALA	2.3
51	C	24	PHE	2.3
55	s5	31	GLU	2.3
62	c2	25	GLU	2.3
79	d9	45	GLU	2.3
15	u	137	LYS	2.3
1	1	1635	G	2.3
25	6	234	G	2.3
25	A	486	G	2.3
25	A	728	U	2.3
51	C	54	LEU	2.3
15	u	9	ALA	2.3
55	s5	77	TYR	2.3
51	C	21	VAL	2.3
69	c9	17	ALA	2.3
79	e	23	VAL	2.3
56	H	186	ARG	2.3
62	N	55	GLY	2.3
82	h	206	PRO	2.3
1	AR	1031	C	2.3
25	6	189	C	2.3
42	AN	121	LEU	2.3
74	Z	63	GLN	2.3
1	1	1353	U	2.3
25	6	242	U	2.3
53	E	25	PHE	2.3
64	P	17	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
75	d5	102	THR	2.3
82	h	182	ASN	2.3
54	F	25	GLY	2.3
82	h	146	GLY	2.3
37	DJ	8	GLU	2.3
56	s6	167	LYS	2.3
62	c2	68	GLU	2.3
69	U	38	LYS	2.3
57	s7	32	PRO	2.3
65	c5	109	PRO	2.3
62	c2	58	LEU	2.3
53	E	27	ARG	2.3
57	s7	89	HIS	2.3
60	L	11	ILE	2.3
75	d5	104	ALA	2.3
25	A	490	C	2.3
29	DB	73	LYS	2.3
62	c2	98	GLY	2.3
65	Q	78	THR	2.3
82	h	77	GLY	2.3
66	c6	89	LEU	2.3
74	d4	32	ARG	2.3
24	lR	137	VAL	2.3
60	L	22	VAL	2.3
82	h	8	VAL	2.3
59	s9	186	GLU	2.3
74	Z	46	GLU	2.3
80	f	52	GLY	2.3
25	A	558	U	2.3
51	s1	98	THR	2.3
62	c2	70	ASN	2.3
82	sR	224	ASN	2.3
10	p	99	PRO	2.3
66	R	105	LEU	2.3
82	h	247	PRO	2.3
14	CN	145	PHE	2.3
69	U	124	ILE	2.3
25	6	188	A	2.3
59	s9	141	VAL	2.3
76	b	62	TYR	2.3
40	DM	60	GLY	2.2
44	AP	90	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
51	C	102	GLY	2.2
56	H	165	GLY	2.2
1	1	3351	U	2.2
49	p0	31	ASP	2.2
53	s3	178	ARG	2.2
57	I	79	ARG	2.2
69	U	101	ASN	2.2
78	d8	61	ARG	2.2
82	h	202	LEU	2.2
54	F	127	LYS	2.2
51	s1	91	VAL	2.2
70	d0	105	GLN	2.2
78	d8	55	VAL	2.2
25	6	1702	A	2.2
55	G	186	ASN	2.2
66	R	62	ASN	2.2
1	1	1582	C	2.2
13	s	90	GLN	2.2
54	s4	258	GLN	2.2
56	H	210	GLN	2.2
57	s7	11	GLN	2.2
81	g	106	TYR	2.2
81	g	110	ALA	2.2
75	d5	38	HIS	2.2
56	H	178	LEU	2.2
25	A	898	A	2.2
67	c7	25	THR	2.2
82	h	312	VAL	2.2
1	1	2209	U	2.2
1	1	3352	U	2.2
20	z	178	ALA	2.2
23	5	94	ARG	2.2
59	s9	182	GLU	2.2
71	W	37	ALA	2.2
71	d1	44	ARG	2.2
25	6	1711	C	2.2
29	DB	96	VAL	2.2
56	H	5	ILE	2.2
46	i	86	ASN	2.2
53	E	93	ASP	2.2
53	E	111	ASN	2.2
74	d4	3	ASP	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
82	sR	165	ASP	2.2
1	1	1245	A	2.2
57	s7	177	THR	2.2
58	s8	117	TYR	2.2
59	s9	112	GLN	2.2
62	N	101	ALA	2.2
71	d1	42	GLU	2.2
82	h	180	ALA	2.2
1	1	2501	U	2.2
25	6	1258	U	2.2
25	A	1688	U	2.2
1	1	1262	G	2.2
70	V	120	SER	2.2
77	c	30	SER	2.2
1	AR	1759	C	2.2
18	CR	171	ARG	2.2
23	5	38	ILE	2.2
29	DB	118	PHE	2.2
50	s0	41	ARG	2.2
64	c4	70	LYS	2.2
7	m	100	ALA	2.2
20	CT	178	ALA	2.2
62	N	84	ASN	2.2
62	c2	20	ALA	2.2
82	h	267	PRO	2.2
82	h	317	THR	2.2
60	L	46	LEU	2.2
49	p0	187	VAL	2.2
62	N	33	ARG	2.2
69	U	40	SER	2.2
82	h	43	ILE	2.2
1	1	1246	G	2.2
9	o	28	ALA	2.2
49	p0	62	ALA	2.2
53	s3	34	TYR	2.2
14	CN	114	GLN	2.2
54	F	171	ASP	2.2
55	s5	28	PRO	2.2
14	CN	116	LEU	2.2
5	k	287	LYS	2.2
25	6	232	U	2.2
25	6	501	U	2.2

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Mol	Chain	Res	Type	RSRZ
25	6	1224	A	2.2
25	A	493	U	2.2
40	DM	26	LYS	2.2
56	s6	175	ILE	2.2
60	c0	10	LYS	2.2
63	c3	25	TRP	2.2
64	c4	83	ILE	2.2
81	g	94	LYS	2.2
29	AA	33	SER	2.2
51	C	65	VAL	2.2
74	d4	27	VAL	2.2
82	sR	315	VAL	2.2
53	E	87	TYR	2.2
23	5	22	PRO	2.2
25	A	682	C	2.2
28	DA	83	ASP	2.2
51	s1	228	LEU	2.2
60	c0	36	ASP	2.2
62	N	69	ALA	2.2
62	N	79	ALA	2.2
25	6	1233	G	2.2
59	K	113	VAL	2.2
78	d8	28	VAL	2.2
1	AR	2508	U	2.2
25	A	280	U	2.2
25	6	579	A	2.2
40	AL	34	ALA	2.2
55	G	198	LEU	2.2
55	s5	158	GLN	2.2
56	H	124	LEU	2.2
76	b	48	ALA	2.2
82	h	27	ALA	2.2
23	5	28	PHE	2.2
69	c9	14	PHE	2.2
1	1	1255	C	2.2
50	B	48	ILE	2.2
75	a	56	THR	2.2
1	1	1573	G	2.2
75	d5	72	GLY	2.2
6	CF	218	ALA	2.2
20	CT	181	ARG	2.2
51	s1	61	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
60	L	44	LYS	2.2
68	T	3	LEU	2.2
23	CW	57	THR	2.2
48	sM	82	THR	2.2
51	C	90	GLU	2.2
51	s1	20	VAL	2.2
57	I	51	VAL	2.2
77	c	36	LYS	2.2
49	p0	289	ALA	2.2
59	K	119	ALA	2.2
73	Y	85	ALA	2.2
83	e1	140	TYR	2.2
1	1	2571	U	2.2
1	1	1953	G	2.2
25	6	1050	G	2.2
68	c8	12	GLN	2.2
40	DM	70	PRO	2.2
36	AH	110	GLU	2.2
49	p0	59	VAL	2.2
51	C	68	VAL	2.2
67	S	88	VAL	2.2
80	e0	45	VAL	2.2
14	CN	130	GLY	2.2
25	6	754	A	2.2
60	c0	19	GLY	2.2
60	c0	28	ASN	2.2
60	c0	96	ASN	2.2
69	c9	32	GLY	2.2
81	g	86	THR	2.2
82	h	306	THR	2.2
7	CG	293	LEU	2.1
57	s7	126	LEU	2.1
59	K	60	LEU	2.1
63	O	53	LEU	2.1
1	1	2572	C	2.1
25	6	1235	C	2.1
82	sR	214	ALA	2.1
49	p0	48	ARG	2.1
64	P	39	ILE	2.1
64	c4	48	VAL	2.1
69	c9	35	ASP	2.1
69	c9	119	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
71	W	40	ASP	2.1
25	A	720	G	2.1
55	G	75	GLY	2.1
29	AA	79	HIS	2.1
57	s7	29	ASN	2.1
59	K	86	LEU	2.1
63	O	138	ASN	2.1
15	u	138	ALA	2.1
23	CW	34	ALA	2.1
75	a	47	TYR	2.1
1	1	2507	C	2.1
7	CG	9	SER	2.1
33	DF	110	GLU	2.1
62	N	106	ILE	2.1
74	Z	69	SER	2.1
77	d7	54	VAL	2.1
1	AR	1630	U	2.1
82	sR	30	PRO	2.1
54	F	144	GLY	2.1
80	f	6	GLY	2.1
51	s1	217	LEU	2.1
55	G	175	LEU	2.1
66	R	52	LEU	2.1
23	CW	100	THR	2.1
79	d9	27	HIS	2.1
83	e1	123	ASN	2.1
1	1	1230	G	2.1
57	I	43	PHE	2.1
12	CL	183	LYS	2.1
56	H	149	LYS	2.1
56	s6	36	VAL	2.1
57	s7	22	GLN	2.1
66	c6	143	ARG	2.1
6	l	2	SER	2.1
40	DM	56	ILE	2.1
58	s8	152	ILE	2.1
12	CL	204	GLY	2.1
25	A	717	C	2.1
4	CD	34	TYR	2.1
66	R	23	LYS	2.1
69	c9	16	ASN	2.1
74	Z	132	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
80	e0	55	ARG	2.1
78	d8	58	GLU	2.1
1	AR	1561	G	2.1
12	CL	205	SER	2.1
25	A	505	A	2.1
49	p0	82	GLY	2.1
51	C	103	MET	2.1
62	c2	82	PRO	2.1
64	P	97	GLY	2.1
64	c4	44	GLY	2.1
69	U	105	LEU	2.1
80	e0	27	PRO	2.1
1	AR	1763	U	2.1
1	AR	2542	U	2.1
23	CW	33	TYR	2.1
25	A	237	C	2.1
27	8	23	ALA	2.1
49	p0	277	ALA	2.1
56	s6	205	ALA	2.1
69	U	80	TYR	2.1
10	CJ	123	GLN	2.1
14	CN	57	VAL	2.1
56	H	162	VAL	2.1
69	U	126	GLU	2.1
69	c9	43	ASN	2.1
82	h	113	VAL	2.1
77	d7	40	CYS	2.1
57	s7	154	LEU	2.1
32	AD	22	LYS	2.1
59	K	120	LYS	2.1
70	d0	102	ARG	2.1
82	h	137	LYS	2.1
5	k	386	ASP	2.1
25	A	1227	A	2.1
51	C	72	ASP	2.1
60	c0	16	PHE	2.1
65	Q	54	ALA	2.1
75	a	101	TYR	2.1
79	d9	43	PHE	2.1
29	AA	40	HIS	2.1
4	j	252	THR	2.1
10	p	201	THR	2.1

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Mol	Chain	Res	Type	RSRZ
56	H	180	THR	2.1
64	c4	65	GLN	2.1
68	c8	20	THR	2.1
75	d5	41	ILE	2.1
79	d9	31	ILE	2.1
49	p0	46	ARG	2.1
69	U	24	ARG	2.1
82	sR	26	SER	2.1
83	e1	122	SER	2.1
29	AA	117	ALA	2.1
44	AP	92	GLU	2.1
69	c9	51	GLU	2.1
1	AR	1356	U	2.1
57	I	11	GLN	2.1
62	c2	78	LEU	2.1
77	c	80	ARG	2.1
79	e	30	LEU	2.1
29	AA	118	PHE	2.1
57	s7	131	PHE	2.1
60	L	59	PHE	2.1
7	m	221	GLU	2.1
46	i	116	GLU	2.1
50	s0	40	ALA	2.1
58	s8	149	SER	2.1
62	N	21	GLU	2.1
68	c8	146	ALA	2.1
69	c9	29	GLU	2.1
69	c9	137	ALA	2.1
78	d8	10	ALA	2.1
77	c	35	VAL	2.1
20	z	181	ARG	2.1
81	g	149	LYS	2.1
50	B	147	THR	2.1
70	V	67	THR	2.1
13	s	167	TYR	2.1
25	A	1237	G	2.1
25	A	1716	C	2.1
51	s1	23	PRO	2.1
20	z	189	ALA	2.1
49	p0	44	GLU	2.1
29	DB	69	LYS	2.1
53	s3	144	ALA	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
82	sR	318	ALA	2.1
54	F	254	ARG	2.1
55	s5	96	SER	2.1
54	s4	253	ASP	2.1
62	N	46	ARG	2.1
66	R	65	ILE	2.1
62	N	126	TRP	2.1
72	d2	56	HIS	2.1
25	A	1240	U	2.1
3	4	80	A	2.1
20	CT	179	GLU	2.1
30	DC	97	GLU	2.1
37	DJ	102	GLU	2.1
82	h	83	ALA	2.1
24	lR	2	SER	2.1
44	AP	22	GLN	2.1
54	F	259	GLN	2.1
57	I	85	PHE	2.1
10	CJ	137	ASN	2.1
54	s4	133	LYS	2.1
56	H	225	GLU	2.1
56	s6	160	ARG	2.1
58	J	141	ARG	2.1
59	K	6	ARG	2.1
60	c0	52	LYS	2.1
75	d5	103	ARG	2.1
8	CH	15	VAL	2.1
1	1	1231	A	2.1
25	6	138	A	2.1
57	s7	66	SER	2.1
62	N	102	GLY	2.1
78	d	56	LEU	2.1
67	S	70	SER	2.1
57	s7	161	GLN	2.0
1	1	1233	G	2.0
1	AR	1268	G	2.0
7	CG	263	GLU	2.0
57	I	17	GLU	2.0
67	S	87	GLU	2.0
40	DM	2	ALA	2.0
25	A	830	U	2.0
28	9	98	ASN	2.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
28	DA	91	ASN	2.0
36	AH	112	ALA	2.0
1	AR	2565	U	2.0
25	6	231	U	2.0
56	H	49	VAL	2.0
56	s6	206	ALA	2.0
66	c6	39	VAL	2.0
70	d0	107	THR	2.0
74	d4	4	ALA	2.0
77	c	42	ASN	2.0
78	d8	19	THR	2.0
56	H	18	ILE	2.0
40	DM	35	GLY	2.0
50	s0	166	GLY	2.0
56	s6	147	LEU	2.0
82	h	73	LEU	2.0
1	1	1263	A	2.0
1	AR	253	A	2.0
29	AA	3	LYS	2.0
51	C	30	PHE	2.0
29	DB	57	HIS	2.0
53	s3	51	ARG	2.0
56	s6	177	ARG	2.0
59	K	63	ASP	2.0
82	h	59	ARG	2.0
82	h	231	MET	2.0
82	sR	205	SER	2.0
25	6	491	C	2.0
56	s6	209	ALA	2.0
59	K	4	ALA	2.0
10	CJ	45	ASN	2.0
10	CJ	67	ILE	2.0
14	CN	133	PRO	2.0
48	sM	50	ASN	2.0
50	B	21	ASN	2.0
50	B	188	LEU	2.0
1	1	250	U	2.0
1	1	1241	U	2.0
1	AR	243	G	2.0
25	A	725	U	2.0
29	AA	130	PHE	2.0
75	d5	58	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
64	P	37	GLU	2.0
7	CG	288	ALA	2.0
80	f	45	VAL	2.0
23	5	93	ILE	2.0
36	DI	59	PRO	2.0
52	D	145	GLY	2.0
59	s9	180	LYS	2.0
78	d8	53	ILE	2.0
82	sR	47	LEU	2.0
62	N	125	ASN	2.0
73	Y	2	GLY	2.0
74	Z	66	GLY	2.0
1	1	545	U	2.0
1	1	1348	U	2.0
40	DM	4	GLU	2.0
49	p0	195	GLN	2.0
55	s5	39	GLU	2.0
22	2	120	LYS	2.0
29	AA	6	LYS	2.0
49	p0	51	VAL	2.0
64	c4	62	LEU	2.0
66	R	30	LYS	2.0
78	d8	30	VAL	2.0
58	J	147	ALA	2.0
66	c6	28	LEU	2.0
81	g	152	ALA	2.0
1	AR	1575	A	2.0
25	A	733	A	2.0
56	H	196	ARG	2.0
60	c0	53	GLY	2.0
69	c9	122	ARG	2.0
60	c0	27	PHE	2.0
68	c8	11	PHE	2.0
8	n	97	ASN	2.0
56	s6	163	THR	2.0
1	AR	1764	U	2.0
25	A	1682	U	2.0
59	K	112	GLN	2.0
46	i	14	ASP	2.0
46	i	83	LYS	2.0
49	p0	43	LYS	2.0
13	s	60	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
67	S	53	TYR	2.0
81	g	116	LYS	2.0
53	E	50	ILE	2.0
56	H	216	LEU	2.0
82	h	214	ALA	2.0
56	H	33	GLY	2.0
7	CG	3	PHE	2.0
25	A	895	G	2.0
29	DB	52	LYS	2.0
50	B	49	ASN	2.0
57	I	33	GLU	2.0
57	I	34	LEU	2.0
61	c1	117	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4126	1/1	0.94	0.97	65.65	33,33,33,33	0
85	MG	AR	4189	1/1	0.92	1.14	55.57	32,32,32,32	0
85	MG	1	4031	1/1	0.99	0.55	52.89	21,21,21,21	0
85	MG	6	2108	1/1	0.94	0.56	50.10	50,50,50,50	0
85	MG	AR	3809	1/1	0.94	0.65	48.65	37,37,37,37	0
85	MG	CE	405	1/1	0.95	0.89	48.12	26,26,26,26	0
85	MG	1	3833	1/1	0.92	0.70	44.59	24,24,24,24	0
85	MG	x	205	1/1	0.90	0.66	44.53	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	A	2078	1/1	0.93	0.68	44.04	54,54,54,54	0
85	MG	AR	3919	1/1	0.96	0.43	39.71	34,34,34,34	0
85	MG	AR	3893	1/1	0.94	0.95	36.88	50,50,50,50	0
85	MG	AR	4102	1/1	0.57	0.97	36.12	30,30,30,30	0
85	MG	AR	3905	1/1	0.93	0.48	34.66	29,29,29,29	0
85	MG	1	3904	1/1	0.98	0.53	34.58	25,25,25,25	0
84	OHX	1	3655	7/7	0.93	0.37	33.37	138,138,138,139	0
85	MG	1	4048	1/1	0.95	0.83	33.02	33,33,33,33	0
85	MG	1	3856	1/1	0.96	0.68	32.97	24,24,24,24	0
85	MG	AT	221	1/1	0.82	0.76	31.91	52,52,52,52	0
85	MG	1	4168	1/1	0.96	0.45	31.18	20,20,20,20	0
85	MG	1	3887	1/1	0.97	0.83	30.98	42,42,42,42	0
85	MG	A	2079	1/1	0.97	0.64	29.07	58,58,58,58	0
85	MG	1	3905	1/1	0.92	0.47	28.94	38,38,38,38	0
85	MG	x	209	1/1	0.87	0.66	28.59	39,39,39,39	0
85	MG	A	2126	1/1	0.92	0.68	28.24	64,64,64,64	0
85	MG	A	2047	1/1	0.84	0.65	28.18	55,55,55,55	0
85	MG	AR	3888	1/1	0.94	0.67	27.41	24,24,24,24	0
85	MG	1	3764	1/1	0.92	0.57	27.14	41,41,41,41	0
85	MG	1	3912	1/1	0.93	0.59	27.00	22,22,22,22	0
85	MG	AR	4230	1/1	0.92	0.55	26.87	18,18,18,18	0
85	MG	AR	4188	1/1	0.84	1.11	26.60	31,31,31,31	0
85	MG	AR	3961	1/1	0.92	0.53	26.48	43,43,43,43	0
85	MG	AR	3912	1/1	0.94	0.54	26.34	23,23,23,23	0
84	OHX	1	3642	7/7	0.90	0.45	26.30	135,135,136,136	0
84	OHX	6	2038	7/7	0.93	0.41	26.26	148,148,148,148	0
85	MG	1	3911	1/1	0.99	0.65	25.89	21,21,21,21	0
85	MG	6	2077	1/1	0.92	0.54	25.02	39,39,39,39	0
85	MG	AR	3937	1/1	0.95	0.67	24.81	27,27,27,27	0
85	MG	1	3885	1/1	0.98	0.49	24.78	20,20,20,20	0
85	MG	AR	3933	1/1	0.96	0.47	24.77	24,24,24,24	0
85	MG	AR	3941	1/1	0.96	0.46	24.54	36,36,36,36	0
84	OHX	AR	3717	7/7	0.84	0.42	24.38	144,144,144,144	0
85	MG	AR	3871	1/1	0.96	0.40	24.21	28,28,28,28	0
85	MG	6	2098	1/1	0.98	0.53	23.94	68,68,68,68	0
85	MG	1	3890	1/1	0.94	0.47	23.87	34,34,34,34	0
85	MG	1	3914	1/1	0.95	0.50	23.81	19,19,19,19	0
85	MG	1	3756	1/1	0.93	0.42	23.71	32,32,32,32	0
85	MG	AR	3879	1/1	0.94	0.64	23.56	22,22,22,22	0
84	OHX	AR	3726	7/7	0.88	0.42	23.26	118,118,118,118	0
85	MG	1	3909	1/1	0.97	0.57	23.15	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3874	1/1	0.96	0.60	22.97	27,27,27,27	0
85	MG	AR	3993	1/1	0.94	0.35	22.96	28,28,28,28	0
84	OHX	A	1953	7/7	0.94	0.41	22.79	146,147,147,147	0
85	MG	1	4195	1/1	0.94	0.46	22.70	29,29,29,29	0
85	MG	A	2053	1/1	0.86	0.72	22.46	57,57,57,57	0
84	OHX	AR	3579	7/7	0.95	0.34	22.03	130,130,130,130	0
85	MG	A	2077	1/1	0.97	0.59	21.99	48,48,48,48	0
84	OHX	AR	3690	7/7	0.88	0.47	21.95	117,118,118,118	0
84	OHX	AR	3648	7/7	0.96	0.55	21.88	130,131,131,131	0
85	MG	AR	4051	1/1	0.88	0.38	21.87	40,40,40,40	0
85	MG	AR	4155	1/1	0.81	0.45	21.63	34,34,34,34	0
85	MG	1	4222	1/1	0.96	0.65	21.62	13,13,13,13	0
85	MG	1	4215	1/1	0.98	0.62	21.48	27,27,27,27	0
85	MG	CE	407	1/1	0.81	0.59	21.42	41,41,41,41	0
85	MG	1	4186	1/1	0.95	0.52	21.28	25,25,25,25	0
85	MG	1	3796	1/1	0.95	0.54	21.03	18,18,18,18	0
85	MG	AR	3940	1/1	0.99	0.49	20.96	21,21,21,21	0
85	MG	AR	3767	1/1	0.94	0.58	20.74	35,35,35,35	0
85	MG	1	3731	1/1	0.85	0.49	20.68	36,36,36,36	0
84	OHX	1	3596	7/7	0.91	0.49	20.67	143,144,144,144	0
85	MG	6	2158	1/1	0.46	0.75	20.63	74,74,74,74	0
85	MG	A	2055	1/1	0.93	0.47	20.45	71,71,71,71	0
85	MG	A	2066	1/1	0.96	0.59	20.38	79,79,79,79	0
85	MG	1	3859	1/1	0.95	0.44	20.02	28,28,28,28	0
85	MG	AR	3906	1/1	0.97	0.36	19.83	33,33,33,33	0
85	MG	AR	3804	1/1	0.92	0.45	19.83	27,27,27,27	0
85	MG	4	221	1/1	0.63	0.54	19.68	51,51,51,51	0
84	OHX	AR	3641	7/7	0.93	0.48	19.59	133,133,133,133	0
85	MG	1	4125	1/1	0.87	0.38	19.56	23,23,23,23	0
85	MG	AR	3930	1/1	0.97	0.62	19.52	29,29,29,29	0
85	MG	1	3860	1/1	0.94	0.47	19.39	36,36,36,36	0
85	MG	1	3875	1/1	0.98	0.46	19.37	23,23,23,23	0
85	MG	1	3891	1/1	0.98	0.60	19.22	17,17,17,17	0
85	MG	AR	3977	1/1	0.92	0.42	19.20	41,41,41,41	0
85	MG	1	3783	1/1	0.98	0.46	19.12	18,18,18,18	0
85	MG	1	3889	1/1	0.98	0.54	19.11	23,23,23,23	0
85	MG	AR	4080	1/1	0.87	0.51	19.07	32,32,32,32	0
85	MG	AR	3763	1/1	0.98	0.59	18.79	17,17,17,17	0
85	MG	AR	3915	1/1	0.95	0.61	18.74	28,28,28,28	0
85	MG	AR	4002	1/1	0.93	0.50	18.59	28,28,28,28	0
85	MG	A	2153	1/1	0.94	0.58	18.55	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	6	2161	1/1	0.86	0.49	18.39	58,58,58,58	0
84	OHX	AR	3592	7/7	0.95	0.34	18.27	114,114,114,114	0
85	MG	AR	3914	1/1	0.90	0.43	18.02	32,32,32,32	0
85	MG	1	3843	1/1	0.83	0.41	17.92	24,24,24,24	0
84	OHX	6	2033	7/7	0.92	0.40	17.86	150,151,151,152	0
85	MG	1	4204	1/1	0.97	0.51	17.83	34,34,34,34	0
84	OHX	1	3640	7/7	0.96	0.35	17.73	124,124,124,125	0
85	MG	1	3828	1/1	0.93	0.55	17.66	30,30,30,30	0
85	MG	1	3732	1/1	0.91	0.44	17.66	26,26,26,26	0
85	MG	1	3962	1/1	0.90	0.41	17.55	39,39,39,39	0
85	MG	1	4196	1/1	0.98	0.42	17.34	30,30,30,30	0
84	OHX	1	3719	7/7	0.90	0.52	17.29	120,120,121,121	0
84	OHX	1	3717	7/7	0.81	0.54	17.26	144,144,144,145	0
85	MG	AR	3859	1/1	0.94	0.49	17.24	29,29,29,29	0
85	MG	1	3801	1/1	0.77	0.54	17.09	37,37,37,37	0
85	MG	4	224	1/1	0.95	0.40	17.09	33,33,33,33	0
85	MG	AR	4247	1/1	0.95	0.46	17.09	22,22,22,22	0
85	MG	k	404	1/1	0.95	0.67	17.04	32,32,32,32	0
85	MG	1	3799	1/1	0.85	0.41	16.98	37,37,37,37	0
84	OHX	A	2012	7/7	0.92	0.37	16.83	139,140,140,140	0
84	OHX	1	3711	7/7	0.93	0.59	16.82	119,120,120,120	0
85	MG	1	4208	1/1	0.95	0.32	16.78	37,37,37,37	0
85	MG	AR	3860	1/1	0.98	0.51	16.70	23,23,23,23	0
85	MG	CR	201	1/1	0.94	0.65	16.63	29,29,29,29	0
84	OHX	A	2026	7/7	0.90	0.40	16.59	123,123,124,124	0
85	MG	AR	4024	1/1	0.74	0.79	16.56	53,53,53,53	0
84	OHX	AR	3652	7/7	0.87	0.43	16.33	112,112,113,113	0
85	MG	6	2107	1/1	0.95	0.55	16.32	43,43,43,43	0
84	OHX	A	2035	7/7	0.91	0.48	16.27	130,131,131,131	0
84	OHX	AR	3660	7/7	0.94	0.43	16.07	123,123,124,124	0
85	MG	6	2140	1/1	0.82	0.40	16.06	69,69,69,69	0
85	MG	AR	4249	1/1	0.96	0.44	15.98	24,24,24,24	0
85	MG	AR	3896	1/1	0.91	0.55	15.96	36,36,36,36	0
85	MG	AR	3909	1/1	0.99	0.57	15.96	25,25,25,25	0
85	MG	AR	3904	1/1	0.95	0.52	15.89	21,21,21,21	0
85	MG	AR	3985	1/1	0.97	0.49	15.81	35,35,35,35	0
85	MG	6	2078	1/1	0.90	0.45	15.79	42,42,42,42	0
85	MG	1	3858	1/1	0.99	0.37	15.77	25,25,25,25	0
85	MG	1	3869	1/1	0.90	0.49	15.63	34,34,34,34	0
85	MG	A	2105	1/1	0.93	0.43	15.57	94,94,94,94	0
84	OHX	1	3695	7/7	0.91	0.61	15.46	154,154,155,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3913	1/1	0.87	0.43	15.31	26,26,26,26	0
84	OHX	AR	3657	7/7	0.92	0.38	15.30	114,114,115,115	0
85	MG	AR	3942	1/1	0.95	0.56	14.97	31,31,31,31	0
85	MG	1	3845	1/1	0.87	0.40	14.88	18,18,18,18	0
85	MG	6	2071	1/1	0.97	0.49	14.88	45,45,45,45	0
85	MG	AT	230	1/1	0.98	0.42	14.78	39,39,39,39	0
84	OHX	AR	3729	7/7	0.89	0.46	14.65	120,120,120,121	0
85	MG	1	3822	1/1	0.97	0.49	14.64	18,18,18,18	0
85	MG	1	3902	1/1	0.95	0.50	14.59	35,35,35,35	0
85	MG	AR	4082	1/1	0.94	0.34	14.52	24,24,24,24	0
85	MG	AR	4241	1/1	0.99	0.39	14.46	17,17,17,17	0
85	MG	6	2053	1/1	0.97	0.57	14.34	41,41,41,41	0
85	MG	6	2057	1/1	0.97	0.56	14.26	51,51,51,51	0
85	MG	AR	3747	1/1	0.92	0.30	14.23	23,23,23,23	0
85	MG	AR	3857	1/1	0.95	0.53	14.19	20,20,20,20	0
85	MG	AR	3918	1/1	0.95	0.48	14.16	27,27,27,27	0
84	OHX	1	3641	7/7	0.94	0.35	14.13	141,141,141,141	0
85	MG	AR	4198	1/1	0.80	0.59	14.07	51,51,51,51	0
85	MG	6	2068	1/1	0.83	0.46	14.06	61,61,61,61	0
85	MG	AR	3926	1/1	0.96	0.37	13.99	33,33,33,33	0
85	MG	AR	4140	1/1	0.85	0.49	13.85	44,44,44,44	0
85	MG	AR	3772	1/1	0.96	0.52	13.85	37,37,37,37	0
85	MG	1	3819	1/1	0.83	0.40	13.70	27,27,27,27	0
85	MG	6	2197	1/1	0.78	0.57	13.64	56,56,56,56	0
85	MG	AR	3938	1/1	0.97	0.39	13.54	34,34,34,34	0
85	MG	AR	3786	1/1	0.97	0.48	13.53	25,25,25,25	0
85	MG	AR	3756	1/1	0.82	0.35	13.47	36,36,36,36	0
85	MG	AK	103	1/1	0.96	0.44	13.43	36,36,36,36	0
85	MG	AR	3810	1/1	0.97	0.51	13.25	27,27,27,27	0
85	MG	1	3829	1/1	0.94	0.53	13.15	16,16,16,16	0
85	MG	A	2062	1/1	0.72	0.71	13.11	65,65,65,65	0
84	OHX	AR	3409	7/7	0.99	0.34	13.07	120,120,120,121	0
85	MG	A	2138	1/1	0.96	0.46	13.06	66,66,66,66	0
84	OHX	AT	201	7/7	0.99	0.33	13.06	109,109,110,110	0
84	OHX	AR	3691	7/7	0.94	0.40	12.93	116,116,116,117	0
84	OHX	6	2046	7/7	0.86	0.36	12.91	151,152,152,152	0
85	MG	A	2119	1/1	0.96	0.35	12.84	57,57,57,57	0
85	MG	1	4193	1/1	0.87	0.37	12.80	23,23,23,23	0
85	MG	1	4189	1/1	0.93	0.36	12.78	27,27,27,27	0
85	MG	AR	4227	1/1	0.94	0.33	12.71	22,22,22,22	0
85	MG	1	4027	1/1	0.81	0.39	12.69	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3841	1/1	0.95	0.59	12.69	29,29,29,29	0
85	MG	1	3779	1/1	0.83	0.48	12.65	55,55,55,55	0
85	MG	1	3746	1/1	0.91	0.41	12.64	26,26,26,26	0
85	MG	AR	4090	1/1	0.83	0.49	12.58	57,57,57,57	0
85	MG	AR	4091	1/1	0.96	0.31	12.50	35,35,35,35	0
85	MG	AR	4252	1/1	0.90	0.37	12.43	50,50,50,50	0
84	OHX	1	3672	7/7	0.92	0.41	12.40	147,147,147,148	0
84	OHX	AR	3732	7/7	0.92	0.52	12.39	146,146,147,147	0
85	MG	1	3886	1/1	0.88	0.41	12.36	21,21,21,21	0
84	OHX	AR	3632	7/7	0.96	0.35	12.25	117,117,118,118	0
85	MG	AR	3863	1/1	0.98	0.57	12.24	21,21,21,21	0
85	MG	1	3868	1/1	0.93	0.42	12.24	29,29,29,29	0
85	MG	AR	4034	1/1	0.73	0.45	12.20	60,60,60,60	0
85	MG	AR	4138	1/1	0.95	0.48	12.16	28,28,28,28	0
85	MG	AB	203	1/1	0.91	0.34	12.15	32,32,32,32	0
85	MG	6	2082	1/1	0.90	0.48	12.13	54,54,54,54	0
84	OHX	AR	3685	7/7	0.94	0.33	12.01	120,121,121,121	0
85	MG	1	3894	1/1	0.95	0.48	11.87	22,22,22,22	0
84	OHX	1	3692	7/7	0.92	0.29	11.87	113,113,113,113	0
84	OHX	1	3661	7/7	0.93	0.32	11.83	119,120,120,120	0
84	OHX	A	1970	7/7	0.91	0.35	11.80	132,132,133,133	0
85	MG	AR	3966	1/1	0.93	0.45	11.80	38,38,38,38	0
85	MG	A	2080	1/1	0.88	0.39	11.79	65,65,65,65	0
84	OHX	1	3723	7/7	0.89	0.35	11.71	113,113,113,113	0
84	OHX	1	3694	7/7	0.93	0.41	11.68	116,116,117,117	0
84	OHX	A	2013	7/7	0.94	0.34	11.65	132,133,133,133	0
85	MG	AR	3901	1/1	0.95	0.45	11.63	29,29,29,29	0
84	OHX	AR	3728	7/7	0.85	0.41	11.63	151,152,152,152	0
85	MG	AR	3873	1/1	0.85	0.46	11.57	31,31,31,31	0
84	OHX	AR	3677	7/7	0.91	0.38	11.48	110,111,111,111	0
85	MG	1	3882	1/1	0.99	0.45	11.38	32,32,32,32	0
84	OHX	6	2039	7/7	0.90	0.62	11.38	132,133,133,134	0
85	MG	A	2057	1/1	0.92	0.46	11.35	70,70,70,70	0
85	MG	AR	4141	1/1	0.78	0.36	11.32	37,37,37,37	0
85	MG	A	2109	1/1	0.86	0.41	11.27	60,60,60,60	0
84	OHX	AR	3626	7/7	0.96	0.30	11.05	122,123,123,123	0
84	OHX	AR	3735	7/7	0.94	0.30	11.04	129,129,129,129	0
85	MG	1	3795	1/1	0.94	0.29	11.03	26,26,26,26	0
85	MG	A	2052	1/1	0.93	0.42	11.00	53,53,53,53	0
84	OHX	AR	3417	7/7	0.98	0.26	10.93	111,112,112,112	0
85	MG	AR	3757	1/1	0.93	0.41	10.81	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3879	1/1	0.95	0.38	10.81	45,45,45,45	0
84	OHX	1	3403	7/7	0.98	0.30	10.74	113,113,113,114	0
84	OHX	x	201	7/7	0.90	0.39	10.74	110,110,110,110	0
84	OHX	AR	3401	7/7	0.98	0.39	10.73	121,121,121,122	0
84	OHX	1	3707	7/7	0.90	0.40	10.72	125,125,126,126	0
84	OHX	AR	3601	7/7	0.95	0.42	10.63	127,127,128,128	0
84	OHX	AR	3402	7/7	0.99	0.39	10.59	113,113,113,113	0
85	MG	AR	3750	1/1	0.90	0.41	10.57	27,27,27,27	0
84	OHX	1	3708	7/7	0.87	0.39	10.55	134,134,134,134	0
84	OHX	6	1901	7/7	0.99	0.34	10.52	119,120,120,120	0
84	OHX	AR	3645	7/7	0.98	0.34	10.47	118,118,118,118	0
84	OHX	AR	3413	7/7	0.99	0.26	10.43	107,107,107,107	0
84	OHX	1	3408	7/7	0.99	0.32	10.36	112,112,112,113	0
85	MG	AR	4226	1/1	0.92	0.41	10.35	24,24,24,24	0
85	MG	AR	3801	1/1	0.94	0.38	10.35	32,32,32,32	0
85	MG	1	4096	1/1	0.96	0.41	10.31	27,27,27,27	0
85	MG	AR	4075	1/1	0.83	0.31	10.29	36,36,36,36	0
84	OHX	AR	3693	7/7	0.96	0.41	10.27	131,131,131,131	0
85	MG	AR	4161	1/1	0.74	0.27	10.26	39,39,39,39	0
84	OHX	1	3409	7/7	0.99	0.30	10.19	116,116,117,117	0
84	OHX	AR	3410	7/7	0.99	0.31	10.09	109,109,109,110	0
85	MG	AR	3850	1/1	0.97	0.28	10.05	24,24,24,24	0
84	OHX	1	3677	7/7	0.96	0.33	10.02	116,116,117,117	0
85	MG	1	3836	1/1	0.97	0.39	9.93	36,36,36,36	0
85	MG	AR	3950	1/1	0.65	0.27	9.89	47,47,47,47	0
85	MG	1	3760	1/1	0.97	0.36	9.85	27,27,27,27	0
84	OHX	1	3401	7/7	0.99	0.38	9.84	114,114,115,115	0
84	OHX	1	3402	7/7	0.99	0.35	9.73	114,115,115,115	0
85	MG	CU	201	1/1	0.87	0.40	9.71	38,38,38,38	0
84	OHX	AR	3411	7/7	0.98	0.30	9.70	106,106,106,106	0
84	OHX	AR	3700	7/7	0.95	0.47	9.58	135,135,135,135	0
84	OHX	1	3705	7/7	0.94	0.38	9.50	131,131,132,132	0
85	MG	1	4142	1/1	0.98	0.26	9.48	38,38,38,38	0
84	OHX	4	201	7/7	0.98	0.35	9.42	108,108,108,108	0
85	MG	CD	302	1/1	0.73	0.49	9.41	36,36,36,36	0
85	MG	1	3866	1/1	0.82	0.39	9.34	34,34,34,34	0
85	MG	AR	4019	1/1	0.84	0.27	9.33	45,45,45,45	0
84	OHX	4	213	7/7	0.91	0.31	9.32	117,117,117,117	0
85	MG	A	2072	1/1	0.93	0.39	9.21	66,66,66,66	0
85	MG	6	2059	1/1	0.86	0.43	9.14	70,70,70,70	0
85	MG	d6	102	1/1	0.97	0.50	9.09	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	6	1980	7/7	0.96	0.34	9.09	116,116,116,116	0
85	MG	AR	4202	1/1	0.95	0.56	9.06	29,29,29,29	0
84	OHX	6	1979	7/7	0.94	0.46	9.06	135,135,136,136	0
84	OHX	A	1990	7/7	0.97	0.27	8.96	135,135,136,136	0
85	MG	1	3899	1/1	0.91	0.35	8.93	39,39,39,39	0
85	MG	AR	3790	1/1	0.96	0.34	8.92	22,22,22,22	0
84	OHX	1	3592	7/7	0.96	0.33	8.88	117,117,117,117	0
85	MG	AR	3865	1/1	0.95	0.41	8.74	24,24,24,24	0
85	MG	AR	3751	1/1	0.82	0.36	8.72	36,36,36,36	0
85	MG	CD	301	1/1	0.90	0.37	8.71	34,34,34,34	0
84	OHX	A	1903	7/7	0.98	0.35	8.68	149,149,150,150	0
85	MG	AR	3936	1/1	0.96	0.52	8.68	20,20,20,20	0
85	MG	A	2131	1/1	0.74	0.43	8.62	64,64,64,64	0
84	OHX	1	3699	7/7	0.97	0.40	8.62	130,131,131,131	0
85	MG	1	3871	1/1	0.92	0.47	8.61	30,30,30,30	0
84	OHX	1	3680	7/7	0.96	0.32	8.58	122,122,122,122	0
85	MG	6	2155	1/1	0.94	0.86	8.54	58,58,58,58	0
85	MG	A	2061	1/1	0.92	0.50	8.53	59,59,59,59	0
85	MG	AR	3994	1/1	0.83	0.32	8.50	25,25,25,25	0
85	MG	AR	4041	1/1	0.93	0.36	8.49	34,34,34,34	0
85	MG	1	3939	1/1	0.88	0.29	8.46	39,39,39,39	0
85	MG	4	225	1/1	0.92	0.32	8.43	25,25,25,25	0
84	OHX	A	2021	7/7	0.91	0.43	8.43	133,133,134,134	0
84	OHX	4	214	7/7	0.94	0.46	8.40	140,140,140,140	0
84	OHX	AM	101	7/7	0.90	0.43	8.37	121,121,121,121	0
84	OHX	AR	3640	7/7	0.87	0.32	8.32	126,126,126,126	0
84	OHX	A	1982	7/7	0.97	0.30	8.30	121,122,122,122	0
84	OHX	AR	3610	7/7	0.95	0.38	8.29	137,138,138,138	0
85	MG	CX	203	1/1	0.97	0.39	8.22	19,19,19,19	0
85	MG	1	3876	1/1	0.96	0.40	8.19	37,37,37,37	0
85	MG	1	3978	1/1	0.94	0.35	8.13	46,46,46,46	0
84	OHX	AR	3658	7/7	0.95	0.35	8.09	122,123,123,123	0
85	MG	1	3730	1/1	0.94	0.34	8.03	36,36,36,36	0
84	OHX	AR	3407	7/7	0.98	0.34	8.01	113,113,113,113	0
84	OHX	6	1902	7/7	0.99	0.34	7.89	136,136,137,137	0
85	MG	1	3725	1/1	0.99	0.38	7.83	34,34,34,34	0
84	OHX	AR	3684	7/7	0.96	0.52	7.80	124,125,125,125	0
85	MG	1	3892	1/1	0.87	0.41	7.78	23,23,23,23	0
85	MG	6	2099	1/1	0.82	0.39	7.77	51,51,51,51	0
85	MG	AR	3897	1/1	0.91	0.44	7.76	51,51,51,51	0
84	OHX	1	3631	7/7	0.94	0.31	7.74	116,116,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	6	2091	1/1	0.92	0.41	7.74	61,61,61,61	0
84	OHX	4	210	7/7	0.95	0.26	7.71	108,108,108,108	0
84	OHX	1	3645	7/7	0.97	0.34	7.68	125,126,126,126	0
85	MG	6	2061	1/1	0.96	0.32	7.67	100,100,100,100	0
85	MG	1	3901	1/1	0.91	0.49	7.67	39,39,39,39	0
84	OHX	1	3657	7/7	0.95	0.28	7.66	123,123,124,124	0
84	OHX	1	3407	7/7	0.98	0.31	7.65	106,106,107,107	0
85	MG	1	3793	1/1	0.90	0.30	7.61	37,37,37,37	0
84	OHX	1	3575	7/7	0.95	0.27	7.58	116,117,117,117	0
84	OHX	1	3539	7/7	0.95	0.28	7.53	119,119,119,119	0
84	OHX	AR	3683	7/7	0.97	0.36	7.49	126,127,127,127	0
84	OHX	AR	3406	7/7	0.98	0.34	7.49	112,112,113,113	0
84	OHX	AR	3654	7/7	0.94	0.50	7.43	137,137,138,138	0
85	MG	AR	4228	1/1	0.95	0.37	7.34	27,27,27,27	0
84	OHX	AR	3415	7/7	0.98	0.35	7.30	109,109,110,110	0
84	OHX	1	3665	7/7	0.92	0.36	7.29	129,129,129,129	0
84	OHX	AR	3403	7/7	0.99	0.28	7.24	110,110,110,110	0
85	MG	1	3846	1/1	0.95	0.28	7.17	39,39,39,39	0
84	OHX	A	2014	7/7	0.94	0.35	7.17	127,128,128,128	0
85	MG	A	2155	1/1	0.61	0.46	7.16	75,75,75,75	0
84	OHX	1	3604	7/7	0.95	0.34	7.16	116,116,117,117	0
84	OHX	1	3601	7/7	0.96	0.30	7.13	112,112,112,112	0
85	MG	AR	3819	1/1	0.98	0.36	7.08	37,37,37,37	0
85	MG	AR	4111	1/1	0.95	0.35	7.04	37,37,37,37	0
84	OHX	AR	3590	7/7	0.94	0.37	7.03	113,113,113,113	0
85	MG	A	2108	1/1	0.97	0.62	6.98	57,57,57,57	0
85	MG	AR	3826	1/1	0.95	0.32	6.84	23,23,23,23	0
85	MG	AR	3753	1/1	0.90	0.33	6.84	26,26,26,26	0
84	OHX	1	3412	7/7	0.99	0.30	6.81	114,114,115,115	0
85	MG	A	2064	1/1	0.95	0.34	6.80	65,65,65,65	0
84	OHX	A	1980	7/7	0.96	0.26	6.76	137,137,138,138	0
84	OHX	6	2019	7/7	0.94	0.30	6.71	140,140,141,141	0
85	MG	1	4188	1/1	0.96	0.37	6.71	28,28,28,28	0
84	OHX	1	3421	7/7	0.99	0.29	6.71	115,115,116,116	0
85	MG	A	2101	1/1	0.85	0.38	6.69	64,64,64,64	0
85	MG	AT	218	1/1	0.69	0.34	6.69	30,30,30,30	0
85	MG	1	3823	1/1	0.65	0.27	6.68	41,41,41,41	0
84	OHX	AR	3644	7/7	0.92	0.31	6.68	126,127,127,127	0
84	OHX	6	1903	7/7	0.99	0.29	6.66	117,118,118,118	0
84	OHX	4	202	7/7	0.99	0.32	6.64	112,112,112,113	0
84	OHX	4	208	7/7	0.97	0.36	6.63	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	6	1987	7/7	0.93	0.28	6.58	137,137,138,138	0
85	MG	1	3837	1/1	0.93	0.33	6.57	26,26,26,26	0
85	MG	AR	3844	1/1	0.96	0.40	6.56	27,27,27,27	0
85	MG	A	2088	1/1	0.87	0.53	6.53	59,59,59,59	0
85	MG	AR	3978	1/1	0.94	0.36	6.52	49,49,49,49	0
84	OHX	AR	3625	7/7	0.97	0.36	6.52	134,134,134,134	0
84	OHX	6	2031	7/7	0.94	0.31	6.48	125,126,126,126	0
84	OHX	AR	3714	7/7	0.95	0.33	6.48	132,132,133,133	0
84	OHX	1	3591	7/7	0.94	0.28	6.47	109,109,109,109	0
84	OHX	6	1972	7/7	0.95	0.42	6.46	142,143,143,144	0
84	OHX	1	3666	7/7	0.92	0.42	6.45	117,118,118,118	0
84	OHX	1	3673	7/7	0.91	0.56	6.44	133,133,133,133	0
85	MG	x	204	1/1	0.92	0.35	6.44	28,28,28,28	0
84	OHX	A	1994	7/7	0.96	0.28	6.40	142,143,144,144	0
84	OHX	AR	3600	7/7	0.94	0.33	6.39	119,119,119,119	0
85	MG	AR	4083	1/1	0.89	0.28	6.36	31,31,31,31	0
84	OHX	A	1901	7/7	0.98	0.29	6.36	127,127,127,128	0
85	MG	1	3867	1/1	0.95	0.43	6.32	35,35,35,35	0
85	MG	1	3740	1/1	0.92	0.36	6.32	30,30,30,30	0
84	OHX	1	3659	7/7	0.91	0.32	6.27	140,140,140,141	0
85	MG	AR	4206	1/1	0.81	0.28	6.23	33,33,33,33	0
85	MG	1	4084	1/1	0.88	0.27	6.19	32,32,32,32	0
84	OHX	AR	3521	7/7	0.96	0.28	6.18	117,118,118,118	0
84	OHX	1	3685	7/7	0.96	0.40	6.14	121,121,121,121	0
84	OHX	AR	3408	7/7	0.99	0.33	6.14	107,107,107,107	0
84	OHX	6	2011	7/7	0.96	0.43	6.10	146,146,147,147	0
85	MG	1	3990	1/1	0.92	0.30	6.10	24,24,24,24	0
84	OHX	AR	3715	7/7	0.96	0.29	6.09	118,118,119,119	0
84	OHX	1	3410	7/7	0.98	0.32	6.08	112,112,112,112	0
84	OHX	6	2001	7/7	0.90	0.28	6.07	119,120,120,120	0
84	OHX	1	3683	7/7	0.96	0.33	6.05	118,118,118,118	0
84	OHX	1	3679	7/7	0.94	0.30	6.00	131,131,132,132	0
84	OHX	AR	3689	7/7	0.94	0.34	5.96	118,118,119,119	0
84	OHX	AR	3414	7/7	0.98	0.30	5.95	113,113,114,114	0
85	MG	x	208	1/1	0.88	0.33	5.92	46,46,46,46	0
84	OHX	1	3582	7/7	0.96	0.29	5.92	121,121,121,121	0
84	OHX	AR	3638	7/7	0.95	0.42	5.89	119,119,119,119	0
85	MG	AR	3841	1/1	0.84	0.29	5.85	54,54,54,54	0
87	GOL	A	2160	6/6	0.82	0.35	5.85	60,60,60,60	0
85	MG	1	4078	1/1	0.98	0.29	5.84	24,24,24,24	0
84	OHX	1	3406	7/7	0.99	0.33	5.80	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	s8	302	1/1	0.97	0.33	5.80	51,51,51,51	0
84	OHX	A	1985	7/7	0.89	0.31	5.79	140,140,141,141	0
84	OHX	AR	3699	7/7	0.96	0.36	5.78	117,117,117,117	0
85	MG	6	2122	1/1	0.86	0.48	5.76	61,61,61,61	0
84	OHX	1	3415	7/7	0.98	0.32	5.75	123,124,124,124	0
84	OHX	1	3462	7/7	0.94	0.21	5.74	119,120,120,120	0
84	OHX	6	2041	7/7	0.90	0.34	5.73	143,144,145,145	0
84	OHX	6	2030	7/7	0.92	0.29	5.73	118,118,118,119	0
85	MG	6	2103	1/1	0.88	0.33	5.72	69,69,69,69	0
84	OHX	1	3431	7/7	0.96	0.30	5.72	114,114,114,114	0
84	OHX	1	3662	7/7	0.95	0.31	5.71	116,116,116,116	0
85	MG	A	2056	1/1	0.91	0.34	5.66	65,65,65,65	0
84	OHX	AR	3613	7/7	0.96	0.29	5.65	112,112,112,112	0
84	OHX	6	2005	7/7	0.92	0.42	5.57	126,126,127,127	0
84	OHX	A	2006	7/7	0.92	0.31	5.57	149,150,150,150	0
84	OHX	A	2017	7/7	0.92	0.31	5.56	158,159,160,160	0
84	OHX	AR	3703	7/7	0.95	0.51	5.54	136,136,136,136	0
84	OHX	6	1910	7/7	0.98	0.26	5.48	119,120,120,120	0
85	MG	1	4127	1/1	0.80	0.26	5.47	45,45,45,45	0
84	OHX	1	3697	7/7	0.98	0.25	5.46	119,119,120,120	0
85	MG	CQ	202	1/1	0.94	0.33	5.45	32,32,32,32	0
84	OHX	AR	3404	7/7	0.99	0.33	5.44	112,112,112,112	0
84	OHX	AR	3688	7/7	0.95	0.29	5.39	136,136,137,137	0
84	OHX	A	1996	7/7	0.93	0.32	5.38	139,140,140,141	0
84	OHX	1	3420	7/7	0.98	0.29	5.38	118,118,118,118	0
84	OHX	AT	202	7/7	0.98	0.30	5.36	106,106,106,106	0
85	MG	4	227	1/1	0.91	0.40	5.35	52,52,52,52	0
84	OHX	1	3608	7/7	0.97	0.25	5.35	118,119,119,119	0
85	MG	v	302	1/1	0.97	0.33	5.34	36,36,36,36	0
84	OHX	AT	208	7/7	0.97	0.31	5.30	114,114,114,114	0
84	OHX	AS	211	7/7	0.91	0.29	5.30	141,141,142,142	0
85	MG	6	2125	1/1	0.93	0.32	5.27	75,75,75,75	0
84	OHX	A	1902	7/7	0.99	0.26	5.27	122,122,123,123	0
84	OHX	AR	3619	7/7	0.96	0.35	5.27	122,123,123,124	0
84	OHX	AR	3552	7/7	0.94	0.28	5.25	114,114,114,114	0
84	OHX	AR	3612	7/7	0.96	0.34	5.22	111,111,111,111	0
85	MG	1	4135	1/1	0.86	0.48	5.20	51,51,51,51	0
85	MG	AF	202	1/1	0.78	0.27	5.19	28,28,28,28	0
84	OHX	1	3620	7/7	0.89	0.35	5.18	118,118,118,118	0
85	MG	1	3809	1/1	0.95	0.27	5.17	39,39,39,39	0
84	OHX	A	2031	7/7	0.95	0.35	5.16	159,160,161,161	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	6	2028	7/7	0.94	0.40	5.16	123,124,124,124	0
84	OHX	AR	3661	7/7	0.97	0.46	5.14	112,112,112,113	0
85	MG	1	4066	1/1	0.94	0.27	5.14	20,20,20,20	0
84	OHX	1	3418	7/7	0.99	0.27	5.10	114,115,115,115	0
85	MG	CP	502	1/1	0.84	0.42	5.05	45,45,45,45	0
85	MG	6	2154	1/1	0.71	0.41	5.02	54,54,54,54	0
85	MG	1	3946	1/1	0.93	0.28	5.00	34,34,34,34	0
84	OHX	1	3643	7/7	0.92	0.39	4.99	114,114,114,114	0
84	OHX	1	3442	7/7	0.97	0.24	4.99	120,121,121,121	0
85	MG	1	3748	1/1	0.99	0.34	4.98	44,44,44,44	0
84	OHX	1	3626	7/7	0.90	0.36	4.98	124,124,124,124	0
85	MG	AR	3764	1/1	0.89	0.34	4.92	33,33,33,33	0
84	OHX	6	2050	7/7	0.92	0.47	4.91	159,159,160,160	0
84	OHX	1	3433	7/7	0.99	0.26	4.89	118,119,119,119	0
84	OHX	6	1906	7/7	0.99	0.29	4.87	122,123,123,124	0
85	MG	b	101	1/1	0.77	0.45	4.87	65,65,65,65	0
84	OHX	1	3506	7/7	0.97	0.29	4.85	109,109,110,110	0
84	OHX	A	2003	7/7	0.96	0.32	4.83	129,130,130,130	0
84	OHX	1	3419	7/7	0.99	0.26	4.82	107,107,107,107	0
85	MG	6	2093	1/1	0.96	0.33	4.80	47,47,47,47	0
86	HN8	AR	4263	22/22	0.95	0.26	4.76	27,27,27,27	22
85	MG	l	404	1/1	0.95	0.34	4.76	35,35,35,35	0
85	MG	AR	3987	1/1	0.97	0.30	4.75	31,31,31,31	0
84	OHX	AR	3524	7/7	0.94	0.29	4.75	118,119,119,119	0
85	MG	AR	4012	1/1	0.95	0.35	4.75	30,30,30,30	0
84	OHX	AR	3737	7/7	0.71	0.46	4.73	158,158,158,159	0
84	OHX	4	212	7/7	0.97	0.28	4.71	128,128,128,128	0
84	OHX	AR	3418	7/7	0.99	0.30	4.71	116,116,117,117	0
84	OHX	1	3650	7/7	0.94	0.27	4.70	128,128,128,128	0
85	MG	AR	4169	1/1	0.81	0.29	4.70	46,46,46,46	0
84	OHX	1	3609	7/7	0.93	0.40	4.68	119,120,120,120	0
85	MG	1	3884	1/1	0.91	0.34	4.66	29,29,29,29	0
85	MG	1	3738	1/1	0.94	0.35	4.64	28,28,28,28	0
84	OHX	A	2030	7/7	0.90	0.47	4.60	142,143,143,144	0
85	MG	AR	3934	1/1	0.91	0.31	4.59	32,32,32,32	0
85	MG	AR	3833	1/1	0.69	0.30	4.58	49,49,49,49	0
84	OHX	6	1986	7/7	0.93	0.32	4.57	147,148,148,148	0
84	OHX	AR	3426	7/7	0.99	0.27	4.57	111,112,112,112	0
85	MG	1	3778	1/1	0.87	0.46	4.56	49,49,49,49	0
84	OHX	6	1968	7/7	0.97	0.26	4.55	122,122,123,123	0
84	OHX	AR	3412	7/7	0.98	0.28	4.55	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4114	1/1	0.94	0.28	4.54	40,40,40,40	0
84	OHX	6	1992	7/7	0.93	0.23	4.52	137,137,138,138	0
84	OHX	AR	3698	7/7	0.94	0.41	4.51	123,123,123,124	0
85	MG	AR	3910	1/1	0.99	0.32	4.49	23,23,23,23	0
85	MG	A	2115	1/1	0.92	0.38	4.48	83,83,83,83	0
85	MG	CR	205	1/1	0.89	0.40	4.46	31,31,31,31	0
85	MG	AR	3895	1/1	0.96	0.28	4.43	43,43,43,43	0
85	MG	1	4207	1/1	0.95	0.28	4.43	36,36,36,36	0
84	OHX	AR	3695	7/7	0.91	0.30	4.41	122,122,123,123	0
84	OHX	AR	3576	7/7	0.97	0.31	4.41	128,128,129,129	0
84	OHX	6	2015	7/7	0.95	0.35	4.36	135,135,136,136	0
84	OHX	A	2009	7/7	0.96	0.38	4.34	126,126,127,127	0
84	OHX	6	2052	7/7	0.90	0.33	4.32	143,144,144,144	0
85	MG	1	4064	1/1	0.85	0.30	4.32	58,58,58,58	0
85	MG	CE	404	1/1	0.88	0.29	4.32	27,27,27,27	0
85	MG	AR	3964	1/1	0.79	0.29	4.32	35,35,35,35	0
84	OHX	AR	3520	7/7	0.97	0.31	4.27	112,112,113,113	0
84	OHX	1	3436	7/7	0.99	0.28	4.26	115,115,115,115	0
84	OHX	AR	3582	7/7	0.98	0.28	4.22	114,114,114,114	0
84	OHX	AR	3607	7/7	0.94	0.30	4.20	113,113,113,113	0
84	OHX	AR	3575	7/7	0.95	0.28	4.17	119,120,120,120	0
84	OHX	1	3432	7/7	0.98	0.27	4.17	117,117,117,117	0
84	OHX	AR	3709	7/7	0.92	0.28	4.08	110,111,111,111	0
84	OHX	AR	3712	7/7	0.94	0.27	4.07	109,109,109,109	0
84	OHX	A	1964	7/7	0.95	0.28	4.07	122,122,123,123	0
84	OHX	1	3690	7/7	0.92	0.41	4.05	122,123,123,123	0
84	OHX	AR	3646	7/7	0.90	0.37	4.03	108,108,108,108	0
85	MG	A	2129	1/1	0.87	0.30	4.02	57,57,57,57	0
84	OHX	AR	3421	7/7	0.99	0.25	4.02	113,113,113,113	0
85	MG	6	2144	1/1	0.89	0.38	4.02	74,74,74,74	0
84	OHX	AR	3643	7/7	0.97	0.30	4.02	120,121,121,121	0
84	OHX	AR	3663	7/7	0.93	0.29	3.97	147,148,148,148	0
84	OHX	AH	201	7/7	0.95	0.44	3.96	129,129,129,130	0
84	OHX	6	1989	7/7	0.93	0.43	3.96	143,144,144,145	0
84	OHX	1	3427	7/7	0.99	0.26	3.95	112,113,113,113	0
84	OHX	AR	3743	7/7	0.96	0.33	3.93	109,109,109,109	0
84	OHX	AR	3606	7/7	0.93	0.31	3.92	113,113,114,114	0
84	OHX	1	3676	7/7	0.91	0.29	3.92	149,150,150,150	0
84	OHX	6	1978	7/7	0.96	0.29	3.91	117,117,117,118	0
85	MG	CI	301	1/1	0.94	0.26	3.91	33,33,33,33	0
84	OHX	AR	3493	7/7	0.97	0.25	3.90	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	A	1918	7/7	0.93	0.23	3.90	128,129,129,129	0
84	OHX	AR	3596	7/7	0.93	0.24	3.85	121,121,122,122	0
84	OHX	6	1991	7/7	0.98	0.29	3.84	133,134,134,135	0
84	OHX	1	3413	7/7	0.99	0.32	3.81	112,113,113,113	0
84	OHX	1	3425	7/7	0.97	0.25	3.79	108,109,109,109	0
85	MG	1	3734	1/1	0.93	0.34	3.78	43,43,43,43	0
84	OHX	1	3577	7/7	0.96	0.31	3.77	118,118,119,119	0
87	GOL	AR	4261	6/6	0.78	0.34	3.75	48,48,48,48	0
85	MG	AR	3864	1/1	0.92	0.29	3.73	40,40,40,40	0
84	OHX	AR	3422	7/7	0.99	0.27	3.72	112,112,112,112	0
85	MG	6	2088	1/1	0.76	0.35	3.72	82,82,82,82	0
85	MG	AR	3939	1/1	0.96	0.31	3.71	31,31,31,31	0
85	MG	A	2100	1/1	0.92	0.44	3.71	92,92,92,92	0
85	MG	DH	203	1/1	0.95	0.29	3.70	31,31,31,31	0
84	OHX	AR	3588	7/7	0.96	0.27	3.69	112,112,112,113	0
84	OHX	1	3426	7/7	0.99	0.28	3.67	120,120,120,120	0
84	OHX	1	3721	7/7	0.89	0.35	3.67	127,127,127,128	0
84	OHX	6	1909	7/7	0.97	0.26	3.66	137,138,138,139	0
84	OHX	AR	3672	7/7	0.98	0.29	3.66	109,110,110,110	0
84	OHX	K	201	7/7	0.93	0.51	3.64	137,137,138,138	0
84	OHX	AR	3573	7/7	0.98	0.21	3.63	123,123,123,123	0
84	OHX	6	2029	7/7	0.96	0.41	3.63	152,153,153,154	0
84	OHX	A	1997	7/7	0.96	0.28	3.61	139,140,140,140	0
84	OHX	1	3445	7/7	0.96	0.26	3.61	111,112,112,112	0
84	OHX	1	3416	7/7	0.99	0.24	3.60	109,109,109,109	0
84	OHX	3	208	7/7	0.97	0.30	3.59	116,116,116,116	0
84	OHX	x	202	7/7	0.93	0.36	3.58	144,144,145,145	0
84	OHX	1	3649	7/7	0.95	0.35	3.57	113,113,113,113	0
84	OHX	1	3703	7/7	0.96	0.46	3.57	131,131,132,132	0
84	OHX	A	1905	7/7	0.99	0.29	3.56	128,129,129,129	0
85	MG	AR	3848	1/1	0.97	0.28	3.56	31,31,31,31	0
84	OHX	A	1947	7/7	0.96	0.27	3.53	129,129,130,130	0
84	OHX	1	3584	7/7	0.96	0.24	3.52	114,114,114,114	0
84	OHX	AC	101	7/7	0.98	0.30	3.51	114,115,115,115	0
84	OHX	1	3605	7/7	0.94	0.33	3.50	129,130,130,130	0
84	OHX	M	201	7/7	0.97	0.38	3.47	137,137,138,138	0
84	OHX	2	201	7/7	0.99	0.31	3.46	119,119,120,120	0
84	OHX	A	2040	7/7	0.93	0.37	3.46	162,162,162,162	0
84	OHX	AR	3424	7/7	0.99	0.27	3.46	112,112,113,113	0
84	OHX	CV	201	7/7	0.99	0.31	3.45	117,117,117,117	0
84	OHX	1	3653	7/7	0.90	0.29	3.42	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	c1	202	1/1	0.93	0.41	3.41	67,67,67,67	0
84	OHX	AR	3653	7/7	0.97	0.30	3.41	120,120,121,121	0
85	MG	6	2086	1/1	0.69	0.25	3.40	82,82,82,82	0
84	OHX	6	2043	7/7	0.93	0.30	3.40	145,145,146,146	0
84	OHX	AR	3420	7/7	0.99	0.29	3.39	113,114,114,114	0
84	OHX	1	3556	7/7	0.93	0.27	3.37	117,117,117,117	0
84	OHX	AR	3405	7/7	0.99	0.34	3.37	119,119,120,120	0
84	OHX	e	101	7/7	0.96	0.41	3.36	143,144,145,145	0
84	OHX	AR	3459	7/7	0.97	0.26	3.34	114,114,115,115	0
84	OHX	1	3414	7/7	0.99	0.27	3.34	109,109,109,109	0
85	MG	AR	4007	1/1	0.96	0.28	3.33	29,29,29,29	0
84	OHX	6	1993	7/7	0.94	0.28	3.32	134,135,135,135	0
84	OHX	1	3687	7/7	0.88	0.42	3.32	149,149,150,150	0
86	HN8	1	4223	22/22	0.95	0.24	3.25	32,32,32,32	0
85	MG	DC	202	1/1	0.86	0.30	3.25	48,48,48,48	0
84	OHX	1	3437	7/7	0.99	0.24	3.25	116,117,117,117	0
84	OHX	1	3551	7/7	0.97	0.27	3.23	118,118,119,119	0
84	OHX	1	3646	7/7	0.97	0.25	3.22	117,118,118,118	0
84	OHX	AR	3416	7/7	0.99	0.29	3.22	114,114,115,115	0
85	MG	AB	206	1/1	0.94	0.27	3.22	26,26,26,26	0
85	MG	AR	3825	1/1	0.94	0.27	3.21	33,33,33,33	0
85	MG	6	2116	1/1	0.93	0.21	3.20	62,62,62,62	0
85	MG	1	4083	1/1	0.94	0.29	3.17	41,41,41,41	0
84	OHX	1	3543	7/7	0.96	0.22	3.17	119,119,120,120	0
84	OHX	6	1907	7/7	0.97	0.32	3.15	135,136,136,137	0
84	OHX	1	3599	7/7	0.95	0.43	3.14	115,116,116,116	0
85	MG	d3	202	1/1	0.95	0.33	3.14	47,47,47,47	0
84	OHX	1	3422	7/7	0.99	0.26	3.12	116,116,117,117	0
84	OHX	AR	3721	7/7	0.92	0.38	3.12	139,139,140,140	0
84	OHX	AR	3722	7/7	0.88	0.31	3.12	140,141,141,141	0
84	OHX	6	2035	7/7	0.93	0.36	3.12	142,142,143,143	0
84	OHX	l	401	7/7	0.92	0.41	3.11	143,143,144,144	0
84	OHX	AR	3423	7/7	0.99	0.28	3.10	110,111,111,111	0
84	OHX	4	209	7/7	0.97	0.23	3.09	113,113,113,113	0
84	OHX	AR	3636	7/7	0.93	0.48	3.08	133,133,134,134	0
84	OHX	AR	3547	7/7	0.97	0.28	3.06	116,116,116,117	0
84	OHX	6	1994	7/7	0.96	0.25	3.04	170,170,170,170	0
85	MG	AR	3814	1/1	0.86	0.31	3.03	105,105,105,105	0
84	OHX	AR	3705	7/7	0.85	0.36	3.03	141,142,142,142	0
84	OHX	1	3623	7/7	0.96	0.22	3.01	114,114,115,115	0
84	OHX	1	3411	7/7	0.99	0.29	3.01	111,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3900	1/1	0.97	0.34	3.01	42,42,42,42	0
84	OHX	1	3638	7/7	0.97	0.33	3.00	122,123,123,123	0
84	OHX	AR	3427	7/7	0.95	0.29	2.99	110,110,111,111	0
84	OHX	1	3612	7/7	0.95	0.31	2.99	122,122,122,122	0
84	OHX	AR	3501	7/7	0.97	0.32	2.97	113,113,114,114	0
84	OHX	AR	3431	7/7	0.99	0.24	2.96	109,109,110,110	0
84	OHX	1	3629	7/7	0.94	0.22	2.94	148,148,148,149	0
84	OHX	1	3572	7/7	0.97	0.27	2.94	118,119,119,119	0
84	OHX	AR	3568	7/7	0.95	0.25	2.91	117,117,117,117	0
84	OHX	AR	3566	7/7	0.97	0.24	2.90	115,115,115,116	0
84	OHX	AR	3616	7/7	0.97	0.34	2.90	109,110,110,110	0
84	OHX	AR	3617	7/7	0.96	0.28	2.89	123,123,123,123	0
85	MG	1	3959	1/1	0.85	0.27	2.88	66,66,66,66	0
85	MG	AR	4179	1/1	0.97	0.27	2.85	43,43,43,43	0
84	OHX	1	3438	7/7	0.97	0.25	2.84	117,117,117,117	0
84	OHX	4	216	7/7	0.93	0.26	2.83	126,126,126,126	0
84	OHX	1	3507	7/7	0.96	0.23	2.82	113,113,114,114	0
85	MG	1	4052	1/1	0.96	0.29	2.81	21,21,21,21	0
84	OHX	6	1971	7/7	0.94	0.24	2.81	136,136,136,137	0
84	OHX	1	3428	7/7	0.99	0.28	2.80	126,126,127,127	0
84	OHX	1	3701	7/7	0.91	0.31	2.80	139,139,140,140	0
84	OHX	A	1940	7/7	0.97	0.29	2.80	137,138,138,139	0
84	OHX	AT	214	7/7	0.95	0.34	2.80	131,131,131,132	0
85	MG	1	3739	1/1	0.83	0.32	2.78	51,51,51,51	0
84	OHX	6	2032	7/7	0.93	0.50	2.76	131,131,132,132	0
84	OHX	6	2025	7/7	0.94	0.39	2.70	120,120,121,121	0
84	OHX	A	1979	7/7	0.97	0.22	2.70	142,143,144,144	0
85	MG	AR	3853	1/1	0.95	0.26	2.69	43,43,43,43	0
85	MG	A	2147	1/1	0.93	0.27	2.69	79,79,79,79	0
84	OHX	6	2027	7/7	0.95	0.47	2.68	146,147,147,148	0
84	OHX	A	1908	7/7	0.98	0.24	2.68	141,142,143,143	0
84	OHX	1	3423	7/7	0.99	0.26	2.67	120,120,121,121	0
85	MG	F	301	1/1	0.92	0.33	2.65	64,64,64,64	0
84	OHX	4	215	7/7	0.91	0.28	2.65	137,138,138,138	0
84	OHX	6	2044	7/7	0.96	0.35	2.65	140,141,141,141	0
85	MG	AR	4038	1/1	0.92	0.23	2.64	35,35,35,35	0
84	OHX	AR	3496	7/7	0.97	0.24	2.61	112,113,113,113	0
84	OHX	1	3417	7/7	0.98	0.31	2.59	116,117,117,117	0
84	OHX	1	3405	7/7	0.99	0.37	2.59	124,125,125,125	0
85	MG	AR	3794	1/1	0.82	0.25	2.59	34,34,34,34	0
84	OHX	1	3606	7/7	0.95	0.39	2.59	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
87	GOL	v	305	6/6	0.86	0.26	2.55	38,38,38,38	0
84	OHX	AR	3603	7/7	0.95	0.24	2.55	107,107,107,107	0
84	OHX	AR	3736	7/7	0.93	0.28	2.53	132,132,132,133	0
84	OHX	6	2013	7/7	0.93	0.33	2.53	121,122,122,122	0
84	OHX	AR	3439	7/7	0.98	0.25	2.52	119,120,120,120	0
85	MG	1	3916	1/1	0.96	0.29	2.51	26,26,26,26	0
85	MG	sM	202	1/1	0.94	0.55	2.49	42,42,42,42	0
84	OHX	AR	3543	7/7	0.96	0.24	2.49	123,123,123,123	0
85	MG	1	3798	1/1	0.98	0.23	2.47	32,32,32,32	0
84	OHX	AR	3667	7/7	0.94	0.38	2.47	146,147,147,147	0
85	MG	1	3917	1/1	0.91	0.26	2.46	30,30,30,30	0
84	OHX	AR	3671	7/7	0.96	0.28	2.46	113,113,113,113	0
85	MG	1	3741	1/1	0.95	0.25	2.45	37,37,37,37	0
84	OHX	1	3541	7/7	0.96	0.25	2.44	119,119,120,120	0
85	MG	A	2095	1/1	0.85	0.25	2.42	96,96,96,96	0
84	OHX	AR	3668	7/7	0.92	0.37	2.42	131,132,132,132	0
84	OHX	1	3675	7/7	0.94	0.30	2.41	140,141,141,141	0
85	MG	w	202	1/1	0.91	0.31	2.41	31,31,31,31	0
84	OHX	6	2051	7/7	0.89	0.29	2.39	172,172,172,173	0
85	MG	1	4100	1/1	0.91	0.27	2.38	53,53,53,53	0
84	OHX	y	201	7/7	0.94	0.32	2.36	128,129,129,129	0
84	OHX	AR	3599	7/7	0.92	0.24	2.35	136,136,136,136	0
84	OHX	AR	3432	7/7	0.97	0.27	2.34	117,117,117,118	0
85	MG	AR	3816	1/1	0.83	0.24	2.33	39,39,39,39	0
85	MG	AR	4203	1/1	0.94	0.24	2.32	29,29,29,29	0
84	OHX	1	3449	7/7	0.97	0.23	2.32	117,117,118,118	0
84	OHX	1	3404	7/7	0.98	0.35	2.29	120,120,121,121	0
85	MG	1	3924	1/1	0.95	0.37	2.29	60,60,60,60	0
84	OHX	1	3616	7/7	0.95	0.31	2.24	146,146,147,147	0
85	MG	c8	202	1/1	0.91	0.33	2.23	79,79,79,79	0
84	OHX	AR	3570	7/7	0.96	0.25	2.23	120,121,121,121	0
84	OHX	1	3636	7/7	0.93	0.33	2.22	126,126,126,126	0
85	MG	1	4167	1/1	0.94	0.23	2.20	23,23,23,23	0
84	OHX	AR	3425	7/7	0.98	0.23	2.20	105,106,106,106	0
84	OHX	A	2018	7/7	0.94	0.34	2.18	155,155,156,156	0
84	OHX	6	1904	7/7	0.99	0.27	2.12	124,124,124,125	0
84	OHX	AR	3455	7/7	0.97	0.22	2.10	111,112,112,112	0
85	MG	r	302	1/1	0.89	0.22	2.09	37,37,37,37	0
84	OHX	c4	201	7/7	0.89	0.53	2.06	152,152,153,153	0
84	OHX	AR	3561	7/7	0.97	0.24	2.04	110,110,110,111	0
84	OHX	1	3704	7/7	0.93	0.32	2.04	116,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3670	7/7	0.96	0.24	1.98	111,111,111,111	0
84	OHX	AR	3704	7/7	0.93	0.38	1.95	133,133,133,133	0
84	OHX	1	3563	7/7	0.93	0.24	1.95	114,114,115,115	0
85	MG	6	2129	1/1	0.91	0.39	1.94	62,62,62,62	0
85	MG	j	302	1/1	0.81	0.25	1.93	35,35,35,35	0
85	MG	1	3873	1/1	0.89	0.23	1.91	48,48,48,48	0
85	MG	AR	3858	1/1	0.98	0.32	1.91	36,36,36,36	0
85	MG	1	4034	1/1	0.98	0.25	1.91	42,42,42,42	0
84	OHX	6	2002	7/7	0.91	0.27	1.90	132,133,133,134	0
85	MG	6	2131	1/1	0.98	0.24	1.89	44,44,44,44	0
85	MG	AR	3956	1/1	0.90	0.22	1.88	29,29,29,29	0
84	OHX	6	2022	7/7	0.93	0.29	1.88	153,154,154,155	0
85	MG	1	3942	1/1	0.92	0.26	1.85	32,32,32,32	0
84	OHX	AR	3611	7/7	0.94	0.23	1.84	126,126,126,126	0
84	OHX	AR	3553	7/7	0.96	0.29	1.80	113,113,113,113	0
84	OHX	AT	215	7/7	0.94	0.20	1.80	137,138,138,138	0
84	OHX	AR	3583	7/7	0.95	0.22	1.78	113,114,114,114	0
85	MG	A	2084	1/1	0.77	0.22	1.78	72,72,72,72	0
85	MG	CM	203	1/1	0.95	0.21	1.77	55,55,55,55	0
84	OHX	A	1909	7/7	0.95	0.24	1.76	151,151,152,153	0
84	OHX	6	1985	7/7	0.96	0.33	1.75	130,130,131,131	0
84	OHX	AR	3621	7/7	0.96	0.35	1.74	135,135,136,136	0
85	MG	A	2149	1/1	0.89	0.25	1.74	60,60,60,60	0
84	OHX	A	1973	7/7	0.95	0.28	1.73	167,168,169,169	0
85	MG	6	2128	1/1	0.95	0.23	1.72	47,47,47,47	0
85	MG	1	3830	1/1	0.90	0.22	1.71	44,44,44,44	0
84	OHX	AR	3438	7/7	0.99	0.22	1.71	108,108,108,108	0
84	OHX	d9	101	7/7	0.92	0.48	1.66	153,153,154,154	0
84	OHX	1	3652	7/7	0.92	0.33	1.65	110,110,110,110	0
84	OHX	AR	3587	7/7	0.95	0.24	1.64	126,126,126,126	0
84	OHX	AR	3562	7/7	0.96	0.24	1.63	124,124,124,124	0
84	OHX	AR	3585	7/7	0.97	0.20	1.62	117,117,117,117	0
84	OHX	1	3630	7/7	0.98	0.33	1.62	113,113,114,114	0
84	OHX	1	3554	7/7	0.95	0.24	1.61	129,129,130,130	0
84	OHX	1	3613	7/7	0.97	0.47	1.59	120,120,121,121	0
84	OHX	1	3424	7/7	0.99	0.23	1.58	115,115,115,115	0
85	MG	1	4163	1/1	0.84	0.24	1.58	44,44,44,44	0
84	OHX	A	2024	7/7	0.95	0.24	1.58	151,152,153,153	0
84	OHX	1	3444	7/7	0.98	0.23	1.56	116,116,117,117	0
85	MG	6	2145	1/1	0.85	0.20	1.56	59,59,59,59	0
85	MG	AR	3752	1/1	0.83	0.21	1.53	37,37,37,37	0
84	OHX	6	1927	7/7	0.97	0.22	1.51	124,124,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3621	7/7	0.95	0.23	1.50	125,126,126,126	0
85	MG	1	4095	1/1	0.96	0.20	1.48	61,61,61,61	0
84	OHX	AR	3730	7/7	0.91	0.33	1.48	176,176,176,176	0
84	OHX	AR	3620	7/7	0.97	0.33	1.45	143,144,144,144	0
84	OHX	AR	3435	7/7	0.98	0.22	1.43	112,113,113,113	0
84	OHX	1	3585	7/7	0.97	0.23	1.43	115,115,116,116	0
84	OHX	c1	201	7/7	0.96	0.41	1.43	147,148,148,149	0
84	OHX	1	3681	7/7	0.95	0.32	1.41	127,127,127,128	0
85	MG	DI	202	1/1	0.79	0.36	1.38	56,56,56,56	0
84	OHX	6	2004	7/7	0.91	0.40	1.38	157,157,158,158	0
84	OHX	CE	402	7/7	0.93	0.38	1.37	138,139,139,139	0
84	OHX	6	2021	7/7	0.90	0.25	1.36	181,181,182,182	0
85	MG	AR	4212	1/1	0.95	0.27	1.31	31,31,31,31	0
84	OHX	1	3524	7/7	0.98	0.21	1.28	116,117,117,117	0
84	OHX	3	207	7/7	0.96	0.20	1.28	137,138,138,138	0
85	MG	AR	4069	1/1	0.89	0.23	1.27	26,26,26,26	0
84	OHX	AR	3701	7/7	0.93	0.29	1.27	128,128,128,128	0
85	MG	AR	4176	1/1	0.91	0.23	1.26	33,33,33,33	0
84	OHX	1	3451	7/7	0.96	0.22	1.25	111,111,111,111	0
84	OHX	CX	202	7/7	0.96	0.27	1.24	117,118,118,118	0
84	OHX	1	3523	7/7	0.98	0.19	1.24	119,119,120,120	0
84	OHX	1	3688	7/7	0.92	0.25	1.23	129,130,130,130	0
84	OHX	6	1932	7/7	0.93	0.23	1.22	132,132,133,133	0
84	OHX	AR	3659	7/7	0.94	0.54	1.22	136,136,137,137	0
84	OHX	1	3574	7/7	0.97	0.28	1.21	116,116,117,117	0
84	OHX	AR	3687	7/7	0.96	0.37	1.19	121,121,122,122	0
84	OHX	AR	3591	7/7	0.97	0.25	1.18	112,112,112,112	0
84	OHX	A	2029	7/7	0.90	0.20	1.16	184,184,184,184	0
84	OHX	AR	3442	7/7	0.97	0.22	1.15	112,112,112,112	0
84	OHX	1	3589	7/7	0.96	0.23	1.14	113,113,113,113	0
85	MG	AR	4175	1/1	0.88	0.25	1.13	35,35,35,35	0
84	OHX	A	2004	7/7	0.97	0.22	1.12	139,139,140,140	0
84	OHX	1	3568	7/7	0.97	0.28	1.11	115,116,116,116	0
85	MG	AB	207	1/1	0.84	0.24	1.11	34,34,34,34	0
84	OHX	AR	3436	7/7	0.98	0.24	1.09	109,109,109,109	0
84	OHX	AR	3428	7/7	0.99	0.21	1.05	115,115,115,116	0
85	MG	z	202	1/1	0.98	0.28	1.03	59,59,59,59	0
84	OHX	1	3519	7/7	0.96	0.22	1.03	116,116,116,116	0
84	OHX	1	3525	7/7	0.95	0.21	0.98	114,114,114,115	0
84	OHX	AR	3593	7/7	0.94	0.23	0.96	113,114,114,114	0
84	OHX	A	1986	7/7	0.95	0.28	0.95	168,169,170,170	0
84	OHX	AR	3515	7/7	0.98	0.22	0.94	113,113,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	6	2012	7/7	0.95	0.21	0.93	136,136,137,137	0
84	OHX	DD	101	7/7	0.98	0.29	0.93	113,114,114,114	0
84	OHX	AR	3441	7/7	0.96	0.18	0.93	116,117,117,117	0
84	OHX	1	3617	7/7	0.96	0.23	0.92	122,122,122,122	0
84	OHX	AS	210	7/7	0.92	0.24	0.92	115,115,116,116	0
84	OHX	AR	3536	7/7	0.96	0.22	0.92	123,124,124,124	0
84	OHX	6	2037	7/7	0.93	0.40	0.88	137,137,138,138	0
84	OHX	AR	3655	7/7	0.94	0.24	0.88	129,129,130,130	0
84	OHX	A	1983	7/7	0.96	0.24	0.84	142,142,143,143	0
84	OHX	AR	3618	7/7	0.95	0.21	0.82	113,113,114,114	0
84	OHX	A	1977	7/7	0.95	0.25	0.82	153,154,154,155	0
85	MG	1	3932	1/1	0.89	0.19	0.82	55,55,55,55	0
84	OHX	AR	3707	7/7	0.88	0.25	0.82	129,129,130,130	0
84	OHX	AR	3565	7/7	0.95	0.20	0.81	113,113,113,113	0
84	OHX	1	3458	7/7	0.96	0.20	0.81	116,116,116,117	0
85	MG	1	4114	1/1	0.97	0.23	0.80	52,52,52,52	0
84	OHX	CF	401	7/7	0.89	0.31	0.80	146,146,147,147	0
84	OHX	1	3467	7/7	0.98	0.17	0.78	123,123,124,124	0
84	OHX	AR	3440	7/7	0.99	0.18	0.77	125,125,125,126	0
84	OHX	1	3429	7/7	0.99	0.22	0.76	110,110,110,110	0
84	OHX	A	1999	7/7	0.96	0.24	0.74	146,146,147,147	0
84	OHX	A	1921	7/7	0.97	0.22	0.74	142,143,144,144	0
84	OHX	1	3537	7/7	0.95	0.24	0.73	115,115,115,116	0
84	OHX	6	1908	7/7	0.99	0.25	0.72	120,120,121,121	0
84	OHX	6	1981	7/7	0.98	0.29	0.72	139,140,140,140	0
84	OHX	AR	3662	7/7	0.96	0.22	0.71	111,111,112,112	0
84	OHX	AR	3545	7/7	0.96	0.24	0.71	108,108,108,108	0
84	OHX	6	1913	7/7	0.98	0.26	0.68	133,134,135,135	0
85	MG	6	2171	1/1	0.88	0.25	0.68	56,56,56,56	0
85	MG	AR	3769	1/1	0.93	0.26	0.68	59,59,59,59	0
85	MG	AR	4027	1/1	0.92	0.23	0.67	76,76,76,76	0
84	OHX	A	1976	7/7	0.96	0.18	0.67	123,124,124,124	0
84	OHX	A	1962	7/7	0.98	0.21	0.66	132,133,133,134	0
84	OHX	A	2002	7/7	0.95	0.31	0.66	147,148,149,149	0
84	OHX	1	3498	7/7	0.94	0.21	0.65	115,116,116,116	0
84	OHX	6	1962	7/7	0.94	0.30	0.64	136,137,137,137	0
84	OHX	6	1911	7/7	0.97	0.24	0.63	134,135,135,135	0
85	MG	1	4134	1/1	0.99	0.20	0.62	63,63,63,63	0
85	MG	AR	4048	1/1	0.97	0.23	0.62	34,34,34,34	0
84	OHX	AR	3528	7/7	0.94	0.21	0.61	108,108,108,108	0
84	OHX	1	3440	7/7	0.98	0.22	0.61	110,110,111,111	0
85	MG	6	2135	1/1	0.95	0.24	0.61	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3982	1/1	0.86	0.24	0.60	53,53,53,53	0
88	ZN	d7	101	1/1	0.79	0.47	0.60	143,143,143,143	0
85	MG	1	3805	1/1	0.85	0.20	0.58	29,29,29,29	0
85	MG	1	4164	1/1	0.99	0.22	0.57	58,58,58,58	0
84	OHX	1	3536	7/7	0.97	0.22	0.55	109,109,109,109	0
84	OHX	A	2043	7/7	0.90	0.19	0.55	155,156,156,157	0
84	OHX	AG	201	7/7	0.97	0.21	0.55	114,115,115,115	0
85	MG	1	4071	1/1	0.95	0.20	0.54	40,40,40,40	0
84	OHX	A	2028	7/7	0.94	0.34	0.54	157,157,158,158	0
88	ZN	c	101	1/1	0.93	0.34	0.54	145,145,145,145	0
85	MG	DA	201	1/1	0.87	0.28	0.53	48,48,48,48	0
84	OHX	6	1977	7/7	0.92	0.25	0.52	150,151,151,152	0
85	MG	A	2092	1/1	0.86	0.27	0.52	91,91,91,91	0
84	OHX	A	2038	7/7	0.91	0.34	0.51	146,147,147,147	0
84	OHX	1	3455	7/7	0.96	0.16	0.51	127,127,127,128	0
84	OHX	AR	3466	7/7	0.96	0.18	0.51	120,120,121,121	0
85	MG	AR	3946	1/1	0.90	0.30	0.50	59,59,59,59	0
84	OHX	AR	3742	7/7	0.93	0.25	0.50	128,129,129,129	0
84	OHX	1	3660	7/7	0.94	0.28	0.50	153,153,154,154	0
84	OHX	A	2016	7/7	0.96	0.28	0.49	142,143,143,144	0
85	MG	AB	204	1/1	0.90	0.29	0.49	52,52,52,52	0
85	MG	AR	3817	1/1	0.72	0.24	0.47	112,112,112,112	0
84	OHX	AR	3511	7/7	0.95	0.26	0.46	108,108,108,108	0
84	OHX	1	3489	7/7	0.96	0.21	0.45	113,113,114,114	0
84	OHX	A	1957	7/7	0.98	0.23	0.45	133,134,134,134	0
84	OHX	1	3499	7/7	0.98	0.23	0.43	111,111,111,111	0
84	OHX	1	3517	7/7	0.95	0.26	0.43	119,119,120,120	0
84	OHX	1	3469	7/7	0.95	0.21	0.42	117,117,118,118	0
85	MG	A	2086	1/1	0.91	0.24	0.42	66,66,66,66	0
84	OHX	A	2015	7/7	0.89	0.40	0.41	169,170,171,172	0
84	OHX	1	3587	7/7	0.98	0.23	0.41	133,133,133,134	0
84	OHX	1	3468	7/7	0.98	0.20	0.40	116,117,117,117	0
84	OHX	6	2034	7/7	0.96	0.19	0.40	155,155,155,155	0
84	OHX	k	401	7/7	0.96	0.27	0.39	118,118,118,118	0
84	OHX	AR	3623	7/7	0.96	0.29	0.38	138,139,139,139	0
85	MG	1	3789	1/1	0.91	0.17	0.36	42,42,42,42	0
84	OHX	AR	3555	7/7	0.96	0.21	0.35	115,115,115,115	0
85	MG	6	2087	1/1	0.86	0.30	0.33	56,56,56,56	0
84	OHX	AR	3531	7/7	0.94	0.19	0.32	115,115,115,115	0
85	MG	CP	505	1/1	0.96	0.28	0.32	71,71,71,71	0
84	OHX	6	1996	7/7	0.96	0.20	0.31	154,154,155,155	0
85	MG	AR	3775	1/1	0.97	0.23	0.30	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	A	1935	7/7	0.95	0.23	0.27	140,140,141,141	0
84	OHX	A	1904	7/7	0.99	0.23	0.27	133,134,134,134	0
85	MG	1	3811	1/1	0.78	0.30	0.27	44,44,44,44	0
84	OHX	A	1998	7/7	0.97	0.25	0.24	158,159,160,160	0
84	OHX	6	1916	7/7	0.98	0.21	0.23	119,120,120,120	0
84	OHX	AR	3437	7/7	0.98	0.23	0.23	108,108,108,108	0
84	OHX	1	3724	7/7	0.86	0.22	0.22	113,113,113,113	0
84	OHX	1	3581	7/7	0.95	0.22	0.22	112,113,113,113	0
85	MG	AS	222	1/1	0.98	0.21	0.20	44,44,44,44	0
85	MG	6	2184	1/1	0.98	0.22	0.19	83,83,83,83	0
84	OHX	A	2033	7/7	0.94	0.25	0.18	146,146,147,147	0
85	MG	1	3757	1/1	0.96	0.19	0.16	38,38,38,38	0
84	OHX	AR	3450	7/7	0.98	0.16	0.16	127,127,127,128	0
85	MG	1	3974	1/1	0.92	0.22	0.16	28,28,28,28	0
84	OHX	1	3607	7/7	0.97	0.17	0.16	122,122,122,122	0
84	OHX	1	3471	7/7	0.96	0.21	0.15	112,112,113,113	0
84	OHX	1	3492	7/7	0.97	0.19	0.14	117,118,118,118	0
84	OHX	6	1919	7/7	0.94	0.21	0.13	121,121,122,122	0
85	MG	A	2144	1/1	0.96	0.39	0.13	69,69,69,69	0
84	OHX	AR	3731	7/7	0.96	0.19	0.13	117,117,117,117	0
84	OHX	AT	213	7/7	0.91	0.25	0.12	137,137,137,137	0
84	OHX	AS	201	7/7	0.98	0.24	0.12	119,119,119,120	0
85	MG	6	2142	1/1	0.91	0.24	0.12	83,83,83,83	0
84	OHX	A	1910	7/7	0.97	0.23	0.10	138,139,139,140	0
84	OHX	1	3593	7/7	0.96	0.15	0.10	166,167,167,167	0
84	OHX	A	1958	7/7	0.95	0.22	0.10	173,173,173,173	0
84	OHX	3	206	7/7	0.94	0.20	0.08	127,127,128,128	0
84	OHX	AR	3460	7/7	0.95	0.20	0.05	112,112,112,112	0
85	MG	1	4103	1/1	0.96	0.27	0.05	60,60,60,60	0
84	OHX	CK	201	7/7	0.96	0.21	0.05	118,118,119,119	0
84	OHX	AR	3433	7/7	0.98	0.21	0.05	110,110,110,111	0
84	OHX	AR	3512	7/7	0.96	0.18	0.02	118,118,119,119	0
84	OHX	1	3578	7/7	0.97	0.19	-0.00	107,107,107,107	0
84	OHX	1	3583	7/7	0.95	0.16	0.00	131,132,132,132	0
85	MG	s4	301	1/1	0.90	0.23	-0.01	59,59,59,59	0
84	OHX	1	3485	7/7	0.93	0.16	-0.01	120,121,121,121	0
84	OHX	AR	3580	7/7	0.96	0.20	-0.03	117,118,118,118	0
85	MG	s6	301	1/1	0.87	0.29	-0.07	77,77,77,77	0
85	MG	6	2056	1/1	0.92	0.22	-0.07	77,77,77,77	0
84	OHX	A	1911	7/7	0.97	0.22	-0.07	139,140,141,141	0
85	MG	AR	4095	1/1	0.96	0.22	-0.07	25,25,25,25	0
84	OHX	AR	3557	7/7	0.96	0.16	-0.08	123,123,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	A	2054	1/1	0.75	0.23	-0.09	66,66,66,66	0
85	MG	3	219	1/1	0.96	0.20	-0.09	56,56,56,56	0
84	OHX	AR	3541	7/7	0.96	0.19	-0.10	125,125,125,125	0
84	OHX	1	3565	7/7	0.96	0.25	-0.12	131,131,131,131	0
84	OHX	6	1999	7/7	0.94	0.26	-0.12	138,139,139,140	0
84	OHX	A	1978	7/7	0.96	0.26	-0.12	143,144,144,145	0
84	OHX	6	1998	7/7	0.96	0.33	-0.14	146,146,147,147	0
84	OHX	1	3671	7/7	0.95	0.24	-0.15	149,150,150,150	0
85	MG	AR	3891	1/1	0.89	0.27	-0.16	69,69,69,69	0
85	MG	6	2063	1/1	0.97	0.20	-0.16	82,82,82,82	0
85	MG	o	302	1/1	0.92	0.21	-0.16	39,39,39,39	0
85	MG	CK	202	1/1	0.96	0.20	-0.17	44,44,44,44	0
84	OHX	AT	212	7/7	0.94	0.30	-0.17	128,128,128,128	0
84	OHX	6	1990	7/7	0.96	0.29	-0.17	129,130,130,130	0
84	OHX	AT	210	7/7	0.96	0.20	-0.19	119,119,120,120	0
84	OHX	6	2047	7/7	0.94	0.32	-0.21	161,162,162,162	0
84	OHX	A	1971	7/7	0.85	0.23	-0.22	149,150,151,151	0
84	OHX	A	1946	7/7	0.86	0.22	-0.24	165,166,166,167	0
84	OHX	1	3441	7/7	0.98	0.20	-0.25	116,116,116,117	0
84	OHX	1	3482	7/7	0.98	0.18	-0.26	117,117,117,117	0
84	OHX	AR	3563	7/7	0.94	0.17	-0.27	122,122,123,123	0
84	OHX	AR	3681	7/7	0.94	0.23	-0.29	140,140,140,141	0
84	OHX	AR	3723	7/7	0.93	0.29	-0.31	146,146,147,147	0
84	OHX	6	1925	7/7	0.97	0.20	-0.32	122,122,122,123	0
84	OHX	1	3481	7/7	0.95	0.19	-0.32	116,117,117,117	0
84	OHX	AR	3505	7/7	0.98	0.20	-0.32	114,114,115,115	0
84	OHX	6	1995	7/7	0.96	0.24	-0.34	133,134,134,135	0
88	ZN	DR	501	1/1	0.99	0.15	-0.34	59,59,59,59	0
84	OHX	A	1914	7/7	0.98	0.23	-0.35	126,127,127,127	0
84	OHX	AR	3484	7/7	0.97	0.19	-0.36	114,114,114,114	0
85	MG	CX	204	1/1	0.91	0.21	-0.37	46,46,46,46	0
84	OHX	6	1960	7/7	0.87	0.22	-0.38	118,118,118,118	0
85	MG	1	3807	1/1	0.80	0.18	-0.38	41,41,41,41	0
84	OHX	1	3579	7/7	0.96	0.17	-0.38	119,120,120,120	0
84	OHX	A	2042	7/7	0.90	0.21	-0.39	172,173,173,174	0
84	OHX	A	1913	7/7	0.97	0.20	-0.39	126,126,127,127	0
84	OHX	A	1963	7/7	0.94	0.18	-0.39	150,151,152,152	0
85	MG	AR	3953	1/1	0.97	0.19	-0.40	34,34,34,34	0
84	OHX	AR	3574	7/7	0.97	0.17	-0.42	112,113,113,113	0
84	OHX	6	1930	7/7	0.98	0.21	-0.42	121,121,122,122	0
84	OHX	AR	3458	7/7	0.97	0.19	-0.43	114,114,114,115	0
85	MG	6	2104	1/1	0.96	0.20	-0.43	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	AR	3448	7/7	0.98	0.17	-0.43	115,115,115,115	0
85	MG	o	301	1/1	0.93	0.19	-0.44	34,34,34,34	0
84	OHX	A	1942	7/7	0.98	0.19	-0.45	133,133,134,134	0
84	OHX	1	3558	7/7	0.97	0.17	-0.45	134,134,135,135	0
84	OHX	Q	201	7/7	0.94	0.26	-0.45	165,165,165,165	0
84	OHX	A	2001	7/7	0.96	0.20	-0.45	136,137,137,138	0
85	MG	1	3839	1/1	0.95	0.20	-0.47	27,27,27,27	0
84	OHX	3	204	7/7	0.97	0.15	-0.48	124,125,125,125	0
84	OHX	s8	301	7/7	0.91	0.32	-0.49	167,167,168,168	0
84	OHX	CL	301	7/7	0.95	0.21	-0.50	121,122,122,122	0
84	OHX	AR	3457	7/7	0.98	0.18	-0.50	108,108,108,109	0
84	OHX	1	3446	7/7	0.97	0.19	-0.52	116,116,116,116	0
84	OHX	AR	3514	7/7	0.96	0.19	-0.52	112,112,112,113	0
85	MG	A	2089	1/1	0.85	0.19	-0.52	90,90,90,90	0
84	OHX	1	3447	7/7	0.98	0.20	-0.52	113,113,113,113	0
84	OHX	1	3461	7/7	0.98	0.18	-0.53	110,110,111,111	0
85	MG	1	4016	1/1	0.93	0.18	-0.54	39,39,39,39	0
84	OHX	AR	3486	7/7	0.98	0.19	-0.55	111,111,111,111	0
84	OHX	A	1954	7/7	0.97	0.17	-0.55	135,136,136,136	0
84	OHX	1	3603	7/7	0.97	0.17	-0.55	123,123,124,124	0
84	OHX	6	2018	7/7	0.88	0.23	-0.57	189,189,189,189	0
84	OHX	6	1912	7/7	0.99	0.18	-0.58	122,122,123,123	0
84	OHX	A	1919	7/7	0.98	0.17	-0.59	121,122,122,122	0
84	OHX	AR	3738	7/7	0.90	0.15	-0.59	141,142,142,142	0
85	MG	CO	201	1/1	0.96	0.19	-0.59	44,44,44,44	0
84	OHX	sR	401	7/7	0.98	0.22	-0.60	161,161,162,162	0
84	OHX	AR	3477	7/7	0.98	0.20	-0.61	112,112,113,113	0
85	MG	1	3769	1/1	0.95	0.19	-0.62	45,45,45,45	0
85	MG	AR	3749	1/1	0.82	0.19	-0.62	42,42,42,42	0
84	OHX	A	1987	7/7	0.97	0.15	-0.62	128,128,129,129	0
84	OHX	CP	501	7/7	0.98	0.20	-0.63	126,126,126,127	0
84	OHX	CG	302	7/7	0.92	0.38	-0.64	147,147,147,148	0
84	OHX	6	1950	7/7	0.93	0.21	-0.67	135,135,136,136	0
84	OHX	6	1973	7/7	0.95	0.22	-0.67	137,138,138,138	0
84	OHX	AR	3462	7/7	0.99	0.16	-0.67	116,116,116,116	0
85	MG	AR	4158	1/1	0.93	0.20	-0.67	29,29,29,29	0
84	OHX	AR	3451	7/7	0.98	0.20	-0.67	114,114,114,114	0
85	MG	1	3897	1/1	0.88	0.21	-0.67	46,46,46,46	0
84	OHX	r	301	7/7	0.94	0.20	-0.68	115,115,115,115	0
84	OHX	CG	301	7/7	0.94	0.16	-0.69	142,143,143,144	0
85	MG	1	3918	1/1	0.97	0.19	-0.71	31,31,31,31	0
84	OHX	A	1952	7/7	0.98	0.20	-0.71	128,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3566	7/7	0.97	0.18	-0.71	113,113,114,114	0
84	OHX	AR	3692	7/7	0.90	0.32	-0.72	170,171,171,171	0
84	OHX	AR	3474	7/7	0.95	0.19	-0.72	114,114,114,115	0
84	OHX	1	3473	7/7	0.96	0.15	-0.73	114,115,115,115	0
84	OHX	6	2000	7/7	0.96	0.17	-0.75	130,130,131,131	0
84	OHX	AR	3508	7/7	0.98	0.21	-0.77	109,109,109,109	0
84	OHX	6	2008	7/7	0.91	0.18	-0.78	136,136,136,136	0
84	OHX	A	1992	7/7	0.97	0.21	-0.78	140,141,142,142	0
84	OHX	AS	207	7/7	0.98	0.16	-0.79	122,122,122,123	0
84	OHX	T	201	7/7	0.96	0.19	-0.79	145,146,146,147	0
84	OHX	AR	3473	7/7	0.97	0.11	-0.79	111,111,112,112	0
84	OHX	6	1982	7/7	0.96	0.17	-0.80	147,147,148,148	0
84	OHX	1	3491	7/7	0.98	0.18	-0.80	120,120,121,121	0
84	OHX	AR	3537	7/7	0.95	0.15	-0.81	131,132,132,132	0
84	OHX	1	3534	7/7	0.97	0.19	-0.81	113,113,113,113	0
84	OHX	6	1976	7/7	0.96	0.13	-0.82	146,147,147,148	0
84	OHX	1	3500	7/7	0.96	0.16	-0.84	119,120,120,120	0
85	MG	j	301	1/1	0.93	0.21	-0.84	29,29,29,29	0
84	OHX	v	301	7/7	0.97	0.20	-0.85	113,113,114,114	0
84	OHX	A	1945	7/7	0.97	0.18	-0.85	143,144,144,145	0
85	MG	AR	3768	1/1	0.94	0.18	-0.87	39,39,39,39	0
84	OHX	A	1916	7/7	0.98	0.18	-0.87	136,137,137,138	0
84	OHX	J	301	7/7	0.97	0.25	-0.88	157,157,158,158	0
84	OHX	1	3542	7/7	0.97	0.17	-0.88	119,119,120,120	0
84	OHX	1	3637	7/7	0.96	0.15	-0.88	140,140,140,141	0
84	OHX	A	1932	7/7	0.97	0.18	-0.88	141,142,142,143	0
84	OHX	1	3502	7/7	0.97	0.18	-0.88	114,114,114,114	0
84	OHX	1	3573	7/7	0.97	0.18	-0.88	131,131,132,132	0
84	OHX	6	1923	7/7	0.98	0.17	-0.89	121,121,122,122	0
84	OHX	6	2009	7/7	0.95	0.17	-0.90	126,127,127,128	0
84	OHX	1	3454	7/7	0.98	0.19	-0.90	111,111,111,111	0
84	OHX	A	1915	7/7	0.95	0.21	-0.92	142,143,143,144	0
88	ZN	d9	102	1/1	0.97	0.13	-0.93	83,83,83,83	0
84	OHX	AR	3605	7/7	0.95	0.16	-0.93	128,128,128,129	0
85	MG	CJ	301	1/1	0.82	0.22	-0.93	78,78,78,78	0
84	OHX	6	1914	7/7	0.99	0.20	-0.94	133,133,134,134	0
85	MG	1	4149	1/1	0.98	0.18	-0.94	54,54,54,54	0
84	OHX	6	1983	7/7	0.97	0.18	-0.96	128,129,129,129	0
84	OHX	6	1942	7/7	0.98	0.16	-0.96	135,135,136,136	0
85	MG	AR	3780	1/1	0.81	0.17	-0.96	88,88,88,88	0
85	MG	CR	203	1/1	0.86	0.15	-0.97	95,95,95,95	0
84	OHX	A	2019	7/7	0.92	0.29	-0.97	176,176,176,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3470	7/7	0.98	0.18	-0.97	115,115,115,115	0
84	OHX	6	2020	7/7	0.95	0.18	-0.97	135,136,136,137	0
85	MG	DI	201	1/1	0.89	0.22	-0.98	68,68,68,68	0
85	MG	AR	3762	1/1	0.97	0.17	-0.99	24,24,24,24	0
84	OHX	AR	3482	7/7	0.98	0.18	-0.99	111,112,112,112	0
88	ZN	AQ	501	1/1	1.00	0.13	-0.99	56,56,56,56	0
84	OHX	AK	102	7/7	0.95	0.18	-0.99	105,105,105,105	0
84	OHX	1	3588	7/7	0.95	0.19	-0.99	128,128,128,128	0
84	OHX	A	1907	7/7	0.99	0.19	-1.00	133,134,134,134	0
84	OHX	1	3501	7/7	0.90	0.17	-1.01	126,126,127,127	0
84	OHX	CE	401	7/7	0.98	0.17	-1.01	114,114,115,115	0
88	ZN	d6	103	1/1	1.00	0.13	-1.01	53,53,53,53	0
84	OHX	AR	3630	7/7	0.97	0.13	-1.02	124,125,125,125	0
84	OHX	6	1940	7/7	0.94	0.13	-1.02	149,150,151,151	0
84	OHX	AR	3494	7/7	0.97	0.15	-1.02	124,125,125,125	0
84	OHX	AT	203	7/7	0.97	0.14	-1.03	117,117,117,117	0
85	MG	AR	3955	1/1	0.66	0.17	-1.05	34,34,34,34	0
84	OHX	1	3516	7/7	0.98	0.12	-1.06	116,117,117,117	0
84	OHX	c5	201	7/7	0.92	0.19	-1.07	161,161,161,161	0
84	OHX	A	1920	7/7	0.99	0.14	-1.08	128,128,129,129	0
84	OHX	1	3634	7/7	0.95	0.17	-1.08	132,132,132,133	0
84	OHX	h	401	7/7	0.97	0.15	-1.08	175,176,177,177	0
84	OHX	1	3544	7/7	0.95	0.16	-1.08	116,117,117,117	0
84	OHX	AR	3478	7/7	0.97	0.17	-1.09	110,110,110,111	0
84	OHX	1	3576	7/7	0.97	0.14	-1.10	131,131,132,132	0
84	OHX	A	1912	7/7	0.98	0.19	-1.11	137,137,138,138	0
84	OHX	1	3430	7/7	0.98	0.19	-1.12	110,110,110,110	0
85	MG	AR	4178	1/1	0.92	0.19	-1.12	24,24,24,24	0
85	MG	1	3933	1/1	0.88	0.11	-1.14	49,49,49,49	0
84	OHX	AT	206	7/7	0.97	0.11	-1.15	123,124,124,124	0
84	OHX	CX	201	7/7	0.98	0.17	-1.15	116,116,116,116	0
85	MG	DA	202	1/1	0.92	0.20	-1.15	45,45,45,45	0
85	MG	AR	3760	1/1	0.81	0.14	-1.16	53,53,53,53	0
84	OHX	6	1922	7/7	0.98	0.18	-1.16	121,122,122,122	0
85	MG	CE	406	1/1	0.94	0.19	-1.20	25,25,25,25	0
84	OHX	A	1966	7/7	0.93	0.19	-1.21	131,131,132,132	0
84	OHX	AS	206	7/7	0.97	0.13	-1.21	124,124,125,125	0
84	OHX	AP	502	7/7	0.97	0.17	-1.22	112,113,113,113	0
84	OHX	AR	3602	7/7	0.89	0.18	-1.23	143,143,144,144	0
84	OHX	1	3450	7/7	0.99	0.17	-1.24	121,122,122,123	0
84	OHX	A	1972	7/7	0.98	0.22	-1.25	148,148,148,148	0
88	ZN	DO	201	1/1	0.99	0.15	-1.26	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	H	301	1/1	0.91	0.10	-1.26	83,83,83,83	0
84	OHX	1	3571	7/7	0.97	0.18	-1.27	111,111,112,112	0
84	OHX	6	1915	7/7	0.99	0.17	-1.27	119,119,120,120	0
84	OHX	AR	3470	7/7	0.98	0.17	-1.27	115,116,116,116	0
84	OHX	6	1963	7/7	0.98	0.15	-1.29	125,125,126,126	0
84	OHX	4	207	7/7	0.98	0.12	-1.29	118,119,119,119	0
84	OHX	A	1937	7/7	0.97	0.16	-1.29	153,154,155,155	0
84	OHX	1	3548	7/7	0.97	0.11	-1.31	134,134,134,134	0
84	OHX	AR	3465	7/7	0.98	0.17	-1.32	118,118,118,118	0
84	OHX	AR	3598	7/7	0.96	0.18	-1.32	117,118,118,118	0
84	OHX	1	3488	7/7	0.92	0.17	-1.33	109,109,109,110	0
84	OHX	1	3495	7/7	0.97	0.14	-1.35	114,115,115,115	0
84	OHX	6	1924	7/7	0.98	0.15	-1.36	134,135,135,135	0
85	MG	AR	3882	1/1	0.89	0.14	-1.36	47,47,47,47	0
84	OHX	AR	3487	7/7	0.98	0.13	-1.37	107,107,107,107	0
84	OHX	1	3479	7/7	0.98	0.17	-1.37	108,109,109,109	0
84	OHX	AR	3523	7/7	0.98	0.14	-1.38	107,108,108,108	0
84	OHX	AR	3469	7/7	0.97	0.14	-1.40	121,122,122,122	0
88	ZN	b	102	1/1	0.99	0.16	-1.44	71,71,71,71	0
84	OHX	AR	3533	7/7	0.97	0.18	-1.45	111,111,111,111	0
84	OHX	AR	3517	7/7	0.88	0.16	-1.47	145,146,146,146	0
84	OHX	A	1931	7/7	0.97	0.10	-1.48	139,140,140,140	0
84	OHX	AR	3551	7/7	0.96	0.14	-1.48	129,129,130,130	0
84	OHX	AR	3558	7/7	0.97	0.16	-1.48	137,137,137,137	0
84	OHX	A	2010	7/7	0.98	0.14	-1.49	157,158,158,159	0
84	OHX	AR	3584	7/7	0.97	0.13	-1.49	131,131,131,132	0
85	MG	AR	4135	1/1	0.89	0.18	-1.50	62,62,62,62	0
84	OHX	1	3527	7/7	0.96	0.12	-1.51	135,135,136,136	0
84	OHX	A	1917	7/7	0.97	0.17	-1.52	130,131,131,131	0
84	OHX	AR	3449	7/7	0.99	0.14	-1.54	116,117,117,117	0
85	MG	1	3777	1/1	0.89	0.17	-1.55	30,30,30,30	0
84	OHX	AR	3454	7/7	0.98	0.17	-1.56	112,112,113,113	0
84	OHX	4	204	7/7	0.97	0.15	-1.56	108,108,108,108	0
84	OHX	AR	3504	7/7	0.97	0.18	-1.57	110,110,110,110	0
84	OHX	1	3547	7/7	0.96	0.11	-1.57	120,121,121,121	0
84	OHX	6	1918	7/7	0.98	0.17	-1.59	116,117,117,117	0
85	MG	AR	4167	1/1	0.93	0.25	-1.61	71,71,71,71	0
84	OHX	1	3505	7/7	0.98	0.18	-1.62	116,116,117,117	0
84	OHX	6	1959	7/7	0.97	0.17	-1.64	137,138,138,139	0
85	MG	sM	201	1/1	0.93	0.12	-1.64	41,41,41,41	0
84	OHX	AS	203	7/7	0.98	0.16	-1.65	116,116,116,116	0
88	ZN	g	501	1/1	0.96	0.06	-1.65	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	A	1933	7/7	0.96	0.13	-1.67	122,122,122,123	0
88	ZN	AN	500	1/1	1.00	0.13	-1.68	38,38,38,38	0
84	OHX	AR	3492	7/7	0.97	0.15	-1.68	116,116,117,117	0
84	OHX	1	3590	7/7	0.98	0.12	-1.68	137,138,138,138	0
84	OHX	AR	3444	7/7	0.98	0.15	-1.70	112,112,112,112	0
84	OHX	AT	209	7/7	0.97	0.11	-1.70	121,121,122,122	0
84	OHX	AR	3577	7/7	0.95	0.09	-1.73	156,157,158,158	0
84	OHX	AR	3452	7/7	0.98	0.18	-1.74	121,121,122,122	0
84	OHX	6	1952	7/7	0.96	0.14	-1.75	148,148,148,148	0
84	OHX	1	3460	7/7	0.98	0.16	-1.76	118,118,118,119	0
84	OHX	AR	3696	7/7	0.97	0.18	-1.77	112,113,113,113	0
84	OHX	AR	3538	7/7	0.95	0.16	-1.79	123,123,124,124	0
84	OHX	6	1947	7/7	0.96	0.14	-1.79	121,122,122,122	0
84	OHX	1	3531	7/7	0.96	0.19	-1.80	114,114,114,114	0
84	OHX	DQ	201	7/7	0.98	0.15	-1.81	111,111,111,111	0
84	OHX	AR	3443	7/7	0.98	0.14	-1.83	116,116,117,117	0
84	OHX	4	205	7/7	0.97	0.17	-1.84	106,106,106,106	0
84	OHX	AR	3594	7/7	0.97	0.20	-1.85	114,114,115,115	0
85	MG	AH	202	1/1	0.90	0.15	-1.86	58,58,58,58	0
85	MG	1	4140	1/1	0.46	0.30	-1.88	187,187,187,187	0
84	OHX	6	1967	7/7	0.97	0.16	-1.88	126,127,127,127	0
84	OHX	AR	3581	7/7	0.96	0.18	-1.91	109,109,109,109	0
84	OHX	1	3529	7/7	0.97	0.17	-1.91	115,115,115,116	0
84	OHX	AR	3532	7/7	0.95	0.14	-1.92	135,136,136,137	0
84	OHX	AR	3527	7/7	0.93	0.20	-1.93	112,112,112,112	0
85	MG	1	4021	1/1	0.91	0.15	-1.94	44,44,44,44	0
84	OHX	6	1961	7/7	0.93	0.19	-1.94	128,129,129,130	0
85	MG	AR	4066	1/1	0.95	0.14	-1.96	56,56,56,56	0
84	OHX	A	2008	7/7	0.97	0.16	-1.97	132,132,133,133	0
84	OHX	AR	3530	7/7	0.96	0.17	-1.97	112,113,113,113	0
84	OHX	AR	3669	7/7	0.96	0.17	-1.98	175,176,176,176	0
88	ZN	AK	101	1/1	1.00	0.15	-2.00	34,34,34,34	0
84	OHX	AR	3429	7/7	0.99	0.19	-2.01	112,112,112,112	0
84	OHX	6	1964	7/7	0.97	0.12	-2.01	123,123,124,124	0
84	OHX	A	1967	7/7	0.98	0.12	-2.02	119,119,120,120	0
84	OHX	AR	3480	7/7	0.97	0.12	-2.02	113,114,114,114	0
84	OHX	1	3715	7/7	0.95	0.09	-2.03	166,166,167,167	0
84	OHX	AR	3499	7/7	0.95	0.15	-2.04	125,126,126,126	0
85	MG	T	202	1/1	0.86	0.09	-2.04	97,97,97,97	0
85	MG	1	4218	1/1	0.92	0.14	-2.04	32,32,32,32	0
84	OHX	6	1946	7/7	0.96	0.17	-2.05	127,128,128,129	0
84	OHX	A	1975	7/7	0.96	0.10	-2.06	156,158,158,158	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3522	7/7	0.98	0.13	-2.06	120,121,121,121	0
84	OHX	AR	3485	7/7	0.98	0.15	-2.08	114,114,115,115	0
84	OHX	AR	3472	7/7	0.95	0.16	-2.08	111,111,111,112	0
84	OHX	6	1988	7/7	0.96	0.14	-2.11	133,133,133,134	0
85	MG	1	3950	1/1	0.94	0.14	-2.12	38,38,38,38	0
84	OHX	6	1929	7/7	0.94	0.11	-2.13	157,158,159,159	0
84	OHX	A	1925	7/7	0.99	0.11	-2.13	136,137,137,137	0
88	ZN	e1	501	1/1	0.96	0.06	-2.13	153,153,153,153	0
85	MG	AR	3875	1/1	0.94	0.16	-2.14	45,45,45,45	0
84	OHX	1	3466	7/7	0.97	0.16	-2.14	114,115,115,115	0
85	MG	1	3977	1/1	0.95	0.14	-2.15	48,48,48,48	0
84	OHX	6	1953	7/7	0.97	0.12	-2.17	132,133,133,134	0
84	OHX	1	3530	7/7	0.98	0.13	-2.18	138,138,139,139	0
84	OHX	4	203	7/7	0.97	0.15	-2.19	106,107,107,107	0
84	OHX	AS	208	7/7	0.97	0.10	-2.20	138,139,139,139	0
84	OHX	1	3552	7/7	0.93	0.10	-2.20	150,150,151,151	0
84	OHX	6	1966	7/7	0.95	0.15	-2.22	133,133,134,134	0
88	ZN	e	102	1/1	0.99	0.09	-2.23	79,79,79,79	0
84	OHX	A	1950	7/7	0.98	0.13	-2.23	127,128,128,128	0
84	OHX	AR	3525	7/7	0.98	0.06	-2.23	119,119,120,120	0
84	OHX	6	1945	7/7	0.98	0.17	-2.24	126,127,127,128	0
84	OHX	1	3493	7/7	0.98	0.17	-2.26	115,116,116,116	0
84	OHX	6	1938	7/7	0.97	0.13	-2.30	130,131,131,131	0
85	MG	6	2137	1/1	0.93	0.12	-2.30	82,82,82,82	0
84	OHX	AR	3489	7/7	0.98	0.15	-2.32	114,114,114,114	0
84	OHX	A	1955	7/7	0.96	0.13	-2.37	145,146,147,147	0
84	OHX	AR	3483	7/7	0.97	0.17	-2.39	111,111,111,111	0
84	OHX	AR	3550	7/7	0.98	0.14	-2.40	107,107,107,107	0
88	ZN	DQ	202	1/1	0.99	0.03	-2.44	63,63,63,63	0
84	OHX	6	1939	7/7	0.97	0.10	-2.45	131,132,132,133	0
84	OHX	AR	3673	7/7	0.95	0.19	-2.45	125,125,125,125	0
84	OHX	6	1920	7/7	0.98	0.14	-2.46	133,133,134,134	0
84	OHX	1	3453	7/7	0.98	0.14	-2.47	120,120,120,120	0
84	OHX	1	3480	7/7	0.97	0.14	-2.49	119,119,119,120	0
84	OHX	6	1933	7/7	0.97	0.13	-2.50	116,116,117,117	0
84	OHX	AR	3589	7/7	0.98	0.13	-2.51	109,110,110,110	0
84	OHX	AR	3481	7/7	0.98	0.20	-2.52	106,106,107,107	0
85	MG	1	4166	1/1	0.94	0.16	-2.52	47,47,47,47	0
84	OHX	6	1958	7/7	0.98	0.15	-2.54	126,127,127,127	0
84	OHX	A	1974	7/7	0.94	0.14	-2.55	167,167,168,168	0
84	OHX	DH	201	7/7	0.98	0.13	-2.56	113,113,113,113	0
85	MG	AR	4192	1/1	0.92	0.19	-2.57	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	6	1917	7/7	0.99	0.16	-2.58	131,131,132,132	0
84	OHX	A	1965	7/7	0.97	0.16	-2.61	134,135,135,136	0
84	OHX	AR	3539	7/7	0.97	0.14	-2.62	127,128,128,128	0
84	OHX	1	3557	7/7	0.98	0.16	-2.65	117,118,118,118	0
84	OHX	AR	3500	7/7	0.98	0.11	-2.66	115,115,115,115	0
88	ZN	DL	101	1/1	0.99	0.20	-2.69	41,41,41,41	0
84	OHX	AR	3507	7/7	0.98	0.08	-2.70	123,123,123,123	0
84	OHX	6	1921	7/7	0.96	0.17	-2.72	141,141,142,143	0
84	OHX	6	1955	7/7	0.97	0.13	-2.75	179,179,179,179	0
85	MG	c9	201	1/1	0.82	0.10	-2.75	79,79,79,79	0
84	OHX	AT	207	7/7	0.97	0.15	-2.78	117,117,117,117	0
84	OHX	1	3546	7/7	0.97	0.17	-2.78	127,127,127,127	0
84	OHX	1	3459	7/7	0.98	0.19	-2.78	108,108,108,108	0
85	MG	6	2150	1/1	0.89	0.13	-2.81	77,77,77,77	0
84	OHX	1	3533	7/7	0.98	0.13	-2.82	149,149,150,150	0
84	OHX	A	1922	7/7	0.98	0.11	-2.84	123,124,124,124	0
84	OHX	AR	3497	7/7	0.98	0.09	-2.88	124,125,125,126	0
85	MG	6	2182	1/1	0.98	0.14	-2.88	83,83,83,83	0
84	OHX	AR	3554	7/7	0.97	0.15	-2.89	112,112,112,112	0
84	OHX	AR	3463	7/7	0.97	0.17	-2.91	110,110,111,111	0
84	OHX	6	1937	7/7	0.98	0.11	-2.92	119,120,120,120	0
84	OHX	AT	204	7/7	0.98	0.11	-2.92	105,105,105,106	0
84	OHX	AR	3464	7/7	0.98	0.17	-2.93	106,106,106,106	0
84	OHX	AR	3498	7/7	0.98	0.15	-2.98	123,123,123,124	0
85	MG	AR	3945	1/1	0.82	0.15	-3.02	40,40,40,40	0
84	OHX	6	1957	7/7	0.97	0.14	-3.02	129,130,130,131	0
84	OHX	AT	205	7/7	0.97	0.15	-3.03	108,108,108,108	0
85	MG	1	3815	1/1	0.97	0.15	-3.04	40,40,40,40	0
84	OHX	1	3510	7/7	0.96	0.16	-3.04	111,111,111,111	0
84	OHX	1	3484	7/7	0.98	0.10	-3.08	125,126,126,126	0
84	OHX	A	1944	7/7	0.96	0.12	-3.11	138,139,139,140	0
85	MG	DC	204	1/1	0.94	0.14	-3.11	35,35,35,35	0
84	OHX	A	1927	7/7	0.97	0.14	-3.14	138,138,139,139	0
84	OHX	6	1951	7/7	0.98	0.14	-3.18	134,134,135,135	0
84	OHX	1	3560	7/7	0.98	0.12	-3.22	111,112,112,112	0
84	OHX	1	3463	7/7	0.97	0.13	-3.24	121,121,122,122	0
84	OHX	1	3487	7/7	0.95	0.17	-3.24	115,115,116,116	0
85	MG	1	4029	1/1	0.89	0.11	-3.24	47,47,47,47	0
84	OHX	A	1923	7/7	0.98	0.13	-3.32	124,125,125,125	0
84	OHX	6	1954	7/7	0.95	0.09	-3.32	178,178,178,178	0
84	OHX	6	1934	7/7	0.97	0.13	-3.33	139,139,140,140	0
84	OHX	6	1956	7/7	0.95	0.12	-3.34	174,174,175,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	A	1961	7/7	0.98	0.11	-3.35	149,150,151,151	0
84	OHX	1	3464	7/7	0.99	0.20	-3.36	109,109,109,109	0
84	OHX	AR	3544	7/7	0.95	0.16	-3.42	109,109,110,110	0
84	OHX	6	1941	7/7	0.96	0.13	-3.47	120,120,121,121	0
85	MG	1	4047	1/1	0.98	0.12	-3.48	57,57,57,57	0
84	OHX	AR	3502	7/7	0.98	0.17	-3.65	113,114,114,114	0
84	OHX	1	3475	7/7	0.98	0.14	-3.67	117,117,118,118	0
84	OHX	1	3528	7/7	0.97	0.12	-3.72	119,120,120,120	0
84	OHX	6	1928	7/7	0.98	0.08	-3.74	126,126,127,127	0
84	OHX	AR	3491	7/7	0.97	0.13	-3.74	108,108,109,109	0
84	OHX	AR	3522	7/7	0.96	0.13	-3.80	114,114,115,115	0
84	OHX	A	1939	7/7	0.97	0.11	-3.82	140,141,141,142	0
84	OHX	AR	3609	7/7	0.98	0.16	-3.83	107,107,107,107	0
84	OHX	1	3555	7/7	0.98	0.17	-3.85	111,111,112,112	0
84	OHX	6	1926	7/7	0.98	0.12	-3.88	120,121,121,121	0
84	OHX	AR	3430	7/7	0.98	0.14	-3.92	107,107,107,107	0
84	OHX	A	1926	7/7	0.97	0.08	-3.93	127,127,127,128	0
84	OHX	6	1944	7/7	0.98	0.10	-3.95	143,143,144,144	0
84	OHX	1	3486	7/7	0.98	0.14	-3.96	116,117,117,117	0
84	OHX	1	3538	7/7	0.97	0.09	-4.07	125,125,125,126	0
88	ZN	AP	501	1/1	0.99	0.04	-4.17	61,61,61,61	0
84	OHX	AR	3560	7/7	0.97	0.19	-4.22	135,135,136,136	0
85	MG	1	3810	1/1	0.98	0.12	-4.24	32,32,32,32	0
84	OHX	1	3476	7/7	0.97	0.14	-4.26	111,111,111,112	0
84	OHX	1	3477	7/7	0.98	0.12	-4.34	109,109,109,109	0
84	OHX	1	3535	7/7	0.98	0.17	-4.37	111,111,111,112	0
84	OHX	AR	3476	7/7	0.98	0.17	-4.37	109,109,109,109	0
84	OHX	A	1948	7/7	0.97	0.13	-4.49	139,140,140,140	0
84	OHX	A	1949	7/7	0.98	0.08	-4.49	148,149,149,149	0
84	OHX	AR	3488	7/7	0.98	0.09	-4.52	118,118,119,119	0
84	OHX	6	1948	7/7	0.98	0.13	-4.53	127,128,128,128	0
84	OHX	AS	204	7/7	0.98	0.15	-4.68	113,113,113,113	0
84	OHX	1	3682	7/7	0.97	0.14	-4.69	110,110,111,111	0
85	MG	1	3921	1/1	0.93	0.12	-4.78	57,57,57,57	0
84	OHX	A	1924	7/7	0.99	0.09	-4.79	132,132,133,133	0
85	MG	1	3925	1/1	0.82	0.13	-4.84	46,46,46,46	0
84	OHX	3	202	7/7	0.97	0.12	-4.85	115,116,116,116	0
84	OHX	AR	3535	7/7	0.97	0.13	-4.87	114,115,115,115	0
84	OHX	1	3513	7/7	0.98	0.11	-4.88	113,113,114,114	0
84	OHX	AR	3479	7/7	0.97	0.15	-4.88	110,110,110,110	0
84	OHX	1	3497	7/7	0.96	0.11	-4.89	125,125,126,126	0
84	OHX	AR	3461	7/7	0.98	0.14	-4.90	110,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	A	1984	7/7	0.98	0.10	-4.97	130,130,131,131	0
84	OHX	A	1928	7/7	0.97	0.13	-5.00	125,126,126,126	0
84	OHX	1	3511	7/7	0.98	0.14	-5.02	109,109,109,109	0
84	OHX	1	3518	7/7	0.96	0.15	-5.06	109,110,110,110	0
84	OHX	1	3483	7/7	0.96	0.12	-5.08	113,113,113,113	0
84	OHX	AR	3490	7/7	0.98	0.12	-5.10	112,112,112,113	0
84	OHX	1	3618	7/7	0.93	0.19	-5.15	190,190,190,190	0
84	OHX	AR	3744	7/7	0.98	0.17	-5.18	109,110,110,110	0
84	OHX	1	3678	7/7	0.97	0.15	-5.31	117,117,118,118	0
84	OHX	AR	3471	7/7	0.98	0.13	-5.46	109,109,109,109	0
84	OHX	AR	3467	7/7	0.97	0.13	-5.48	108,109,109,109	0
84	OHX	6	2003	7/7	0.97	0.13	-5.64	126,126,127,127	0
84	OHX	AR	3519	7/7	0.97	0.15	-5.66	108,109,109,109	0
84	OHX	AR	3529	7/7	0.98	0.12	-5.70	108,109,109,109	0
84	OHX	A	1941	7/7	0.97	0.12	-5.74	136,137,137,137	0
84	OHX	1	3532	7/7	0.98	0.07	-5.88	159,159,159,159	0
84	OHX	AR	3495	7/7	0.95	0.17	-5.93	113,113,114,114	0
84	OHX	AR	3513	7/7	0.97	0.09	-6.19	150,151,151,151	0
84	OHX	3	203	7/7	0.97	0.11	-6.21	118,118,118,119	0
84	OHX	A	1956	7/7	0.97	0.14	-6.47	133,133,134,134	0
84	OHX	AS	205	7/7	0.98	0.11	-6.74	113,113,114,114	0
84	OHX	A	1938	7/7	0.98	0.14	-6.82	126,127,127,127	0
85	MG	1	3920	1/1	0.91	0.10	-8.18	41,41,41,41	0
84	OHX	1	3472	7/7	0.98	0.17	-8.24	110,111,111,111	0
84	OHX	AR	3509	7/7	0.99	0.10	-8.36	106,106,106,106	0
84	OHX	1	3515	7/7	0.98	0.10	-8.47	110,110,110,110	0
85	MG	AR	4089	1/1	0.83	0.10	-9.56	62,62,62,62	0
84	OHX	AR	3578	7/7	0.99	0.14	-10.49	109,109,110,110	0
85	MG	AR	4164	1/1	0.86	0.22	-	41,41,41,41	0
85	MG	6	2159	1/1	0.94	0.08	-	82,82,82,82	0
84	OHX	AR	3597	7/7	0.93	0.30	-	150,151,151,151	0
85	MG	1	3936	1/1	0.86	0.54	-	61,61,61,61	0
85	MG	1	3751	1/1	0.79	0.35	-	40,40,40,40	0
84	OHX	1	3714	7/7	0.86	0.51	-	146,147,147,148	0
85	MG	1	4105	1/1	0.96	0.49	-	26,26,26,26	0
85	MG	AR	3861	1/1	0.88	0.37	-	30,30,30,30	0
85	MG	A	2151	1/1	0.69	0.69	-	52,52,52,52	0
84	OHX	1	3663	7/7	0.94	0.19	-	111,111,111,111	0
84	OHX	6	1975	7/7	0.89	0.42	-	120,120,120,120	0
85	MG	6	2179	1/1	0.95	0.36	-	43,43,43,43	0
85	MG	A	2099	1/1	0.69	0.69	-	71,71,71,71	0
85	MG	A	2044	1/1	0.93	0.80	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3569	7/7	0.97	0.28	-	111,111,111,111	0
85	MG	AR	3951	1/1	0.96	0.53	-	29,29,29,29	0
85	MG	1	4011	1/1	0.91	0.37	-	44,44,44,44	0
85	MG	6	2133	1/1	0.70	0.66	-	61,61,61,61	0
85	MG	1	3954	1/1	0.81	0.15	-	46,46,46,46	0
85	MG	6	2194	1/1	0.62	0.15	-	108,108,108,108	0
85	MG	CF	403	1/1	0.87	0.40	-	34,34,34,34	0
85	MG	1	4036	1/1	0.89	0.42	-	70,70,70,70	0
87	GOL	6	2199	6/6	0.79	0.44	-	49,49,49,49	0
84	OHX	AR	3665	7/7	0.91	0.39	-	133,133,133,133	0
85	MG	1	4015	1/1	0.90	0.37	-	67,67,67,67	0
85	MG	6	2070	1/1	0.83	0.38	-	73,73,73,73	0
84	OHX	1	3478	7/7	0.99	0.14	-	125,125,125,126	0
85	MG	AR	4100	1/1	0.91	0.28	-	57,57,57,57	0
85	MG	AR	4185	1/1	0.93	0.37	-	38,38,38,38	0
85	MG	AB	201	1/1	0.91	0.28	-	34,34,34,34	0
85	MG	AR	3813	1/1	0.94	0.16	-	55,55,55,55	0
85	MG	1	3808	1/1	0.94	0.47	-	43,43,43,43	0
85	MG	AR	4124	1/1	0.86	0.18	-	39,39,39,39	0
85	MG	k	402	1/1	0.91	0.37	-	37,37,37,37	0
84	OHX	AR	3642	7/7	0.97	0.24	-	122,122,122,122	0
85	MG	AR	4190	1/1	0.98	0.19	-	30,30,30,30	0
85	MG	AR	4043	1/1	0.89	0.38	-	37,37,37,37	0
85	MG	A	2142	1/1	0.85	0.12	-	80,80,80,80	0
85	MG	AR	3995	1/1	0.75	0.34	-	65,65,65,65	0
85	MG	1	4041	1/1	0.93	0.16	-	45,45,45,45	0
85	MG	1	3781	1/1	0.96	0.39	-	33,33,33,33	0
85	MG	1	3784	1/1	0.97	0.46	-	26,26,26,26	0
85	MG	6	2089	1/1	0.95	0.44	-	44,44,44,44	0
85	MG	4	218	1/1	0.95	0.60	-	49,49,49,49	0
85	MG	6	2177	1/1	0.96	0.19	-	68,68,68,68	0
85	MG	AR	3829	1/1	0.86	0.66	-	66,66,66,66	0
85	MG	6	2139	1/1	0.90	0.22	-	45,45,45,45	0
85	MG	AR	3766	1/1	0.96	0.14	-	96,96,96,96	0
85	MG	1	3788	1/1	0.95	0.53	-	45,45,45,45	0
85	MG	1	3792	1/1	0.96	0.52	-	37,37,37,37	0
84	OHX	1	3545	7/7	0.95	0.21	-	120,120,120,120	0
84	OHX	1	3435	7/7	0.96	0.27	-	114,114,114,114	0
85	MG	AR	3822	1/1	0.95	0.32	-	46,46,46,46	0
85	MG	1	3934	1/1	0.88	0.44	-	54,54,54,54	0
85	MG	AR	4014	1/1	0.82	0.39	-	57,57,57,57	0
85	MG	1	4090	1/1	0.94	0.21	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3886	1/1	0.95	0.70	-	30,30,30,30	0
84	OHX	AR	3706	7/7	0.93	0.34	-	155,155,155,156	0
85	MG	1	4150	1/1	0.58	0.26	-	49,49,49,49	0
85	MG	1	4156	1/1	0.90	0.19	-	44,44,44,44	0
85	MG	6	2168	1/1	0.61	0.31	-	132,132,132,132	0
85	MG	1	4089	1/1	0.92	0.21	-	42,42,42,42	0
84	OHX	AR	3637	7/7	0.95	0.40	-	129,129,129,129	0
85	MG	AR	4070	1/1	0.90	0.19	-	50,50,50,50	0
84	OHX	AR	3548	7/7	0.96	0.16	-	121,121,122,122	0
85	MG	A	2065	1/1	0.90	0.73	-	57,57,57,57	0
85	MG	AR	3827	1/1	0.75	0.34	-	58,58,58,58	0
84	OHX	AR	3542	7/7	0.97	0.11	-	152,152,152,153	0
85	MG	4	234	1/1	0.83	0.43	-	44,44,44,44	0
84	OHX	1	3700	7/7	0.90	0.37	-	148,148,149,149	0
85	MG	AR	4086	1/1	0.84	0.40	-	42,42,42,42	0
85	MG	1	3893	1/1	0.98	0.26	-	26,26,26,26	0
85	MG	1	4221	1/1	0.96	0.52	-	35,35,35,35	0
84	OHX	1	3686	7/7	0.93	0.58	-	156,156,157,157	0
84	OHX	AR	3711	7/7	0.93	0.37	-	144,144,145,145	0
85	MG	A	2063	1/1	0.95	0.50	-	51,51,51,51	0
84	OHX	1	3456	7/7	0.98	0.16	-	111,111,111,111	0
85	MG	AR	4103	1/1	0.85	0.19	-	47,47,47,47	0
84	OHX	CM	201	7/7	0.94	0.34	-	150,150,151,151	0
85	MG	1	3767	1/1	0.87	0.12	-	60,60,60,60	0
85	MG	AR	3970	1/1	0.97	0.23	-	50,50,50,50	0
84	OHX	A	2034	7/7	0.83	0.20	-	231,232,232,232	0
85	MG	1	3971	1/1	0.87	0.46	-	35,35,35,35	0
85	MG	AR	4112	1/1	0.96	0.15	-	54,54,54,54	0
85	MG	A	2123	1/1	0.93	0.50	-	55,55,55,55	0
85	MG	AR	4025	1/1	0.85	0.25	-	31,31,31,31	0
85	MG	6	2138	1/1	0.83	0.30	-	73,73,73,73	0
85	MG	AR	4005	1/1	0.78	0.62	-	40,40,40,40	0
85	MG	AR	3770	1/1	0.91	0.44	-	32,32,32,32	0
85	MG	AR	4044	1/1	0.84	0.56	-	60,60,60,60	0
85	MG	6	2081	1/1	0.77	0.25	-	55,55,55,55	0
85	MG	1	3935	1/1	0.98	0.23	-	47,47,47,47	0
84	OHX	A	2037	7/7	0.92	0.44	-	153,154,154,155	0
85	MG	A	2127	1/1	0.83	0.29	-	83,83,83,83	0
84	OHX	A	1936	7/7	0.96	0.17	-	126,127,127,128	0
85	MG	AR	3948	1/1	0.90	0.54	-	40,40,40,40	0
85	MG	x	203	1/1	0.82	0.39	-	63,63,63,63	0
84	OHX	A	2011	7/7	0.92	0.23	-	149,149,150,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	A	2025	7/7	0.87	0.48	-	173,173,173,173	0
85	MG	1	4012	1/1	0.78	0.44	-	50,50,50,50	0
85	MG	A	2094	1/1	0.83	0.38	-	110,110,110,110	0
85	MG	6	2075	1/1	0.96	0.14	-	76,76,76,76	0
85	MG	6	2096	1/1	0.94	0.57	-	68,68,68,68	0
85	MG	AR	3973	1/1	0.83	0.23	-	40,40,40,40	0
85	MG	v	303	1/1	0.83	0.24	-	44,44,44,44	0
85	MG	A	2118	1/1	0.75	0.92	-	80,80,80,80	0
85	MG	AR	4218	1/1	0.93	0.27	-	54,54,54,54	0
85	MG	A	2157	1/1	0.92	0.79	-	75,75,75,75	0
85	MG	AR	4046	1/1	0.84	0.26	-	46,46,46,46	0
85	MG	6	2110	1/1	0.85	0.54	-	54,54,54,54	0
84	OHX	A	1995	7/7	0.95	0.17	-	151,152,152,152	0
84	OHX	1	3684	7/7	0.96	0.41	-	141,141,141,141	0
85	MG	A	2075	1/1	0.86	0.43	-	74,74,74,74	0
85	MG	6	2198	1/1	0.90	0.56	-	49,49,49,49	0
85	MG	AR	4106	1/1	0.98	0.07	-	46,46,46,46	0
85	MG	A	2113	1/1	0.90	0.48	-	73,73,73,73	0
85	MG	6	2064	1/1	0.83	0.68	-	53,53,53,53	0
85	MG	AR	4209	1/1	0.92	0.41	-	74,74,74,74	0
85	MG	1	3999	1/1	0.89	0.33	-	41,41,41,41	0
85	MG	AR	3797	1/1	0.97	0.27	-	31,31,31,31	0
85	MG	1	3844	1/1	0.98	0.41	-	28,28,28,28	0
85	MG	AR	4020	1/1	0.87	0.23	-	41,41,41,41	0
85	MG	AR	3849	1/1	0.97	0.45	-	35,35,35,35	0
85	MG	AT	227	1/1	0.86	0.88	-	79,79,79,79	0
85	MG	A	2085	1/1	0.70	0.40	-	63,63,63,63	0
85	MG	3	212	1/1	0.88	0.44	-	62,62,62,62	0
85	MG	CR	204	1/1	0.86	0.21	-	46,46,46,46	0
85	MG	1	3949	1/1	0.92	0.47	-	44,44,44,44	0
85	MG	AR	4159	1/1	0.86	0.38	-	36,36,36,36	0
85	MG	AR	4115	1/1	0.97	0.33	-	46,46,46,46	0
84	OHX	AR	3639	7/7	0.91	0.22	-	138,139,139,139	0
84	OHX	1	3526	7/7	0.96	0.29	-	114,115,115,115	0
85	MG	AR	3823	1/1	0.92	0.51	-	39,39,39,39	0
85	MG	1	4023	1/1	0.79	0.48	-	57,57,57,57	0
85	MG	6	2163	1/1	0.77	0.42	-	48,48,48,48	0
84	OHX	1	3452	7/7	0.98	0.16	-	109,109,109,109	0
85	MG	AR	4253	1/1	0.84	0.17	-	41,41,41,41	0
85	MG	A	2114	1/1	0.81	0.39	-	76,76,76,76	0
84	OHX	AR	3628	7/7	0.96	0.32	-	147,148,148,148	0
85	MG	1	4025	1/1	0.94	0.48	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	A	1969	7/7	0.95	0.34	-	144,144,145,145	0
85	MG	1	3854	1/1	0.96	0.62	-	34,34,34,34	0
85	MG	1	4123	1/1	0.94	0.22	-	51,51,51,51	0
85	MG	AR	4081	1/1	0.98	0.24	-	55,55,55,55	0
85	MG	CG	304	1/1	0.81	0.25	-	56,56,56,56	0
84	OHX	A	1959	7/7	0.94	0.20	-	137,138,139,139	0
85	MG	1	4118	1/1	0.83	0.34	-	43,43,43,43	0
85	MG	1	3771	1/1	0.90	0.42	-	33,33,33,33	0
84	OHX	1	3494	7/7	0.97	0.13	-	119,119,120,120	0
85	MG	AR	3989	1/1	0.95	0.23	-	44,44,44,44	0
85	MG	A	2141	1/1	0.99	0.31	-	101,101,101,101	0
84	OHX	1	3651	7/7	0.92	0.26	-	130,130,131,131	0
85	MG	AS	213	1/1	0.90	0.45	-	26,26,26,26	0
85	MG	A	2087	1/1	0.88	0.49	-	78,78,78,78	0
85	MG	A	2104	1/1	0.93	0.15	-	137,137,137,137	0
85	MG	1	4119	1/1	0.82	0.28	-	35,35,35,35	0
85	MG	1	4180	1/1	0.98	0.35	-	45,45,45,45	0
85	MG	A	2097	1/1	0.94	0.57	-	53,53,53,53	0
85	MG	A	2106	1/1	0.90	0.49	-	58,58,58,58	0
85	MG	1	4202	1/1	0.84	0.56	-	19,19,19,19	0
85	MG	6	2193	1/1	0.79	0.45	-	55,55,55,55	0
85	MG	1	3992	1/1	0.91	0.24	-	40,40,40,40	0
85	MG	A	2048	1/1	0.83	0.33	-	52,52,52,52	0
84	OHX	AR	3503	7/7	0.95	0.17	-	120,120,121,121	0
85	MG	AB	205	1/1	0.91	0.22	-	40,40,40,40	0
85	MG	1	3820	1/1	0.68	0.60	-	65,65,65,65	0
85	MG	1	4191	1/1	0.97	0.44	-	29,29,29,29	0
85	MG	3	217	1/1	0.91	0.36	-	40,40,40,40	0
85	MG	AR	3838	1/1	0.88	0.37	-	27,27,27,27	0
85	MG	4	238	1/1	0.79	0.26	-	35,35,35,35	0
84	OHX	AR	3702	7/7	0.94	0.40	-	139,139,140,140	0
85	MG	AR	3996	1/1	0.92	0.33	-	56,56,56,56	0
84	OHX	A	1989	7/7	0.96	0.36	-	154,155,155,155	0
85	MG	AR	3781	1/1	0.98	0.25	-	23,23,23,23	0
85	MG	1	3872	1/1	0.95	0.59	-	32,32,32,32	0
85	MG	DH	202	1/1	0.96	0.26	-	40,40,40,40	0
84	OHX	1	3716	7/7	0.91	0.45	-	138,138,139,139	0
85	MG	6	2065	1/1	0.93	0.58	-	40,40,40,40	0
84	OHX	1	3540	7/7	0.94	0.18	-	111,111,111,111	0
85	MG	AR	4110	1/1	0.80	0.50	-	46,46,46,46	0
84	OHX	6	1970	7/7	0.98	0.26	-	126,126,127,127	0
85	MG	A	2103	1/1	0.69	0.55	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AT	228	1/1	0.82	0.37	-	47,47,47,47	0
85	MG	1	4094	1/1	0.96	0.15	-	78,78,78,78	0
85	MG	AR	4130	1/1	0.88	0.15	-	31,31,31,31	0
85	MG	AR	4036	1/1	0.94	0.27	-	41,41,41,41	0
85	MG	AR	3921	1/1	0.77	0.31	-	38,38,38,38	0
85	MG	1	3787	1/1	0.88	0.46	-	46,46,46,46	0
85	MG	AR	4132	1/1	0.97	0.15	-	49,49,49,49	0
84	OHX	1	3696	7/7	0.90	0.39	-	146,146,147,147	0
85	MG	AR	4162	1/1	0.94	0.60	-	56,56,56,56	0
85	MG	AR	4207	1/1	0.87	0.50	-	48,48,48,48	0
85	MG	AR	4125	1/1	0.64	0.28	-	82,82,82,82	0
85	MG	1	4216	1/1	0.96	0.39	-	23,23,23,23	0
84	OHX	AR	3447	7/7	0.97	0.25	-	112,112,112,112	0
84	OHX	AR	3569	7/7	0.97	0.29	-	137,137,137,138	0
84	OHX	AR	3633	7/7	0.96	0.28	-	124,125,125,125	0
85	MG	AR	3962	1/1	0.93	0.19	-	93,93,93,93	0
85	MG	1	3994	1/1	0.79	0.27	-	47,47,47,47	0
85	MG	AR	4033	1/1	0.90	0.26	-	40,40,40,40	0
84	OHX	A	1988	7/7	0.97	0.23	-	139,140,141,141	0
84	OHX	AR	3675	7/7	0.93	0.33	-	138,139,139,139	0
85	MG	1	4179	1/1	0.95	0.23	-	38,38,38,38	0
85	MG	AR	4177	1/1	0.91	0.30	-	32,32,32,32	0
85	MG	1	3896	1/1	0.93	0.30	-	36,36,36,36	0
85	MG	1	4006	1/1	0.84	0.58	-	47,47,47,47	0
85	MG	A	2091	1/1	0.80	0.43	-	71,71,71,71	0
84	OHX	6	2040	7/7	0.87	0.29	-	184,184,185,185	0
85	MG	1	4130	1/1	0.89	0.27	-	45,45,45,45	0
85	MG	AR	3968	1/1	0.78	0.32	-	30,30,30,30	0
85	MG	AR	4181	1/1	0.72	0.24	-	50,50,50,50	0
85	MG	1	4141	1/1	0.95	0.38	-	64,64,64,64	0
85	MG	1	3785	1/1	0.88	0.45	-	25,25,25,25	0
85	MG	6	2157	1/1	0.78	0.28	-	56,56,56,56	0
85	MG	6	2109	1/1	0.91	0.42	-	56,56,56,56	0
85	MG	1	3780	1/1	0.97	0.33	-	17,17,17,17	0
85	MG	d4	201	1/1	0.87	0.38	-	53,53,53,53	0
85	MG	A	2102	1/1	0.90	0.49	-	58,58,58,58	0
85	MG	V	201	1/1	0.77	0.50	-	70,70,70,70	0
84	OHX	1	3710	7/7	0.90	0.33	-	136,137,137,137	0
85	MG	6	2196	1/1	0.91	0.76	-	48,48,48,48	0
85	MG	1	3938	1/1	0.92	0.21	-	34,34,34,34	0
84	OHX	AS	209	7/7	0.93	0.31	-	140,140,140,140	0
85	MG	1	3888	1/1	0.98	0.40	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	6	1905	7/7	0.97	0.34	-	132,133,133,134	0
85	MG	1	4185	1/1	0.97	0.50	-	27,27,27,27	0
85	MG	AR	4153	1/1	0.89	0.19	-	88,88,88,88	0
84	OHX	1	3632	7/7	0.94	0.34	-	156,156,156,156	0
85	MG	6	2060	1/1	0.92	0.34	-	47,47,47,47	0
85	MG	6	2118	1/1	0.84	0.15	-	93,93,93,93	0
85	MG	AR	3965	1/1	0.93	0.25	-	50,50,50,50	0
85	MG	AR	4235	1/1	0.97	0.37	-	26,26,26,26	0
84	OHX	1	3713	7/7	0.93	0.26	-	138,138,138,139	0
85	MG	3	221	1/1	0.89	0.46	-	34,34,34,34	0
84	OHX	1	3549	7/7	0.97	0.15	-	120,120,120,120	0
85	MG	6	2170	1/1	0.98	0.17	-	64,64,64,64	0
85	MG	1	3804	1/1	0.93	0.50	-	35,35,35,35	0
85	MG	6	2188	1/1	0.76	0.54	-	66,66,66,66	0
84	OHX	AR	3720	7/7	0.89	0.33	-	152,152,152,152	0
85	MG	t	202	1/1	0.68	0.26	-	101,101,101,101	0
85	MG	AR	3999	1/1	0.88	0.30	-	44,44,44,44	0
85	MG	A	2143	1/1	0.92	0.38	-	106,106,106,106	0
85	MG	1	4058	1/1	0.92	0.31	-	51,51,51,51	0
85	MG	A	2120	1/1	0.95	0.22	-	85,85,85,85	0
84	OHX	6	1943	7/7	0.97	0.09	-	124,124,125,125	0
85	MG	A	2076	1/1	0.93	0.35	-	51,51,51,51	0
85	MG	AR	3796	1/1	0.91	0.41	-	64,64,64,64	0
85	MG	1	4060	1/1	0.82	0.36	-	44,44,44,44	0
85	MG	1	4077	1/1	0.85	0.27	-	33,33,33,33	0
84	OHX	AR	3627	7/7	0.96	0.32	-	127,128,128,128	0
85	MG	6	2187	1/1	0.96	0.18	-	82,82,82,82	0
84	OHX	AR	3664	7/7	0.83	0.43	-	180,180,181,181	0
84	OHX	1	3615	7/7	0.94	0.37	-	133,133,133,134	0
85	MG	1	4139	1/1	0.94	0.28	-	31,31,31,31	0
85	MG	AR	4061	1/1	0.92	0.53	-	50,50,50,50	0
85	MG	1	4201	1/1	0.94	0.49	-	28,28,28,28	0
85	MG	AR	4042	1/1	0.90	0.12	-	57,57,57,57	0
85	MG	6	2105	1/1	0.86	0.48	-	64,64,64,64	0
85	MG	1	3842	1/1	0.96	0.55	-	25,25,25,25	0
85	MG	6	2183	1/1	0.79	0.58	-	71,71,71,71	0
85	MG	CR	202	1/1	0.84	0.28	-	29,29,29,29	0
84	OHX	AR	3631	7/7	0.90	0.18	-	175,176,177,177	0
85	MG	AR	4154	1/1	0.89	0.31	-	39,39,39,39	0
85	MG	6	2101	1/1	0.96	0.51	-	53,53,53,53	0
84	OHX	1	3614	7/7	0.93	0.27	-	133,133,133,134	0
85	MG	k	403	1/1	0.94	0.20	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3828	1/1	0.96	0.61	-	60,60,60,60	0
84	OHX	6	2014	7/7	0.95	0.34	-	129,129,129,130	0
85	MG	1	3744	1/1	0.77	0.42	-	83,83,83,83	0
85	MG	AR	4107	1/1	0.94	0.13	-	78,78,78,78	0
85	MG	AR	3969	1/1	0.94	0.13	-	60,60,60,60	0
85	MG	3	222	1/1	0.93	0.38	-	52,52,52,52	0
85	MG	AR	3975	1/1	0.83	0.27	-	31,31,31,31	0
85	MG	1	4110	1/1	0.88	0.24	-	30,30,30,30	0
85	MG	1	3776	1/1	0.96	0.49	-	43,43,43,43	0
85	MG	1	4155	1/1	0.77	0.23	-	53,53,53,53	0
85	MG	AS	224	1/1	0.88	0.24	-	55,55,55,55	0
85	MG	1	4172	1/1	0.96	0.40	-	67,67,67,67	0
85	MG	1	4214	1/1	0.92	0.39	-	43,43,43,43	0
85	MG	1	4128	1/1	0.87	0.45	-	51,51,51,51	0
85	MG	AR	4133	1/1	0.96	0.27	-	25,25,25,25	0
85	MG	1	3735	1/1	0.94	0.35	-	24,24,24,24	0
85	MG	1	4175	1/1	0.96	0.45	-	39,39,39,39	0
85	MG	6	2124	1/1	0.73	0.28	-	66,66,66,66	0
85	MG	6	2085	1/1	0.90	0.47	-	75,75,75,75	0
84	OHX	1	3658	7/7	0.97	0.34	-	142,143,143,143	0
85	MG	4	231	1/1	0.90	0.23	-	58,58,58,58	0
85	MG	1	4112	1/1	0.97	0.43	-	32,32,32,32	0
85	MG	1	3947	1/1	0.92	0.21	-	26,26,26,26	0
85	MG	AR	4128	1/1	0.81	0.21	-	55,55,55,55	0
85	MG	1	3733	1/1	0.95	0.49	-	26,26,26,26	0
85	MG	AR	3947	1/1	0.87	0.50	-	44,44,44,44	0
85	MG	1	3985	1/1	0.82	0.60	-	50,50,50,50	0
85	MG	1	4033	1/1	0.88	0.21	-	58,58,58,58	0
84	OHX	A	1960	7/7	0.95	0.18	-	151,151,151,152	0
85	MG	1	4092	1/1	0.78	0.64	-	54,54,54,54	0
85	MG	AR	3890	1/1	0.60	0.42	-	29,29,29,29	0
84	OHX	AR	3656	7/7	0.97	0.31	-	134,134,134,134	0
84	OHX	AR	3635	7/7	0.93	0.22	-	137,138,138,138	0
85	MG	1	4049	1/1	0.94	0.25	-	32,32,32,32	0
85	MG	AR	3795	1/1	0.96	0.66	-	49,49,49,49	0
85	MG	1	4121	1/1	0.98	0.10	-	64,64,64,64	0
85	MG	1	4190	1/1	0.73	0.56	-	25,25,25,25	0
85	MG	AR	3856	1/1	0.95	0.71	-	27,27,27,27	0
85	MG	1	3919	1/1	0.95	0.27	-	33,33,33,33	0
84	OHX	1	3567	7/7	0.95	0.24	-	128,129,129,129	0
85	MG	AR	4233	1/1	0.92	0.33	-	31,31,31,31	0
85	MG	AR	3881	1/1	0.95	0.29	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	DE	201	1/1	0.81	0.28	-	72,72,72,72	0
85	MG	AR	4210	1/1	0.88	0.71	-	54,54,54,54	0
85	MG	AR	4186	1/1	0.89	0.21	-	33,33,33,33	0
85	MG	1	4020	1/1	0.90	0.38	-	34,34,34,34	0
84	OHX	AR	3719	7/7	0.84	0.42	-	133,133,133,133	0
85	MG	AR	3907	1/1	0.88	0.63	-	25,25,25,25	0
85	MG	1	4081	1/1	0.74	0.39	-	29,29,29,29	0
85	MG	1	4183	1/1	0.86	0.17	-	44,44,44,44	0
85	MG	AG	202	1/1	0.91	0.20	-	43,43,43,43	0
85	MG	AR	4234	1/1	0.84	0.45	-	32,32,32,32	0
85	MG	1	3755	1/1	0.92	0.42	-	36,36,36,36	0
85	MG	6	2175	1/1	0.99	0.10	-	118,118,118,118	0
85	MG	AR	3812	1/1	0.83	0.42	-	32,32,32,32	0
84	OHX	AR	3718	7/7	0.91	0.46	-	166,167,167,167	0
85	MG	AS	229	1/1	0.96	0.24	-	46,46,46,46	0
85	MG	AT	222	1/1	0.75	0.35	-	43,43,43,43	0
85	MG	6	2121	1/1	0.92	0.28	-	41,41,41,41	0
85	MG	A	2098	1/1	0.81	0.48	-	65,65,65,65	0
84	OHX	1	3669	7/7	0.94	0.39	-	131,131,131,131	0
85	MG	AR	3986	1/1	0.80	0.21	-	56,56,56,56	0
85	MG	AR	4148	1/1	0.89	0.28	-	43,43,43,43	0
84	OHX	6	1931	7/7	0.98	0.10	-	115,116,116,116	0
85	MG	A	2073	1/1	0.95	0.57	-	50,50,50,50	0
84	OHX	1	3633	7/7	0.97	0.30	-	134,134,135,135	0
85	MG	AR	3765	1/1	0.90	0.39	-	71,71,71,71	0
85	MG	AR	4216	1/1	0.91	0.20	-	44,44,44,44	0
85	MG	4	230	1/1	0.93	0.34	-	35,35,35,35	0
85	MG	1	3728	1/1	0.92	0.61	-	52,52,52,52	0
85	MG	1	4220	1/1	0.94	0.57	-	35,35,35,35	0
85	MG	1	4187	1/1	0.78	0.35	-	43,43,43,43	0
85	MG	A	2051	1/1	0.90	0.47	-	67,67,67,67	0
85	MG	A	2130	1/1	0.46	0.62	-	74,74,74,74	0
85	MG	1	3803	1/1	0.88	0.42	-	41,41,41,41	0
85	MG	AT	231	1/1	0.80	0.83	-	52,52,52,52	0
85	MG	1	3937	1/1	0.93	0.12	-	68,68,68,68	0
85	MG	AR	4031	1/1	0.92	0.20	-	39,39,39,39	0
85	MG	AR	3831	1/1	0.94	0.23	-	44,44,44,44	0
84	OHX	AR	3740	7/7	0.93	0.25	-	161,161,161,162	0
85	MG	AS	216	1/1	0.96	0.50	-	23,23,23,23	0
85	MG	AR	3867	1/1	0.95	0.55	-	18,18,18,18	0
84	OHX	1	3706	7/7	0.95	0.30	-	136,137,137,138	0
85	MG	1	4067	1/1	0.98	0.09	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3824	1/1	0.91	0.13	-	77,77,77,77	0
85	MG	1	4070	1/1	0.85	0.20	-	68,68,68,68	0
85	MG	6	2115	1/1	0.86	0.41	-	85,85,85,85	0
85	MG	1	3745	1/1	0.99	0.67	-	31,31,31,31	0
85	MG	AR	4165	1/1	0.92	0.21	-	43,43,43,43	0
85	MG	AP	503	1/1	0.96	0.28	-	27,27,27,27	0
85	MG	AR	3832	1/1	0.91	0.53	-	30,30,30,30	0
85	MG	1	3928	1/1	0.89	0.27	-	34,34,34,34	0
85	MG	AS	231	1/1	0.97	0.19	-	56,56,56,56	0
85	MG	1	3863	1/1	0.82	0.21	-	55,55,55,55	0
85	MG	1	4122	1/1	0.97	0.25	-	78,78,78,78	0
85	MG	AR	3894	1/1	0.86	0.53	-	45,45,45,45	0
85	MG	A	2137	1/1	0.96	0.49	-	58,58,58,58	0
85	MG	1	4124	1/1	0.69	0.22	-	48,48,48,48	0
85	MG	4	240	1/1	0.89	0.57	-	32,32,32,32	0
85	MG	CE	403	1/1	0.82	0.32	-	22,22,22,22	0
85	MG	AR	3974	1/1	0.97	0.42	-	81,81,81,81	0
85	MG	AR	4223	1/1	0.80	0.30	-	61,61,61,61	0
85	MG	AR	4224	1/1	0.82	0.49	-	47,47,47,47	0
85	MG	1	3775	1/1	0.96	0.29	-	32,32,32,32	0
85	MG	1	4160	1/1	0.84	0.32	-	34,34,34,34	0
85	MG	1	3861	1/1	0.91	0.24	-	34,34,34,34	0
85	MG	6	2080	1/1	0.90	0.64	-	69,69,69,69	0
84	OHX	AR	3745	7/7	0.91	0.35	-	128,128,128,128	0
84	OHX	1	3644	7/7	0.90	0.25	-	166,167,167,167	0
85	MG	AR	3988	1/1	0.85	0.81	-	50,50,50,50	0
85	MG	AR	3748	1/1	0.93	0.38	-	44,44,44,44	0
85	MG	1	3825	1/1	0.99	0.41	-	31,31,31,31	0
85	MG	1	4042	1/1	0.85	0.41	-	48,48,48,48	0
84	OHX	1	3702	7/7	0.86	0.22	-	219,219,219,219	0
85	MG	1	4205	1/1	0.97	0.24	-	31,31,31,31	0
84	OHX	6	2016	7/7	0.94	0.25	-	120,120,121,121	0
85	MG	AR	4134	1/1	0.90	0.27	-	44,44,44,44	0
85	MG	AR	4187	1/1	0.86	0.43	-	36,36,36,36	0
84	OHX	1	3448	7/7	0.98	0.21	-	117,117,117,117	0
85	MG	AR	3872	1/1	0.94	0.34	-	43,43,43,43	0
84	OHX	1	3611	7/7	0.96	0.21	-	119,119,119,120	0
85	MG	6	2114	1/1	0.96	0.47	-	46,46,46,46	0
85	MG	1	3752	1/1	0.86	0.43	-	57,57,57,57	0
85	MG	1	4152	1/1	0.59	0.80	-	111,111,111,111	0
85	MG	1	4169	1/1	0.94	0.27	-	30,30,30,30	0
85	MG	AR	4000	1/1	0.96	0.44	-	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	6	2048	7/7	0.91	0.35	-	173,174,174,174	0
85	MG	6	2186	1/1	0.82	0.31	-	107,107,107,107	0
85	MG	AR	4113	1/1	0.84	0.57	-	37,37,37,37	0
85	MG	AR	4196	1/1	0.55	0.43	-	43,43,43,43	0
85	MG	1	4145	1/1	0.84	0.33	-	42,42,42,42	0
85	MG	1	3923	1/1	0.94	0.39	-	51,51,51,51	0
85	MG	s	300	1/1	0.72	0.27	-	70,70,70,70	0
85	MG	1	4091	1/1	0.84	0.32	-	47,47,47,47	0
85	MG	1	3984	1/1	0.85	0.27	-	70,70,70,70	0
85	MG	A	2050	1/1	0.85	0.39	-	67,67,67,67	0
84	OHX	A	2000	7/7	0.95	0.24	-	140,141,141,141	0
85	MG	1	4129	1/1	0.74	0.43	-	33,33,33,33	0
85	MG	6	2192	1/1	0.74	0.67	-	74,74,74,74	0
85	MG	AR	4237	1/1	0.95	0.20	-	39,39,39,39	0
85	MG	AR	3787	1/1	0.95	0.69	-	31,31,31,31	0
84	OHX	6	1935	7/7	0.97	0.14	-	121,121,121,122	0
85	MG	6	2195	1/1	0.86	0.65	-	35,35,35,35	0
85	MG	AR	4191	1/1	0.99	0.17	-	58,58,58,58	0
85	MG	AR	3774	1/1	0.98	0.15	-	30,30,30,30	0
85	MG	6	2117	1/1	0.75	0.28	-	65,65,65,65	0
84	OHX	1	3635	7/7	0.97	0.28	-	122,122,123,123	0
85	MG	AR	4120	1/1	0.86	0.27	-	31,31,31,31	0
85	MG	1	3851	1/1	0.90	0.36	-	34,34,34,34	0
85	MG	AR	3778	1/1	0.91	0.26	-	42,42,42,42	0
84	OHX	1	3628	7/7	0.96	0.26	-	144,145,145,145	0
85	MG	AR	4254	1/1	0.61	0.38	-	56,56,56,56	0
84	OHX	1	3648	7/7	0.94	0.25	-	119,120,120,120	0
85	MG	CM	202	1/1	0.76	0.15	-	62,62,62,62	0
85	MG	1	4211	1/1	0.87	0.63	-	42,42,42,42	0
85	MG	AR	4022	1/1	0.75	0.44	-	30,30,30,30	0
85	MG	AR	3883	1/1	0.94	0.54	-	32,32,32,32	0
85	MG	1	3940	1/1	0.85	0.37	-	43,43,43,43	0
85	MG	A	2049	1/1	0.94	0.50	-	54,54,54,54	0
85	MG	1	3743	1/1	0.96	0.28	-	79,79,79,79	0
85	MG	1	4148	1/1	0.76	0.18	-	53,53,53,53	0
85	MG	1	3812	1/1	0.96	0.64	-	64,64,64,64	0
85	MG	4	241	1/1	0.94	0.58	-	45,45,45,45	0
85	MG	6	2100	1/1	0.92	0.51	-	36,36,36,36	0
85	MG	AR	3845	1/1	0.87	0.41	-	23,23,23,23	0
84	OHX	AR	3564	7/7	0.94	0.14	-	155,155,155,155	0
85	MG	AR	3835	1/1	0.92	0.41	-	45,45,45,45	0
85	MG	1	3877	1/1	0.92	0.72	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3998	1/1	0.82	0.34	-	36,36,36,36	0
84	OHX	1	3709	7/7	0.86	0.35	-	157,158,158,158	0
84	OHX	3	209	7/7	0.90	0.28	-	152,152,152,152	0
85	MG	1	3883	1/1	0.97	0.41	-	22,22,22,22	0
85	MG	3	216	1/1	0.86	0.40	-	58,58,58,58	0
85	MG	1	4111	1/1	0.85	0.55	-	44,44,44,44	0
85	MG	1	3929	1/1	0.91	0.30	-	34,34,34,34	0
84	OHX	AR	3741	7/7	0.87	0.38	-	207,208,208,208	0
85	MG	A	2128	1/1	0.73	0.50	-	78,78,78,78	0
85	MG	AR	4076	1/1	0.83	0.32	-	48,48,48,48	0
85	MG	x	206	1/1	0.78	0.58	-	35,35,35,35	0
85	MG	1	3957	1/1	0.94	0.39	-	37,37,37,37	0
85	MG	6	2160	1/1	0.62	0.38	-	85,85,85,85	0
85	MG	6	2169	1/1	0.87	0.63	-	49,49,49,49	0
85	MG	1	3970	1/1	0.92	0.30	-	31,31,31,31	0
85	MG	AR	4088	1/1	0.95	0.40	-	25,25,25,25	0
85	MG	1	3951	1/1	0.45	0.33	-	69,69,69,69	0
85	MG	1	3881	1/1	0.89	0.55	-	31,31,31,31	0
84	OHX	1	3712	7/7	0.89	0.34	-	133,133,133,133	0
85	MG	1	3948	1/1	0.55	0.23	-	73,73,73,73	0
85	MG	AR	4127	1/1	0.86	0.16	-	77,77,77,77	0
84	OHX	AR	3614	7/7	0.96	0.20	-	114,114,114,114	0
85	MG	1	3853	1/1	0.84	0.55	-	48,48,48,48	0
85	MG	6	2164	1/1	0.87	0.35	-	53,53,53,53	0
84	OHX	AR	3733	7/7	0.89	0.33	-	187,188,188,188	0
84	OHX	AR	3647	7/7	0.92	0.30	-	126,126,127,127	0
85	MG	AR	4003	1/1	0.72	0.44	-	45,45,45,45	0
85	MG	AR	4222	1/1	0.73	0.39	-	58,58,58,58	0
85	MG	l	402	1/1	0.92	0.33	-	57,57,57,57	0
85	MG	1	4165	1/1	0.82	0.40	-	24,24,24,24	0
85	MG	AR	4056	1/1	0.82	0.38	-	44,44,44,44	0
85	MG	6	2152	1/1	0.82	0.43	-	62,62,62,62	0
85	MG	AR	3808	1/1	0.92	0.34	-	28,28,28,28	0
85	MG	AR	4011	1/1	0.73	0.39	-	58,58,58,58	0
85	MG	1	3747	1/1	0.94	0.34	-	37,37,37,37	0
85	MG	1	3964	1/1	0.93	0.46	-	68,68,68,68	0
85	MG	AR	4251	1/1	0.88	0.41	-	59,59,59,59	0
85	MG	1	3758	1/1	0.88	0.50	-	32,32,32,32	0
84	OHX	6	2023	7/7	0.92	0.38	-	161,161,162,162	0
84	OHX	1	3512	7/7	0.98	0.17	-	110,110,110,110	0
84	OHX	CF	402	7/7	0.92	0.34	-	145,146,146,146	0
85	MG	AR	4018	1/1	0.92	0.21	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4117	1/1	0.90	0.31	-	41,41,41,41	0
85	MG	A	2096	1/1	0.94	0.41	-	62,62,62,62	0
84	OHX	A	1993	7/7	0.91	0.38	-	151,151,152,152	0
84	OHX	AR	3595	7/7	0.95	0.31	-	131,131,131,132	0
85	MG	6	2146	1/1	0.81	1.00	-	80,80,80,80	0
84	OHX	A	2022	7/7	0.94	0.36	-	167,167,167,167	0
85	MG	AR	4084	1/1	0.90	0.22	-	34,34,34,34	0
85	MG	AR	3862	1/1	0.85	0.21	-	56,56,56,56	0
85	MG	AR	4260	1/1	0.98	0.52	-	6,6,6,6	0
84	OHX	1	3693	7/7	0.96	0.27	-	118,118,118,118	0
85	MG	AR	3922	1/1	0.91	0.49	-	31,31,31,31	0
85	MG	1	3855	1/1	0.82	0.31	-	44,44,44,44	0
85	MG	AR	3811	1/1	0.82	0.20	-	50,50,50,50	0
85	MG	1	3832	1/1	0.86	0.41	-	26,26,26,26	0
85	MG	AR	4147	1/1	0.91	0.23	-	31,31,31,31	0
85	MG	6	2090	1/1	0.86	0.31	-	49,49,49,49	0
85	MG	AT	224	1/1	0.73	0.22	-	68,68,68,68	0
84	OHX	1	3625	7/7	0.97	0.22	-	135,135,135,135	0
85	MG	AR	3791	1/1	0.94	0.26	-	34,34,34,34	0
85	MG	6	2074	1/1	0.78	0.37	-	62,62,62,62	0
85	MG	AR	3928	1/1	0.93	0.46	-	39,39,39,39	0
85	MG	1	4057	1/1	0.94	0.23	-	26,26,26,26	0
84	OHX	1	3647	7/7	0.97	0.23	-	118,118,118,118	0
85	MG	1	4035	1/1	0.91	0.60	-	47,47,47,47	0
84	OHX	1	3562	7/7	0.97	0.14	-	121,121,121,121	0
84	OHX	AR	3694	7/7	0.92	0.33	-	146,147,147,147	0
85	MG	1	4206	1/1	0.94	0.30	-	30,30,30,30	0
84	OHX	AR	3567	7/7	0.96	0.15	-	121,121,121,121	0
84	OHX	AR	3518	7/7	0.98	0.10	-	118,119,119,119	0
85	MG	1	3922	1/1	0.94	0.45	-	45,45,45,45	0
85	MG	AR	4049	1/1	0.72	0.19	-	50,50,50,50	0
85	MG	1	4072	1/1	0.97	0.18	-	46,46,46,46	0
85	MG	A	2059	1/1	0.95	0.61	-	53,53,53,53	0
85	MG	1	3726	1/1	0.89	0.84	-	54,54,54,54	0
85	MG	AR	4229	1/1	0.97	0.70	-	34,34,34,34	0
85	MG	6	2141	1/1	0.87	0.32	-	52,52,52,52	0
85	MG	1	3895	1/1	0.97	0.42	-	28,28,28,28	0
84	OHX	6	2045	7/7	0.83	0.34	-	141,141,142,142	0
85	MG	6	2095	1/1	0.92	0.43	-	41,41,41,41	0
85	MG	1	4099	1/1	0.92	0.23	-	44,44,44,44	0
85	MG	AR	4259	1/1	0.95	0.49	-	16,16,16,16	0
85	MG	AR	4166	1/1	0.90	0.16	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3639	7/7	0.94	0.32	-	132,132,132,132	0
84	OHX	6	1936	7/7	0.97	0.15	-	116,116,117,117	0
85	MG	A	2071	1/1	0.94	0.33	-	64,64,64,64	0
85	MG	1	3763	1/1	0.94	0.66	-	29,29,29,29	0
85	MG	A	2152	1/1	0.81	0.70	-	43,43,43,43	0
84	OHX	3	201	7/7	0.98	0.19	-	121,121,121,122	0
85	MG	AR	4023	1/1	0.88	0.23	-	31,31,31,31	0
85	MG	6	2113	1/1	0.94	0.23	-	77,77,77,77	0
85	MG	A	2124	1/1	0.61	0.30	-	68,68,68,68	0
85	MG	1	4019	1/1	0.97	0.24	-	42,42,42,42	0
85	MG	AR	4129	1/1	0.95	0.36	-	26,26,26,26	0
84	OHX	A	2007	7/7	0.87	0.26	-	200,200,201,201	0
85	MG	AR	4047	1/1	0.88	0.14	-	54,54,54,54	0
85	MG	1	4002	1/1	0.92	0.55	-	37,37,37,37	0
85	MG	A	2133	1/1	0.88	0.20	-	72,72,72,72	0
85	MG	AR	3990	1/1	0.95	0.08	-	39,39,39,39	0
85	MG	AR	3836	1/1	0.82	0.45	-	48,48,48,48	0
85	MG	AR	3923	1/1	0.94	0.66	-	38,38,38,38	0
85	MG	AR	4231	1/1	0.91	0.35	-	32,32,32,32	0
85	MG	4	220	1/1	0.85	0.34	-	64,64,64,64	0
85	MG	1	4055	1/1	0.90	0.17	-	33,33,33,33	0
85	MG	A	2135	1/1	0.74	0.56	-	55,55,55,55	0
85	MG	1	3966	1/1	0.81	0.18	-	69,69,69,69	0
85	MG	AS	215	1/1	0.88	0.36	-	58,58,58,58	0
85	MG	AR	4201	1/1	0.93	0.26	-	35,35,35,35	0
85	MG	1	4069	1/1	0.96	0.43	-	46,46,46,46	0
85	MG	1	3772	1/1	0.61	0.20	-	35,35,35,35	0
85	MG	1	3996	1/1	0.87	0.44	-	64,64,64,64	0
85	MG	1	4014	1/1	0.80	0.37	-	57,57,57,57	0
85	MG	1	3813	1/1	0.48	0.37	-	61,61,61,61	0
85	MG	1	4107	1/1	0.92	0.16	-	40,40,40,40	0
85	MG	4	217	1/1	0.93	0.56	-	52,52,52,52	0
85	MG	AR	3916	1/1	0.96	0.58	-	19,19,19,19	0
85	MG	AS	226	1/1	0.85	0.21	-	67,67,67,67	0
85	MG	AR	4163	1/1	0.89	0.23	-	62,62,62,62	0
85	MG	1	3816	1/1	0.75	0.34	-	44,44,44,44	0
85	MG	AR	4060	1/1	0.81	0.27	-	70,70,70,70	0
84	OHX	A	1968	7/7	0.97	0.34	-	125,125,126,126	0
84	OHX	1	3503	7/7	0.97	0.10	-	127,128,128,129	0
85	MG	1	4054	1/1	0.92	0.21	-	56,56,56,56	0
84	OHX	6	2036	7/7	0.93	0.39	-	135,135,136,136	0
85	MG	A	2083	1/1	0.81	0.18	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3759	1/1	0.86	0.12	-	41,41,41,41	0
85	MG	1	3850	1/1	0.92	0.48	-	31,31,31,31	0
84	OHX	AR	3679	7/7	0.96	0.25	-	153,153,153,154	0
85	MG	1	3980	1/1	0.96	0.27	-	73,73,73,73	0
85	MG	CP	503	1/1	0.97	0.41	-	38,38,38,38	0
85	MG	A	2146	1/1	0.72	0.16	-	120,120,120,120	0
85	MG	A	2110	1/1	0.87	0.67	-	116,116,116,116	0
84	OHX	4	211	7/7	0.96	0.14	-	138,139,139,140	0
85	MG	AR	4236	1/1	0.91	0.42	-	23,23,23,23	0
85	MG	1	3963	1/1	0.81	0.24	-	45,45,45,45	0
85	MG	1	4053	1/1	0.49	0.41	-	74,74,74,74	0
85	MG	A	2122	1/1	0.90	0.17	-	86,86,86,86	0
85	MG	6	2058	1/1	0.97	0.43	-	45,45,45,45	0
85	MG	4	229	1/1	0.56	0.41	-	54,54,54,54	0
85	MG	AR	4123	1/1	0.78	0.36	-	57,57,57,57	0
84	OHX	6	2042	7/7	0.94	0.34	-	151,151,151,151	0
84	OHX	AR	3650	7/7	0.93	0.44	-	118,118,118,118	0
84	OHX	6	2010	7/7	0.94	0.33	-	154,155,155,155	0
84	OHX	1	3602	7/7	0.97	0.23	-	128,128,128,129	0
85	MG	1	4098	1/1	0.83	0.27	-	47,47,47,47	0
84	OHX	A	1934	7/7	0.97	0.12	-	132,132,133,133	0
85	MG	1	4050	1/1	0.83	0.36	-	31,31,31,31	0
85	MG	A	2060	1/1	0.93	0.62	-	55,55,55,55	0
85	MG	6	2055	1/1	0.96	0.73	-	49,49,49,49	0
85	MG	AR	3944	1/1	0.83	0.17	-	38,38,38,38	0
84	OHX	AR	3676	7/7	0.96	0.29	-	122,122,123,123	0
85	MG	AR	3830	1/1	0.98	0.46	-	42,42,42,42	0
85	MG	6	2181	1/1	0.99	0.11	-	95,95,95,95	0
84	OHX	4	206	7/7	0.96	0.16	-	116,116,116,116	0
85	MG	1	3903	1/1	0.99	0.67	-	21,21,21,21	0
85	MG	1	3831	1/1	0.94	0.47	-	26,26,26,26	0
85	MG	1	3961	1/1	0.87	0.19	-	40,40,40,40	0
85	MG	A	2067	1/1	0.91	0.81	-	64,64,64,64	0
85	MG	1	3908	1/1	0.87	0.50	-	62,62,62,62	0
85	MG	1	3818	1/1	0.90	0.43	-	39,39,39,39	0
85	MG	6	2054	1/1	0.94	0.39	-	49,49,49,49	0
85	MG	4	235	1/1	0.76	0.50	-	70,70,70,70	0
85	MG	1	4030	1/1	0.91	0.72	-	72,72,72,72	0
84	OHX	1	3595	7/7	0.96	0.11	-	140,140,140,140	0
85	MG	AR	3967	1/1	0.89	0.55	-	42,42,42,42	0
85	MG	AR	4004	1/1	0.94	0.16	-	32,32,32,32	0
85	MG	6	2123	1/1	0.89	0.24	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	6	1965	7/7	0.97	0.24	-	116,117,117,117	0
85	MG	1	4079	1/1	0.92	0.21	-	97,97,97,97	0
85	MG	1	3907	1/1	0.95	0.33	-	40,40,40,40	0
84	OHX	AT	216	7/7	0.95	0.40	-	132,132,132,132	0
85	MG	6	2147	1/1	0.95	0.12	-	57,57,57,57	0
85	MG	AR	4087	1/1	0.76	0.36	-	63,63,63,63	0
85	MG	1	4194	1/1	0.94	0.50	-	22,22,22,22	0
84	OHX	AR	3419	7/7	0.99	0.27	-	122,122,123,123	0
85	MG	6	2176	1/1	0.32	0.67	-	93,93,93,93	0
85	MG	AR	4180	1/1	0.91	0.39	-	48,48,48,48	0
84	OHX	AR	3674	7/7	0.93	0.46	-	130,130,130,131	0
85	MG	1	4176	1/1	0.96	0.62	-	34,34,34,34	0
84	OHX	c3	201	7/7	0.91	0.24	-	155,156,156,157	0
85	MG	1	3817	1/1	0.98	0.26	-	23,23,23,23	0
85	MG	AR	4142	1/1	0.85	0.31	-	46,46,46,46	0
84	OHX	1	3439	7/7	0.98	0.19	-	109,109,109,109	0
84	OHX	AR	3510	7/7	0.98	0.13	-	117,118,118,118	0
84	OHX	AR	3540	7/7	0.97	0.16	-	108,108,108,108	0
85	MG	AR	3792	1/1	0.92	0.51	-	43,43,43,43	0
85	MG	AR	4215	1/1	0.75	0.28	-	70,70,70,70	0
85	MG	1	4022	1/1	0.91	0.59	-	53,53,53,53	0
85	MG	1	4161	1/1	0.73	0.25	-	69,69,69,69	0
84	OHX	A	2023	7/7	0.91	0.26	-	144,145,145,145	0
85	MG	1	3981	1/1	0.86	0.49	-	50,50,50,50	0
85	MG	6	2180	1/1	0.61	0.60	-	64,64,64,64	0
85	MG	1	4080	1/1	0.89	0.22	-	35,35,35,35	0
85	MG	AS	225	1/1	0.74	0.35	-	58,58,58,58	0
85	MG	AR	3788	1/1	0.93	0.50	-	28,28,28,28	0
85	MG	CQ	203	1/1	0.95	0.15	-	34,34,34,34	0
85	MG	1	4146	1/1	0.92	0.17	-	48,48,48,48	0
85	MG	AR	3798	1/1	0.93	0.33	-	33,33,33,33	0
84	OHX	6	2026	7/7	0.95	0.26	-	146,146,147,147	0
85	MG	1	4028	1/1	0.90	0.16	-	46,46,46,46	0
85	MG	AR	4072	1/1	0.91	0.25	-	70,70,70,70	0
85	MG	6	2174	1/1	0.70	0.44	-	58,58,58,58	0
84	OHX	AR	3546	7/7	0.96	0.21	-	123,124,124,124	0
85	MG	AR	3911	1/1	0.83	0.42	-	40,40,40,40	0
85	MG	AR	4017	1/1	0.85	0.31	-	95,95,95,95	0
85	MG	AR	3931	1/1	0.96	0.29	-	17,17,17,17	0
85	MG	AR	4093	1/1	0.85	0.37	-	46,46,46,46	0
85	MG	A	2090	1/1	0.93	0.20	-	57,57,57,57	0
85	MG	1	3736	1/1	0.97	0.60	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3984	1/1	0.82	0.65	-	50,50,50,50	0
85	MG	1	3862	1/1	0.93	0.46	-	52,52,52,52	0
85	MG	3	210	1/1	0.92	0.39	-	59,59,59,59	0
85	MG	lR	201	1/1	0.96	0.36	-	26,26,26,26	0
85	MG	1	3824	1/1	0.95	0.39	-	25,25,25,25	0
84	OHX	1	3664	7/7	0.93	0.35	-	124,124,124,124	0
85	MG	AR	4032	1/1	0.84	0.37	-	48,48,48,48	0
85	MG	AT	226	1/1	0.84	0.30	-	63,63,63,63	0
84	OHX	1	3622	7/7	0.96	0.27	-	153,154,154,154	0
85	MG	1	3857	1/1	0.76	0.25	-	56,56,56,56	0
85	MG	1	4153	1/1	0.93	0.18	-	39,39,39,39	0
85	MG	AR	3866	1/1	0.99	0.23	-	34,34,34,34	0
85	MG	1	4005	1/1	0.89	0.35	-	36,36,36,36	0
85	MG	AR	4173	1/1	0.83	0.31	-	53,53,53,53	0
85	MG	AS	219	1/1	0.77	0.24	-	58,58,58,58	0
85	MG	4	239	1/1	0.96	0.70	-	43,43,43,43	0
85	MG	1	3910	1/1	0.98	0.58	-	19,19,19,19	0
85	MG	1	3753	1/1	0.94	0.54	-	35,35,35,35	0
85	MG	AR	4116	1/1	0.82	0.30	-	99,99,99,99	0
84	OHX	AR	3608	7/7	0.94	0.34	-	131,131,132,132	0
85	MG	6	2079	1/1	0.87	0.24	-	45,45,45,45	0
85	MG	1	4097	1/1	0.99	0.22	-	70,70,70,70	0
85	MG	AR	4170	1/1	0.70	0.27	-	32,32,32,32	0
85	MG	AR	4006	1/1	0.94	0.55	-	47,47,47,47	0
85	MG	d6	101	1/1	0.91	0.33	-	49,49,49,49	0
84	OHX	1	3514	7/7	0.94	0.18	-	112,112,112,112	0
84	OHX	A	2020	7/7	0.93	0.23	-	147,148,148,148	0
85	MG	1	4217	1/1	0.93	0.92	-	58,58,58,58	0
85	MG	CG	303	1/1	0.93	0.13	-	62,62,62,62	0
85	MG	AR	3852	1/1	0.87	0.24	-	37,37,37,37	0
85	MG	AR	3960	1/1	0.84	0.21	-	41,41,41,41	0
85	MG	AR	4160	1/1	0.77	0.26	-	78,78,78,78	0
85	MG	AR	3899	1/1	0.89	0.60	-	45,45,45,45	0
85	MG	1	4182	1/1	0.97	0.30	-	25,25,25,25	0
84	OHX	A	1943	7/7	0.97	0.21	-	133,133,134,134	0
84	OHX	6	1969	7/7	0.94	0.15	-	127,127,128,128	0
85	MG	1	3972	1/1	0.83	0.85	-	45,45,45,45	0
85	MG	6	2106	1/1	0.92	0.39	-	50,50,50,50	0
85	MG	3	213	1/1	0.96	0.45	-	48,48,48,48	0
85	MG	6	2072	1/1	0.82	0.70	-	40,40,40,40	0
85	MG	1	4046	1/1	0.78	0.34	-	37,37,37,37	0
85	MG	AR	4037	1/1	0.71	0.34	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4245	1/1	0.83	0.22	-	26,26,26,26	0
85	MG	AR	4194	1/1	0.80	0.27	-	53,53,53,53	0
85	MG	1	3834	1/1	0.92	0.51	-	22,22,22,22	0
84	OHX	AR	3734	7/7	0.86	0.54	-	148,148,148,149	0
85	MG	AR	3892	1/1	0.91	0.48	-	31,31,31,31	0
85	MG	1	4004	1/1	0.64	0.26	-	44,44,44,44	0
84	OHX	6	2007	7/7	0.92	0.28	-	145,146,146,146	0
85	MG	DC	201	1/1	0.89	0.45	-	30,30,30,30	0
85	MG	1	4026	1/1	0.92	0.40	-	65,65,65,65	0
85	MG	1	3774	1/1	0.95	0.54	-	43,43,43,43	0
85	MG	AR	3870	1/1	0.98	0.70	-	33,33,33,33	0
84	OHX	1	3600	7/7	0.98	0.15	-	150,150,150,150	0
85	MG	DC	203	1/1	0.73	0.30	-	47,47,47,47	0
85	MG	1	4008	1/1	0.92	0.29	-	37,37,37,37	0
85	MG	6	2119	1/1	0.98	0.47	-	74,74,74,74	0
85	MG	6	2069	1/1	0.94	0.35	-	65,65,65,65	0
85	MG	1	4045	1/1	0.82	0.34	-	39,39,39,39	0
85	MG	AR	3782	1/1	0.74	0.35	-	36,36,36,36	0
85	MG	1	3768	1/1	0.94	0.41	-	36,36,36,36	0
85	MG	AR	4097	1/1	0.79	0.58	-	40,40,40,40	0
85	MG	AR	3971	1/1	0.78	0.42	-	57,57,57,57	0
85	MG	3	214	1/1	0.92	0.52	-	34,34,34,34	0
84	OHX	A	2032	7/7	0.94	0.20	-	154,154,155,155	0
85	MG	AS	212	1/1	0.95	0.33	-	41,41,41,41	0
85	MG	A	2132	1/1	0.90	0.26	-	98,98,98,98	0
84	OHX	3	205	7/7	0.91	0.21	-	127,128,128,128	0
85	MG	1	4197	1/1	0.96	0.34	-	32,32,32,32	0
85	MG	AR	4137	1/1	0.91	0.48	-	79,79,79,79	0
84	OHX	1	3691	7/7	0.77	0.31	-	201,201,201,201	0
84	OHX	AR	3678	7/7	0.93	0.42	-	137,137,137,138	0
85	MG	AS	228	1/1	0.56	0.43	-	84,84,84,84	0
85	MG	AR	3958	1/1	0.85	0.56	-	38,38,38,38	0
85	MG	AR	4145	1/1	0.86	0.20	-	70,70,70,70	0
85	MG	1	4120	1/1	0.96	0.40	-	27,27,27,27	0
85	MG	AR	4213	1/1	0.94	0.14	-	53,53,53,53	0
84	OHX	AR	3713	7/7	0.94	0.24	-	178,178,179,179	0
85	MG	1	4143	1/1	0.96	0.21	-	29,29,29,29	0
85	MG	AR	4068	1/1	0.91	0.12	-	99,99,99,99	0
85	MG	1	3826	1/1	0.93	0.25	-	33,33,33,33	0
84	OHX	AR	3680	7/7	0.95	0.41	-	141,141,142,142	0
85	MG	A	2045	1/1	0.75	0.79	-	58,58,58,58	0
85	MG	6	2092	1/1	0.79	0.57	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	A	2139	1/1	0.70	0.36	-	64,64,64,64	0
85	MG	1	3956	1/1	0.89	0.54	-	34,34,34,34	0
85	MG	AR	3943	1/1	0.89	0.10	-	41,41,41,41	0
85	MG	AR	3761	1/1	0.81	0.33	-	31,31,31,31	0
85	MG	t	201	1/1	0.90	0.17	-	51,51,51,51	0
85	MG	AR	4101	1/1	0.82	0.25	-	48,48,48,48	0
85	MG	1	3749	1/1	0.95	0.26	-	24,24,24,24	0
85	MG	1	3750	1/1	0.79	0.18	-	55,55,55,55	0
85	MG	AR	3880	1/1	0.95	0.47	-	42,42,42,42	0
85	MG	AR	3957	1/1	0.86	0.13	-	55,55,55,55	0
85	MG	AR	4217	1/1	0.96	0.60	-	80,80,80,80	0
85	MG	U	201	1/1	0.86	0.42	-	76,76,76,76	0
84	OHX	AR	3670	7/7	0.93	0.19	-	143,143,144,144	0
85	MG	DL	102	1/1	0.88	0.50	-	39,39,39,39	0
85	MG	AR	3903	1/1	0.82	0.69	-	39,39,39,39	0
85	MG	AR	3773	1/1	0.90	0.29	-	41,41,41,41	0
85	MG	A	2082	1/1	0.94	0.23	-	61,61,61,61	0
85	MG	1	4043	1/1	0.97	0.32	-	27,27,27,27	0
84	OHX	1	3720	7/7	0.91	0.28	-	128,128,129,129	0
85	MG	c6	201	1/1	0.82	0.22	-	89,89,89,89	0
84	OHX	1	3559	7/7	0.95	0.17	-	143,143,143,144	0
85	MG	AR	3799	1/1	0.99	0.36	-	22,22,22,22	0
85	MG	AR	4121	1/1	0.96	0.30	-	27,27,27,27	0
85	MG	A	2112	1/1	0.70	0.37	-	86,86,86,86	0
85	MG	d3	201	1/1	0.94	0.25	-	49,49,49,49	0
85	MG	4	226	1/1	0.96	0.59	-	42,42,42,42	0
85	MG	1	3849	1/1	0.91	0.44	-	23,23,23,23	0
85	MG	6	2062	1/1	0.95	0.42	-	51,51,51,51	0
84	OHX	6	2006	7/7	0.89	0.29	-	151,151,152,152	0
84	OHX	AR	3682	7/7	0.96	0.52	-	144,144,144,145	0
85	MG	1	3742	1/1	0.94	0.47	-	38,38,38,38	0
85	MG	AR	3834	1/1	0.89	0.47	-	33,33,33,33	0
85	MG	1	3865	1/1	0.91	0.32	-	45,45,45,45	0
85	MG	1	4144	1/1	0.95	0.16	-	53,53,53,53	0
85	MG	1	4177	1/1	0.96	0.44	-	27,27,27,27	0
85	MG	AR	4150	1/1	0.88	0.17	-	44,44,44,44	0
85	MG	1	4138	1/1	0.87	0.28	-	33,33,33,33	0
85	MG	AR	4193	1/1	0.93	0.32	-	38,38,38,38	0
85	MG	1	3993	1/1	0.83	0.62	-	42,42,42,42	0
85	MG	CQ	201	1/1	0.93	0.38	-	34,34,34,34	0
85	MG	3	215	1/1	0.96	0.57	-	31,31,31,31	0
85	MG	1	4101	1/1	0.72	0.51	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	6	2151	1/1	0.96	0.15	-	60,60,60,60	0
85	MG	1	3852	1/1	0.80	0.33	-	38,38,38,38	0
84	OHX	A	1929	7/7	0.98	0.15	-	123,123,124,124	0
85	MG	A	2070	1/1	0.88	0.53	-	79,79,79,79	0
85	MG	6	2126	1/1	0.95	0.29	-	53,53,53,53	0
84	OHX	AR	3453	7/7	0.98	0.10	-	106,106,107,107	0
84	OHX	AT	217	7/7	0.93	0.37	-	128,128,128,128	0
85	MG	1	4009	1/1	0.86	0.66	-	42,42,42,42	0
84	OHX	AS	202	7/7	0.98	0.22	-	124,124,125,125	0
85	MG	AR	4039	1/1	0.82	0.38	-	56,56,56,56	0
84	OHX	1	3667	7/7	0.95	0.30	-	127,127,128,128	0
84	OHX	1	3668	7/7	0.81	0.45	-	124,124,124,124	0
84	OHX	A	2039	7/7	0.91	0.41	-	166,167,168,168	0
85	MG	1	3945	1/1	0.88	0.29	-	57,57,57,57	0
85	MG	1	3770	1/1	0.94	0.25	-	29,29,29,29	0
85	MG	AR	3908	1/1	0.97	0.53	-	25,25,25,25	0
85	MG	AR	4030	1/1	0.72	0.57	-	59,59,59,59	0
85	MG	1	4056	1/1	0.74	0.30	-	51,51,51,51	0
85	MG	1	3986	1/1	0.94	0.26	-	42,42,42,42	0
85	MG	v	304	1/1	0.86	0.62	-	52,52,52,52	0
85	MG	AS	221	1/1	0.95	0.16	-	60,60,60,60	0
85	MG	1	4162	1/1	0.88	0.25	-	40,40,40,40	0
85	MG	AR	3789	1/1	0.91	0.39	-	36,36,36,36	0
85	MG	1	4044	1/1	0.80	0.32	-	47,47,47,47	0
85	MG	AR	4058	1/1	0.93	0.53	-	61,61,61,61	0
85	MG	1	4116	1/1	0.90	0.52	-	44,44,44,44	0
85	MG	A	2134	1/1	0.87	0.35	-	70,70,70,70	0
85	MG	1	3821	1/1	0.92	0.52	-	66,66,66,66	0
84	OHX	AR	3445	7/7	0.97	0.18	-	107,107,107,107	0
85	MG	1	3766	1/1	0.90	0.16	-	73,73,73,73	0
85	MG	1	4173	1/1	0.95	0.54	-	36,36,36,36	0
85	MG	1	3786	1/1	0.87	0.20	-	40,40,40,40	0
85	MG	AR	4094	1/1	0.83	0.31	-	43,43,43,43	0
85	MG	1	3835	1/1	0.98	0.47	-	30,30,30,30	0
85	MG	A	2068	1/1	0.84	0.56	-	84,84,84,84	0
85	MG	1	3983	1/1	0.74	0.52	-	55,55,55,55	0
85	MG	3	211	1/1	0.89	0.35	-	38,38,38,38	0
85	MG	AR	4104	1/1	0.57	0.39	-	66,66,66,66	0
84	OHX	A	2005	7/7	0.96	0.32	-	131,132,132,132	0
85	MG	Y	201	1/1	0.70	0.20	-	61,61,61,61	0
85	MG	1	4068	1/1	0.93	0.46	-	42,42,42,42	0
85	MG	AR	3800	1/1	0.93	0.65	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3627	7/7	0.92	0.28	-	141,142,142,143	0
85	MG	AT	219	1/1	0.98	0.35	-	36,36,36,36	0
85	MG	AR	4242	1/1	0.93	0.46	-	35,35,35,35	0
85	MG	AS	227	1/1	0.92	0.32	-	45,45,45,45	0
85	MG	1	4192	1/1	0.97	0.67	-	21,21,21,21	0
85	MG	1	3754	1/1	0.85	0.52	-	37,37,37,37	0
85	MG	1	3840	1/1	0.81	0.31	-	78,78,78,78	0
85	MG	6	2165	1/1	0.91	0.35	-	51,51,51,51	0
85	MG	AR	4063	1/1	0.79	0.12	-	54,54,54,54	0
85	MG	AR	4099	1/1	0.89	0.16	-	41,41,41,41	0
84	OHX	AR	3634	7/7	0.94	0.26	-	112,112,113,113	0
85	MG	6	2083	1/1	0.75	0.45	-	63,63,63,63	0
85	MG	AR	3805	1/1	0.93	0.44	-	36,36,36,36	0
85	MG	4	232	1/1	0.80	0.28	-	37,37,37,37	0
85	MG	1	3791	1/1	0.94	0.60	-	54,54,54,54	0
85	MG	AR	4021	1/1	0.84	0.17	-	82,82,82,82	0
85	MG	AR	4098	1/1	0.90	0.20	-	46,46,46,46	0
85	MG	AT	225	1/1	0.86	0.90	-	53,53,53,53	0
85	MG	1	3988	1/1	0.73	0.37	-	34,34,34,34	0
85	MG	AR	4146	1/1	0.86	0.19	-	34,34,34,34	0
85	MG	6	2156	1/1	0.95	0.16	-	101,101,101,101	0
85	MG	AR	4171	1/1	0.77	0.17	-	88,88,88,88	0
85	MG	1	4132	1/1	0.98	0.12	-	86,86,86,86	0
85	MG	AR	3932	1/1	0.97	0.28	-	63,63,63,63	0
84	OHX	AR	3629	7/7	0.96	0.14	-	141,141,141,142	0
84	OHX	AR	3710	7/7	0.94	0.34	-	137,137,137,138	0
85	MG	1	3960	1/1	0.89	0.21	-	33,33,33,33	0
85	MG	AR	3842	1/1	0.87	0.16	-	47,47,47,47	0
85	MG	6	2073	1/1	0.95	0.52	-	48,48,48,48	0
85	MG	3	218	1/1	0.97	0.22	-	54,54,54,54	0
85	MG	AB	202	1/1	0.86	0.31	-	29,29,29,29	0
84	OHX	A	1981	7/7	0.92	0.16	-	194,195,195,195	0
84	OHX	1	3465	7/7	0.98	0.18	-	117,117,117,117	0
85	MG	6	2185	1/1	0.61	0.46	-	89,89,89,89	0
84	OHX	AR	3615	7/7	0.94	0.36	-	132,133,133,133	0
85	MG	6	2136	1/1	0.97	0.23	-	52,52,52,52	0
85	MG	AR	3902	1/1	0.92	0.57	-	42,42,42,42	0
85	MG	1	3797	1/1	0.85	0.18	-	79,79,79,79	0
85	MG	AR	3976	1/1	0.77	0.44	-	81,81,81,81	0
85	MG	AR	4257	1/1	0.76	0.32	-	51,51,51,51	0
85	MG	AR	3851	1/1	0.87	0.29	-	38,38,38,38	0
85	MG	A	2046	1/1	0.71	0.29	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4073	1/1	0.89	0.39	-	40,40,40,40	0
85	MG	AR	3779	1/1	0.80	0.38	-	73,73,73,73	0
85	MG	1	4059	1/1	0.97	0.42	-	51,51,51,51	0
85	MG	AR	4105	1/1	0.95	0.14	-	42,42,42,42	0
84	OHX	AR	3475	7/7	0.98	0.14	-	116,116,116,116	0
84	OHX	AR	3556	7/7	0.96	0.21	-	109,109,109,109	0
85	MG	1	3965	1/1	0.51	0.57	-	94,94,94,94	0
85	MG	6	2149	1/1	0.89	0.32	-	46,46,46,46	0
85	MG	A	2107	1/1	0.82	0.31	-	80,80,80,80	0
85	MG	1	3727	1/1	0.94	0.28	-	37,37,37,37	0
85	MG	4	223	1/1	0.94	0.59	-	27,27,27,27	0
85	MG	1	3827	1/1	0.98	0.73	-	32,32,32,32	0
85	MG	1	3955	1/1	0.82	0.43	-	51,51,51,51	0
85	MG	AR	3746	1/1	0.95	0.26	-	58,58,58,58	0
85	MG	AR	4184	1/1	0.91	0.16	-	69,69,69,69	0
85	MG	1	4032	1/1	0.96	0.31	-	42,42,42,42	0
85	MG	AR	4258	1/1	0.96	0.54	-	34,34,34,34	0
85	MG	6	2189	1/1	0.76	0.34	-	63,63,63,63	0
85	MG	1	3967	1/1	0.85	0.20	-	38,38,38,38	0
85	MG	1	3915	1/1	0.89	0.13	-	36,36,36,36	0
85	MG	1	4062	1/1	0.93	0.16	-	45,45,45,45	0
85	MG	AR	4151	1/1	0.95	0.11	-	148,148,148,148	0
85	MG	6	2127	1/1	0.91	0.47	-	54,54,54,54	0
85	MG	1	4087	1/1	0.78	0.23	-	59,59,59,59	0
85	MG	1	4171	1/1	0.95	0.23	-	85,85,85,85	0
85	MG	AR	4156	1/1	0.77	1.08	-	72,72,72,72	0
84	OHX	1	3490	7/7	0.99	0.17	-	113,113,113,113	0
85	MG	A	2117	1/1	0.71	0.19	-	71,71,71,71	0
84	OHX	1	3457	7/7	0.98	0.18	-	126,127,127,128	0
84	OHX	AR	3686	7/7	0.83	0.38	-	156,156,156,157	0
85	MG	1	3995	1/1	0.89	0.30	-	34,34,34,34	0
84	OHX	AR	3526	7/7	0.96	0.18	-	117,117,117,118	0
85	MG	A	2159	1/1	0.84	0.93	-	64,64,64,64	0
85	MG	d5	201	1/1	0.89	0.09	-	71,71,71,71	0
85	MG	AS	218	1/1	0.90	0.30	-	33,33,33,33	0
85	MG	AR	4256	1/1	0.91	0.43	-	49,49,49,49	0
85	MG	1	3973	1/1	0.93	0.47	-	37,37,37,37	0
85	MG	AR	3839	1/1	0.93	0.43	-	33,33,33,33	0
84	OHX	1	3718	7/7	0.90	0.39	-	149,149,149,149	0
85	MG	AR	4168	1/1	1.00	0.19	-	65,65,65,65	0
85	MG	AR	4108	1/1	0.94	0.19	-	36,36,36,36	0
85	MG	AR	4172	1/1	0.99	0.12	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4200	1/1	0.81	0.25	-	48,48,48,48	0
85	MG	1	403	1/1	0.71	0.47	-	37,37,37,37	0
85	MG	AR	4071	1/1	0.86	0.27	-	39,39,39,39	0
85	MG	1	4147	1/1	0.90	0.21	-	48,48,48,48	0
85	MG	AR	4053	1/1	0.97	0.40	-	30,30,30,30	0
85	MG	AR	3959	1/1	0.94	0.28	-	32,32,32,32	0
85	MG	A	2136	1/1	0.75	0.70	-	74,74,74,74	0
85	MG	6	2084	1/1	0.96	0.22	-	48,48,48,48	0
85	MG	AR	4085	1/1	0.77	0.46	-	35,35,35,35	0
85	MG	AR	3887	1/1	0.99	0.46	-	21,21,21,21	0
84	OHX	AR	3446	7/7	0.99	0.17	-	112,113,113,113	0
85	MG	AR	4040	1/1	0.90	0.26	-	43,43,43,43	0
84	OHX	1	3580	7/7	0.97	0.34	-	115,116,116,116	0
85	MG	6	2153	1/1	0.95	0.27	-	97,97,97,97	0
85	MG	AR	3952	1/1	0.96	0.36	-	28,28,28,28	0
85	MG	A	2069	1/1	0.84	0.49	-	58,58,58,58	0
85	MG	AR	3846	1/1	0.96	0.56	-	33,33,33,33	0
85	MG	AR	3889	1/1	0.91	0.36	-	35,35,35,35	0
85	MG	1	4131	1/1	0.74	0.32	-	48,48,48,48	0
85	MG	AR	4204	1/1	0.93	0.30	-	38,38,38,38	0
85	MG	AR	4045	1/1	0.84	0.30	-	55,55,55,55	0
85	MG	AR	4026	1/1	0.91	0.33	-	60,60,60,60	0
85	MG	1	4108	1/1	0.87	0.21	-	42,42,42,42	0
85	MG	AR	4035	1/1	0.84	0.38	-	43,43,43,43	0
84	OHX	AR	3651	7/7	0.94	0.31	-	150,151,151,151	0
85	MG	6	2112	1/1	0.93	0.53	-	46,46,46,46	0
85	MG	1	3806	1/1	0.97	0.46	-	51,51,51,51	0
85	MG	1	3794	1/1	0.94	0.53	-	34,34,34,34	0
85	MG	1	4000	1/1	0.87	0.23	-	43,43,43,43	0
84	OHX	6	2049	7/7	0.93	0.33	-	170,171,171,171	0
85	MG	AR	3954	1/1	0.86	0.30	-	44,44,44,44	0
85	MG	AR	3777	1/1	0.89	0.31	-	37,37,37,37	0
84	OHX	1	3561	7/7	0.97	0.26	-	124,124,125,125	0
84	OHX	6	1949	7/7	0.96	0.11	-	135,136,136,136	0
85	MG	AR	4009	1/1	0.90	0.34	-	37,37,37,37	0
84	OHX	1	3521	7/7	0.98	0.14	-	116,117,117,117	0
84	OHX	1	3619	7/7	0.94	0.22	-	127,127,127,127	0
85	MG	AR	3949	1/1	0.94	0.19	-	32,32,32,32	0
85	MG	A	2121	1/1	0.51	0.31	-	62,62,62,62	0
85	MG	AR	4096	1/1	0.85	0.32	-	54,54,54,54	0
85	MG	AR	4208	1/1	0.98	0.21	-	57,57,57,57	0
85	MG	AR	4079	1/1	0.96	0.31	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	1	4109	1/1	0.91	0.14	-	66,66,66,66	0
84	OHX	AR	3666	7/7	0.94	0.27	-	130,131,131,131	0
85	MG	6	2173	1/1	0.84	0.73	-	48,48,48,48	0
85	MG	A	2148	1/1	0.95	0.37	-	64,64,64,64	0
85	MG	1	4010	1/1	0.94	0.46	-	30,30,30,30	0
85	MG	AR	3784	1/1	0.94	0.24	-	51,51,51,51	0
84	OHX	AR	3622	7/7	0.94	0.24	-	130,131,131,131	0
85	MG	1	3930	1/1	0.69	0.57	-	40,40,40,40	0
84	OHX	AR	3434	7/7	0.99	0.22	-	111,111,111,111	0
85	MG	AR	3980	1/1	0.92	0.86	-	40,40,40,40	0
85	MG	4	222	1/1	0.88	0.28	-	33,33,33,33	0
85	MG	AR	4064	1/1	0.90	0.24	-	38,38,38,38	0
85	MG	1	4037	1/1	0.91	0.30	-	30,30,30,30	0
84	OHX	AR	3708	7/7	0.93	0.26	-	138,138,139,139	0
85	MG	6	2076	1/1	0.78	0.58	-	105,105,105,105	0
85	MG	AR	3963	1/1	0.94	0.20	-	49,49,49,49	0
85	MG	1	3989	1/1	0.60	0.26	-	55,55,55,55	0
85	MG	AR	4074	1/1	0.68	0.23	-	77,77,77,77	0
85	MG	1	4013	1/1	0.82	0.33	-	52,52,52,52	0
85	MG	AR	4182	1/1	0.81	0.37	-	79,79,79,79	0
84	OHX	1	3553	7/7	0.96	0.29	-	121,122,122,122	0
84	OHX	1	3674	7/7	0.95	0.28	-	136,136,137,137	0
85	MG	AR	3972	1/1	0.95	0.53	-	39,39,39,39	0
85	MG	AR	3981	1/1	0.94	0.14	-	33,33,33,33	0
85	MG	A	2140	1/1	0.82	0.82	-	82,82,82,82	0
84	OHX	1	3586	7/7	0.96	0.23	-	121,122,122,122	0
84	OHX	AR	3604	7/7	0.90	0.19	-	158,159,159,159	0
85	MG	AT	220	1/1	0.92	0.47	-	53,53,53,53	0
87	GOL	AR	4262	6/6	0.80	0.34	-	48,48,48,48	0
85	MG	AR	4205	1/1	0.91	0.24	-	59,59,59,59	0
85	MG	6	2148	1/1	0.95	0.43	-	48,48,48,48	0
85	MG	1	4024	1/1	0.95	0.21	-	61,61,61,61	0
85	MG	AR	4243	1/1	0.93	0.59	-	30,30,30,30	0
85	MG	t	203	1/1	0.92	0.42	-	29,29,29,29	0
85	MG	AR	3806	1/1	0.97	0.29	-	57,57,57,57	0
85	MG	1	4181	1/1	0.94	0.35	-	23,23,23,23	0
85	MG	AR	4067	1/1	0.89	0.34	-	34,34,34,34	0
85	MG	AR	3802	1/1	0.95	0.12	-	40,40,40,40	0
85	MG	1	3737	1/1	0.90	0.93	-	57,57,57,57	0
85	MG	AR	3758	1/1	0.93	0.30	-	37,37,37,37	0
85	MG	AR	3869	1/1	0.97	0.40	-	31,31,31,31	0
84	OHX	AR	3559	7/7	0.97	0.31	-	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3594	7/7	0.94	0.20	-	131,131,132,132	0
85	MG	1	4209	1/1	0.90	0.66	-	48,48,48,48	0
85	MG	1	3802	1/1	0.92	0.18	-	86,86,86,86	0
85	MG	1	4038	1/1	0.86	0.72	-	41,41,41,41	0
84	OHX	1	3570	7/7	0.98	0.09	-	144,144,145,145	0
85	MG	1	4065	1/1	0.84	0.31	-	48,48,48,48	0
85	MG	1	3800	1/1	0.79	0.61	-	45,45,45,45	0
85	MG	AR	3793	1/1	0.95	0.31	-	29,29,29,29	0
85	MG	AR	3754	1/1	0.93	0.31	-	40,40,40,40	0
85	MG	1	4040	1/1	0.80	0.30	-	74,74,74,74	0
85	MG	CL	302	1/1	0.87	0.36	-	68,68,68,68	0
85	MG	1	4178	1/1	0.93	0.40	-	28,28,28,28	0
85	MG	1	4085	1/1	0.91	0.39	-	51,51,51,51	0
85	MG	AR	3776	1/1	0.76	0.33	-	76,76,76,76	0
85	MG	1	3906	1/1	0.93	0.36	-	42,42,42,42	0
85	MG	AT	223	1/1	0.93	0.79	-	45,45,45,45	0
85	MG	AR	3840	1/1	0.86	0.31	-	47,47,47,47	0
85	MG	AR	3803	1/1	0.78	0.51	-	35,35,35,35	0
85	MG	1	3782	1/1	0.91	0.45	-	58,58,58,58	0
85	MG	AR	3920	1/1	0.93	0.50	-	27,27,27,27	0
84	OHX	1	3689	7/7	0.94	0.52	-	140,140,141,141	0
85	MG	AR	4052	1/1	0.99	0.12	-	86,86,86,86	0
85	MG	AR	3898	1/1	0.97	0.62	-	28,28,28,28	0
85	MG	AR	3900	1/1	0.94	0.81	-	37,37,37,37	0
84	OHX	c8	201	7/7	0.97	0.20	-	146,147,147,148	0
85	MG	AR	3843	1/1	0.93	0.35	-	30,30,30,30	0
85	MG	1	3814	1/1	0.72	0.22	-	77,77,77,77	0
85	MG	AR	4246	1/1	0.87	0.41	-	22,22,22,22	0
84	OHX	z	201	7/7	0.87	0.39	-	155,156,157,157	0
84	OHX	6	1974	7/7	0.97	0.15	-	121,121,122,122	0
85	MG	6	2191	1/1	0.65	0.44	-	87,87,87,87	0
85	MG	AR	4055	1/1	0.92	0.17	-	40,40,40,40	0
85	MG	A	2156	1/1	0.86	0.62	-	45,45,45,45	0
85	MG	AR	4054	1/1	0.98	0.14	-	55,55,55,55	0
85	MG	1	4151	1/1	0.74	0.28	-	41,41,41,41	0
85	MG	1	4154	1/1	0.87	0.21	-	46,46,46,46	0
84	OHX	AR	3468	7/7	0.98	0.16	-	124,124,125,125	0
85	MG	w	201	1/1	0.95	0.42	-	37,37,37,37	0
84	OHX	AR	3724	7/7	0.95	0.27	-	130,130,131,131	0
85	MG	1	4174	1/1	0.91	0.83	-	55,55,55,55	0
84	OHX	1	3474	7/7	0.98	0.16	-	122,122,123,123	0
84	OHX	AR	3739	7/7	0.93	0.51	-	148,149,149,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	6	2167	1/1	0.80	0.50	-	53,53,53,53	0
85	MG	AR	3929	1/1	0.91	0.37	-	25,25,25,25	0
85	MG	AR	4062	1/1	0.95	0.17	-	42,42,42,42	0
85	MG	AR	3877	1/1	0.95	0.34	-	22,22,22,22	0
85	MG	6	2134	1/1	0.89	0.22	-	80,80,80,80	0
85	MG	4	237	1/1	0.89	0.20	-	38,38,38,38	0
84	OHX	A	1930	7/7	0.97	0.10	-	122,122,123,123	0
85	MG	AR	3925	1/1	0.93	0.41	-	34,34,34,34	0
84	OHX	AR	3727	7/7	0.91	0.23	-	187,188,188,188	0
85	MG	AR	4092	1/1	0.86	0.31	-	47,47,47,47	0
85	MG	AR	4028	1/1	0.89	0.19	-	41,41,41,41	0
85	MG	AR	4136	1/1	0.91	0.27	-	36,36,36,36	0
85	MG	AR	4255	1/1	0.66	0.64	-	57,57,57,57	0
85	MG	1	4051	1/1	0.97	0.23	-	44,44,44,44	0
85	MG	1	4093	1/1	0.76	0.37	-	57,57,57,57	0
85	MG	1	4133	1/1	0.98	0.09	-	51,51,51,51	0
85	MG	AR	4225	1/1	0.77	0.35	-	34,34,34,34	0
85	MG	AR	3983	1/1	0.99	0.12	-	33,33,33,33	0
85	MG	AR	4122	1/1	0.60	0.25	-	68,68,68,68	0
85	MG	AR	4010	1/1	0.94	0.30	-	30,30,30,30	0
85	MG	AR	4078	1/1	0.93	0.52	-	60,60,60,60	0
85	MG	1	4115	1/1	0.88	0.23	-	36,36,36,36	0
84	OHX	1	3624	7/7	0.96	0.20	-	136,136,136,137	0
85	MG	AR	4073	1/1	0.89	0.39	-	40,40,40,40	0
85	MG	1	4076	1/1	0.99	0.24	-	64,64,64,64	0
85	MG	AR	3991	1/1	0.86	0.14	-	98,98,98,98	0
85	MG	AR	4152	1/1	0.93	0.22	-	38,38,38,38	0
84	OHX	1	3434	7/7	0.98	0.25	-	126,127,127,127	0
85	MG	AR	3935	1/1	0.86	0.62	-	49,49,49,49	0
84	OHX	A	1906	7/7	0.99	0.23	-	142,143,143,143	0
85	MG	AR	4057	1/1	0.93	0.39	-	41,41,41,41	0
85	MG	1	3997	1/1	0.82	0.17	-	54,54,54,54	0
85	MG	1	3790	1/1	0.76	0.12	-	43,43,43,43	0
85	MG	AR	3785	1/1	0.92	0.47	-	57,57,57,57	0
85	MG	6	2102	1/1	0.94	0.46	-	45,45,45,45	0
85	MG	1	4136	1/1	0.93	0.27	-	40,40,40,40	0
85	MG	A	2150	1/1	0.57	0.16	-	86,86,86,86	0
85	MG	1	3987	1/1	0.81	0.68	-	65,65,65,65	0
85	MG	1	3913	1/1	0.91	0.59	-	28,28,28,28	0
85	MG	1	4063	1/1	0.98	0.09	-	38,38,38,38	0
85	MG	AR	4139	1/1	0.91	0.35	-	46,46,46,46	0
85	MG	AR	3878	1/1	0.99	0.36	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4088	1/1	0.81	0.25	-	44,44,44,44	0
85	MG	1	3975	1/1	0.93	0.33	-	42,42,42,42	0
84	OHX	1	3509	7/7	0.96	0.14	-	119,120,120,120	0
85	MG	6	2143	1/1	0.91	0.31	-	75,75,75,75	0
85	MG	AR	3783	1/1	0.75	0.32	-	44,44,44,44	0
85	MG	1	4184	1/1	0.89	0.26	-	36,36,36,36	0
85	MG	AR	4109	1/1	0.93	0.16	-	39,39,39,39	0
85	MG	AR	3884	1/1	0.98	0.45	-	22,22,22,22	0
85	MG	AR	4077	1/1	0.93	0.32	-	40,40,40,40	0
84	OHX	AR	3716	7/7	0.92	0.37	-	143,143,143,143	0
85	MG	AR	4244	1/1	0.77	0.40	-	45,45,45,45	0
85	MG	6	2190	1/1	0.89	0.48	-	66,66,66,66	0
85	MG	1	4137	1/1	0.88	0.17	-	55,55,55,55	0
85	MG	1	3927	1/1	0.88	0.24	-	42,42,42,42	0
85	MG	1	3952	1/1	0.69	0.24	-	77,77,77,77	0
85	MG	AR	4157	1/1	0.86	0.28	-	75,75,75,75	0
85	MG	1	4170	1/1	0.81	0.49	-	41,41,41,41	0
85	MG	1	4039	1/1	0.92	0.48	-	40,40,40,40	0
85	MG	1	3878	1/1	0.97	0.58	-	24,24,24,24	0
85	MG	1	4159	1/1	0.80	0.40	-	43,43,43,43	0
84	OHX	A	1951	7/7	0.97	0.24	-	145,145,146,146	0
85	MG	AR	4029	1/1	0.86	0.22	-	42,42,42,42	0
85	MG	1	4075	1/1	0.95	0.43	-	41,41,41,41	0
84	OHX	1	3598	7/7	0.97	0.27	-	127,127,127,127	0
85	MG	1	4061	1/1	0.71	0.31	-	54,54,54,54	0
85	MG	AR	4174	1/1	0.69	0.42	-	39,39,39,39	0
85	MG	1	3969	1/1	0.92	0.21	-	41,41,41,41	0
85	MG	1	3953	1/1	0.86	0.20	-	46,46,46,46	0
85	MG	1	3979	1/1	0.91	0.31	-	39,39,39,39	0
85	MG	AR	4240	1/1	0.83	0.55	-	70,70,70,70	0
85	MG	AR	4118	1/1	0.86	0.41	-	31,31,31,31	0
84	OHX	1	3508	7/7	0.98	0.10	-	113,114,114,114	0
85	MG	AR	4001	1/1	0.94	0.22	-	38,38,38,38	0
84	OHX	AR	3549	7/7	0.97	0.20	-	116,117,117,117	0
85	MG	1	3880	1/1	0.94	0.59	-	31,31,31,31	0
85	MG	1	4074	1/1	0.80	0.24	-	37,37,37,37	0
85	MG	AR	3771	1/1	0.91	0.36	-	42,42,42,42	0
84	OHX	A	1991	7/7	0.94	0.24	-	157,157,158,158	0
85	MG	AR	3847	1/1	0.93	0.16	-	38,38,38,38	0
85	MG	AR	4199	1/1	0.95	0.36	-	45,45,45,45	0
85	MG	1	4082	1/1	0.85	0.30	-	35,35,35,35	0
85	MG	AR	4149	1/1	0.88	0.38	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	A	2116	1/1	0.79	0.61	-	67,67,67,67	0
85	MG	1	4213	1/1	0.91	0.64	-	50,50,50,50	0
85	MG	AR	3820	1/1	0.92	0.26	-	43,43,43,43	0
84	OHX	1	3656	7/7	0.90	0.50	-	143,143,143,144	0
85	MG	AR	4059	1/1	0.89	0.20	-	47,47,47,47	0
85	MG	AR	4214	1/1	0.73	0.24	-	55,55,55,55	0
85	MG	AR	4008	1/1	0.94	0.25	-	26,26,26,26	0
85	MG	AR	3927	1/1	0.92	0.45	-	35,35,35,35	0
85	MG	A	2111	1/1	0.94	0.26	-	90,90,90,90	0
85	MG	1	4018	1/1	0.93	0.33	-	38,38,38,38	0
85	MG	AR	4238	1/1	0.85	0.39	-	36,36,36,36	0
84	OHX	A	2041	7/7	0.88	0.46	-	139,139,140,140	0
84	OHX	1	3597	7/7	0.96	0.39	-	117,117,118,118	0
85	MG	AR	4232	1/1	0.83	0.43	-	28,28,28,28	0
85	MG	AR	4248	1/1	0.86	0.94	-	45,45,45,45	0
85	MG	1	4157	1/1	0.97	0.49	-	60,60,60,60	0
85	MG	1	3848	1/1	0.92	0.41	-	60,60,60,60	0
85	MG	AR	4013	1/1	0.60	0.29	-	65,65,65,65	0
85	MG	1	3761	1/1	0.83	0.30	-	41,41,41,41	0
85	MG	A	2081	1/1	0.84	0.31	-	66,66,66,66	0
84	OHX	AR	3456	7/7	0.97	0.19	-	117,117,117,117	0
85	MG	AR	3992	1/1	0.92	0.64	-	67,67,67,67	0
85	MG	AR	4050	1/1	0.89	0.31	-	91,91,91,91	0
85	MG	1	3944	1/1	0.87	0.48	-	32,32,32,32	0
84	OHX	AT	211	7/7	0.96	0.11	-	137,138,138,138	0
84	OHX	AR	3649	7/7	0.93	0.50	-	144,144,144,144	0
85	MG	3	220	1/1	0.88	0.17	-	68,68,68,68	0
85	MG	6	2162	1/1	0.77	0.27	-	60,60,60,60	0
85	MG	AR	3868	1/1	0.88	0.47	-	25,25,25,25	0
85	MG	1	3729	1/1	0.93	0.32	-	90,90,90,90	0
85	MG	AR	4126	1/1	0.88	0.69	-	83,83,83,83	0
85	MG	A	2154	1/1	0.97	0.93	-	45,45,45,45	0
84	OHX	1	3443	7/7	0.98	0.19	-	119,120,120,120	0
85	MG	x	207	1/1	0.89	0.30	-	33,33,33,33	0
85	MG	n	201	1/1	0.87	0.26	-	43,43,43,43	0
85	MG	CP	504	1/1	0.95	0.23	-	46,46,46,46	0
85	MG	6	2111	1/1	0.83	0.42	-	61,61,61,61	0
84	OHX	1	3654	7/7	0.96	0.14	-	136,136,136,137	0
85	MG	1	4104	1/1	0.60	0.45	-	53,53,53,53	0
85	MG	AR	4211	1/1	0.93	0.14	-	73,73,73,73	0
85	MG	AR	3755	1/1	0.90	0.19	-	56,56,56,56	0
84	OHX	AR	3624	7/7	0.95	0.33	-	150,150,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4239	1/1	0.82	0.42	-	39,39,39,39	0
85	MG	1	3991	1/1	0.98	0.17	-	66,66,66,66	0
84	OHX	1	3564	7/7	0.97	0.24	-	126,126,127,127	0
85	MG	1	4102	1/1	0.90	0.37	-	57,57,57,57	0
85	MG	4	236	1/1	0.79	0.19	-	50,50,50,50	0
84	OHX	6	1997	7/7	0.95	0.36	-	132,132,133,133	0
85	MG	1	3898	1/1	0.90	0.46	-	33,33,33,33	0
85	MG	1	3765	1/1	0.90	0.49	-	21,21,21,21	0
85	MG	1	3976	1/1	0.78	0.14	-	61,61,61,61	0
85	MG	A	2074	1/1	0.96	0.41	-	55,55,55,55	0
85	MG	1	3773	1/1	0.93	0.21	-	38,38,38,38	0
85	MG	A	2145	1/1	0.99	0.21	-	92,92,92,92	0
85	MG	AR	3979	1/1	0.91	0.57	-	41,41,41,41	0
85	MG	AR	3876	1/1	0.98	0.55	-	27,27,27,27	0
85	MG	1	3864	1/1	0.92	0.25	-	38,38,38,38	0
85	MG	AR	4197	1/1	0.90	0.27	-	35,35,35,35	0
84	OHX	6	2017	7/7	0.96	0.29	-	135,135,136,136	0
84	OHX	AR	3571	7/7	0.93	0.18	-	125,125,125,125	0
85	MG	6	2172	1/1	0.96	0.26	-	38,38,38,38	0
85	MG	A	2125	1/1	0.89	0.85	-	56,56,56,56	0
84	OHX	AR	3586	7/7	0.96	0.24	-	119,119,120,120	0
85	MG	1	4113	1/1	0.88	0.26	-	57,57,57,57	0
85	MG	1	4017	1/1	0.93	0.21	-	101,101,101,101	0
84	OHX	A	2036	7/7	0.88	0.15	-	252,253,253,253	0
85	MG	6	2166	1/1	0.90	0.48	-	53,53,53,53	0
85	MG	AR	4065	1/1	0.95	0.25	-	31,31,31,31	0
85	MG	AS	220	1/1	0.64	0.37	-	68,68,68,68	0
85	MG	AR	4219	1/1	0.68	0.17	-	67,67,67,67	0
85	MG	AR	4221	1/1	0.83	0.28	-	35,35,35,35	0
84	OHX	1	3722	1/7	0.92	0.12	-	136,136,136,136	0
85	MG	DQ	203	1/1	0.86	0.22	-	45,45,45,45	0
85	MG	DQ	204	1/1	0.91	0.35	-	32,32,32,32	0
85	MG	1	4203	1/1	0.81	0.24	-	31,31,31,31	0
85	MG	1	3870	1/1	0.83	0.28	-	47,47,47,47	0
85	MG	AR	4183	1/1	0.85	0.23	-	55,55,55,55	0
85	MG	AR	4016	1/1	0.93	0.36	-	33,33,33,33	0
85	MG	1	3838	1/1	0.96	0.57	-	33,33,33,33	0
85	MG	A	2093	1/1	0.88	0.13	-	100,100,100,100	0
85	MG	1	4001	1/1	0.79	0.45	-	47,47,47,47	0
85	MG	1	4086	1/1	0.93	0.29	-	32,32,32,32	0
85	MG	1	3926	1/1	0.86	0.16	-	37,37,37,37	0
85	MG	6	2067	1/1	0.93	0.30	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4195	1/1	0.99	0.18	-	63,63,63,63	0
85	MG	1	3931	1/1	0.84	0.53	-	32,32,32,32	0
84	OHX	1	3504	7/7	0.97	0.18	-	127,127,127,128	0
85	MG	AR	3924	1/1	0.92	0.49	-	27,27,27,27	0
85	MG	AR	3855	1/1	0.95	0.43	-	33,33,33,33	0
85	MG	AS	217	1/1	0.81	0.47	-	44,44,44,44	0
85	MG	AR	3998	1/1	0.80	0.45	-	40,40,40,40	0
85	MG	6	2132	1/1	0.92	0.35	-	42,42,42,42	0
85	MG	6	2178	1/1	0.83	0.36	-	57,57,57,57	0
85	MG	AR	3759	1/1	0.85	0.62	-	34,34,34,34	0
85	MG	1	3968	1/1	0.96	0.47	-	29,29,29,29	0
85	MG	1	3958	1/1	0.49	0.38	-	44,44,44,44	0
85	MG	AR	3807	1/1	0.90	0.38	-	25,25,25,25	0
85	MG	1	4199	1/1	0.96	0.59	-	24,24,24,24	0
85	MG	AR	4119	1/1	0.71	0.39	-	91,91,91,91	0
84	OHX	1	3610	7/7	0.94	0.23	-	130,130,131,131	0
84	OHX	AR	3697	7/7	0.96	0.25	-	114,115,115,115	0
85	MG	1	3762	1/1	0.90	0.56	-	30,30,30,30	0
84	OHX	AR	3725	7/7	0.93	0.20	-	165,165,165,165	0
85	MG	6	2120	1/1	0.87	0.42	-	69,69,69,69	0
85	MG	AR	4250	1/1	0.87	0.80	-	59,59,59,59	0
85	MG	AR	3997	1/1	0.94	0.12	-	44,44,44,44	0
85	MG	6	2130	1/1	0.80	0.31	-	66,66,66,66	0
85	MG	6	2094	1/1	0.93	0.22	-	37,37,37,37	0
85	MG	1	4212	1/1	0.94	0.42	-	39,39,39,39	0
84	OHX	AR	3516	7/7	0.97	0.15	-	112,112,112,112	0
85	MG	AT	229	1/1	0.89	0.42	-	55,55,55,55	0
85	MG	AR	4131	1/1	0.98	0.09	-	39,39,39,39	0
84	OHX	AR	3572	7/7	0.98	0.28	-	118,119,119,119	0
84	OHX	AR	3534	7/7	0.96	0.16	-	109,109,109,109	0
84	OHX	AR	3506	7/7	0.92	0.21	-	112,112,112,112	0
84	OHX	1	3698	7/7	0.92	0.30	-	162,163,163,163	0
85	MG	AR	4220	1/1	0.78	0.39	-	44,44,44,44	0
84	OHX	A	2027	7/7	0.95	0.33	-	159,160,161,161	0
85	MG	1	4003	1/1	0.84	0.35	-	79,79,79,79	0
84	OHX	6	2024	7/7	0.93	0.35	-	151,152,152,153	0
84	OHX	O	201	7/7	0.96	0.28	-	158,159,159,160	0
85	MG	AF	201	1/1	0.93	0.30	-	41,41,41,41	0
84	OHX	6	1984	7/7	0.95	0.26	-	150,150,151,151	0
85	MG	6	2066	1/1	0.86	0.35	-	74,74,74,74	0
85	MG	1	4219	1/1	0.89	0.26	-	98,98,98,98	0
85	MG	AS	230	1/1	0.94	0.42	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3496	7/7	0.98	0.16	-	115,115,115,115	0
85	MG	AR	3854	1/1	0.94	0.40	-	48,48,48,48	0
85	MG	CQ	204	1/1	0.85	0.41	-	30,30,30,30	0
85	MG	DO	202	1/1	0.93	0.26	-	42,42,42,42	0
85	MG	4	219	1/1	0.95	0.68	-	42,42,42,42	0
84	OHX	1	3550	7/7	0.95	0.18	-	115,115,115,116	0
85	MG	6	2097	1/1	0.94	0.42	-	46,46,46,46	0
85	MG	4	233	1/1	0.71	0.20	-	48,48,48,48	0
85	MG	1	3847	1/1	0.91	0.54	-	28,28,28,28	0
85	MG	A	2158	1/1	0.93	0.34	-	67,67,67,67	0
85	MG	1	4200	1/1	0.97	0.49	-	22,22,22,22	0
85	MG	1	4210	1/1	0.87	0.30	-	24,24,24,24	0
85	MG	1	3941	1/1	0.78	0.41	-	78,78,78,78	0
85	MG	1	3982	1/1	0.89	0.37	-	32,32,32,32	0
85	MG	D	301	1/1	0.89	0.58	-	58,58,58,58	0
85	MG	AR	3837	1/1	0.97	0.59	-	19,19,19,19	0
85	MG	AR	4117	1/1	0.74	0.31	-	64,64,64,64	0
85	MG	1	4106	1/1	0.95	0.34	-	67,67,67,67	0
85	MG	4	228	1/1	0.89	0.26	-	54,54,54,54	0
85	MG	AR	3917	1/1	0.94	0.50	-	42,42,42,42	0
85	MG	AR	3821	1/1	0.90	0.21	-	42,42,42,42	0
85	MG	AR	4015	1/1	0.93	0.16	-	45,45,45,45	0
85	MG	AR	3815	1/1	0.91	0.24	-	32,32,32,32	0
85	MG	AR	4143	1/1	0.93	0.26	-	34,34,34,34	0
85	MG	A	2058	1/1	0.97	0.67	-	46,46,46,46	0
85	MG	AS	223	1/1	0.88	0.28	-	41,41,41,41	0
84	OHX	1	3520	7/7	0.96	0.18	-	123,123,124,124	0
85	MG	1	4007	1/1	0.86	0.42	-	29,29,29,29	0
85	MG	AR	4144	1/1	0.93	0.33	-	41,41,41,41	0
85	MG	AS	214	1/1	0.92	0.30	-	52,52,52,52	0
85	MG	AR	3818	1/1	0.98	0.79	-	37,37,37,37	0
85	MG	1	4198	1/1	0.90	0.60	-	43,43,43,43	0
85	MG	1	4158	1/1	0.75	0.45	-	47,47,47,47	0
85	MG	AR	3885	1/1	0.97	0.37	-	33,33,33,33	0
85	MG	1	3943	1/1	0.92	0.54	-	37,37,37,37	0
85	MG	1	3874	1/1	0.85	0.55	-	49,49,49,49	0

## 6.5 Other polymers

There are no such residues in this entry.