



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 11, 2025 – 09:49 pm GMT

PDB ID : 7AZS  
Title : 70S thermus thermophilus ribosome with bound antibiotic lead SEQ-569  
Authors : Jenner, L.B.; Yusupov, M.; Yusupova, G.; Rak, A.  
Deposited on : 2020-11-17  
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

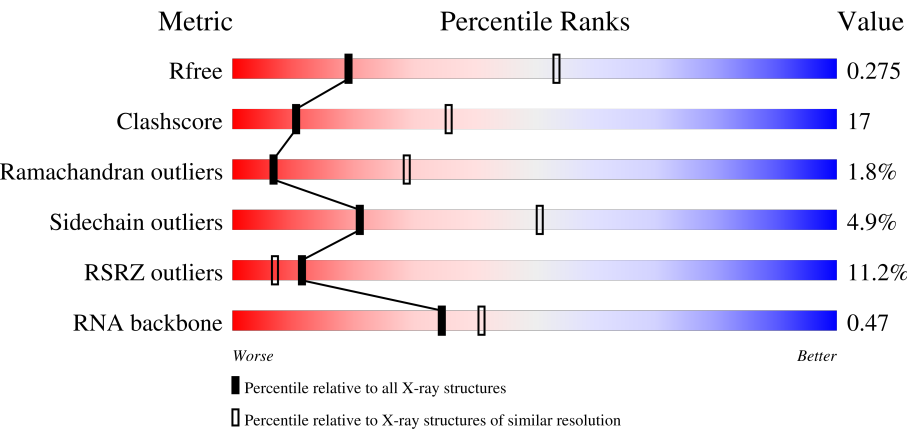
# 1 Overall quality at a glance i

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 <sub>free</sub>	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)
RNA backbone	3690	1021 (3.36-2.84)

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

Mol	Chain	Length	Quality of chain
1	16SA	1512	<div><div>3%</div><div></div><div>71%</div><div>24%</div><div></div></div>
1	16SB	1512	<div><div>%</div><div></div><div>71%</div><div>25%</div><div></div></div>
2	S2A	256	<div><div>31%</div><div></div><div>53%</div><div>35%</div><div>5%</div><div>7%</div></div>
2	S2B	256	<div><div>30%</div><div></div><div>46%</div><div>43%</div><div></div><div>7%</div></div>

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Mol	Chain	Length	Quality of chain
3	S3A	239	
3	S3B	239	
4	S4A	209	
4	S4B	209	
5	S5A	162	
5	S5B	162	
6	S6A	101	
6	S6B	101	
7	S7A	156	
7	S7B	156	
8	S8A	138	
8	S8B	138	
9	S9A	128	
9	S9B	128	
10	S10A	105	
10	S10B	105	
11	S11A	129	
11	S11B	129	
12	S12A	132	
12	S12B	132	
13	S13A	126	
13	S13B	126	
14	S14A	61	
14	S14B	61	
15	S15A	89	

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Mol	Chain	Length	Quality of chain
15	S15B	89	
16	S16A	88	
16	S16B	88	
17	S17A	105	
17	S17B	105	
18	S18A	88	
18	S18B	88	
19	S19A	93	
19	S19B	93	
20	S20A	106	
20	S20B	106	
21	THXA	27	
21	THXB	27	
22	ASIA	76	
23	PSIA	76	
23	PSIB	76	
24	ESIA	76	
24	ESIB	76	
25	MRNA	30	
25	MRNB	30	
26	TRNA	76	
27	23SA	2911	
27	23SB	2911	
28	5SA	124	
28	5SB	124	

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Mol	Chain	Length	Quality of chain
29	L2A	276	
29	L2B	276	
30	L3A	206	
30	L3B	206	
31	L4A	210	
31	L4B	210	
32	L5A	182	
32	L5B	182	
33	L6A	180	
33	L6B	180	
34	L9A	148	
34	L9B	148	
35	L13A	140	
35	L13B	140	
36	L14A	122	
36	L14B	122	
37	L15A	150	
37	L15B	150	
38	L16A	141	
38	L16B	141	
39	L17A	118	
39	L17B	118	
40	L18A	112	
40	L18B	112	
41	L19A	146	

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Mol	Chain	Length	Quality of chain
41	L19B	146	
42	L20A	118	
42	L20B	118	
43	L21A	101	
43	L21B	101	
44	L22A	113	
44	L22B	113	
45	L23A	96	
45	L23B	96	
46	L24A	110	
46	L24B	110	
47	L25A	206	
47	L25B	206	
48	L27A	85	
48	L27B	85	
49	L28A	98	
49	L28B	98	
50	L29A	72	
50	L29B	72	
51	L30A	60	
51	L30B	60	
52	L31A	71	
52	L31B	71	
53	L32A	60	
53	L32B	60	

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Mol	Chain	Length	Quality of chain
54	L33A	54	
54	L33B	54	
55	L34A	49	
55	L34B	49	
56	L35A	65	
56	L35B	65	
57	ASIB	76	

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
58	MG	16SA	2217	-	-	-	X
58	MG	16SB	2248	-	-	-	X
58	MG	23SA	3015	-	-	-	X
58	MG	23SB	3087	-	-	-	X
59	K	23SA	3390	-	-	-	X

## 2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 306277 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 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	16SA	1511	Total	C	N	O	P	0	0	0
			32489	14469	6014	10495	1511			
1	16SB	1507	Total	C	N	O	P	0	0	0
			32409	14433	6005	10464	1507			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S2A	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
2	S2B	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S3A	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	S3B	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	S4A	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			
4	S4B	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	S5A	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	S5B	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	S6A	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			
6	S6B	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	S7A	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	6			
7	S7B	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	S8A	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			
8	S8B	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	S9A	127	Total	C	N	O		0	0	0
			1009	639	197	173				
9	S9B	127	Total	C	N	O		0	0	0
			1009	639	197	173				

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	S10A	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	S10B	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	S11A	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			
11	S11B	117	Total	C	N	O	S	0	0	0
			873	543	166	161	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	S12A	125	Total	C	N	O	S	0	0	0
			977	615	196	164	2			
12	S12B	125	Total	C	N	O	S	0	0	0
			977	615	196	164	2			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	S13A	119	Total	C	N	O	S	0	0	0
			946	585	195	164	2			
13	S13B	121	Total	C	N	O	S	0	0	0
			964	597	199	166	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	S14A	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			
14	S14B	59	Total	C	N	O	S	0	0	0
			486	309	103	70	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	S15A	88	Total	C	N	O	S	0	0	0
			733	459	147	125	2			
15	S15B	88	Total	C	N	O	S	0	0	0
			733	459	147	125	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	S16A	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
16	S16B	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	S17A	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	S17B	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	S18A	71	Total	C	N	O	0	0	0
			584	373	116	95			
18	S18B	70	Total	C	N	O	0	0	0
			573	367	112	94			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S19A	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			
19	S19B	86	Total	C	N	O	S	0	0	0
			684	436	126	120	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S20A	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			
20	S20B	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	THXA	24	Total	C	N	O	0	0	0
			208	128	50	30			
21	THXB	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called Phe-tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	ASIA	76	Total	C	N	O	P	S	0	0	0
			1628	731	290	530	75	2			

- Molecule 23 is a RNA chain called Phe-tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	PSIA	76	Total	C	N	O	P	S	0	0	0
			1635	735	291	532	75	2			
23	PSIB	76	Total	C	N	O	P	S	0	0	0
			1635	735	291	532	75	2			

- Molecule 24 is a RNA chain called Phe-tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	ESIA	76	Total	C	N	O	P	S	0	0	0
			1626	729	290	531	75	1			
24	ESIB	76	Total	C	N	O	P	S	0	0	0
			1626	729	290	531	75	1			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	MRNA	30	Total	C	N	O	P	0	0	0
			621	279	88	225	29			
25	MRNB	30	Total	C	N	O	P	0	0	0
			621	279	88	225	29			

- Molecule 26 is a RNA chain called Phe-tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
26	TRNA	73	Total	C	N	O	P	S	0	0	0
			1565	702	279	510	72	2			

- Molecule 27 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	23SA	2889	Total	C	N	O	P	0	0	0
			62225	27699	11629	20008	2889			
27	23SB	2875	Total	C	N	O	P	0	0	0
			61926	27566	11578	19907	2875			

- Molecule 28 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	5SA	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
28	5SB	121	Total	C	N	O	P	0	0	0
			2598	1156	481	840	121			

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	L2A	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
29	L2B	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	L3A	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
30	L3B	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 31 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	L4A	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
31	L4B	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 32 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	L5A	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	L5B	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			

- Molecule 33 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	L6A	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
33	L6B	173	Total	C	N	O	S	0	0	0
			1327	842	249	235	1			

- Molecule 34 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	L9A	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
34	L9B	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	L13A	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
35	L13B	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	L14A	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			
36	L14B	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	L15A	150	Total	C	N	O	S	0	0	0
			1144	712	232	197	3			
37	L15B	150	Total	C	N	O	S	0	0	0
			1144	712	232	197	3			

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	L16A	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			
38	L16B	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L17A	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
39	L17B	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	L18A	112	Total	C	N	O	S	0	0	0
			889	561	177	150	1			
40	L18B	111	Total	C	N	O		0	0	0
			881	556	176	149				

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	L19A	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
41	L19B	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	L20A	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			
42	L20B	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	L21A	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			
43	L21B	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	L22A	113	Total	C	N	O	S	0	0	0
			899	566	177	154	2			
44	L22B	113	Total	C	N	O	S	0	0	0
			899	566	177	154	2			

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L23A	95	Total	C	N	O	S	0	0	0
			747	485	135	126	1			
45	L23B	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	L24A	108	Total	C	N	O	S	0	0	0
			824	528	153	138	5			
46	L24B	106	Total	C	N	O	S	0	0	0
			775	494	147	129	5			

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	L25A	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			
47	L25B	176	Total	C	N	O	S	0	0	0
			1404	897	252	252	3			

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	L27A	84	Total	C	N	O	S	0	0	0
			661	410	140	110	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	L27B	84	Total	C	N	O	S	0	0	0
			661	410	140	110	1			

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	L28A	97	Total	C	N	O	S	0	0	0
			762	481	150	130	1			
49	L28B	97	Total	C	N	O	S	0	0	0
			762	481	150	130	1			

- Molecule 50 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	L29A	69	Total	C	N	O	S	0	0	0
			583	363	117	101	2			
50	L29B	68	Total	C	N	O	S	0	0	0
			575	358	116	100	1			

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	L30A	59	Total	C	N	O	0	0	0
			468	298	90	80			
51	L30B	59	Total	C	N	O	0	0	0
			468	298	90	80			

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	L31A	71	Total	C	N	O	S	0	0	0
			580	364	108	103	5			
52	L31B	71	Total	C	N	O	S	0	0	0
			580	364	108	103	5			

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	L32A	56	Total	C	N	O	S	0	0	0
			434	272	87	70	5			
53	L32B	56	Total	C	N	O	S	0	0	0
			434	272	87	70	5			

- Molecule 54 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	L33A	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
54	L33B	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 55 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	L34A	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
55	L34B	49	Total	C	N	O	S	0	0	0
			429	263	108	56	2			

- Molecule 56 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	L35A	64	Total	C	N	O	S	0	0	0
			516	331	102	81	2			
56	L35B	64	Total	C	N	O	S	0	0	0
			516	331	102	81	2			

- Molecule 57 is a RNA chain called Phe-tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
57	ASIB	76	Total	C	N	O	P	S	0	0	0
			1627	730	290	531	75	1			

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	16SA	90	Total	Mg	0	0
			90	90		
58	S4A	1	Total	Mg	0	0
			1	1		
58	PSIA	2	Total	Mg	0	0
			2	2		
58	MRNA	1	Total	Mg	0	0
			1	1		
58	23SA	334	Total	Mg	0	0
			334	334		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	5SA	6	Total 6	Mg 6	0	0
58	L3A	2	Total 2	Mg 2	0	0
58	L4A	2	Total 2	Mg 2	0	0
58	L5A	1	Total 1	Mg 1	0	0
58	L15A	2	Total 2	Mg 2	0	0
58	L17A	1	Total 1	Mg 1	0	0
58	L23A	1	Total 1	Mg 1	0	0
58	L27A	2	Total 2	Mg 2	0	0
58	L30A	1	Total 1	Mg 1	0	0
58	L32A	1	Total 1	Mg 1	0	0
58	L33A	1	Total 1	Mg 1	0	0
58	L34A	1	Total 1	Mg 1	0	0
58	L35A	1	Total 1	Mg 1	0	0
58	16SB	85	Total 86	Mg 86	0	1
58	S5B	2	Total 2	Mg 2	0	0
58	PSIB	3	Total 3	Mg 3	0	0
58	23SB	239	Total 240	Mg 240	0	1
58	5SB	4	Total 4	Mg 4	0	0
58	L2B	1	Total 1	Mg 1	0	0
58	L3B	2	Total 2	Mg 2	0	0
58	L5B	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	L27B	1	Total 1	Mg 1	0	0
58	L35B	2	Total 2	Mg 2	0	0

- Molecule 59 is POTASSIUM ION (three-letter code: K) (formula: K).

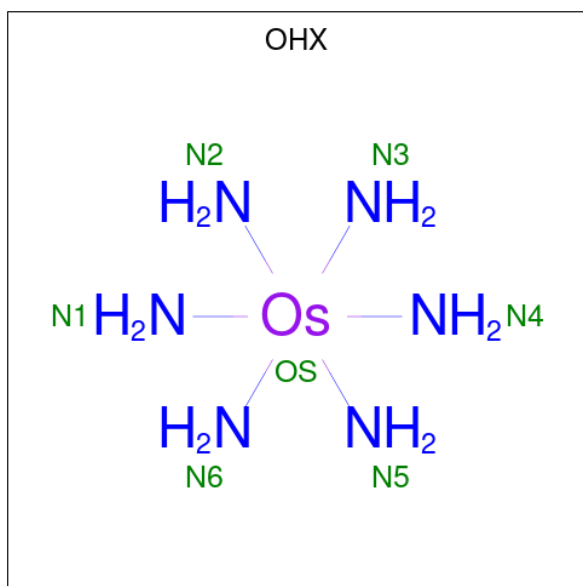
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	16SA	46	Total 46	K 46	0	0
59	S6A	1	Total 1	K 1	0	0
59	S13A	1	Total 1	K 1	0	0
59	S20A	1	Total 1	K 1	0	0
59	PSIA	2	Total 2	K 2	0	0
59	23SA	101	Total 101	K 101	0	0
59	5SA	2	Total 2	K 2	0	0
59	L2A	1	Total 1	K 1	0	0
59	L3A	1	Total 1	K 1	0	0
59	L4A	1	Total 1	K 1	0	0
59	L5A	1	Total 1	K 1	0	0
59	L16A	1	Total 1	K 1	0	0
59	16SB	36	Total 36	K 36	0	0
59	S4B	1	Total 1	K 1	0	0
59	S6B	1	Total 1	K 1	0	0
59	S13B	1	Total 1	K 1	0	0
59	S20B	1	Total 1	K 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	23SB	83	Total	K	0	0
			83	83		
59	5SB	1	Total	K	0	0
			1	1		
59	L2B	1	Total	K	0	0
			1	1		
59	L3B	1	Total	K	0	0
			1	1		
59	L4B	1	Total	K	0	0
			1	1		
59	L5B	1	Total	K	0	0
			1	1		
59	L16B	1	Total	K	0	0
			1	1		

- Molecule 60 is osmium (III) hexammine (three-letter code: OHX) (formula:  $\text{H}_{12}\text{N}_6\text{Os}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	16SA	1	Total	N	Os	0	0
			7	6	1		
60	S19A	1	Total	N	Os	0	0
			7	6	1		
60	ASIA	1	Total	N	Os	0	0
			7	6	1		
60	ASIA	1	Total	N	Os	0	0
			7	6	1		
60	ASIA	1	Total	N	Os	0	0
			7	6	1		
60	PSIA	1	Total	N	Os	0	0
			7	6	1		
60	ESIA	1	Total	N	Os	0	0
			7	6	1		
60	MRNA	1	Total	N	Os	0	0
			7	6	1		
60	TRNA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	TRNA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
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			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
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60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
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60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
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60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	23SA	1	Total	N	Os	0	0
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60	23SA	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
60	23SA	1	Total	N	Os	0	0
			7	6	1		
60	5SA	1	Total	N	Os	0	0
			7	6	1		
60	5SA	1	Total	N	Os	0	0
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60	5SA	1	Total	N	Os	0	0
			7	6	1		
60	5SA	1	Total	N	Os	0	0
			7	6	1		
60	5SA	1	Total	N	Os	0	0
			7	6	1		
60	5SA	1	Total	N	Os	0	0
			7	6	1		
60	5SA	1	Total	N	Os	0	0
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60	5SA	1	Total	N	Os	0	0
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60	5SA	1	Total	N	Os	0	0
			7	6	1		
60	L4A	1	Total	N	Os	0	0
			7	6	1		
60	L15A	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	L17A	1	Total	N	Os	0	0
			7	6	1		
60	L19A	1	Total	N	Os	0	0
			7	6	1		
60	L27A	1	Total	N	Os	0	0
			7	6	1		
60	L27A	1	Total	N	Os	0	0
			7	6	1		
60	L28A	1	Total	N	Os	0	0
			7	6	1		
60	L35A	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
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60	16SB	1	Total	N	Os	0	0
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60	16SB	1	Total	N	Os	0	0
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60	16SB	1	Total	N	Os	0	0
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60	16SB	1	Total	N	Os	0	0
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60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
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60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
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60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
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60	16SB	1	Total	N	Os	0	0
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			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
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60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		
60	16SB	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	S4B	1	Total	N	Os	0	0
			7	6	1		
60	S8B	1	Total	N	Os	0	0
			7	6	1		
60	S14B	1	Total	N	Os	0	0
			7	6	1		
60	ASIB	1	Total	N	Os	0	0
			7	6	1		
60	ASIB	1	Total	N	Os	0	0
			7	6	1		
60	ASIB	1	Total	N	Os	0	0
			7	6	1		
60	PSIB	1	Total	N	Os	0	0
			7	6	1		
60	PSIB	1	Total	N	Os	0	0
			7	6	1		
60	PSIB	1	Total	N	Os	0	0
			7	6	1		
60	ESIB	1	Total	N	Os	0	0
			7	6	1		
60	MRNB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
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60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
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60	23SB	1	Total	N	Os	0	0
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60	23SB	1	Total	N	Os	0	0
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60	23SB	1	Total	N	Os	0	0
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60	23SB	1	Total	N	Os	0	0
			7	6	1		
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60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
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60	23SB	1	Total	N	Os	0	0
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60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
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60	23SB	1	Total	N	Os	0	0
			7	6	1		
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60	23SB	1	Total	N	Os	0	0
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			7	6	1		
60	23SB	1	Total	N	Os	0	0
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			7	6	1		
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			7	6	1		
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			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
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60	23SB	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
60	23SB	1	Total	N	Os	0	0
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			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
60	23SB	1	Total	N	Os	0	0
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60	23SB	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	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		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	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		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
60	23SB	1	Total	N	Os	0	0
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60	23SB	1	Total	N	Os	0	0
			7	6	1		

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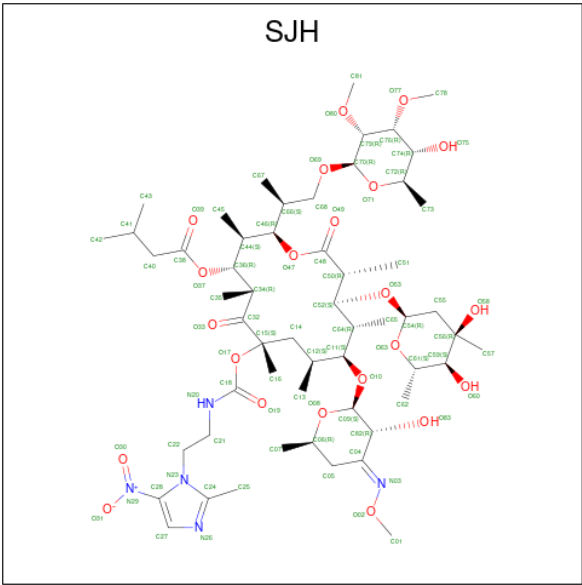
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	5SB	1	Total	N	Os	0	0
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60	5SB	1	Total	N	Os	0	0
			7	6	1		
60	5SB	1	Total	N	Os	0	0
			7	6	1		
60	5SB	1	Total	N	Os	0	0
			7	6	1		
60	5SB	1	Total	N	Os	0	0
			7	6	1		
60	5SB	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O		
60	5SB	1	7	6	1	0	0
60	5SB	1	7	6	1	0	0
60	5SB	1	7	6	1	0	0
60	L17B	1	7	6	1	0	0
60	L20B	1	7	6	1	0	0
60	L35B	1	7	6	1	0	0

- Molecule 61 is (2R,3S,4R,5R,7S,9S,10S,11R,12S,13R)-12-(((2R,4R,5S,6S)-4,5-dihydroxy-4,6-dimethyltetrahydro-2H-pyran-2-yl)oxy)-2-(((S)-1-(((2R,3R,4R,5R,6R)-5-hydroxy-3,4-dimethoxy-6-methyltetrahydro-2H-pyran-2-yl)oxy)propan-2-yl)-10-(((2S,3R,6R,E)-3-hydroxy-4-(methoxyimino)-6-methyltetrahydro-2H-pyran-2-yl)oxy)-3,5,7,9,11,13-hexamethyl-7-(((2-(2-methyl-5-nitro-1H-imidazol-1-yl)ethyl)carbamoyl)oxy)-6,14-dioxooxacyclotetradecan-4-yl 3-methylbutanoate (three-letter code: SJH) (formula: C<sub>56</sub>H<sub>93</sub>N<sub>5</sub>O<sub>22</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
61	23SA	1	83	56	5	22	0	0
61	23SB	1	83	56	5	22	0	0

- Molecule 62 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	16SA	173	Total O 173 173	0	0
62	S4A	2	Total O 2 2	0	0
62	S5A	1	Total O 1 1	0	0
62	S13A	1	Total O 1 1	0	0
62	S14A	1	Total O 1 1	0	0
62	S16A	1	Total O 1 1	0	0
62	S17A	1	Total O 1 1	0	0
62	THXA	3	Total O 3 3	0	0
62	PSIA	6	Total O 6 6	0	0
62	ESIA	1	Total O 1 1	0	0
62	23SA	801	Total O 801 801	0	0
62	5SA	14	Total O 14 14	0	0
62	L2A	9	Total O 9 9	0	0
62	L3A	7	Total O 7 7	0	0
62	L4A	6	Total O 6 6	0	0
62	L15A	10	Total O 10 10	0	0
62	L16A	1	Total O 1 1	0	0
62	L17A	2	Total O 2 2	0	0
62	L18A	2	Total O 2 2	0	0
62	L19A	1	Total O 1 1	0	0
62	L23A	1	Total O 1 1	0	0
62	L27A	3	Total O 3 3	0	0

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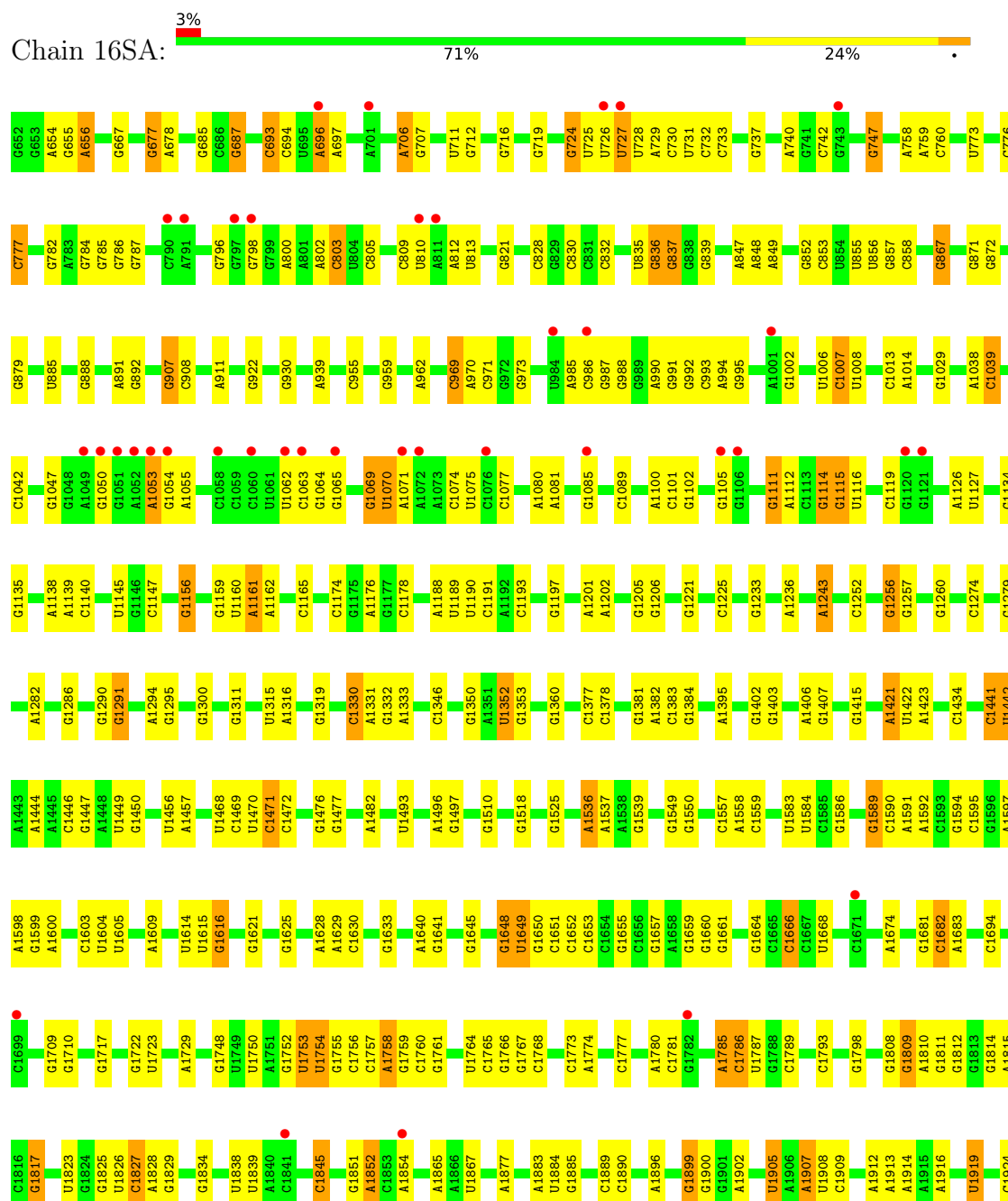
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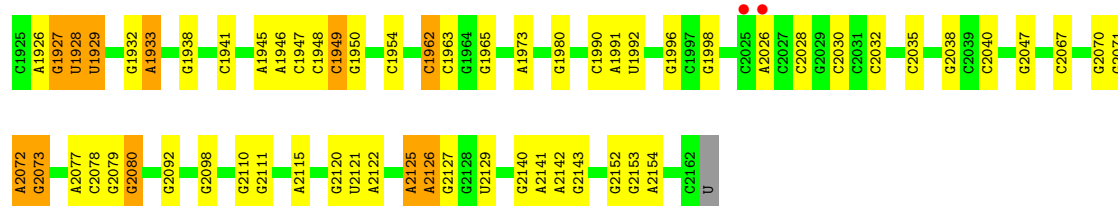
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	L30A	1	Total 1	O 1	0	0
62	L34A	1	Total 1	O 1	0	0
62	L35A	1	Total 1	O 1	0	0
62	16SB	158	Total 158	O 158	0	0
62	S4B	1	Total 1	O 1	0	0
62	S5B	1	Total 1	O 1	0	0
62	S9B	1	Total 1	O 1	0	0
62	S12B	2	Total 2	O 2	0	0
62	S14B	2	Total 2	O 2	0	0
62	23SB	518	Total 518	O 518	0	0
62	5SB	5	Total 5	O 5	0	0
62	L2B	13	Total 13	O 13	0	0
62	L3B	6	Total 6	O 6	0	0
62	L4B	1	Total 1	O 1	0	0
62	L15B	7	Total 7	O 7	0	0
62	L27B	2	Total 2	O 2	0	0
62	L28B	1	Total 1	O 1	0	0
62	L30B	2	Total 2	O 2	0	0
62	L35B	6	Total 6	O 6	0	0

### 3 Residue-property plots

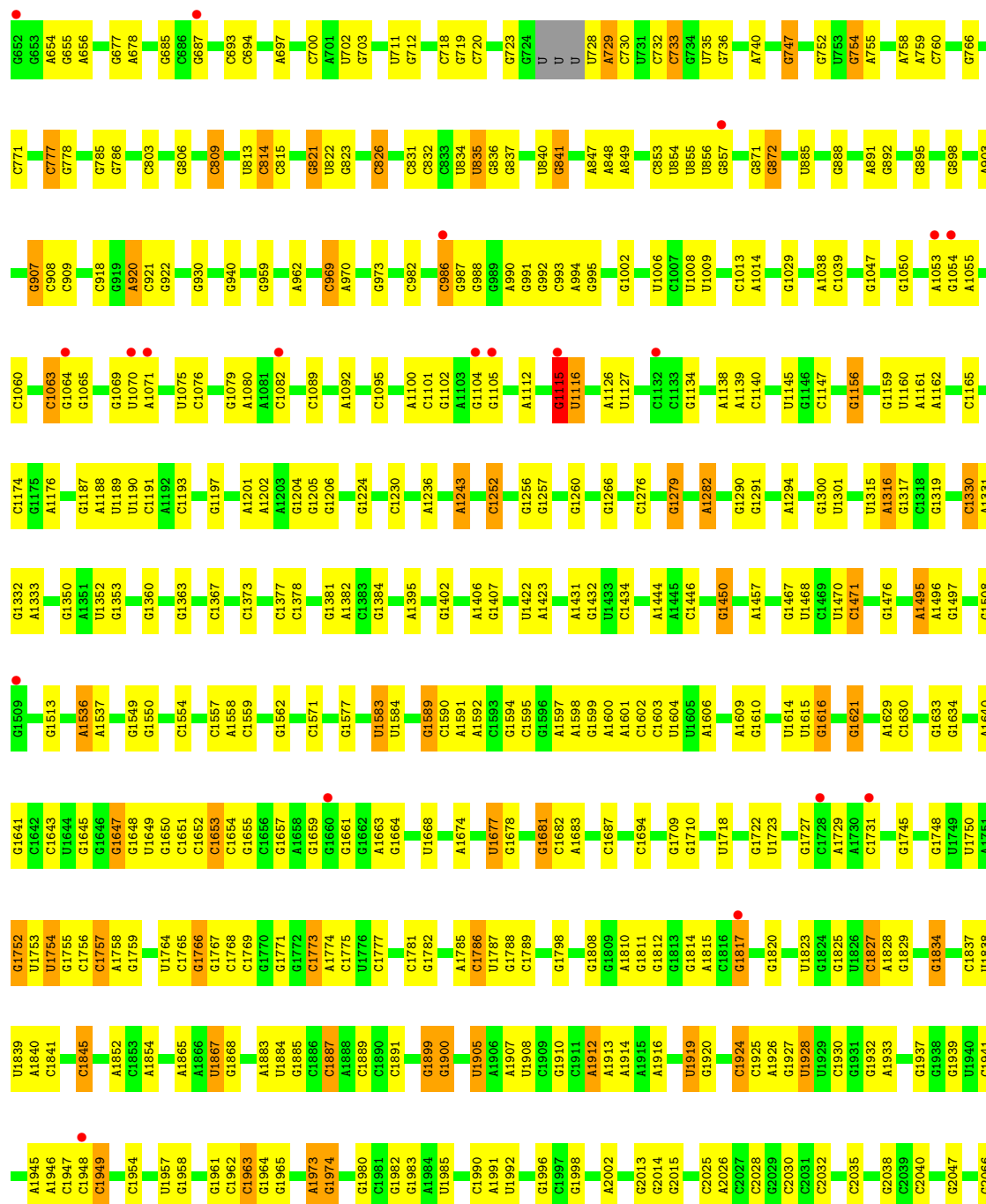
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 16S rRNA



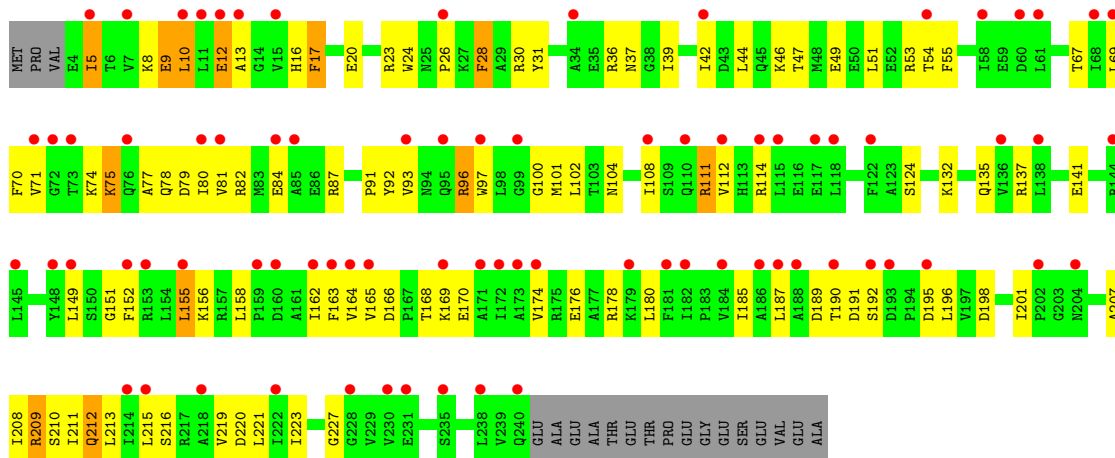


• Molecule 1: 16S rRNA

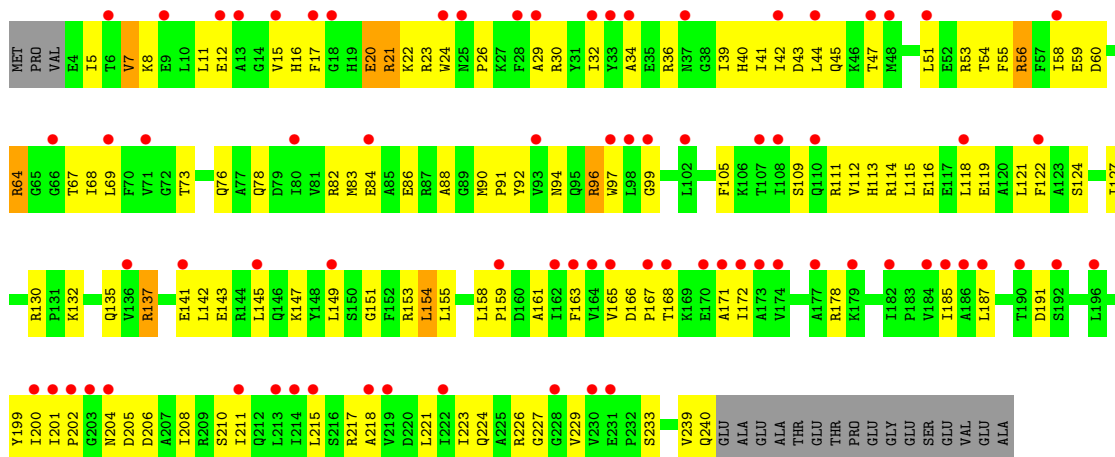




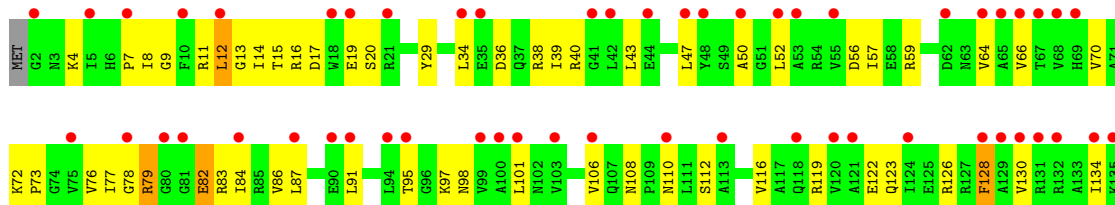
- Molecule 2: 30S ribosomal protein S2

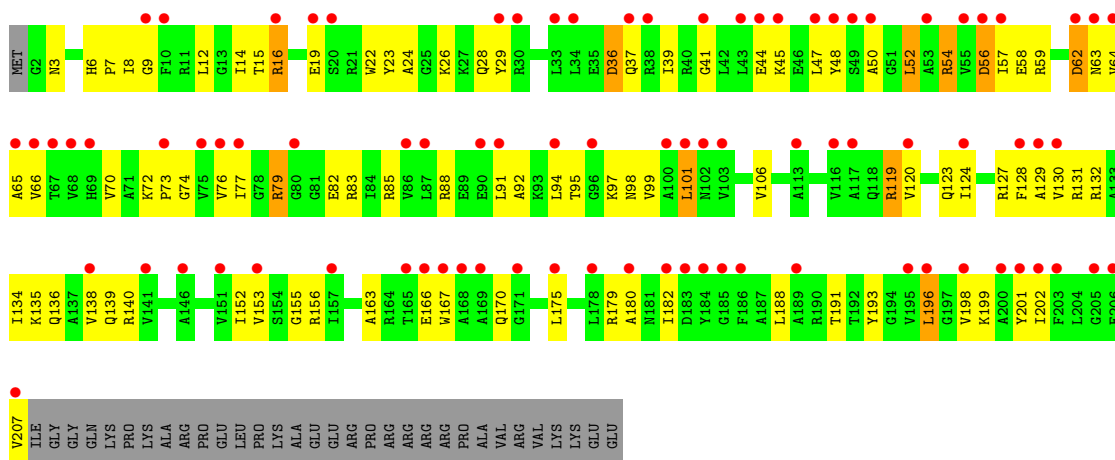
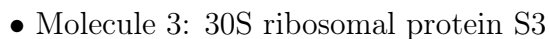


- Molecule 2: 30S ribosomal protein S2

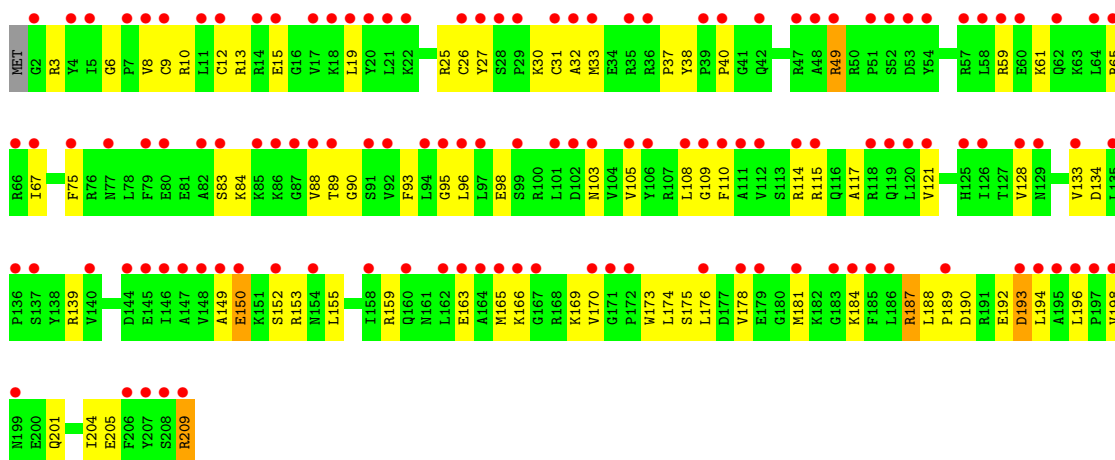


- Molecule 3: 30S ribosomal protein S3

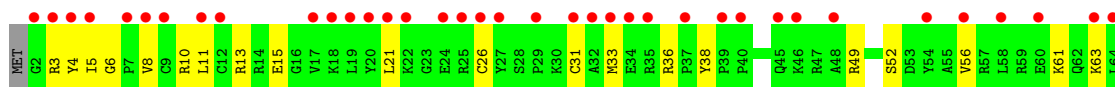




- Molecule 4: 30S ribosomal protein S4



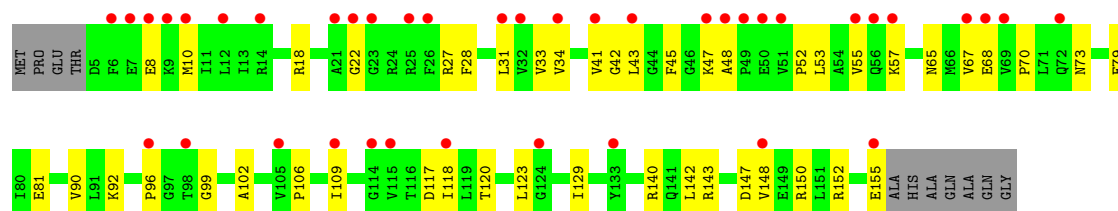
- Molecule 4: 30S ribosomal protein S4



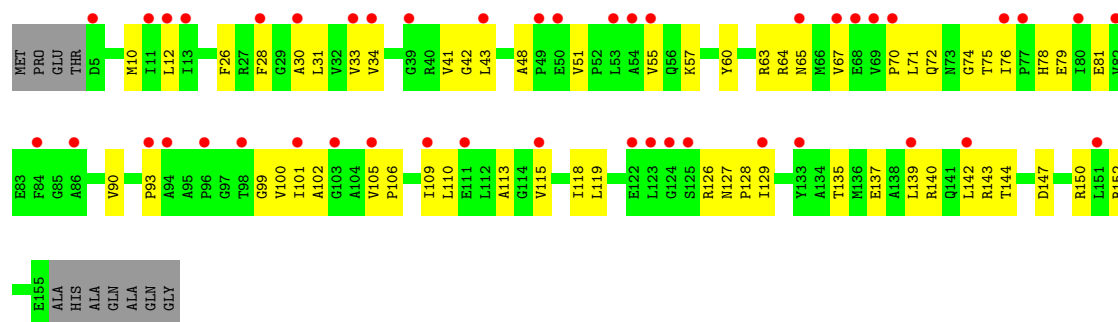




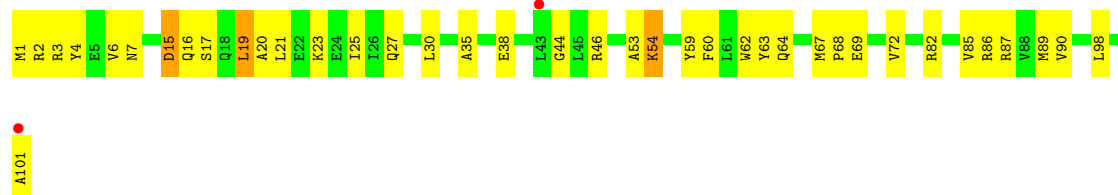
• Molecule 5: 30S ribosomal protein S5



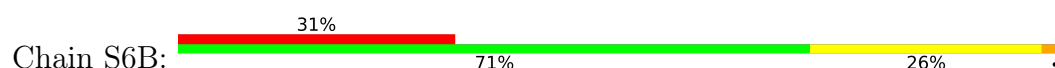
• Molecule 5: 30S ribosomal protein S5

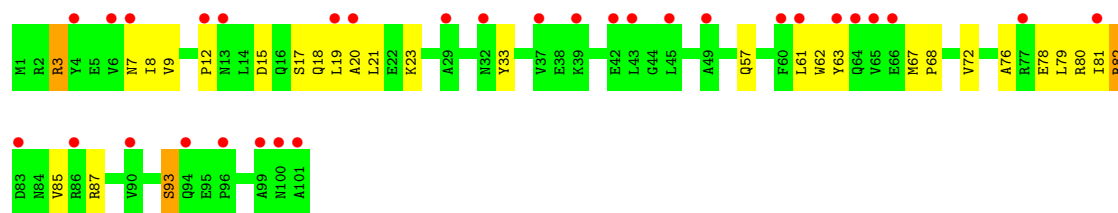


• Molecule 6: 30S ribosomal protein S6

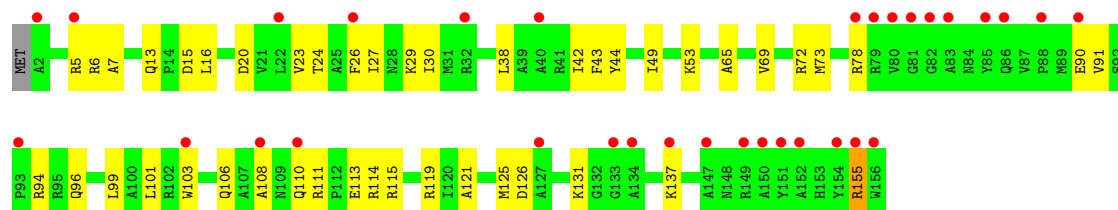
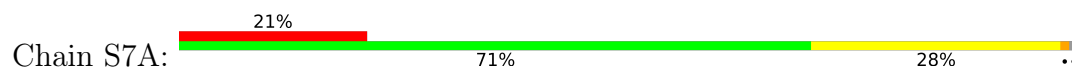


• Molecule 6: 30S ribosomal protein S6

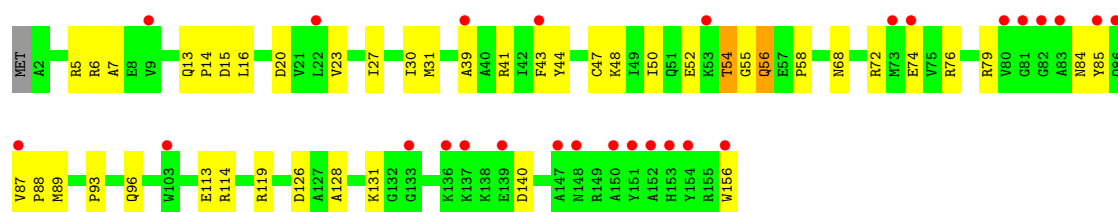
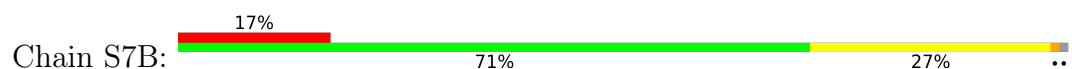




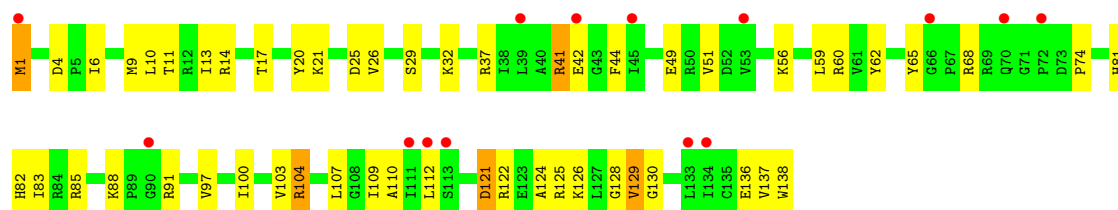
• Molecule 7: 30S ribosomal protein S7



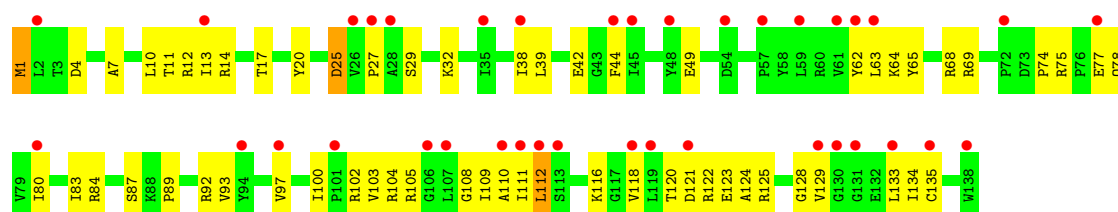
• Molecule 7: 30S ribosomal protein S7



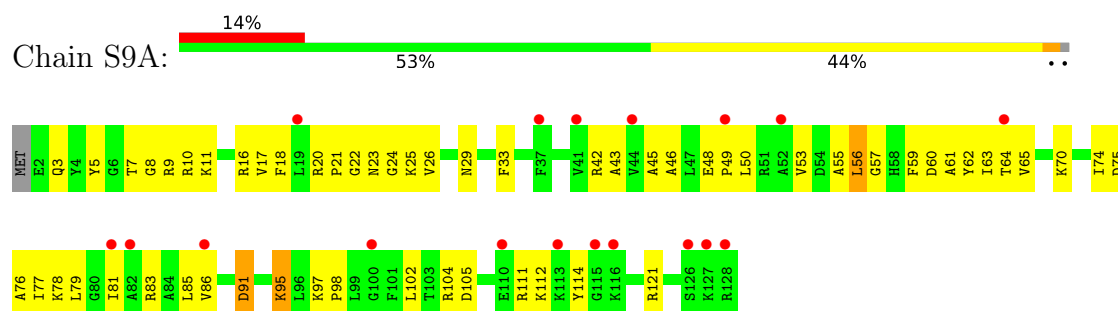
• Molecule 8: 30S ribosomal protein S8



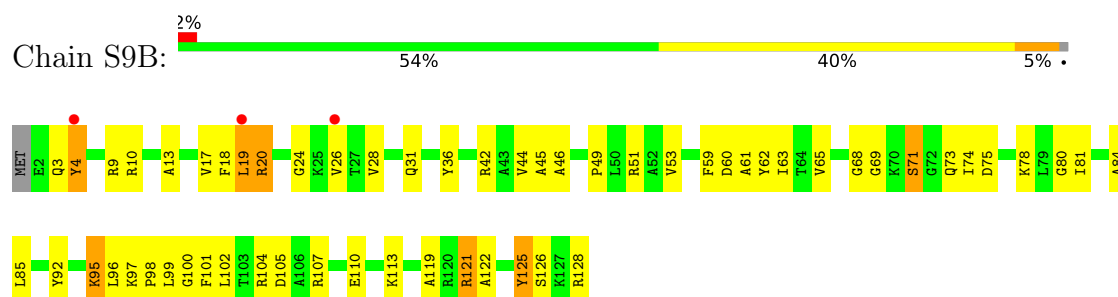
• Molecule 8: 30S ribosomal protein S8



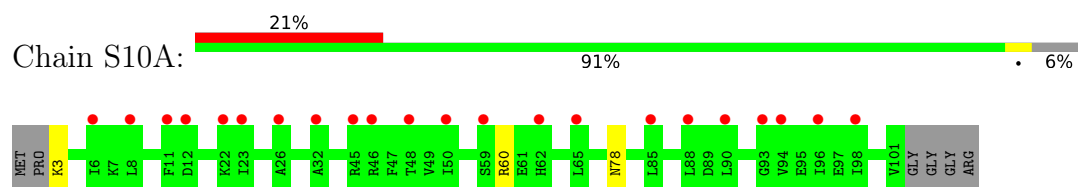
- Molecule 9: 30S ribosomal protein S9



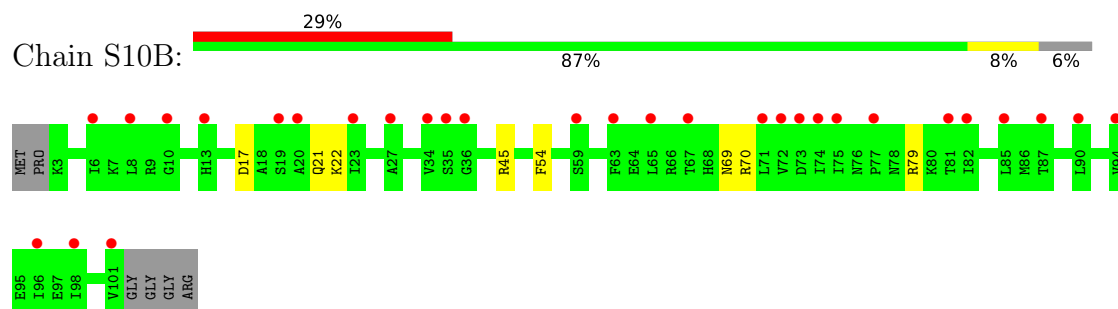
- Molecule 9: 30S ribosomal protein S9



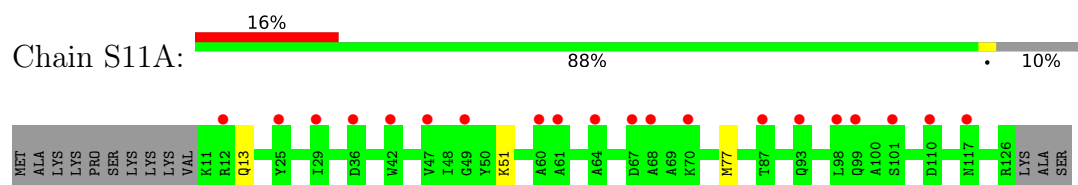
- Molecule 10: 30S ribosomal protein S10



- Molecule 10: 30S ribosomal protein S10

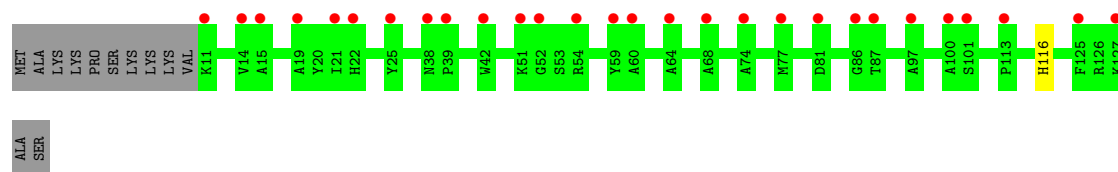


- Molecule 11: 30S ribosomal protein S11

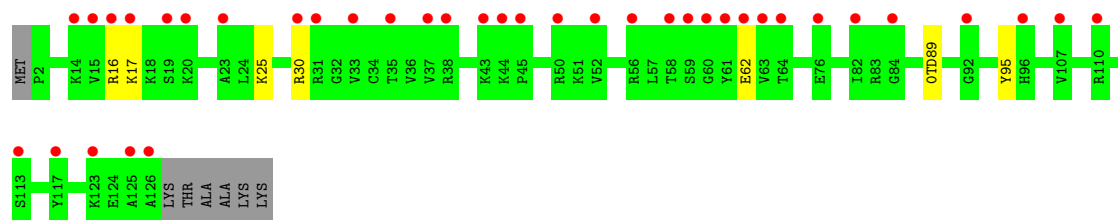


- Molecule 11: 30S ribosomal protein S11

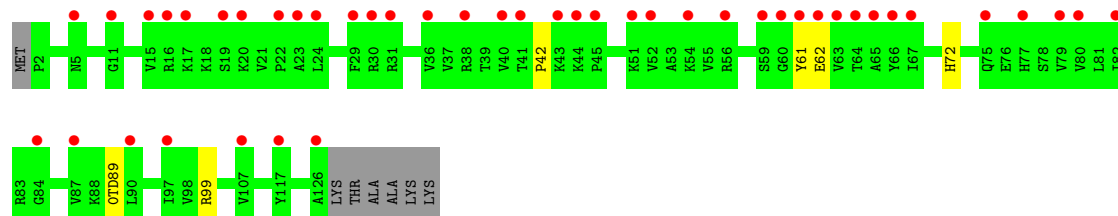




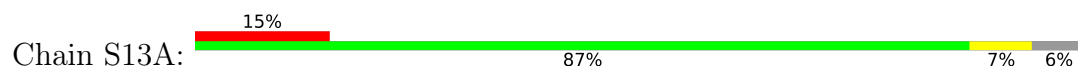
- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12



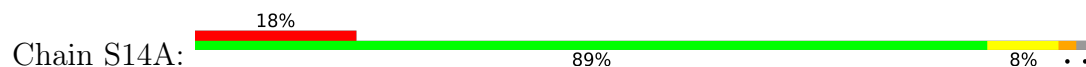
- Molecule 13: 30S ribosomal protein S13



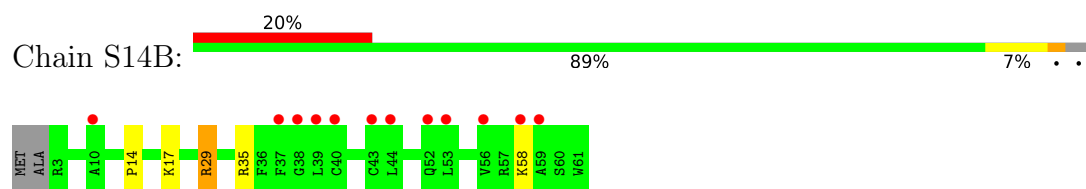
- Molecule 13: 30S ribosomal protein S13



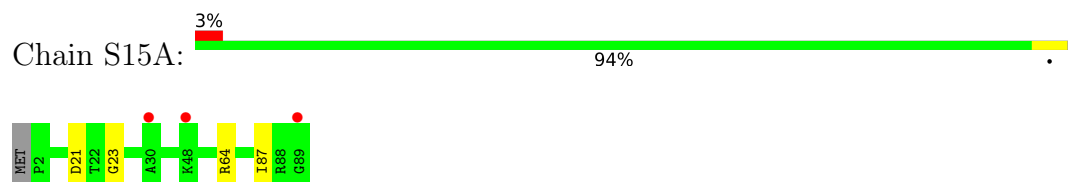
- Molecule 14: 30S ribosomal protein S14 type Z



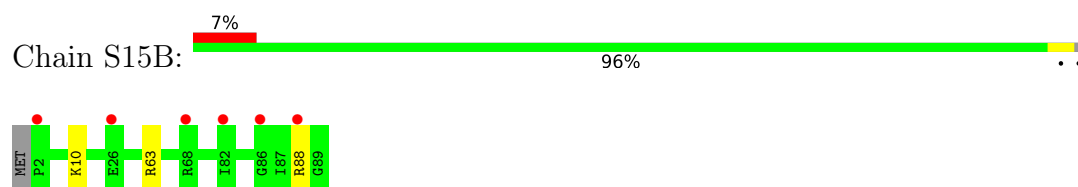
- Molecule 14: 30S ribosomal protein S14 type Z



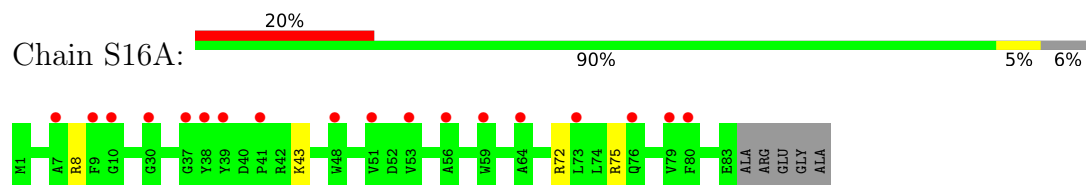
- Molecule 15: 30S ribosomal protein S15



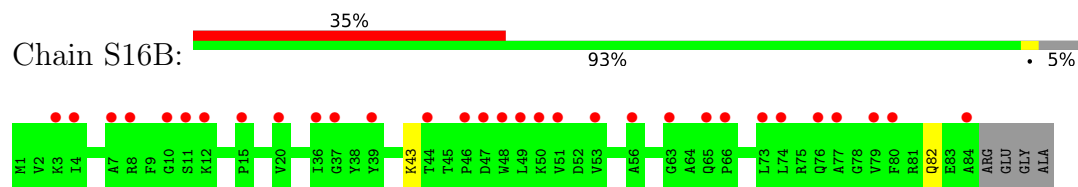
- Molecule 15: 30S ribosomal protein S15



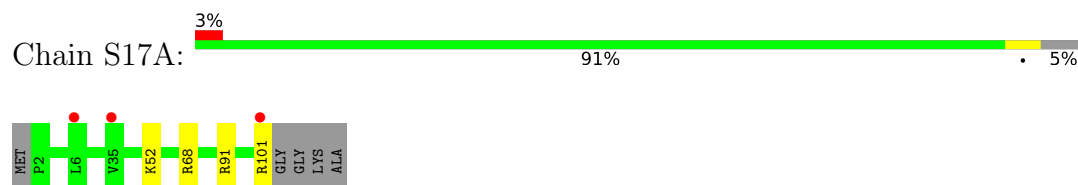
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16

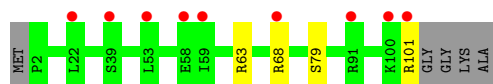


- Molecule 17: 30S ribosomal protein S17

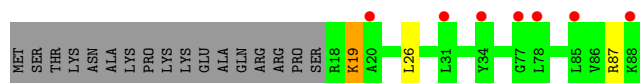
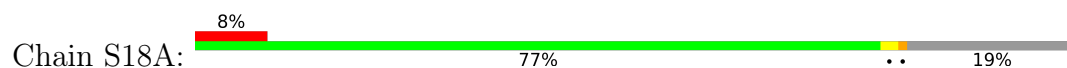


- Molecule 17: 30S ribosomal protein S17

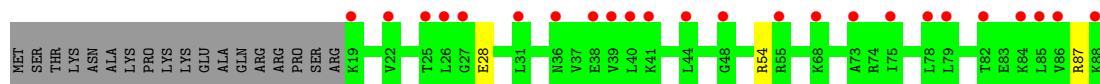
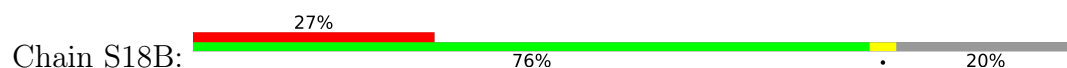




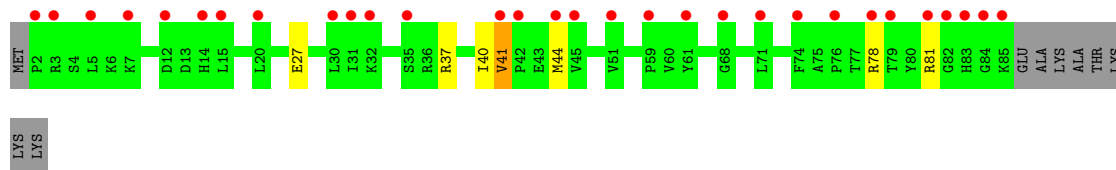
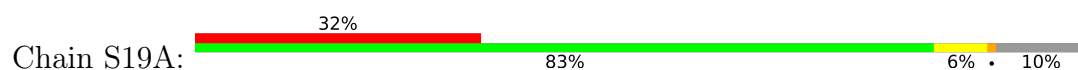
- Molecule 18: 30S ribosomal protein S18



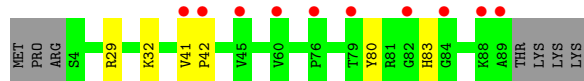
- Molecule 18: 30S ribosomal protein S18



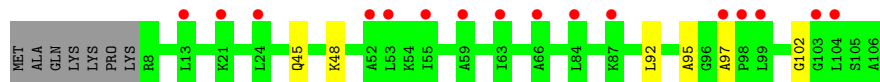
- Molecule 19: 30S ribosomal protein S19



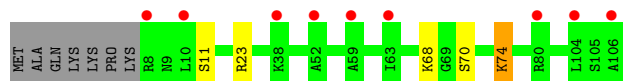
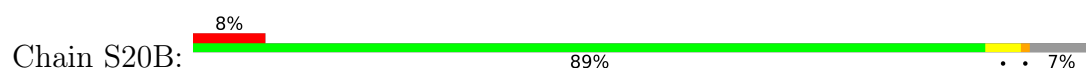
- Molecule 19: 30S ribosomal protein S19



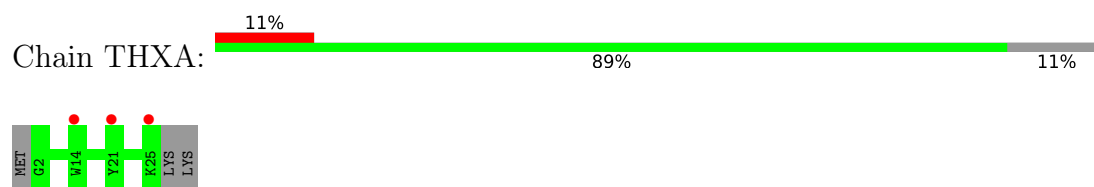
- Molecule 20: 30S ribosomal protein S20



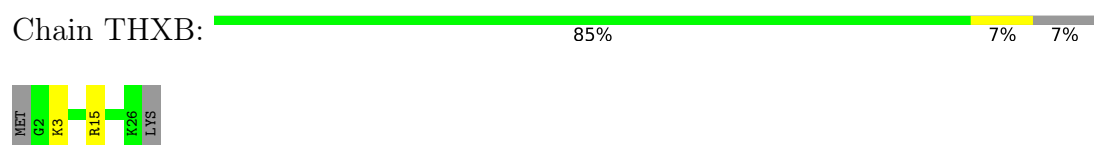
- Molecule 20: 30S ribosomal protein S20



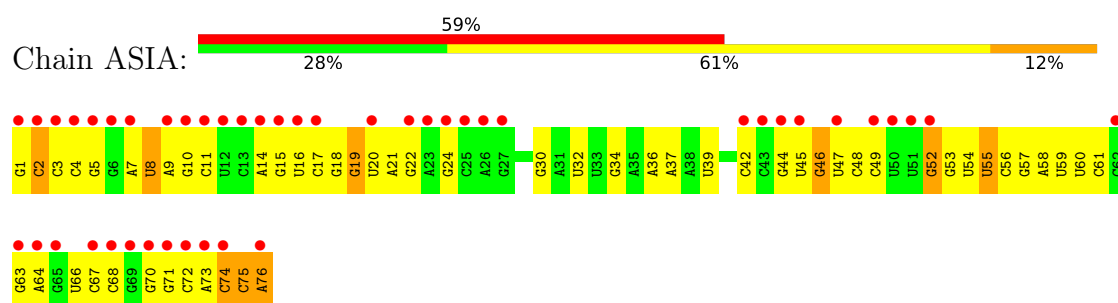
- Molecule 21: 30S ribosomal protein Thx



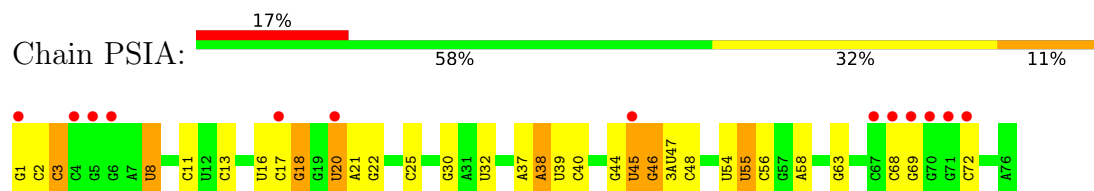
- Molecule 21: 30S ribosomal protein Thx



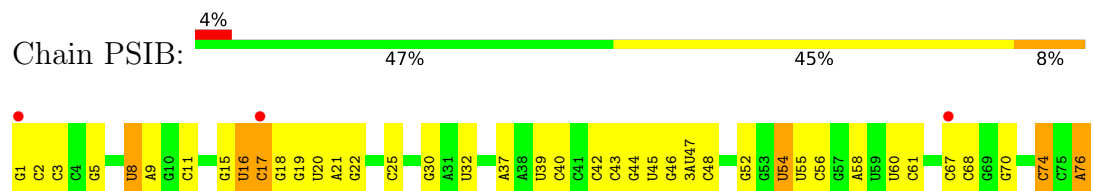
- Molecule 22: Phe-tRNA



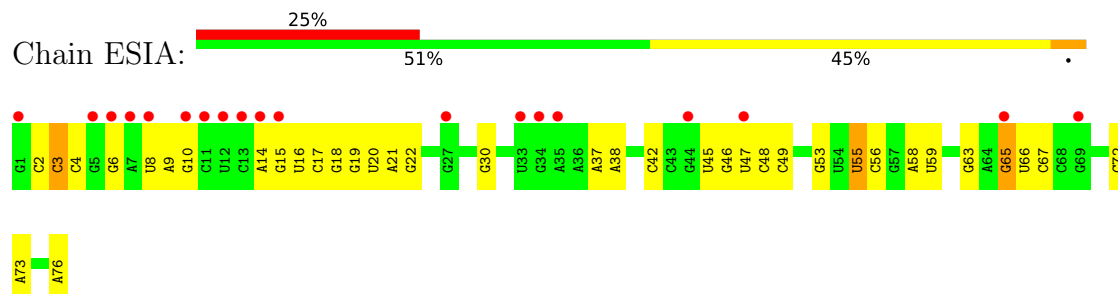
- Molecule 23: Phe-tRNA



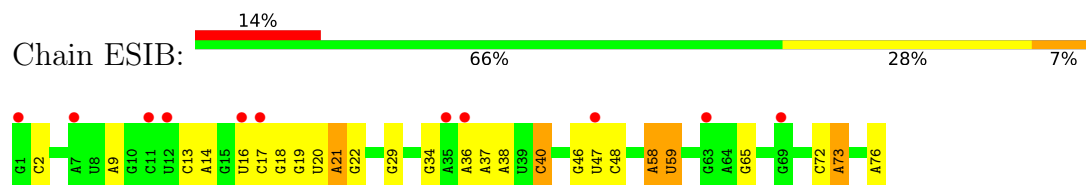
- Molecule 23: Phe-tRNA



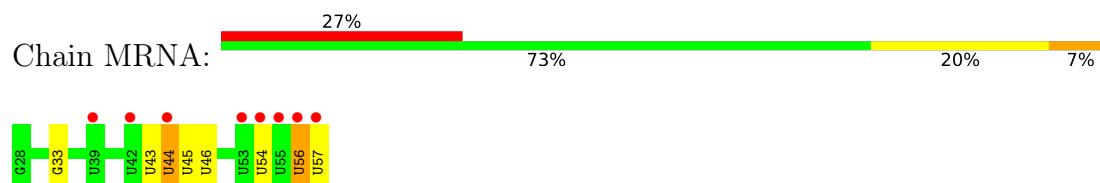
- Molecule 24: Phe-tRNA



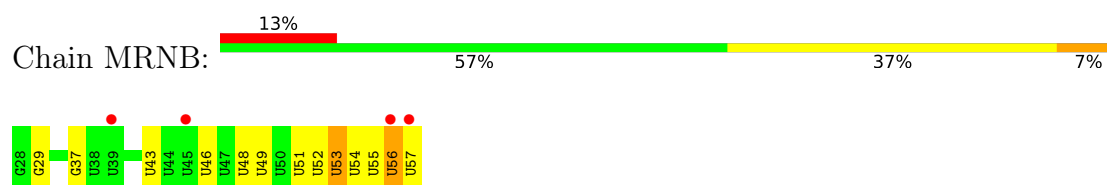
- Molecule 24: Phe-tRNA



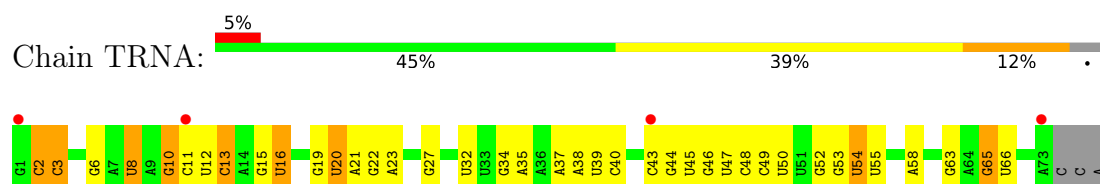
- Molecule 25: mRNA



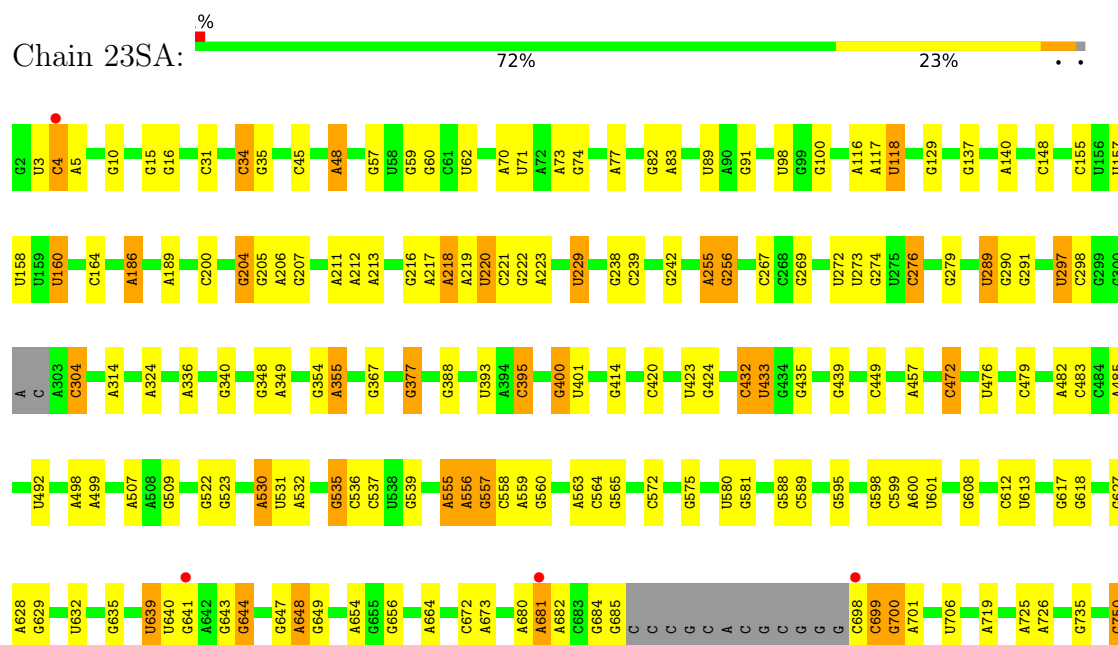
- Molecule 25: mRNA



- Molecule 26: Phe-tRNA

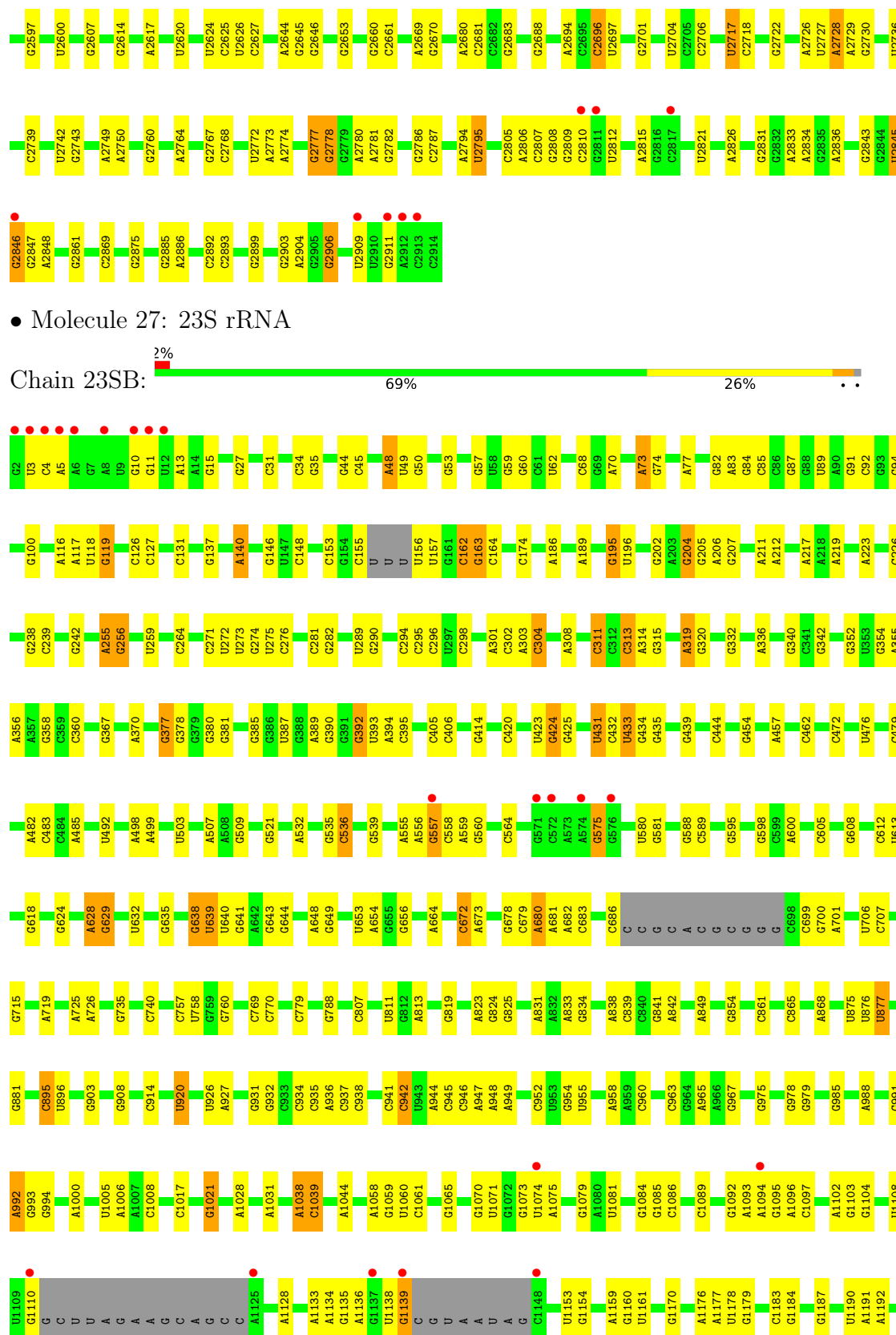


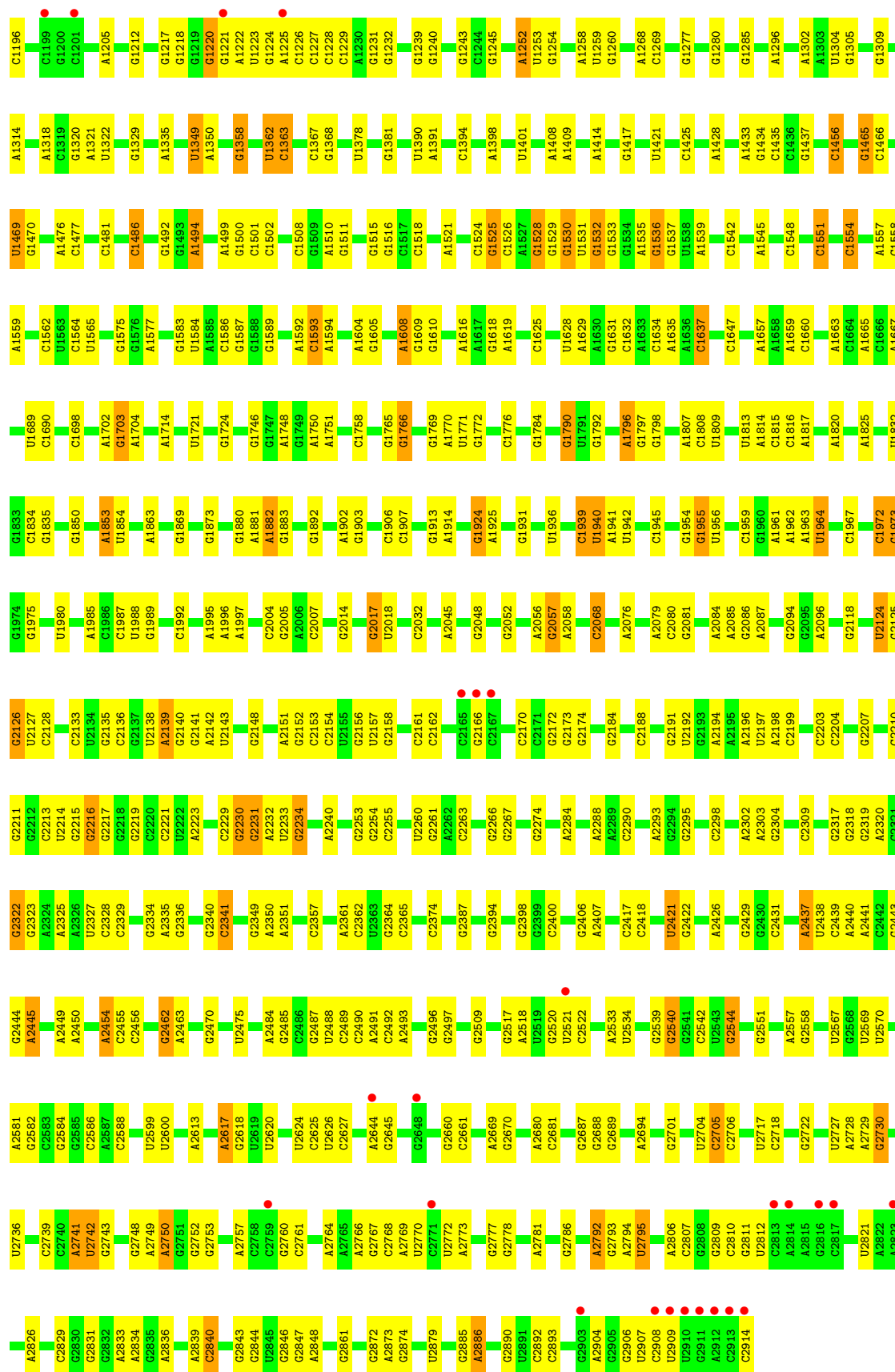
- Molecule 27: 23S rRNA



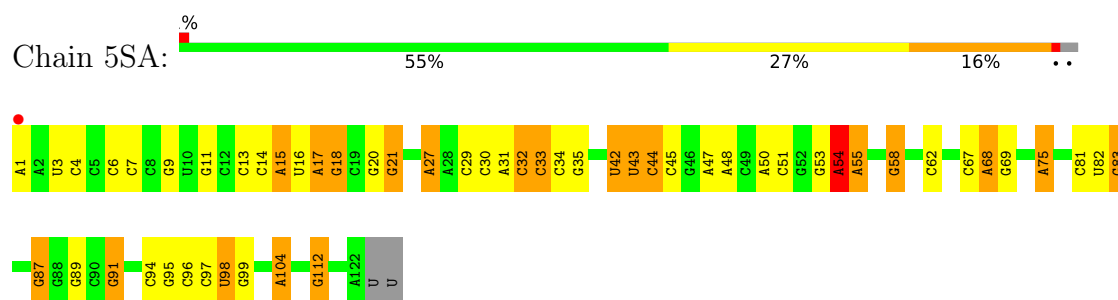


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A2302	A2303	G2304	G2319	A2320	C2321	G2322	G2323	A2326	U2327	C2328	C2329	G2333	G2334	A2335	G2336	G2340	C2341	G2349	A2350	A2351	A2361	C2362	C2365	G2394	C2395	G2398	A2518	C2400	G2406	A2407	C2417	G2420	U2421	G2422	G2425	A2426	C2435	G2436	A2437	U2438	C2439	A2440	A2441	C2442	G2443				
G2191	U2192	A2193	A2194	A2195	A2196	U2197	A2198	C2200	A2201	G2202	C2203	G2206	G2207	C2208	U2214	G2215	G2216	G2217	U2221	C2222	A2223	G2230	A2231	U2232	G2233	G2234	A2240	G2253	G2254	G2261	A2262	C2263	G2266	G2267	A2282	U2287	A2288	C2289	G2290	G2291	A2292	C2293	G2294	G2295	C2298	G2299	A2301		
C2090	G2094	G2108	G2118	U2124	G2125	G2126	C2130	C2133	C2136	G2137	U2138	A2139	G2140	G2141	A2142	U2143	A2144	G2145	C2150	A2151	C2152	C2153	C2154	U2157	C2158	C2161	C2162	C2165	G2166	U2169	C2170	G2171	G2172	G2173	G2177	G2180	A2183	G2184	G2185	C2188	C2189	G2190							
G1954	G1955	U1956	A1961	A1962	A1963	U1964	C1967	G1975	U1980	A1985	C1986	C1987	U1988	G1989	C1992	G1993	A1994	A1995	A1996	A1997	C2007	G2014	C2015	U2016	G2017	U2018	G2022	A2045	G2048	G2052	A2056	G2057	A2058	C2068	A2076	A2079	C2080	G2081	A2084	A2085	G2086								
C1808	U1809	U1813	C1815	C1816	A1825	U1832	G1833	C1834	G1835	G1850	A1853	U1854	A1863	G1873	G1880	A1881	A1882	G1883	G1889	A1902	G1903	C1907	G1913	A1914	G1924	A1925	C1926	C1927	G1928	G1929	C1930	G1931	U1936	C1939	U1940	A1941	U1942	C1945											
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C1542	U1546	C1553	C1554	C1555	A1556	A1557	C1558	A1559	C1562	U1563	A1564	U1565	G1574	A1577	C1582	G1583	U1584	A1585	C1586	G1587	G1588	A1592	C1593	A1594	A1604	G1605	A1608	G1609	G1610	A1616	A1619	U1628	C1629	G1635	G1642	G1643	G1644	C1647	A1652	A1657	A1658	A1659							
U1443	C1456	C1460	A1461	G1462	G1465	A1466	A1468	U1469	G1470	A1476	C1477	G1478	C1486	G1492	G1493	A1494	G1495	C1496	G1497	G1498	A1499	G1500	C1501	C1502	G1505	C1508	G1509	A1510	G1511	C1517	A1521	C1524	G1525	C1526	A1527	G1528	U1531	G1532	G1533	A1534	A1535	G1536	A1539						
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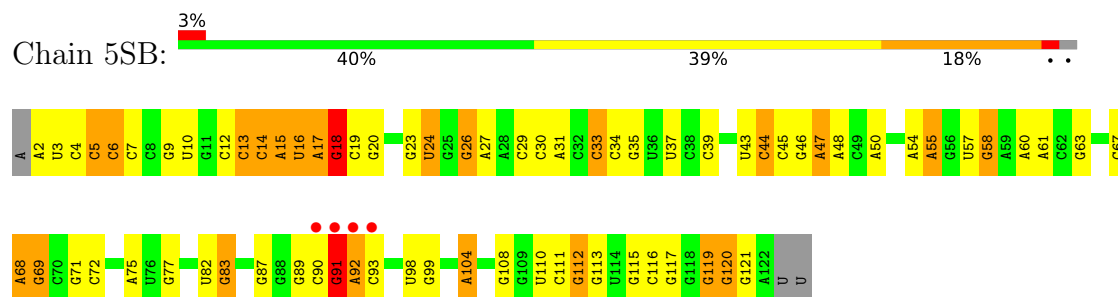




• Molecule 28: 5S rRNA



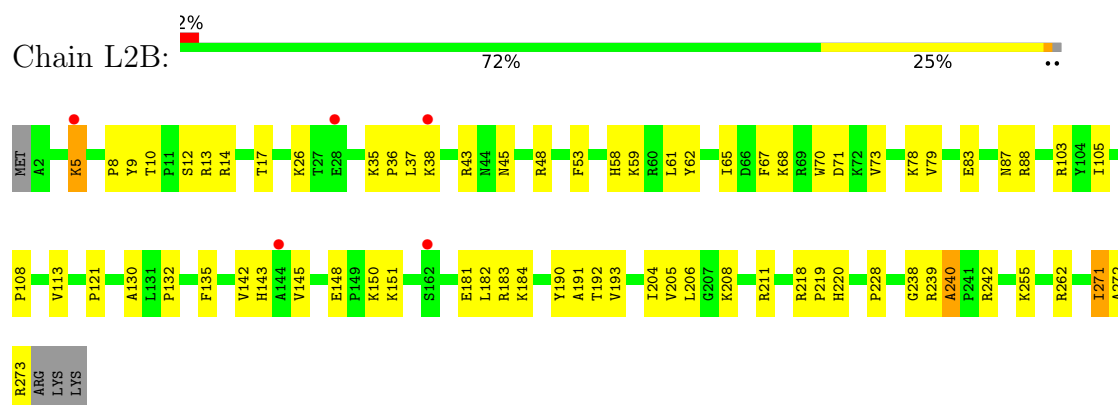
• Molecule 28: 5S rRNA



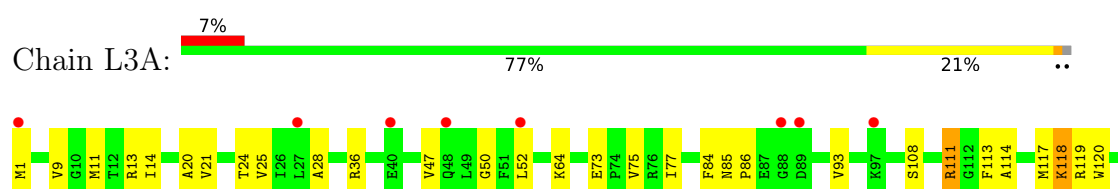
• Molecule 29: 50S ribosomal protein L2



• Molecule 29: 50S ribosomal protein L2

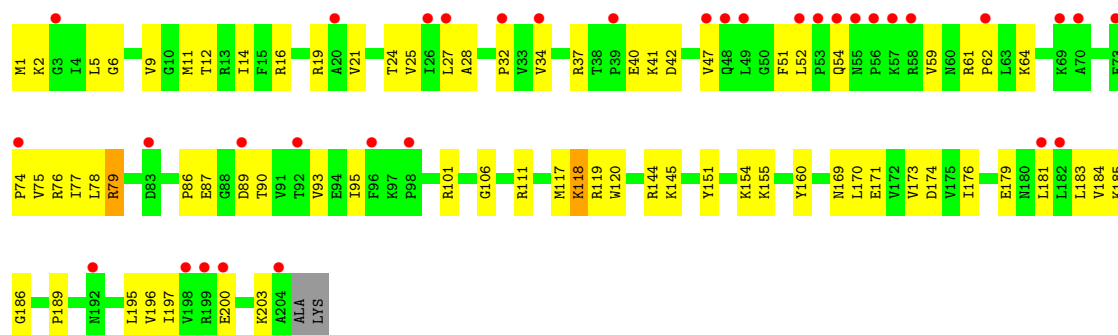


• Molecule 30: 50S ribosomal protein L3

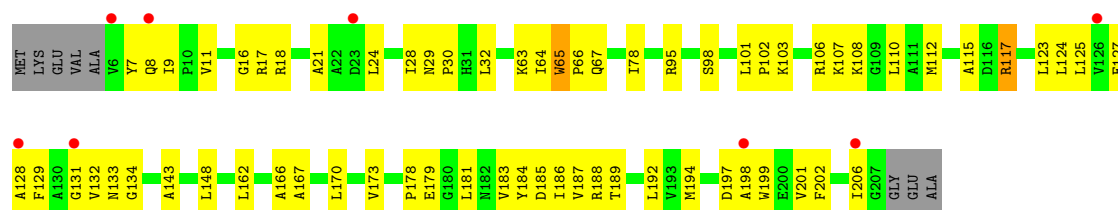




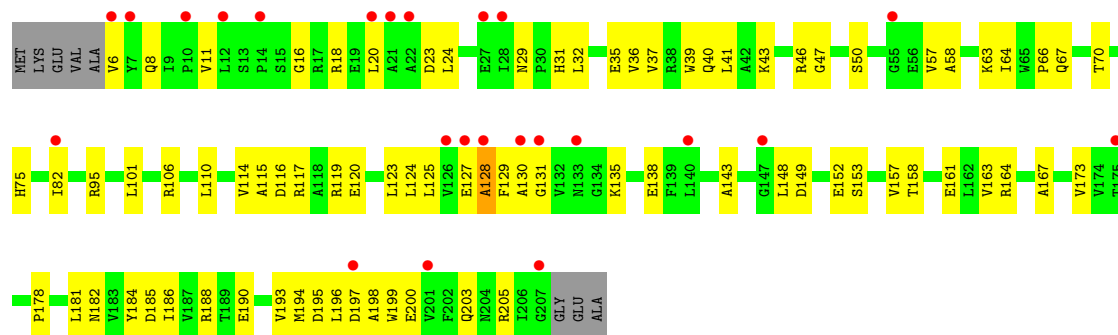
• Molecule 30: 50S ribosomal protein L3



• Molecule 31: 50S ribosomal protein L4



• Molecule 31: 50S ribosomal protein L4

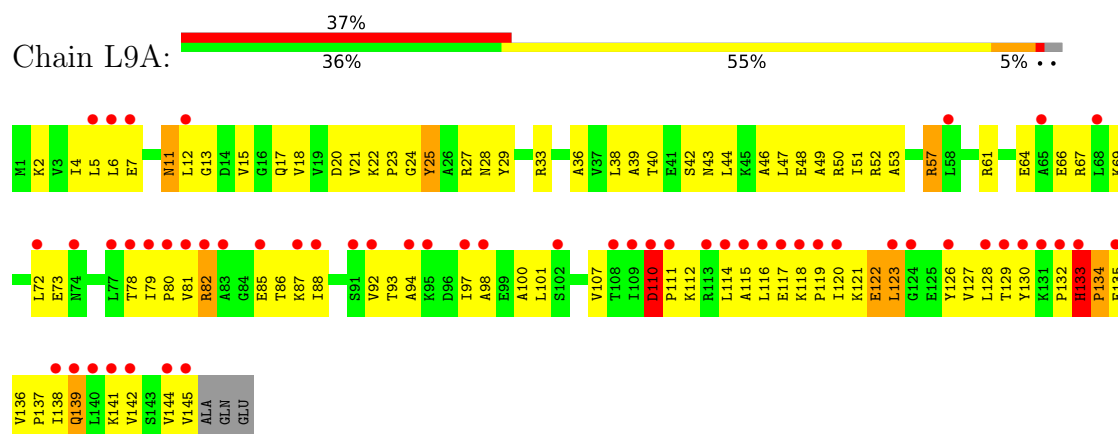


• Molecule 32: 50S ribosomal protein L5

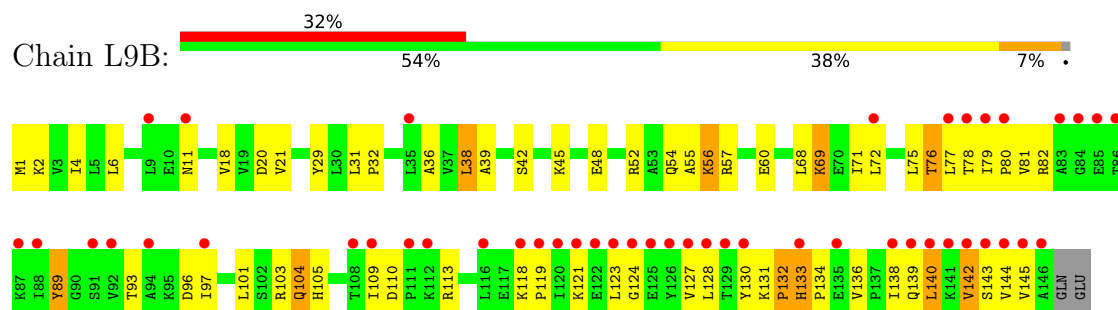




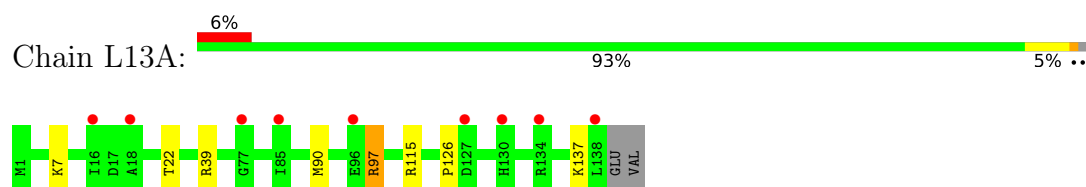
- Molecule 34: 50S ribosomal protein L9



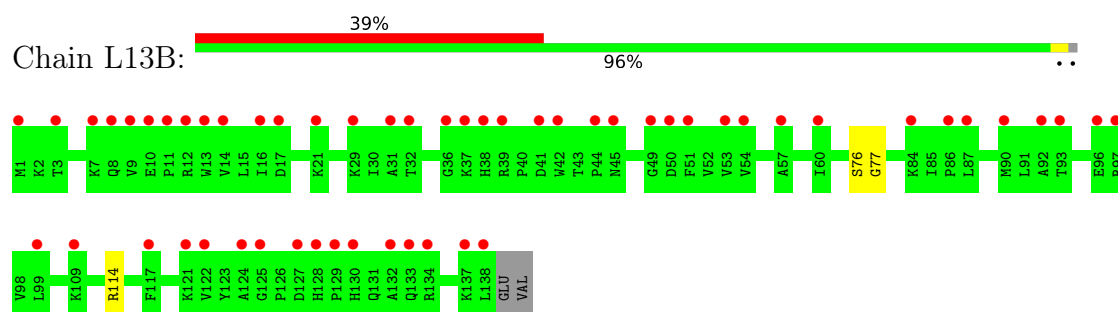
- Molecule 34: 50S ribosomal protein L9



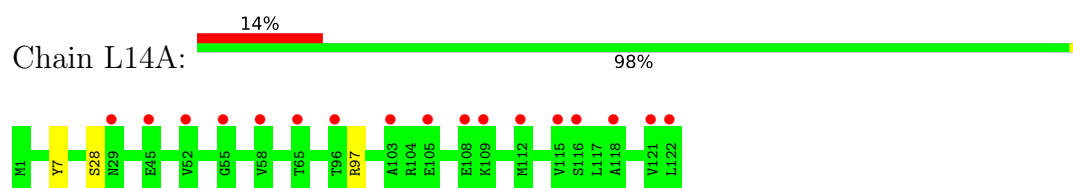
- Molecule 35: 50S ribosomal protein L13



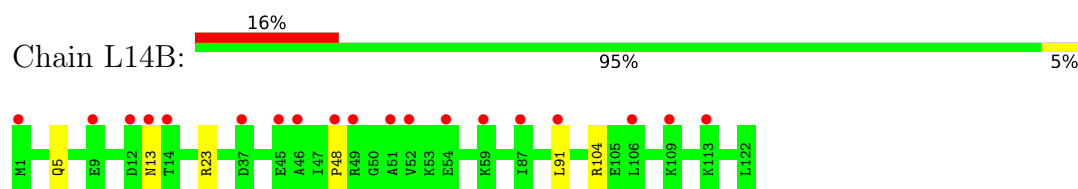
- Molecule 35: 50S ribosomal protein L13



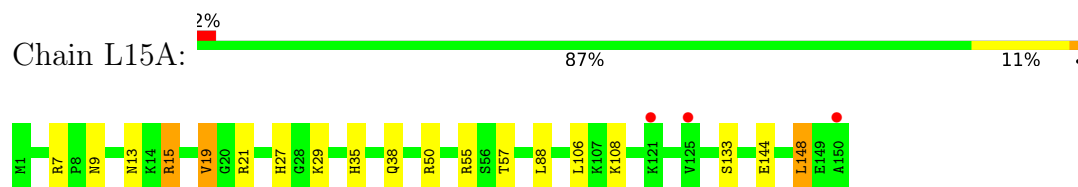
- Molecule 36: 50S ribosomal protein L14



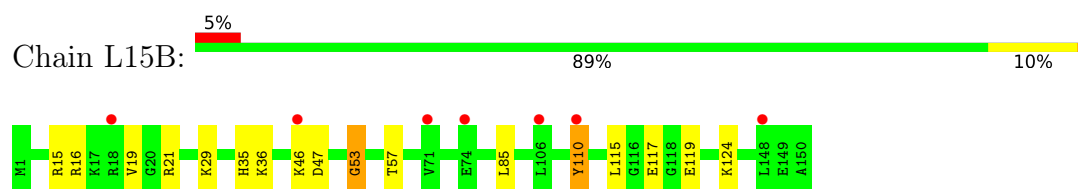
## • Molecule 36: 50S ribosomal protein L14



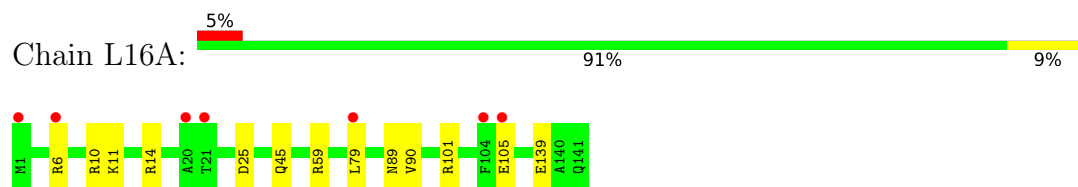
## • Molecule 37: 50S ribosomal protein L15



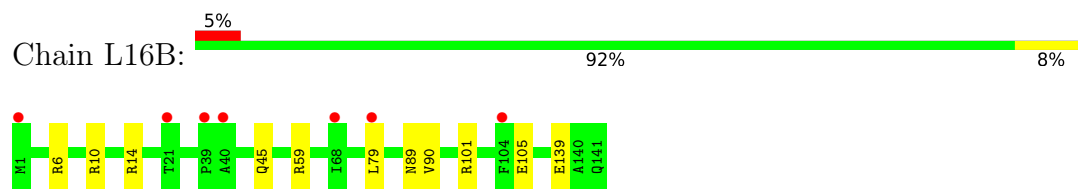
## • Molecule 37: 50S ribosomal protein L15



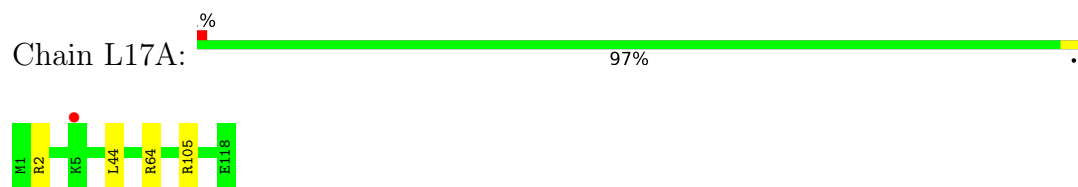
## • Molecule 38: 50S ribosomal protein L16



## • Molecule 38: 50S ribosomal protein L16



## • Molecule 39: 50S ribosomal protein L17



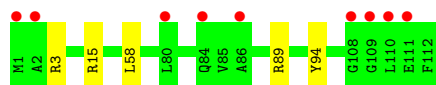
## • Molecule 39: 50S ribosomal protein L17



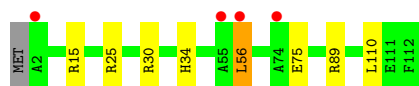




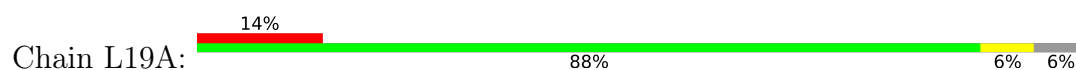
- Molecule 40: 50S ribosomal protein L18



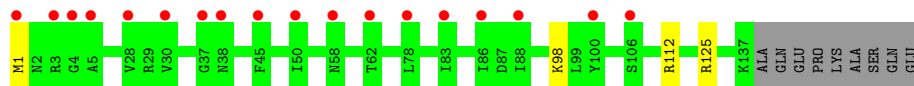
- Molecule 40: 50S ribosomal protein L18



- Molecule 41: 50S ribosomal protein L19



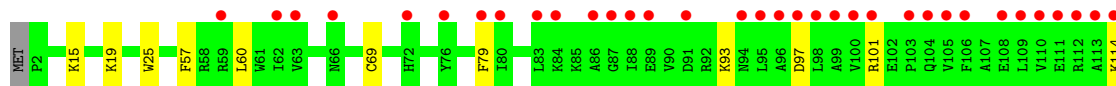
- Molecule 41: 50S ribosomal protein L19



- Molecule 42: 50S ribosomal protein L20

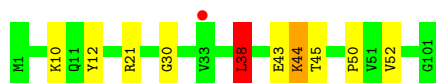


- Molecule 42: 50S ribosomal protein L20

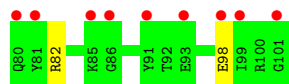
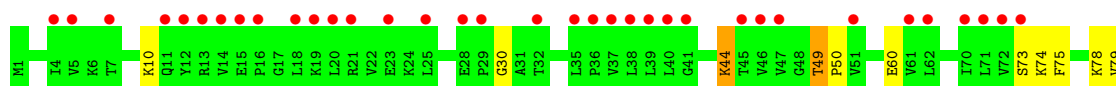




- Molecule 43: 50S ribosomal protein L21



- Molecule 43: 50S ribosomal protein L21



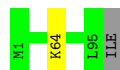
- Molecule 44: 50S ribosomal protein L22



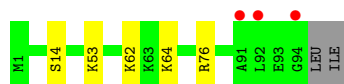
- Molecule 44: 50S ribosomal protein L22



- Molecule 45: 50S ribosomal protein L23

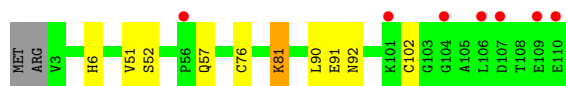


- Molecule 45: 50S ribosomal protein L23




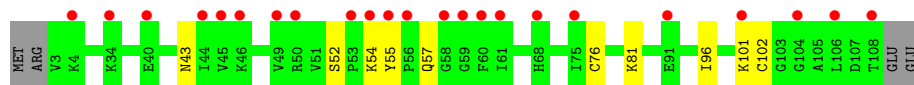
- Molecule 46: 50S ribosomal protein L24

Chain L24A: 




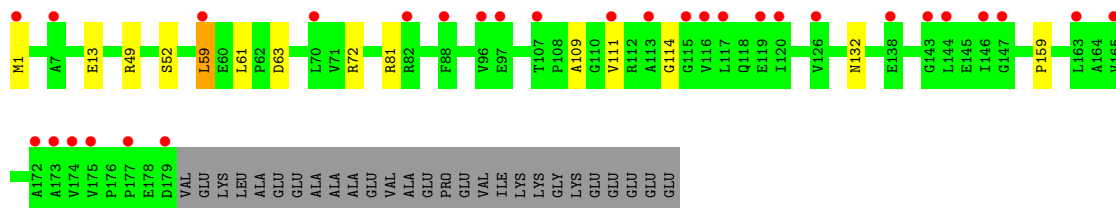
- Molecule 46: 50S ribosomal protein L24

Chain L24B: 




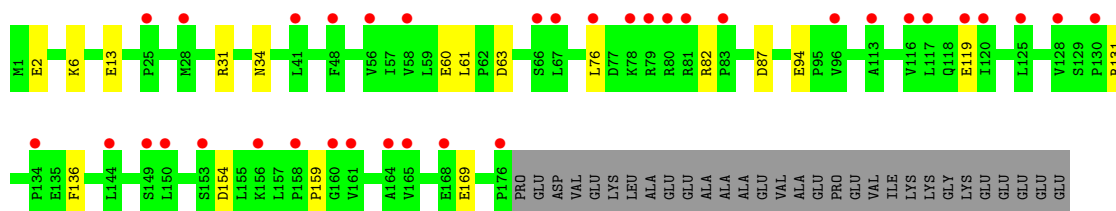
- Molecule 47: 50S ribosomal protein L25

Chain L25A: 



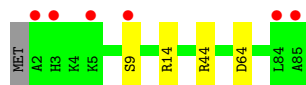
- Molecule 47: 50S ribosomal protein L25

Chain L25B: 



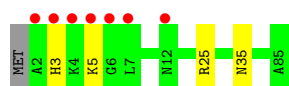
- Molecule 48: 50S ribosomal protein L27

Chain L27A: 

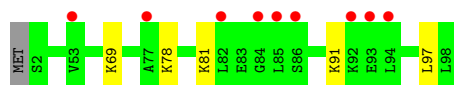


- Molecule 48: 50S ribosomal protein L27

Chain L27B: 



- Molecule 49: 50S ribosomal protein L28



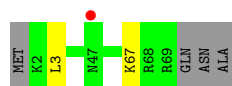
- Molecule 49: 50S ribosomal protein L28



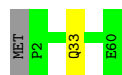
- Molecule 50: 50S ribosomal protein L29



- Molecule 50: 50S ribosomal protein L29



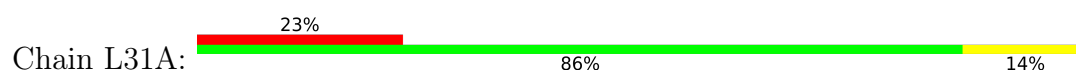
- Molecule 51: 50S ribosomal protein L30



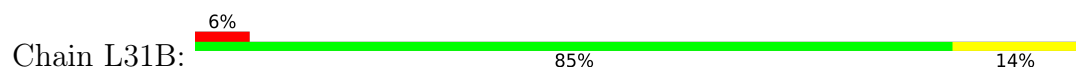
- Molecule 51: 50S ribosomal protein L30



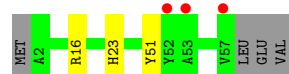
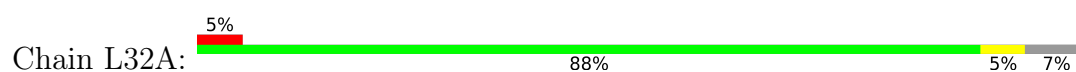
- Molecule 52: 50S ribosomal protein L31



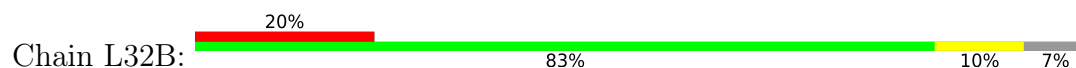
- Molecule 52: 50S ribosomal protein L31



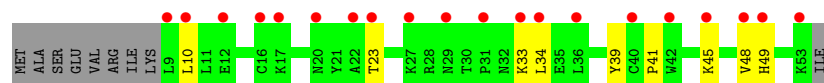
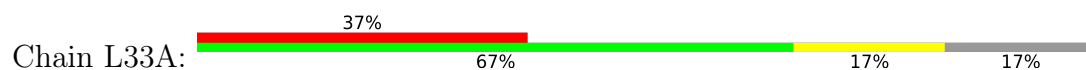
- Molecule 53: 50S ribosomal protein L32



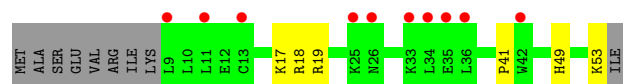
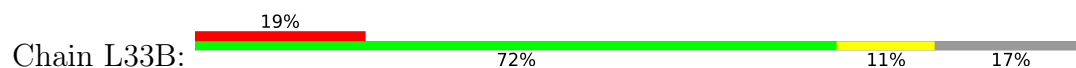
- Molecule 53: 50S ribosomal protein L32



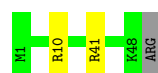
- Molecule 54: 50S ribosomal protein L33



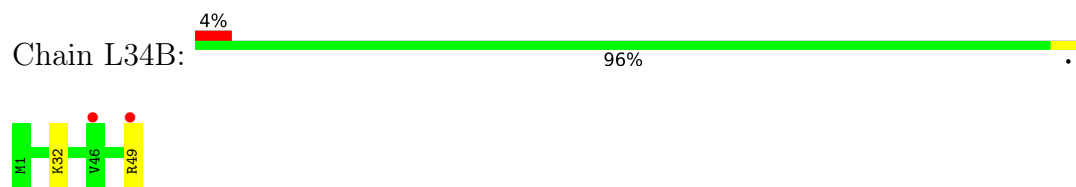
- Molecule 54: 50S ribosomal protein L33



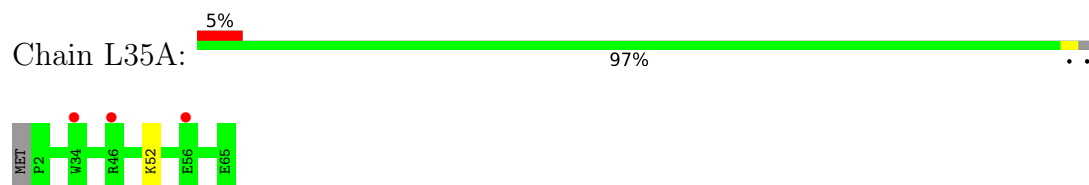
- Molecule 55: 50S ribosomal protein L34



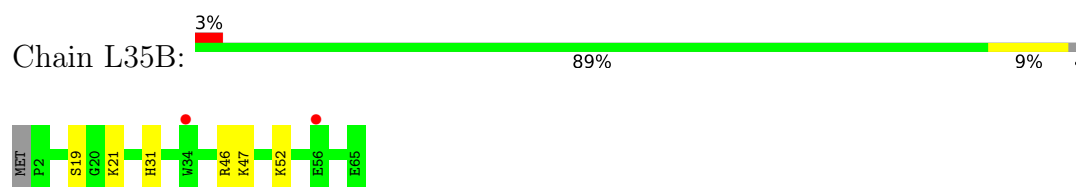
- Molecule 55: 50S ribosomal protein L34



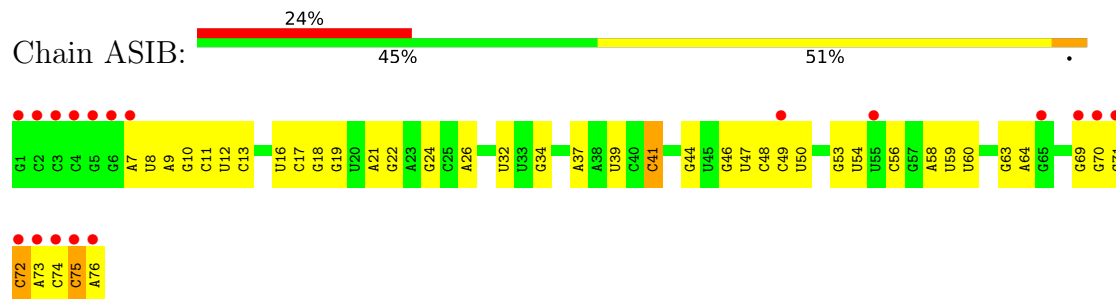
- Molecule 56: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L35



- Molecule 57: Phe-tRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.40Å 450.10Å 626.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	256.98 – 3.10 256.98 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (256.98-3.10) 94.2 (256.98-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.247 , 0.275 0.247 , 0.275	Depositor DCC
$R_{free}$ test set	31853 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.5	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 58.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	306277	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.38% 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: 4OC, OMG, MG, K, 5MC, 3AU, 4SU, 2MG, OMU, SJH, 2MA, 5MU, PSU, MIA, UR3, OHX, 7MG, MA6, OMC, 0TD, M2G

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	16SA	0.49	4/36066 (0.0%)	1.26	276/56286 (0.5%)
1	16SB	0.48	1/35977 (0.0%)	1.25	278/56146 (0.5%)
2	S2A	0.34	0/1959	0.69	0/2642
2	S2B	0.32	0/1959	0.67	0/2642
3	S3A	0.33	0/1629	0.72	0/2195
3	S3B	0.30	0/1636	0.71	2/2205 (0.1%)
4	S4A	0.38	0/1732	0.75	0/2318
4	S4B	0.33	0/1732	0.70	0/2318
5	S5A	0.38	0/1171	0.74	0/1576
5	S5B	0.32	0/1171	0.69	0/1576
6	S6A	0.31	0/855	0.69	0/1154
6	S6B	0.31	0/855	0.65	0/1154
7	S7A	0.34	0/1275	0.68	0/1709
7	S7B	0.29	0/1274	0.64	0/1706
8	S8A	0.34	0/1135	0.71	0/1527
8	S8B	0.31	0/1135	0.66	0/1527
9	S9A	0.33	0/1028	0.73	1/1379 (0.1%)
9	S9B	0.32	0/1028	0.74	1/1379 (0.1%)
10	S10A	0.32	0/814	0.68	0/1095
10	S10B	0.31	0/814	0.71	0/1095
11	S11A	0.33	0/879	0.61	0/1187
11	S11B	0.30	0/888	0.62	0/1198
12	S12A	0.34	0/982	0.75	0/1313
12	S12B	0.34	0/982	0.67	0/1313
13	S13A	0.31	0/956	0.73	0/1281
13	S13B	0.29	0/974	0.68	0/1303
14	S14A	0.44	0/500	0.76	1/664 (0.2%)
14	S14B	0.33	0/495	0.74	0/657
15	S15A	0.30	0/744	0.64	0/992
15	S15B	0.28	0/744	0.59	0/992
16	S16A	0.31	0/716	0.73	0/963



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	S16B	0.33	0/721	0.67	0/970
17	S17A	0.32	0/847	0.69	0/1131
17	S17B	0.29	0/847	0.65	0/1131
18	S18A	0.32	0/589	0.75	0/782
18	S18B	0.32	0/578	0.72	0/768
19	S19A	0.35	0/689	0.81	2/926 (0.2%)
19	S19B	0.31	0/698	0.66	0/938
20	S20A	0.33	0/764	0.72	0/1007
20	S20B	0.29	0/764	0.66	0/1007
21	THXA	0.30	0/212	0.78	0/277
21	THXB	0.28	0/221	0.75	0/288
22	ASIA	0.54	0/1647	1.49	35/2565 (1.4%)
23	PSIA	0.97	9/1624 (0.6%)	1.45	21/2527 (0.8%)
23	PSIB	0.78	5/1624 (0.3%)	1.30	15/2527 (0.6%)
24	ESIA	0.48	0/1783	1.22	12/2776 (0.4%)
24	ESIB	0.44	0/1783	1.16	7/2776 (0.3%)
25	MRNA	0.41	0/689	1.12	4/1069 (0.4%)
25	MRNB	0.43	0/689	1.19	7/1069 (0.7%)
26	TRNA	0.97	11/1604 (0.7%)	1.36	24/2499 (1.0%)
27	23SA	0.47	2/69430 (0.0%)	1.22	441/108380 (0.4%)
27	23SB	0.47	5/69097 (0.0%)	1.21	520/107863 (0.5%)
28	5SA	0.50	1/2928 (0.0%)	1.27	26/4568 (0.6%)
28	5SB	0.51	0/2906	1.33	35/4533 (0.8%)
29	L2A	0.33	0/2165	0.72	1/2919 (0.0%)
29	L2B	0.33	0/2165	0.72	0/2919
30	L3A	0.34	0/1596	0.67	0/2153
30	L3B	0.31	0/1596	0.66	0/2153
31	L4A	0.35	0/1620	0.69	0/2194
31	L4B	0.32	0/1620	0.67	0/2194
32	L5A	0.31	0/1498	0.68	1/2016 (0.0%)
32	L5B	0.32	0/1498	0.67	0/2016
33	L6A	0.34	0/1362	0.74	1/1841 (0.1%)
33	L6B	0.33	0/1353	0.71	0/1830
34	L9A	0.37	0/1146	0.82	1/1551 (0.1%)
34	L9B	0.34	0/1151	0.71	1/1558 (0.1%)
35	L13A	0.34	0/1131	0.71	0/1525
35	L13B	0.29	0/1131	0.66	0/1525
36	L14A	0.37	0/942	0.72	0/1269
36	L14B	0.35	0/942	0.67	1/1269 (0.1%)
37	L15A	0.37	0/1161	0.88	1/1544 (0.1%)
37	L15B	0.34	0/1161	0.85	2/1544 (0.1%)
38	L16A	0.31	0/1142	0.68	0/1527
38	L16B	0.33	0/1142	0.67	0/1527

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	L17A	0.32	0/981	0.74	0/1312
39	L17B	0.30	0/981	0.72	0/1312
40	L18A	0.32	0/899	0.82	0/1197
40	L18B	0.32	0/891	0.77	1/1187 (0.1%)
41	L19A	0.35	0/1155	0.73	0/1542
41	L19B	0.33	0/1155	0.71	0/1542
42	L20A	0.34	0/981	0.72	1/1306 (0.1%)
42	L20B	0.31	0/981	0.67	0/1306
43	L21A	0.35	0/789	0.80	1/1057 (0.1%)
43	L21B	0.35	0/789	0.75	0/1057
44	L22A	0.33	0/910	0.69	0/1220
44	L22B	0.30	0/910	0.64	0/1220
45	L23A	0.36	0/761	0.68	0/1021
45	L23B	0.33	0/756	0.64	0/1014
46	L24A	0.34	0/837	0.70	0/1118
46	L24B	0.34	0/787	0.72	0/1056
47	L25A	0.32	0/1460	0.75	1/1982 (0.1%)
47	L25B	0.31	0/1435	0.71	0/1947
48	L27A	0.34	0/670	0.77	0/892
48	L27B	0.35	0/670	0.70	0/892
49	L28A	0.35	0/769	0.70	0/1022
49	L28B	0.34	0/769	0.77	1/1022 (0.1%)
50	L29A	0.30	0/585	0.67	0/773
50	L29B	0.31	0/577	0.69	0/763
51	L30A	0.32	0/473	0.72	0/635
51	L30B	0.28	0/473	0.71	1/635 (0.2%)
52	L31A	0.33	0/593	0.76	0/795
52	L31B	0.32	0/593	0.70	0/795
53	L32A	0.39	0/448	0.68	0/606
53	L32B	0.37	0/448	0.72	0/606
54	L33A	0.39	0/396	0.91	1/529 (0.2%)
54	L33B	0.39	0/396	0.87	0/529
55	L34A	0.31	0/426	0.79	0/561
55	L34B	0.29	0/437	0.78	0/575
56	L35A	0.32	0/524	0.69	0/691
56	L35B	0.31	0/524	0.68	0/691
57	ASIB	0.46	0/1717	1.23	8/2674 (0.3%)
All	All	0.45	38/323307 (0.0%)	1.12	1732/484025 (0.4%)

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
13	S13A	0	1
19	S19B	0	1
20	S20A	0	1
29	L2A	0	1
29	L2B	0	1
31	L4A	0	2
33	L6A	0	1
33	L6B	0	2
34	L9A	0	1
37	L15A	0	2
39	L17A	0	1
41	L19A	0	1
43	L21A	0	2
43	L21B	0	1
48	L27A	0	1
50	L29A	0	1
All	All	0	20

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	TRNA	20	U	C5-C6	17.65	1.50	1.34
23	PSIB	16	U	C5-C6	17.49	1.49	1.34
23	PSIA	16	U	C5-C6	17.25	1.49	1.34
23	PSIA	20	U	C5-C6	17.19	1.49	1.34
26	TRNA	16	U	C5-C6	17.18	1.49	1.34
23	PSIB	16	U	C2-N3	11.13	1.45	1.37
26	TRNA	20	U	C2-N3	10.71	1.45	1.37
23	PSIA	20	U	C2-N3	10.28	1.45	1.37
26	TRNA	16	U	C2-N3	10.28	1.45	1.37
23	PSIA	16	U	C2-N3	9.22	1.44	1.37
23	PSIA	16	U	C4-C5	8.34	1.51	1.43
27	23SB	1065	G	C6-N1	8.25	1.45	1.39
23	PSIA	20	U	C4-C5	8.18	1.50	1.43
26	TRNA	20	U	C4-C5	8.07	1.50	1.43
1	16SA	727	U	C2-N3	8.02	1.43	1.37
26	TRNA	16	U	C4-C5	7.94	1.50	1.43
23	PSIB	16	U	C4-C5	7.89	1.50	1.43
26	TRNA	20	U	N1-C2	7.86	1.45	1.38
1	16SB	785	G	C6-N1	7.43	1.44	1.39
1	16SA	1221	G	C6-N1	6.66	1.44	1.39
1	16SA	798	G	C6-N1	6.65	1.44	1.39
23	PSIA	20	U	N1-C2	6.42	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	23SB	760	G	C6-N1	6.42	1.44	1.39
27	23SB	44	G	C6-N1	6.35	1.44	1.39
27	23SA	1924	G	N9-C4	-6.07	1.33	1.38
23	PSIB	16	U	N1-C2	5.97	1.44	1.38
23	PSIA	16	U	N1-C2	5.93	1.43	1.38
26	TRNA	16	U	N1-C2	5.90	1.43	1.38
27	23SB	380	G	C6-N1	5.86	1.43	1.39
23	PSIB	16	U	N3-C4	5.81	1.43	1.38
28	5SA	20	G	C6-N1	5.55	1.43	1.39
23	PSIA	20	U	N3-C4	5.49	1.43	1.38
26	TRNA	16	U	N3-C4	5.47	1.43	1.38
27	23SB	53	G	C6-N1	5.33	1.43	1.39
26	TRNA	20	U	N1-C6	5.22	1.42	1.38
27	23SA	1462	G	C6-N1	5.17	1.43	1.39
1	16SA	1717	G	C6-N1	5.15	1.43	1.39
26	TRNA	20	U	N3-C4	5.08	1.43	1.38

All (1732) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16SA	727	U	N3-C4-O4	16.49	130.94	119.40
27	23SB	1065	G	N3-C2-N2	-15.07	109.35	119.90
1	16SA	727	U	C5-C4-O4	-13.95	117.53	125.90
27	23SA	995	G	O5'-P-OP1	-13.62	93.44	105.70
27	23SA	836	U	O5'-P-OP1	-13.48	93.56	105.70
1	16SA	798	G	N3-C2-N2	-12.74	110.98	119.90
27	23SB	44	G	N1-C6-O6	12.26	127.26	119.90
1	16SA	1221	G	N1-C6-O6	12.25	127.25	119.90
27	23SB	1689	U	O5'-P-OP2	-12.10	94.81	105.70
26	TRNA	16	U	C5-C4-O4	-12.06	118.67	125.90
27	23SB	2840	C	C2-N1-C1'	11.96	131.96	118.80
1	16SA	1221	G	C5-C6-O6	-11.90	121.46	128.60
27	23SB	44	G	N3-C2-N2	-11.82	111.63	119.90
1	16SA	1717	G	N3-C2-N2	-11.75	111.68	119.90
23	PSIA	16	U	N3-C4-C5	11.71	121.63	114.60
1	16SA	1826	U	O5'-P-OP1	-11.53	95.32	105.70
23	PSIB	16	U	C5-C4-O4	-11.53	118.98	125.90
27	23SB	1065	G	N1-C6-O6	11.47	126.78	119.90
26	TRNA	16	U	N3-C4-C5	11.40	121.44	114.60
27	23SB	2617	A	O5'-P-OP1	-11.37	95.47	105.70
23	PSIA	16	U	C2-N3-C4	-11.35	120.19	127.00
27	23SB	2829	C	C6-N1-C2	-11.34	115.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SB	760	G	N3-C2-N2	-11.34	111.97	119.90
26	TRNA	16	U	C2-N3-C4	-11.33	120.20	127.00
1	16SA	1682	C	C2-N1-C1'	11.18	131.10	118.80
23	PSIA	20	U	C5-C4-O4	-11.15	119.21	125.90
27	23SB	44	G	C5-C6-O6	-11.12	121.93	128.60
27	23SA	700	G	C5-C6-O6	-10.99	122.01	128.60
23	PSIA	20	U	N3-C4-C5	10.97	121.18	114.60
27	23SB	2840	C	C5-C6-N1	10.94	126.47	121.00
27	23SA	1663	A	O5'-P-OP1	-10.93	95.86	105.70
27	23SB	1212	G	N3-C2-N2	-10.86	112.30	119.90
1	16SB	785	G	N3-C2-N2	-10.79	112.35	119.90
27	23SB	2207	G	N3-C2-N2	-10.74	112.38	119.90
27	23SB	1924	G	N3-C4-N9	-10.54	119.68	126.00
1	16SB	1900	G	N3-C2-N2	-10.49	112.56	119.90
27	23SB	2843	G	N3-C2-N2	-10.40	112.62	119.90
27	23SB	1065	G	C5-C6-O6	-10.38	122.38	128.60
23	PSIA	20	U	C2-N3-C4	-10.32	120.81	127.00
1	16SA	727	U	C2-N1-C1'	10.24	129.99	117.70
1	16SB	785	G	C5-C6-O6	-10.14	122.51	128.60
27	23SA	700	G	N1-C6-O6	10.13	125.98	119.90
27	23SA	1462	G	N3-C2-N2	-10.08	112.84	119.90
26	TRNA	20	U	C5-C4-O4	-10.05	119.87	125.90
27	23SA	1924	G	N3-C4-N9	-10.04	119.98	126.00
28	5SA	20	G	N3-C2-N2	-10.03	112.88	119.90
27	23SB	760	G	C5-C6-O6	-10.02	122.59	128.60
27	23SA	1924	G	N3-C2-N2	-10.00	112.90	119.90
1	16SB	1616	G	C6-C5-N7	-9.95	124.43	130.40
27	23SA	1924	G	C4-N9-C1'	-9.90	113.62	126.50
27	23SA	395	C	C2-N1-C1'	9.82	129.60	118.80
27	23SB	380	G	N3-C2-N2	-9.79	113.05	119.90
22	ASIA	71	G	N1-C6-O6	9.79	125.77	119.90
26	TRNA	20	U	N3-C4-C5	9.76	120.46	114.60
23	PSIA	16	U	C5-C4-O4	-9.70	120.08	125.90
1	16SA	1682	C	C6-N1-C1'	-9.69	109.17	120.80
26	TRNA	20	U	C2-N3-C4	-9.69	121.19	127.00
25	MRNB	56	U	C2-N1-C1'	9.65	129.28	117.70
22	ASIA	71	G	C5-C6-O6	-9.64	122.81	128.60
1	16SA	1221	G	N3-C2-N2	-9.64	113.15	119.90
1	16SA	1905	U	O5'-P-OP1	-9.62	97.04	105.70
27	23SB	420	C	O5'-P-OP1	-9.56	97.09	105.70
1	16SA	1584	U	C2-N3-C4	-9.52	121.29	127.00
23	PSIB	16	U	C2-N3-C4	-9.50	121.30	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SB	380	G	C5-C6-O6	-9.49	122.90	128.60
23	PSIB	16	U	N3-C4-C5	9.42	120.25	114.60
26	TRNA	20	U	N1-C2-N3	9.35	120.51	114.90
1	16SA	798	G	N9-C4-C5	9.34	109.14	105.40
27	23SA	1988	U	N3-C2-O2	-9.33	115.67	122.20
22	ASIA	71	G	C4-C5-N7	9.31	114.52	110.80
27	23SA	1155	G	N3-C2-N2	-9.27	113.41	119.90
1	16SB	1771	G	N3-C4-N9	-9.26	120.44	126.00
22	ASIA	19	G	N3-C4-N9	-9.25	120.45	126.00
27	23SA	1988	U	N1-C2-O2	9.23	129.26	122.80
1	16SB	1653	C	C5-C4-N4	-9.21	113.75	120.20
27	23SB	760	G	N1-C6-O6	9.20	125.42	119.90
27	23SB	53	G	N3-C2-N2	-9.15	113.50	119.90
27	23SB	2840	C	C6-N1-C2	-9.13	116.65	120.30
1	16SB	1647	G	N9-C4-C5	-9.13	101.75	105.40
27	23SB	2445	A	O5'-P-OP2	-9.12	97.49	105.70
27	23SB	380	G	N1-C6-O6	9.10	125.36	119.90
1	16SB	1771	G	N9-C4-C5	9.08	109.03	105.40
27	23SA	1228	C	C2-N1-C1'	9.07	128.78	118.80
1	16SB	1562	G	N3-C2-N2	-9.04	113.57	119.90
27	23SA	2483	G	O4'-C1'-N9	9.03	115.42	108.20
22	ASIA	71	G	N9-C4-C5	-9.02	101.79	105.40
1	16SB	1919	U	O5'-P-OP1	-9.01	97.59	105.70
27	23SB	1017	C	C6-N1-C2	-9.00	116.70	120.30
27	23SA	2490	C	N1-C2-O2	9.00	124.30	118.90
27	23SA	1924	G	C8-N9-C1'	8.99	138.69	127.00
27	23SA	433	U	O5'-P-OP1	-8.96	97.64	105.70
27	23SA	1110	G	N3-C4-N9	-8.95	120.63	126.00
27	23SB	2211	G	N3-C2-N2	-8.94	113.64	119.90
27	23SA	2421	U	C2-N1-C1'	8.84	128.30	117.70
27	23SA	255	A	O4'-C1'-N9	8.82	115.26	108.20
1	16SA	1717	G	C5-C6-O6	-8.81	123.31	128.60
27	23SA	2490	C	C2-N1-C1'	8.80	128.48	118.80
43	L21A	38	LEU	CA-CB-CG	8.78	135.50	115.30
1	16SA	1621	G	N3-C2-N2	-8.77	113.76	119.90
1	16SB	1647	G	C4-C5-N7	8.77	114.31	110.80
1	16SB	1616	G	C4-C5-N7	8.71	114.29	110.80
28	5SA	20	G	C5-C6-O6	-8.71	123.37	128.60
1	16SA	1421	A	O4'-C1'-N9	8.68	115.15	108.20
27	23SB	1240	G	N1-C6-O6	-8.67	114.70	119.90
1	16SB	1616	G	N3-C4-N9	8.66	131.19	126.00
1	16SB	1899	G	N1-C6-O6	8.64	125.09	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SB	849	A	O5'-P-OP1	-8.64	97.92	105.70
1	16SB	1616	G	N9-C4-C5	-8.62	101.95	105.40
1	16SB	1069	G	N3-C4-N9	-8.61	120.83	126.00
22	ASIA	71	G	C6-C5-N7	-8.61	125.24	130.40
27	23SA	1228	C	C6-N1-C1'	-8.61	110.47	120.80
27	23SB	2207	G	N9-C4-C5	8.60	108.84	105.40
27	23SB	202	G	N3-C2-N2	-8.58	113.89	119.90
27	23SA	1532	G	C5-C6-O6	-8.57	123.46	128.60
23	PSIA	16	U	N1-C2-N3	8.56	120.04	114.90
27	23SA	1924	G	N3-C4-C5	8.56	132.88	128.60
1	16SB	1116	U	O5'-P-OP1	-8.55	98.00	105.70
27	23SA	1907	C	C6-N1-C2	-8.55	116.88	120.30
27	23SA	700	G	C6-C5-N7	-8.53	125.28	130.40
26	TRNA	16	U	N1-C2-N3	8.52	120.01	114.90
1	16SA	798	G	C4-C5-N7	-8.52	107.39	110.80
28	5SB	69	G	N1-C6-O6	8.52	125.01	119.90
1	16SB	754	G	N3-C4-C5	-8.52	124.34	128.60
1	16SA	1584	U	N1-C2-N3	8.50	120.00	114.90
28	5SB	69	G	C5-C6-O6	-8.50	123.50	128.60
1	16SA	1851	G	N3-C2-N2	-8.49	113.96	119.90
27	23SA	929	G	N3-C4-N9	-8.46	120.92	126.00
1	16SA	1471	C	C2-N1-C1'	8.45	128.09	118.80
1	16SB	1757	C	C2-N1-C1'	8.44	128.09	118.80
1	16SA	1929	U	C2-N1-C1'	8.43	127.82	117.70
28	5SA	20	G	N1-C6-O6	8.43	124.96	119.90
27	23SB	2829	C	N3-C4-C5	-8.41	118.53	121.90
23	PSIB	16	U	N1-C2-N3	8.40	119.94	114.90
1	16SB	1653	C	N3-C4-N4	8.39	123.87	118.00
1	16SB	1899	G	C4-C5-N7	8.38	114.15	110.80
1	16SA	1471	C	N3-C4-N4	8.37	123.86	118.00
27	23SB	1924	G	C4-N9-C1'	-8.35	115.64	126.50
1	16SB	1905	U	O5'-P-OP2	-8.35	98.19	105.70
27	23SA	2521	U	N3-C2-O2	-8.34	116.36	122.20
27	23SA	118	U	C4-C5-C6	8.33	124.70	119.70
27	23SA	1155	G	N9-C4-C5	8.33	108.73	105.40
27	23SB	1634	C	C2-N1-C1'	8.32	127.95	118.80
27	23SA	895	C	P-O3'-C3'	8.31	129.67	119.70
27	23SA	1101	C	C2-N1-C1'	8.31	127.94	118.80
1	16SB	785	G	C6-N1-C2	-8.31	120.11	125.10
27	23SA	929	G	N3-C2-N2	-8.30	114.09	119.90
27	23SB	352	G	N3-C2-N2	-8.27	114.11	119.90
27	23SA	395	C	C5-C6-N1	8.26	125.13	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	TRNA	20	U	N3-C2-O2	-8.23	116.44	122.20
27	23SB	1924	G	C8-N9-C1'	8.23	137.70	127.00
27	23SB	942	C	C2-N1-C1'	8.22	127.84	118.80
1	16SA	1817	G	N9-C4-C5	-8.21	102.11	105.40
27	23SA	1058	A	O5'-P-OP2	-8.19	98.33	105.70
57	ASIB	72	C	N3-C2-O2	-8.18	116.18	121.90
1	16SB	1257	G	N3-C2-N2	-8.15	114.19	119.90
1	16SA	1717	G	N1-C6-O6	8.14	124.78	119.90
27	23SA	229	U	O5'-P-OP2	-8.14	98.37	105.70
27	23SB	1065	G	N1-C2-N2	8.13	123.52	116.20
27	23SA	1744	C	P-O3'-C3'	8.12	129.45	119.70
27	23SA	700	G	C4-C5-N7	8.12	114.05	110.80
27	23SB	2840	C	C6-N1-C1'	-8.12	111.06	120.80
1	16SA	1352	U	C2-N1-C1'	8.11	127.43	117.70
1	16SB	1899	G	C6-C5-N7	-8.10	125.54	130.40
27	23SB	1551	C	C5-C6-N1	8.08	125.04	121.00
22	ASIA	19	G	N9-C4-C5	8.04	108.62	105.40
1	16SB	1837	C	C2-N1-C1'	8.04	127.64	118.80
1	16SB	1899	G	C5-C6-O6	-8.03	123.78	128.60
1	16SB	1115	G	O4'-C1'-N9	8.00	114.60	108.20
27	23SA	91	G	N3-C4-N9	-7.99	121.21	126.00
27	23SB	392	G	N9-C4-C5	7.99	108.59	105.40
27	23SB	392	G	N3-C2-N2	-7.97	114.32	119.90
27	23SB	788	G	O5'-P-OP1	-7.96	98.53	105.70
27	23SB	1021	G	C4-N9-C1'	-7.96	116.15	126.50
1	16SB	736	G	N3-C2-N2	-7.95	114.34	119.90
27	23SB	581	G	N7-C8-N9	7.94	117.07	113.10
1	16SB	1771	G	C6-C5-N7	7.93	135.16	130.40
27	23SA	909	U	C4-C5-C6	7.93	124.45	119.70
27	23SB	256	G	N9-C4-C5	-7.92	102.23	105.40
27	23SA	1228	C	C5-C4-N4	-7.92	114.66	120.20
1	16SB	1252	C	C2-N1-C1'	7.90	127.49	118.80
1	16SA	1002	G	C4-C5-N7	7.89	113.96	110.80
27	23SA	1532	G	N1-C6-O6	7.88	124.62	119.90
27	23SA	1907	C	C2-N1-C1'	7.87	127.46	118.80
1	16SB	1402	G	N9-C4-C5	7.87	108.55	105.40
1	16SB	785	G	N1-C6-O6	7.83	124.60	119.90
27	23SA	2322	G	O4'-C1'-N9	7.83	114.47	108.20
27	23SB	1820	A	N7-C8-N9	7.83	117.72	113.80
1	16SB	1928	U	N1-C2-O2	7.83	128.28	122.80
1	16SA	867	G	N1-C6-O6	7.81	124.59	119.90
1	16SA	1471	C	C5-C6-N1	7.81	124.91	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	PSIA	20	U	N1-C2-N3	7.81	119.58	114.90
1	16SB	826	C	C2-N1-C1'	7.80	127.38	118.80
27	23SB	2213	C	C2-N1-C1'	-7.80	110.22	118.80
27	23SA	1988	U	C2-N1-C1'	7.80	127.06	117.70
27	23SA	2808	G	N3-C2-N2	-7.80	114.44	119.90
27	23SA	2177	G	C5-C6-O6	-7.79	123.93	128.60
29	L2A	111	LEU	CA-CB-CG	7.78	133.19	115.30
27	23SB	1232	G	N3-C2-N2	-7.78	114.46	119.90
1	16SA	787	G	N1-C6-O6	-7.76	115.24	119.90
1	16SA	1927	G	C4-N9-C1'	-7.76	116.41	126.50
24	ESIA	3	C	C6-N1-C2	-7.75	117.20	120.30
1	16SB	1754	U	N3-C2-O2	-7.74	116.78	122.20
1	16SA	724	G	N3-C4-N9	-7.71	121.38	126.00
1	16SB	1899	G	N9-C4-C5	-7.69	102.32	105.40
1	16SA	1809	G	C4-N9-C1'	-7.68	116.52	126.50
28	5SA	21	G	C4-C5-N7	7.62	113.85	110.80
1	16SB	1781	C	C6-N1-C2	-7.62	117.25	120.30
27	23SB	1456	C	C2-N1-C1'	7.62	127.18	118.80
27	23SB	903	G	N3-C2-N2	-7.62	114.57	119.90
27	23SB	264	C	N1-C2-O2	-7.60	114.34	118.90
1	16SA	730	C	C6-N1-C2	-7.59	117.26	120.30
1	16SB	1562	G	N9-C4-C5	7.58	108.43	105.40
27	23SB	1065	G	C6-N1-C2	-7.58	120.55	125.10
1	16SA	796	G	N3-C2-N2	-7.57	114.60	119.90
1	16SB	1889	C	C6-N1-C2	-7.57	117.27	120.30
22	ASIA	19	G	C8-N9-C1'	7.56	136.83	127.00
27	23SB	31	C	O5'-P-OP1	-7.55	98.90	105.70
27	23SB	2211	G	N3-C4-N9	-7.55	121.47	126.00
27	23SA	1780	G	N3-C2-N2	-7.54	114.62	119.90
1	16SA	716	G	O4'-C1'-N9	7.54	114.23	108.20
27	23SA	2483	G	C4-N9-C1'	7.54	136.30	126.50
1	16SA	1899	G	N9-C4-C5	-7.54	102.39	105.40
27	23SB	1924	G	C6-C5-N7	7.53	134.92	130.40
27	23SA	2521	U	N1-C2-O2	7.53	128.07	122.80
27	23SB	1239	G	N9-C4-C5	-7.52	102.39	105.40
27	23SA	1443	U	O5'-P-OP1	-7.52	98.93	105.70
27	23SB	1079	G	N3-C2-N2	-7.52	114.64	119.90
1	16SA	798	G	N3-C4-N9	-7.51	121.49	126.00
27	23SA	256	G	N9-C4-C5	-7.51	102.40	105.40
27	23SA	700	G	N9-C4-C5	-7.51	102.40	105.40
27	23SA	220	U	O5'-P-OP2	-7.50	98.95	105.70
28	5SB	120	G	N3-C2-N2	-7.50	114.65	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SA	895	C	C2-N1-C1'	7.50	127.04	118.80
27	23SB	146	G	C4-C5-N7	-7.49	107.80	110.80
27	23SA	1362	U	C2-N1-C1'	7.49	126.69	117.70
27	23SB	1021	G	C8-N9-C1'	7.49	136.74	127.00
27	23SB	2184	G	O4'-C1'-N9	-7.49	102.21	108.20
23	PSIB	1	G	N3-C4-N9	7.47	130.48	126.00
27	23SB	146	G	N9-C4-C5	7.46	108.39	105.40
22	ASIA	56	C	C2-N1-C1'	7.46	127.00	118.80
27	23SB	1808	C	N3-C2-O2	-7.45	116.68	121.90
1	16SA	1899	G	C4-C5-N7	7.45	113.78	110.80
27	23SB	2317	G	N9-C4-C5	7.45	108.38	105.40
22	ASIA	75	C	C5-C6-N1	7.45	124.72	121.00
1	16SA	1442	U	O5'-P-OP1	-7.44	99.00	105.70
27	23SA	1462	G	C5-C6-O6	-7.44	124.14	128.60
27	23SB	1551	C	C2-N1-C1'	7.43	126.98	118.80
1	16SB	1647	G	C6-C5-N7	-7.43	125.94	130.40
27	23SB	1808	C	N1-C2-O2	7.43	123.36	118.90
27	23SA	2490	C	N3-C2-O2	-7.42	116.70	121.90
1	16SB	1754	U	C2-N1-C1'	7.42	126.61	117.70
28	5SA	21	G	N1-C6-O6	7.42	124.35	119.90
1	16SB	1187	G	O5'-P-OP1	-7.41	99.03	105.70
1	16SA	1441	C	P-O3'-C3'	7.41	128.59	119.70
27	23SA	946	C	N1-C2-O2	7.41	123.35	118.90
26	TRNA	3	C	N3-C4-N4	7.41	123.19	118.00
27	23SA	952	C	C2-N1-C1'	7.41	126.95	118.80
27	23SB	942	C	C5-C6-N1	7.40	124.70	121.00
28	5SB	69	G	C6-C5-N7	-7.39	125.96	130.40
1	16SA	727	U	N1-C2-O2	-7.39	117.63	122.80
1	16SA	1929	U	N1-C2-O2	7.39	127.97	122.80
1	16SA	1927	G	C8-N9-C1'	7.39	136.60	127.00
1	16SA	1002	G	N9-C4-C5	-7.38	102.45	105.40
27	23SA	2421	U	P-O3'-C3'	7.38	128.56	119.70
27	23SA	1882	A	O5'-P-OP2	-7.37	99.07	105.70
27	23SB	2318	G	N3-C2-N2	-7.37	114.74	119.90
1	16SA	1781	C	C6-N1-C2	-7.36	117.36	120.30
27	23SB	2221	C	C6-N1-C2	-7.35	117.36	120.30
27	23SB	377	G	C4-C5-N7	-7.34	107.87	110.80
1	16SA	1621	G	N9-C4-C5	7.33	108.33	105.40
22	ASIA	56	C	C6-N1-C2	-7.33	117.37	120.30
27	23SB	1817	A	O5'-P-OP1	7.32	119.49	110.70
27	23SB	2211	G	N9-C4-C5	7.32	108.33	105.40
27	23SB	423	U	O4'-C1'-N1	7.31	114.05	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SB	2207	G	N3-C4-N9	-7.31	121.61	126.00
1	16SB	814	C	C6-N1-C2	-7.31	117.38	120.30
1	16SB	2085	G	N9-C4-C5	-7.30	102.48	105.40
27	23SB	281	C	C2-N1-C1'	7.30	126.83	118.80
27	23SB	1924	G	N3-C4-C5	7.30	132.25	128.60
27	23SA	2130	C	N1-C2-O2	-7.30	114.52	118.90
27	23SA	2333	G	O4'-C1'-N9	7.30	114.04	108.20
1	16SA	867	G	C5-C6-O6	-7.29	124.23	128.60
1	16SB	1900	G	N9-C4-C5	7.29	108.31	105.40
27	23SA	256	G	C8-N9-C4	7.29	109.31	106.40
27	23SB	1924	G	N3-C2-N2	-7.29	114.80	119.90
27	23SA	2177	G	N3-C4-N9	7.28	130.37	126.00
22	ASIA	19	G	N3-C2-N2	-7.27	114.81	119.90
27	23SA	700	G	N3-C4-N9	7.26	130.35	126.00
1	16SA	727	U	C6-N1-C1'	-7.25	111.06	121.20
27	23SB	1637	C	C2-N1-C1'	7.24	126.77	118.80
1	16SA	1786	C	C2-N1-C1'	7.24	126.77	118.80
1	16SB	2085	G	C4-C5-N7	7.24	113.69	110.80
1	16SA	1817	G	N3-C4-N9	7.23	130.34	126.00
27	23SB	2341	C	C6-N1-C2	-7.23	117.41	120.30
27	23SB	1280	G	N3-C4-N9	-7.22	121.67	126.00
1	16SB	1562	G	N3-C4-N9	-7.21	121.67	126.00
27	23SB	757	C	C2-N1-C1'	7.21	126.73	118.80
1	16SA	2040	C	C6-N1-C2	-7.21	117.42	120.30
27	23SB	2617	A	O5'-P-OP2	7.21	119.35	110.70
27	23SB	294	C	C6-N1-C2	-7.19	117.42	120.30
1	16SB	986	C	C2-N1-C1'	7.18	126.70	118.80
27	23SA	789	U	O5'-P-OP2	-7.17	99.25	105.70
27	23SA	1421	U	C5-C6-N1	7.17	126.29	122.70
27	23SB	942	C	C6-N1-C2	-7.16	117.44	120.30
27	23SB	1882	A	O5'-P-OP1	-7.16	99.25	105.70
22	ASIA	19	G	C4-N9-C1'	-7.16	117.19	126.50
27	23SA	164	C	C6-N1-C2	-7.16	117.44	120.30
27	23SB	1039	C	C6-N1-C2	-7.15	117.44	120.30
1	16SA	727	U	N3-C2-O2	7.15	127.20	122.20
27	23SB	2886	A	N1-C2-N3	7.15	132.88	129.30
27	23SB	2128	C	C2-N1-C1'	7.15	126.66	118.80
27	23SA	1462	G	N1-C6-O6	7.14	124.18	119.90
28	5SA	21	G	C6-C5-N7	-7.14	126.12	130.40
27	23SA	2728	A	C8-N9-C4	-7.13	102.95	105.80
27	23SB	1231	G	N3-C2-N2	-7.13	114.91	119.90
27	23SA	2696	C	P-O3'-C3'	7.13	128.26	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16SA	1867	U	N1-C2-O2	7.12	127.79	122.80
27	23SA	1975	G	O4'-C1'-N9	7.12	113.89	108.20
1	16SB	1771	G	C4-C5-N7	-7.11	107.96	110.80
1	16SA	971	C	N1-C2-O2	7.10	123.16	118.90
27	23SA	1381	G	N3-C4-N9	7.10	130.26	126.00
27	23SA	118	U	N3-C2-O2	-7.10	117.23	122.20
27	23SA	1808	C	N3-C2-O2	-7.09	116.94	121.90
27	23SA	2184	G	C5-C6-O6	-7.09	124.35	128.60
27	23SA	1228	C	N3-C4-N4	7.08	122.96	118.00
27	23SB	1084	G	N3-C2-N2	-7.07	114.95	119.90
27	23SA	1101	C	C6-N1-C1'	-7.07	112.32	120.80
27	23SB	2128	C	C6-N1-C2	-7.06	117.47	120.30
1	16SB	1937	G	N3-C2-N2	-7.06	114.96	119.90
1	16SB	1402	G	C4-C5-N7	-7.05	107.98	110.80
22	ASIA	57	G	O4'-C1'-N9	7.05	113.84	108.20
27	23SB	332	G	N3-C4-N9	7.05	130.23	126.00
27	23SB	1349	U	P-O3'-C3'	7.05	128.16	119.70
27	23SB	1381	G	C4-N9-C1'	7.04	135.65	126.50
27	23SB	2322	G	O4'-C1'-N9	7.04	113.83	108.20
27	23SB	385	G	N3-C2-N2	-7.04	114.98	119.90
27	23SB	2127	U	C2-N3-C4	-7.03	122.78	127.00
1	16SA	1119	C	C2-N1-C1'	7.03	126.53	118.80
27	23SA	2177	G	C6-C5-N7	-7.03	126.18	130.40
27	23SB	1212	G	N1-C2-N2	7.03	122.52	116.20
27	23SB	1545	A	N7-C8-N9	7.03	117.31	113.80
27	23SB	1809	U	N3-C4-O4	7.02	124.31	119.40
27	23SB	1533	G	C6-C5-N7	-7.01	126.19	130.40
28	5SB	68	A	P-O3'-C3'	7.01	128.12	119.70
19	S19A	41	VAL	C-N-CD	-7.00	105.19	120.60
27	23SA	1532	G	N3-C4-N9	7.00	130.20	126.00
27	23SA	395	C	C6-N1-C1'	-7.00	112.40	120.80
1	16SA	798	G	N1-C2-N2	6.97	122.47	116.20
26	TRNA	20	U	C2-N1-C1'	6.97	126.07	117.70
27	23SB	903	G	N9-C4-C5	6.97	108.19	105.40
27	23SA	1466	C	C6-N1-C2	-6.97	117.51	120.30
1	16SA	1867	U	C2-N1-C1'	6.96	126.05	117.70
27	23SB	2184	G	C2-N3-C4	-6.96	108.42	111.90
22	ASIA	56	C	N3-C2-O2	-6.96	117.03	121.90
27	23SB	1212	G	N3-C4-N9	-6.95	121.83	126.00
27	23SB	1363	C	C2-N1-C1'	6.95	126.44	118.80
1	16SB	1606	A	N1-C2-N3	6.95	132.77	129.30
27	23SA	928	G	C4-C5-N7	6.94	113.58	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16SA	1403	G	N3-C2-N2	-6.92	115.05	119.90
23	PSIA	20	U	C4-C5-C6	-6.92	115.55	119.70
1	16SB	895	G	O5'-P-OP1	-6.92	99.47	105.70
27	23SB	146	G	N3-C2-N2	-6.92	115.06	119.90
27	23SB	163	G	C5-C6-O6	-6.92	124.45	128.60
1	16SA	785	G	N9-C4-C5	-6.92	102.63	105.40
1	16SA	747	G	C4-N9-C1'	6.91	135.49	126.50
27	23SB	358	G	C4-C5-N7	6.91	113.56	110.80
28	5SA	21	G	N9-C4-C5	-6.90	102.64	105.40
1	16SB	1402	G	N3-C4-N9	-6.90	121.86	126.00
27	23SB	1562	C	C6-N1-C2	-6.90	117.54	120.30
1	16SA	693	C	C6-N1-C2	6.90	123.06	120.30
1	16SB	814	C	C2-N1-C1'	6.90	126.39	118.80
1	16SB	1069	G	C8-N9-C1'	6.90	135.97	127.00
25	MRNB	56	U	C6-N1-C1'	-6.90	111.55	121.20
27	23SA	1217	G	C5-C6-O6	-6.90	124.46	128.60
27	23SA	1217	G	N1-C6-O6	6.89	124.04	119.90
28	5SB	69	G	C4-C5-N7	6.89	113.56	110.80
27	23SB	377	G	C5-C6-N1	-6.89	108.05	111.50
1	16SB	777	C	C2-N1-C1'	6.88	126.37	118.80
26	TRNA	3	C	C2-N1-C1'	6.88	126.37	118.80
27	23SA	1381	G	C4-N9-C1'	6.88	135.44	126.50
27	23SB	2213	C	C6-N1-C1'	6.87	129.05	120.80
1	16SA	867	G	C4-C5-N7	6.87	113.55	110.80
27	23SA	2208	C	C6-N1-C2	-6.87	117.55	120.30
28	5SB	91	G	C4-N9-C1'	6.87	135.43	126.50
27	23SA	877	U	C2-N1-C1'	6.87	125.94	117.70
22	ASIA	71	G	N3-C4-N9	6.86	130.12	126.00
27	23SA	2154	C	N3-C4-N4	-6.86	113.20	118.00
27	23SA	1532	G	N9-C4-C5	-6.85	102.66	105.40
27	23SB	2462	G	P-O3'-C3'	6.85	127.92	119.70
1	16SB	1973	A	P-O3'-C3'	6.85	127.92	119.70
27	23SB	557	G	C8-N9-C1'	-6.85	118.10	127.00
27	23SB	875	U	OP1-P-O3'	6.85	120.27	105.20
1	16SA	1471	C	C5-C4-N4	-6.85	115.41	120.20
1	16SB	1748	G	C6-C5-N7	6.85	134.51	130.40
1	16SA	1928	U	C2-N1-C1'	6.84	125.91	117.70
24	ESIB	59	U	O5'-P-OP1	-6.84	99.54	105.70
1	16SA	1221	G	C6-N1-C2	-6.84	121.00	125.10
27	23SB	377	G	C5-C6-O6	6.84	132.70	128.60
27	23SA	1532	G	C6-C5-N7	-6.83	126.30	130.40
24	ESIA	6	G	N3-C2-N2	-6.83	115.12	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	5SB	120	G	N3-C4-N9	-6.83	121.90	126.00
1	16SA	1225	C	O5'-P-OP2	-6.82	99.56	105.70
27	23SB	2421	U	O5'-P-OP1	-6.81	99.57	105.70
26	TRNA	3	C	C5-C4-N4	-6.80	115.44	120.20
24	ESIB	29	G	N3-C2-N2	-6.80	115.14	119.90
27	23SB	1634	C	C6-N1-C1'	-6.80	112.64	120.80
27	23SA	267	C	C6-N1-C2	-6.80	117.58	120.30
1	16SA	1929	U	N3-C2-O2	-6.79	117.45	122.20
1	16SB	1583	U	C2-N1-C1'	6.77	125.83	117.70
1	16SA	1403	G	N9-C4-C5	6.76	108.11	105.40
27	23SB	148	C	C6-N1-C2	-6.76	117.59	120.30
27	23SB	557	G	C4-N9-C1'	6.76	135.29	126.50
27	23SB	1239	G	C4-C5-N7	6.76	113.50	110.80
27	23SB	332	G	N9-C4-C5	-6.76	102.70	105.40
1	16SB	1974	G	N9-C4-C5	-6.75	102.70	105.40
1	16SA	1471	C	C6-N1-C1'	-6.75	112.70	120.80
27	23SB	1972	C	C6-N1-C2	-6.74	117.61	120.30
1	16SA	724	G	N9-C4-C5	6.73	108.09	105.40
27	23SB	1663	A	O4'-C1'-N9	6.73	113.58	108.20
1	16SA	796	G	N3-C4-N9	-6.72	121.97	126.00
27	23SB	44	G	C6-N1-C2	-6.72	121.07	125.10
27	23SA	2180	G	N3-C4-N9	-6.72	121.97	126.00
26	TRNA	16	U	C4-C5-C6	-6.72	115.67	119.70
27	23SA	2490	C	C6-N1-C2	-6.71	117.61	120.30
1	16SB	733	C	C2-N1-C1'	6.71	126.19	118.80
1	16SB	1069	G	C4-N9-C1'	-6.71	117.77	126.50
1	16SB	1748	G	C4-C5-N7	-6.71	108.11	110.80
27	23SA	1460	C	C2-N1-C1'	6.71	126.18	118.80
1	16SA	867	G	N9-C4-C5	-6.70	102.72	105.40
23	PSIA	16	U	C4-C5-C6	-6.70	115.68	119.70
1	16SB	1757	C	C6-N1-C2	-6.70	117.62	120.30
27	23SA	269	G	N3-C2-N2	-6.70	115.21	119.90
25	MRNA	56	U	C2-N1-C1'	6.69	125.73	117.70
27	23SB	311	C	C2-N1-C1'	6.69	126.16	118.80
28	5SB	69	G	N9-C4-C5	-6.69	102.72	105.40
27	23SB	2317	G	C6-C5-N7	6.69	134.41	130.40
24	ESIA	6	G	C8-N9-C4	-6.68	103.73	106.40
27	23SB	295	C	C2-N1-C1'	6.68	126.15	118.80
27	23SB	760	G	N1-C2-N2	6.68	122.21	116.20
27	23SB	1924	G	N9-C4-C5	6.68	108.07	105.40
27	23SA	2728	A	N7-C8-N9	6.67	117.14	113.80
27	23SA	699	C	N3-C4-N4	6.66	122.66	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16SB	1257	G	N9-C4-C5	6.66	108.06	105.40
1	16SB	1224	G	N3-C4-N9	6.66	130.00	126.00
27	23SB	557	G	C6-C5-N7	-6.66	126.41	130.40
1	16SA	1717	G	C6-N1-C2	-6.65	121.11	125.10
1	16SA	1793	C	N1-C2-O2	-6.65	114.91	118.90
23	PSIA	68	C	C2-N1-C1'	-6.64	111.49	118.80
1	16SA	867	G	C6-C5-N7	-6.64	126.42	130.40
27	23SA	1695	G	P-O3'-C3'	6.64	127.67	119.70
27	23SA	1927	C	C4-C5-C6	6.64	120.72	117.40
14	S14A	27	CYS	CA-CB-SG	6.63	125.94	114.00
27	23SB	202	G	N9-C4-C5	6.63	108.05	105.40
1	16SA	959	G	C4-C5-N7	-6.63	108.15	110.80
28	5SA	62	C	C2-N1-C1'	6.63	126.09	118.80
40	L18B	56	LEU	CA-CB-CG	6.62	130.53	115.30
27	23SA	1362	U	C5-C6-N1	6.62	126.01	122.70
27	23SA	2221	C	C6-N1-C2	-6.62	117.65	120.30
27	23SA	757	C	C2-N1-C1'	6.62	126.08	118.80
1	16SA	879	G	N3-C4-N9	-6.61	122.03	126.00
27	23SA	221	C	C2-N1-C1'	6.61	126.07	118.80
1	16SB	1616	G	C8-N9-C1'	-6.61	118.41	127.00
27	23SB	1065	G	N9-C4-C5	6.60	108.04	105.40
1	16SA	1002	G	C6-C5-N7	-6.60	126.44	130.40
1	16SB	733	C	C5-C4-N4	-6.59	115.58	120.20
1	16SB	1817	G	C8-N9-C4	-6.59	103.76	106.40
1	16SB	1899	G	N3-C4-N9	6.59	129.96	126.00
27	23SB	2492	C	C6-N1-C2	-6.59	117.66	120.30
37	L15A	88	LEU	CA-CB-CG	6.59	130.46	115.30
27	23SA	91	G	C6-C5-N7	6.59	134.35	130.40
1	16SA	727	U	C4-C5-C6	6.58	123.65	119.70
24	ESIA	6	G	N9-C4-C5	6.58	108.03	105.40
1	16SA	1286	G	N3-C2-N2	-6.58	115.30	119.90
1	16SB	1224	G	C8-N9-C1'	-6.57	118.46	127.00
27	23SB	332	G	C5-C6-N1	6.57	114.78	111.50
27	23SB	629	G	C5-C6-O6	-6.57	124.66	128.60
27	23SB	1784	G	C4-C5-N7	-6.57	108.17	110.80
1	16SA	2126	A	P-O3'-C3'	6.57	127.58	119.70
27	23SB	2328	C	N3-C2-O2	-6.57	117.30	121.90
24	ESIA	3	C	C5-C6-N1	6.56	124.28	121.00
1	16SA	1007	C	P-O3'-C3'	6.56	127.57	119.70
1	16SB	1754	U	N1-C2-O2	6.56	127.39	122.80
1	16SA	805	C	C5-C6-N1	6.55	124.27	121.00
1	16SB	1471	C	C6-N1-C2	-6.55	117.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SB	153	C	C2-N1-C1'	6.55	126.00	118.80
27	23SA	928	G	C6-C5-N7	-6.54	126.47	130.40
27	23SA	279	G	N1-C6-O6	-6.54	115.97	119.90
27	23SB	1381	G	C8-N9-C1'	-6.54	118.50	127.00
27	23SB	2124	U	C2-N1-C1'	6.54	125.55	117.70
27	23SA	1157	C	P-O3'-C3'	6.53	127.54	119.70
27	23SA	2154	C	N3-C2-O2	-6.53	117.33	121.90
27	23SA	2808	G	N9-C4-C5	6.53	108.01	105.40
27	23SB	1784	G	N9-C4-C5	6.53	108.01	105.40
1	16SA	2038	G	N3-C2-N2	-6.52	115.33	119.90
23	PSIB	16	U	C4-C5-C6	-6.52	115.79	119.70
1	16SA	803	C	C2-N1-C1'	6.52	125.97	118.80
27	23SB	1589	G	N3-C2-N2	-6.52	115.34	119.90
27	23SA	1421	U	C2-N3-C4	6.52	130.91	127.00
22	ASIA	75	C	C6-N1-C2	-6.51	117.69	120.30
1	16SB	1616	G	C4-N9-C1'	6.51	134.97	126.50
27	23SB	1097	C	C2-N1-C1'	6.51	125.96	118.80
25	MRNB	48	U	O5'-P-OP2	-6.51	99.84	105.70
27	23SB	2613	A	O5'-P-OP1	-6.50	99.85	105.70
27	23SA	1021	G	C4-N9-C1'	-6.49	118.06	126.50
1	16SB	1009	U	O4'-C1'-N1	6.49	113.39	108.20
1	16SB	1928	U	C2-N1-C1'	6.49	125.49	117.70
27	23SB	1515	G	C4-C5-N7	-6.49	108.20	110.80
1	16SB	1279	G	N3-C2-N2	-6.49	115.36	119.90
27	23SB	2207	G	C4-C5-N7	-6.49	108.20	110.80
27	23SA	800	A	O5'-P-OP1	-6.49	99.86	105.70
27	23SB	2488	U	C2-N1-C1'	6.49	125.48	117.70
28	5SB	33	C	N1-C2-O2	6.48	122.79	118.90
1	16SA	796	G	N9-C4-C5	6.48	107.99	105.40
27	23SA	2180	G	N9-C4-C5	6.48	107.99	105.40
1	16SA	777	C	C2-N1-C1'	6.47	125.92	118.80
27	23SB	1882	A	O5'-P-OP2	6.47	118.47	110.70
1	16SA	1660	G	C4-C5-N7	6.47	113.39	110.80
27	23SA	1936	PSU	OP2-P-O3'	6.47	119.43	105.20
27	23SB	1515	G	N9-C4-C5	6.47	107.99	105.40
1	16SA	1013	C	C2-N1-C1'	6.47	125.92	118.80
27	23SA	160	U	C2-N1-C1'	6.47	125.46	117.70
27	23SB	581	G	C4-N9-C1'	6.47	134.91	126.50
1	16SA	1899	G	N3-C4-N9	6.47	129.88	126.00
27	23SA	2774	A	N1-C6-N6	-6.47	114.72	118.60
27	23SB	624	G	N3-C4-N9	-6.47	122.12	126.00
27	23SA	1465	G	O4'-C1'-N9	6.46	113.37	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	MRNB	53	U	O4'-C1'-N1	6.46	113.36	108.20
1	16SB	1905	U	O5'-P-OP1	6.46	118.45	110.70
1	16SA	1938	G	N3-C2-N2	-6.45	115.39	119.90
27	23SB	174	C	C6-N1-C2	-6.45	117.72	120.30
27	23SB	2096	A	N1-C6-N6	6.45	122.47	118.60
1	16SB	754	G	P-O3'-C3'	6.44	127.43	119.70
27	23SA	1381	G	C8-N9-C1'	-6.44	118.63	127.00
27	23SA	2085	A	P-O3'-C3'	6.43	127.42	119.70
1	16SB	1939	G	N3-C2-N2	-6.43	115.40	119.90
27	23SA	2177	G	C4-C5-N7	6.43	113.37	110.80
1	16SB	1115	G	C4-N9-C1'	-6.43	118.14	126.50
1	16SB	1928	U	N3-C2-O2	-6.42	117.71	122.20
27	23SB	1021	G	C6-C5-N7	6.42	134.25	130.40
27	23SA	2126	G	N3-C4-N9	-6.41	122.15	126.00
27	23SB	392	G	C4-C5-N7	-6.41	108.23	110.80
27	23SB	1039	C	N3-C4-C5	-6.41	119.33	121.90
27	23SA	186	A	O4'-C1'-N9	6.41	113.33	108.20
27	23SA	1703	G	C8-N9-C4	-6.41	103.84	106.40
27	23SB	425	G	N3-C2-N2	-6.41	115.42	119.90
22	ASIA	19	G	C6-C5-N7	6.41	134.24	130.40
1	16SA	907	G	C4-N9-C1'	6.40	134.82	126.50
1	16SB	785	G	N1-C2-N2	6.40	121.96	116.20
27	23SB	1634	C	N1-C2-O2	6.39	122.74	118.90
27	23SA	1128	A	N9-C4-C5	-6.39	103.24	105.80
1	16SA	1682	C	C5-C6-N1	6.38	124.19	121.00
1	16SA	1809	G	C8-N9-C1'	6.38	135.30	127.00
1	16SB	1781	C	C2-N1-C1'	6.38	125.82	118.80
1	16SA	724	G	N3-C2-N2	-6.38	115.44	119.90
27	23SA	1435	C	C6-N1-C2	-6.37	117.75	120.30
27	23SB	624	G	C6-C5-N7	6.37	134.22	130.40
27	23SA	2441	A	P-O3'-C3'	6.37	127.34	119.70
27	23SA	432	C	C2-N1-C1'	6.37	125.80	118.80
27	23SB	605	C	C6-N1-C2	-6.36	117.75	120.30
27	23SA	160	U	N1-C2-O2	6.36	127.25	122.80
28	5SB	91	G	C8-N9-C1'	-6.36	118.73	127.00
27	23SA	91	G	N9-C4-C5	6.36	107.94	105.40
1	16SB	1554	C	N1-C2-O2	-6.36	115.09	118.90
27	23SB	392	G	C8-N9-C4	-6.36	103.86	106.40
27	23SB	2357	C	C6-N1-C2	-6.36	117.76	120.30
27	23SB	2317	G	C4-C5-N7	-6.35	108.26	110.80
27	23SA	2126	G	N3-C4-C5	6.35	131.78	128.60
1	16SA	955	C	C2-N1-C1'	6.35	125.78	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16SA	1845	C	C6-N1-C2	-6.35	117.76	120.30
27	23SA	929	G	C8-N9-C1'	6.35	135.25	127.00
27	23SA	2162	C	C6-N1-C2	-6.35	117.76	120.30
27	23SB	1955	G	C4-N9-C1'	-6.34	118.25	126.50
57	ASIB	34	G	C4-N9-C1'	6.34	134.75	126.50
27	23SB	624	G	C4-C5-N7	-6.34	108.26	110.80
27	23SA	1775	C	C6-N1-C2	-6.34	117.76	120.30
1	16SB	1845	C	C6-N1-C2	-6.34	117.77	120.30
27	23SA	1744	C	C2-N1-C1'	6.34	125.77	118.80
1	16SA	1933	A	N7-C8-N9	6.33	116.97	113.80
27	23SA	1217	G	C6-C5-N7	-6.33	126.60	130.40
27	23SB	1593	C	C2-N1-C1'	6.33	125.76	118.80
27	23SA	2177	G	N1-C6-O6	6.33	123.70	119.90
27	23SB	1139	G	N3-C4-N9	-6.33	122.20	126.00
27	23SA	2417	C	C5-C6-N1	6.32	124.16	121.00
1	16SA	1472	C	C6-N1-C2	-6.32	117.77	120.30
27	23SB	153	C	C6-N1-C1'	-6.32	113.22	120.80
1	16SB	1867	U	P-O3'-C3'	6.32	127.28	119.70
27	23SB	895	C	N3-C2-O2	-6.32	117.48	121.90
27	23SA	1685	G	C4-C5-N7	6.31	113.32	110.80
1	16SA	1717	G	N9-C4-C5	6.31	107.92	105.40
1	16SB	1771	G	N1-C6-O6	-6.31	116.12	119.90
1	16SB	1434	C	N1-C2-O2	6.30	122.68	118.90
27	23SB	1362	U	C2-N1-C1'	6.30	125.26	117.70
27	23SB	760	G	C6-N1-C2	-6.29	121.32	125.10
1	16SA	2073	G	N3-C4-N9	6.29	129.78	126.00
27	23SA	2521	U	C2-N1-C1'	6.29	125.25	117.70
1	16SA	1648	G	O4'-C1'-N9	6.29	113.23	108.20
1	16SA	2098	G	N1-C6-O6	-6.29	116.12	119.90
22	ASIA	74	C	C2-N1-C1'	6.29	125.72	118.80
27	23SA	2483	G	C8-N9-C1'	-6.28	118.83	127.00
27	23SB	255	A	O4'-C1'-N9	6.28	113.22	108.20
1	16SA	1660	G	N9-C4-C5	-6.26	102.90	105.40
27	23SA	2184	G	N1-C6-O6	6.26	123.66	119.90
1	16SB	1495	A	O4'-C1'-N9	-6.26	103.19	108.20
27	23SB	1813	U	O5'-P-OP2	-6.26	100.06	105.70
1	16SA	1536	A	P-O3'-C3'	6.25	127.21	119.70
27	23SA	2483	G	N7-C8-N9	6.25	116.23	113.10
1	16SB	1471	C	C5-C6-N1	6.25	124.13	121.00
23	PSIA	1	G	C4-N9-C1'	6.25	134.63	126.50
22	ASIA	67	C	C5-C4-N4	-6.25	115.83	120.20
27	23SB	1227	C	C2-N1-C1'	6.25	125.67	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SB	2184	G	C5-C6-N1	-6.25	108.38	111.50
57	ASIB	72	C	N1-C2-O2	6.24	122.65	118.90
27	23SB	1421	U	C5-C6-N1	6.24	125.82	122.70
27	23SB	2544	G	C4-N9-C1'	6.24	134.62	126.50
26	TRNA	20	U	C4-C5-C6	-6.24	115.95	119.70
1	16SA	1434	C	C6-N1-C2	-6.24	117.80	120.30
27	23SA	1110	G	N3-C4-C5	6.24	131.72	128.60
1	16SB	1069	G	N9-C4-C5	6.24	107.89	105.40
47	L25A	59	LEU	CA-CB-CG	6.23	129.63	115.30
1	16SB	1647	G	O4'-C1'-N9	6.23	113.19	108.20
1	16SB	1252	C	C6-N1-C1'	-6.23	113.33	120.80
1	16SA	969	C	C2-N1-C1'	6.23	125.65	118.80
1	16SB	1653	C	N1-C2-O2	-6.23	115.16	118.90
1	16SB	1467	G	C6-C5-N7	6.22	134.13	130.40
27	23SB	431	U	P-O3'-C3'	6.22	127.17	119.70
27	23SA	1258	A	P-O3'-C3'	6.22	127.16	119.70
1	16SB	1089	C	C2-N1-C1'	6.21	125.64	118.80
27	23SB	895	C	C6-N1-C2	-6.21	117.81	120.30
1	16SA	858	C	C2-N1-C1'	6.21	125.63	118.80
27	23SA	2022	G	O5'-P-OP2	-6.21	100.11	105.70
1	16SA	1256	G	N3-C2-N2	-6.21	115.55	119.90
1	16SB	1115	G	C8-N9-C1'	6.21	135.07	127.00
1	16SA	1793	C	C2-N3-C4	-6.21	116.80	119.90
1	16SA	2072	A	O4'-C1'-N9	6.21	113.17	108.20
27	23SB	1232	G	N3-C4-N9	-6.21	122.27	126.00
27	23SB	1381	G	N7-C8-N9	6.21	116.20	113.10
27	23SA	2173	G	N1-C6-O6	6.21	123.62	119.90
1	16SA	1114	G	P-O3'-C3'	6.20	127.14	119.70
1	16SB	754	G	C4-N9-C1'	6.20	134.56	126.50
27	23SB	1038	A	O5'-P-OP2	-6.20	100.12	105.70
28	5SB	119	G	N3-C4-N9	-6.20	122.28	126.00
1	16SA	1717	G	N1-C2-N2	6.20	121.78	116.20
27	23SA	432	C	P-O3'-C3'	6.20	127.14	119.70
27	23SA	1155	G	C4-C5-N7	-6.20	108.32	110.80
1	16SB	959	G	N3-C2-N2	-6.20	115.56	119.90
28	5SB	119	G	N3-C2-N2	-6.20	115.56	119.90
25	MRNB	56	U	N1-C2-O2	6.20	127.14	122.80
1	16SA	1089	C	C6-N1-C2	-6.19	117.83	120.30
27	23SA	1833	G	P-O3'-C3'	6.19	127.12	119.70
27	23SB	1533	G	C4-C5-N7	6.19	113.28	110.80
22	ASIA	2	C	N1-C2-O2	6.19	122.61	118.90
27	23SB	2322	G	C4-N9-C1'	6.18	134.53	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16SB	2085	G	C6-C5-N7	-6.17	126.70	130.40
27	23SB	1784	G	C6-C5-N7	6.17	134.10	130.40
27	23SA	98	U	C2-N1-C1'	6.17	125.10	117.70
24	ESIA	65	G	C4-C5-N7	6.17	113.27	110.80
27	23SA	1381	G	C6-C5-N7	-6.16	126.70	130.40
27	23SB	92	C	C2-N1-C1'	6.16	125.57	118.80
1	16SB	1076	C	C6-N1-C2	-6.15	117.84	120.30
1	16SB	1224	G	N9-C4-C5	-6.15	102.94	105.40
27	23SA	1894	G	N3-C4-N9	-6.15	122.31	126.00
27	23SB	1097	C	N1-C2-O2	6.15	122.59	118.90
1	16SA	830	C	N1-C2-O2	-6.14	115.22	118.90
27	23SB	877	U	C2-N1-C1'	6.14	125.06	117.70
27	23SB	1533	G	N9-C4-C5	-6.13	102.95	105.40
1	16SB	1634	G	N3-C2-N2	-6.13	115.61	119.90
1	16SB	1508	G	N9-C4-C5	6.12	107.85	105.40
27	23SB	295	C	C6-N1-C1'	-6.12	113.45	120.80
28	5SB	72	C	C6-N1-C2	-6.12	117.85	120.30
27	23SB	87	G	N9-C4-C5	-6.12	102.95	105.40
27	23SA	377	G	C5-C6-O6	-6.12	124.93	128.60
27	23SB	1562	C	C5-C6-N1	6.12	124.06	121.00
27	23SA	929	G	C4-N9-C1'	-6.12	118.55	126.50
27	23SA	945	C	C5-C4-N4	-6.12	115.92	120.20
27	23SB	992	A	O4'-C1'-N9	6.12	113.09	108.20
27	23SA	1584	U	N3-C2-O2	-6.11	117.92	122.20
27	23SA	2425	G	C4-C5-N7	-6.11	108.36	110.80
27	23SB	1190	U	C6-N1-C1'	-6.11	112.64	121.20
1	16SA	839	G	N3-C2-N2	-6.11	115.62	119.90
1	16SB	754	G	C2-N3-C4	6.11	114.95	111.90
27	23SB	2032	C	C6-N1-C2	-6.11	117.86	120.30
1	16SB	677	G	N3-C4-C5	6.11	131.65	128.60
27	23SB	1748	A	O4'-C1'-N9	6.11	113.08	108.20
27	23SA	2607	G	O5'-P-OP1	-6.10	100.21	105.70
1	16SA	1013	C	C6-N1-C2	-6.10	117.86	120.30
1	16SA	706	A	P-O3'-C3'	6.10	127.02	119.70
27	23SB	1421	U	C2-N3-C4	6.10	130.66	127.00
27	23SA	2717	U	O4'-C1'-N1	6.09	113.08	108.20
36	L14B	91	LEU	CA-CB-CG	6.09	129.32	115.30
1	16SA	2080	G	N3-C4-N9	-6.09	122.34	126.00
27	23SB	1939	C	C6-N1-C2	-6.09	117.86	120.30
22	ASIA	56	C	N1-C2-O2	6.09	122.55	118.90
1	16SB	872	G	N3-C2-N2	-6.09	115.64	119.90
1	16SA	1649	U	P-O3'-C3'	6.09	127.00	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16SB	831	C	N1-C2-O2	-6.08	115.25	118.90
27	23SA	1159	A	O4'-C1'-N9	6.08	113.07	108.20
27	23SA	2459	G	O5'-P-OP2	-6.08	100.22	105.70
27	23SB	119	G	C4-N9-C1'	6.08	134.41	126.50
1	16SA	1899	G	C6-C5-N7	-6.08	126.75	130.40
27	23SB	1551	C	C6-N1-C2	-6.08	117.87	120.30
1	16SA	1383	C	C6-N1-C2	-6.08	117.87	120.30
27	23SA	1363	C	C2-N1-C1'	6.07	125.48	118.80
1	16SA	1817	G	C5-C6-O6	-6.07	124.96	128.60
1	16SA	687	G	C8-N9-C4	-6.07	103.97	106.40
1	16SA	907	G	O4'-C1'-N9	-6.07	103.34	108.20
1	16SA	1257	G	N3-C2-N2	-6.07	115.65	119.90
27	23SB	2139	A	O4'-C1'-N9	6.07	113.06	108.20
27	23SA	1532	G	C4-C5-N7	6.07	113.23	110.80
27	23SB	819	G	N9-C4-C5	6.07	107.83	105.40
1	16SA	747	G	C8-N9-C1'	-6.07	119.11	127.00
27	23SA	1217	G	C4-C5-N7	6.06	113.23	110.80
1	16SA	1929	U	C5-C6-N1	6.06	125.73	122.70
23	PSIB	1	G	C6-C5-N7	-6.06	126.76	130.40
27	23SB	406	C	C6-N1-C2	-6.06	117.88	120.30
27	23SA	639	U	C2-N1-C1'	6.06	124.97	117.70
1	16SA	1069	G	P-O3'-C3'	6.06	126.97	119.70
1	16SB	1748	G	N9-C4-C5	6.06	107.82	105.40
1	16SA	2040	C	C5-C6-N1	6.05	124.03	121.00
1	16SA	1753	U	OP1-P-O3'	6.05	118.51	105.20
27	23SA	1924	G	C6-C5-N7	6.05	134.03	130.40
1	16SB	1069	G	N3-C2-N2	-6.05	115.66	119.90
27	23SB	1469	U	P-O3'-C3'	6.05	126.96	119.70
27	23SA	160	U	N3-C2-O2	-6.05	117.97	122.20
27	23SA	395	C	C6-N1-C2	-6.05	117.88	120.30
28	5SA	6	C	C6-N1-C2	-6.05	117.88	120.30
27	23SA	2231	G	C4-N9-C1'	6.04	134.36	126.50
27	23SB	380	G	C6-N1-C2	-6.04	121.47	125.10
1	16SB	785	G	C4-C5-N7	-6.04	108.38	110.80
1	16SB	1718	U	C6-N1-C2	-6.04	117.37	121.00
27	23SB	629	G	N3-C4-N9	6.04	129.63	126.00
1	16SB	1513	G	O4'-C1'-N9	6.04	113.03	108.20
27	23SB	377	G	N9-C4-C5	6.04	107.82	105.40
1	16SA	805	C	C6-N1-C2	-6.04	117.88	120.30
27	23SA	2301	A	O5'-P-OP2	-6.04	100.26	105.70
27	23SB	48	A	P-O3'-C3'	6.04	126.95	119.70
27	23SA	2231	G	C8-N9-C1'	-6.04	119.15	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16SB	1224	G	C4-N9-C1'	6.04	134.35	126.50
27	23SB	195	G	P-O3'-C3'	6.03	126.94	119.70
1	16SA	858	C	N3-C4-N4	6.03	122.22	118.00
1	16SA	1748	G	N9-C4-C5	6.03	107.81	105.40
1	16SA	1584	U	N3-C2-O2	-6.03	117.98	122.20
22	ASIA	19	G	C4-C5-N7	-6.02	108.39	110.80
28	5SB	34	C	C2-N1-C1'	6.02	125.42	118.80
27	23SA	557	G	C8-N9-C1'	6.02	134.82	127.00
27	23SA	2326	A	C2-N3-C4	-6.01	107.59	110.60
27	23SB	202	G	C4-C5-N7	-6.01	108.39	110.80
1	16SB	1837	C	N1-C2-O2	6.01	122.51	118.90
27	23SB	1097	C	C6-N1-C1'	-6.01	113.58	120.80
24	ESIB	58	A	OP1-P-O3'	6.01	118.43	105.20
27	23SB	575	G	N3-C4-N9	6.01	129.61	126.00
1	16SA	1243	A	N9-C4-C5	-6.01	103.40	105.80
1	16SA	1809	G	N3-C4-C5	6.00	131.60	128.60
1	16SB	754	G	C8-N9-C4	-6.00	104.00	106.40
1	16SB	1887	C	C6-N1-C2	-6.00	117.90	120.30
1	16SA	1330	C	P-O3'-C3'	6.00	126.90	119.70
1	16SA	1754	U	N3-C2-O2	-6.00	118.00	122.20
1	16SB	1079	G	C5-C6-O6	-6.00	125.00	128.60
1	16SB	1771	G	C5-C6-O6	5.99	132.20	128.60
27	23SB	2128	C	C5-C6-N1	5.99	124.00	121.00
27	23SB	424	G	C8-N9-C4	-5.99	104.00	106.40
27	23SB	1501	C	N1-C2-O2	-5.99	115.31	118.90
1	16SA	677	G	P-O3'-C3'	5.99	126.89	119.70
27	23SB	1809	U	C5-C4-O4	-5.99	122.31	125.90
27	23SB	2211	G	C8-N9-C1'	5.99	134.78	127.00
1	16SB	1319	G	O4'-C1'-N9	5.99	112.99	108.20
27	23SB	1252	A	P-O3'-C3'	5.99	126.88	119.70
23	PSIA	45	U	O4'-C1'-N1	5.98	112.99	108.20
1	16SB	1621	G	N3-C2-N2	-5.98	115.71	119.90
27	23SB	1820	A	C8-N9-C4	-5.98	103.41	105.80
1	16SA	1809	G	N3-C4-N9	-5.98	122.41	126.00
1	16SB	1963	C	P-O3'-C3'	5.98	126.88	119.70
27	23SB	1530	G	N9-C4-C5	5.98	107.79	105.40
27	23SA	1110	G	C2-N3-C4	-5.98	108.91	111.90
27	23SB	332	G	N3-C2-N2	5.98	124.08	119.90
27	23SB	2437	A	P-O3'-C3'	5.97	126.87	119.70
1	16SB	1562	G	C4-C5-N7	-5.97	108.41	110.80
27	23SA	2361	A	P-O3'-C3'	5.97	126.86	119.70
27	23SB	44	G	N1-C2-N2	5.97	121.57	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SB	2753	G	N9-C4-C5	5.97	107.79	105.40
27	23SA	946	C	N3-C2-O2	-5.96	117.73	121.90
27	23SA	4	C	C6-N1-C2	-5.96	117.92	120.30
27	23SA	1703	G	P-O3'-C3'	5.96	126.85	119.70
1	16SA	1752	G	C6-N1-C2	-5.96	121.53	125.10
1	16SB	754	G	N3-C4-N9	5.96	129.57	126.00
27	23SB	740	C	C6-N1-C2	-5.96	117.92	120.30
27	23SA	2017	G	P-O3'-C3'	5.96	126.85	119.70
27	23SB	975	G	N3-C2-N2	-5.96	115.73	119.90
27	23SB	2127	U	C5-C4-O4	-5.96	122.33	125.90
1	16SA	1510	G	N9-C4-C5	5.95	107.78	105.40
27	23SA	1110	G	N3-C2-N2	-5.95	115.73	119.90
27	23SA	685	G	N3-C4-N9	-5.95	122.43	126.00
27	23SB	2454	A	P-O3'-C3'	5.95	126.83	119.70
24	ESIB	73	A	O4'-C1'-N9	-5.94	103.44	108.20
1	16SA	796	G	C6-C5-N7	5.94	133.96	130.40
1	16SB	1982	G	N3-C2-N2	-5.94	115.74	119.90
1	16SA	2111	G	N9-C4-C5	5.93	107.77	105.40
27	23SA	1808	C	C6-N1-C2	-5.93	117.93	120.30
27	23SA	2124	U	N3-C2-O2	-5.93	118.05	122.20
1	16SA	969	C	C6-N1-C2	-5.93	117.93	120.30
27	23SB	1277	G	N3-C2-N2	-5.93	115.75	119.90
27	23SB	2255	C	C6-N1-C2	-5.93	117.93	120.30
27	23SA	2173	G	C4-C5-N7	5.93	113.17	110.80
24	ESIB	40	C	C6-N1-C2	-5.93	117.93	120.30
27	23SB	1975	G	O4'-C1'-N9	5.93	112.94	108.20
27	23SB	2216	G	P-O3'-C3'	5.93	126.81	119.70
27	23SA	1765	G	C5-C6-O6	-5.93	125.04	128.60
27	23SB	1481	C	C6-N1-C2	-5.93	117.93	120.30
1	16SA	1616	G	N3-C4-N9	5.92	129.56	126.00
27	23SA	648	A	N1-C2-N3	5.92	132.26	129.30
27	23SB	581	G	C8-N9-C4	-5.92	104.03	106.40
27	23SB	1456	C	C6-N1-C1'	-5.92	113.69	120.80
27	23SB	1703	G	P-O3'-C3'	5.92	126.81	119.70
27	23SB	2874	G	N3-C4-N9	5.92	129.56	126.00
1	16SB	1827	C	N3-C2-O2	-5.92	117.75	121.90
27	23SB	1391	A	O4'-C1'-N9	5.92	112.94	108.20
27	23SB	1528	G	C6-C5-N7	-5.92	126.85	130.40
1	16SA	1817	G	C4-C5-N7	5.92	113.17	110.80
1	16SB	766	G	N9-C4-C5	-5.92	103.03	105.40
27	23SB	204	G	O4'-C1'-N9	5.92	112.94	108.20
27	23SB	2057	G	C8-N9-C4	5.92	108.77	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16SB	1536	A	P-O3'-C3'	5.92	126.80	119.70
27	23SA	2533	A	C4-N9-C1'	5.91	136.94	126.30
27	23SB	624	G	N9-C4-C5	5.91	107.77	105.40
27	23SA	1562	C	C2-N1-C1'	5.91	125.30	118.80
1	16SA	907	G	P-O3'-C3'	5.91	126.79	119.70
1	16SA	1777	C	N3-C2-O2	-5.91	117.76	121.90
27	23SB	202	G	N3-C4-N9	-5.91	122.45	126.00
1	16SB	1771	G	N3-C2-N2	-5.91	115.77	119.90
1	16SB	736	G	C6-N1-C2	-5.91	121.56	125.10
1	16SB	1985	U	C2-N3-C4	-5.91	123.46	127.00
1	16SA	828	C	N1-C2-O2	-5.90	115.36	118.90
27	23SA	1956	U	N1-C2-O2	5.90	126.93	122.80
1	16SB	747	G	C4-N9-C1'	5.90	134.17	126.50
27	23SB	769	C	C2-N1-C1'	5.90	125.29	118.80
27	23SB	1955	G	P-O3'-C3'	5.90	126.78	119.70
27	23SB	2234	G	N3-C2-N2	-5.90	115.77	119.90
27	23SA	2173	G	C6-C5-N7	-5.90	126.86	130.40
28	5SA	20	G	N1-C2-N2	5.90	121.51	116.20
27	23SB	454	G	N9-C4-C5	-5.90	103.04	105.40
27	23SA	148	C	O5'-P-OP2	-5.90	100.39	105.70
1	16SA	1477	G	N3-C2-N2	-5.90	115.77	119.90
1	16SA	1777	C	N1-C2-O2	5.90	122.44	118.90
1	16SB	806	G	C6-C5-N7	5.89	133.94	130.40
27	23SB	1528	G	N9-C4-C5	-5.89	103.04	105.40
27	23SB	367	G	N3-C2-N2	-5.89	115.78	119.90
27	23SA	1010	U	O5'-P-OP2	-5.89	100.40	105.70
1	16SB	1616	G	N1-C6-O6	5.89	123.43	119.90
57	ASIB	7	A	O4'-C1'-N9	-5.89	103.49	108.20
1	16SA	836	G	P-O3'-C3'	5.89	126.77	119.70
1	16SA	1456	U	C2-N1-C1'	5.89	124.76	117.70
24	ESIA	65	G	N9-C4-C5	-5.89	103.05	105.40
27	23SB	294	C	N3-C4-C5	-5.89	119.55	121.90
1	16SA	1352	U	N1-C2-O2	5.88	126.92	122.80
27	23SA	2869	C	C6-N1-C2	-5.88	117.95	120.30
1	16SB	1900	G	N1-C2-N2	5.88	121.50	116.20
27	23SB	2357	C	C2-N1-C1'	5.88	125.27	118.80
27	23SB	2017	G	P-O3'-C3'	5.88	126.76	119.70
27	23SA	2683	G	N3-C4-N9	-5.88	122.47	126.00
1	16SB	1643	C	N3-C2-O2	-5.88	117.79	121.90
27	23SB	575	G	C5-C6-O6	-5.87	125.08	128.60
27	23SB	1456	C	C5-C6-N1	5.87	123.94	121.00
27	23SA	522	G	N9-C4-C5	5.87	107.75	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SA	2322	G	C8-N9-C1'	-5.87	119.37	127.00
1	16SB	2085	G	N1-C6-O6	5.87	123.42	119.90
27	23SB	2014	G	N3-C2-N2	-5.87	115.79	119.90
27	23SB	1939	C	C2-N1-C1'	5.87	125.25	118.80
1	16SA	805	C	C2-N1-C1'	5.87	125.25	118.80
22	ASIA	68	C	O4'-C1'-N1	5.86	112.89	108.20
1	16SA	1928	U	N3-C2-O2	-5.86	118.10	122.20
27	23SA	2845	U	C2-N1-C1'	5.86	124.73	117.70
27	23SB	1766	G	C4-N9-C1'	5.86	134.12	126.50
27	23SA	2333	G	C4-N9-C1'	5.86	134.12	126.50
24	ESIB	29	G	N9-C4-C5	5.86	107.74	105.40
27	23SA	1213	G	N9-C4-C5	5.86	107.74	105.40
27	23SA	1421	U	N1-C2-N3	-5.86	111.39	114.90
1	16SB	986	C	N1-C2-O2	5.86	122.41	118.90
27	23SB	725	A	O4'-C1'-N9	5.86	112.88	108.20
27	23SA	2162	C	N3-C2-O2	-5.85	117.80	121.90
1	16SB	1752	G	N3-C2-N2	-5.85	115.80	119.90
1	16SA	1013	C	N1-C2-O2	5.85	122.41	118.90
27	23SA	1939	C	C2-N1-C1'	5.85	125.23	118.80
1	16SB	1330	C	P-O3'-C3'	5.85	126.72	119.70
27	23SB	770	C	C2-N1-C1'	5.85	125.23	118.80
1	16SA	1851	G	N9-C4-C5	5.84	107.73	105.40
1	16SA	1074	C	C6-N1-C2	-5.83	117.97	120.30
27	23SB	672	C	O4'-C1'-N1	5.83	112.86	108.20
27	23SB	1869	G	N9-C4-C5	-5.83	103.07	105.40
22	ASIA	4	C	C6-N1-C2	-5.83	117.97	120.30
27	23SB	557	G	N9-C4-C5	-5.83	103.07	105.40
27	23SA	2165	C	N1-C2-O2	-5.83	115.41	118.90
27	23SB	1518	C	O5'-P-OP1	5.83	117.69	110.70
27	23SB	1329	G	N9-C4-C5	-5.82	103.07	105.40
28	5SB	5	C	C6-N1-C2	-5.82	117.97	120.30
1	16SB	2140	G	O5'-P-OP1	-5.82	100.46	105.70
28	5SA	45	C	C6-N1-C2	-5.82	117.97	120.30
27	23SA	1652	A	O5'-P-OP1	-5.82	100.46	105.70
27	23SA	1780	G	C6-N1-C2	-5.82	121.61	125.10
27	23SB	2274	G	N9-C4-C5	-5.82	103.07	105.40
27	23SA	965	A	O4'-C1'-N9	5.81	112.85	108.20
1	16SB	1610	G	N3-C4-N9	-5.81	122.51	126.00
1	16SA	1256	G	N9-C4-C5	5.81	107.72	105.40
1	16SA	971	C	N3-C2-O2	-5.81	117.83	121.90
1	16SA	1161	A	O4'-C1'-N9	5.81	112.85	108.20
28	5SA	68	A	O5'-P-OP2	-5.81	100.47	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16SA	1621	G	C6-N1-C2	-5.81	121.61	125.10
1	16SA	2073	G	C6-C5-N7	-5.81	126.92	130.40
27	23SA	539	G	O4'-C1'-N9	5.81	112.85	108.20
27	23SA	2322	G	C4-N9-C1'	5.81	134.05	126.50
1	16SB	1266	G	N9-C4-C5	5.81	107.72	105.40
1	16SA	1471	C	C2-N3-C4	5.80	122.80	119.90
27	23SA	1770	A	O4'-C1'-N9	5.80	112.84	108.20
27	23SA	2173	G	N9-C4-C5	-5.80	103.08	105.40
3	S3B	94	LEU	CA-CB-CG	5.80	128.65	115.30
1	16SA	716	G	C4-N9-C1'	5.80	134.04	126.50
1	16SB	1837	C	C6-N1-C1'	-5.80	113.84	120.80
27	23SB	87	G	C4-C5-N7	5.80	113.12	110.80
23	PSIA	40	C	C6-N1-C2	-5.80	117.98	120.30
28	5SA	21	G	C8-N9-C1'	-5.80	119.46	127.00
27	23SB	2255	C	N3-C2-O2	-5.80	117.84	121.90
27	23SA	140	A	N7-C8-N9	5.80	116.70	113.80
27	23SB	629	G	C6-C5-N7	-5.80	126.92	130.40
27	23SB	1154	G	N3-C4-N9	5.79	129.48	126.00
27	23SA	699	C	C5-C4-N4	-5.79	116.15	120.20
27	23SA	1228	C	C5-C6-N1	5.79	123.89	121.00
27	23SA	2180	G	N3-C2-N2	-5.79	115.85	119.90
9	S9A	85	LEU	CA-CB-CG	5.79	128.62	115.30
27	23SA	929	G	N9-C4-C5	5.79	107.72	105.40
27	23SA	1685	G	C6-C5-N7	-5.79	126.93	130.40
27	23SA	2142	A	O4'-C1'-N9	5.79	112.83	108.20
28	5SA	62	C	C6-N1-C2	-5.79	117.99	120.30
27	23SB	1103	G	C8-N9-C1'	-5.79	119.48	127.00
1	16SB	1974	G	N3-C4-N9	5.78	129.47	126.00
27	23SB	629	G	N1-C6-O6	5.78	123.37	119.90
27	23SB	680	A	OP2-P-O3'	5.78	117.92	105.20
1	16SA	737	G	C6-C5-N7	-5.78	126.93	130.40
22	ASIA	19	G	O4'-C1'-N9	-5.78	103.58	108.20
28	5SA	58	G	N3-C4-C5	-5.78	125.71	128.60
27	23SB	994	G	N9-C4-C5	5.78	107.71	105.40
27	23SB	1906	C	C2-N1-C1'	5.78	125.16	118.80
27	23SB	119	G	C8-N9-C1'	-5.77	119.50	127.00
27	23SA	2124	U	N1-C2-O2	5.77	126.84	122.80
1	16SB	841	G	N9-C4-C5	5.77	107.71	105.40
27	23SA	1700	G	N3-C4-N9	-5.77	122.54	126.00
27	23SB	555	A	N1-C2-N3	5.77	132.18	129.30
1	16SA	1867	U	C6-N1-C1'	-5.77	113.12	121.20
27	23SA	1894	G	N9-C4-C5	5.77	107.71	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16SB	1508	G	N3-C4-N9	-5.77	122.54	126.00
1	16SB	1985	U	N1-C2-N3	5.77	118.36	114.90
22	ASIA	76	A	O4'-C1'-N9	5.76	112.81	108.20
1	16SB	1495	A	C4-N9-C1'	5.76	136.67	126.30
27	23SA	1469	U	P-O3'-C3'	5.76	126.61	119.70
27	23SB	1239	G	C8-N9-C4	5.76	108.70	106.40
1	16SB	752	G	N3-C4-N9	5.75	129.45	126.00
27	23SA	1703	G	C4-N9-C1'	5.75	133.98	126.50
1	16SB	826	C	C6-N1-C1'	-5.75	113.90	120.80
1	16SB	1827	C	N1-C2-O2	5.75	122.35	118.90
27	23SB	2229	C	C6-N1-C2	-5.75	118.00	120.30
27	23SA	1907	C	C5-C6-N1	5.75	123.88	121.00
27	23SB	1217	G	N9-C4-C5	-5.75	103.10	105.40
27	23SA	2490	C	C6-N1-C1'	-5.75	113.90	120.80
23	PSIA	3	C	C6-N1-C2	-5.75	118.00	120.30
27	23SA	945	C	C5-C6-N1	5.75	123.87	121.00
1	16SB	1781	C	C5-C6-N1	5.75	123.87	121.00
1	16SA	777	C	C6-N1-C1'	-5.75	113.91	120.80
27	23SA	1079	G	N3-C2-N2	-5.75	115.88	119.90
1	16SA	798	G	N1-C6-O6	5.74	123.35	119.90
27	23SB	1285	G	N1-C6-O6	-5.74	116.45	119.90
27	23SB	2844	G	C6-C5-N7	5.74	133.85	130.40
27	23SB	1021	G	N3-C4-N9	-5.74	122.56	126.00
27	23SB	2492	C	C2-N1-C1'	5.74	125.12	118.80
28	5SB	23	G	C6-C5-N7	5.74	133.84	130.40
1	16SB	1777	C	C6-N1-C2	-5.74	118.00	120.30
27	23SA	2421	U	C5-C6-N1	5.74	125.57	122.70
27	23SA	2683	G	N9-C4-C5	5.74	107.70	105.40
27	23SB	1196	C	N1-C2-O2	-5.74	115.46	118.90
27	23SB	2293	A	O4'-C1'-N9	5.74	112.79	108.20
1	16SB	2038	G	N3-C4-N9	-5.73	122.56	126.00
27	23SB	2422	G	C4-C5-N7	5.73	113.09	110.80
27	23SB	2540	G	N9-C4-C5	5.73	107.69	105.40
27	23SB	2761	C	OP1-P-O3'	5.73	117.81	105.20
27	23SB	424	G	N7-C8-N9	5.73	115.96	113.10
27	23SA	1533	G	N9-C4-C5	-5.73	103.11	105.40
27	23SA	2191	G	N3-C4-N9	-5.73	122.56	126.00
1	16SA	959	G	N9-C4-C5	5.72	107.69	105.40
27	23SA	1809	U	N3-C4-O4	5.72	123.41	119.40
27	23SB	1391	A	C2-N3-C4	-5.72	107.74	110.60
27	23SB	1545	A	C8-N9-C4	-5.72	103.51	105.80
27	23SB	131	C	C6-N1-C2	-5.72	118.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SA	276	C	C5-C6-N1	5.72	123.86	121.00
27	23SA	1899	G	O4'-C1'-N9	-5.72	103.62	108.20
1	16SB	809	C	C6-N1-C2	-5.72	118.01	120.30
27	23SA	2177	G	N9-C4-C5	-5.71	103.11	105.40
27	23SB	2204	C	N3-C4-N4	5.71	122.00	118.00
1	16SA	1291	G	O4'-C1'-N9	5.70	112.76	108.20
1	16SA	2073	G	N3-C4-C5	-5.70	125.75	128.60
1	16SB	1983	G	N3-C4-C5	-5.70	125.75	128.60
27	23SB	281	C	C5-C6-N1	5.70	123.85	121.00
28	5SB	69	G	N3-C4-N9	5.70	129.42	126.00
1	16SA	1586	G	N9-C4-C5	5.70	107.68	105.40
27	23SA	400	G	N3-C4-N9	-5.70	122.58	126.00
27	23SB	707	C	C6-N1-C2	-5.70	118.02	120.30
1	16SA	1616	G	C6-C5-N7	-5.69	126.98	130.40
1	16SA	879	G	N3-C2-N2	-5.69	115.92	119.90
27	23SB	1103	G	C4-N9-C1'	5.69	133.90	126.50
27	23SA	2845	U	P-O3'-C3'	5.69	126.53	119.70
1	16SB	1316	A	P-O3'-C3'	5.69	126.53	119.70
23	PSIB	1	G	N9-C4-C5	-5.69	103.12	105.40
1	16SA	1905	U	C5-C6-N1	5.69	125.54	122.70
27	23SB	2211	G	N1-C2-N2	5.68	121.31	116.20
27	23SB	352	G	N9-C4-C5	5.68	107.67	105.40
27	23SA	1702	A	P-O3'-C3'	5.68	126.51	119.70
1	16SA	1352	U	C6-N1-C1'	-5.68	113.25	121.20
27	23SA	952	C	C6-N1-C1'	-5.68	113.99	120.80
27	23SA	1155	G	N3-C4-N9	-5.68	122.59	126.00
27	23SB	2204	C	C5-C4-N4	-5.68	116.23	120.20
27	23SA	877	U	N1-C2-O2	5.67	126.77	122.80
1	16SB	2013	G	C4-C5-N7	5.67	113.07	110.80
27	23SA	1765	G	N3-C4-N9	5.67	129.40	126.00
1	16SB	990	A	N9-C4-C5	-5.67	103.53	105.80
1	16SB	1924	C	P-O3'-C3'	5.67	126.50	119.70
27	23SA	644	G	O5'-P-OP2	-5.67	100.60	105.70
23	PSIB	5	G	N1-C6-O6	5.67	123.30	119.90
27	23SB	1065	G	C4-C5-N7	-5.67	108.53	110.80
1	16SA	1899	G	C8-N9-C1'	-5.67	119.64	127.00
1	16SA	1070	U	C5-C4-O4	-5.66	122.50	125.90
27	23SA	535	G	C4-N9-C1'	5.66	133.86	126.50
1	16SB	1773	C	P-O3'-C3'	5.66	126.49	119.70
27	23SA	1101	C	C5-C6-N1	5.66	123.83	121.00
27	23SA	778	G	O5'-P-OP1	-5.65	100.61	105.70
27	23SB	1632	C	C6-N1-C2	-5.65	118.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SB	2317	G	N3-C4-N9	-5.65	122.61	126.00
27	23SA	2646	G	C6-C5-N7	5.65	133.79	130.40
1	16SB	733	C	C6-N1-C1'	-5.65	114.02	120.80
28	5SA	87	G	N3-C4-N9	5.65	129.39	126.00
27	23SA	1021	G	C8-N9-C1'	5.64	134.34	127.00
27	23SA	2417	C	C6-N1-C2	-5.64	118.04	120.30
27	23SA	348	G	C4-C5-N7	5.64	113.06	110.80
27	23SB	1562	C	C2-N1-C1'	5.64	125.01	118.80
1	16SA	1346	C	C2-N1-C1'	5.64	125.00	118.80
27	23SA	2454	A	P-O3'-C3'	5.64	126.47	119.70
27	23SA	2490	C	C5-C6-N1	5.64	123.82	121.00
57	ASIB	34	G	C6-C5-N7	-5.64	127.02	130.40
23	PSIB	74	C	N1-C2-O2	5.64	122.28	118.90
1	16SB	1769	C	C6-N1-C1'	5.64	127.56	120.80
1	16SA	1928	U	N1-C2-O2	5.63	126.75	122.80
27	23SA	400	G	OP2-P-O3'	5.63	117.60	105.20
27	23SB	319	A	P-O3'-C3'	5.63	126.46	119.70
1	16SA	1518	G	N3-C4-N9	-5.63	122.62	126.00
1	16SB	1687	C	C6-N1-C2	-5.63	118.05	120.30
25	MRNA	56	U	N1-C2-O2	5.63	126.74	122.80
1	16SB	733	C	N3-C4-N4	5.63	121.94	118.00
1	16SB	1900	G	C6-N1-C2	-5.63	121.72	125.10
1	16SB	1402	G	C6-C5-N7	5.63	133.78	130.40
57	ASIB	41	C	C2-N1-C1'	5.63	124.99	118.80
27	23SB	462	C	C6-N1-C2	-5.63	118.05	120.30
27	23SA	1486	C	C2-N1-C1'	5.62	124.99	118.80
1	16SA	858	C	C5-C4-N4	-5.62	116.26	120.20
22	ASIA	1	G	N9-C4-C5	-5.62	103.15	105.40
27	23SA	1110	G	N9-C4-C5	5.62	107.65	105.40
1	16SB	718	C	C6-N1-C2	-5.62	118.05	120.30
27	23SB	2162	C	N1-C2-O2	5.62	122.27	118.90
1	16SA	1754	U	N1-C2-O2	5.62	126.73	122.80
28	5SA	62	C	C5-C6-N1	5.62	123.81	121.00
27	23SA	2421	U	C6-N1-C1'	-5.62	113.34	121.20
1	16SB	1095	C	C2-N1-C1'	5.62	124.98	118.80
27	23SB	1975	G	C4-N9-C1'	5.62	133.80	126.50
27	23SB	358	G	C6-C5-N7	-5.61	127.03	130.40
26	TRNA	3	C	C6-N1-C1'	-5.61	114.07	120.80
1	16SA	871	G	C4-C5-N7	-5.61	108.56	110.80
27	23SA	2483	G	C6-C5-N7	-5.61	127.04	130.40
28	5SA	54	A	O4'-C1'-N9	5.61	112.69	108.20
1	16SB	1554	C	O4'-C1'-N1	5.61	112.69	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16SA	1852	A	O4'-C1'-N9	5.61	112.68	108.20
27	23SB	2705	C	O5'-P-OP2	-5.61	100.66	105.70
27	23SB	2890	G	N3-C2-N2	-5.61	115.98	119.90
27	23SA	556	A	N7-C8-N9	5.60	116.60	113.80
27	23SA	2230	G	N3-C4-C5	-5.60	125.80	128.60
28	5SB	46	G	C6-C5-N7	5.60	133.76	130.40
27	23SA	2777	G	N3-C4-C5	-5.60	125.80	128.60
1	16SB	1467	G	N3-C4-N9	-5.60	122.64	126.00
27	23SB	946	C	O4'-C1'-N1	5.60	112.68	108.20
1	16SB	1827	C	P-O3'-C3'	5.59	126.41	119.70
27	23SA	1217	G	C8-N9-C1'	-5.59	119.73	127.00
27	23SA	1748	A	O4'-C1'-N9	5.59	112.67	108.20
51	L30B	53	LEU	CA-CB-CG	5.59	128.16	115.30
27	23SA	2533	A	C8-N9-C1'	-5.59	117.64	127.70
27	23SB	1227	C	C6-N1-C1'	-5.59	114.09	120.80
27	23SB	2570	U	C5-C4-O4	-5.59	122.55	125.90
1	16SB	986	C	C6-N1-C1'	-5.59	114.10	120.80
42	L20A	98	LEU	CA-CB-CG	5.58	128.15	115.30
1	16SA	667	G	C8-N9-C4	-5.58	104.17	106.40
1	16SA	837	G	N3-C4-N9	5.58	129.35	126.00
27	23SA	535	G	C8-N9-C1'	-5.58	119.75	127.00
1	16SB	2014	G	N3-C2-N2	-5.58	115.99	119.90
1	16SB	826	C	C5-C6-N1	5.58	123.79	121.00
27	23SB	1280	G	N9-C4-C5	5.58	107.63	105.40
23	PSIB	68	C	N1-C2-O2	-5.57	115.56	118.90
27	23SB	536	C	C6-N1-C2	-5.57	118.07	120.30
27	23SA	1584	U	N1-C2-O2	5.57	126.70	122.80
27	23SA	2521	U	C6-N1-C2	-5.57	117.66	121.00
27	23SA	1466	C	C5-C6-N1	5.57	123.78	121.00
27	23SB	581	G	C6-C5-N7	-5.57	127.06	130.40
1	16SA	969	C	N1-C2-O2	5.56	122.24	118.90
27	23SB	53	G	C5-C6-O6	-5.56	125.26	128.60
27	23SB	757	C	C6-N1-C1'	-5.56	114.13	120.80
27	23SB	2005	G	N9-C4-C5	-5.56	103.18	105.40
27	23SB	2769	A	OP2-P-O3'	5.56	117.43	105.20
1	16SB	1006	U	C2-N1-C1'	5.56	124.37	117.70
1	16SB	1786	C	C2-N1-C1'	5.56	124.91	118.80
1	16SB	1963	C	OP2-P-O3'	5.56	117.42	105.20
27	23SB	2599	U	N3-C2-O2	-5.56	118.31	122.20
1	16SA	871	G	N9-C4-C5	5.55	107.62	105.40
27	23SA	400	G	N3-C4-C5	5.55	131.38	128.60
27	23SB	2126	G	N9-C4-C5	-5.55	103.18	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SA	530	A	P-O3'-C3'	5.55	126.36	119.70
27	23SB	358	G	N9-C4-C5	-5.55	103.18	105.40
27	23SB	2422	G	N9-C4-C5	-5.55	103.18	105.40
27	23SB	1820	A	C4-N9-C1'	5.55	136.29	126.30
1	16SA	879	G	N9-C4-C5	5.55	107.62	105.40
27	23SA	1583	G	N3-C4-C5	-5.55	125.83	128.60
27	23SB	2741	A	P-O3'-C3'	5.55	126.36	119.70
27	23SA	1217	G	C4-N9-C1'	5.54	133.71	126.50
27	23SB	2210	C	N1-C2-O2	-5.54	115.57	118.90
1	16SB	1434	C	N3-C2-O2	-5.54	118.02	121.90
1	16SA	1402	G	O5'-P-OP2	-5.54	100.71	105.70
1	16SA	1621	G	C4-C5-N7	-5.54	108.58	110.80
27	23SA	1070	G	C8-N9-C4	-5.54	104.19	106.40
27	23SB	2068	C	C2-N1-C1'	5.54	124.89	118.80
1	16SB	1900	G	N3-C4-N9	-5.54	122.68	126.00
27	23SB	2322	G	C8-N9-C1'	-5.54	119.80	127.00
27	23SB	392	G	N3-C4-N9	-5.53	122.68	126.00
27	23SB	683	C	C6-N1-C2	-5.53	118.09	120.30
27	23SB	1212	G	N9-C4-C5	5.53	107.61	105.40
27	23SA	557	G	C4-N9-C1'	-5.53	119.31	126.50
27	23SA	1776	C	C5-C6-N1	5.53	123.76	121.00
27	23SA	1924	G	N1-C2-N2	5.53	121.17	116.20
1	16SA	1441	C	OP2-P-O3'	5.53	117.36	105.20
27	23SB	281	C	C6-N1-C1'	-5.53	114.17	120.80
27	23SB	2492	C	N3-C4-C5	-5.53	119.69	121.90
27	23SB	405	C	C6-N1-C2	-5.52	118.09	120.30
24	ESIA	6	G	C6-N1-C2	-5.52	121.79	125.10
27	23SA	555	A	C4-N9-C1'	-5.52	116.36	126.30
27	23SA	2533	A	N9-C1'-C2'	-5.52	105.92	112.00
1	16SB	1367	C	C6-N1-C2	-5.52	118.09	120.30
27	23SA	1582	C	C2-N1-C1'	5.52	124.87	118.80
27	23SA	2909	U	N3-C4-O4	5.52	123.26	119.40
23	PSIB	17	C	C6-N1-C2	-5.52	118.09	120.30
27	23SB	256	G	C8-N9-C4	5.52	108.61	106.40
27	23SB	1358	G	O5'-P-OP2	5.52	117.32	110.70
27	23SA	1635	A	O5'-P-OP1	-5.52	100.74	105.70
27	23SA	895	C	C6-N1-C2	-5.51	118.10	120.30
27	23SA	2014	G	N3-C2-N2	-5.51	116.04	119.90
27	23SB	226	C	N1-C2-O2	-5.51	115.59	118.90
27	23SA	2188	C	O5'-P-OP2	-5.51	100.74	105.70
27	23SA	1462	G	N1-C2-N2	5.50	121.15	116.20
27	23SB	1190	U	N1-C2-O2	5.50	126.65	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	5SB	46	G	N3-C4-N9	-5.50	122.70	126.00
27	23SA	1744	C	C6-N1-C1'	-5.50	114.20	120.80
1	16SA	730	C	C5-C4-N4	5.50	124.05	120.20
28	5SA	21	G	O4'-C1'-N9	-5.50	103.80	108.20
27	23SA	952	C	C5-C6-N1	5.50	123.75	121.00
32	L5A	34	LEU	CA-CB-CG	5.50	127.94	115.30
27	23SA	1217	G	N9-C4-C5	-5.49	103.20	105.40
27	23SA	1593	C	C2-N1-C1'	5.49	124.84	118.80
27	23SA	1765	G	N9-C4-C5	-5.49	103.20	105.40
27	23SA	929	G	N1-C2-N2	5.49	121.14	116.20
27	23SB	1231	G	C5-C6-O6	-5.49	125.31	128.60
27	23SB	2886	A	N7-C8-N9	5.49	116.55	113.80
27	23SB	994	G	C4-C5-N7	-5.49	108.61	110.80
27	23SB	1766	G	C8-N9-C1'	-5.49	119.86	127.00
22	ASIA	67	C	N3-C4-N4	5.49	121.84	118.00
27	23SA	348	G	N9-C4-C5	-5.49	103.21	105.40
27	23SA	2130	C	C2-N1-C1'	-5.49	112.77	118.80
27	23SA	2395	C	C6-N1-C2	-5.48	118.11	120.30
27	23SB	380	G	N1-C2-N2	5.48	121.13	116.20
27	23SB	2231	G	OP2-P-O3'	5.48	117.26	105.20
28	5SB	18	G	N9-C4-C5	5.48	107.59	105.40
27	23SB	256	G	C4-C5-N7	5.48	112.99	110.80
27	23SA	1703	G	N3-C4-C5	-5.48	125.86	128.60
1	16SB	814	C	N1-C2-O2	5.47	122.18	118.90
27	23SB	1758	C	C6-N1-C2	-5.47	118.11	120.30
27	23SB	2551	G	N9-C4-C5	5.47	107.59	105.40
27	23SB	153	C	C5-C4-N4	-5.47	116.37	120.20
27	23SB	2096	A	N9-C4-C5	-5.47	103.61	105.80
1	16SB	814	C	N3-C2-O2	-5.47	118.07	121.90
27	23SB	146	G	N3-C4-N9	-5.47	122.72	126.00
27	23SB	1494	A	O4'-C1'-N9	5.47	112.58	108.20
27	23SB	1220	G	P-O3'-C3'	5.47	126.26	119.70
28	5SB	108	G	N3-C2-N2	-5.47	116.07	119.90
27	23SA	1252	A	N1-C2-N3	5.46	132.03	129.30
27	23SA	1588	G	C5-C6-O6	-5.46	125.33	128.60
27	23SB	140	A	N7-C8-N9	5.46	116.53	113.80
27	23SB	2795	U	C2-N1-C1'	5.46	124.25	117.70
27	23SA	2425	G	N9-C4-C5	5.46	107.58	105.40
27	23SB	53	G	N1-C2-N2	5.46	121.11	116.20
27	23SA	48	A	C5-N7-C8	5.45	106.63	103.90
24	ESIA	4	C	C6-N1-C2	-5.45	118.12	120.30
27	23SA	221	C	C6-N1-C1'	-5.45	114.26	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SA	2333	G	C8-N9-C4	-5.45	104.22	106.40
1	16SB	1583	U	N1-C2-O2	5.45	126.61	122.80
27	23SA	355	A	N1-C2-N3	5.45	132.03	129.30
1	16SA	796	G	C8-N9-C1'	5.45	134.08	127.00
22	ASIA	1	G	C4-C5-N7	5.45	112.98	110.80
27	23SA	2263	C	O5'-P-OP2	-5.45	100.80	105.70
27	23SA	2475	U	N1-C2-O2	5.45	126.61	122.80
27	23SA	2488	U	O5'-P-OP1	-5.45	100.80	105.70
27	23SB	994	G	C6-C5-N7	5.45	133.67	130.40
27	23SB	1820	A	C6-C5-N7	-5.45	128.49	132.30
27	23SB	163	G	N1-C6-O6	5.45	123.17	119.90
27	23SB	1190	U	C2-N1-C1'	5.45	124.23	117.70
27	23SB	378	G	N9-C4-C5	-5.44	103.22	105.40
27	23SB	2207	G	N1-C2-N2	5.44	121.10	116.20
1	16SA	1616	G	C4-N9-C1'	5.44	133.57	126.50
1	16SB	703	G	N3-C2-N2	-5.44	116.09	119.90
1	16SB	871	G	N3-C2-N2	-5.44	116.09	119.90
27	23SB	1381	G	C6-C5-N7	-5.44	127.14	130.40
1	16SB	1769	C	C2-N1-C1'	-5.44	112.82	118.80
25	MRNA	44	U	C5-C6-N1	5.44	125.42	122.70
27	23SB	1217	G	C5-C6-O6	-5.44	125.34	128.60
27	23SB	1703	G	C8-N9-C4	-5.44	104.22	106.40
26	TRNA	10	G	N3-C4-N9	5.43	129.26	126.00
27	23SA	2173	G	C5-C6-O6	-5.43	125.34	128.60
27	23SB	2742	U	C6-N1-C1'	-5.43	113.59	121.20
27	23SB	1089	C	C6-N1-C2	-5.43	118.13	120.30
27	23SA	699	C	C5-C6-N1	5.43	123.72	121.00
27	23SB	433	U	N1-C2-O2	5.43	126.60	122.80
1	16SB	786	G	C4-C5-N7	-5.43	108.63	110.80
27	23SB	423	U	C2-N1-C1'	-5.43	111.18	117.70
27	23SB	1869	G	N3-C4-N9	5.43	129.26	126.00
27	23SA	2906	G	O4'-C1'-N9	5.43	112.54	108.20
25	MRNB	56	U	C5-C6-N1	5.43	125.41	122.70
27	23SB	1637	C	C5-C6-N1	5.43	123.71	121.00
1	16SA	828	C	C2-N1-C1'	-5.42	112.83	118.80
27	23SA	377	G	N1-C6-O6	5.42	123.16	119.90
27	23SA	2207	G	N3-C2-N2	-5.42	116.10	119.90
28	5SB	68	A	C4-N9-C1'	5.42	136.06	126.30
1	16SA	1621	G	N3-C4-N9	-5.42	122.75	126.00
1	16SB	1206	G	N9-C4-C5	5.42	107.57	105.40
1	16SB	1647	G	N3-C4-N9	5.42	129.25	126.00
1	16SB	1757	C	C6-N1-C1'	-5.42	114.29	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SB	991	G	C4-N9-C1'	5.42	133.55	126.50
27	23SB	1637	C	C6-N1-C1'	-5.42	114.30	120.80
27	23SB	2127	U	N1-C2-O2	-5.42	119.01	122.80
27	23SA	2875	G	N9-C4-C5	5.42	107.57	105.40
1	16SB	1577	G	C6-N1-C2	-5.42	121.85	125.10
27	23SB	1532	G	C4-C5-N7	5.42	112.97	110.80
49	L28B	80	LEU	CA-CB-CG	5.42	127.76	115.30
28	5SB	18	G	N3-C4-N9	-5.42	122.75	126.00
1	16SA	1510	G	C4-C5-N7	-5.41	108.64	110.80
27	23SA	1956	U	N3-C2-O2	-5.41	118.41	122.20
28	5SA	58	G	C8-N9-C4	-5.41	104.23	106.40
27	23SA	2287	U	N3-C4-O4	-5.41	115.61	119.40
27	23SA	1462	G	C6-N1-C2	-5.41	121.86	125.10
24	ESIA	67	C	C6-N1-C2	-5.40	118.14	120.30
27	23SB	2124	U	C6-N1-C1'	-5.40	113.64	121.20
1	16SB	1206	G	C4-C5-N7	-5.40	108.64	110.80
27	23SB	2211	G	C4-N9-C1'	-5.40	119.48	126.50
27	23SA	2292	G	N3-C2-N2	-5.40	116.12	119.90
1	16SB	1063	C	C6-N1-C2	-5.40	118.14	120.30
23	PSIB	76	A	O4'-C1'-N9	-5.40	103.88	108.20
27	23SB	557	G	N3-C4-N9	5.40	129.24	126.00
27	23SB	1154	G	N9-C4-C5	-5.40	103.24	105.40
27	23SB	1381	G	C5-N7-C8	-5.39	101.60	104.30
27	23SB	2374	C	C6-N1-C2	-5.39	118.14	120.30
27	23SB	1790	G	N3-C4-N9	-5.39	122.76	126.00
1	16SA	776	C	C2-N1-C1'	5.39	124.73	118.80
27	23SA	1155	G	C6-N1-C2	-5.39	121.87	125.10
27	23SB	91	G	C6-N1-C2	-5.39	121.87	125.10
27	23SB	2843	G	N1-C2-N2	5.39	121.05	116.20
27	23SA	34	C	P-O3'-C3'	5.38	126.16	119.70
1	16SB	1495	A	C8-N9-C1'	-5.38	118.01	127.70
27	23SB	2211	G	C6-C5-N7	5.38	133.63	130.40
26	TRNA	10	G	C4-N9-C1'	5.38	133.50	126.50
27	23SA	2461	G	N3-C2-N2	-5.38	116.13	119.90
27	23SB	1065	G	N1-C2-N3	5.38	127.13	123.90
27	23SA	699	C	C2-N1-C1'	5.38	124.72	118.80
1	16SB	1301	U	N1-C2-O2	-5.38	119.03	122.80
27	23SA	1894	G	C6-C5-N7	5.38	133.63	130.40
1	16SB	766	G	C4-C5-N7	5.38	112.95	110.80
27	23SA	928	G	N9-C4-C5	-5.38	103.25	105.40
27	23SA	2326	A	N1-C2-N3	5.38	131.99	129.30
1	16SB	729	A	P-O3'-C3'	5.38	126.15	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16SA	656	A	C8-N9-C4	-5.37	103.65	105.80
1	16SA	1753	U	P-O3'-C3'	5.37	126.15	119.70
27	23SA	1714	A	O5'-P-OP2	-5.37	100.86	105.70
1	16SA	1584	U	C5-C6-N1	-5.37	120.01	122.70
27	23SA	2846	G	O4'-C1'-N9	5.37	112.50	108.20
22	ASIA	74	C	O4'-C1'-N1	5.37	112.50	108.20
22	ASIA	52	G	C4-N9-C1'	5.37	133.48	126.50
27	23SB	1593	C	O4'-C1'-N1	5.37	112.49	108.20
1	16SA	1089	C	C2-N1-C1'	5.37	124.70	118.80
1	16SA	1666	C	C5-C4-N4	-5.37	116.44	120.20
27	23SA	1685	G	N9-C4-C5	-5.37	103.25	105.40
27	23SB	1869	G	C4-C5-N7	5.37	112.95	110.80
27	23SA	1975	G	C4-N9-C1'	5.36	133.47	126.50
27	23SA	2736	U	N3-C4-O4	5.36	123.16	119.40
27	23SB	1545	A	O4'-C1'-N9	5.36	112.49	108.20
28	5SB	6	C	C2-N1-C1'	5.36	124.70	118.80
27	23SA	1767	G	C4-C5-N7	-5.36	108.66	110.80
27	23SB	1329	G	C4-C5-N7	5.36	112.94	110.80
1	16SA	785	G	N3-C4-N9	5.36	129.22	126.00
1	16SA	1456	U	N3-C2-O2	-5.36	118.45	122.20
1	16SA	1919	U	O5'-P-OP2	-5.36	100.88	105.70
1	16SB	1647	G	C8-N9-C1'	-5.36	120.04	127.00
27	23SA	1704	A	O5'-P-OP1	-5.36	100.88	105.70
27	23SA	2795	U	C2-N1-C1'	5.36	124.13	117.70
27	23SB	378	G	C4-C5-N7	5.35	112.94	110.80
23	PSIA	68	C	C6-N1-C2	5.35	122.44	120.30
1	16SB	920	A	P-O3'-C3'	5.35	126.12	119.70
23	PSIA	38	A	O5'-P-OP2	-5.35	100.88	105.70
1	16SB	1677	U	P-O3'-C3'	5.35	126.12	119.70
27	23SB	1853	A	P-O3'-C3'	5.35	126.12	119.70
27	23SA	2808	G	N3-C4-N9	-5.35	122.79	126.00
1	16SB	720	C	N3-C4-N4	5.35	121.74	118.00
27	23SB	2004	C	C6-N1-C2	-5.35	118.16	120.30
27	23SA	988	A	O5'-P-OP1	-5.35	100.89	105.70
1	16SA	1477	G	N9-C4-C5	5.35	107.54	105.40
27	23SB	87	G	C6-C5-N7	-5.34	127.19	130.40
1	16SA	1758	A	O4'-C1'-N9	-5.34	103.93	108.20
22	ASIA	1	G	N3-C4-N9	5.34	129.21	126.00
27	23SB	2792	A	P-O3'-C3'	5.34	126.11	119.70
27	23SB	433	U	N3-C2-O2	-5.34	118.46	122.20
27	23SB	1217	G	N3-C4-N9	5.34	129.20	126.00
27	23SB	1765	G	N3-C2-N2	-5.34	116.16	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SB	1796	A	OP2-P-O3'	5.34	116.95	105.20
1	16SA	1039	C	C2-N1-C1'	-5.34	112.93	118.80
27	23SA	929	G	N3-C4-C5	5.34	131.27	128.60
1	16SB	1912	A	P-O3'-C3'	5.34	126.10	119.70
27	23SB	423	U	C6-N1-C1'	5.34	128.67	121.20
27	23SB	992	A	C4-N9-C1'	5.34	135.90	126.30
27	23SA	1258	A	C3'-C2'-C1'	5.33	105.77	101.50
27	23SA	681	A	O5'-P-OP2	-5.33	100.90	105.70
1	16SB	1069	G	N3-C4-C5	5.33	131.27	128.60
1	16SA	991	G	N9-C4-C5	5.33	107.53	105.40
1	16SA	1111	G	P-O3'-C3'	5.33	126.09	119.70
27	23SA	1155	G	C8-N9-C4	-5.33	104.27	106.40
27	23SB	377	G	C8-N9-C4	-5.33	104.27	106.40
27	23SA	2184	G	N9-C4-C5	-5.32	103.27	105.40
1	16SB	1508	G	C6-C5-N7	5.32	133.59	130.40
1	16SA	1115	G	OP2-P-O3'	5.32	116.90	105.20
1	16SB	1069	G	C6-C5-N7	5.32	133.59	130.40
1	16SB	2085	G	C5-C6-O6	-5.32	125.41	128.60
27	23SB	2742	U	C2-N1-C1'	5.32	124.08	117.70
23	PSIA	72	C	O4'-C1'-N1	5.32	112.45	108.20
27	23SB	2544	G	C8-N9-C1'	-5.32	120.09	127.00
27	23SB	2689	G	C4-C5-N7	5.32	112.93	110.80
27	23SA	2726	A	O5'-P-OP2	-5.31	100.92	105.70
1	16SB	815	C	C2-N1-C1'	5.31	124.64	118.80
27	23SB	1280	G	C6-C5-N7	5.31	133.59	130.40
34	L9A	123	LEU	CA-CB-CG	5.31	127.51	115.30
1	16SB	1450	G	OP2-P-O3'	5.30	116.87	105.20
1	16SB	821	G	P-O3'-C3'	5.30	126.06	119.70
1	16SA	1666	C	C2-N1-C1'	5.30	124.63	118.80
1	16SB	1069	G	C4-C5-N7	-5.30	108.68	110.80
27	23SB	256	G	N3-C4-N9	5.30	129.18	126.00
27	23SB	2431	C	C6-N1-C2	-5.30	118.18	120.30
27	23SA	204	G	O4'-C1'-N9	5.30	112.44	108.20
27	23SA	601	U	O5'-P-OP1	-5.30	100.93	105.70
1	16SA	2067	C	C2-N1-C1'	5.30	124.63	118.80
28	5SB	46	G	N9-C4-C5	5.30	107.52	105.40
1	16SA	786	G	N3-C2-N2	-5.29	116.19	119.90
27	23SA	2180	G	C8-N9-C1'	5.29	133.88	127.00
57	ASIB	72	C	N3-C4-N4	-5.29	114.29	118.00
1	16SB	1508	G	C4-C5-N7	-5.29	108.68	110.80
28	5SA	81	C	C6-N1-C2	-5.29	118.18	120.30
27	23SB	360	C	C6-N1-C2	-5.29	118.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SB	1703	G	C4-N9-C1'	5.29	133.38	126.50
1	16SB	2066	G	N3-C4-N9	5.29	129.17	126.00
27	23SB	1906	C	C6-N1-C2	-5.29	118.19	120.30
1	16SA	2125	A	N7-C8-N9	5.29	116.44	113.80
26	TRNA	2	C	N1-C2-O2	-5.29	115.73	118.90
27	23SA	420	C	C2-N1-C1'	5.29	124.61	118.80
27	23SA	1780	G	C5-C6-O6	-5.29	125.43	128.60
26	TRNA	65	G	P-O3'-C3'	5.28	126.04	119.70
27	23SA	1665	A	O4'-C1'-N9	5.28	112.43	108.20
27	23SA	2505	G	C4-N9-C1'	5.28	133.37	126.50
1	16SA	1346	C	C6-N1-C2	-5.28	118.19	120.30
27	23SA	2232	A	O5'-P-OP1	5.28	117.04	110.70
1	16SB	1279	G	N9-C4-C5	5.28	107.51	105.40
27	23SB	1525	G	C4-N9-C1'	5.28	133.36	126.50
27	23SB	11	G	O4'-C1'-N9	5.28	112.42	108.20
27	23SB	259	U	O5'-P-OP2	-5.28	100.95	105.70
27	23SB	1363	C	C6-N1-C1'	-5.28	114.47	120.80
1	16SB	1687	C	N3-C2-O2	-5.28	118.21	121.90
1	16SA	1233	G	C6-C5-N7	-5.27	127.24	130.40
27	23SA	291	G	C5-C6-O6	-5.27	125.44	128.60
27	23SB	1525	G	C8-N9-C1'	-5.27	120.15	127.00
27	23SB	2263	C	N1-C2-O2	5.27	122.06	118.90
27	23SA	91	G	C4-C5-N7	-5.27	108.69	110.80
27	23SA	881	G	N3-C4-C5	-5.27	125.97	128.60
1	16SA	1748	G	C4-C5-N7	-5.27	108.69	110.80
1	16SA	1851	G	N1-C2-N2	5.27	120.94	116.20
27	23SA	1928	G	C4-C5-N7	5.27	112.91	110.80
28	5SB	113	G	C6-C5-N7	5.27	133.56	130.40
1	16SB	1562	G	N1-C2-N2	5.27	120.94	116.20
1	16SB	1845	C	C2-N1-C1'	5.26	124.59	118.80
1	16SB	1748	G	N1-C6-O6	-5.26	116.74	119.90
27	23SB	53	G	N1-C6-O6	5.26	123.06	119.90
27	23SA	992	A	P-O3'-C3'	5.26	126.02	119.70
27	23SB	1608	A	P-O3'-C3'	5.26	126.01	119.70
23	PSIA	18	G	O5'-P-OP1	-5.26	100.97	105.70
27	23SA	1776	C	C2-N1-C1'	5.26	124.59	118.80
1	16SB	1928	U	C6-N1-C1'	-5.26	113.84	121.20
1	16SB	1983	G	N3-C4-N9	5.26	129.16	126.00
27	23SA	2108	G	C4-C5-N7	5.26	112.90	110.80
57	ASIB	75	C	O4'-C1'-N1	5.26	112.41	108.20
1	16SB	969	C	C6-N1-C2	-5.25	118.20	120.30
1	16SA	1785	A	C2-N3-C4	5.25	113.23	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SA	2017	G	O4'-C1'-N9	-5.25	104.00	108.20
1	16SB	2066	G	C6-C5-N7	-5.25	127.25	130.40
27	23SB	2211	G	C4-C5-N7	-5.25	108.70	110.80
27	23SB	1285	G	N3-C2-N2	5.25	123.58	119.90
27	23SB	2154	C	C6-N1-C2	-5.25	118.20	120.30
27	23SB	1973	G	C4-N9-C1'	5.25	133.32	126.50
1	16SA	955	C	C6-N1-C1'	-5.25	114.50	120.80
27	23SB	895	C	P-O3'-C3'	5.25	126.00	119.70
27	23SB	2328	C	C6-N1-C2	-5.25	118.20	120.30
1	16SA	969	C	P-O3'-C3'	5.25	125.99	119.70
27	23SB	162	C	C5-C4-N4	-5.25	116.53	120.20
1	16SA	1933	A	C8-N9-C4	-5.24	103.70	105.80
27	23SB	73	A	N1-C2-N3	5.24	131.92	129.30
27	23SB	1665	A	O4'-C1'-N9	5.24	112.39	108.20
1	16SB	1910	G	N3-C2-N2	-5.24	116.23	119.90
27	23SA	2583	C	C6-N1-C2	-5.24	118.20	120.30
27	23SA	200	C	C6-N1-C2	5.24	122.39	120.30
28	5SB	77	G	C4-N9-C1'	5.24	133.31	126.50
27	23SB	1618	G	N3-C4-C5	5.23	131.22	128.60
1	16SA	2121	UR3	P-O3'-C3'	5.23	125.98	119.70
1	16SB	677	G	N3-C4-N9	-5.23	122.86	126.00
27	23SA	725	A	O4'-C1'-N9	5.23	112.38	108.20
23	PSIA	1	G	C8-N9-C1'	-5.23	120.20	127.00
27	23SB	769	C	C6-N1-C2	-5.23	118.21	120.30
1	16SB	1786	C	N1-C2-O2	5.23	122.04	118.90
1	16SA	742	C	N1-C2-O2	-5.22	115.77	118.90
27	23SA	218	A	OP1-P-O3'	5.22	116.69	105.20
27	23SA	2911	G	C6-C5-N7	5.22	133.53	130.40
27	23SB	2890	G	N9-C4-C5	5.22	107.49	105.40
28	5SB	18	G	C8-N9-C4	-5.22	104.31	106.40
27	23SA	1700	G	C4-C5-N7	-5.22	108.71	110.80
27	23SA	2173	G	C8-N9-C1'	-5.22	120.21	127.00
27	23SA	2778	G	N3-C4-C5	-5.22	125.99	128.60
27	23SB	2126	G	C4-C5-N7	5.22	112.89	110.80
28	5SB	113	G	C4-C5-N7	-5.22	108.71	110.80
1	16SB	1104	G	C5-C6-O6	5.22	131.73	128.60
27	23SB	1486	C	C2-N1-C1'	5.22	124.54	118.80
27	23SA	750	G	O4'-C1'-N9	-5.22	104.03	108.20
27	23SA	909	U	C2-N1-C1'	5.22	123.96	117.70
27	23SA	1690	C	O4'-C1'-N1	5.22	112.37	108.20
27	23SB	264	C	O4'-C1'-N1	5.21	112.37	108.20
27	23SB	454	G	C4-C5-N7	5.21	112.89	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SB	2284	A	OP2-P-O3'	5.21	116.67	105.20
27	23SB	1381	G	O4'-C1'-N9	-5.21	104.03	108.20
27	23SA	279	G	C6-C5-N7	5.21	133.53	130.40
27	23SA	1883	G	N3-C2-N2	-5.21	116.25	119.90
27	23SB	1973	G	C8-N9-C1'	-5.21	120.22	127.00
1	16SA	1042	C	N1-C2-O2	-5.21	115.77	118.90
27	23SA	2217	G	C8-N9-C1'	-5.21	120.23	127.00
27	23SA	2435	C	O5'-P-OP1	-5.21	101.01	105.70
1	16SA	1867	U	N3-C2-O2	-5.21	118.56	122.20
27	23SA	2778	G	C4-N9-C1'	5.21	133.27	126.50
1	16SB	1681	G	N3-C4-C5	5.21	131.20	128.60
27	23SB	960	C	C6-N1-C2	-5.21	118.22	120.30
27	23SA	216	G	O4'-C1'-N9	5.21	112.36	108.20
27	23SA	877	U	C6-N1-C1'	-5.21	113.91	121.20
27	23SB	2274	G	C4-C5-N7	5.21	112.88	110.80
27	23SB	2542	C	C6-N1-C2	-5.21	118.22	120.30
27	23SA	1217	G	N3-C4-N9	5.21	129.12	126.00
27	23SA	1930	C	C6-N1-C2	-5.21	118.22	120.30
1	16SB	1616	G	C5-C6-O6	-5.21	125.48	128.60
27	23SB	760	G	N9-C4-C5	5.21	107.48	105.40
27	23SB	1924	G	C4-C5-N7	-5.21	108.72	110.80
27	23SA	1021	G	N3-C4-C5	5.20	131.20	128.60
1	16SA	2111	G	C4-C5-N7	-5.20	108.72	110.80
23	PSIA	1	G	N3-C4-C5	-5.20	126.00	128.60
1	16SA	1077	C	C6-N1-C2	-5.20	118.22	120.30
27	23SA	2287	U	C5-C4-O4	5.20	129.02	125.90
27	23SB	1309	G	N9-C4-C5	5.20	107.48	105.40
1	16SA	1777	C	C2-N1-C1'	5.20	124.52	118.80
1	16SB	1282	A	O4'-C1'-N9	5.20	112.36	108.20
1	16SB	1562	G	C8-N9-C1'	5.20	133.76	127.00
27	23SB	628	A	P-O3'-C3'	5.20	125.94	119.70
1	16SA	1053	A	P-O3'-C3'	5.20	125.94	119.70
27	23SB	2230	G	N3-C4-C5	-5.20	126.00	128.60
27	23SB	2431	C	C5-C6-N1	5.20	123.60	121.00
1	16SA	1135	G	N9-C4-C5	-5.19	103.32	105.40
27	23SB	1536	G	N9-C4-C5	5.19	107.48	105.40
24	ESIA	6	G	C4-C5-N7	-5.19	108.72	110.80
1	16SB	1974	G	OP1-P-O3'	5.19	116.62	105.20
1	16SA	907	G	C8-N9-C1'	-5.19	120.26	127.00
27	23SA	1498	G	N9-C4-C5	5.19	107.47	105.40
27	23SA	1553	C	C2-N1-C1'	5.19	124.51	118.80
1	16SA	1752	G	N9-C4-C5	5.18	107.47	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S19A	41	VAL	C-N-CA	5.18	143.78	122.00
27	23SA	1228	C	N3-C2-O2	5.18	125.53	121.90
27	23SA	2540	G	O4'-C1'-N9	5.18	112.35	108.20
27	23SB	895	C	N1-C2-O2	5.18	122.01	118.90
27	23SB	2492	C	N3-C4-N4	5.18	121.63	118.00
27	23SB	2736	U	C2-N3-C4	5.18	130.11	127.00
1	16SB	747	G	C8-N9-C1'	-5.18	120.26	127.00
1	16SB	1230	C	C6-N1-C2	-5.18	118.23	120.30
1	16SA	1274	C	C2-N1-C1'	5.18	124.50	118.80
26	TRNA	10	G	N3-C4-C5	-5.18	126.01	128.60
1	16SB	1204	G	O4'-C1'-N9	-5.18	104.06	108.20
27	23SA	782	G	N3-C4-N9	5.18	129.11	126.00
26	TRNA	13	C	C2-N1-C1'	-5.18	113.11	118.80
27	23SA	1554	C	C6-N1-C1'	-5.18	114.59	120.80
1	16SB	1373	C	C5-C6-N1	5.18	123.59	121.00
27	23SB	311	C	C6-N1-C2	-5.18	118.23	120.30
27	23SB	557	G	C4-C5-N7	5.18	112.87	110.80
34	L9B	140	LEU	CA-CB-CG	5.18	127.21	115.30
27	23SA	2581	A	P-O3'-C3'	5.17	125.91	119.70
27	23SB	352	G	N3-C4-N9	-5.17	122.89	126.00
1	16SB	736	G	N9-C4-C5	5.17	107.47	105.40
27	23SA	297	U	C5-C4-O4	-5.17	122.80	125.90
27	23SB	1465	G	C6-C5-N7	5.17	133.50	130.40
1	16SA	667	G	O5'-P-OP1	-5.17	101.05	105.70
27	23SA	1809	U	C5-C4-O4	-5.17	122.80	125.90
27	23SA	2177	G	C4-N9-C1'	5.17	133.22	126.50
27	23SA	2361	A	OP2-P-O3'	5.17	116.57	105.20
27	23SB	1465	G	C4-N9-C1'	-5.17	119.78	126.50
27	23SB	2230	G	N3-C4-N9	5.17	129.10	126.00
27	23SB	2689	G	N9-C4-C5	-5.17	103.33	105.40
28	5SB	12	C	C2-N1-C1'	5.17	124.48	118.80
27	23SA	1907	C	N3-C4-C5	-5.17	119.83	121.90
27	23SA	2090	C	C5-C6-N1	5.17	123.58	121.00
26	TRNA	13	C	O4'-C1'-N1	5.16	112.33	108.20
27	23SA	1238	G	C4-C5-N7	5.16	112.87	110.80
1	16SA	1233	G	N9-C4-C5	-5.16	103.34	105.40
27	23SB	2230	G	P-O3'-C3'	5.16	125.89	119.70
27	23SB	2739	C	C6-N1-C2	-5.16	118.24	120.30
1	16SB	1536	A	OP2-P-O3'	5.16	116.55	105.20
27	23SA	2739	C	C6-N1-C2	-5.16	118.24	120.30
27	23SA	2014	G	N3-C4-N9	-5.15	122.91	126.00
27	23SA	1700	G	N9-C4-C5	5.15	107.46	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16SB	1276	C	N1-C2-O2	-5.15	115.81	118.90
27	23SB	304	C	C6-N1-C2	-5.15	118.24	120.30
1	16SA	1311	G	C6-C5-N7	5.15	133.49	130.40
27	23SA	965	A	N1-C2-N3	5.15	131.88	129.30
28	5SA	32	C	C6-N1-C2	-5.15	118.24	120.30
1	16SB	1900	G	C4-C5-N7	-5.15	108.74	110.80
27	23SB	2551	G	C4-C5-N7	-5.15	108.74	110.80
1	16SA	1949	C	C6-N1-C2	-5.15	118.24	120.30
27	23SA	1044	A	N1-C6-N6	5.15	121.69	118.60
27	23SB	740	C	C5-C6-N1	5.15	123.57	121.00
27	23SB	1229	C	C2-N1-C1'	5.15	124.46	118.80
27	23SA	1021	G	N3-C4-N9	-5.14	122.91	126.00
28	5SA	7	C	C6-N1-C2	-5.14	118.24	120.30
23	PSIB	40	C	C6-N1-C2	-5.14	118.24	120.30
27	23SB	1381	G	C4-C5-N7	5.14	112.86	110.80
27	23SB	2192	U	C2-N1-C1'	5.14	123.87	117.70
1	16SA	1006	U	C2-N1-C1'	5.14	123.87	117.70
1	16SB	777	C	C5-C6-N1	5.14	123.57	121.00
27	23SB	1084	G	N3-C4-N9	-5.14	122.91	126.00
22	ASIA	34	G	C8-N9-C4	-5.14	104.34	106.40
1	16SB	1653	C	N3-C2-O2	5.14	125.50	121.90
1	16SA	1786	C	C6-N1-C2	-5.14	118.24	120.30
1	16SA	1929	U	C6-N1-C1'	-5.14	114.01	121.20
1	16SA	1899	G	C4-N9-C1'	5.14	133.18	126.50
27	23SA	16	G	C5-C6-O6	5.14	131.68	128.60
27	23SB	1551	C	C6-N1-C1'	-5.14	114.64	120.80
1	16SA	727	U	N3-C4-C5	-5.13	111.52	114.60
27	23SA	698	C	N1-C2-O2	-5.13	115.82	118.90
1	16SB	1961	G	N1-C6-O6	-5.13	116.82	119.90
27	23SB	91	G	N3-C2-N2	-5.13	116.31	119.90
27	23SB	1955	G	C8-N9-C1'	5.13	133.67	127.00
27	23SB	281	C	N1-C2-O2	5.13	121.98	118.90
27	23SB	1229	C	N1-C2-O2	5.13	121.98	118.90
27	23SB	2753	G	C4-C5-N7	-5.13	108.75	110.80
28	5SA	21	G	C4-N9-C1'	5.13	133.17	126.50
9	S9B	19	LEU	C-N-CA	5.13	134.52	121.70
1	16SB	1973	A	OP2-P-O3'	5.12	116.47	105.20
1	16SA	1962	C	O4'-C1'-N1	5.12	112.30	108.20
27	23SA	1496	C	C6-N1-C2	-5.12	118.25	120.30
27	23SB	1425	C	O5'-P-OP2	-5.12	101.09	105.70
27	23SA	2516	C	C6-N1-C1'	5.12	126.94	120.80
27	23SA	2533	A	C3'-C2'-C1'	5.12	105.60	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	5SA	67	C	C2-N1-C1'	5.12	124.43	118.80
1	16SB	1002	G	C4-C5-N7	5.12	112.85	110.80
1	16SA	798	G	C6-N1-C2	-5.12	122.03	125.10
1	16SA	1472	C	C2-N1-C1'	5.12	124.43	118.80
1	16SA	1781	C	C2-N1-C1'	5.12	124.43	118.80
1	16SB	1647	G	N1-C6-O6	5.12	122.97	119.90
1	16SA	1415	G	N3-C2-N2	-5.12	116.32	119.90
1	16SB	786	G	C6-C5-N7	5.11	133.47	130.40
27	23SB	27	G	N3-C4-N9	-5.11	122.93	126.00
27	23SA	1381	G	N9-C4-C5	-5.11	103.36	105.40
1	16SA	796	G	C4-N9-C1'	-5.11	119.86	126.50
1	16SA	1002	G	N3-C4-N9	5.11	129.07	126.00
1	16SA	1319	G	O4'-C1'-N9	5.11	112.29	108.20
27	23SA	2180	G	C4-C5-N7	-5.11	108.76	110.80
27	23SA	2808	G	C4-C5-N7	-5.11	108.76	110.80
1	16SA	747	G	O4'-C1'-N9	5.11	112.28	108.20
27	23SA	2861	G	O4'-C1'-N9	5.11	112.28	108.20
1	16SB	1731	C	C6-N1-C2	-5.11	118.26	120.30
27	23SB	2231	G	P-O3'-C3'	5.11	125.83	119.70
27	23SA	16	G	N1-C6-O6	-5.10	116.84	119.90
27	23SA	2326	A	O4'-C1'-N9	5.10	112.28	108.20
27	23SB	2431	C	C2-N1-C1'	5.10	124.41	118.80
27	23SA	1924	G	C2-N3-C4	-5.10	109.35	111.90
27	23SB	2017	G	O4'-C1'-N9	-5.10	104.12	108.20
27	23SA	2909	U	C5-C4-O4	-5.10	122.84	125.90
1	16SB	1554	C	C2-N3-C4	-5.10	117.35	119.90
1	16SB	2040	C	C2-N1-C1'	5.10	124.41	118.80
27	23SB	638	G	C4-N9-C1'	5.10	133.13	126.50
27	23SB	1089	C	C2-N1-C1'	5.10	124.41	118.80
27	23SB	2318	G	N9-C4-C5	5.10	107.44	105.40
1	16SA	1907	A	O4'-C1'-N9	5.10	112.28	108.20
27	23SA	2217	G	N3-C4-N9	5.10	129.06	126.00
1	16SB	898	G	C6-C5-N7	-5.10	127.34	130.40
1	16SB	1571	C	C6-N1-C2	-5.10	118.26	120.30
1	16SB	1757	C	N3-C4-C5	-5.10	119.86	121.90
3	S3B	188	LEU	CA-CB-CG	5.10	127.03	115.30
27	23SB	2742	U	O4'-C1'-N1	5.10	112.28	108.20
28	5SB	5	C	C2-N1-C1'	5.10	124.41	118.80
27	23SB	1231	G	N1-C2-N2	5.10	120.79	116.20
1	16SA	696	A	P-O3'-C3'	5.09	125.81	119.70
1	16SB	907	G	C8-N9-C1'	-5.09	120.38	127.00
1	16SA	1085	G	C6-C5-N7	5.09	133.46	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SA	1780	G	N9-C4-C5	5.09	107.44	105.40
27	23SA	31	C	O5'-P-OP1	-5.09	101.12	105.70
27	23SB	2470	G	N3-C2-N2	-5.09	116.34	119.90
27	23SB	1554	C	C2-N1-C1'	-5.09	113.20	118.80
28	5SB	5	C	C5-C6-N1	5.09	123.55	121.00
1	16SA	803	C	C6-N1-C2	-5.09	118.27	120.30
1	16SA	839	G	O4'-C1'-N9	5.09	112.27	108.20
27	23SA	555	A	P-O3'-C3'	5.09	125.81	119.70
27	23SA	685	G	N3-C4-C5	5.09	131.14	128.60
1	16SB	940	G	N1-C6-O6	5.09	122.95	119.90
27	23SA	291	G	N9-C4-C5	-5.09	103.37	105.40
27	23SA	881	G	C8-N9-C4	-5.09	104.36	106.40
54	L33A	10	LEU	CA-CB-CG	5.09	127.00	115.30
24	ESIB	21	A	O4'-C1'-N9	-5.09	104.13	108.20
27	23SB	1817	A	O5'-P-OP2	-5.09	101.12	105.70
27	23SA	1813	U	O4'-C1'-N1	5.08	112.27	108.20
1	16SB	1930	C	C2-N1-C1'	5.08	124.39	118.80
27	23SB	264	C	C2-N1-C1'	-5.08	113.21	118.80
27	23SB	332	G	C2-N3-C4	5.08	114.44	111.90
27	23SB	865	C	C6-N1-C2	-5.08	118.27	120.30
27	23SA	1456	C	C5-C6-N1	5.08	123.54	121.00
1	16SA	1256	G	C8-N9-C4	-5.08	104.37	106.40
27	23SB	629	G	C4-N9-C1'	5.08	133.10	126.50
27	23SB	1536	G	N3-C4-N9	-5.08	122.95	126.00
24	ESIA	55	U	C5-C6-N1	5.08	125.24	122.70
1	16SB	1937	G	C5-C6-O6	-5.08	125.55	128.60
27	23SB	264	C	C2-N3-C4	-5.08	117.36	119.90
27	23SB	1296	A	O5'-P-OP2	5.08	116.79	110.70
26	TRNA	13	C	C6-N1-C1'	5.08	126.89	120.80
27	23SA	757	C	C6-N1-C1'	-5.08	114.71	120.80
27	23SB	942	C	C6-N1-C1'	-5.08	114.71	120.80
1	16SA	796	G	N1-C2-N2	5.07	120.77	116.20
27	23SA	204	G	N1-C6-O6	-5.07	116.86	119.90
27	23SA	895	C	C6-N1-C1'	-5.07	114.71	120.80
27	23SB	1501	C	C2-N3-C4	-5.07	117.36	119.90
28	5SB	120	G	N1-C2-N2	5.07	120.77	116.20
1	16SA	1851	G	C6-N1-C2	-5.07	122.06	125.10
27	23SA	1478	G	C6-C5-N7	-5.07	127.36	130.40
1	16SB	1089	C	O4'-C1'-N1	5.07	112.26	108.20
1	16SB	1920	G	N9-C4-C5	5.07	107.43	105.40
27	23SA	725	A	C2-N3-C4	-5.07	108.06	110.60
1	16SB	1634	G	N9-C4-C5	5.07	107.43	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	MRNA	56	U	N3-C2-O2	-5.06	118.66	122.20
27	23SB	444	C	C6-N1-C1'	-5.06	114.73	120.80
27	23SA	1460	C	C5-C6-N1	5.06	123.53	121.00
1	16SB	2075	C	C2-N3-C4	-5.06	117.37	119.90
22	ASIA	34	G	N3-C4-C5	-5.06	126.07	128.60
1	16SA	939	A	C8-N9-C4	-5.06	103.78	105.80
1	16SA	852	G	C5-C6-N1	5.05	114.03	111.50
27	23SB	1532	G	N9-C4-C5	-5.05	103.38	105.40
27	23SB	1632	C	C5-C4-N4	5.05	123.74	120.20
27	23SA	629	G	N9-C4-C5	-5.05	103.38	105.40
28	5SA	6	C	N3-C4-C5	-5.05	119.88	121.90
23	PSIB	1	G	C4-C5-N7	5.05	112.82	110.80
27	23SA	1128	A	C4-C5-N7	5.05	113.22	110.70
27	23SA	839	C	O5'-P-OP2	-5.05	101.16	105.70
1	16SB	918	C	C6-N1-C2	-5.05	118.28	120.30
1	16SB	1243	A	N9-C4-C5	-5.05	103.78	105.80
27	23SB	119	G	C6-C5-N7	-5.05	127.37	130.40
27	23SA	2787	C	C6-N1-C2	-5.04	118.28	120.30
1	16SB	835	U	O4'-C1'-N1	-5.04	104.16	108.20
27	23SB	2127	U	N1-C2-N3	5.04	117.93	114.90
28	5SB	91	G	C6-C5-N7	-5.04	127.37	130.40
27	23SB	2730	G	C4-C5-N7	5.04	112.82	110.80
27	23SB	2861	G	O4'-C1'-N9	5.04	112.23	108.20
1	16SB	1577	G	N3-C2-N2	-5.04	116.37	119.90
1	16SB	1432	G	N9-C4-C5	5.04	107.42	105.40
27	23SA	1784	G	O4'-C1'-N9	5.04	112.23	108.20
25	MRNB	53	U	OP1-P-O3'	5.04	116.28	105.20
27	23SB	1721	U	C5-C4-O4	5.04	128.92	125.90
37	L15B	53	GLY	N-CA-C	5.04	125.69	113.10
1	16SA	730	C	C2-N1-C1'	5.03	124.34	118.80
27	23SA	289	U	C2-N1-C1'	-5.03	111.66	117.70
27	23SA	2190	G	C4-N9-C1'	5.03	133.04	126.50
27	23SB	931	G	C6-C5-N7	5.03	133.42	130.40
1	16SB	1949	C	N1-C2-O2	5.03	121.92	118.90
27	23SB	1593	C	C6-N1-C1'	-5.03	114.76	120.80
1	16SA	785	G	C6-C5-N7	-5.03	127.38	130.40
27	23SA	2683	G	C6-C5-N7	5.03	133.42	130.40
1	16SB	2121	UR3	P-O3'-C3'	5.03	125.74	119.70
27	23SB	313	C	C2-N1-C1'	5.03	124.33	118.80
27	23SB	2750	A	N7-C8-N9	5.03	116.31	113.80
27	23SB	2809	G	N3-C2-N2	-5.03	116.38	119.90
27	23SA	304	C	C2-N1-C1'	5.03	124.33	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SA	2805	C	O4'-C1'-N1	5.03	112.22	108.20
1	16SB	778	G	N9-C4-C5	-5.03	103.39	105.40
1	16SB	1330	C	OP2-P-O3'	5.03	116.26	105.20
1	16SA	785	G	C4-C5-N7	5.03	112.81	110.80
27	23SB	920	U	O5'-P-OP2	-5.03	101.18	105.70
1	16SB	1766	G	O5'-P-OP1	-5.02	101.18	105.70
27	23SB	202	G	N1-C2-N2	5.02	120.72	116.20
27	23SA	472	C	C2-N1-C1'	-5.02	113.28	118.80
27	23SB	2617	A	N1-C6-N6	5.02	121.61	118.60
1	16SA	1649	U	OP2-P-O3'	5.02	116.25	105.20
27	23SB	73	A	C2-N3-C4	-5.02	108.09	110.60
27	23SA	2505	G	C8-N9-C1'	-5.02	120.48	127.00
1	16SB	909	C	C6-N1-C2	-5.02	118.29	120.30
1	16SA	1827	C	P-O3'-C3'	5.01	125.72	119.70
27	23SA	1925	A	O4'-C1'-N9	-5.01	104.19	108.20
27	23SB	715	G	N3-C2-N2	-5.01	116.39	119.90
27	23SA	599	C	O5'-P-OP2	-5.01	101.19	105.70
33	L6A	9	ILE	CG1-CB-CG2	-5.01	100.38	111.40
1	16SB	752	G	N3-C4-C5	-5.01	126.09	128.60
27	23SB	639	U	C2-N1-C1'	5.01	123.71	117.70
27	23SB	1721	U	N3-C4-O4	-5.01	115.89	119.40
27	23SB	1796	A	N1-C2-N3	5.01	131.81	129.30
27	23SB	2829	C	C5-C6-N1	5.01	123.50	121.00
1	16SB	2002	A	O4'-C1'-N9	5.01	112.21	108.20
37	L15B	47	ASP	C-N-CD	-5.01	109.58	120.60
27	23SB	1465	G	N3-C4-N9	-5.01	123.00	126.00
27	23SB	1139	G	C4-N9-C1'	-5.00	120.00	126.50
27	23SB	1252	A	OP2-P-O3'	5.00	116.21	105.20
27	23SA	2133	C	C2-N1-C1'	-5.00	113.30	118.80
1	16SB	1961	G	C6-C5-N7	5.00	133.40	130.40

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
37	L15A	35	HIS	Peptide
37	L15A	9	ASN	Peptide
39	L17A	2	ARG	Peptide
41	L19A	58	ASN	Peptide
43	L21A	43	GLU	Peptide
43	L21A	44	LYS	Peptide
43	L21B	49	THR	Peptide

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Mol	Chain	Res	Type	Group
48	L27A	9	SER	Peptide
50	L29A	15	LYS	Peptide
29	L2A	45	ASN	Peptide
29	L2B	45	ASN	Peptide
31	L4A	132	VAL	Peptide
31	L4A	65	TRP	Peptide
33	L6A	172	LYS	Peptide
33	L6B	100	GLY	Peptide
33	L6B	11	VAL	Peptide
34	L9A	110	ASP	Peptide
13	S13A	105	THR	Peptide
19	S19B	41	VAL	Peptide
20	S20A	95	ALA	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	16SA	32489	0	0	0	0
1	16SB	32409	0	0	0	9
2	S2A	1924	0	1975	80	0
2	S2B	1924	0	1975	96	0
3	S3A	1605	0	1668	56	0
3	S3B	1612	0	1677	60	0
4	S4A	1702	0	1767	63	0
4	S4B	1702	0	1764	51	0
5	S5A	1155	0	1213	31	0
5	S5B	1155	0	1212	33	0
6	S6A	842	0	857	27	0
6	S6B	842	0	857	22	0
7	S7A	1256	0	1296	27	0
7	S7B	1256	0	1295	25	0
8	S8A	1115	0	1177	45	0
8	S8B	1115	0	1177	40	0
9	S9A	1009	0	1037	43	0
9	S9B	1009	0	1037	53	0
10	S10A	801	0	0	0	0
10	S10B	801	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	S11A	864	0	0	0	0
11	S11B	873	0	0	0	0
12	S12A	977	0	0	0	0
12	S12B	977	0	0	0	0
13	S13A	946	0	0	0	0
13	S13B	964	0	0	0	0
14	S14A	491	0	0	0	0
14	S14B	486	0	0	0	0
15	S15A	733	0	0	0	0
15	S15B	733	0	0	0	0
16	S16A	700	0	0	0	0
16	S16B	705	0	0	0	0
17	S17A	834	0	0	0	0
17	S17B	834	0	0	0	0
18	S18A	584	0	0	0	0
18	S18B	573	0	0	0	0
19	S19A	674	0	0	0	0
19	S19B	684	0	0	0	0
20	S20A	762	0	0	0	0
20	S20B	762	0	0	0	0
21	THXA	208	0	0	0	0
21	THXB	217	0	0	0	0
22	ASIA	1628	0	0	0	0
23	PSIA	1635	0	0	0	0
23	PSIB	1635	0	0	0	0
24	ESIA	1626	0	0	0	0
24	ESIB	1626	0	0	0	0
25	MRNA	621	0	0	0	0
25	MRNB	621	0	0	0	0
26	TRNA	1565	0	0	0	0
27	23SA	62225	0	0	0	1
27	23SB	61926	0	0	0	0
28	5SA	2617	0	1328	35	0
28	5SB	2598	0	1316	43	0
29	L2A	2115	0	2195	35	0
29	L2B	2115	0	2195	47	0
30	L3A	1563	0	1629	26	0
30	L3B	1563	0	1629	51	0
31	L4A	1585	0	1632	46	0
31	L4B	1585	0	1632	60	0
32	L5A	1473	0	1535	58	0
32	L5B	1473	0	1534	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	L6A	1336	0	1418	61	0
33	L6B	1327	0	1405	72	0
34	L9A	1131	0	1218	78	9
34	L9B	1136	0	1223	56	0
35	L13A	1104	0	0	0	0
35	L13B	1104	0	0	0	0
36	L14A	932	0	0	0	0
36	L14B	932	0	0	0	0
37	L15A	1144	0	0	0	0
37	L15B	1144	0	0	0	0
38	L16A	1121	0	0	0	0
38	L16B	1121	0	0	0	0
39	L17A	967	0	0	0	0
39	L17B	967	0	0	0	0
40	L18A	889	0	0	0	0
40	L18B	881	0	0	0	0
41	L19A	1141	0	0	0	0
41	L19B	1141	0	0	0	0
42	L20A	963	0	0	0	0
42	L20B	963	0	0	0	0
43	L21A	778	0	0	0	0
43	L21B	778	0	0	0	0
44	L22A	899	0	0	0	0
44	L22B	899	0	0	0	0
45	L23A	747	0	0	0	0
45	L23B	742	0	0	0	0
46	L24A	824	0	0	0	0
46	L24B	775	0	0	0	1
47	L25A	1428	0	0	0	0
47	L25B	1404	0	0	0	0
48	L27A	661	0	0	0	0
48	L27B	661	0	0	0	0
49	L28A	762	0	0	0	0
49	L28B	762	0	0	0	0
50	L29A	583	0	0	0	0
50	L29B	575	0	0	0	0
51	L30A	468	0	0	0	0
51	L30B	468	0	0	0	0
52	L31A	580	0	0	0	0
52	L31B	580	0	0	0	0
53	L32A	434	0	0	0	0
53	L32B	434	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	L33A	389	0	0	0	0
54	L33B	389	0	0	0	0
55	L34A	418	0	0	0	0
55	L34B	429	0	0	0	0
56	L35A	516	0	0	0	0
56	L35B	516	0	0	0	0
57	ASIB	1627	0	0	0	0
58	16SA	90	0	0	0	0
58	16SB	86	0	0	0	0
58	23SA	334	0	0	0	0
58	23SB	240	0	0	0	0
58	5SA	6	0	0	0	0
58	5SB	4	0	0	0	0
58	L15A	2	0	0	0	0
58	L17A	1	0	0	0	0
58	L23A	1	0	0	0	0
58	L27A	2	0	0	0	0
58	L27B	1	0	0	0	0
58	L2B	1	0	0	0	0
58	L30A	1	0	0	0	0
58	L32A	1	0	0	0	0
58	L33A	1	0	0	0	0
58	L34A	1	0	0	0	0
58	L35A	1	0	0	0	0
58	L35B	2	0	0	0	0
58	L3A	2	0	0	0	0
58	L3B	2	0	0	0	0
58	L4A	2	0	0	0	0
58	L5A	1	0	0	0	0
58	L5B	1	0	0	0	0
58	MRNA	1	0	0	0	0
58	PSIA	2	0	0	0	0
58	PSIB	3	0	0	0	0
58	S4A	1	0	0	0	0
58	S5B	2	0	0	0	0
59	16SA	46	0	0	0	0
59	16SB	36	0	0	0	0
59	23SA	101	0	0	0	0
59	23SB	83	0	0	0	0
59	5SA	2	0	0	0	0
59	5SB	1	0	0	0	0
59	L16A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	L16B	1	0	0	0	0
59	L2A	1	0	0	0	0
59	L2B	1	0	0	0	0
59	L3A	1	0	0	0	0
59	L3B	1	0	0	0	0
59	L4A	1	0	0	0	0
59	L4B	1	0	0	0	0
59	L5A	1	0	0	0	0
59	L5B	1	0	0	0	0
59	PSIA	2	0	0	0	0
59	S13A	1	0	0	0	0
59	S13B	1	0	0	0	0
59	S20A	1	0	0	0	0
59	S20B	1	0	0	0	0
59	S4B	1	0	0	0	0
59	S6A	1	0	0	0	0
59	S6B	1	0	0	0	0
60	16SA	560	0	0	0	0
60	16SB	546	0	0	0	0
60	23SA	1379	0	0	0	0
60	23SB	1344	0	0	0	0
60	5SA	70	0	0	0	0
60	5SB	70	0	0	0	0
60	ASIA	21	0	0	0	0
60	ASIB	21	0	0	0	0
60	ESIA	7	0	0	0	0
60	ESIB	7	0	0	0	0
60	L15A	7	0	0	0	0
60	L17A	7	0	0	0	0
60	L17B	7	0	0	0	0
60	L19A	7	0	0	0	0
60	L20B	7	0	0	0	0
60	L27A	14	0	0	0	0
60	L28A	7	0	0	0	0
60	L35A	7	0	0	0	0
60	L35B	7	0	0	0	0
60	L4A	7	0	0	0	0
60	MRNA	7	0	0	0	0
60	MRNB	7	0	0	0	0
60	PSIA	7	0	0	0	0
60	PSIB	21	0	0	0	0
60	S14B	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	S19A	7	0	0	0	0
60	S4B	7	0	0	0	0
60	S8B	7	0	0	0	0
60	TRNA	14	0	0	0	0
61	23SA	83	0	0	0	0
61	23SB	83	0	0	0	0
62	16SA	173	0	0	0	0
62	16SB	158	0	0	0	0
62	23SA	801	0	0	0	0
62	23SB	518	0	0	0	0
62	5SA	14	0	0	4	0
62	5SB	5	0	0	1	0
62	ESIA	1	0	0	0	0
62	L15A	10	0	0	0	0
62	L15B	7	0	0	0	0
62	L16A	1	0	0	0	0
62	L17A	2	0	0	0	0
62	L18A	2	0	0	0	0
62	L19A	1	0	0	0	0
62	L23A	1	0	0	0	0
62	L27A	3	0	0	0	0
62	L27B	2	0	0	0	0
62	L28B	1	0	0	0	0
62	L2A	9	0	0	1	0
62	L2B	13	0	0	1	0
62	L30A	1	0	0	0	0
62	L30B	2	0	0	0	0
62	L34A	1	0	0	0	0
62	L35A	1	0	0	0	0
62	L35B	6	0	0	0	0
62	L3A	7	0	0	0	0
62	L3B	6	0	0	0	0
62	L4A	6	0	0	0	0
62	L4B	1	0	0	0	0
62	PSIA	6	0	0	0	0
62	S12B	2	0	0	0	0
62	S13A	1	0	0	0	0
62	S14A	1	0	0	0	0
62	S14B	2	0	0	0	0
62	S16A	1	0	0	0	0
62	S17A	1	0	0	0	0
62	S4A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	S4B	1	0	0	0	0
62	S5A	1	0	0	0	0
62	S5B	1	0	0	0	0
62	S9B	1	0	0	0	0
62	THXA	3	0	0	0	0
All	All	306277	0	43873	1447	10

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 17.

All (1447) 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)
34:L9A:115:ALA:CB	34:L9A:128:LEU:HD21	1.50	1.39
2:S2B:55:PHE:CE1	2:S2B:221:LEU:HD22	1.82	1.15
34:L9A:115:ALA:HB2	34:L9A:128:LEU:HD21	1.14	1.05
34:L9A:115:ALA:HB3	34:L9A:128:LEU:HD21	1.33	1.02
34:L9A:115:ALA:CB	34:L9A:128:LEU:CD2	2.41	0.97
34:L9A:114:LEU:CD1	34:L9A:129:THR:O	2.14	0.95
2:S2B:69:LEU:HD13	2:S2B:159:PRO:HG3	1.45	0.95
3:S3B:50:ALA:HB2	3:S3B:76:VAL:HG11	1.46	0.94
34:L9A:114:LEU:HD12	34:L9A:129:THR:O	1.70	0.92
29:L2A:60:ARG:HD3	29:L2A:86:PRO:HB2	1.51	0.91
29:L2A:242:ARG:O	62:L2A:401:HOH:O	1.90	0.89
28:5SB:54:A:O2'	28:5SB:55:A:N7	2.06	0.88
31:L4B:167:ALA:HB1	31:L4B:173:VAL:HG11	1.56	0.88
34:L9A:115:ALA:HB3	34:L9A:128:LEU:CD2	2.01	0.88
2:S2B:5:ILE:HG12	2:S2B:55:PHE:CD1	2.08	0.88
30:L3B:119:ARG:HD3	30:L3B:160:TYR:HB2	1.54	0.88
2:S2B:132:LYS:HA	2:S2B:135:GLN:HB2	1.55	0.87
2:S2B:127:ILE:O	2:S2B:135:GLN:NE2	2.08	0.86
2:S2A:168:THR:HG23	2:S2A:169:LYS:N	1.90	0.85
34:L9A:123:LEU:HD23	34:L9A:142:VAL:HG12	1.58	0.85
28:5SA:82:U:H2'	28:5SA:83:G:H21	1.40	0.84
28:5SB:17:A:H5'	28:5SB:18:G:H8	1.42	0.84
2:S2A:178:ARG:HH21	8:S8A:74:PRO:HG3	1.43	0.84
31:L4B:127:GLU:O	31:L4B:129:PHE:N	2.09	0.84
31:L4A:103:LYS:HA	31:L4A:106:ARG:HD3	1.60	0.83
30:L3B:9:VAL:HG11	30:L3B:27:LEU:HD23	1.61	0.83
31:L4A:65:TRP:HB2	31:L4A:66:PRO:HD3	1.61	0.82
28:5SA:75:A:OP2	62:5SA:302:HOH:O	1.97	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:L5B:64:THR:HG23	32:L5B:66:GLN:H	1.43	0.82
2:S2B:20:GLU:HB3	2:S2B:23:ARG:HB2	1.61	0.81
28:5SB:17:A:H5'	28:5SB:18:G:C8	2.15	0.81
2:S2A:168:THR:CG2	2:S2A:169:LYS:N	2.43	0.81
33:L6A:41:MET:HG3	33:L6A:54:ARG:HA	1.63	0.80
34:L9A:115:ALA:HB2	34:L9A:128:LEU:CD2	2.06	0.79
30:L3B:47:VAL:HG11	30:L3B:86:PRO:HD2	1.65	0.79
28:5SA:27:A:OP1	62:5SA:303:HOH:O	2.01	0.79
5:S5A:152:ARG:NH2	8:S8A:107:LEU:O	2.16	0.78
34:L9A:127:VAL:HG22	34:L9A:139:GLN:HB3	1.64	0.78
28:5SB:35:G:H5'	32:L5B:2:PRO:HD3	1.64	0.78
4:S4A:96:LEU:HG	4:S4A:139:ARG:HH22	1.48	0.77
2:S2A:82:ARG:NH2	2:S2A:92:TYR:OH	2.17	0.77
34:L9A:86:THR:H	34:L9A:123:LEU:HD12	1.50	0.77
33:L6B:27:LYS:HA	33:L6B:32:GLU:HB3	1.65	0.77
31:L4A:127:GLU:O	31:L4A:129:PHE:N	2.17	0.77
34:L9A:115:ALA:C	34:L9A:117:GLU:H	1.88	0.77
9:S9B:19:LEU:HB2	9:S9B:59:PHE:HE1	1.49	0.77
28:5SA:104:A:OP2	62:5SA:304:HOH:O	2.03	0.77
30:L3A:36:ARG:NH1	30:L3A:85:ASN:OD1	2.18	0.77
2:S2A:20:GLU:HB3	2:S2A:23:ARG:HG3	1.66	0.76
7:S7B:5:ARG:C	7:S7B:7:ALA:HB2	2.06	0.76
4:S4A:33:MET:HE2	4:S4A:37:PRO:HA	1.68	0.75
5:S5B:78:HIS:HB2	8:S8B:104:ARG:HD2	1.67	0.75
2:S2A:53:ARG:NH2	2:S2A:198:ASP:O	2.20	0.75
33:L6B:86:GLU:HA	33:L6B:132:ARG:HB2	1.66	0.75
3:S3B:9:GLY:HA2	3:S3B:12:LEU:HG	1.69	0.75
28:5SA:54:A:O2'	28:5SA:55:A:N7	2.20	0.75
34:L9B:118:LYS:HG2	34:L9B:119:PRO:HD2	1.69	0.74
2:S2B:137:ARG:NH1	2:S2B:137:ARG:O	2.20	0.74
2:S2B:224:GLN:HG2	2:S2B:229:VAL:HG22	1.69	0.74
3:S3B:91:LEU:O	3:S3B:95:THR:OG1	2.04	0.74
28:5SB:104:A:N7	62:5SB:301:HOH:O	2.20	0.74
3:S3B:135:LYS:O	3:S3B:139:GLN:NE2	2.20	0.74
34:L9A:73:GLU:HG3	34:L9A:136:VAL:HG23	1.68	0.74
30:L3B:11:MET:HG2	30:L3B:24:THR:HG22	1.70	0.73
33:L6B:73:ALA:O	33:L6B:77:LYS:N	2.19	0.73
30:L3A:111:ARG:HG3	30:L3A:160:TYR:CD2	2.23	0.73
3:S3A:20:SER:HB3	3:S3A:40:ARG:HH22	1.52	0.73
33:L6B:23:ARG:HG3	33:L6B:25:LYS:HE3	1.70	0.73
33:L6A:7:LEU:HD22	33:L6A:69:ARG:HH21	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S9A:83:ARG:HA	9:S9A:86:VAL:HG12	1.70	0.72
2:S2B:55:PHE:CD1	2:S2B:221:LEU:HD22	2.23	0.72
8:S8A:129:VAL:HG23	8:S8A:130:GLY:H	1.53	0.72
34:L9A:133:HIS:CB	34:L9A:134:PRO:HD2	2.19	0.72
6:S6B:15:ASP:HB2	6:S6B:18:GLN:H	1.52	0.72
30:L3A:119:ARG:HD3	30:L3A:160:TYR:HB2	1.70	0.72
2:S2B:16:HIS:HB3	2:S2B:210:SER:HB2	1.72	0.72
32:L5A:161:THR:HG22	32:L5A:163:ALA:H	1.55	0.71
2:S2B:32:ILE:HD11	2:S2B:40:HIS:CD2	2.25	0.71
34:L9A:64:GLU:HB3	34:L9A:67:ARG:HH21	1.54	0.71
33:L6B:41:MET:HG2	33:L6B:55:PRO:HD3	1.71	0.71
5:S5B:102:ALA:HB1	5:S5B:106:PRO:HG2	1.72	0.71
33:L6A:124:GLU:HG2	33:L6A:126:PRO:HD3	1.72	0.71
28:5SB:17:A:H1'	28:5SB:112:G:C5	2.25	0.71
29:L2B:182:LEU:H	29:L2B:272:ALA:HB3	1.56	0.71
3:S3A:36:ASP:HA	3:S3A:39:ILE:HD12	1.72	0.71
4:S4A:26:CYS:HA	4:S4A:31:CYS:HB2	1.73	0.70
34:L9A:133:HIS:HB2	34:L9A:134:PRO:HD2	1.73	0.70
28:5SA:11:G:O2'	62:5SA:305:HOH:O	2.08	0.70
4:S4A:169:LYS:HE2	6:S6B:21:LEU:HD12	1.73	0.70
33:L6B:33:LEU:HD21	33:L6B:136:ILE:HG22	1.74	0.70
2:S2B:5:ILE:HG12	2:S2B:55:PHE:HD1	1.52	0.70
9:S9B:28:VAL:HG22	9:S9B:63:ILE:HB	1.73	0.70
5:S5B:142:LEU:O	5:S5B:143:ARG:NH1	2.25	0.70
7:S7A:91:VAL:HG23	7:S7A:96:GLN:HG2	1.73	0.70
29:L2A:96:HIS:HD2	29:L2A:102:LYS:HG2	1.57	0.70
29:L2B:5:LYS:H	29:L2B:5:LYS:HD2	1.56	0.70
33:L6B:98:LEU:HD21	33:L6B:105:LEU:HB3	1.74	0.70
2:S2A:77:ALA:HB2	2:S2A:211:ILE:HD13	1.74	0.70
31:L4A:117:ARG:NH2	31:L4A:189:THR:O	2.25	0.70
2:S2A:168:THR:CG2	2:S2A:169:LYS:H	2.05	0.69
34:L9A:94:ALA:O	34:L9A:111:PRO:HG3	1.92	0.69
9:S9B:10:ARG:HE	9:S9B:105:ASP:HB3	1.57	0.69
6:S6A:27:GLN:HA	6:S6A:30:LEU:HD12	1.74	0.69
9:S9A:16:ARG:O	9:S9A:63:ILE:HA	1.93	0.69
29:L2A:142:VAL:HG23	29:L2A:193:VAL:HA	1.72	0.69
33:L6B:121:ILE:HG23	33:L6B:133:VAL:HG11	1.72	0.69
29:L2B:130:ALA:HB2	29:L2B:192:THR:HG22	1.75	0.69
4:S4B:187:ARG:NH2	4:S4B:193:ASP:OD2	2.26	0.69
7:S7B:23:VAL:HG13	7:S7B:43:PHE:HE2	1.56	0.69
2:S2A:12:GLU:O	2:S2A:16:HIS:HB2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S9A:61:ALA:HB1	9:S9A:63:ILE:HD13	1.73	0.69
7:S7B:113:GLU:HB2	7:S7B:119:ARG:HG3	1.74	0.69
32:L5B:47:LYS:HD2	32:L5B:81:LYS:HB2	1.73	0.69
30:L3A:47:VAL:HG11	30:L3A:86:PRO:HD2	1.75	0.69
33:L6B:98:LEU:O	33:L6B:99:VAL:HG23	1.93	0.69
4:S4B:191:ARG:NH1	4:S4B:191:ARG:O	2.24	0.69
34:L9B:54:GLN:HA	34:L9B:57:ARG:HB2	1.74	0.69
29:L2A:166:GLN:HB2	29:L2A:174:ILE:HG22	1.75	0.68
5:S5B:34:VAL:HG11	5:S5B:63:ARG:HG2	1.75	0.68
28:5SB:82:U:H2'	28:5SB:83:G:H21	1.58	0.68
8:S8B:100:ILE:O	8:S8B:125:ARG:NH1	2.26	0.68
34:L9A:72:LEU:HD13	34:L9A:107:VAL:HG11	1.75	0.68
2:S2B:54:THR:HG23	2:S2B:199:TYR:HB3	1.76	0.68
3:S3B:152:ILE:HB	3:S3B:199:LYS:HB2	1.76	0.68
34:L9A:94:ALA:HB1	34:L9A:111:PRO:HG2	1.76	0.68
4:S4A:25:ARG:HG3	4:S4A:30:LYS:HG3	1.75	0.67
29:L2A:136:ILE:O	29:L2A:168:ARG:NH2	2.27	0.67
28:5SB:15:A:N1	28:5SB:71:G:O2'	2.23	0.67
9:S9B:96:LEU:HD12	9:S9B:101:PHE:HB2	1.75	0.67
2:S2A:87:ARG:HH11	2:S2A:219:VAL:HB	1.59	0.67
2:S2B:215:LEU:HA	2:S2B:218:ALA:HB3	1.77	0.67
34:L9B:113:ARG:HD2	34:L9B:131:LYS:HD2	1.76	0.67
34:L9A:144:VAL:HG22	34:L9A:145:VAL:HG23	1.75	0.67
3:S3B:120:VAL:HG13	3:S3B:124:ILE:HD13	1.77	0.67
7:S7B:68:ASN:ND2	7:S7B:128:ALA:O	2.27	0.67
5:S5A:48:ALA:HB2	5:S5A:57:LYS:HD3	1.77	0.67
2:S2B:78:GLN:O	2:S2B:94:ASN:ND2	2.28	0.67
9:S9B:46:ALA:HA	9:S9B:78:LYS:HE3	1.77	0.67
33:L6A:3:ARG:HG3	33:L6A:6:ARG:H	1.60	0.67
31:L4B:197:ASP:HA	31:L4B:200:GLU:HB2	1.77	0.67
3:S3A:84:ILE:HG13	3:S3A:101:LEU:HD22	1.76	0.67
3:S3A:188:LEU:HD11	3:S3A:195:VAL:HG13	1.76	0.67
7:S7A:106:GLN:O	7:S7A:110:GLN:NE2	2.21	0.67
33:L6B:157:TYR:HA	33:L6B:171:LEU:HG	1.78	0.66
34:L9A:93:THR:HA	34:L9A:119:PRO:HB3	1.75	0.66
7:S7B:16:LEU:HD11	9:S9B:42:ARG:HA	1.78	0.66
29:L2A:71:ASP:OD1	29:L2A:103:ARG:NH2	2.27	0.66
7:S7A:38:LEU:O	7:S7A:42:ILE:HG13	1.95	0.66
31:L4B:184:TYR:CE2	31:L4B:188:ARG:HD2	2.30	0.66
28:5SB:47:A:OP2	32:L5B:96:ARG:NH1	2.28	0.66
29:L2A:182:LEU:H	29:L2A:272:ALA:HB3	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:L3B:54:GLN:HG2	30:L3B:59:VAL:HG23	1.77	0.66
34:L9A:110:ASP:OD1	34:L9A:110:ASP:N	2.17	0.66
9:S9B:110:GLU:HG2	9:S9B:119:ALA:HB1	1.78	0.66
7:S7B:6:ARG:O	7:S7B:7:ALA:O	2.14	0.66
4:S4A:128:VAL:HB	4:S4A:133:VAL:HG21	1.78	0.65
9:S9A:21:PRO:HA	9:S9A:59:PHE:HA	1.77	0.65
33:L6B:8:PRO:HG2	33:L6B:69:ARG:HG2	1.78	0.65
28:5SA:42:U:H3'	28:5SA:43:U:C5'	2.27	0.65
2:S2B:55:PHE:CE1	2:S2B:221:LEU:CD2	2.72	0.65
8:S8A:29:SER:HB3	8:S8A:32:LYS:HG3	1.79	0.65
29:L2A:72:LYS:NZ	29:L2A:99:ASP:OD2	2.28	0.65
3:S3B:119:ARG:HH22	3:S3B:140:ARG:HG3	1.60	0.65
31:L4B:40:GLN:NE2	31:L4B:182:ASN:HB2	2.12	0.65
31:L4A:101:LEU:HD12	31:L4A:102:PRO:HD2	1.77	0.65
9:S9B:17:VAL:HG21	9:S9B:80:GLY:HA3	1.79	0.65
5:S5A:67:VAL:HG21	5:S5A:140:ARG:HA	1.79	0.65
7:S7B:44:TYR:HA	7:S7B:47:CYS:HB3	1.78	0.65
9:S9B:28:VAL:HA	9:S9B:63:ILE:O	1.97	0.65
29:L2B:228:PRO:O	62:L2B:402:HOH:O	2.14	0.65
4:S4A:109:GLY:HA3	4:S4A:165:MET:SD	2.37	0.65
3:S3B:136:GLN:O	3:S3B:140:ARG:HG2	1.96	0.65
34:L9A:110:ASP:HB2	34:L9A:112:LYS:HG3	1.79	0.64
28:5SB:44:C:O3'	32:L5B:67:LYS:HE2	1.97	0.64
32:L5A:66:GLN:OE1	32:L5A:98:ARG:NH1	2.30	0.64
8:S8B:29:SER:HB3	8:S8B:32:LYS:HG3	1.78	0.64
2:S2A:67:THR:HG21	2:S2A:155:LEU:HD11	1.78	0.64
6:S6A:62:TRP:CH2	6:S6A:64:GLN:HB2	2.33	0.64
5:S5A:68:GLU:HG2	5:S5A:70:PRO:HD3	1.79	0.64
3:S3B:155:GLY:HA2	3:S3B:163:ALA:HB1	1.78	0.64
8:S8B:69:ARG:NH1	8:S8B:75:ARG:O	2.30	0.64
2:S2A:5:ILE:HD12	2:S2A:221:LEU:HD23	1.80	0.64
28:5SA:17:A:H5'	28:5SA:18:G:C8	2.32	0.64
33:L6A:130:ARG:HG2	33:L6A:130:ARG:HH11	1.61	0.64
34:L9A:85:GLU:OE2	34:L9A:86:THR:OG1	2.10	0.64
31:L4B:40:GLN:HE22	31:L4B:182:ASN:HB2	1.63	0.64
31:L4A:134:GLY:HA2	31:L4A:166:ALA:HB2	1.78	0.64
5:S5B:31:LEU:HD11	5:S5B:43:LEU:HD11	1.80	0.64
34:L9B:81:VAL:HG13	34:L9B:144:VAL:H	1.63	0.64
28:5SB:16:U:O2'	28:5SB:110:U:O2'	2.13	0.64
4:S4A:90:GLY:HA3	4:S4A:204:ILE:HD11	1.79	0.64
8:S8A:42:GLU:HG3	8:S8A:109:ILE:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S9A:46:ALA:HB2	9:S9A:74:ILE:HG23	1.79	0.64
33:L6A:45:VAL:HA	33:L6A:50:VAL:HG12	1.79	0.64
8:S8B:42:GLU:HG3	8:S8B:109:ILE:HD12	1.81	0.63
34:L9B:68:LEU:HA	34:L9B:71:ILE:HG22	1.78	0.63
32:L5A:47:LYS:HD3	32:L5A:81:LYS:HB2	1.79	0.63
5:S5B:76:ILE:HD13	5:S5B:118:ILE:HD13	1.80	0.63
9:S9B:24:GLY:HA2	9:S9B:59:PHE:O	1.98	0.63
33:L6B:20:ALA:HB1	33:L6B:23:ARG:NH1	2.14	0.63
33:L6B:77:LYS:HE2	33:L6B:138:LYS:HB2	1.81	0.63
9:S9A:7:THR:O	9:S9A:83:ARG:HD2	1.98	0.63
9:S9A:91:ASP:OD1	9:S9A:91:ASP:N	2.31	0.63
28:5SA:17:A:H1'	28:5SA:112:G:C8	2.33	0.63
30:L3A:13:ARG:HD2	30:L3A:20:ALA:HB1	1.80	0.63
34:L9A:69:LYS:HG3	34:L9A:136:VAL:HB	1.80	0.63
2:S2A:92:TYR:CZ	2:S2A:151:GLY:HA3	2.35	0.62
34:L9A:29:TYR:O	34:L9A:33:ARG:HG2	1.98	0.62
4:S4A:13:ARG:NH1	4:S4A:38:TYR:O	2.31	0.62
31:L4A:133:ASN:HA	31:L4A:162:LEU:HD22	1.81	0.62
2:S2B:223:ILE:HA	2:S2B:226:ARG:HG2	1.80	0.62
4:S4B:100:ARG:HE	4:S4B:137:SER:HA	1.63	0.62
7:S7B:54:THR:O	7:S7B:56:GLN:N	2.32	0.62
30:L3A:117:MET:O	30:L3A:118:LYS:HB3	1.98	0.62
3:S3B:95:THR:HG22	3:S3B:97:LYS:HG2	1.81	0.62
8:S8B:17:THR:O	8:S8B:78:GLN:NE2	2.31	0.62
30:L3B:170:LEU:HD23	30:L3B:184:VAL:HB	1.82	0.62
31:L4A:9:ILE:HD11	31:L4A:125:LEU:HG	1.82	0.62
29:L2B:8:PRO:HB3	29:L2B:14:ARG:HB3	1.80	0.62
3:S3A:73:PRO:HA	3:S3A:76:VAL:HG22	1.82	0.62
31:L4B:124:LEU:HB3	31:L4B:193:VAL:HG22	1.81	0.62
33:L6B:138:LYS:HA	33:L6B:141:VAL:HG12	1.81	0.62
6:S6A:82:ARG:HB2	6:S6A:85:VAL:HG23	1.82	0.62
8:S8A:10:LEU:HD22	8:S8A:83:ILE:HD11	1.81	0.62
3:S3A:95:THR:HG23	3:S3A:97:LYS:HE2	1.81	0.62
2:S2B:178:ARG:NH2	8:S8B:68:ARG:HH22	1.98	0.62
31:L4B:24:LEU:HD23	31:L4B:115:ALA:HA	1.82	0.62
34:L9B:110:ASP:H	34:L9B:130:TYR:HH	1.47	0.62
5:S5A:8:GLU:HG2	5:S5A:34:VAL:HG22	1.82	0.62
32:L5B:37:VAL:HG23	32:L5B:99:MET:HE3	1.81	0.62
30:L3A:11:MET:HG2	30:L3A:24:THR:HB	1.80	0.61
5:S5B:74:GLY:O	5:S5B:115:VAL:HG23	1.99	0.61
29:L2A:96:HIS:CD2	29:L2A:102:LYS:HG2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S9B:19:LEU:HA	9:S9B:61:ALA:HA	1.81	0.61
29:L2B:70:TRP:CH2	29:L2B:150:LYS:HA	2.36	0.61
33:L6A:87:LEU:HB2	33:L6A:131:VAL:HG12	1.82	0.61
9:S9B:44:VAL:O	9:S9B:51:ARG:NH2	2.29	0.61
2:S2B:56:ARG:O	2:S2B:60:ASP:HB2	2.01	0.61
9:S9B:71:SER:HA	9:S9B:74:ILE:HD12	1.82	0.61
2:S2B:153:ARG:O	2:S2B:155:LEU:N	2.34	0.61
34:L9B:76:THR:HA	34:L9B:139:GLN:HB2	1.81	0.61
33:L6B:25:LYS:N	33:L6B:25:LYS:HD2	2.15	0.61
34:L9B:79:ILE:HG12	34:L9B:104:GLN:OE1	2.01	0.61
3:S3A:7:PRO:O	3:S3A:11:ARG:HG2	2.00	0.61
31:L4B:117:ARG:NH1	31:L4B:120:GLU:OE2	2.34	0.61
32:L5B:114:ILE:HD13	32:L5B:140:ILE:HG21	1.83	0.61
4:S4A:13:ARG:HB2	4:S4A:40:PRO:HD3	1.83	0.61
3:S3B:36:ASP:HA	3:S3B:39:ILE:HD12	1.83	0.61
8:S8A:83:ILE:HG13	8:S8A:137:VAL:HG22	1.83	0.60
32:L5B:56:ALA:HB2	32:L5B:153:ARG:HE	1.66	0.60
33:L6B:121:ILE:HG23	33:L6B:133:VAL:CG1	2.30	0.60
4:S4A:149:ALA:O	4:S4A:153:ARG:HG2	2.01	0.60
32:L5A:37:VAL:HG22	32:L5A:159:VAL:HG12	1.82	0.60
3:S3A:11:ARG:O	3:S3A:13:GLY:N	2.34	0.60
29:L2A:10:THR:HG23	29:L2A:13:ARG:HB2	1.83	0.60
4:S4A:8:VAL:HG21	4:S4A:115:ARG:NH2	2.16	0.60
7:S7A:113:GLU:HB2	7:S7A:119:ARG:HG2	1.83	0.60
8:S8B:100:ILE:HD12	8:S8B:125:ARG:HG3	1.83	0.60
8:S8A:21:LYS:O	8:S8A:65:TYR:OH	2.14	0.60
8:S8A:49:GLU:HG2	8:S8A:62:TYR:HE2	1.64	0.60
2:S2B:8:LYS:HE3	2:S2B:11:LEU:HD22	1.84	0.60
2:S2B:223:ILE:O	2:S2B:227:GLY:N	2.33	0.60
5:S5B:51:VAL:O	5:S5B:55:VAL:HG23	2.00	0.60
2:S2B:121:LEU:HA	2:S2B:124:SER:HB3	1.83	0.60
6:S6B:20:ALA:HA	6:S6B:23:LYS:HB2	1.84	0.60
7:S7B:27:ILE:HA	7:S7B:30:ILE:HD12	1.82	0.60
9:S9B:18:PHE:O	9:S9B:62:TYR:N	2.30	0.60
9:S9A:70:LYS:O	9:S9A:74:ILE:HG13	2.02	0.60
32:L5A:27:ASN:HB3	32:L5A:30:GLU:HG3	1.82	0.60
31:L4B:23:ASP:OD1	31:L4B:203:GLN:NE2	2.34	0.60
4:S4A:9:CYS:HB3	4:S4A:32:ALA:HB3	1.84	0.60
5:S5B:105:VAL:HG21	5:S5B:128:PRO:HB3	1.82	0.60
5:S5A:102:ALA:HB1	5:S5A:106:PRO:HG2	1.84	0.59
28:5SA:82:U:H2'	28:5SA:83:G:N2	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:L3B:34:VAL:HG21	30:L3B:78:LEU:HD11	1.83	0.59
32:L5B:6:ALA:HB3	32:L5B:104:GLU:OE2	2.01	0.59
33:L6B:70:THR:HG22	33:L6B:74:ASN:ND2	2.17	0.59
3:S3B:37:GLN:O	3:S3B:41:GLY:N	2.31	0.59
33:L6B:87:LEU:HB3	33:L6B:162:ILE:HG22	1.84	0.59
29:L2A:70:TRP:O	29:L2A:73:VAL:HG23	2.01	0.59
34:L9A:21:VAL:HG21	34:L9A:25:TYR:HD2	1.67	0.59
31:L4B:149:ASP:N	31:L4B:149:ASP:OD1	2.35	0.59
4:S4A:187:ARG:NH2	4:S4A:190:ASP:H	1.99	0.59
28:5SA:43:U:C5	32:L5A:69:ALA:HB1	2.38	0.59
8:S8B:104:ARG:HB3	8:S8B:108:GLY:H	1.66	0.59
9:S9B:19:LEU:HD21	9:S9B:84:ALA:HB1	1.84	0.59
33:L6B:6:ARG:C	33:L6B:8:PRO:HD3	2.22	0.59
3:S3A:57:ILE:HG12	3:S3A:66:VAL:HG22	1.83	0.59
2:S2B:105:PHE:O	2:S2B:109:SER:N	2.35	0.59
2:S2B:224:GLN:HG2	2:S2B:229:VAL:CG2	2.33	0.59
5:S5A:90:VAL:O	5:S5A:120:THR:HA	2.02	0.59
9:S9A:8:GLY:HA3	9:S9A:76:ALA:O	2.02	0.59
29:L2B:206:LEU:O	29:L2B:211:ARG:HD3	2.03	0.59
30:L3B:40:GLU:HG3	30:L3B:41:LYS:N	2.18	0.59
29:L2B:142:VAL:HG23	29:L2B:193:VAL:HA	1.85	0.59
4:S4A:13:ARG:HA	4:S4A:33:MET:HE3	1.84	0.58
4:S4A:98:GLU:OE2	4:S4A:103:ASN:ND2	2.30	0.58
2:S2B:178:ARG:NH2	8:S8B:74:PRO:HG3	2.17	0.58
28:5SB:2:A:C8	28:5SB:3:U:C5	2.91	0.58
30:L3B:24:THR:HG23	30:L3B:186:GLY:O	2.03	0.58
3:S3A:122:GLU:O	3:S3A:126:ARG:HG2	2.04	0.58
8:S8B:103:VAL:HG21	8:S8B:110:ALA:HB2	1.85	0.58
34:L9A:92:VAL:HG13	34:L9A:120:ILE:HG23	1.85	0.58
33:L6B:87:LEU:HA	33:L6B:163:TYR:O	2.02	0.58
3:S3A:150:LYS:HE2	3:S3A:152:ILE:HD11	1.84	0.58
32:L5A:97:ASP:H	32:L5A:100:TRP:HD1	1.51	0.58
4:S4B:70:ILE:CG1	4:S4B:74:GLN:HG3	2.33	0.58
29:L2A:70:TRP:CH2	29:L2A:150:LYS:HA	2.38	0.58
32:L5B:151:ALA:O	32:L5B:153:ARG:NH1	2.36	0.58
33:L6A:172:LYS:O	33:L6A:174:GLY:N	2.36	0.58
34:L9A:40:THR:HG22	34:L9A:42:SER:H	1.67	0.58
32:L5B:66:GLN:OE1	32:L5B:98:ARG:NH1	2.35	0.58
3:S3A:8:ILE:HG23	3:S3A:16:ARG:HG2	1.86	0.58
8:S8A:9:MET:HG3	8:S8A:26:VAL:HG11	1.84	0.58
34:L9A:79:ILE:HG22	34:L9A:141:LYS:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:L9B:78:THR:HG21	34:L9B:140:LEU:HD13	1.85	0.58
2:S2A:79:ASP:O	2:S2A:82:ARG:HB3	2.04	0.58
34:L9A:79:ILE:HD12	34:L9A:80:PRO:HD2	1.85	0.58
2:S2B:167:PRO:O	2:S2B:171:ALA:HB2	2.03	0.58
8:S8A:13:ILE:O	8:S8A:17:THR:HG23	2.04	0.58
28:5SA:16:U:H4'	28:5SA:17:A:OP2	2.04	0.58
33:L6B:33:LEU:HB2	33:L6B:75:ALA:HB1	1.85	0.57
4:S4B:70:ILE:HG13	4:S4B:74:GLN:HG3	1.86	0.57
28:5SB:16:U:HO2'	28:5SB:17:A:P	2.27	0.57
32:L5B:64:THR:OG1	32:L5B:94:LEU:HD13	2.05	0.57
4:S4A:103:ASN:OD1	4:S4A:114:ARG:NH2	2.33	0.57
9:S9A:77:ILE:O	9:S9A:81:ILE:HG12	2.04	0.57
33:L6A:15:VAL:HG12	33:L6A:29:PRO:HD2	1.85	0.57
32:L5A:49:ASP:OD1	32:L5A:51:ARG:HG3	2.04	0.57
9:S9A:25:LYS:HB2	9:S9A:60:ASP:OD2	2.04	0.57
31:L4A:63:LYS:HE3	31:L4A:67:GLN:HB2	1.86	0.57
31:L4A:107:LYS:HE3	31:L4A:206:ILE:HD12	1.86	0.57
3:S3B:44:GLU:HA	3:S3B:52:LEU:HD11	1.86	0.57
31:L4B:185:ASP:HA	31:L4B:188:ARG:HD3	1.86	0.57
32:L5B:106:LEU:HD12	32:L5B:110:ALA:HB3	1.87	0.57
6:S6A:30:LEU:HD11	6:S6A:63:TYR:HE2	1.70	0.57
34:L9A:115:ALA:C	34:L9A:117:GLU:N	2.54	0.57
28:5SB:17:A:H3'	28:5SB:18:G:H5'	1.86	0.57
30:L3B:176:ILE:HD12	30:L3B:181:LEU:HD23	1.86	0.57
5:S5A:33:VAL:HG11	5:S5A:109:ILE:HA	1.87	0.57
34:L9A:93:THR:O	34:L9A:97:ILE:HG13	2.05	0.57
2:S2A:31:TYR:HB3	2:S2A:42:ILE:HD11	1.87	0.57
8:S8A:124:ALA:O	8:S8A:128:GLY:N	2.38	0.57
2:S2B:7:VAL:HG22	2:S2B:8:LYS:H	1.70	0.57
29:L2A:182:LEU:HB2	29:L2A:271:ILE:HG13	1.87	0.57
34:L9A:57:ARG:NH1	34:L9A:61:ARG:HD2	2.19	0.57
34:L9B:110:ASP:N	34:L9B:130:TYR:OH	2.29	0.57
29:L2B:35:LYS:HG3	29:L2B:36:PRO:HD2	1.87	0.56
2:S2A:168:THR:HG22	2:S2A:169:LYS:H	1.70	0.56
9:S9A:8:GLY:HA2	9:S9A:79:LEU:HD12	1.87	0.56
6:S6B:8:ILE:HB	6:S6B:61:LEU:HB2	1.87	0.56
8:S8B:112:LEU:HB3	8:S8B:133:LEU:HA	1.87	0.56
31:L4B:31:HIS:NE2	31:L4B:35:GLU:OE2	2.36	0.56
3:S3A:8:ILE:HD12	3:S3A:16:ARG:HE	1.71	0.56
4:S4A:13:ARG:HD3	4:S4A:32:ALA:HB1	1.87	0.56
4:S4A:61:LYS:HE3	4:S4A:65:ARG:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S8A:81:HIS:HB2	8:S8A:138:TRP:CZ3	2.41	0.56
3:S3B:70:VAL:O	3:S3B:106:VAL:N	2.27	0.56
29:L2B:53:PHE:CE2	29:L2B:220:HIS:ND1	2.73	0.56
5:S5A:45:PHE:CE2	5:S5A:47:LYS:HD2	2.40	0.56
3:S3A:83:ARG:O	3:S3A:86:VAL:HG22	2.05	0.56
4:S4A:153:ARG:NE	4:S4A:181:MET:SD	2.69	0.56
32:L5A:72:ARG:HD3	32:L5A:87:PRO:HA	1.86	0.56
34:L9A:6:LEU:HB2	34:L9A:36:ALA:HA	1.88	0.56
34:L9B:71:ILE:HG23	34:L9B:72:LEU:HG	1.88	0.56
9:S9A:10:ARG:HG3	9:S9A:10:ARG:O	2.05	0.56
6:S6A:6:VAL:HG22	6:S6A:90:VAL:HG22	1.86	0.56
6:S6A:16:GLN:HA	6:S6A:19:LEU:HB3	1.87	0.56
28:5SA:50:A:H2'	28:5SA:51:C:C6	2.41	0.56
31:L4A:129:PHE:O	31:L4A:131:GLY:N	2.34	0.56
33:L6B:78:GLY:HA3	33:L6B:136:ILE:O	2.06	0.56
33:L6B:154:PRO:HA	33:L6B:161:GLY:HA3	1.87	0.56
31:L4A:66:PRO:O	31:L4A:67:GLN:HB3	2.05	0.56
31:L4A:185:ASP:OD1	31:L4A:188:ARG:NH1	2.38	0.56
34:L9A:88:ILE:HG12	34:L9A:122:GLU:N	2.21	0.56
4:S4B:172:PRO:HB2	4:S4B:187:ARG:HH22	1.71	0.56
9:S9B:19:LEU:HD23	9:S9B:19:LEU:H	1.69	0.56
7:S7A:49:ILE:O	7:S7A:53:LYS:HB3	2.05	0.56
8:S8A:4:ASP:OD2	8:S8A:85:ARG:NH1	2.39	0.56
2:S2B:172:ILE:H	2:S2B:172:ILE:HD12	1.70	0.56
5:S5B:101:ILE:HG13	5:S5B:119:LEU:HD23	1.88	0.56
6:S6B:17:SER:O	6:S6B:21:LEU:HD23	2.06	0.56
28:5SA:42:U:H3'	28:5SA:43:U:H5''	1.88	0.56
30:L3A:24:THR:HG22	30:L3A:186:GLY:O	2.06	0.56
33:L6A:115:VAL:HG11	33:L6A:148:ILE:HD11	1.87	0.56
3:S3B:91:LEU:HB3	3:S3B:99:VAL:HG11	1.88	0.55
30:L3B:1:MET:N	30:L3B:200:GLU:HG2	2.21	0.55
32:L5B:49:ASP:HB3	32:L5B:52:ILE:HG22	1.88	0.55
7:S7A:65:ALA:O	7:S7A:69:VAL:HG23	2.06	0.55
7:S7B:79:ARG:HG2	7:S7B:84:ASN:HB2	1.87	0.55
31:L4B:11:VAL:HG22	31:L4B:125:LEU:HB2	1.87	0.55
33:L6B:76:VAL:HA	33:L6B:79:VAL:HG22	1.88	0.55
2:S2A:54:THR:HG21	2:S2A:201:ILE:HD11	1.88	0.55
7:S7A:111:ARG:NH1	7:S7A:113:GLU:OE2	2.38	0.55
3:S3B:28:GLN:OE1	3:S3B:28:GLN:N	2.39	0.55
30:L3B:77:ILE:HG12	30:L3B:195:LEU:HD22	1.89	0.55
33:L6B:20:ALA:HB3	33:L6B:23:ARG:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:L9A:115:ALA:O	34:L9A:117:GLU:N	2.39	0.55
3:S3B:63:ASN:HB3	3:S3B:98:ASN:HB3	1.88	0.55
8:S8B:89:PRO:HA	8:S8B:92:ARG:HH11	1.71	0.55
9:S9B:74:ILE:O	9:S9B:78:LYS:NZ	2.39	0.55
33:L6A:86:GLU:N	33:L6A:86:GLU:OE2	2.39	0.55
8:S8A:121:ASP:OD1	8:S8A:121:ASP:N	2.38	0.55
31:L4A:123:LEU:HD12	31:L4A:124:LEU:H	1.70	0.55
28:5SB:15:A:O2'	28:5SB:17:A:O5'	2.24	0.55
2:S2B:137:ARG:HH11	2:S2B:137:ARG:C	2.10	0.55
3:S3B:156:ARG:HD2	3:S3B:193:TYR:CD1	2.42	0.55
30:L3B:106:GLY:HA3	30:L3B:189:PRO:HB2	1.88	0.55
31:L4A:28:ILE:HD13	31:L4A:30:PRO:HD3	1.89	0.55
34:L9A:2:LYS:HE3	34:L9A:20:ASP:HB3	1.89	0.55
29:L2B:12:SER:HB2	29:L2B:208:LYS:HB3	1.89	0.55
9:S9A:3:GLN:HB3	9:S9A:20:ARG:HG2	1.88	0.55
4:S4B:121:VAL:HG22	4:S4B:126:ILE:HG13	1.88	0.55
5:S5A:31:LEU:HD22	5:S5A:43:LEU:HD11	1.89	0.55
6:S6A:69:GLU:O	6:S6A:72:VAL:HG12	2.06	0.55
34:L9A:40:THR:HB	34:L9A:43:ASN:H	1.71	0.55
34:L9A:130:TYR:O	34:L9A:135:GLU:HG3	2.06	0.55
9:S9B:19:LEU:CB	9:S9B:59:PHE:HE1	2.17	0.55
34:L9B:109:ILE:HB	34:L9B:130:TYR:OH	2.07	0.55
2:S2A:93:VAL:HG11	2:S2A:97:TRP:HA	1.89	0.54
31:L4A:8:GLN:OE1	31:L4A:8:GLN:N	2.37	0.54
4:S4B:102:ASP:HB3	4:S4B:136:PRO:HB3	1.87	0.54
9:S9B:19:LEU:HB2	9:S9B:59:PHE:CE1	2.35	0.54
28:5SB:47:A:C4	28:5SB:48:A:C8	2.95	0.54
34:L9A:87:LYS:HA	34:L9A:122:GLU:HA	1.89	0.54
3:S3B:50:ALA:HB1	3:S3B:70:VAL:HG11	1.89	0.54
30:L3B:87:GLU:H	30:L3B:87:GLU:CD	2.11	0.54
34:L9B:123:LEU:HA	34:L9B:142:VAL:HG11	1.89	0.54
2:S2B:119:GLU:HA	2:S2B:122:PHE:HB2	1.88	0.54
30:L3B:174:ASP:HB3	30:L3B:183:LEU:HD22	1.90	0.54
4:S4A:15:GLU:OE2	4:S4A:59:ARG:NE	2.35	0.54
7:S7A:26:PHE:O	7:S7A:30:ILE:HG13	2.06	0.54
9:S9A:3:GLN:OE1	9:S9A:20:ARG:NH1	2.40	0.54
31:L4A:11:VAL:HG22	31:L4A:125:LEU:HB2	1.89	0.54
33:L6A:88:LEU:HD11	33:L6A:130:ARG:HD3	1.90	0.54
3:S3B:50:ALA:HB2	3:S3B:76:VAL:CG1	2.30	0.54
34:L9B:52:ARG:HA	34:L9B:55:ALA:HB3	1.89	0.54
8:S8A:97:VAL:HG23	8:S8A:100:ILE:HD12	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S3B:58:GLU:HB3	3:S3B:65:ALA:HB3	1.88	0.54
4:S4B:100:ARG:O	4:S4B:104:VAL:HG23	2.07	0.54
6:S6B:9:VAL:HB	6:S6B:87:ARG:HB2	1.88	0.54
9:S9B:13:ALA:HB2	9:S9B:68:GLY:HA3	1.89	0.54
4:S4B:3:ARG:HD2	4:S4B:118:ARG:CZ	2.38	0.54
5:S5B:48:ALA:HB2	5:S5B:57:LYS:HD3	1.90	0.54
31:L4B:129:PHE:O	31:L4B:131:GLY:N	2.37	0.54
2:S2A:10:LEU:O	2:S2A:13:ALA:N	2.39	0.54
2:S2A:178:ARG:HH22	8:S8A:68:ARG:HH22	1.56	0.54
31:L4B:101:LEU:O	31:L4B:106:ARG:NH1	2.41	0.54
34:L9B:31:LEU:HD21	34:L9B:38:LEU:HG	1.88	0.54
34:L9B:78:THR:HB	34:L9B:80:PRO:HD3	1.89	0.54
4:S4A:187:ARG:NH2	4:S4A:189:PRO:HA	2.23	0.54
7:S7A:126:ASP:HB3	7:S7A:131:LYS:HG3	1.89	0.54
31:L4A:123:LEU:HD13	31:L4A:192:LEU:HB3	1.90	0.54
34:L9A:6:LEU:H	34:L9A:36:ALA:HA	1.73	0.54
4:S4B:152:SER:HA	4:S4B:155:LEU:HD23	1.90	0.54
6:S6B:3:ARG:HG3	6:S6B:93:SER:HB3	1.90	0.54
9:S9B:3:GLN:HB3	9:S9B:20:ARG:HD2	1.90	0.54
32:L5B:32:PRO:HB2	32:L5B:172:LEU:HD22	1.89	0.54
32:L5B:61:ALA:HA	32:L5B:66:GLN:O	2.07	0.54
33:L6B:122:THR:HG22	33:L6B:123:PHE:H	1.72	0.54
2:S2A:75:LYS:HA	2:S2A:78:GLN:HB2	1.90	0.54
8:S8A:25:ASP:HA	8:S8A:59:LEU:O	2.08	0.54
5:S5A:142:LEU:O	5:S5A:143:ARG:NH1	2.35	0.54
34:L9A:98:ALA:HB2	34:L9A:111:PRO:HD3	1.90	0.54
3:S3B:6:HIS:HD2	3:S3B:8:ILE:H	1.54	0.54
4:S4B:15:GLU:OE1	4:S4B:66:ARG:NH1	2.39	0.54
2:S2A:219:VAL:O	2:S2A:223:ILE:HG13	2.07	0.53
28:5SB:91:G:N2	28:5SB:92:A:N1	2.34	0.53
33:L6B:87:LEU:HD22	33:L6B:149:ARG:HG3	1.90	0.53
7:S7A:13:GLN:O	7:S7A:24:THR:HG21	2.09	0.53
33:L6A:98:LEU:HD22	33:L6A:125:VAL:HB	1.91	0.53
9:S9B:10:ARG:HH11	9:S9B:10:ARG:HG3	1.74	0.53
31:L4B:24:LEU:HD21	31:L4B:114:VAL:HG12	1.89	0.53
31:L4B:143:ALA:HB1	31:L4B:148:LEU:HB2	1.91	0.53
31:L4B:178:PRO:HB3	31:L4B:198:ALA:CB	2.38	0.53
2:S2A:87:ARG:NH1	2:S2A:220:ASP:OD1	2.41	0.53
4:S4A:201:GLN:O	4:S4A:205:GLU:HG3	2.07	0.53
34:L9A:4:ILE:HD11	34:L9A:44:LEU:HD12	1.90	0.53
5:S5B:28:PHE:CD2	5:S5B:51:VAL:HG22	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5SB:19:C:H2'	28:5SB:20:G:O4'	2.07	0.53
31:L4B:66:PRO:O	31:L4B:67:GLN:HB3	2.08	0.53
33:L6B:46:GLU:HB3	33:L6B:49:VAL:HG23	1.89	0.53
4:S4A:173:TRP:CD2	4:S4A:189:PRO:HB3	2.44	0.53
34:L9A:135:GLU:OE1	34:L9A:135:GLU:N	2.40	0.53
7:S7B:50:ILE:HB	7:S7B:58:PRO:HG3	1.90	0.53
8:S8B:120:THR:HG23	8:S8B:123:GLU:OE1	2.07	0.53
28:5SB:4:C:H2'	28:5SB:5:C:H6	1.74	0.53
9:S9A:65:VAL:HG21	9:S9A:77:ILE:HD11	1.91	0.53
32:L5B:37:VAL:O	32:L5B:94:LEU:HD23	2.09	0.53
30:L3A:176:ILE:HB	30:L3A:181:LEU:HB2	1.90	0.53
2:S2B:59:GLU:HB2	2:S2B:221:LEU:HD21	1.90	0.53
3:S3B:74:GLY:O	3:S3B:79:ARG:NH2	2.41	0.53
34:L9B:48:GLU:O	34:L9B:52:ARG:HG3	2.08	0.53
32:L5A:11:TYR:HA	32:L5A:15:VAL:HB	1.90	0.53
2:S2B:55:PHE:HE1	2:S2B:221:LEU:HD22	1.62	0.53
3:S3A:150:LYS:HG3	3:S3A:169:ALA:HB2	1.90	0.53
29:L2B:132:PRO:HD3	29:L2B:190:TYR:CE2	2.44	0.53
2:S2A:84:GLU:HB3	2:S2A:219:VAL:HG21	1.91	0.53
32:L5A:55:LYS:HE3	32:L5A:59:GLU:OE2	2.09	0.53
4:S4B:80:GLU:OE2	4:S4B:84:LYS:NZ	2.40	0.53
9:S9B:45:ALA:HA	9:S9B:51:ARG:HH12	1.74	0.53
28:5SB:45:C:P	32:L5B:67:LYS:HE2	2.49	0.53
30:L3B:28:ALA:HB3	30:L3B:93:VAL:HG12	1.90	0.53
2:S2A:5:ILE:CD1	2:S2A:221:LEU:HD23	2.39	0.52
7:S7A:23:VAL:HG13	7:S7A:43:PHE:CE2	2.43	0.52
29:L2A:60:ARG:HD3	29:L2A:86:PRO:CB	2.33	0.52
30:L3B:21:VAL:HG23	30:L3B:185:LYS:HD3	1.91	0.52
4:S4A:150:GLU:OE2	4:S4A:153:ARG:NH1	2.42	0.52
30:L3A:50:GLY:HA3	30:L3A:75:VAL:HG21	1.91	0.52
28:5SB:4:C:H2'	28:5SB:5:C:C6	2.44	0.52
29:L2B:181:GLU:HA	29:L2B:272:ALA:HB3	1.91	0.52
2:S2A:223:ILE:O	2:S2A:227:GLY:N	2.38	0.52
3:S3A:39:ILE:O	3:S3A:43:LEU:HG	2.08	0.52
4:S4B:106:TYR:HE1	4:S4B:112:VAL:O	1.92	0.52
28:5SB:4:C:C2	28:5SB:5:C:C5	2.97	0.52
3:S3A:20:SER:HB3	3:S3A:40:ARG:NH2	2.22	0.52
28:5SA:17:A:H5'	28:5SA:18:G:H8	1.73	0.52
29:L2A:17:THR:HB	29:L2A:205:VAL:H	1.73	0.52
33:L6A:26:VAL:HG21	33:L6A:75:ALA:HB1	1.90	0.52
33:L6A:113:VAL:HG11	33:L6A:151:ILE:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S5B:33:VAL:HG11	5:S5B:109:ILE:HA	1.91	0.52
28:5SA:42:U:H1'	28:5SA:47:A:H61	1.74	0.52
32:L5A:146:TYR:O	32:L5A:149:VAL:HG22	2.10	0.52
2:S2B:21:ARG:HA	2:S2B:39:ILE:HA	1.91	0.52
5:S5A:18:ARG:CZ	5:S5A:27:ARG:HH21	2.22	0.52
8:S8A:6:ILE:HB	8:S8A:85:ARG:NH1	2.25	0.52
32:L5A:43:LEU:HD21	32:L5A:153:ARG:HD2	1.90	0.52
29:L2B:242:ARG:H	29:L2B:242:ARG:HD2	1.75	0.52
5:S5A:31:LEU:HD11	5:S5A:129:ILE:HA	1.90	0.52
34:L9A:11:ASN:O	34:L9A:12:LEU:HB2	2.10	0.52
34:L9A:48:GLU:O	34:L9A:52:ARG:HG2	2.10	0.52
29:L2B:145:VAL:HG13	29:L2B:191:ALA:HB2	1.92	0.52
30:L3B:179:GLU:HB3	30:L3B:181:LEU:HB2	1.92	0.52
9:S9A:10:ARG:HD3	9:S9A:75:ASP:HB2	1.91	0.52
9:S9A:97:LYS:HB2	9:S9A:102:LEU:HD12	1.91	0.52
3:S3B:44:GLU:HA	3:S3B:52:LEU:HD21	1.91	0.52
3:S3B:156:ARG:NH1	3:S3B:193:TYR:O	2.42	0.52
4:S4B:26:CYS:HA	4:S4B:31:CYS:HB2	1.92	0.52
4:S4B:101:LEU:CB	4:S4B:138:TYR:HB3	2.40	0.52
2:S2A:209:ARG:O	2:S2A:213:LEU:HG	2.10	0.52
3:S3B:14:ILE:O	3:S3B:15:THR:HG22	2.09	0.52
3:S3A:87:LEU:O	3:S3A:91:LEU:HG	2.10	0.52
8:S8B:38:ILE:HD11	8:S8B:118:VAL:O	2.09	0.52
28:5SB:16:U:O2'	28:5SB:17:A:OP1	2.27	0.52
33:L6B:92:ILE:HG13	33:L6B:160:LYS:HD3	1.92	0.52
34:L9B:75:LEU:O	34:L9B:77:LEU:N	2.43	0.52
3:S3A:188:LEU:CD1	3:S3A:195:VAL:HG13	2.38	0.51
33:L6A:30:LYS:HD2	33:L6A:81:GLU:H	1.75	0.51
34:L9A:86:THR:N	34:L9A:123:LEU:HD12	2.21	0.51
3:S3B:47:LEU:HB3	3:S3B:52:LEU:HD13	1.92	0.51
8:S8B:13:ILE:O	8:S8B:17:THR:HG23	2.10	0.51
29:L2B:238:GLY:O	29:L2B:240:ALA:N	2.43	0.51
6:S6A:15:ASP:OD2	6:S6A:17:SER:HB2	2.09	0.51
6:S6A:30:LEU:HD11	6:S6A:63:TYR:CE2	2.45	0.51
7:S7A:27:ILE:HA	7:S7A:30:ILE:HD12	1.93	0.51
30:L3B:101:ARG:CZ	30:L3B:171:GLU:HB2	2.41	0.51
31:L4B:135:LYS:HB3	31:L4B:138:GLU:HG3	1.93	0.51
33:L6B:69:ARG:NH1	33:L6B:73:ALA:HB2	2.25	0.51
31:L4A:65:TRP:HB2	31:L4A:66:PRO:CD	2.38	0.51
31:L4A:107:LYS:HG2	31:L4A:206:ILE:HA	1.92	0.51
2:S2A:47:THR:O	2:S2A:51:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2A:55:PHE:HD1	2:S2A:221:LEU:HG	1.75	0.51
4:S4A:190:ASP:HB2	4:S4A:193:ASP:OD1	2.11	0.51
28:5SA:89:G:C2	28:5SA:91:G:H5"	2.45	0.51
8:S8B:124:ALA:O	8:S8B:128:GLY:N	2.44	0.51
9:S9B:125:TYR:HD1	9:S9B:126:SER:N	2.09	0.51
33:L6B:74:ASN:HA	33:L6B:77:LYS:HB3	1.92	0.51
33:L6B:89:ILE:HG22	33:L6B:94:TYR:CD2	2.46	0.51
32:L5A:4:ASP:OD2	32:L5A:9:ARG:NH1	2.43	0.51
32:L5A:55:LYS:O	32:L5A:58:GLN:HG3	2.10	0.51
33:L6A:18:GLU:HB2	33:L6A:25:LYS:HB2	1.93	0.51
33:L6A:169:VAL:HG22	33:L6A:171:LEU:HD11	1.92	0.51
29:L2B:79:VAL:HG12	29:L2B:113:VAL:HA	1.92	0.51
30:L3B:9:VAL:HG22	30:L3B:25:VAL:O	2.10	0.51
34:L9B:118:LYS:HG2	34:L9B:119:PRO:CD	2.39	0.51
5:S5A:18:ARG:NH2	5:S5A:27:ARG:HE	2.07	0.51
2:S2B:56:ARG:NH1	2:S2B:56:ARG:HB3	2.26	0.51
3:S3A:134:ILE:HG22	3:S3A:168:ALA:HB3	1.92	0.51
4:S4A:12:CYS:HB3	4:S4A:33:MET:CG	2.41	0.51
31:L4A:127:GLU:C	31:L4A:129:PHE:H	2.14	0.51
31:L4A:178:PRO:HG2	31:L4A:179:GLU:OE2	2.10	0.51
3:S3B:138:VAL:HG11	3:S3B:170:GLN:HG3	1.92	0.51
30:L3B:119:ARG:CD	30:L3B:160:TYR:HB2	2.32	0.51
2:S2A:71:VAL:HG23	2:S2A:164:VAL:HA	1.93	0.51
33:L6A:131:VAL:HG22	33:L6A:132:ARG:H	1.76	0.51
3:S3B:36:ASP:OD1	3:S3B:57:ILE:HD13	2.11	0.51
9:S9B:24:GLY:N	9:S9B:60:ASP:OD1	2.37	0.51
30:L3B:5:LEU:HD22	30:L3B:197:ILE:HG12	1.93	0.51
4:S4A:98:GLU:OE1	4:S4A:194:LEU:HD11	2.12	0.51
31:L4A:110:LEU:HG	31:L4A:202:PHE:HE1	1.76	0.51
3:S3A:78:GLY:C	3:S3A:79:ARG:HD3	2.31	0.50
3:S3A:108:ASN:OD1	3:S3A:110:ASN:HB2	2.11	0.50
3:S3A:123:GLN:O	3:S3A:128:PHE:HB2	2.11	0.50
3:S3A:136:GLN:HG2	3:S3A:140:ARG:NH2	2.26	0.50
4:S4A:8:VAL:HG21	4:S4A:115:ARG:CZ	2.40	0.50
2:S2B:187:LEU:HD11	2:S2B:204:ASN:N	2.26	0.50
29:L2B:17:THR:HG22	29:L2B:205:VAL:H	1.76	0.50
32:L5B:67:LYS:CD	32:L5B:67:LYS:N	2.74	0.50
9:S9A:57:GLY:C	9:S9A:59:PHE:H	2.14	0.50
31:L4A:167:ALA:HB1	31:L4A:173:VAL:HG11	1.94	0.50
31:L4A:181:LEU:HD22	31:L4A:186:ILE:HD11	1.93	0.50
33:L6A:9:ILE:HG22	33:L6A:69:ARG:NE	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:L4B:75:HIS:HD2	31:L4B:82:ILE:HD11	1.75	0.50
32:L5B:6:ALA:O	32:L5B:10:LYS:N	2.25	0.50
4:S4A:12:CYS:HB3	4:S4A:33:MET:HG2	1.91	0.50
5:S5A:28:PHE:O	5:S5A:47:LYS:HA	2.12	0.50
6:S6A:46:ARG:HB3	6:S6A:60:PHE:CE1	2.47	0.50
7:S7A:20:ASP:OD2	7:S7A:23:VAL:N	2.42	0.50
7:S7A:115:ARG:O	7:S7A:119:ARG:HG3	2.11	0.50
8:S8A:82:HIS:HE1	8:S8A:136:GLU:HG3	1.76	0.50
33:L6A:4:ILE:O	33:L6A:69:ARG:HG2	2.11	0.50
33:L6A:127:GLU:O	33:L6A:129:THR:N	2.44	0.50
34:L9A:4:ILE:HG12	34:L9A:18:VAL:HG22	1.93	0.50
8:S8B:11:THR:HG23	8:S8B:14:ARG:NH1	2.27	0.50
9:S9B:19:LEU:HD21	9:S9B:84:ALA:CB	2.40	0.50
29:L2B:71:ASP:N	29:L2B:71:ASP:OD1	2.43	0.50
31:L4B:123:LEU:HD12	31:L4B:124:LEU:H	1.76	0.50
32:L5B:129:GLY:HA2	32:L5B:166:ASP:HA	1.93	0.50
34:L9B:42:SER:HA	34:L9B:45:LYS:HE3	1.92	0.50
4:S4A:88:VAL:O	4:S4A:89:THR:HB	2.12	0.50
4:S4A:150:GLU:C	4:S4A:152:SER:H	2.13	0.50
8:S8A:51:VAL:HG21	8:S8A:60:ARG:HG2	1.94	0.50
28:5SA:17:A:H1'	28:5SA:112:G:N9	2.26	0.50
2:S2B:73:THR:HB	2:S2B:96:ARG:H	1.76	0.50
4:S4B:61:LYS:HD2	4:S4B:206:PHE:CE2	2.46	0.50
4:S4B:63:LYS:O	4:S4B:67:ILE:HG13	2.12	0.50
4:S4B:176:LEU:HG	4:S4B:178:VAL:HG22	1.93	0.50
8:S8B:122:ARG:HA	8:S8B:125:ARG:HB2	1.92	0.50
30:L3B:11:MET:CG	30:L3B:24:THR:HG22	2.39	0.50
31:L4B:197:ASP:N	31:L4B:197:ASP:OD1	2.43	0.50
7:S7A:5:ARG:HB3	7:S7A:7:ALA:H	1.77	0.50
7:S7A:91:VAL:CG2	7:S7A:96:GLN:HG2	2.41	0.50
28:5SA:98:U:H2'	28:5SA:99:G:H8	1.77	0.50
33:L6A:24:VAL:HG22	33:L6A:35:VAL:HB	1.92	0.50
34:L9A:110:ASP:HB2	34:L9A:112:LYS:H	1.76	0.50
28:5SB:89:G:N2	28:5SB:92:A:OP2	2.44	0.50
29:L2A:10:THR:CG2	29:L2A:13:ARG:HB2	2.42	0.50
31:L4A:178:PRO:HB3	31:L4A:198:ALA:CB	2.41	0.50
32:L5A:106:LEU:HD12	32:L5A:110:ALA:HB3	1.93	0.50
32:L5A:131:TYR:HB3	32:L5A:159:VAL:HG22	1.93	0.50
2:S2B:76:GLN:O	2:S2B:208:ILE:HG12	2.12	0.50
4:S4B:3:ARG:O	4:S4B:5:ILE:HD12	2.12	0.50
3:S3A:64:VAL:HG12	3:S3A:66:VAL:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S9A:46:ALA:HA	9:S9A:78:LYS:HB2	1.94	0.50
5:S5B:67:VAL:HG21	5:S5B:140:ARG:HA	1.94	0.50
32:L5B:7:LEU:HA	32:L5B:10:LYS:HB3	1.93	0.50
2:S2A:158:LEU:HD12	2:S2A:158:LEU:O	2.12	0.50
4:S4A:166:LYS:HG3	4:S4A:178:VAL:HG11	1.94	0.50
5:S5A:148:VAL:HG21	8:S8A:107:LEU:HD22	1.94	0.50
9:S9A:43:ALA:HA	9:S9A:74:ILE:HD13	1.94	0.50
30:L3A:28:ALA:HB3	30:L3A:93:VAL:HG12	1.93	0.50
33:L6A:27:LYS:HA	33:L6A:32:GLU:HB3	1.94	0.50
34:L9A:94:ALA:O	34:L9A:111:PRO:CG	2.60	0.50
8:S8B:116:LYS:HD2	8:S8B:129:VAL:HG11	1.94	0.50
32:L5B:60:LEU:HD12	32:L5B:63:ILE:HD11	1.93	0.50
34:L9B:1:MET:HB3	34:L9B:21:VAL:O	2.12	0.50
2:S2A:17:PHE:HB3	2:S2A:44:LEU:HD21	1.93	0.49
2:S2A:80:ILE:HD11	2:S2A:208:ILE:HG23	1.93	0.49
5:S5A:96:PRO:HA	5:S5A:117:ASP:OD2	2.12	0.49
34:L9B:75:LEU:HD21	34:L9B:105:HIS:CE1	2.47	0.49
29:L2A:130:ALA:HB2	29:L2A:192:THR:HG22	1.93	0.49
28:5SB:17:A:H3'	28:5SB:18:G:C5'	2.43	0.49
34:L9B:144:VAL:HG22	34:L9B:145:VAL:H	1.77	0.49
4:S4A:19:LEU:HD12	4:S4A:67:ILE:CG1	2.41	0.49
9:S9A:17:VAL:HG11	9:S9A:81:ILE:HA	1.94	0.49
28:5SA:31:A:H2'	28:5SA:32:C:O4'	2.13	0.49
33:L6A:74:ASN:HA	33:L6A:77:LYS:HB3	1.93	0.49
30:L3B:6:GLY:N	30:L3B:196:VAL:O	2.42	0.49
31:L4B:6:VAL:HG21	31:L4B:119:ARG:HG3	1.94	0.49
32:L5B:80:PHE:O	32:L5B:82:LEU:HB2	2.11	0.49
7:S7A:99:LEU:HD22	7:S7A:103:TRP:CZ2	2.47	0.49
31:L4A:184:TYR:O	31:L4A:188:ARG:HB2	2.12	0.49
31:L4A:197:ASP:O	31:L4A:198:ALA:HB3	2.11	0.49
34:L9A:88:ILE:O	34:L9A:121:LYS:HE3	2.12	0.49
28:5SB:60:A:H5'	28:5SB:61:A:OP2	2.12	0.49
29:L2B:17:THR:HG22	29:L2B:205:VAL:HB	1.94	0.49
32:L5B:43:LEU:HD21	32:L5B:153:ARG:HD2	1.95	0.49
33:L6B:30:LYS:HB3	33:L6B:79:VAL:HA	1.93	0.49
3:S3A:9:GLY:HA2	3:S3A:12:LEU:HG	1.95	0.49
9:S9A:26:VAL:HB	9:S9A:33:PHE:HB2	1.94	0.49
32:L5A:133:LEU:CD2	32:L5A:157:ILE:HB	2.43	0.49
5:S5B:70:PRO:HB3	5:S5B:144:THR:CG2	2.42	0.49
8:S8B:20:TYR:HA	8:S8B:65:TYR:CZ	2.48	0.49
9:S9B:99:LEU:HB3	9:S9B:101:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:L5B:67:LYS:N	32:L5B:67:LYS:HD3	2.27	0.49
33:L6B:7:LEU:HB3	33:L6B:65:HIS:HE1	1.77	0.49
3:S3A:20:SER:HB2	3:S3A:57:ILE:HB	1.93	0.49
30:L3A:73:GLU:OE1	30:L3A:73:GLU:N	2.43	0.49
2:S2B:165:VAL:HA	2:S2B:187:LEU:HB3	1.93	0.49
5:S5B:144:THR:N	5:S5B:147:ASP:OD1	2.45	0.49
34:L9B:82:ARG:NH2	34:L9B:96:ASP:OD2	2.45	0.49
3:S3A:119:ARG:O	3:S3A:123:GLN:HG3	2.13	0.49
5:S5A:147:ASP:HA	5:S5A:150:ARG:NH1	2.28	0.49
8:S8A:97:VAL:HA	8:S8A:100:ILE:HG13	1.94	0.49
33:L6A:15:VAL:HG12	33:L6A:29:PRO:CD	2.41	0.49
33:L6A:20:ALA:HB3	33:L6A:23:ARG:HG3	1.94	0.49
3:S3B:179:ARG:HD2	3:S3B:207:VAL:H	1.78	0.49
5:S5B:42:GLY:HA3	5:S5B:65:ASN:O	2.13	0.49
9:S9B:10:ARG:NH2	9:S9B:105:ASP:OD2	2.41	0.49
31:L4B:116:ASP:OD1	31:L4B:119:ARG:NH2	2.39	0.49
33:L6B:124:GLU:O	33:L6B:125:VAL:HB	2.13	0.49
2:S2A:24:TRP:HB2	2:S2A:190:THR:HB	1.95	0.49
3:S3A:182:ILE:HG13	3:S3A:203:PHE:HD1	1.76	0.49
4:S4A:83:SER:HA	4:S4A:89:THR:HG23	1.95	0.49
7:S7A:73:MET:HG2	7:S7A:90:GLU:HA	1.95	0.49
2:S2B:91:PRO:HA	2:S2B:154:LEU:HD12	1.94	0.49
8:S8B:17:THR:HG22	8:S8B:63:LEU:HD23	1.93	0.49
5:S5A:81:GLU:CG	5:S5A:90:VAL:HG22	2.42	0.49
9:S9A:50:LEU:HD22	9:S9A:55:ALA:HB3	1.95	0.49
32:L5A:133:LEU:HD21	32:L5A:157:ILE:HB	1.95	0.49
9:S9B:10:ARG:NE	9:S9B:105:ASP:HB3	2.26	0.49
6:S6B:33:TYR:OH	6:S6B:78:GLU:HG3	2.12	0.49
32:L5B:135:LEU:HD11	32:L5B:155:MET:HG2	1.94	0.49
33:L6B:60:ARG:O	33:L6B:64:LEU:HG	2.13	0.49
9:S9A:29:ASN:OD1	9:S9A:64:THR:HA	2.12	0.48
30:L3B:120:TRP:CG	30:L3B:155:LYS:HB3	2.48	0.48
32:L5B:102:PHE:HE1	32:L5B:141:PHE:HE1	1.59	0.48
34:L9B:80:PRO:O	34:L9B:143:SER:HB2	2.12	0.48
3:S3A:70:VAL:HG12	3:S3A:72:LYS:H	1.78	0.48
31:L4A:125:LEU:HD11	31:L4A:199:TRP:CD2	2.47	0.48
33:L6A:157:TYR:CE1	33:L6A:172:LYS:HB2	2.47	0.48
5:S5B:72:GLN:O	5:S5B:75:THR:HG22	2.13	0.48
34:L9B:89:TYR:N	34:L9B:89:TYR:CD1	2.81	0.48
34:L9B:143:SER:OG	34:L9B:144:VAL:N	2.46	0.48
4:S4A:65:ARG:HG2	4:S4A:75:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S6A:53:ALA:O	6:S6A:54:LYS:HG2	2.12	0.48
32:L5A:16:ARG:HB3	32:L5A:17:PRO:HD3	1.96	0.48
2:S2B:200:ILE:O	2:S2B:201:ILE:HD13	2.12	0.48
9:S9B:49:PRO:O	9:S9B:53:VAL:HG22	2.13	0.48
33:L6B:101:ARG:O	33:L6B:101:ARG:HD3	2.12	0.48
5:S5A:52:PRO:O	5:S5A:55:VAL:HG12	2.13	0.48
6:S6A:20:ALA:HA	6:S6A:23:LYS:HB2	1.94	0.48
31:L4A:143:ALA:HB1	31:L4A:148:LEU:HB2	1.95	0.48
34:L9A:81:VAL:HG21	34:L9A:88:ILE:HD12	1.95	0.48
34:L9B:127:VAL:HA	34:L9B:138:ILE:O	2.13	0.48
5:S5A:81:GLU:HG3	5:S5A:90:VAL:HG22	1.95	0.48
33:L6A:15:VAL:HG12	33:L6A:28:GLY:HA3	1.95	0.48
34:L9A:129:THR:HA	34:L9A:137:PRO:HA	1.94	0.48
2:S2B:92:TYR:CE2	2:S2B:151:GLY:HA3	2.49	0.48
3:S3B:129:ALA:HB3	3:S3B:132:ARG:HB3	1.94	0.48
9:S9B:63:ILE:HD11	9:S9B:81:ILE:HD11	1.96	0.48
28:5SB:26:G:H2'	28:5SB:58:G:N7	2.28	0.48
2:S2A:170:GLU:O	2:S2A:174:VAL:HG23	2.13	0.48
2:S2B:221:LEU:HG	2:S2B:221:LEU:O	2.12	0.48
4:S4B:81:GLU:HG2	4:S4B:96:LEU:HD21	1.95	0.48
29:L2B:105:ILE:HD11	29:L2B:192:THR:HG21	1.95	0.48
30:L3B:59:VAL:HG21	30:L3B:74:PRO:HB2	1.96	0.48
33:L6B:35:VAL:HG11	33:L6B:71:LEU:HB3	1.95	0.48
34:L9B:38:LEU:H	34:L9B:38:LEU:HD12	1.79	0.48
2:S2A:37:ASN:C	2:S2A:39:ILE:H	2.17	0.48
3:S3A:155:GLY:HA3	3:S3A:196:LEU:HD13	1.96	0.48
7:S7B:113:GLU:HG3	7:S7B:119:ARG:HA	1.94	0.48
29:L2B:58:HIS:ND1	29:L2B:59:LYS:O	2.37	0.48
29:L2B:148:GLU:HB2	29:L2B:151:LYS:HD2	1.96	0.48
32:L5B:111:LEU:HB2	32:L5B:112:PRO:HD3	1.94	0.48
33:L6B:144:VAL:O	33:L6B:147:ASN:HB2	2.13	0.48
2:S2A:36:ARG:HD3	2:S2A:36:ARG:HA	1.71	0.48
2:S2A:69:LEU:HB3	2:S2A:162:ILE:HG22	1.96	0.48
6:S6A:44:GLY:HA2	6:S6A:59:TYR:CE1	2.48	0.48
32:L5A:124:SER:HB2	32:L5A:131:TYR:CE1	2.49	0.48
2:S2B:158:LEU:H	2:S2B:158:LEU:HD12	1.78	0.48
7:S7B:13:GLN:HG2	7:S7B:14:PRO:HD2	1.95	0.48
33:L6B:139:GLN:O	33:L6B:139:GLN:NE2	2.47	0.48
3:S3B:182:ILE:HA	3:S3B:202:ILE:O	2.13	0.48
6:S6B:76:ALA:HB1	6:S6B:80:ARG:HH21	1.79	0.48
8:S8B:97:VAL:HA	8:S8B:100:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:L6B:130:ARG:O	33:L6B:131:VAL:HG23	2.13	0.48
34:L9B:29:TYR:O	34:L9B:32:PRO:HD2	2.14	0.48
9:S9A:48:GLU:N	9:S9A:49:PRO:HD2	2.29	0.48
2:S2B:51:LEU:HG	2:S2B:201:ILE:HG23	1.96	0.48
2:S2B:54:THR:O	2:S2B:58:ILE:HG12	2.14	0.48
2:S2B:69:LEU:HG	2:S2B:91:PRO:HB2	1.94	0.48
3:S3B:6:HIS:CD2	3:S3B:7:PRO:HD2	2.49	0.48
29:L2B:183:ARG:HG3	29:L2B:184:LYS:N	2.28	0.48
33:L6B:76:VAL:O	33:L6B:79:VAL:HG22	2.14	0.48
33:L6A:7:LEU:HB3	33:L6A:69:ARG:HE	1.77	0.47
9:S9B:4:TYR:HB2	9:S9B:19:LEU:CD2	2.44	0.47
9:S9B:17:VAL:HA	9:S9B:63:ILE:HG23	1.96	0.47
34:L9B:97:ILE:HG22	34:L9B:101:LEU:HD23	1.96	0.47
3:S3A:76:VAL:O	3:S3A:83:ARG:HG2	2.14	0.47
6:S6A:62:TRP:C	6:S6A:63:TYR:HD1	2.17	0.47
7:S7A:15:ASP:OD1	7:S7A:44:TYR:OH	2.31	0.47
9:S9A:42:ARG:NH1	9:S9A:75:ASP:OD2	2.46	0.47
29:L2A:33:LEU:O	29:L2A:64:ILE:HG22	2.14	0.47
2:S2A:9:GLU:N	2:S2A:9:GLU:OE1	2.47	0.47
2:S2B:68:ILE:HA	2:S2B:161:ALA:O	2.13	0.47
5:S5B:152:ARG:O	8:S8B:64:LYS:NZ	2.46	0.47
31:L4B:39:TRP:O	31:L4B:43:LYS:HG2	2.14	0.47
31:L4B:47:GLY:HA3	31:L4B:95:ARG:O	2.14	0.47
2:S2A:212:GLN:OE1	2:S2A:216:SER:HB2	2.13	0.47
3:S3A:70:VAL:O	3:S3A:106:VAL:N	2.45	0.47
5:S5A:31:LEU:HG	5:S5A:45:PHE:CD1	2.49	0.47
6:S6A:30:LEU:HB3	6:S6A:35:ALA:HB3	1.95	0.47
2:S2B:91:PRO:HG3	2:S2B:154:LEU:HB2	1.97	0.47
2:S2B:143:GLU:O	2:S2B:147:LYS:HB2	2.13	0.47
4:S4B:173:TRP:O	4:S4B:186:LEU:HB2	2.15	0.47
3:S3A:56:ASP:O	3:S3A:66:VAL:HA	2.15	0.47
32:L5A:170:ARG:HE	32:L5A:174:GLU:HG2	1.79	0.47
2:S2B:60:ASP:O	2:S2B:64:ARG:HD3	2.14	0.47
2:S2A:92:TYR:CE1	2:S2A:151:GLY:HA3	2.49	0.47
4:S4A:170:VAL:HG11	4:S4A:176:LEU:HD23	1.95	0.47
8:S8B:39:LEU:HD12	8:S8B:44:PHE:CB	2.44	0.47
28:5SB:39:C:N3	28:5SB:50:A:O2'	2.44	0.47
30:L3B:144:ARG:HB3	30:L3B:145:LYS:H	1.57	0.47
34:L9B:2:LYS:HG3	34:L9B:39:ALA:HB3	1.97	0.47
4:S4A:33:MET:CE	4:S4A:37:PRO:HA	2.42	0.47
7:S7A:155:ARG:HD3	7:S7A:155:ARG:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:L3A:174:ASP:HB3	30:L3A:183:LEU:HD22	1.95	0.47
3:S3B:73:PRO:O	3:S3B:77:ILE:HG22	2.14	0.47
3:S3B:82:GLU:H	3:S3B:85:ARG:NH1	2.13	0.47
4:S4B:156:GLU:O	4:S4B:159:ARG:HG2	2.14	0.47
4:S4B:177:ASP:HB3	4:S4B:182:LYS:HG3	1.95	0.47
7:S7B:15:ASP:OD1	7:S7B:16:LEU:N	2.44	0.47
9:S9B:4:TYR:O	9:S9B:18:PHE:HA	2.15	0.47
31:L4B:181:LEU:HD23	31:L4B:181:LEU:HA	1.76	0.47
32:L5B:84:LYS:HE2	32:L5B:84:LYS:HB3	1.74	0.47
33:L6B:91:GLY:HA3	33:L6B:94:TYR:CD2	2.50	0.47
2:S2B:32:ILE:HD11	2:S2B:40:HIS:NE2	2.29	0.47
2:S2B:83:MET:CE	2:S2B:84:GLU:HG2	2.44	0.47
4:S4B:8:VAL:CG1	4:S4B:21:LEU:HB2	2.45	0.47
6:S6B:82:ARG:HB2	6:S6B:85:VAL:HG23	1.96	0.47
28:5SB:44:C:C4	32:L5B:91:ARG:NH2	2.82	0.47
30:L3B:77:ILE:HD11	30:L3B:79:ARG:NH2	2.29	0.47
2:S2A:209:ARG:HE	2:S2A:209:ARG:HB3	1.27	0.47
4:S4A:170:VAL:HG13	4:S4A:174:LEU:HB2	1.97	0.47
2:S2B:17:PHE:CE2	2:S2B:44:LEU:HB3	2.50	0.47
3:S3B:8:ILE:HG23	3:S3B:16:ARG:HG2	1.96	0.47
3:S3B:88:ARG:HA	3:S3B:91:LEU:HD12	1.97	0.47
5:S5B:79:GLU:HG3	5:S5B:93:PRO:HD2	1.97	0.47
6:S6B:79:LEU:O	6:S6B:85:VAL:HG11	2.14	0.47
9:S9B:9:ARG:O	9:S9B:104:ARG:HG2	2.15	0.47
9:S9B:53:VAL:HG13	9:S9B:95:LYS:HD3	1.95	0.47
30:L3B:117:MET:O	30:L3B:118:LYS:HG2	2.15	0.47
31:L4B:129:PHE:CD2	31:L4B:163:VAL:HG21	2.50	0.47
32:L5B:60:LEU:O	32:L5B:64:THR:HG22	2.15	0.47
2:S2A:108:ILE:O	2:S2A:112:VAL:HG23	2.15	0.47
5:S5A:92:LYS:O	5:S5A:118:ILE:HD12	2.14	0.47
28:5SA:34:C:C2	28:5SA:53:G:N2	2.83	0.47
33:L6A:30:LYS:O	33:L6A:136:ILE:HG21	2.15	0.47
2:S2B:17:PHE:HB3	2:S2B:42:ILE:HG23	1.97	0.47
7:S7B:15:ASP:HB3	7:S7B:20:ASP:H	1.79	0.47
7:S7B:76:ARG:N	7:S7B:87:VAL:O	2.48	0.47
29:L2B:218:ARG:HB3	29:L2B:219:PRO:HD2	1.96	0.47
2:S2A:165:VAL:HG23	2:S2A:166:ASP:H	1.80	0.46
8:S8A:37:ARG:O	8:S8A:41:ARG:HB2	2.14	0.46
29:L2A:16:MET:HG3	29:L2A:207:GLY:HA3	1.97	0.46
29:L2A:175:LEU:HD23	29:L2A:175:LEU:HA	1.79	0.46
2:S2B:205:ASP:OD1	2:S2B:206:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S3B:58:GLU:O	3:S3B:65:ALA:N	2.41	0.46
29:L2B:62:TYR:HA	29:L2B:87:ASN:OD1	2.15	0.46
31:L4B:110:LEU:HD11	31:L4B:181:LEU:HB3	1.97	0.46
32:L5B:59:GLU:HG3	32:L5B:144:ILE:HD11	1.97	0.46
33:L6B:87:LEU:N	33:L6B:131:VAL:O	2.44	0.46
2:S2A:132:LYS:HA	2:S2A:135:GLN:HB2	1.96	0.46
34:L9A:39:ALA:HB1	34:L9A:44:LEU:HD11	1.97	0.46
3:S3B:119:ARG:NH2	3:S3B:140:ARG:HG3	2.30	0.46
30:L3B:32:PRO:HA	30:L3B:90:THR:HA	1.97	0.46
30:L3B:169:ASN:HD22	30:L3B:203:LYS:HB2	1.81	0.46
31:L4B:185:ASP:OD1	31:L4B:188:ARG:NH1	2.43	0.46
5:S5A:34:VAL:O	5:S5A:41:VAL:HA	2.14	0.46
28:5SA:47:A:OP1	32:L5A:96:ARG:NH1	2.49	0.46
29:L2A:111:LEU:HA	29:L2A:115:GLN:NE2	2.30	0.46
4:S4B:81:GLU:CD	4:S4B:139:ARG:HH22	2.19	0.46
34:L9B:69:LYS:HG2	34:L9B:136:VAL:HB	1.97	0.46
34:L9B:79:ILE:N	34:L9B:80:PRO:HD3	2.29	0.46
2:S2A:24:TRP:CZ3	2:S2A:26:PRO:HA	2.51	0.46
9:S9A:5:TYR:OH	9:S9A:16:ARG:HD3	2.14	0.46
2:S2B:22:LYS:HA	2:S2B:24:TRP:HD1	1.81	0.46
3:S3B:123:GLN:HG2	3:S3B:128:PHE:CD2	2.50	0.46
32:L5B:11:TYR:HE1	32:L5B:172:LEU:HD11	1.80	0.46
33:L6B:46:GLU:OE1	33:L6B:51:ARG:NH1	2.47	0.46
4:S4A:175:SER:HB3	4:S4A:184:LYS:HB2	1.98	0.46
9:S9A:18:PHE:HB2	9:S9A:62:TYR:O	2.16	0.46
30:L3A:179:GLU:HB3	30:L3A:181:LEU:HD13	1.98	0.46
3:S3B:153:VAL:HG22	3:S3B:198:VAL:HG13	1.96	0.46
28:5SB:119:G:H2'	28:5SB:120:G:O4'	2.15	0.46
29:L2B:70:TRP:O	29:L2B:73:VAL:HG23	2.16	0.46
6:S6A:54:LYS:HE2	6:S6A:54:LYS:HB3	1.57	0.46
31:L4A:11:VAL:HB	31:L4A:18:ARG:HG3	1.97	0.46
31:L4A:24:LEU:HD23	31:L4A:115:ALA:HA	1.97	0.46
29:L2B:182:LEU:HB3	29:L2B:271:ILE:HG13	1.97	0.46
3:S3A:19:GLU:O	3:S3A:56:ASP:HA	2.16	0.46
3:S3A:130:VAL:O	3:S3A:134:ILE:HG12	2.16	0.46
8:S8A:121:ASP:HB2	8:S8A:125:ARG:NH2	2.30	0.46
28:5SA:98:U:H2'	28:5SA:99:G:C8	2.49	0.46
30:L3A:9:VAL:HG22	30:L3A:25:VAL:O	2.15	0.46
33:L6A:9:ILE:HD13	33:L6A:9:ILE:HG21	1.70	0.46
4:S4B:173:TRP:CD2	4:S4B:189:PRO:HB3	2.51	0.46
7:S7B:31:MET:HA	7:S7B:39:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S8B:49:GLU:HG2	8:S8B:62:TYR:HE2	1.81	0.46
30:L3B:2:LYS:NZ	30:L3B:95:ILE:O	2.39	0.46
30:L3B:181:LEU:HD12	30:L3B:181:LEU:HA	1.72	0.46
31:L4B:153:SER:OG	31:L4B:190:GLU:HG3	2.15	0.46
34:L9B:93:THR:O	34:L9B:97:ILE:HG13	2.16	0.46
3:S3A:77:ILE:HG12	3:S3A:84:ILE:HB	1.98	0.46
4:S4A:27:TYR:CE1	6:S6B:15:ASP:OD1	2.68	0.46
4:S4A:93:PHE:O	4:S4A:96:LEU:HB2	2.16	0.46
5:S5A:52:PRO:HA	5:S5A:55:VAL:HG12	1.97	0.46
9:S9A:10:ARG:NH2	9:S9A:11:LYS:HE3	2.31	0.46
30:L3A:1:MET:O	30:L3A:84:PHE:HB2	2.16	0.46
31:L4A:101:LEU:HD23	31:L4A:106:ARG:HG3	1.98	0.46
32:L5A:64:THR:HB	32:L5A:94:LEU:HD11	1.97	0.46
33:L6A:154:PRO:HD3	33:L6A:162:ILE:O	2.16	0.46
2:S2B:82:ARG:O	2:S2B:86:GLU:HG3	2.15	0.46
2:S2B:113:HIS:O	2:S2B:116:GLU:HG2	2.16	0.46
2:S2B:239:VAL:HG12	2:S2B:240:GLN:HG3	1.98	0.46
29:L2B:26:LYS:HB3	29:L2B:83:GLU:HG2	1.98	0.46
34:L9B:81:VAL:HA	34:L9B:143:SER:CB	2.45	0.46
2:S2A:44:LEU:O	2:S2A:47:THR:HB	2.16	0.46
2:S2A:70:PHE:HB2	2:S2A:92:TYR:HB3	1.97	0.46
4:S4A:194:LEU:HD12	4:S4A:194:LEU:HA	1.65	0.46
7:S7A:29:LYS:HG3	7:S7A:101:LEU:HD13	1.98	0.46
32:L5A:102:PHE:HA	32:L5A:105:LYS:HE2	1.98	0.46
32:L5A:107:LEU:HD22	32:L5A:178:PHE:HA	1.98	0.46
33:L6A:16:SER:O	33:L6A:26:VAL:O	2.33	0.46
34:L9A:7:GLU:HA	34:L9A:15:VAL:HG12	1.97	0.46
2:S2B:30:ARG:H	2:S2B:30:ARG:HG3	1.42	0.46
2:S2B:56:ARG:HB3	2:S2B:56:ARG:CZ	2.46	0.46
4:S4B:13:ARG:HD2	4:S4B:36:ARG:O	2.16	0.46
5:S5B:12:LEU:O	5:S5B:30:ALA:HA	2.16	0.46
28:5SB:111:C:H5'	28:5SB:112:G:H5'	1.98	0.46
2:S2A:51:LEU:HA	2:S2A:54:THR:HB	1.98	0.46
3:S3A:16:ARG:NH2	3:S3A:183:ASP:HA	2.31	0.46
4:S4A:163:GLU:O	4:S4A:166:LYS:HB2	2.16	0.46
28:5SA:15:A:O2'	28:5SA:17:A:O5'	2.34	0.46
32:L5A:60:LEU:O	32:L5A:64:THR:HG23	2.16	0.46
33:L6A:41:MET:HA	33:L6A:53:GLU:O	2.15	0.46
33:L6A:68:THR:O	33:L6A:72:ILE:HG12	2.16	0.46
2:S2B:7:VAL:HG13	2:S2B:8:LYS:N	2.31	0.46
2:S2B:34:ALA:HB1	2:S2B:36:ARG:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2B:34:ALA:O	2:S2B:41:ILE:HB	2.16	0.46
2:S2A:17:PHE:HD2	2:S2A:44:LEU:HD11	1.81	0.45
7:S7A:16:LEU:HD11	9:S9A:45:ALA:HB2	1.98	0.45
9:S9A:50:LEU:HA	9:S9A:53:VAL:HG12	1.98	0.45
30:L3A:200:GLU:HG2	30:L3A:201:THR:N	2.30	0.45
3:S3B:23:TYR:CG	3:S3B:24:ALA:N	2.84	0.45
4:S4B:108:LEU:HD21	4:S4B:183:GLY:HA3	1.97	0.45
31:L4B:157:VAL:HB	31:L4B:194:MET:HG2	1.99	0.45
33:L6B:88:LEU:HG	33:L6B:163:TYR:HB2	1.97	0.45
3:S3A:50:ALA:HB1	3:S3A:76:VAL:HG11	1.98	0.45
4:S4A:173:TRP:HB2	4:S4A:187:ARG:O	2.15	0.45
31:L4A:29:ASN:HB3	31:L4A:32:LEU:HB3	1.98	0.45
2:S2B:43:ASP:OD1	2:S2B:44:LEU:N	2.49	0.45
3:S3A:34:LEU:O	3:S3A:38:ARG:HG3	2.15	0.45
6:S6A:98:LEU:HB2	6:S6A:101:ALA:HB2	1.98	0.45
34:L9A:21:VAL:HG22	34:L9A:22:LYS:H	1.80	0.45
5:S5B:41:VAL:HG13	5:S5B:113:ALA:HA	1.97	0.45
5:S5B:81:GLU:HB3	5:S5B:90:VAL:HG12	1.99	0.45
5:S5B:147:ASP:HA	5:S5B:150:ARG:HD2	1.97	0.45
28:5SB:44:C:H4'	32:L5B:67:LYS:HG2	1.99	0.45
29:L2B:182:LEU:HD23	29:L2B:182:LEU:HA	1.77	0.45
34:L9B:142:VAL:HG23	34:L9B:143:SER:H	1.81	0.45
2:S2A:9:GLU:HA	2:S2A:12:GLU:OE2	2.16	0.45
2:S2A:195:ASP:O	8:S8A:68:ARG:NH2	2.49	0.45
4:S4A:6:GLY:O	4:S4A:8:VAL:HG23	2.16	0.45
8:S8A:97:VAL:HB	8:S8A:129:VAL:O	2.17	0.45
28:5SA:35:G:H5'	32:L5A:2:PRO:HD3	1.97	0.45
32:L5A:63:ILE:O	32:L5A:105:LYS:NZ	2.38	0.45
2:S2B:97:TRP:HZ3	2:S2B:99:GLY:HA2	1.81	0.45
3:S3B:36:ASP:OD1	3:S3B:57:ILE:HG21	2.16	0.45
6:S6B:3:ARG:HB3	6:S6B:3:ARG:CZ	2.46	0.45
7:S7B:52:GLU:H	7:S7B:52:GLU:HG2	1.61	0.45
31:L4B:37:VAL:O	31:L4B:41:LEU:HG	2.17	0.45
31:L4B:152:GLU:HA	31:L4B:190:GLU:OE2	2.17	0.45
34:L9B:4:ILE:HG12	34:L9B:18:VAL:HG22	1.98	0.45
6:S6A:16:GLN:H	6:S6A:16:GLN:CD	2.19	0.45
28:5SA:3:U:H2'	28:5SA:4:C:C6	2.51	0.45
29:L2A:78:LYS:HB2	29:L2A:78:LYS:HE3	1.65	0.45
31:L4A:178:PRO:HB3	31:L4A:198:ALA:HB1	1.98	0.45
33:L6A:59:ARG:HA	33:L6A:62:LYS:HE2	1.98	0.45
2:S2B:47:THR:HG23	2:S2B:202:PRO:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S9B:95:LYS:HA	9:S9B:98:PRO:HG2	1.99	0.45
31:L4B:32:LEU:O	31:L4B:36:VAL:HG23	2.16	0.45
29:L2A:148:GLU:HB2	29:L2A:151:LYS:HD2	1.98	0.45
32:L5A:56:ALA:HB2	32:L5A:153:ARG:CZ	2.47	0.45
4:S4B:88:VAL:O	4:S4B:90:GLY:N	2.41	0.45
7:S7B:44:TYR:O	7:S7B:48:LYS:HG2	2.17	0.45
29:L2B:10:THR:OG1	29:L2B:13:ARG:HB2	2.17	0.45
31:L4B:157:VAL:O	31:L4B:194:MET:HA	2.16	0.45
6:S6A:3:ARG:HD3	6:S6A:38:GLU:OE1	2.17	0.45
31:L4A:16:GLY:O	31:L4A:18:ARG:N	2.47	0.45
33:L6A:27:LYS:HE3	33:L6A:27:LYS:HB2	1.77	0.45
33:L6A:103:LEU:HB3	33:L6A:115:VAL:HB	1.98	0.45
3:S3B:166:GLU:HG3	3:S3B:167:TRP:H	1.81	0.45
6:S6B:12:PRO:HG3	6:S6B:57:GLN:O	2.17	0.45
29:L2B:130:ALA:HA	29:L2B:192:THR:HA	1.99	0.45
33:L6B:137:ASP:HB3	33:L6B:140:LYS:HB2	1.99	0.45
31:L4A:63:LYS:CE	31:L4A:67:GLN:HB2	2.47	0.45
32:L5A:28:VAL:O	32:L5A:31:VAL:HG12	2.16	0.45
32:L5A:118:ARG:HA	32:L5A:118:ARG:HE	1.81	0.45
3:S3B:22:TRP:HB3	3:S3B:59:ARG:HB2	1.99	0.45
8:S8B:1:MET:SD	8:S8B:1:MET:N	2.89	0.45
28:5SB:6:C:H2'	28:5SB:7:C:O4'	2.16	0.45
33:L6B:21:PRO:HD2	33:L6B:23:ARG:HH12	1.81	0.45
33:L6B:91:GLY:HA3	33:L6B:94:TYR:CG	2.52	0.45
34:L9B:133:HIS:ND1	34:L9B:134:PRO:HD3	2.31	0.45
2:S2A:189:ASP:OD1	2:S2A:191:ASP:HB2	2.17	0.45
32:L5A:18:GLU:CD	32:L5A:21:ARG:HH21	2.21	0.45
33:L6A:85:LYS:HE3	33:L6A:142:GLY:HA2	1.99	0.45
34:L9A:97:ILE:O	34:L9A:101:LEU:N	2.48	0.45
2:S2B:12:GLU:HG2	2:S2B:12:GLU:O	2.15	0.45
29:L2B:65:ILE:HD11	29:L2B:67:PHE:CZ	2.52	0.45
30:L3B:1:MET:H3	30:L3B:200:GLU:HG2	1.81	0.45
31:L4B:123:LEU:HD12	31:L4B:124:LEU:N	2.32	0.45
6:S6A:2:ARG:HD3	6:S6A:4:TYR:OH	2.17	0.45
9:S9A:45:ALA:O	9:S9A:78:LYS:HE3	2.16	0.45
33:L6A:15:VAL:HG11	33:L6A:79:VAL:HG23	1.98	0.45
8:S8B:87:SER:HB2	8:S8B:93:VAL:HB	1.98	0.45
28:5SB:47:A:H8	28:5SB:47:A:OP1	2.00	0.45
32:L5B:94:LEU:HD23	32:L5B:94:LEU:H	1.81	0.45
33:L6B:72:ILE:O	33:L6B:76:VAL:HG23	2.17	0.45
33:L6B:148:ILE:H	33:L6B:148:ILE:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2A:77:ALA:HA	2:S2A:80:ILE:HD12	1.99	0.44
8:S8A:103:VAL:HG21	8:S8A:110:ALA:HB2	1.99	0.44
33:L6A:41:MET:HB3	33:L6A:52:VAL:HG23	1.99	0.44
3:S3B:19:GLU:HA	3:S3B:54:ARG:HH12	1.82	0.44
4:S4B:13:ARG:NH1	4:S4B:38:TYR:O	2.50	0.44
6:S6B:67:MET:HB2	6:S6B:68:PRO:HD2	1.99	0.44
7:S7B:43:PHE:O	7:S7B:47:CYS:N	2.35	0.44
33:L6B:125:VAL:H	33:L6B:126:PRO:HD3	1.82	0.44
34:L9B:138:ILE:HG12	34:L9B:139:GLN:H	1.82	0.44
29:L2A:17:THR:HG22	29:L2A:204:ILE:HA	1.99	0.44
30:L3A:188:VAL:HG13	30:L3A:189:PRO:HD2	1.99	0.44
30:L3B:61:ARG:HB2	30:L3B:62:PRO:HD3	1.98	0.44
30:L3B:101:ARG:NH1	30:L3B:171:GLU:HB2	2.33	0.44
32:L5B:43:LEU:HD12	32:L5B:43:LEU:HA	1.79	0.44
33:L6B:5:GLY:O	33:L6B:8:PRO:HG3	2.18	0.44
2:S2A:178:ARG:NH2	8:S8A:74:PRO:HG3	2.22	0.44
9:S9A:5:TYR:HA	9:S9A:17:VAL:O	2.17	0.44
29:L2A:46:GLN:H	29:L2A:46:GLN:HG3	1.64	0.44
31:L4A:183:VAL:O	31:L4A:187:VAL:HG23	2.17	0.44
34:L9A:24:GLY:O	34:L9A:28:ASN:HB2	2.18	0.44
3:S3B:153:VAL:HG12	3:S3B:196:LEU:HD12	1.98	0.44
33:L6B:149:ARG:HD2	33:L6B:164:TYR:HE1	1.81	0.44
34:L9B:128:LEU:HD12	34:L9B:128:LEU:HA	1.80	0.44
8:S8A:104:ARG:O	8:S8A:107:LEU:HB2	2.16	0.44
30:L3A:108:SER:O	30:L3A:162:ALA:HA	2.17	0.44
4:S4B:119:GLN:HG3	4:S4B:123:HIS:CE1	2.52	0.44
9:S9B:53:VAL:HG11	9:S9B:92:TYR:CZ	2.52	0.44
32:L5B:135:LEU:HD22	32:L5B:140:ILE:HD11	1.98	0.44
33:L6B:156:ALA:O	33:L6B:171:LEU:HA	2.17	0.44
4:S4A:108:LEU:HB3	4:S4A:110:PHE:CE1	2.53	0.44
5:S5A:31:LEU:HG	5:S5A:45:PHE:HD1	1.82	0.44
6:S6A:20:ALA:HA	6:S6A:23:LYS:HD3	2.00	0.44
9:S9A:48:GLU:HB2	9:S9A:78:LYS:HE2	1.99	0.44
32:L5A:126:ASP:CG	32:L5A:127:GLY:H	2.21	0.44
31:L4B:8:GLN:HA	31:L4B:20:LEU:O	2.17	0.44
28:5SA:44:C:O5'	32:L5A:67:LYS:NZ	2.47	0.44
34:L9A:46:ALA:O	34:L9A:50:ARG:HD3	2.18	0.44
34:L9A:64:GLU:HA	34:L9A:67:ARG:HE	1.83	0.44
28:5SB:20:G:H1	28:5SB:67:C:H42	1.65	0.44
32:L5B:146:TYR:O	32:L5B:149:VAL:HG22	2.17	0.44
34:L9B:81:VAL:HA	34:L9B:143:SER:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2A:87:ARG:O	2:S2A:87:ARG:HG2	2.17	0.44
4:S4A:155:LEU:O	4:S4A:159:ARG:HG2	2.18	0.44
6:S6A:21:LEU:O	6:S6A:25:ILE:HG12	2.18	0.44
9:S9A:42:ARG:HH12	9:S9A:75:ASP:CG	2.20	0.44
32:L5A:64:THR:HG21	32:L5A:92:VAL:HG11	2.00	0.44
2:S2B:187:LEU:HD22	2:S2B:201:ILE:O	2.18	0.44
4:S4B:101:LEU:HB2	4:S4B:138:TYR:HB3	1.99	0.44
5:S5B:129:ILE:H	5:S5B:129:ILE:HD12	1.82	0.44
5:S5B:135:THR:O	5:S5B:139:LEU:HG	2.17	0.44
30:L3B:54:GLN:HB2	30:L3B:76:ARG:HG2	1.99	0.44
2:S2A:87:ARG:NH1	2:S2A:216:SER:O	2.42	0.44
5:S5A:123:LEU:HD23	5:S5A:123:LEU:HA	1.79	0.44
2:S2B:44:LEU:HD12	2:S2B:45:GLN:N	2.31	0.44
29:L2B:9:TYR:CD1	29:L2B:10:THR:HG23	2.53	0.44
30:L3B:151:TYR:CE1	30:L3B:154:LYS:HD3	2.53	0.44
31:L4B:116:ASP:O	31:L4B:120:GLU:HG2	2.18	0.44
31:L4B:161:GLU:OE2	31:L4B:164:ARG:NH2	2.50	0.44
32:L5B:106:LEU:HA	32:L5B:110:ALA:HB3	2.00	0.44
7:S7A:121:ALA:O	7:S7A:125:MET:HG3	2.18	0.44
8:S8A:51:VAL:HG11	8:S8A:60:ARG:HG3	1.99	0.44
30:L3A:119:ARG:CD	30:L3A:160:TYR:HB2	2.44	0.44
31:L4A:198:ALA:HA	31:L4A:201:VAL:HB	2.00	0.44
6:S6B:15:ASP:O	6:S6B:19:LEU:N	2.29	0.44
33:L6B:125:VAL:O	33:L6B:125:VAL:HG13	2.18	0.44
2:S2A:46:LYS:HA	2:S2A:49:GLU:HB2	2.00	0.43
3:S3A:12:LEU:C	3:S3A:14:ILE:H	2.21	0.43
5:S5A:99:GLY:O	5:S5A:117:ASP:HA	2.18	0.43
6:S6A:67:MET:HB2	6:S6A:68:PRO:HD2	2.00	0.43
29:L2A:70:TRP:CZ2	29:L2A:150:LYS:HD3	2.53	0.43
30:L3A:77:ILE:HD12	30:L3A:77:ILE:HA	1.86	0.43
30:L3A:195:LEU:HD12	30:L3A:196:VAL:H	1.83	0.43
34:L9A:57:ARG:O	34:L9A:61:ARG:HG2	2.18	0.43
9:S9B:19:LEU:HD23	9:S9B:19:LEU:N	2.32	0.43
30:L3B:14:ILE:HD11	30:L3B:173:VAL:HG11	1.99	0.43
32:L5B:173:LEU:HD23	32:L5B:173:LEU:HA	1.80	0.43
34:L9B:2:LYS:HA	34:L9B:20:ASP:HA	1.99	0.43
28:5SA:1:A:H2'	28:5SA:1:A:N3	2.33	0.43
29:L2A:105:ILE:HD12	29:L2A:105:ILE:HA	1.84	0.43
30:L3A:120:TRP:CD1	30:L3A:155:LYS:HB3	2.52	0.43
32:L5B:129:GLY:HA3	32:L5B:163:ALA:HB3	2.00	0.43
3:S3A:79:ARG:O	3:S3A:79:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S7A:108:ALA:O	7:S7A:111:ARG:HG3	2.18	0.43
8:S8A:100:ILE:HG22	8:S8A:125:ARG:NH1	2.32	0.43
31:L4A:170:LEU:HD13	31:L4A:170:LEU:HA	1.87	0.43
32:L5A:60:LEU:HD23	32:L5A:60:LEU:HA	1.81	0.43
2:S2B:82:ARG:HB2	2:S2B:94:ASN:HD22	1.83	0.43
2:S2B:91:PRO:HD3	2:S2B:155:LEU:HD23	1.99	0.43
2:S2B:178:ARG:NH2	8:S8B:68:ARG:NH2	2.65	0.43
4:S4B:94:LEU:O	4:S4B:98:GLU:N	2.39	0.43
4:S4B:129:ASN:OD1	4:S4B:145:GLU:N	2.45	0.43
3:S3A:16:ARG:HH22	3:S3A:183:ASP:HA	1.84	0.43
6:S6A:1:MET:HG2	6:S6A:68:PRO:HA	2.00	0.43
2:S2B:112:VAL:O	2:S2B:115:LEU:HB3	2.18	0.43
2:S2B:215:LEU:HA	2:S2B:215:LEU:HD13	1.89	0.43
4:S4B:145:GLU:OE2	4:S4B:182:LYS:HD2	2.19	0.43
28:5SB:13:C:H3'	28:5SB:14:C:C5	2.53	0.43
28:5SB:82:U:H2'	28:5SB:83:G:N2	2.30	0.43
30:L3B:120:TRP:CD1	30:L3B:155:LYS:HB3	2.53	0.43
31:L4B:178:PRO:HB3	31:L4B:198:ALA:HB2	2.00	0.43
32:L5B:16:ARG:NH2	32:L5B:31:VAL:HB	2.33	0.43
33:L6B:58:GLU:O	33:L6B:62:LYS:HG3	2.19	0.43
3:S3A:91:LEU:HD11	3:S3A:101:LEU:HD12	2.00	0.43
3:S3A:181:ASN:OD1	3:S3A:204:LEU:HD12	2.18	0.43
32:L5A:33:ARG:O	32:L5A:162:THR:HG23	2.18	0.43
2:S2B:67:THR:HA	2:S2B:90:MET:SD	2.59	0.43
4:S4B:13:ARG:HB3	4:S4B:38:TYR:O	2.18	0.43
5:S5B:60:TYR:HB3	5:S5B:64:ARG:NH2	2.33	0.43
29:L2B:17:THR:HG23	29:L2B:204:ILE:HA	2.00	0.43
30:L3B:51:PHE:O	30:L3B:75:VAL:HB	2.18	0.43
31:L4B:57:VAL:HG22	31:L4B:58:ALA:H	1.83	0.43
31:L4B:117:ARG:HD3	31:L4B:117:ARG:HA	1.78	0.43
32:L5B:124:SER:HB2	32:L5B:131:TYR:CE1	2.54	0.43
4:S4A:196:LEU:O	4:S4A:198:VAL:N	2.47	0.43
5:S5A:42:GLY:HA2	5:S5A:65:ASN:O	2.18	0.43
28:5SA:30:C:H2'	28:5SA:31:A:C8	2.54	0.43
32:L5A:120:LEU:O	32:L5A:181:ARG:HB2	2.18	0.43
33:L6A:121:ILE:HG12	33:L6A:140:LYS:HD3	1.99	0.43
34:L9A:49:ALA:O	34:L9A:53:ALA:N	2.44	0.43
34:L9A:78:THR:HA	34:L9A:141:LYS:HB2	2.00	0.43
34:L9A:79:ILE:HG23	34:L9A:81:VAL:HG13	2.01	0.43
3:S3B:50:ALA:CB	3:S3B:76:VAL:HG11	2.34	0.43
8:S8B:104:ARG:HB3	8:S8B:108:GLY:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:L2B:71:ASP:CG	29:L2B:103:ARG:HH22	2.22	0.43
30:L3B:21:VAL:CG2	30:L3B:185:LYS:HD3	2.48	0.43
32:L5B:75:LYS:HA	32:L5B:84:LYS:HG2	1.99	0.43
8:S8A:83:ILE:HA	8:S8A:136:GLU:O	2.18	0.43
28:5SA:47:A:C4	28:5SA:48:A:C8	3.07	0.43
33:L6A:54:ARG:NE	33:L6A:57:ASP:OD1	2.45	0.43
33:L6A:117:PRO:HB3	33:L6A:123:PHE:CE2	2.53	0.43
2:S2B:88:ALA:O	2:S2B:226:ARG:NH1	2.51	0.43
8:S8B:121:ASP:OD1	8:S8B:121:ASP:N	2.52	0.43
31:L4B:64:ILE:HD12	31:L4B:64:ILE:HA	1.88	0.43
4:S4A:13:ARG:HA	4:S4A:33:MET:CE	2.47	0.43
8:S8A:122:ARG:HG2	8:S8A:126:LYS:NZ	2.33	0.43
28:5SA:3:U:H2'	28:5SA:4:C:H6	1.84	0.43
31:L4A:179:GLU:CD	31:L4A:179:GLU:H	2.22	0.43
32:L5A:97:ASP:HA	32:L5A:100:TRP:HB2	2.01	0.43
32:L5A:99:MET:HE3	32:L5A:99:MET:HB2	1.90	0.43
33:L6A:91:GLY:C	33:L6A:93:GLY:H	2.22	0.43
34:L9A:5:LEU:HD12	34:L9A:17:GLN:HB3	2.00	0.43
34:L9A:47:LEU:O	34:L9A:51:ILE:HG13	2.19	0.43
2:S2B:185:ILE:HG22	2:S2B:199:TYR:HB2	2.00	0.43
2:S2B:208:ILE:HA	2:S2B:211:ILE:HD12	2.01	0.43
5:S5B:71:LEU:HD23	5:S5B:71:LEU:HA	1.77	0.43
8:S8B:112:LEU:HA	8:S8B:134:ILE:H	1.84	0.43
30:L3B:37:ARG:HA	30:L3B:42:ASP:OD2	2.18	0.43
31:L4B:129:PHE:C	31:L4B:131:GLY:H	2.20	0.43
34:L9B:75:LEU:C	34:L9B:77:LEU:H	2.22	0.43
31:L4A:125:LEU:HA	31:L4A:194:MET:O	2.19	0.43
33:L6A:125:VAL:HG22	33:L6A:131:VAL:HG23	1.99	0.43
3:S3B:123:GLN:HG2	3:S3B:128:PHE:HD2	1.83	0.43
4:S4B:101:LEU:HB3	4:S4B:138:TYR:HB3	2.00	0.43
9:S9B:31:GLN:HG2	9:S9B:36:TYR:HB2	2.01	0.43
28:5SB:30:C:H2'	28:5SB:31:A:C8	2.54	0.43
33:L6B:10:PRO:HB2	33:L6B:50:VAL:HG13	2.00	0.43
2:S2A:69:LEU:HA	2:S2A:91:PRO:HG2	2.01	0.43
29:L2A:232:PRO:HB3	29:L2A:244:ARG:NH1	2.34	0.43
33:L6A:98:LEU:HD12	33:L6A:98:LEU:HA	1.90	0.43
2:S2B:111:ARG:HD3	2:S2B:111:ARG:HA	1.76	0.43
4:S4B:63:LYS:HE3	4:S4B:63:LYS:HB2	1.80	0.43
4:S4B:74:GLN:H	4:S4B:74:GLN:HG2	1.59	0.43
8:S8B:12:ARG:NH1	8:S8B:27:PRO:HD3	2.34	0.43
9:S9B:96:LEU:HB3	9:S9B:102:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:L3B:9:VAL:CG1	30:L3B:27:LEU:HD23	2.42	0.43
2:S2A:101:MET:HA	2:S2A:108:ILE:HG13	2.01	0.42
2:S2A:165:VAL:O	2:S2A:187:LEU:O	2.37	0.42
9:S9A:9:ARG:HG2	9:S9A:104:ARG:CZ	2.49	0.42
9:S9A:50:LEU:HB3	9:S9A:55:ALA:O	2.19	0.42
28:5SA:33:C:C2	28:5SA:34:C:C5	3.07	0.42
28:5SA:94:C:H2'	28:5SA:95:G:H8	1.84	0.42
33:L6A:77:LYS:HE2	33:L6A:138:LYS:HD2	2.00	0.42
3:S3B:56:ASP:O	3:S3B:66:VAL:HA	2.18	0.42
4:S4B:4:TYR:O	4:S4B:115:ARG:NH1	2.51	0.42
9:S9B:3:GLN:CB	9:S9B:20:ARG:HD2	2.49	0.42
32:L5B:95:ARG:HE	32:L5B:95:ARG:HB3	1.69	0.42
34:L9B:29:TYR:C	34:L9B:32:PRO:HD2	2.39	0.42
2:S2A:55:PHE:CD1	2:S2A:221:LEU:HG	2.54	0.42
4:S4A:117:ALA:O	4:S4A:121:VAL:HG23	2.20	0.42
4:S4A:163:GLU:HG3	4:S4A:166:LYS:HE3	2.00	0.42
8:S8A:11:THR:HG23	8:S8A:14:ARG:NH1	2.34	0.42
33:L6A:30:LYS:HE3	33:L6A:80:SER:HA	2.01	0.42
33:L6A:41:MET:H	33:L6A:55:PRO:HG3	1.84	0.42
33:L6A:126:PRO:O	33:L6A:127:GLU:C	2.57	0.42
34:L9A:38:LEU:HD12	34:L9A:40:THR:OG1	2.18	0.42
2:S2B:178:ARG:HH21	8:S8B:74:PRO:HG3	1.83	0.42
3:S3B:127:ARG:HH21	3:S3B:191:THR:HB	1.84	0.42
4:S4B:162:LEU:HD13	4:S4B:181:MET:HE2	2.01	0.42
6:S6B:7:ASN:OD1	6:S6B:62:TRP:HD1	2.02	0.42
28:5SB:57:U:O3'	32:L5B:27:ASN:ND2	2.51	0.42
34:L9B:89:TYR:N	34:L9B:89:TYR:HD1	2.15	0.42
32:L5A:99:MET:HG3	32:L5A:100:TRP:N	2.34	0.42
33:L6A:9:ILE:HG22	33:L6A:69:ARG:CZ	2.48	0.42
34:L9A:66:GLU:HA	34:L9A:69:LYS:HB3	2.02	0.42
3:S3B:130:VAL:O	3:S3B:134:ILE:HG12	2.19	0.42
3:S3B:175:LEU:HD11	3:S3B:201:TYR:CE2	2.53	0.42
4:S4B:160:GLN:O	4:S4B:163:GLU:HB3	2.19	0.42
7:S7B:6:ARG:O	7:S7B:7:ALA:C	2.48	0.42
29:L2B:61:LEU:HD12	29:L2B:61:LEU:HA	1.90	0.42
30:L3B:64:LYS:HB2	30:L3B:64:LYS:HE2	1.95	0.42
31:L4B:20:LEU:HD12	31:L4B:20:LEU:HA	1.90	0.42
33:L6B:89:ILE:HG12	33:L6B:162:ILE:HG23	2.01	0.42
3:S3A:72:LYS:O	3:S3A:76:VAL:HG13	2.19	0.42
4:S4A:209:ARG:HE	4:S4A:209:ARG:HB3	1.67	0.42
6:S6A:86:ARG:O	6:S6A:87:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S6A:89:MET:HB2	6:S6A:89:MET:HE3	1.94	0.42
29:L2A:133:LEU:HG	29:L2A:189:CYS:O	2.20	0.42
34:L9A:138:ILE:HG12	34:L9A:139:GLN:H	1.85	0.42
2:S2B:73:THR:HB	2:S2B:96:ARG:N	2.34	0.42
4:S4B:121:VAL:HG12	4:S4B:134:ASP:HA	2.01	0.42
6:S6B:61:LEU:HB3	6:S6B:63:TYR:HE1	1.83	0.42
29:L2B:43:ARG:HA	29:L2B:48:ARG:O	2.19	0.42
31:L4B:16:GLY:O	31:L4B:18:ARG:N	2.45	0.42
31:L4B:196:LEU:HD23	31:L4B:196:LEU:HA	1.71	0.42
33:L6B:18:GLU:O	33:L6B:24:VAL:HG23	2.19	0.42
33:L6B:46:GLU:HG2	33:L6B:47:GLU:H	1.82	0.42
2:S2A:8:LYS:HD3	2:S2A:10:LEU:HB2	2.02	0.42
4:S4A:27:TYR:HE1	6:S6B:15:ASP:OD1	2.01	0.42
34:L9A:97:ILE:HA	34:L9A:100:ALA:HB3	2.01	0.42
2:S2B:137:ARG:HH12	2:S2B:141:GLU:H	1.68	0.42
32:L5B:34:LEU:HD23	32:L5B:34:LEU:HA	1.89	0.42
2:S2A:149:LEU:HD22	2:S2A:152:PHE:HB3	2.02	0.42
3:S3A:11:ARG:HH22	3:S3A:175:LEU:HA	1.85	0.42
3:S3A:77:ILE:HG23	3:S3A:84:ILE:HG22	2.01	0.42
3:S3A:186:PHE:HD1	3:S3A:198:VAL:O	2.03	0.42
32:L5A:62:LEU:HD12	32:L5A:62:LEU:HA	1.88	0.42
33:L6A:46:GLU:CD	33:L6A:51:ARG:HH12	2.23	0.42
33:L6A:86:GLU:N	33:L6A:86:GLU:CD	2.73	0.42
2:S2B:137:ARG:HH12	2:S2B:141:GLU:N	2.16	0.42
2:S2B:145:LEU:O	2:S2B:149:LEU:HB2	2.20	0.42
28:5SB:47:A:C5	28:5SB:48:A:N7	2.88	0.42
31:L4B:196:LEU:O	31:L4B:199:TRP:HB3	2.20	0.42
3:S3A:14:ILE:HG12	3:S3A:15:THR:OG1	2.20	0.42
4:S4A:152:SER:HA	4:S4A:155:LEU:HG	2.01	0.42
9:S9B:128:ARG:HD3	9:S9B:128:ARG:HA	1.72	0.42
30:L3B:11:MET:O	30:L3B:12:THR:HG23	2.20	0.42
34:L9B:2:LYS:HE2	34:L9B:2:LYS:HB3	1.91	0.42
2:S2A:162:ILE:O	2:S2A:185:ILE:HD12	2.20	0.42
3:S3A:116:VAL:HG21	3:S3A:202:ILE:HD11	2.01	0.42
4:S4A:187:ARG:HH21	4:S4A:190:ASP:H	1.64	0.42
5:S5A:53:LEU:O	5:S5A:57:LYS:HG2	2.20	0.42
8:S8A:1:MET:HE3	8:S8A:1:MET:H3	1.84	0.42
8:S8A:103:VAL:CG2	8:S8A:110:ALA:HB2	2.50	0.42
9:S9A:22:GLY:O	9:S9A:23:ASN:ND2	2.53	0.42
34:L9A:92:VAL:CG1	34:L9A:120:ILE:HG23	2.49	0.42
2:S2B:187:LEU:HD11	2:S2B:204:ASN:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S4B:201:GLN:HE21	5:S5B:99:GLY:HA2	1.84	0.42
9:S9B:4:TYR:HB2	9:S9B:19:LEU:HD23	2.02	0.42
29:L2B:78:LYS:HB2	29:L2B:78:LYS:HE3	1.87	0.42
31:L4B:46:ARG:HA	31:L4B:46:ARG:HD2	1.90	0.42
32:L5B:41:GLN:O	32:L5B:89:GLY:HA2	2.20	0.42
34:L9B:11:ASN:ND2	34:L9B:11:ASN:O	2.52	0.42
2:S2A:91:PRO:HG3	2:S2A:155:LEU:HG	2.01	0.42
4:S4A:108:LEU:HD11	4:S4A:174:LEU:HD22	2.02	0.42
29:L2A:181:GLU:HA	29:L2A:272:ALA:HB3	2.01	0.42
32:L5A:16:ARG:NH1	32:L5A:31:VAL:HG11	2.35	0.42
32:L5A:43:LEU:HD11	32:L5A:153:ARG:HD2	2.02	0.42
32:L5A:96:ARG:O	32:L5A:98:ARG:N	2.50	0.42
31:L4B:182:ASN:O	31:L4B:186:ILE:HG13	2.20	0.42
29:L2A:70:TRP:CE2	29:L2A:150:LYS:HD3	2.55	0.42
2:S2B:15:VAL:HG23	2:S2B:16:HIS:CE1	2.54	0.42
3:S3B:92:ALA:HB2	3:S3B:99:VAL:HG22	2.01	0.42
4:S4B:6:GLY:O	4:S4B:8:VAL:HG23	2.20	0.42
7:S7B:93:PRO:HA	7:S7B:96:GLN:HB2	2.01	0.42
28:5SB:24:U:H3	28:5SB:63:G:H1	1.67	0.42
29:L2B:255:LYS:HA	29:L2B:255:LYS:HD2	1.77	0.42
33:L6B:12:PRO:HG3	33:L6B:48:GLY:O	2.18	0.42
4:S4A:25:ARG:NH2	4:S4A:30:LYS:HB2	2.34	0.41
8:S8A:20:TYR:HD1	8:S8A:65:TYR:CD2	2.38	0.41
32:L5A:67:LYS:HG3	32:L5A:67:LYS:H	1.76	0.41
6:S6B:67:MET:SD	6:S6B:72:VAL:HG12	2.60	0.41
31:L4B:23:ASP:OD1	31:L4B:23:ASP:N	2.41	0.41
31:L4B:63:LYS:NZ	31:L4B:67:GLN:HB2	2.34	0.41
2:S2A:87:ARG:HD3	2:S2A:223:ILE:HD11	2.01	0.41
4:S4A:150:GLU:C	4:S4A:152:SER:N	2.73	0.41
8:S8A:6:ILE:O	8:S8A:10:LEU:HG	2.19	0.41
2:S2B:114:ARG:O	2:S2B:118:LEU:HG	2.20	0.41
28:5SB:60:A:H3'	28:5SB:61:A:H8	1.84	0.41
31:L4B:63:LYS:HZ1	31:L4B:67:GLN:HB2	1.85	0.41
32:L5B:75:LYS:HE2	32:L5B:75:LYS:HB3	1.86	0.41
2:S2A:97:TRP:HH2	2:S2A:176:GLU:CD	2.23	0.41
2:S2A:111:ARG:NH2	2:S2A:114:ARG:HG2	2.35	0.41
2:S2A:176:GLU:O	2:S2A:180:LEU:HD12	2.21	0.41
8:S8A:82:HIS:O	8:S8A:137:VAL:HA	2.21	0.41
31:L4A:7:TYR:O	31:L4A:21:ALA:HA	2.19	0.41
32:L5A:28:VAL:HG23	32:L5A:29:TRP:CD1	2.55	0.41
33:L6A:41:MET:HE2	33:L6A:41:MET:HB2	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S4B:52:SER:O	4:S4B:56:VAL:HG23	2.20	0.41
30:L3B:89:ASP:OD1	30:L3B:89:ASP:N	2.49	0.41
9:S9A:20:ARG:HH21	9:S9A:62:TYR:CB	2.33	0.41
33:L6A:83:TYR:HD2	33:L6A:132:ARG:HH12	1.69	0.41
3:S3B:62:ASP:O	3:S3B:97:LYS:HB2	2.20	0.41
3:S3B:120:VAL:HA	3:S3B:123:GLN:HB2	2.02	0.41
9:S9B:28:VAL:HG11	9:S9B:65:VAL:HG12	2.02	0.41
31:L4B:158:THR:HA	31:L4B:195:ASP:OD1	2.21	0.41
33:L6B:118:PRO:HB2	33:L6B:119:GLU:H	1.70	0.41
2:S2A:28:PHE:HE2	2:S2A:42:ILE:HD12	1.85	0.41
28:5SA:82:U:C2	28:5SA:83:G:N2	2.89	0.41
29:L2A:77:ALA:HB2	29:L2A:97:TYR:CD1	2.55	0.41
32:L5A:82:LEU:HD23	32:L5A:82:LEU:HA	1.90	0.41
34:L9A:120:ILE:HG13	34:L9A:121:LYS:O	2.21	0.41
4:S4B:103:ASN:OD1	4:S4B:114:ARG:NH2	2.53	0.41
9:S9B:49:PRO:HB2	9:S9B:85:LEU:HD21	2.02	0.41
32:L5B:103:LEU:O	32:L5B:107:LEU:HG	2.20	0.41
32:L5B:135:LEU:CD1	32:L5B:155:MET:HG2	2.51	0.41
33:L6B:30:LYS:HB3	33:L6B:79:VAL:CA	2.50	0.41
34:L9B:76:THR:HG22	34:L9B:139:GLN:OE1	2.20	0.41
2:S2A:189:ASP:C	2:S2A:191:ASP:H	2.24	0.41
8:S8A:109:ILE:CG2	8:S8A:137:VAL:HB	2.50	0.41
9:S9A:22:GLY:O	9:S9A:24:GLY:N	2.49	0.41
30:L3A:114:ALA:HB3	30:L3A:119:ARG:HG2	2.02	0.41
31:L4A:29:ASN:H	31:L4A:112:MET:HE3	1.85	0.41
2:S2B:215:LEU:HD13	2:S2B:218:ALA:HB3	2.03	0.41
3:S3B:101:LEU:HD23	3:S3B:101:LEU:HA	1.95	0.41
5:S5B:79:GLU:OE2	8:S8B:105:ARG:HG2	2.21	0.41
30:L3B:11:MET:SD	30:L3B:24:THR:HG22	2.61	0.41
32:L5B:13:GLU:O	32:L5B:17:PRO:HG3	2.21	0.41
5:S5A:152:ARG:HD3	8:S8A:44:PHE:CZ	2.55	0.41
7:S7A:72:ARG:HA	7:S7A:72:ARG:HD3	1.88	0.41
9:S9A:56:LEU:HB3	9:S9A:57:GLY:H	1.31	0.41
29:L2A:268:ARG:HE	29:L2A:268:ARG:HB3	1.68	0.41
31:L4A:63:LYS:NZ	31:L4A:67:GLN:HB2	2.36	0.41
32:L5A:81:LYS:HD3	32:L5A:81:LYS:N	2.35	0.41
32:L5A:101:ILE:O	32:L5A:105:LYS:HG3	2.20	0.41
32:L5A:111:LEU:HB2	32:L5A:112:PRO:HD3	2.02	0.41
4:S4B:4:TYR:CE2	4:S4B:11:LEU:HD11	2.54	0.41
5:S5B:100:VAL:HG12	5:S5B:118:ILE:HG22	2.03	0.41
9:S9B:19:LEU:HD12	9:S9B:59:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S9B:96:LEU:O	9:S9B:100:GLY:N	2.53	0.41
32:L5B:102:PHE:HE1	32:L5B:141:PHE:CE1	2.38	0.41
2:S2A:96:ARG:HD2	2:S2A:96:ARG:N	2.36	0.41
4:S4A:49:ARG:H	4:S4A:49:ARG:HD3	1.85	0.41
32:L5A:118:ARG:HA	32:L5A:118:ARG:NE	2.35	0.41
34:L9A:23:PRO:O	34:L9A:27:ARG:HG2	2.21	0.41
34:L9A:94:ALA:CB	34:L9A:111:PRO:HG2	2.48	0.41
6:S6B:81:ILE:H	6:S6B:81:ILE:HG13	1.67	0.41
9:S9B:46:ALA:HA	9:S9B:78:LYS:HB3	2.03	0.41
33:L6B:90:LYS:O	33:L6B:160:LYS:HA	2.20	0.41
33:L6B:153:LYS:HB2	33:L6B:154:PRO:HD2	2.03	0.41
34:L9B:6:LEU:H	34:L9B:36:ALA:HA	1.86	0.41
4:S4A:95:GLY:HA3	4:S4A:188:LEU:HD11	2.03	0.41
9:S9A:95:LYS:HA	9:S9A:98:PRO:HG2	2.02	0.41
28:5SA:96:C:H2'	28:5SA:97:C:H6	1.85	0.41
29:L2A:79:VAL:HG12	29:L2A:113:VAL:HA	2.03	0.41
32:L5A:3:LEU:HA	32:L5A:3:LEU:HD23	1.74	0.41
2:S2B:53:ARG:HA	2:S2B:56:ARG:HE	1.86	0.41
3:S3B:180:ALA:HB1	3:S3B:182:ILE:HG13	2.02	0.41
4:S4B:120:LEU:HD23	4:S4B:120:LEU:HA	1.88	0.41
9:S9B:26:VAL:HG13	9:S9B:61:ALA:HB3	2.03	0.41
9:S9B:121:ARG:HD3	9:S9B:122:ALA:O	2.21	0.41
29:L2B:37:LEU:HD13	29:L2B:62:TYR:HB2	2.01	0.41
29:L2B:68:LYS:HB2	29:L2B:70:TRP:CH2	2.56	0.41
29:L2B:121:PRO:HB3	29:L2B:135:PHE:CE2	2.56	0.41
29:L2B:242:ARG:HD2	29:L2B:242:ARG:N	2.36	0.41
30:L3B:195:LEU:HG	30:L3B:196:VAL:N	2.36	0.41
33:L6B:164:TYR:HB2	33:L6B:167:GLU:HG3	2.03	0.41
34:L9B:130:TYR:HB3	34:L9B:136:VAL:HG13	2.02	0.41
2:S2A:114:ARG:NH2	2:S2A:141:GLU:OE1	2.54	0.41
3:S3A:47:LEU:HB2	3:S3A:52:LEU:HD13	2.01	0.41
4:S4A:105:VAL:HG13	4:S4A:110:PHE:HB2	2.02	0.41
6:S6A:62:TRP:O	6:S6A:63:TYR:HD1	2.04	0.41
8:S8A:11:THR:HG23	8:S8A:14:ARG:HH12	1.85	0.41
31:L4A:64:ILE:CD1	31:L4A:78:ILE:HD11	2.51	0.41
34:L9A:121:LYS:HB3	34:L9A:122:GLU:HG3	2.03	0.41
2:S2B:118:LEU:HB2	2:S2B:142:LEU:HD12	2.03	0.41
2:S2B:154:LEU:O	2:S2B:155:LEU:HD22	2.21	0.41
7:S7B:76:ARG:HD3	7:S7B:89:MET:HG3	2.02	0.41
8:S8B:4:ASP:HB3	8:S8B:7:ALA:HB3	2.03	0.41
8:S8B:10:LEU:HD22	8:S8B:83:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5SB:116:C:H2'	28:5SB:117:G:C8	2.56	0.41
29:L2B:108:PRO:HG3	29:L2B:143:HIS:CE1	2.55	0.41
31:L4B:66:PRO:HD2	31:L4B:70:THR:HG21	2.02	0.41
32:L5B:173:LEU:HD13	32:L5B:178:PHE:CD2	2.56	0.41
34:L9B:77:LEU:HD12	34:L9B:104:GLN:HE22	1.86	0.41
2:S2A:97:TRP:HZ2	2:S2A:102:LEU:HD13	1.87	0.40
3:S3A:79:ARG:NH2	3:S3A:82:GLU:HG3	2.35	0.40
7:S7A:26:PHE:CE2	7:S7A:30:ILE:HD11	2.57	0.40
8:S8A:49:GLU:HG2	8:S8A:62:TYR:CE2	2.51	0.40
32:L5A:97:ASP:O	32:L5A:101:ILE:N	2.31	0.40
33:L6A:7:LEU:HD23	33:L6A:8:PRO:HD2	2.03	0.40
33:L6A:55:PRO:HD2	33:L6A:61:HIS:ND1	2.36	0.40
33:L6A:149:ARG:O	33:L6A:149:ARG:HG2	2.22	0.40
34:L9A:78:THR:HG22	34:L9A:141:LYS:HB2	2.01	0.40
3:S3B:59:ARG:HG2	3:S3B:64:VAL:HG23	2.03	0.40
8:S8B:111:ILE:HB	8:S8B:135:CYS:SG	2.60	0.40
29:L2B:5:LYS:HD2	29:L2B:5:LYS:N	2.30	0.40
31:L4B:128:ALA:O	31:L4B:130:ALA:N	2.51	0.40
33:L6B:151:ILE:H	33:L6B:151:ILE:HG13	1.64	0.40
4:S4A:192:GLU:HG2	4:S4A:193:ASP:H	1.87	0.40
30:L3A:14:ILE:HG13	30:L3A:21:VAL:HG13	2.01	0.40
32:L5A:170:ARG:HE	32:L5A:174:GLU:CG	2.34	0.40
33:L6A:3:ARG:HD3	33:L6A:5:GLY:H	1.85	0.40
2:S2B:166:ASP:C	2:S2B:168:THR:H	2.25	0.40
8:S8B:25:ASP:N	8:S8B:25:ASP:OD1	2.54	0.40
30:L3B:171:GLU:O	30:L3B:184:VAL:HA	2.21	0.40
31:L4B:197:ASP:O	31:L4B:198:ALA:HB3	2.21	0.40
32:L5B:47:LYS:HD2	32:L5B:81:LYS:CB	2.49	0.40
32:L5B:80:PHE:O	32:L5B:81:LYS:C	2.59	0.40
34:L9B:56:LYS:O	34:L9B:60:GLU:N	2.36	0.40
2:S2A:100:GLY:O	2:S2A:104:ASN:N	2.42	0.40
2:S2A:112:VAL:HG22	2:S2A:149:LEU:HD13	2.04	0.40
3:S3A:59:ARG:HG2	3:S3A:64:VAL:HG22	2.03	0.40
30:L3A:111:ARG:HG2	30:L3A:160:TYR:O	2.21	0.40
3:S3B:50:ALA:HB1	3:S3B:70:VAL:CG1	2.51	0.40
4:S4B:162:LEU:HD13	4:S4B:181:MET:CE	2.50	0.40
5:S5B:127:ASN:HA	5:S5B:128:PRO:HD3	1.94	0.40
9:S9B:69:GLY:O	9:S9B:73:GLN:HG3	2.21	0.40
33:L6B:149:ARG:HD2	33:L6B:164:TYR:CE1	2.56	0.40
33:L6B:172:LYS:N	33:L6B:173:PRO:HA	2.37	0.40
34:L9B:144:VAL:HG13	34:L9B:145:VAL:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2A:156:LYS:H	2:S2A:156:LYS:HD2	1.86	0.40
7:S7A:24:THR:HA	7:S7A:27:ILE:HD12	2.03	0.40
32:L5A:126:ASP:N	32:L5A:126:ASP:OD1	2.55	0.40
32:L5A:173:LEU:O	32:L5A:178:PHE:HB2	2.21	0.40
34:L9A:61:ARG:NH2	34:L9A:64:GLU:OE2	2.55	0.40
2:S2B:44:LEU:O	2:S2B:47:THR:HB	2.22	0.40
6:S6B:15:ASP:HB2	6:S6B:18:GLN:HB2	2.04	0.40
8:S8B:44:PHE:CD1	8:S8B:80:ILE:HG12	2.57	0.40
9:S9B:42:ARG:NH1	9:S9B:75:ASP:OD1	2.43	0.40
29:L2B:67:PHE:HD1	29:L2B:67:PHE:HA	1.81	0.40
30:L3B:16:ARG:O	30:L3B:19:ARG:HB3	2.22	0.40
33:L6B:83:TYR:HD2	33:L6B:132:ARG:HH22	1.69	0.40
2:S2A:70:PHE:H	2:S2A:92:TYR:HA	1.87	0.40
2:S2A:77:ALA:O	2:S2A:81:VAL:HG23	2.22	0.40
3:S3A:83:ARG:O	3:S3A:83:ARG:HG3	2.20	0.40
3:S3A:137:ALA:O	3:S3A:141:VAL:HG23	2.21	0.40
8:S8A:20:TYR:HA	8:S8A:65:TYR:CE2	2.56	0.40
2:S2B:26:PRO:O	2:S2B:29:ALA:HB2	2.22	0.40
5:S5B:110:LEU:HD23	5:S5B:110:LEU:HA	1.86	0.40
7:S7B:74:GLU:O	7:S7B:88:PRO:HA	2.21	0.40
7:S7B:126:ASP:O	7:S7B:131:LYS:N	2.54	0.40
32:L5B:133:LEU:HD11	32:L5B:157:ILE:HD12	2.04	0.40
33:L6B:4:ILE:HG21	33:L6B:6:ARG:CZ	2.52	0.40
34:L9B:124:GLY:H	34:L9B:142:VAL:CG2	2.35	0.40
34:L9B:132:PRO:HB2	34:L9B:133:HIS:H	1.68	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:L9A:112:LYS:NZ	1:16SB:1115:G:C1'[4_555]	0.88	1.32
34:L9A:112:LYS:CE	1:16SB:1115:G:N3[4_555]	1.44	0.76
34:L9A:112:LYS:CE	1:16SB:1115:G:C4[4_555]	1.53	0.67
34:L9A:112:LYS:NZ	1:16SB:1115:G:O4'[4_555]	1.54	0.66
34:L9A:112:LYS:NZ	1:16SB:1115:G:N9[4_555]	1.66	0.54
34:L9A:82:ARG:NH1	1:16SB:702:U:O2'[4_555]	1.79	0.41
34:L9A:112:LYS:CE	1:16SB:1115:G:N9[4_555]	1.99	0.21
27:23SA:314:A:OP1	46:L24B:57:GLN:NE2[2_564]	2.07	0.13
34:L9A:112:LYS:NZ	1:16SB:1115:G:C4[4_555]	2.10	0.10
34:L9A:112:LYS:NZ	1:16SB:1115:G:N3[4_555]	2.16	0.04

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
2	S2A	235/256 (92%)	194 (83%)	37 (16%)	4 (2%)	7	30
2	S2B	235/256 (92%)	196 (83%)	33 (14%)	6 (3%)	4	21
3	S3A	203/239 (85%)	177 (87%)	23 (11%)	3 (2%)	8	33
3	S3B	204/239 (85%)	184 (90%)	19 (9%)	1 (0%)	25	58
4	S4A	206/209 (99%)	188 (91%)	18 (9%)	0	100	100
4	S4B	206/209 (99%)	189 (92%)	17 (8%)	0	100	100
5	S5A	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	19	51
5	S5B	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
6	S6A	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
6	S6B	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
7	S7A	153/156 (98%)	142 (93%)	11 (7%)	0	100	100
7	S7B	151/156 (97%)	140 (93%)	10 (7%)	1 (1%)	19	51
8	S8A	136/138 (99%)	122 (90%)	13 (10%)	1 (1%)	19	51
8	S8B	136/138 (99%)	124 (91%)	12 (9%)	0	100	100
9	S9A	125/128 (98%)	104 (83%)	20 (16%)	1 (1%)	16	48
9	S9B	125/128 (98%)	107 (86%)	18 (14%)	0	100	100
10	S10A	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
10	S10B	97/105 (92%)	81 (84%)	14 (14%)	2 (2%)	5	25
11	S11A	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
11	S11B	115/129 (89%)	104 (90%)	11 (10%)	0	100	100
12	S12A	122/132 (92%)	105 (86%)	16 (13%)	1 (1%)	16	48
12	S12B	122/132 (92%)	109 (89%)	11 (9%)	2 (2%)	8	31
13	S13A	117/126 (93%)	100 (86%)	13 (11%)	4 (3%)	3	17
13	S13B	119/126 (94%)	95 (80%)	20 (17%)	4 (3%)	3	17
14	S14A	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	S14B	57/61 (93%)	48 (84%)	6 (10%)	3 (5%)	1	10
15	S15A	86/89 (97%)	81 (94%)	3 (4%)	2 (2%)	5	23
15	S15B	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	11	38
16	S16A	81/88 (92%)	77 (95%)	4 (5%)	0	100	100
16	S16B	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	S17A	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
17	S17B	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
18	S18A	69/88 (78%)	63 (91%)	4 (6%)	2 (3%)	3	20
18	S18B	68/88 (77%)	62 (91%)	6 (9%)	0	100	100
19	S19A	82/93 (88%)	61 (74%)	19 (23%)	2 (2%)	5	22
19	S19B	84/93 (90%)	66 (79%)	17 (20%)	1 (1%)	11	38
20	S20A	97/106 (92%)	83 (86%)	11 (11%)	3 (3%)	3	19
20	S20B	97/106 (92%)	83 (86%)	11 (11%)	3 (3%)	3	19
21	THXA	22/27 (82%)	20 (91%)	2 (9%)	0	100	100
21	THXB	23/27 (85%)	20 (87%)	2 (9%)	1 (4%)	2	13
29	L2A	270/276 (98%)	244 (90%)	21 (8%)	5 (2%)	6	27
29	L2B	270/276 (98%)	246 (91%)	21 (8%)	3 (1%)	12	39
30	L3A	202/206 (98%)	187 (93%)	13 (6%)	2 (1%)	13	42
30	L3B	202/206 (98%)	187 (93%)	13 (6%)	2 (1%)	13	42
31	L4A	200/210 (95%)	183 (92%)	16 (8%)	1 (0%)	25	58
31	L4B	200/210 (95%)	179 (90%)	20 (10%)	1 (0%)	25	58
32	L5A	179/182 (98%)	153 (86%)	20 (11%)	6 (3%)	3	17
32	L5B	179/182 (98%)	155 (87%)	19 (11%)	5 (3%)	4	20
33	L6A	172/180 (96%)	141 (82%)	25 (14%)	6 (4%)	3	16
33	L6B	171/180 (95%)	126 (74%)	36 (21%)	9 (5%)	1	10
34	L9A	143/148 (97%)	116 (81%)	18 (13%)	9 (6%)	1	7
34	L9B	144/148 (97%)	121 (84%)	20 (14%)	3 (2%)	5	25
35	L13A	136/140 (97%)	115 (85%)	17 (12%)	4 (3%)	3	20
35	L13B	136/140 (97%)	118 (87%)	17 (12%)	1 (1%)	19	51
36	L14A	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16	48
36	L14B	120/122 (98%)	107 (89%)	11 (9%)	2 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	L15A	148/150 (99%)	115 (78%)	25 (17%)	8 (5%)	1	9
37	L15B	148/150 (99%)	115 (78%)	23 (16%)	10 (7%)	1	6
38	L16A	139/141 (99%)	115 (83%)	18 (13%)	6 (4%)	2	13
38	L16B	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	3	16
39	L17A	116/118 (98%)	103 (89%)	13 (11%)	0	100	100
39	L17B	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
40	L18A	110/112 (98%)	90 (82%)	18 (16%)	2 (2%)	7	29
40	L18B	109/112 (97%)	88 (81%)	21 (19%)	0	100	100
41	L19A	135/146 (92%)	118 (87%)	15 (11%)	2 (2%)	8	33
41	L19B	135/146 (92%)	118 (87%)	17 (13%)	0	100	100
42	L20A	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
42	L20B	115/118 (98%)	105 (91%)	7 (6%)	3 (3%)	4	21
43	L21A	99/101 (98%)	86 (87%)	9 (9%)	4 (4%)	2	14
43	L21B	99/101 (98%)	78 (79%)	16 (16%)	5 (5%)	1	10
44	L22A	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
44	L22B	111/113 (98%)	100 (90%)	10 (9%)	1 (1%)	14	45
45	L23A	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
45	L23B	92/96 (96%)	85 (92%)	7 (8%)	0	100	100
46	L24A	106/110 (96%)	83 (78%)	16 (15%)	7 (7%)	1	6
46	L24B	104/110 (94%)	83 (80%)	16 (15%)	5 (5%)	2	11
47	L25A	177/206 (86%)	136 (77%)	32 (18%)	9 (5%)	1	10
47	L25B	174/206 (84%)	136 (78%)	32 (18%)	6 (3%)	3	17
48	L27A	82/85 (96%)	72 (88%)	10 (12%)	0	100	100
48	L27B	82/85 (96%)	70 (85%)	11 (13%)	1 (1%)	11	38
49	L28A	95/98 (97%)	83 (87%)	10 (10%)	2 (2%)	5	25
49	L28B	95/98 (97%)	79 (83%)	14 (15%)	2 (2%)	5	25
50	L29A	67/72 (93%)	61 (91%)	6 (9%)	0	100	100
50	L29B	66/72 (92%)	61 (92%)	5 (8%)	0	100	100
51	L30A	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
51	L30B	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
52	L31A	69/71 (97%)	43 (62%)	22 (32%)	4 (6%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	L31B	69/71 (97%)	46 (67%)	18 (26%)	5 (7%)	1	5
53	L32A	54/60 (90%)	43 (80%)	11 (20%)	0	100	100
53	L32B	54/60 (90%)	47 (87%)	6 (11%)	1 (2%)	6	27
54	L33A	43/54 (80%)	27 (63%)	11 (26%)	5 (12%)	0	1
54	L33B	43/54 (80%)	30 (70%)	10 (23%)	3 (7%)	1	5
55	L34A	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
55	L34B	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
56	L35A	62/65 (95%)	55 (89%)	7 (11%)	0	100	100
56	L35B	62/65 (95%)	56 (90%)	6 (10%)	0	100	100
All	All	11387/12054 (94%)	9910 (87%)	1271 (11%)	206 (2%)	7	29

All (206) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S3A	12	LEU
12	S12A	62	GLU
13	S13A	67	GLU
13	S13A	101	GLN
14	S14A	24	CYS
19	S19A	41	VAL
20	S20A	48	LYS
29	L2A	122	ASP
29	L2A	123	ALA
30	L3A	118	LYS
31	L4A	128	ALA
32	L5A	96	ARG
33	L6A	81	GLU
33	L6A	173	PRO
34	L9A	134	PRO
35	L13A	97	ARG
35	L13A	137	LYS
36	L14A	97	ARG
37	L15A	7	ARG
37	L15A	15	ARG
37	L15A	29	LYS
37	L15A	38	GLN
37	L15A	57	THR
37	L15A	106	LEU
38	L16A	105	GLU

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Mol	Chain	Res	Type
38	L16A	139	GLU
40	L18A	3	ARG
41	L19A	18	ASP
43	L21A	45	THR
43	L21A	50	PRO
46	L24A	81	LYS
46	L24A	90	LEU
46	L24A	92	ASN
47	L25A	13	GLU
47	L25A	111	VAL
54	L33A	45	LYS
54	L33A	48	VAL
54	L33A	49	HIS
2	S2B	20	GLU
2	S2B	154	LEU
7	S7B	55	GLY
10	S10B	17	ASP
12	S12B	62	GLU
13	S13B	83	ASP
13	S13B	106	ASN
14	S14B	14	PRO
14	S14B	17	LYS
20	S20B	70	SER
20	S20B	74	LYS
21	THXB	3	LYS
29	L2B	239	ARG
31	L4B	128	ALA
32	L5B	5	VAL
32	L5B	81	LYS
32	L5B	96	ARG
33	L6B	99	VAL
34	L9B	76	THR
34	L9B	142	VAL
35	L13B	77	GLY
37	L15B	15	ARG
37	L15B	19	VAL
37	L15B	36	LYS
37	L15B	46	LYS
37	L15B	53	GLY
37	L15B	110	TYR
38	L16B	105	GLU
38	L16B	139	GLU

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Mol	Chain	Res	Type
42	L20B	93	LYS
43	L21B	44	LYS
46	L24B	81	LYS
47	L25B	60	GLU
47	L25B	63	ASP
49	L28B	91	LYS
52	L31B	67	TYR
54	L33B	19	ARG
2	S2A	10	LEU
2	S2A	207	ALA
13	S13A	14	ARG
20	S20A	102	GLY
32	L5A	49	ASP
33	L6A	92	ILE
34	L9A	13	GLY
34	L9A	122	GLU
35	L13A	22	THR
37	L15A	19	VAL
47	L25A	59	LEU
47	L25A	63	ASP
47	L25A	109	ALA
47	L25A	159	PRO
10	S10B	54	PHE
14	S14B	29	ARG
15	S15B	88	ARG
30	L3B	118	LYS
32	L5B	117	PHE
33	L6B	118	PRO
37	L15B	29	LYS
38	L16B	90	VAL
42	L20B	101	ARG
43	L21B	50	PRO
43	L21B	79	VAL
53	L32B	50	GLY
54	L33B	49	HIS
2	S2A	5	ILE
3	S3A	82	GLU
9	S9A	56	LEU
29	L2A	239	ARG
32	L5A	127	GLY
33	L6A	127	GLU
34	L9A	116	LEU

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Mol	Chain	Res	Type
37	L15A	148	LEU
38	L16A	6	ARG
38	L16A	79	LEU
38	L16A	90	VAL
41	L19A	124	ASP
43	L21A	30	GLY
49	L28A	91	LYS
2	S2B	191	ASP
3	S3B	3	ASN
19	S19B	42	PRO
33	L6B	12	PRO
33	L6B	21	PRO
33	L6B	125	VAL
36	L14B	48	PRO
37	L15B	16	ARG
37	L15B	57	THR
2	S2A	155	LEU
15	S15A	23	GLY
15	S15A	87	ILE
18	S18A	19	LYS
30	L3A	52	LEU
32	L5A	126	ASP
34	L9A	82	ARG
46	L24A	91	GLU
52	L31A	40	HIS
54	L33A	41	PRO
13	S13B	120	LYS
30	L3B	52	LEU
33	L6B	108	GLY
37	L15B	119	GLU
43	L21B	30	GLY
43	L21B	49	THR
44	L22B	67	ASP
46	L24B	76	CYS
47	L25B	6	LYS
47	L25B	61	LEU
52	L31B	41	PRO
52	L31B	49	PHE
8	S8A	129	VAL
20	S20A	97	ALA
29	L2A	240	ALA
32	L5A	82	LEU

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Mol	Chain	Res	Type
32	L5A	86	MET
40	L18A	94	TYR
43	L21A	38	LEU
46	L24A	52	SER
47	L25A	52	SER
49	L28A	97	LEU
52	L31A	43	TYR
54	L33A	23	THR
2	S2B	96	ARG
2	S2B	130	ARG
12	S12B	42	PRO
20	S20B	68	LYS
29	L2B	240	ALA
33	L6B	127	GLU
38	L16B	6	ARG
38	L16B	79	LEU
48	L27B	3	HIS
3	S3A	4	LYS
13	S13A	4	ILE
18	S18A	87	ARG
33	L6A	93	GLY
34	L9A	11	ASN
38	L16A	11	LYS
46	L24A	76	CYS
52	L31A	34	GLU
52	L31A	46	GLN
2	S2B	7	VAL
13	S13B	5	ALA
29	L2B	271	ILE
32	L5B	36	LYS
36	L14B	5	GLN
42	L20B	116	ALA
46	L24B	52	SER
46	L24B	54	LYS
47	L25B	13	GLU
52	L31B	42	PHE
5	S5A	22	GLY
19	S19A	40	ILE
33	L6A	126	PRO
34	L9A	132	PRO
46	L24A	51	VAL
34	L9A	133	HIS

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Mol	Chain	Res	Type
47	L25A	61	LEU
33	L6B	120	GLY
46	L24B	96	ILE
54	L33B	41	PRO
29	L2A	271	ILE
49	L28B	55	GLY
52	L31B	29	PRO
34	L9A	118	LYS
35	L13A	126	PRO
47	L25A	114	GLY
33	L6B	151	ILE
47	L25B	159	PRO
34	L9B	132	PRO

### 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	
2	S2A	205/220 (93%)	187 (91%)	18 (9%)	8	30
2	S2B	205/220 (93%)	198 (97%)	7 (3%)	32	62
3	S3A	159/188 (85%)	152 (96%)	7 (4%)	24	54
3	S3B	160/188 (85%)	143 (89%)	17 (11%)	5	21
4	S4A	180/181 (99%)	171 (95%)	9 (5%)	20	50
4	S4B	180/181 (99%)	174 (97%)	6 (3%)	33	62
5	S5A	116/123 (94%)	112 (97%)	4 (3%)	32	62
5	S5B	116/123 (94%)	112 (97%)	4 (3%)	32	62
6	S6A	90/90 (100%)	86 (96%)	4 (4%)	24	54
6	S6B	90/90 (100%)	87 (97%)	3 (3%)	33	62
7	S7A	126/127 (99%)	120 (95%)	6 (5%)	21	51
7	S7B	126/127 (99%)	118 (94%)	8 (6%)	15	42
8	S8A	119/119 (100%)	111 (93%)	8 (7%)	13	40
8	S8B	119/119 (100%)	113 (95%)	6 (5%)	20	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	S9A	98/99 (99%)	91 (93%)	7 (7%)	12	39
9	S9B	98/99 (99%)	89 (91%)	9 (9%)	7	28
10	S10A	89/92 (97%)	86 (97%)	3 (3%)	32	62
10	S10B	89/92 (97%)	83 (93%)	6 (7%)	13	40
11	S11A	88/99 (89%)	85 (97%)	3 (3%)	32	62
11	S11B	89/99 (90%)	88 (99%)	1 (1%)	70	84
12	S12A	103/108 (95%)	98 (95%)	5 (5%)	21	51
12	S12B	103/108 (95%)	100 (97%)	3 (3%)	37	65
13	S13A	95/101 (94%)	91 (96%)	4 (4%)	25	56
13	S13B	97/101 (96%)	93 (96%)	4 (4%)	26	57
14	S14A	49/50 (98%)	44 (90%)	5 (10%)	6	23
14	S14B	49/50 (98%)	46 (94%)	3 (6%)	15	43
15	S15A	79/80 (99%)	77 (98%)	2 (2%)	42	69
15	S15B	79/80 (99%)	77 (98%)	2 (2%)	42	69
16	S16A	72/74 (97%)	68 (94%)	4 (6%)	17	46
16	S16B	72/74 (97%)	70 (97%)	2 (3%)	38	66
17	S17A	95/97 (98%)	91 (96%)	4 (4%)	25	56
17	S17B	95/97 (98%)	91 (96%)	4 (4%)	25	56
18	S18A	62/77 (80%)	60 (97%)	2 (3%)	34	63
18	S18B	61/77 (79%)	58 (95%)	3 (5%)	21	51
19	S19A	73/80 (91%)	68 (93%)	5 (7%)	13	40
19	S19B	73/80 (91%)	69 (94%)	4 (6%)	18	47
20	S20A	76/82 (93%)	74 (97%)	2 (3%)	41	68
20	S20B	76/82 (93%)	73 (96%)	3 (4%)	27	58
21	THXA	19/22 (86%)	19 (100%)	0	100	100
21	THXB	20/22 (91%)	19 (95%)	1 (5%)	20	50
29	L2A	214/218 (98%)	209 (98%)	5 (2%)	45	70
29	L2B	214/218 (98%)	209 (98%)	5 (2%)	45	70
30	L3A	165/166 (99%)	161 (98%)	4 (2%)	44	70
30	L3B	165/166 (99%)	163 (99%)	2 (1%)	67	83
31	L4A	161/166 (97%)	156 (97%)	5 (3%)	35	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	L4B	161/166 (97%)	158 (98%)	3 (2%)	52	75
32	L5A	155/156 (99%)	148 (96%)	7 (4%)	23	53
32	L5B	155/156 (99%)	143 (92%)	12 (8%)	10	35
33	L6A	145/148 (98%)	140 (97%)	5 (3%)	32	62
33	L6B	144/148 (97%)	128 (89%)	16 (11%)	5	20
34	L9A	122/124 (98%)	116 (95%)	6 (5%)	21	51
34	L9B	122/124 (98%)	114 (93%)	8 (7%)	14	41
35	L13A	117/119 (98%)	112 (96%)	5 (4%)	25	55
35	L13B	117/119 (98%)	115 (98%)	2 (2%)	56	78
36	L14A	100/100 (100%)	98 (98%)	2 (2%)	50	74
36	L14B	100/100 (100%)	97 (97%)	3 (3%)	36	64
37	L15A	116/116 (100%)	105 (90%)	11 (10%)	7	26
37	L15B	116/116 (100%)	109 (94%)	7 (6%)	16	44
38	L16A	111/111 (100%)	104 (94%)	7 (6%)	15	42
38	L16B	111/111 (100%)	105 (95%)	6 (5%)	18	47
39	L17A	101/101 (100%)	98 (97%)	3 (3%)	36	64
39	L17B	101/101 (100%)	97 (96%)	4 (4%)	27	58
40	L18A	88/88 (100%)	85 (97%)	3 (3%)	32	62
40	L18B	87/88 (99%)	79 (91%)	8 (9%)	7	28
41	L19A	120/127 (94%)	114 (95%)	6 (5%)	20	50
41	L19B	120/127 (94%)	116 (97%)	4 (3%)	33	62
42	L20A	93/94 (99%)	90 (97%)	3 (3%)	34	63
42	L20B	93/94 (99%)	84 (90%)	9 (10%)	6	25
43	L21A	82/82 (100%)	76 (93%)	6 (7%)	11	37
43	L21B	82/82 (100%)	73 (89%)	9 (11%)	5	21
44	L22A	92/92 (100%)	87 (95%)	5 (5%)	18	47
44	L22B	92/92 (100%)	87 (95%)	5 (5%)	18	47
45	L23A	76/78 (97%)	75 (99%)	1 (1%)	65	82
45	L23B	76/78 (97%)	71 (93%)	5 (7%)	14	41
46	L24A	89/91 (98%)	85 (96%)	4 (4%)	23	53
46	L24B	79/91 (87%)	75 (95%)	4 (5%)	20	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	L25A	158/179 (88%)	153 (97%)	5 (3%)	34	63
47	L25B	155/179 (87%)	143 (92%)	12 (8%)	10	35
48	L27A	66/67 (98%)	63 (96%)	3 (4%)	23	53
48	L27B	66/67 (98%)	63 (96%)	3 (4%)	23	53
49	L28A	82/83 (99%)	79 (96%)	3 (4%)	29	59
49	L28B	82/83 (99%)	81 (99%)	1 (1%)	67	83
50	L29A	65/67 (97%)	64 (98%)	1 (2%)	60	80
50	L29B	64/67 (96%)	62 (97%)	2 (3%)	35	63
51	L30A	51/52 (98%)	50 (98%)	1 (2%)	50	74
51	L30B	51/52 (98%)	50 (98%)	1 (2%)	50	74
52	L31A	63/63 (100%)	57 (90%)	6 (10%)	7	26
52	L31B	63/63 (100%)	56 (89%)	7 (11%)	5	20
53	L32A	48/52 (92%)	45 (94%)	3 (6%)	15	42
53	L32B	48/52 (92%)	43 (90%)	5 (10%)	5	22
54	L33A	44/52 (85%)	41 (93%)	3 (7%)	13	40
54	L33B	44/52 (85%)	41 (93%)	3 (7%)	13	40
55	L34A	41/42 (98%)	39 (95%)	2 (5%)	21	51
55	L34B	42/42 (100%)	40 (95%)	2 (5%)	21	51
56	L35A	54/55 (98%)	53 (98%)	1 (2%)	52	75
56	L35B	54/55 (98%)	48 (89%)	6 (11%)	5	20
All	All	9613/9996 (96%)	9145 (95%)	468 (5%)	21	51

All (468) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S2A	9	GLU
2	S2A	12	GLU
2	S2A	17	PHE
2	S2A	28	PHE
2	S2A	30	ARG
2	S2A	74	LYS
2	S2A	75	LYS
2	S2A	96	ARG
2	S2A	111	ARG
2	S2A	124	SER

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Mol	Chain	Res	Type
2	S2A	137	ARG
2	S2A	163	PHE
2	S2A	192	SER
2	S2A	196	LEU
2	S2A	209	ARG
2	S2A	210	SER
2	S2A	212	GLN
2	S2A	215	LEU
3	S3A	17	ASP
3	S3A	29	TYR
3	S3A	79	ARG
3	S3A	98	ASN
3	S3A	112	SER
3	S3A	128	PHE
3	S3A	167	TRP
4	S4A	3	ARG
4	S4A	10	ARG
4	S4A	49	ARG
4	S4A	84	LYS
4	S4A	134	ASP
4	S4A	150	GLU
4	S4A	187	ARG
4	S4A	193	ASP
4	S4A	209	ARG
5	S5A	10	MET
5	S5A	73	ASN
5	S5A	79	GLU
5	S5A	155	GLU
6	S6A	7	ASN
6	S6A	15	ASP
6	S6A	19	LEU
6	S6A	54	LYS
7	S7A	6	ARG
7	S7A	78	ARG
7	S7A	94	ARG
7	S7A	114	ARG
7	S7A	137	LYS
7	S7A	155	ARG
8	S8A	1	MET
8	S8A	41	ARG
8	S8A	56	LYS
8	S8A	88	LYS

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Mol	Chain	Res	Type
8	S8A	91	ARG
8	S8A	104	ARG
8	S8A	112	LEU
8	S8A	121	ASP
9	S9A	91	ASP
9	S9A	95	LYS
9	S9A	105	ASP
9	S9A	111	ARG
9	S9A	112	LYS
9	S9A	114	TYR
9	S9A	121	ARG
10	S10A	3	LYS
10	S10A	60	ARG
10	S10A	78	ASN
11	S11A	13	GLN
11	S11A	51	LYS
11	S11A	77	MET
12	S12A	16	ARG
12	S12A	17	LYS
12	S12A	25	LYS
12	S12A	30	ARG
12	S12A	95	TYR
13	S13A	48	LEU
13	S13A	64	TRP
13	S13A	65	LYS
13	S13A	69	GLU
14	S14A	16	PHE
14	S14A	23	ARG
14	S14A	24	CYS
14	S14A	35	ARG
14	S14A	41	ARG
15	S15A	21	ASP
15	S15A	64	ARG
16	S16A	8	ARG
16	S16A	43	LYS
16	S16A	72	ARG
16	S16A	75	ARG
17	S17A	52	LYS
17	S17A	68	ARG
17	S17A	91	ARG
17	S17A	101	ARG
18	S18A	19	LYS

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Mol	Chain	Res	Type
18	S18A	26	LEU
19	S19A	27	GLU
19	S19A	37	ARG
19	S19A	44	MET
19	S19A	78	ARG
19	S19A	81	ARG
20	S20A	45	GLN
20	S20A	92	LEU
29	L2A	13	ARG
29	L2A	14	ARG
29	L2A	38	LYS
29	L2A	212	SER
29	L2A	237	GLU
30	L3A	64	LYS
30	L3A	111	ARG
30	L3A	113	PHE
30	L3A	154	LYS
31	L4A	17	ARG
31	L4A	95	ARG
31	L4A	98	SER
31	L4A	108	LYS
31	L4A	117	ARG
32	L5A	18	GLU
32	L5A	51	ARG
32	L5A	58	GLN
32	L5A	67	LYS
32	L5A	80	PHE
32	L5A	86	MET
32	L5A	174	GLU
33	L6A	77	LYS
33	L6A	86	GLU
33	L6A	104	GLU
33	L6A	149	ARG
33	L6A	155	SER
34	L9A	25	TYR
34	L9A	57	ARG
34	L9A	110	ASP
34	L9A	126	TYR
34	L9A	133	HIS
34	L9A	139	GLN
35	L13A	7	LYS
35	L13A	39	ARG

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Mol	Chain	Res	Type
35	L13A	90	MET
35	L13A	97	ARG
35	L13A	115	ARG
36	L14A	7	TYR
36	L14A	28	SER
37	L15A	13	ASN
37	L15A	15	ARG
37	L15A	19	VAL
37	L15A	21	ARG
37	L15A	27	HIS
37	L15A	50	ARG
37	L15A	55	ARG
37	L15A	108	LYS
37	L15A	133	SER
37	L15A	144	GLU
37	L15A	148	LEU
38	L16A	10	ARG
38	L16A	14	ARG
38	L16A	25	ASP
38	L16A	45	GLN
38	L16A	59	ARG
38	L16A	89	ASN
38	L16A	101	ARG
39	L17A	44	LEU
39	L17A	64	ARG
39	L17A	105	ARG
40	L18A	15	ARG
40	L18A	58	LEU
40	L18A	89	ARG
41	L19A	1	MET
41	L19A	51	ARG
41	L19A	78	LEU
41	L19A	96	ARG
41	L19A	111	ARG
41	L19A	112	ARG
42	L20A	5	LYS
42	L20A	92	ARG
42	L20A	104	GLN
43	L21A	10	LYS
43	L21A	12	TYR
43	L21A	21	ARG
43	L21A	38	LEU

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Mol	Chain	Res	Type
43	L21A	44	LYS
43	L21A	52	VAL
44	L22A	11	ARG
44	L22A	37	ARG
44	L22A	67	ASP
44	L22A	70	TYR
44	L22A	92	ARG
45	L23A	64	LYS
46	L24A	6	HIS
46	L24A	57	GLN
46	L24A	81	LYS
46	L24A	102	CYS
47	L25A	1	MET
47	L25A	49	ARG
47	L25A	72	ARG
47	L25A	81	ARG
47	L25A	132	ASN
48	L27A	14	ARG
48	L27A	44	ARG
48	L27A	64	ASP
49	L28A	69	LYS
49	L28A	78	LYS
49	L28A	81	LYS
50	L29A	8	LYS
51	L30A	33	GLN
52	L31A	18	CYS
52	L31A	38	LYS
52	L31A	55	ARG
52	L31A	61	ARG
52	L31A	63	TYR
52	L31A	67	TYR
53	L32A	16	ARG
53	L32A	23	HIS
53	L32A	51	TYR
54	L33A	33	LYS
54	L33A	34	LEU
54	L33A	39	TYR
55	L34A	10	ARG
55	L34A	41	ARG
56	L35A	52	LYS
2	S2B	21	ARG
2	S2B	56	ARG

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Mol	Chain	Res	Type
2	S2B	64	ARG
2	S2B	137	ARG
2	S2B	163	PHE
2	S2B	217	ARG
2	S2B	233	SER
3	S3B	16	ARG
3	S3B	26	LYS
3	S3B	29	TYR
3	S3B	36	ASP
3	S3B	45	LYS
3	S3B	48	TYR
3	S3B	52	LEU
3	S3B	54	ARG
3	S3B	56	ASP
3	S3B	62	ASP
3	S3B	72	LYS
3	S3B	79	ARG
3	S3B	83	ARG
3	S3B	101	LEU
3	S3B	119	ARG
3	S3B	131	ARG
3	S3B	196	LEU
4	S4B	10	ARG
4	S4B	33	MET
4	S4B	49	ARG
4	S4B	118	ARG
4	S4B	162	LEU
4	S4B	181	MET
5	S5B	10	MET
5	S5B	26	PHE
5	S5B	126	ARG
5	S5B	137	GLU
6	S6B	3	ARG
6	S6B	82	ARG
6	S6B	93	SER
7	S7B	41	ARG
7	S7B	54	THR
7	S7B	56	GLN
7	S7B	72	ARG
7	S7B	85	TYR
7	S7B	114	ARG
7	S7B	140	ASP

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Mol	Chain	Res	Type
7	S7B	156	TRP
8	S8B	1	MET
8	S8B	25	ASP
8	S8B	77	GLU
8	S8B	84	ARG
8	S8B	102	ARG
8	S8B	112	LEU
9	S9B	4	TYR
9	S9B	20	ARG
9	S9B	71	SER
9	S9B	95	LYS
9	S9B	97	LYS
9	S9B	107	ARG
9	S9B	113	LYS
9	S9B	121	ARG
9	S9B	125	TYR
10	S10B	21	GLN
10	S10B	22	LYS
10	S10B	45	ARG
10	S10B	69	ASN
10	S10B	70	ARG
10	S10B	79	ARG
11	S11B	116	HIS
12	S12B	61	TYR
12	S12B	72	HIS
12	S12B	99	ARG
13	S13B	47	ASP
13	S13B	64	TRP
13	S13B	88	ARG
13	S13B	94	ARG
14	S14B	29	ARG
14	S14B	35	ARG
14	S14B	58	LYS
15	S15B	10	LYS
15	S15B	63	ARG
16	S16B	43	LYS
16	S16B	82	GLN
17	S17B	63	ARG
17	S17B	68	ARG
17	S17B	79	SER
17	S17B	101	ARG
18	S18B	28	GLU

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Mol	Chain	Res	Type
18	S18B	54	ARG
18	S18B	87	ARG
19	S19B	29	ARG
19	S19B	32	LYS
19	S19B	80	TYR
19	S19B	83	HIS
20	S20B	11	SER
20	S20B	23	ARG
20	S20B	74	LYS
21	THXB	15	ARG
29	L2B	5	LYS
29	L2B	38	LYS
29	L2B	88	ARG
29	L2B	262	ARG
29	L2B	273	ARG
30	L3B	79	ARG
30	L3B	111	ARG
31	L4B	29	ASN
31	L4B	50	SER
31	L4B	205	ARG
32	L5B	4	ASP
32	L5B	10	LYS
32	L5B	21	ARG
32	L5B	33	ARG
32	L5B	47	LYS
32	L5B	51	ARG
32	L5B	67	LYS
32	L5B	80	PHE
32	L5B	91	ARG
32	L5B	95	ARG
32	L5B	118	ARG
32	L5B	153	ARG
33	L6B	23	ARG
33	L6B	25	LYS
33	L6B	59	ARG
33	L6B	67	LEU
33	L6B	77	LYS
33	L6B	83	TYR
33	L6B	86	GLU
33	L6B	88	LEU
33	L6B	97	ARG
33	L6B	101	ARG

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Mol	Chain	Res	Type
33	L6B	111	HIS
33	L6B	147	ASN
33	L6B	152	ARG
33	L6B	153	LYS
33	L6B	155	SER
33	L6B	167	GLU
34	L9B	38	LEU
34	L9B	56	LYS
34	L9B	69	LYS
34	L9B	89	TYR
34	L9B	103	ARG
34	L9B	104	GLN
34	L9B	121	LYS
34	L9B	133	HIS
35	L13B	76	SER
35	L13B	114	ARG
36	L14B	13	ASN
36	L14B	23	ARG
36	L14B	104	ARG
37	L15B	21	ARG
37	L15B	35	HIS
37	L15B	85	LEU
37	L15B	110	TYR
37	L15B	115	LEU
37	L15B	117	GLU
37	L15B	124	LYS
38	L16B	10	ARG
38	L16B	14	ARG
38	L16B	45	GLN
38	L16B	59	ARG
38	L16B	89	ASN
38	L16B	101	ARG
39	L17B	1	MET
39	L17B	2	ARG
39	L17B	88	ARG
39	L17B	91	GLN
40	L18B	15	ARG
40	L18B	25	ARG
40	L18B	30	ARG
40	L18B	34	HIS
40	L18B	56	LEU
40	L18B	75	GLU

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Mol	Chain	Res	Type
40	L18B	89	ARG
40	L18B	110	LEU
41	L19B	1	MET
41	L19B	98	LYS
41	L19B	112	ARG
41	L19B	125	ARG
42	L20B	15	LYS
42	L20B	19	LYS
42	L20B	25	TRP
42	L20B	57	PHE
42	L20B	60	LEU
42	L20B	69	CYS
42	L20B	79	PHE
42	L20B	97	ASP
42	L20B	114	LYS
43	L21B	10	LYS
43	L21B	44	LYS
43	L21B	60	GLU
43	L21B	73	SER
43	L21B	74	LYS
43	L21B	75	PHE
43	L21B	78	LYS
43	L21B	82	ARG
43	L21B	98	GLU
44	L22B	11	ARG
44	L22B	67	ASP
44	L22B	70	TYR
44	L22B	111	HIS
44	L22B	113	LYS
45	L23B	14	SER
45	L23B	53	LYS
45	L23B	62	LYS
45	L23B	64	LYS
45	L23B	76	ARG
46	L24B	43	ASN
46	L24B	55	TYR
46	L24B	101	LYS
46	L24B	102	CYS
47	L25B	2	GLU
47	L25B	31	ARG
47	L25B	34	ASN
47	L25B	76	LEU

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Mol	Chain	Res	Type
47	L25B	82	ARG
47	L25B	87	ASP
47	L25B	94	GLU
47	L25B	119	GLU
47	L25B	131	ARG
47	L25B	136	PHE
47	L25B	154	ASP
47	L25B	169	GLU
48	L27B	5	LYS
48	L27B	25	ARG
48	L27B	35	ASN
49	L28B	88	LYS
50	L29B	3	LEU
50	L29B	67	LYS
51	L30B	30	ARG
52	L31B	40	HIS
52	L31B	49	PHE
52	L31B	53	GLU
52	L31B	58	ARG
52	L31B	61	ARG
52	L31B	62	ARG
52	L31B	69	LYS
53	L32B	21	SER
53	L32B	33	CYS
53	L32B	40	LYS
53	L32B	52	TYR
53	L32B	55	ARG
54	L33B	17	LYS
54	L33B	18	ARG
54	L33B	53	LYS
55	L34B	32	LYS
55	L34B	49	ARG
56	L35B	19	SER
56	L35B	21	LYS
56	L35B	31	HIS
56	L35B	46	ARG
56	L35B	47	LYS
56	L35B	52	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

## 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16SA	1507/1512 (99%)	330 (21%)	52 (3%)
1	16SB	1503/1512 (99%)	332 (22%)	48 (3%)
22	ASIA	74/76 (97%)	43 (58%)	2 (2%)
23	PSIA	73/76 (96%)	22 (30%)	2 (2%)
23	PSIB	73/76 (96%)	29 (39%)	2 (2%)
24	ESIA	74/76 (97%)	33 (44%)	1 (1%)
24	ESIB	74/76 (97%)	23 (31%)	3 (4%)
25	MRNA	29/30 (96%)	7 (24%)	2 (6%)
25	MRNB	29/30 (96%)	11 (37%)	2 (6%)
26	TRNA	71/76 (93%)	33 (46%)	3 (4%)
27	23SA	2883/2911 (99%)	643 (22%)	66 (2%)
27	23SB	2870/2911 (98%)	666 (23%)	67 (2%)
28	5SA	121/124 (97%)	25 (20%)	1 (0%)
28	5SB	120/124 (96%)	32 (26%)	5 (4%)
57	ASIB	74/76 (97%)	36 (48%)	2 (2%)
All	All	9575/9686 (98%)	2265 (23%)	258 (2%)

All (2265) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16SA	654	A
1	16SA	655	G
1	16SA	656	A
1	16SA	678	A
1	16SA	685	G
1	16SA	687	G
1	16SA	693	C
1	16SA	694	C
1	16SA	697	A
1	16SA	707	G
1	16SA	711	U
1	16SA	712	G
1	16SA	719	G
1	16SA	724	G
1	16SA	725	U
1	16SA	726	U
1	16SA	727	U
1	16SA	728	U
1	16SA	729	A
1	16SA	732	C
1	16SA	733	C

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Mol	Chain	Res	Type
1	16SA	740	A
1	16SA	747	G
1	16SA	759	A
1	16SA	760	C
1	16SA	773	U
1	16SA	777	C
1	16SA	782	G
1	16SA	784	G
1	16SA	800	A
1	16SA	802	A
1	16SA	803	C
1	16SA	809	C
1	16SA	810	U
1	16SA	812	A
1	16SA	813	U
1	16SA	821	G
1	16SA	832	C
1	16SA	835	U
1	16SA	836	G
1	16SA	837	G
1	16SA	847	A
1	16SA	848	A
1	16SA	849	A
1	16SA	853	C
1	16SA	855	U
1	16SA	856	U
1	16SA	857	G
1	16SA	867	G
1	16SA	872	G
1	16SA	885	U
1	16SA	888	G
1	16SA	892	G
1	16SA	907	G
1	16SA	908	C
1	16SA	911	A
1	16SA	922	G
1	16SA	930	G
1	16SA	962	A
1	16SA	969	C
1	16SA	970	A
1	16SA	973	G
1	16SA	985	A

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Mol	Chain	Res	Type
1	16SA	986	C
1	16SA	987	G
1	16SA	988	G
1	16SA	990	A
1	16SA	992	G
1	16SA	993	C
1	16SA	994	A
1	16SA	995	G
1	16SA	1008	U
1	16SA	1014	A
1	16SA	1029	G
1	16SA	1038	A
1	16SA	1039	C
1	16SA	1047	G
1	16SA	1050	G
1	16SA	1053	A
1	16SA	1054	G
1	16SA	1055	A
1	16SA	1062	U
1	16SA	1063	C
1	16SA	1064	G
1	16SA	1065	G
1	16SA	1070	U
1	16SA	1071	A
1	16SA	1075	U
1	16SA	1080	A
1	16SA	1081	A
1	16SA	1100	A
1	16SA	1101	C
1	16SA	1102	G
1	16SA	1105	G
1	16SA	1112	A
1	16SA	1115	G
1	16SA	1116	U
1	16SA	1126	A
1	16SA	1127	U
1	16SA	1134	G
1	16SA	1138	A
1	16SA	1139	A
1	16SA	1140	C
1	16SA	1147	C
1	16SA	1156	7MG

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Mol	Chain	Res	Type
1	16SA	1160	U
1	16SA	1161	A
1	16SA	1162	A
1	16SA	1165	C
1	16SA	1174	C
1	16SA	1176	A
1	16SA	1178	C
1	16SA	1188	A
1	16SA	1190	U
1	16SA	1191	C
1	16SA	1193	C
1	16SA	1197	G
1	16SA	1201	A
1	16SA	1202	A
1	16SA	1205	G
1	16SA	1206	G
1	16SA	1236	A
1	16SA	1243	A
1	16SA	1252	C
1	16SA	1256	G
1	16SA	1260	G
1	16SA	1279	G
1	16SA	1282	A
1	16SA	1290	G
1	16SA	1291	G
1	16SA	1294	A
1	16SA	1295	G
1	16SA	1300	G
1	16SA	1316	A
1	16SA	1330	C
1	16SA	1331	A
1	16SA	1332	G
1	16SA	1333	A
1	16SA	1350	G
1	16SA	1352	U
1	16SA	1353	G
1	16SA	1360	G
1	16SA	1377	C
1	16SA	1378	C
1	16SA	1382	A
1	16SA	1384	G
1	16SA	1395	A

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Mol	Chain	Res	Type
1	16SA	1406	A
1	16SA	1407	G
1	16SA	1421	A
1	16SA	1422	U
1	16SA	1423	A
1	16SA	1442	U
1	16SA	1444	A
1	16SA	1446	C
1	16SA	1447	G
1	16SA	1449	U
1	16SA	1450	G
1	16SA	1457	A
1	16SA	1468	U
1	16SA	1469	C
1	16SA	1470	U
1	16SA	1471	C
1	16SA	1476	G
1	16SA	1482	A
1	16SA	1493	U
1	16SA	1496	A
1	16SA	1497	G
1	16SA	1525	G
1	16SA	1536	A
1	16SA	1537	A
1	16SA	1539	G
1	16SA	1549	G
1	16SA	1550	G
1	16SA	1557	C
1	16SA	1558	A
1	16SA	1559	C
1	16SA	1583	U
1	16SA	1589	M2G
1	16SA	1591	A
1	16SA	1592	A
1	16SA	1594	G
1	16SA	1595	C
1	16SA	1597	A
1	16SA	1598	A
1	16SA	1599	G
1	16SA	1600	A
1	16SA	1603	C
1	16SA	1604	U

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Mol	Chain	Res	Type
1	16SA	1605	U
1	16SA	1609	A
1	16SA	1614	U
1	16SA	1615	U
1	16SA	1616	G
1	16SA	1625	G
1	16SA	1628	A
1	16SA	1629	A
1	16SA	1630	C
1	16SA	1633	G
1	16SA	1640	A
1	16SA	1641	G
1	16SA	1645	G
1	16SA	1648	G
1	16SA	1649	U
1	16SA	1650	G
1	16SA	1652	C
1	16SA	1653	C
1	16SA	1655	G
1	16SA	1657	G
1	16SA	1659	G
1	16SA	1661	G
1	16SA	1664	G
1	16SA	1666	C
1	16SA	1668	U
1	16SA	1674	A
1	16SA	1681	G
1	16SA	1682	C
1	16SA	1683	A
1	16SA	1694	C
1	16SA	1709	G
1	16SA	1710	G
1	16SA	1722	G
1	16SA	1723	U
1	16SA	1729	A
1	16SA	1750	U
1	16SA	1753	U
1	16SA	1754	U
1	16SA	1755	G
1	16SA	1756	C
1	16SA	1757	C
1	16SA	1758	A

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Mol	Chain	Res	Type
1	16SA	1759	G
1	16SA	1760	C
1	16SA	1761	G
1	16SA	1764	U
1	16SA	1765	C
1	16SA	1766	G
1	16SA	1767	G
1	16SA	1768	C
1	16SA	1774	A
1	16SA	1780	A
1	16SA	1785	A
1	16SA	1786	C
1	16SA	1787	U
1	16SA	1789	C
1	16SA	1798	G
1	16SA	1808	G
1	16SA	1809	G
1	16SA	1810	A
1	16SA	1811	G
1	16SA	1812	G
1	16SA	1814	G
1	16SA	1815	A
1	16SA	1823	U
1	16SA	1825	G
1	16SA	1827	C
1	16SA	1828	A
1	16SA	1829	G
1	16SA	1839	U
1	16SA	1845	C
1	16SA	1852	A
1	16SA	1854	A
1	16SA	1865	A
1	16SA	1877	A
1	16SA	1883	A
1	16SA	1884	U
1	16SA	1885	G
1	16SA	1889	C
1	16SA	1890	C
1	16SA	1896	A
1	16SA	1899	G
1	16SA	1900	G
1	16SA	1902	A

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Mol	Chain	Res	Type
1	16SA	1905	U
1	16SA	1907	A
1	16SA	1908	U
1	16SA	1909	C
1	16SA	1912	A
1	16SA	1913	A
1	16SA	1914	A
1	16SA	1916	A
1	16SA	1919	U
1	16SA	1924	C
1	16SA	1926	A
1	16SA	1927	G
1	16SA	1928	U
1	16SA	1929	U
1	16SA	1932	G
1	16SA	1933	A
1	16SA	1941	C
1	16SA	1945	A
1	16SA	1946	A
1	16SA	1947	C
1	16SA	1948	C
1	16SA	1949	C
1	16SA	1950	G
1	16SA	1954	C
1	16SA	1962	C
1	16SA	1963	C
1	16SA	1965	G
1	16SA	1973	A
1	16SA	1980	G
1	16SA	1990	C
1	16SA	1991	A
1	16SA	1992	U
1	16SA	1996	G
1	16SA	1998	G
1	16SA	2026	A
1	16SA	2047	G
1	16SA	2070	G
1	16SA	2071	G
1	16SA	2072	A
1	16SA	2073	G
1	16SA	2077	A
1	16SA	2078	C

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Mol	Chain	Res	Type
1	16SA	2079	G
1	16SA	2080	G
1	16SA	2092	G
1	16SA	2110	G
1	16SA	2115	A
1	16SA	2120	G
1	16SA	2122	A
1	16SA	2125	A
1	16SA	2127	G
1	16SA	2129	U
1	16SA	2140	G
1	16SA	2143	G
1	16SA	2152	G
1	16SA	2153	G
1	16SA	2154	A
22	ASIA	2	C
22	ASIA	3	C
22	ASIA	5	G
22	ASIA	7	A
22	ASIA	8	4SU
22	ASIA	9	A
22	ASIA	10	G
22	ASIA	11	C
22	ASIA	14	A
22	ASIA	15	G
22	ASIA	16	U
22	ASIA	17	C
22	ASIA	18	G
22	ASIA	19	G
22	ASIA	20	U
22	ASIA	21	A
22	ASIA	22	G
22	ASIA	24	G
22	ASIA	30	G
22	ASIA	36	A
22	ASIA	42	C
22	ASIA	44	G
22	ASIA	45	U
22	ASIA	46	7MG
22	ASIA	47	U
22	ASIA	48	C
22	ASIA	49	C

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Mol	Chain	Res	Type
22	ASIA	52	G
22	ASIA	53	G
22	ASIA	55	PSU
22	ASIA	58	A
22	ASIA	59	U
22	ASIA	60	U
22	ASIA	61	C
22	ASIA	63	G
22	ASIA	64	A
22	ASIA	66	U
22	ASIA	70	G
22	ASIA	72	C
22	ASIA	73	A
22	ASIA	74	C
22	ASIA	75	C
22	ASIA	76	A
23	PSIA	2	C
23	PSIA	3	C
23	PSIA	8	4SU
23	PSIA	11	C
23	PSIA	13	C
23	PSIA	17	C
23	PSIA	18	G
23	PSIA	20	U
23	PSIA	21	A
23	PSIA	22	G
23	PSIA	25	C
23	PSIA	30	G
23	PSIA	38	A
23	PSIA	44	G
23	PSIA	45	U
23	PSIA	46	7MG
23	PSIA	48	C
23	PSIA	55	PSU
23	PSIA	56	C
23	PSIA	58	A
23	PSIA	63	G
23	PSIA	69	G
24	ESIA	2	C
24	ESIA	3	C
24	ESIA	8	U
24	ESIA	9	A

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Mol	Chain	Res	Type
24	ESIA	10	G
24	ESIA	14	A
24	ESIA	15	G
24	ESIA	16	U
24	ESIA	17	C
24	ESIA	18	G
24	ESIA	19	G
24	ESIA	20	U
24	ESIA	21	A
24	ESIA	22	G
24	ESIA	30	G
24	ESIA	38	A
24	ESIA	42	C
24	ESIA	45	U
24	ESIA	46	G
24	ESIA	47	U
24	ESIA	48	C
24	ESIA	49	C
24	ESIA	53	G
24	ESIA	55	U
24	ESIA	56	C
24	ESIA	58	A
24	ESIA	59	U
24	ESIA	63	G
24	ESIA	65	G
24	ESIA	66	U
24	ESIA	72	C
24	ESIA	73	A
24	ESIA	76	A
25	MRNA	33	G
25	MRNA	43	U
25	MRNA	45	U
25	MRNA	46	U
25	MRNA	54	U
25	MRNA	56	U
25	MRNA	57	U
26	TRNA	2	C
26	TRNA	3	C
26	TRNA	6	G
26	TRNA	8	4SU
26	TRNA	10	G
26	TRNA	11	C

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Mol	Chain	Res	Type
26	TRNA	12	U
26	TRNA	13	C
26	TRNA	15	G
26	TRNA	16	U
26	TRNA	19	G
26	TRNA	20	U
26	TRNA	21	A
26	TRNA	22	G
26	TRNA	23	A
26	TRNA	27	G
26	TRNA	35	A
26	TRNA	38	A
26	TRNA	40	C
26	TRNA	43	C
26	TRNA	44	G
26	TRNA	45	U
26	TRNA	46	G
26	TRNA	47	U
26	TRNA	48	C
26	TRNA	49	C
26	TRNA	50	U
26	TRNA	52	G
26	TRNA	53	G
26	TRNA	54	5MU
26	TRNA	58	A
26	TRNA	63	G
26	TRNA	66	U
27	23SA	3	U
27	23SA	4	C
27	23SA	5	A
27	23SA	10	G
27	23SA	15	G
27	23SA	34	C
27	23SA	35	G
27	23SA	45	C
27	23SA	48	A
27	23SA	57	G
27	23SA	59	G
27	23SA	60	G
27	23SA	62	U
27	23SA	70	A
27	23SA	71	U

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Mol	Chain	Res	Type
27	23SA	73	A
27	23SA	74	G
27	23SA	77	A
27	23SA	82	G
27	23SA	83	A
27	23SA	89	U
27	23SA	100	G
27	23SA	116	A
27	23SA	117	A
27	23SA	118	U
27	23SA	129	G
27	23SA	137	G
27	23SA	155	C
27	23SA	157	U
27	23SA	158	U
27	23SA	160	U
27	23SA	186	A
27	23SA	189	A
27	23SA	204	G
27	23SA	205	G
27	23SA	206	A
27	23SA	207	G
27	23SA	211	A
27	23SA	212	A
27	23SA	213	A
27	23SA	217	A
27	23SA	218	A
27	23SA	219	A
27	23SA	220	U
27	23SA	222	G
27	23SA	223	A
27	23SA	229	U
27	23SA	238	G
27	23SA	239	C
27	23SA	242	G
27	23SA	255	A
27	23SA	256	G
27	23SA	272	U
27	23SA	273	U
27	23SA	274	G
27	23SA	276	C
27	23SA	289	U

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Mol	Chain	Res	Type
27	23SA	290	G
27	23SA	297	U
27	23SA	298	C
27	23SA	304	C
27	23SA	324	A
27	23SA	336	A
27	23SA	340	G
27	23SA	349	A
27	23SA	354	G
27	23SA	355	A
27	23SA	367	G
27	23SA	377	G
27	23SA	388	G
27	23SA	393	U
27	23SA	395	C
27	23SA	400	G
27	23SA	401	U
27	23SA	414	G
27	23SA	424	G
27	23SA	432	C
27	23SA	433	U
27	23SA	435	G
27	23SA	439	G
27	23SA	449	C
27	23SA	457	A
27	23SA	472	C
27	23SA	476	U
27	23SA	479	C
27	23SA	482	A
27	23SA	483	C
27	23SA	485	A
27	23SA	492	U
27	23SA	498	A
27	23SA	499	A
27	23SA	507	A
27	23SA	509	G
27	23SA	523	G
27	23SA	531	U
27	23SA	532	A
27	23SA	535	G
27	23SA	536	C
27	23SA	537	C

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Mol	Chain	Res	Type
27	23SA	555	A
27	23SA	556	A
27	23SA	557	G
27	23SA	558	C
27	23SA	559	A
27	23SA	560	G
27	23SA	563	A
27	23SA	564	C
27	23SA	565	G
27	23SA	572	C
27	23SA	575	G
27	23SA	581	G
27	23SA	588	G
27	23SA	589	C
27	23SA	595	G
27	23SA	598	G
27	23SA	600	A
27	23SA	608	G
27	23SA	613	U
27	23SA	617	G
27	23SA	618	G
27	23SA	627	G
27	23SA	628	A
27	23SA	632	U
27	23SA	635	G
27	23SA	639	U
27	23SA	640	U
27	23SA	641	G
27	23SA	643	G
27	23SA	644	G
27	23SA	647	G
27	23SA	648	A
27	23SA	649	G
27	23SA	654	A
27	23SA	656	G
27	23SA	664	A
27	23SA	672	C
27	23SA	673	A
27	23SA	681	A
27	23SA	682	A
27	23SA	684	G
27	23SA	699	C

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Mol	Chain	Res	Type
27	23SA	700	G
27	23SA	701	A
27	23SA	706	U
27	23SA	719	A
27	23SA	726	A
27	23SA	735	G
27	23SA	750	G
27	23SA	758	U
27	23SA	779	C
27	23SA	789	U
27	23SA	811	U
27	23SA	824	G
27	23SA	825	G
27	23SA	831	A
27	23SA	833	A
27	23SA	834	G
27	23SA	839	C
27	23SA	841	G
27	23SA	842	A
27	23SA	854	G
27	23SA	861	C
27	23SA	868	A
27	23SA	876	U
27	23SA	877	U
27	23SA	881	G
27	23SA	895	C
27	23SA	896	U
27	23SA	908	G
27	23SA	926	U
27	23SA	927	A
27	23SA	929	G
27	23SA	930	G
27	23SA	931	G
27	23SA	932	G
27	23SA	933	C
27	23SA	934	C
27	23SA	935	C
27	23SA	936	A
27	23SA	937	C
27	23SA	938	C
27	23SA	939	A
27	23SA	940	G

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Mol	Chain	Res	Type
27	23SA	941	C
27	23SA	944	A
27	23SA	945	C
27	23SA	946	C
27	23SA	947	A
27	23SA	948	A
27	23SA	952	C
27	23SA	954	G
27	23SA	958	A
27	23SA	959	A
27	23SA	963	C
27	23SA	965	A
27	23SA	967	G
27	23SA	978	G
27	23SA	979	G
27	23SA	985	G
27	23SA	988	A
27	23SA	992	A
27	23SA	993	G
27	23SA	1000	A
27	23SA	1006	A
27	23SA	1008	C
27	23SA	1021	G
27	23SA	1028	A
27	23SA	1031	A
27	23SA	1038	A
27	23SA	1039	C
27	23SA	1044	A
27	23SA	1058	A
27	23SA	1059	G
27	23SA	1060	U
27	23SA	1061	C
27	23SA	1070	G
27	23SA	1071	U
27	23SA	1073	G
27	23SA	1074	U
27	23SA	1075	A
27	23SA	1081	U
27	23SA	1086	C
27	23SA	1093	A
27	23SA	1095	G
27	23SA	1098	A

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Mol	Chain	Res	Type
27	23SA	1106	U
27	23SA	1108	U
27	23SA	1110	G
27	23SA	1119	G
27	23SA	1122	G
27	23SA	1124	C
27	23SA	1125	A
27	23SA	1126	U
27	23SA	1127	C
27	23SA	1130	U
27	23SA	1131	U
27	23SA	1132	A
27	23SA	1133	A
27	23SA	1134	A
27	23SA	1135	G
27	23SA	1136	A
27	23SA	1138	U
27	23SA	1139	G
27	23SA	1158	G
27	23SA	1159	A
27	23SA	1160	G
27	23SA	1170	G
27	23SA	1177	A
27	23SA	1178	U
27	23SA	1179	G
27	23SA	1183	C
27	23SA	1184	G
27	23SA	1186	G
27	23SA	1187	G
27	23SA	1190	U
27	23SA	1191	A
27	23SA	1192	A
27	23SA	1198	G
27	23SA	1205	A
27	23SA	1206	G
27	23SA	1208	U
27	23SA	1217	G
27	23SA	1221	G
27	23SA	1223	U
27	23SA	1224	G
27	23SA	1225	A
27	23SA	1227	C

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Mol	Chain	Res	Type
27	23SA	1228	C
27	23SA	1243	G
27	23SA	1245	G
27	23SA	1252	A
27	23SA	1253	U
27	23SA	1254	G
27	23SA	1259	U
27	23SA	1268	A
27	23SA	1269	C
27	23SA	1276	G
27	23SA	1293	G
27	23SA	1302	A
27	23SA	1305	G
27	23SA	1314	A
27	23SA	1318	A
27	23SA	1320	G
27	23SA	1321	A
27	23SA	1322	U
27	23SA	1335	A
27	23SA	1349	U
27	23SA	1350	A
27	23SA	1358	G
27	23SA	1362	U
27	23SA	1363	C
27	23SA	1368	G
27	23SA	1378	U
27	23SA	1390	U
27	23SA	1394	C
27	23SA	1398	A
27	23SA	1401	U
27	23SA	1408	A
27	23SA	1409	A
27	23SA	1414	A
27	23SA	1419	C
27	23SA	1428	A
27	23SA	1433	A
27	23SA	1434	G
27	23SA	1435	C
27	23SA	1437	G
27	23SA	1460	C
27	23SA	1465	G
27	23SA	1466	C

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Mol	Chain	Res	Type
27	23SA	1468	A
27	23SA	1469	U
27	23SA	1470	G
27	23SA	1477	C
27	23SA	1486	C
27	23SA	1492	G
27	23SA	1494	A
27	23SA	1499	A
27	23SA	1500	G
27	23SA	1502	C
27	23SA	1505	G
27	23SA	1508	C
27	23SA	1509	G
27	23SA	1511	G
27	23SA	1517	C
27	23SA	1521	A
27	23SA	1524	C
27	23SA	1525	G
27	23SA	1526	C
27	23SA	1528	G
27	23SA	1531	U
27	23SA	1532	G
27	23SA	1534	G
27	23SA	1535	A
27	23SA	1536	G
27	23SA	1539	A
27	23SA	1542	C
27	23SA	1546	U
27	23SA	1554	C
27	23SA	1555	C
27	23SA	1557	A
27	23SA	1558	C
27	23SA	1559	A
27	23SA	1563	U
27	23SA	1564	C
27	23SA	1565	U
27	23SA	1574	G
27	23SA	1577	A
27	23SA	1582	C
27	23SA	1583	G
27	23SA	1584	U
27	23SA	1586	C

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Mol	Chain	Res	Type
27	23SA	1587	G
27	23SA	1592	A
27	23SA	1593	C
27	23SA	1594	A
27	23SA	1604	A
27	23SA	1605	G
27	23SA	1608	A
27	23SA	1609	G
27	23SA	1610	G
27	23SA	1616	A
27	23SA	1619	A
27	23SA	1628	U
27	23SA	1629	A
27	23SA	1635	A
27	23SA	1642	G
27	23SA	1644	G
27	23SA	1647	C
27	23SA	1657	A
27	23SA	1659	A
27	23SA	1660	C
27	23SA	1666	C
27	23SA	1667	A
27	23SA	1671	G
27	23SA	1696	C
27	23SA	1698	C
27	23SA	1703	G
27	23SA	1704	A
27	23SA	1724	G
27	23SA	1745	G
27	23SA	1753	G
27	23SA	1766	G
27	23SA	1769	G
27	23SA	1770	A
27	23SA	1771	U
27	23SA	1772	G
27	23SA	1773	A
27	23SA	1776	C
27	23SA	1784	G
27	23SA	1792	G
27	23SA	1796	A
27	23SA	1797	G
27	23SA	1798	G

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Mol	Chain	Res	Type
27	23SA	1807	A
27	23SA	1814	A
27	23SA	1816	C
27	23SA	1825	A
27	23SA	1832	U
27	23SA	1833	G
27	23SA	1834	C
27	23SA	1835	G
27	23SA	1850	G
27	23SA	1854	U
27	23SA	1863	A
27	23SA	1873	G
27	23SA	1880	G
27	23SA	1881	A
27	23SA	1882	A
27	23SA	1883	G
27	23SA	1892	G
27	23SA	1899	G
27	23SA	1902	A
27	23SA	1903	G
27	23SA	1907	C
27	23SA	1913	G
27	23SA	1914	A
27	23SA	1925	A
27	23SA	1931	G
27	23SA	1939	C
27	23SA	1954	G
27	23SA	1955	G
27	23SA	1961	A
27	23SA	1962	A
27	23SA	1963	A
27	23SA	1964	5MU
27	23SA	1980	U
27	23SA	1985	A
27	23SA	1988	U
27	23SA	1989	G
27	23SA	1992	C
27	23SA	1994	A
27	23SA	1995	A
27	23SA	1996	A
27	23SA	1997	A
27	23SA	2007	C

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Mol	Chain	Res	Type
27	23SA	2016	U
27	23SA	2018	U
27	23SA	2045	A
27	23SA	2048	G
27	23SA	2052	G
27	23SA	2056	A
27	23SA	2057	G
27	23SA	2058	A
27	23SA	2068	C
27	23SA	2076	A
27	23SA	2079	A
27	23SA	2080	C
27	23SA	2081	G
27	23SA	2084	A
27	23SA	2085	A
27	23SA	2086	G
27	23SA	2094	G
27	23SA	2118	G
27	23SA	2124	U
27	23SA	2125	G
27	23SA	2126	G
27	23SA	2136	C
27	23SA	2138	U
27	23SA	2139	A
27	23SA	2140	G
27	23SA	2141	G
27	23SA	2142	A
27	23SA	2143	U
27	23SA	2144	A
27	23SA	2145	G
27	23SA	2150	G
27	23SA	2152	G
27	23SA	2153	C
27	23SA	2154	C
27	23SA	2157	U
27	23SA	2158	G
27	23SA	2161	C
27	23SA	2170	C
27	23SA	2171	C
27	23SA	2172	G
27	23SA	2173	G
27	23SA	2183	A

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Mol	Chain	Res	Type
27	23SA	2185	G
27	23SA	2188	C
27	23SA	2191	G
27	23SA	2193	G
27	23SA	2194	A
27	23SA	2195	A
27	23SA	2196	A
27	23SA	2197	U
27	23SA	2198	A
27	23SA	2199	C
27	23SA	2201	A
27	23SA	2203	C
27	23SA	2206	G
27	23SA	2214	U
27	23SA	2215	G
27	23SA	2217	G
27	23SA	2223	A
27	23SA	2230	G
27	23SA	2231	G
27	23SA	2232	A
27	23SA	2233	U
27	23SA	2234	G
27	23SA	2240	A
27	23SA	2253	G
27	23SA	2254	G
27	23SA	2261	G
27	23SA	2267	G
27	23SA	2282	A
27	23SA	2288	A
27	23SA	2290	C
27	23SA	2293	A
27	23SA	2295	G
27	23SA	2298	C
27	23SA	2302	A
27	23SA	2303	A
27	23SA	2304	G
27	23SA	2319	G
27	23SA	2320	A
27	23SA	2322	G
27	23SA	2323	G
27	23SA	2327	U
27	23SA	2329	C

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Mol	Chain	Res	Type
27	23SA	2334	G
27	23SA	2335	A
27	23SA	2336	G
27	23SA	2340	G
27	23SA	2341	C
27	23SA	2349	G
27	23SA	2351	A
27	23SA	2361	A
27	23SA	2362	C
27	23SA	2365	C
27	23SA	2394	G
27	23SA	2398	G
27	23SA	2400	C
27	23SA	2406	G
27	23SA	2407	A
27	23SA	2421	U
27	23SA	2422	G
27	23SA	2426	A
27	23SA	2437	A
27	23SA	2438	U
27	23SA	2439	C
27	23SA	2440	A
27	23SA	2441	A
27	23SA	2442	C
27	23SA	2443	G
27	23SA	2444	G
27	23SA	2445	A
27	23SA	2450	A
27	23SA	2454	A
27	23SA	2455	C
27	23SA	2456	C
27	23SA	2463	A
27	23SA	2475	U
27	23SA	2484	A
27	23SA	2485	G
27	23SA	2488	U
27	23SA	2489	C
27	23SA	2490	C
27	23SA	2491	A
27	23SA	2497	G
27	23SA	2509	G
27	23SA	2517	G

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Mol	Chain	Res	Type
27	23SA	2519	U
27	23SA	2520	G
27	23SA	2522	C
27	23SA	2533	A
27	23SA	2534	U
27	23SA	2540	G
27	23SA	2544	G
27	23SA	2558	G
27	23SA	2569	U
27	23SA	2581	A
27	23SA	2582	G
27	23SA	2588	C
27	23SA	2597	G
27	23SA	2600	U
27	23SA	2614	G
27	23SA	2617	A
27	23SA	2624	U
27	23SA	2625	C
27	23SA	2626	U
27	23SA	2627	C
27	23SA	2644	A
27	23SA	2645	G
27	23SA	2661	C
27	23SA	2669	A
27	23SA	2670	G
27	23SA	2680	A
27	23SA	2681	C
27	23SA	2688	G
27	23SA	2694	A
27	23SA	2697	U
27	23SA	2701	G
27	23SA	2704	U
27	23SA	2706	C
27	23SA	2717	U
27	23SA	2718	C
27	23SA	2722	G
27	23SA	2727	U
27	23SA	2728	A
27	23SA	2729	A
27	23SA	2730	G
27	23SA	2742	U
27	23SA	2743	G

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Mol	Chain	Res	Type
27	23SA	2749	A
27	23SA	2750	A
27	23SA	2760	G
27	23SA	2764	A
27	23SA	2767	G
27	23SA	2768	C
27	23SA	2773	A
27	23SA	2777	G
27	23SA	2778	G
27	23SA	2780	A
27	23SA	2781	A
27	23SA	2782	G
27	23SA	2786	G
27	23SA	2794	A
27	23SA	2795	U
27	23SA	2806	A
27	23SA	2807	C
27	23SA	2809	G
27	23SA	2810	C
27	23SA	2812	U
27	23SA	2815	A
27	23SA	2821	U
27	23SA	2826	A
27	23SA	2831	G
27	23SA	2833	A
27	23SA	2834	A
27	23SA	2836	A
27	23SA	2843	G
27	23SA	2845	U
27	23SA	2846	G
27	23SA	2847	G
27	23SA	2848	A
27	23SA	2885	G
27	23SA	2886	A
27	23SA	2892	C
27	23SA	2893	C
27	23SA	2899	G
27	23SA	2903	G
27	23SA	2904	A
27	23SA	2906	G
28	5SA	9	G
28	5SA	13	C

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Mol	Chain	Res	Type
28	5SA	14	C
28	5SA	15	A
28	5SA	17	A
28	5SA	18	G
28	5SA	21	G
28	5SA	27	A
28	5SA	29	C
28	5SA	33	C
28	5SA	42	U
28	5SA	43	U
28	5SA	44	C
28	5SA	54	A
28	5SA	55	A
28	5SA	58	G
28	5SA	68	A
28	5SA	69	G
28	5SA	75	A
28	5SA	83	G
28	5SA	87	G
28	5SA	91	G
28	5SA	98	U
28	5SA	104	A
28	5SA	112	G
1	16SB	654	A
1	16SB	655	G
1	16SB	656	A
1	16SB	678	A
1	16SB	685	G
1	16SB	687	G
1	16SB	693	C
1	16SB	694	C
1	16SB	697	A
1	16SB	700	C
1	16SB	711	U
1	16SB	712	G
1	16SB	719	G
1	16SB	723	G
1	16SB	729	A
1	16SB	730	C
1	16SB	732	C
1	16SB	733	C
1	16SB	735	U

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Mol	Chain	Res	Type
1	16SB	740	A
1	16SB	747	G
1	16SB	755	A
1	16SB	759	A
1	16SB	760	C
1	16SB	771	C
1	16SB	777	C
1	16SB	803	C
1	16SB	809	C
1	16SB	814	C
1	16SB	821	G
1	16SB	822	U
1	16SB	823	G
1	16SB	826	C
1	16SB	832	C
1	16SB	834	U
1	16SB	835	U
1	16SB	836	G
1	16SB	837	G
1	16SB	840	U
1	16SB	841	G
1	16SB	847	A
1	16SB	848	A
1	16SB	849	A
1	16SB	854	U
1	16SB	855	U
1	16SB	856	U
1	16SB	857	G
1	16SB	872	G
1	16SB	885	U
1	16SB	888	G
1	16SB	892	G
1	16SB	903	A
1	16SB	907	G
1	16SB	908	C
1	16SB	921	C
1	16SB	922	G
1	16SB	930	G
1	16SB	962	A
1	16SB	969	C
1	16SB	970	A
1	16SB	973	G

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Mol	Chain	Res	Type
1	16SB	982	C
1	16SB	986	C
1	16SB	987	G
1	16SB	988	G
1	16SB	991	G
1	16SB	992	G
1	16SB	993	C
1	16SB	994	A
1	16SB	995	G
1	16SB	1008	U
1	16SB	1013	C
1	16SB	1014	A
1	16SB	1029	G
1	16SB	1038	A
1	16SB	1039	C
1	16SB	1047	G
1	16SB	1050	G
1	16SB	1053	A
1	16SB	1054	G
1	16SB	1055	A
1	16SB	1060	C
1	16SB	1063	C
1	16SB	1064	G
1	16SB	1065	G
1	16SB	1070	U
1	16SB	1071	A
1	16SB	1075	U
1	16SB	1080	A
1	16SB	1082	C
1	16SB	1092	A
1	16SB	1100	A
1	16SB	1101	C
1	16SB	1102	G
1	16SB	1105	G
1	16SB	1112	A
1	16SB	1115	G
1	16SB	1116	U
1	16SB	1126	A
1	16SB	1127	U
1	16SB	1134	G
1	16SB	1138	A
1	16SB	1139	A

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Mol	Chain	Res	Type
1	16SB	1140	C
1	16SB	1147	C
1	16SB	1156	7MG
1	16SB	1159	G
1	16SB	1160	U
1	16SB	1161	A
1	16SB	1162	A
1	16SB	1165	C
1	16SB	1174	C
1	16SB	1176	A
1	16SB	1188	A
1	16SB	1190	U
1	16SB	1191	C
1	16SB	1193	C
1	16SB	1197	G
1	16SB	1201	A
1	16SB	1202	A
1	16SB	1205	G
1	16SB	1236	A
1	16SB	1243	A
1	16SB	1252	C
1	16SB	1256	G
1	16SB	1260	G
1	16SB	1279	G
1	16SB	1282	A
1	16SB	1290	G
1	16SB	1291	G
1	16SB	1294	A
1	16SB	1300	G
1	16SB	1316	A
1	16SB	1317	G
1	16SB	1330	C
1	16SB	1331	A
1	16SB	1332	G
1	16SB	1333	A
1	16SB	1350	G
1	16SB	1352	U
1	16SB	1353	G
1	16SB	1360	G
1	16SB	1363	G
1	16SB	1377	C
1	16SB	1378	C

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Mol	Chain	Res	Type
1	16SB	1381	G
1	16SB	1382	A
1	16SB	1384	G
1	16SB	1395	A
1	16SB	1406	A
1	16SB	1407	G
1	16SB	1422	U
1	16SB	1423	A
1	16SB	1431	A
1	16SB	1444	A
1	16SB	1446	C
1	16SB	1450	G
1	16SB	1457	A
1	16SB	1468	U
1	16SB	1470	U
1	16SB	1471	C
1	16SB	1476	G
1	16SB	1495	A
1	16SB	1496	A
1	16SB	1497	G
1	16SB	1536	A
1	16SB	1537	A
1	16SB	1549	G
1	16SB	1550	G
1	16SB	1557	C
1	16SB	1558	A
1	16SB	1559	C
1	16SB	1583	U
1	16SB	1584	U
1	16SB	1589	M2G
1	16SB	1591	A
1	16SB	1592	A
1	16SB	1594	G
1	16SB	1595	C
1	16SB	1597	A
1	16SB	1598	A
1	16SB	1599	G
1	16SB	1600	A
1	16SB	1601	A
1	16SB	1602	C
1	16SB	1603	C
1	16SB	1604	U

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Mol	Chain	Res	Type
1	16SB	1609	A
1	16SB	1614	U
1	16SB	1615	U
1	16SB	1616	G
1	16SB	1621	G
1	16SB	1629	A
1	16SB	1630	C
1	16SB	1633	G
1	16SB	1640	A
1	16SB	1641	G
1	16SB	1645	G
1	16SB	1647	G
1	16SB	1648	G
1	16SB	1649	U
1	16SB	1650	G
1	16SB	1652	C
1	16SB	1653	C
1	16SB	1654	C
1	16SB	1655	G
1	16SB	1657	G
1	16SB	1659	G
1	16SB	1661	G
1	16SB	1663	A
1	16SB	1664	G
1	16SB	1668	U
1	16SB	1674	A
1	16SB	1678	G
1	16SB	1681	G
1	16SB	1682	C
1	16SB	1683	A
1	16SB	1694	C
1	16SB	1709	G
1	16SB	1710	G
1	16SB	1722	G
1	16SB	1723	U
1	16SB	1727	G
1	16SB	1729	A
1	16SB	1745	G
1	16SB	1750	U
1	16SB	1752	G
1	16SB	1753	U
1	16SB	1755	G

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Mol	Chain	Res	Type
1	16SB	1756	C
1	16SB	1757	C
1	16SB	1758	A
1	16SB	1759	G
1	16SB	1764	U
1	16SB	1765	C
1	16SB	1766	G
1	16SB	1767	G
1	16SB	1768	C
1	16SB	1774	A
1	16SB	1775	C
1	16SB	1782	G
1	16SB	1785	A
1	16SB	1786	C
1	16SB	1787	U
1	16SB	1788	G
1	16SB	1789	C
1	16SB	1798	G
1	16SB	1808	G
1	16SB	1810	A
1	16SB	1811	G
1	16SB	1812	G
1	16SB	1814	G
1	16SB	1815	A
1	16SB	1817	G
1	16SB	1820	G
1	16SB	1823	U
1	16SB	1825	G
1	16SB	1827	C
1	16SB	1828	A
1	16SB	1829	G
1	16SB	1834	2MG
1	16SB	1838	U
1	16SB	1839	U
1	16SB	1840	A
1	16SB	1841	C
1	16SB	1845	C
1	16SB	1852	A
1	16SB	1854	A
1	16SB	1865	A
1	16SB	1868	G
1	16SB	1883	A

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Mol	Chain	Res	Type
1	16SB	1884	U
1	16SB	1885	G
1	16SB	1887	C
1	16SB	1891	C
1	16SB	1899	G
1	16SB	1900	G
1	16SB	1905	U
1	16SB	1907	A
1	16SB	1908	U
1	16SB	1912	A
1	16SB	1913	A
1	16SB	1914	A
1	16SB	1916	A
1	16SB	1919	U
1	16SB	1924	C
1	16SB	1925	C
1	16SB	1926	A
1	16SB	1928	U
1	16SB	1932	G
1	16SB	1933	A
1	16SB	1941	C
1	16SB	1945	A
1	16SB	1946	A
1	16SB	1947	C
1	16SB	1948	C
1	16SB	1949	C
1	16SB	1954	C
1	16SB	1958	G
1	16SB	1962	C
1	16SB	1963	C
1	16SB	1964	G
1	16SB	1965	G
1	16SB	1973	A
1	16SB	1974	G
1	16SB	1980	G
1	16SB	1990	C
1	16SB	1991	A
1	16SB	1992	U
1	16SB	1996	G
1	16SB	1998	G
1	16SB	2015	G
1	16SB	2025	C

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Mol	Chain	Res	Type
1	16SB	2026	A
1	16SB	2047	G
1	16SB	2070	G
1	16SB	2071	G
1	16SB	2072	A
1	16SB	2076	U
1	16SB	2077	A
1	16SB	2078	C
1	16SB	2079	G
1	16SB	2110	G
1	16SB	2115	A
1	16SB	2122	A
1	16SB	2129	U
1	16SB	2140	G
1	16SB	2143	G
1	16SB	2152	G
1	16SB	2153	G
1	16SB	2160	U
1	16SB	2161	C
57	ASIB	8	U
57	ASIB	9	A
57	ASIB	10	G
57	ASIB	11	C
57	ASIB	12	U
57	ASIB	13	C
57	ASIB	16	U
57	ASIB	17	C
57	ASIB	18	G
57	ASIB	19	G
57	ASIB	21	A
57	ASIB	22	G
57	ASIB	24	G
57	ASIB	26	A
57	ASIB	41	C
57	ASIB	44	G
57	ASIB	46	G
57	ASIB	47	U
57	ASIB	48	C
57	ASIB	49	C
57	ASIB	50	U
57	ASIB	53	G
57	ASIB	56	C

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Mol	Chain	Res	Type
57	ASIB	58	A
57	ASIB	59	U
57	ASIB	60	U
57	ASIB	63	G
57	ASIB	64	A
57	ASIB	69	G
57	ASIB	70	G
57	ASIB	71	G
57	ASIB	72	C
57	ASIB	73	A
57	ASIB	74	C
57	ASIB	75	C
57	ASIB	76	A
23	PSIB	2	C
23	PSIB	3	C
23	PSIB	8	4SU
23	PSIB	9	A
23	PSIB	11	C
23	PSIB	15	G
23	PSIB	16	U
23	PSIB	17	C
23	PSIB	18	G
23	PSIB	19	G
23	PSIB	20	U
23	PSIB	21	A
23	PSIB	22	G
23	PSIB	25	C
23	PSIB	30	G
23	PSIB	42	C
23	PSIB	43	C
23	PSIB	44	G
23	PSIB	45	U
23	PSIB	48	C
23	PSIB	52	G
23	PSIB	54	5MU
23	PSIB	56	C
23	PSIB	58	A
23	PSIB	61	C
23	PSIB	67	C
23	PSIB	70	G
23	PSIB	74	C
23	PSIB	76	A

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Mol	Chain	Res	Type
24	ESIB	2	C
24	ESIB	9	A
24	ESIB	13	C
24	ESIB	14	A
24	ESIB	16	U
24	ESIB	17	C
24	ESIB	18	G
24	ESIB	19	G
24	ESIB	20	U
24	ESIB	21	A
24	ESIB	22	G
24	ESIB	34	G
24	ESIB	36	A
24	ESIB	38	A
24	ESIB	40	C
24	ESIB	46	G
24	ESIB	48	C
24	ESIB	58	A
24	ESIB	59	U
24	ESIB	65	G
24	ESIB	72	C
24	ESIB	73	A
24	ESIB	76	A
25	MRNB	29	G
25	MRNB	37	G
25	MRNB	43	U
25	MRNB	46	U
25	MRNB	49	U
25	MRNB	51	U
25	MRNB	52	U
25	MRNB	54	U
25	MRNB	55	U
25	MRNB	56	U
25	MRNB	57	U
27	23SB	3	U
27	23SB	4	C
27	23SB	5	A
27	23SB	10	G
27	23SB	13	A
27	23SB	15	G
27	23SB	34	C
27	23SB	35	G

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Mol	Chain	Res	Type
27	23SB	45	C
27	23SB	48	A
27	23SB	49	U
27	23SB	50	G
27	23SB	57	G
27	23SB	59	G
27	23SB	60	G
27	23SB	62	U
27	23SB	68	C
27	23SB	70	A
27	23SB	73	A
27	23SB	74	G
27	23SB	77	A
27	23SB	82	G
27	23SB	83	A
27	23SB	84	G
27	23SB	85	C
27	23SB	89	U
27	23SB	94	G
27	23SB	100	G
27	23SB	116	A
27	23SB	117	A
27	23SB	118	U
27	23SB	119	G
27	23SB	127	C
27	23SB	137	G
27	23SB	140	A
27	23SB	155	C
27	23SB	156	U
27	23SB	157	U
27	23SB	162	C
27	23SB	163	G
27	23SB	164	C
27	23SB	186	A
27	23SB	189	A
27	23SB	196	U
27	23SB	204	G
27	23SB	205	G
27	23SB	206	A
27	23SB	207	G
27	23SB	211	A
27	23SB	212	A

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Mol	Chain	Res	Type
27	23SB	217	A
27	23SB	219	A
27	23SB	223	A
27	23SB	238	G
27	23SB	239	C
27	23SB	242	G
27	23SB	255	A
27	23SB	256	G
27	23SB	271	C
27	23SB	272	U
27	23SB	273	U
27	23SB	274	G
27	23SB	275	U
27	23SB	276	C
27	23SB	282	G
27	23SB	289	U
27	23SB	290	G
27	23SB	296	C
27	23SB	298	C
27	23SB	301	A
27	23SB	302	C
27	23SB	303	A
27	23SB	304	C
27	23SB	308	A
27	23SB	311	C
27	23SB	313	C
27	23SB	314	A
27	23SB	315	G
27	23SB	320	G
27	23SB	336	A
27	23SB	340	G
27	23SB	342	G
27	23SB	354	G
27	23SB	355	A
27	23SB	356	A
27	23SB	370	A
27	23SB	377	G
27	23SB	381	G
27	23SB	387	U
27	23SB	389	A
27	23SB	390	G
27	23SB	392	G

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Mol	Chain	Res	Type
27	23SB	393	U
27	23SB	394	A
27	23SB	395	C
27	23SB	414	G
27	23SB	424	G
27	23SB	432	C
27	23SB	433	U
27	23SB	434	G
27	23SB	435	G
27	23SB	439	G
27	23SB	457	A
27	23SB	472	C
27	23SB	476	U
27	23SB	479	C
27	23SB	482	A
27	23SB	483	C
27	23SB	485	A
27	23SB	492	U
27	23SB	498	A
27	23SB	499	A
27	23SB	503	U
27	23SB	507	A
27	23SB	509	G
27	23SB	521	G
27	23SB	532	A
27	23SB	535	G
27	23SB	536	C
27	23SB	539	G
27	23SB	556	A
27	23SB	557	G
27	23SB	558	C
27	23SB	559	A
27	23SB	560	G
27	23SB	564	C
27	23SB	575	G
27	23SB	588	G
27	23SB	589	C
27	23SB	595	G
27	23SB	598	G
27	23SB	600	A
27	23SB	608	G
27	23SB	613	U

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Mol	Chain	Res	Type
27	23SB	618	G
27	23SB	628	A
27	23SB	629	G
27	23SB	632	U
27	23SB	635	G
27	23SB	638	G
27	23SB	639	U
27	23SB	640	U
27	23SB	641	G
27	23SB	643	G
27	23SB	644	G
27	23SB	648	A
27	23SB	649	G
27	23SB	653	U
27	23SB	654	A
27	23SB	656	G
27	23SB	664	A
27	23SB	672	C
27	23SB	673	A
27	23SB	678	G
27	23SB	679	C
27	23SB	680	A
27	23SB	681	A
27	23SB	682	A
27	23SB	686	C
27	23SB	699	C
27	23SB	700	G
27	23SB	701	A
27	23SB	706	U
27	23SB	719	A
27	23SB	726	A
27	23SB	735	G
27	23SB	758	U
27	23SB	779	C
27	23SB	807	C
27	23SB	811	U
27	23SB	824	G
27	23SB	825	G
27	23SB	831	A
27	23SB	833	A
27	23SB	834	G
27	23SB	838	A

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Mol	Chain	Res	Type
27	23SB	839	C
27	23SB	841	G
27	23SB	842	A
27	23SB	854	G
27	23SB	861	C
27	23SB	868	A
27	23SB	876	U
27	23SB	877	U
27	23SB	881	G
27	23SB	895	C
27	23SB	896	U
27	23SB	908	G
27	23SB	914	C
27	23SB	920	U
27	23SB	927	A
27	23SB	932	G
27	23SB	934	C
27	23SB	935	C
27	23SB	936	A
27	23SB	937	C
27	23SB	938	C
27	23SB	942	C
27	23SB	944	A
27	23SB	945	C
27	23SB	947	A
27	23SB	948	A
27	23SB	949	A
27	23SB	952	C
27	23SB	954	G
27	23SB	955	U
27	23SB	958	A
27	23SB	963	C
27	23SB	965	A
27	23SB	967	G
27	23SB	978	G
27	23SB	979	G
27	23SB	985	G
27	23SB	988	A
27	23SB	992	A
27	23SB	993	G
27	23SB	1000	A
27	23SB	1005	U

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Mol	Chain	Res	Type
27	23SB	1006	A
27	23SB	1008	C
27	23SB	1021	G
27	23SB	1028	A
27	23SB	1031	A
27	23SB	1038	A
27	23SB	1039	C
27	23SB	1044	A
27	23SB	1058	A
27	23SB	1059	G
27	23SB	1060	U
27	23SB	1061	C
27	23SB	1070	G
27	23SB	1071	U
27	23SB	1073	G
27	23SB	1074	U
27	23SB	1075	A
27	23SB	1081	U
27	23SB	1085	G
27	23SB	1086	C
27	23SB	1092	G
27	23SB	1093	A
27	23SB	1094	A
27	23SB	1095	G
27	23SB	1096	A
27	23SB	1102	A
27	23SB	1104	G
27	23SB	1108	U
27	23SB	1110	G
27	23SB	1128	A
27	23SB	1133	A
27	23SB	1134	A
27	23SB	1135	G
27	23SB	1136	A
27	23SB	1138	U
27	23SB	1139	G
27	23SB	1153	U
27	23SB	1159	A
27	23SB	1160	G
27	23SB	1161	U
27	23SB	1170	G
27	23SB	1176	A

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Mol	Chain	Res	Type
27	23SB	1177	A
27	23SB	1178	U
27	23SB	1179	G
27	23SB	1183	C
27	23SB	1184	G
27	23SB	1187	G
27	23SB	1191	A
27	23SB	1192	A
27	23SB	1205	A
27	23SB	1218	G
27	23SB	1221	G
27	23SB	1222	A
27	23SB	1223	U
27	23SB	1224	G
27	23SB	1225	A
27	23SB	1226	C
27	23SB	1228	C
27	23SB	1243	G
27	23SB	1245	G
27	23SB	1253	U
27	23SB	1254	G
27	23SB	1258	A
27	23SB	1259	U
27	23SB	1260	G
27	23SB	1268	A
27	23SB	1269	C
27	23SB	1302	A
27	23SB	1304	U
27	23SB	1305	G
27	23SB	1314	A
27	23SB	1318	A
27	23SB	1320	G
27	23SB	1321	A
27	23SB	1322	U
27	23SB	1335	A
27	23SB	1349	U
27	23SB	1350	A
27	23SB	1358	G
27	23SB	1362	U
27	23SB	1363	C
27	23SB	1367	C
27	23SB	1368	G

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Mol	Chain	Res	Type
27	23SB	1378	U
27	23SB	1390	U
27	23SB	1394	C
27	23SB	1398	A
27	23SB	1401	U
27	23SB	1408	A
27	23SB	1409	A
27	23SB	1414	A
27	23SB	1417	G
27	23SB	1428	A
27	23SB	1433	A
27	23SB	1434	G
27	23SB	1435	C
27	23SB	1437	G
27	23SB	1456	C
27	23SB	1465	G
27	23SB	1466	C
27	23SB	1469	U
27	23SB	1470	G
27	23SB	1477	C
27	23SB	1486	C
27	23SB	1492	G
27	23SB	1494	A
27	23SB	1499	A
27	23SB	1500	G
27	23SB	1502	C
27	23SB	1508	C
27	23SB	1510	A
27	23SB	1511	G
27	23SB	1516	G
27	23SB	1521	A
27	23SB	1524	C
27	23SB	1525	G
27	23SB	1526	C
27	23SB	1528	G
27	23SB	1529	G
27	23SB	1530	G
27	23SB	1531	U
27	23SB	1532	G
27	23SB	1535	A
27	23SB	1536	G
27	23SB	1537	G

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Mol	Chain	Res	Type
27	23SB	1539	A
27	23SB	1542	C
27	23SB	1548	C
27	23SB	1551	C
27	23SB	1554	C
27	23SB	1557	A
27	23SB	1558	C
27	23SB	1559	A
27	23SB	1564	C
27	23SB	1565	U
27	23SB	1577	A
27	23SB	1583	G
27	23SB	1584	U
27	23SB	1586	C
27	23SB	1587	G
27	23SB	1592	A
27	23SB	1593	C
27	23SB	1594	A
27	23SB	1604	A
27	23SB	1605	G
27	23SB	1608	A
27	23SB	1609	G
27	23SB	1610	G
27	23SB	1616	A
27	23SB	1619	A
27	23SB	1625	C
27	23SB	1628	U
27	23SB	1629	A
27	23SB	1631	G
27	23SB	1635	A
27	23SB	1637	C
27	23SB	1647	C
27	23SB	1657	A
27	23SB	1659	A
27	23SB	1660	C
27	23SB	1667	A
27	23SB	1690	C
27	23SB	1698	C
27	23SB	1703	G
27	23SB	1704	A
27	23SB	1714	A
27	23SB	1724	G

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Mol	Chain	Res	Type
27	23SB	1746	G
27	23SB	1750	A
27	23SB	1751	A
27	23SB	1766	G
27	23SB	1769	G
27	23SB	1770	A
27	23SB	1771	U
27	23SB	1772	G
27	23SB	1776	C
27	23SB	1790	G
27	23SB	1792	G
27	23SB	1796	A
27	23SB	1797	G
27	23SB	1798	G
27	23SB	1807	A
27	23SB	1814	A
27	23SB	1815	C
27	23SB	1816	C
27	23SB	1825	A
27	23SB	1832	U
27	23SB	1834	C
27	23SB	1835	G
27	23SB	1850	G
27	23SB	1854	U
27	23SB	1863	A
27	23SB	1873	G
27	23SB	1880	G
27	23SB	1881	A
27	23SB	1882	A
27	23SB	1883	G
27	23SB	1892	G
27	23SB	1902	A
27	23SB	1903	G
27	23SB	1907	C
27	23SB	1913	G
27	23SB	1914	A
27	23SB	1925	A
27	23SB	1931	G
27	23SB	1939	C
27	23SB	1941	A
27	23SB	1954	G
27	23SB	1955	G

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Mol	Chain	Res	Type
27	23SB	1956	U
27	23SB	1959	C
27	23SB	1961	A
27	23SB	1962	A
27	23SB	1963	A
27	23SB	1964	5MU
27	23SB	1972	C
27	23SB	1973	G
27	23SB	1980	U
27	23SB	1985	A
27	23SB	1988	U
27	23SB	1989	G
27	23SB	1992	C
27	23SB	1995	A
27	23SB	1996	A
27	23SB	1997	A
27	23SB	2007	C
27	23SB	2018	U
27	23SB	2045	A
27	23SB	2048	G
27	23SB	2052	G
27	23SB	2056	A
27	23SB	2057	G
27	23SB	2058	A
27	23SB	2068	C
27	23SB	2076	A
27	23SB	2079	A
27	23SB	2080	C
27	23SB	2081	G
27	23SB	2084	A
27	23SB	2085	A
27	23SB	2086	G
27	23SB	2087	A
27	23SB	2094	G
27	23SB	2118	G
27	23SB	2124	U
27	23SB	2125	G
27	23SB	2126	G
27	23SB	2133	C
27	23SB	2135	G
27	23SB	2136	C
27	23SB	2138	U

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Mol	Chain	Res	Type
27	23SB	2139	A
27	23SB	2140	G
27	23SB	2141	G
27	23SB	2142	A
27	23SB	2143	U
27	23SB	2148	G
27	23SB	2151	A
27	23SB	2152	G
27	23SB	2153	C
27	23SB	2156	G
27	23SB	2157	U
27	23SB	2158	G
27	23SB	2161	C
27	23SB	2166	G
27	23SB	2172	G
27	23SB	2173	G
27	23SB	2174	G
27	23SB	2188	C
27	23SB	2191	G
27	23SB	2194	A
27	23SB	2196	A
27	23SB	2197	U
27	23SB	2198	A
27	23SB	2199	C
27	23SB	2203	C
27	23SB	2214	U
27	23SB	2215	G
27	23SB	2217	G
27	23SB	2219	G
27	23SB	2223	A
27	23SB	2230	G
27	23SB	2231	G
27	23SB	2232	A
27	23SB	2233	U
27	23SB	2234	G
27	23SB	2240	A
27	23SB	2253	G
27	23SB	2254	G
27	23SB	2260	U
27	23SB	2261	G
27	23SB	2267	G
27	23SB	2288	A

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Mol	Chain	Res	Type
27	23SB	2290	C
27	23SB	2295	G
27	23SB	2298	C
27	23SB	2302	A
27	23SB	2303	A
27	23SB	2304	G
27	23SB	2309	C
27	23SB	2319	G
27	23SB	2320	A
27	23SB	2322	G
27	23SB	2323	G
27	23SB	2325	A
27	23SB	2327	U
27	23SB	2329	C
27	23SB	2334	G
27	23SB	2335	A
27	23SB	2336	G
27	23SB	2340	G
27	23SB	2341	C
27	23SB	2349	G
27	23SB	2351	A
27	23SB	2361	A
27	23SB	2362	C
27	23SB	2364	G
27	23SB	2365	C
27	23SB	2387	G
27	23SB	2394	G
27	23SB	2398	G
27	23SB	2400	C
27	23SB	2406	G
27	23SB	2407	A
27	23SB	2417	C
27	23SB	2418	C
27	23SB	2421	U
27	23SB	2426	A
27	23SB	2429	G
27	23SB	2438	U
27	23SB	2439	C
27	23SB	2440	A
27	23SB	2441	A
27	23SB	2443	G
27	23SB	2444	G

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Mol	Chain	Res	Type
27	23SB	2445	A
27	23SB	2449	A
27	23SB	2450	A
27	23SB	2454	A
27	23SB	2455	C
27	23SB	2456	C
27	23SB	2463	A
27	23SB	2475	U
27	23SB	2484	A
27	23SB	2485	G
27	23SB	2487	G
27	23SB	2489	C
27	23SB	2490	C
27	23SB	2491	A
27	23SB	2493	A
27	23SB	2497	G
27	23SB	2509	G
27	23SB	2517	G
27	23SB	2520	G
27	23SB	2521	U
27	23SB	2522	C
27	23SB	2533	A
27	23SB	2534	U
27	23SB	2539	G
27	23SB	2540	G
27	23SB	2544	G
27	23SB	2557	A
27	23SB	2558	G
27	23SB	2569	U
27	23SB	2581	A
27	23SB	2582	G
27	23SB	2584	G
27	23SB	2586	C
27	23SB	2588	C
27	23SB	2600	U
27	23SB	2617	A
27	23SB	2618	G
27	23SB	2624	U
27	23SB	2625	C
27	23SB	2626	U
27	23SB	2627	C
27	23SB	2644	A

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Mol	Chain	Res	Type
27	23SB	2645	G
27	23SB	2660	G
27	23SB	2661	C
27	23SB	2669	A
27	23SB	2670	G
27	23SB	2680	A
27	23SB	2681	C
27	23SB	2687	G
27	23SB	2688	G
27	23SB	2694	A
27	23SB	2701	G
27	23SB	2704	U
27	23SB	2705	C
27	23SB	2706	C
27	23SB	2717	U
27	23SB	2718	C
27	23SB	2722	G
27	23SB	2727	U
27	23SB	2728	A
27	23SB	2729	A
27	23SB	2730	G
27	23SB	2742	U
27	23SB	2743	G
27	23SB	2748	G
27	23SB	2749	A
27	23SB	2750	A
27	23SB	2752	G
27	23SB	2757	A
27	23SB	2760	G
27	23SB	2764	A
27	23SB	2766	A
27	23SB	2767	G
27	23SB	2768	C
27	23SB	2770	U
27	23SB	2773	A
27	23SB	2777	G
27	23SB	2778	G
27	23SB	2781	A
27	23SB	2786	G
27	23SB	2793	G
27	23SB	2794	A
27	23SB	2795	U

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Mol	Chain	Res	Type
27	23SB	2806	A
27	23SB	2807	C
27	23SB	2810	C
27	23SB	2811	G
27	23SB	2812	U
27	23SB	2821	U
27	23SB	2826	A
27	23SB	2831	G
27	23SB	2833	A
27	23SB	2834	A
27	23SB	2836	A
27	23SB	2839	A
27	23SB	2840	C
27	23SB	2846	G
27	23SB	2847	G
27	23SB	2848	A
27	23SB	2873	A
27	23SB	2879	U
27	23SB	2885	G
27	23SB	2886	A
27	23SB	2892	C
27	23SB	2893	C
27	23SB	2904	A
27	23SB	2906	G
27	23SB	2907	U
27	23SB	2908	C
27	23SB	2909	U
27	23SB	2914	C
28	5SB	9	G
28	5SB	10	U
28	5SB	14	C
28	5SB	15	A
28	5SB	17	A
28	5SB	18	G
28	5SB	24	U
28	5SB	26	G
28	5SB	27	A
28	5SB	29	C
28	5SB	33	C
28	5SB	37	U
28	5SB	43	U
28	5SB	44	C

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Mol	Chain	Res	Type
28	5SB	47	A
28	5SB	55	A
28	5SB	58	G
28	5SB	68	A
28	5SB	69	G
28	5SB	75	A
28	5SB	83	G
28	5SB	87	G
28	5SB	90	C
28	5SB	91	G
28	5SB	92	A
28	5SB	93	C
28	5SB	98	U
28	5SB	99	G
28	5SB	104	A
28	5SB	112	G
28	5SB	115	G
28	5SB	121	G

All (258) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	16SA	677	G
1	16SA	696	A
1	16SA	706	A
1	16SA	731	U
1	16SA	758	A
1	16SA	813	U
1	16SA	836	G
1	16SA	891	A
1	16SA	907	G
1	16SA	969	C
1	16SA	1007	C
1	16SA	1053	A
1	16SA	1063	C
1	16SA	1069	G
1	16SA	1070	U
1	16SA	1111	G
1	16SA	1114	G
1	16SA	1115	G
1	16SA	1138	A
1	16SA	1159	G

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Mol	Chain	Res	Type
1	16SA	1161	A
1	16SA	1189	U
1	16SA	1315	U
1	16SA	1330	C
1	16SA	1332	G
1	16SA	1377	C
1	16SA	1381	G
1	16SA	1422	U
1	16SA	1441	C
1	16SA	1536	A
1	16SA	1614	U
1	16SA	1615	U
1	16SA	1649	U
1	16SA	1651	C
1	16SA	1753	U
1	16SA	1757	C
1	16SA	1767	G
1	16SA	1773	C
1	16SA	1785	A
1	16SA	1810	A
1	16SA	1817	G
1	16SA	1827	C
1	16SA	1838	U
1	16SA	1907	A
1	16SA	1912	A
1	16SA	1927	G
1	16SA	1928	U
1	16SA	1932	G
1	16SA	1946	A
1	16SA	1949	C
1	16SA	2078	C
1	16SA	2126	A
22	ASIA	10	G
22	ASIA	19	G
23	PSIA	20	U
23	PSIA	45	U
24	ESIA	45	U
25	MRNA	44	U
25	MRNA	56	U
26	TRNA	20	U
26	TRNA	34	G
26	TRNA	65	G

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Mol	Chain	Res	Type
27	23SA	34	C
27	23SA	186	A
27	23SA	218	A
27	23SA	219	A
27	23SA	400	G
27	23SA	423	U
27	23SA	432	C
27	23SA	530	A
27	23SA	555	A
27	23SA	557	G
27	23SA	580	U
27	23SA	612	C
27	23SA	672	C
27	23SA	680	A
27	23SA	700	G
27	23SA	813	A
27	23SA	823	A
27	23SA	895	C
27	23SA	929	G
27	23SA	992	A
27	23SA	1070	G
27	23SA	1074	U
27	23SA	1105	A
27	23SA	1133	A
27	23SA	1157	C
27	23SA	1189	U
27	23SA	1226	C
27	23SA	1252	A
27	23SA	1258	A
27	23SA	1469	U
27	23SA	1476	A
27	23SA	1608	A
27	23SA	1657	A
27	23SA	1695	G
27	23SA	1702	A
27	23SA	1703	G
27	23SA	1744	C
27	23SA	1770	A
27	23SA	1833	G
27	23SA	1853	A
27	23SA	1924	G
27	23SA	1964	5MU

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Mol	Chain	Res	Type
27	23SA	2017	G
27	23SA	2085	A
27	23SA	2192	U
27	23SA	2231	G
27	23SA	2322	G
27	23SA	2335	A
27	23SA	2361	A
27	23SA	2420	G
27	23SA	2421	U
27	23SA	2437	A
27	23SA	2441	A
27	23SA	2454	A
27	23SA	2496	G
27	23SA	2533	A
27	23SA	2581	A
27	23SA	2653	G
27	23SA	2660	G
27	23SA	2696	C
27	23SA	2727	U
27	23SA	2742	U
27	23SA	2767	G
27	23SA	2772	U
27	23SA	2806	A
27	23SA	2845	U
28	5SA	68	A
1	16SB	728	U
1	16SB	729	A
1	16SB	754	G
1	16SB	758	A
1	16SB	813	U
1	16SB	821	G
1	16SB	853	C
1	16SB	855	U
1	16SB	891	A
1	16SB	920	A
1	16SB	969	C
1	16SB	1053	A
1	16SB	1063	C
1	16SB	1070	U
1	16SB	1138	A
1	16SB	1161	A
1	16SB	1189	U

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Mol	Chain	Res	Type
1	16SB	1315	U
1	16SB	1316	A
1	16SB	1330	C
1	16SB	1332	G
1	16SB	1377	C
1	16SB	1381	G
1	16SB	1422	U
1	16SB	1495	A
1	16SB	1536	A
1	16SB	1583	U
1	16SB	1615	U
1	16SB	1651	C
1	16SB	1677	U
1	16SB	1754	U
1	16SB	1765	C
1	16SB	1773	C
1	16SB	1785	A
1	16SB	1827	C
1	16SB	1867	U
1	16SB	1883	A
1	16SB	1908	U
1	16SB	1912	A
1	16SB	1924	C
1	16SB	1927	G
1	16SB	1932	G
1	16SB	1946	A
1	16SB	1949	C
1	16SB	1957	U
1	16SB	1963	C
1	16SB	1973	A
1	16SB	2078	C
57	ASIB	10	G
57	ASIB	69	G
23	PSIB	8	4SU
23	PSIB	60	U
24	ESIB	9	A
24	ESIB	47	U
24	ESIB	58	A
25	MRNB	53	U
25	MRNB	56	U
27	23SB	34	C
27	23SB	48	A

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Mol	Chain	Res	Type
27	23SB	49	U
27	23SB	126	C
27	23SB	186	A
27	23SB	195	G
27	23SB	301	A
27	23SB	302	C
27	23SB	303	A
27	23SB	319	A
27	23SB	355	A
27	23SB	431	U
27	23SB	557	G
27	23SB	580	U
27	23SB	612	C
27	23SB	680	A
27	23SB	700	G
27	23SB	813	A
27	23SB	823	A
27	23SB	876	U
27	23SB	895	C
27	23SB	926	U
27	23SB	935	C
27	23SB	937	C
27	23SB	941	C
27	23SB	1133	A
27	23SB	1191	A
27	23SB	1220	G
27	23SB	1252	A
27	23SB	1258	A
27	23SB	1349	U
27	23SB	1350	A
27	23SB	1469	U
27	23SB	1476	A
27	23SB	1510	A
27	23SB	1575	G
27	23SB	1608	A
27	23SB	1657	A
27	23SB	1702	A
27	23SB	1703	G
27	23SB	1770	A
27	23SB	1853	A
27	23SB	1924	G
27	23SB	1940	5MU

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Mol	Chain	Res	Type
27	23SB	1955	G
27	23SB	2017	G
27	23SB	2135	G
27	23SB	2170	C
27	23SB	2216	G
27	23SB	2230	G
27	23SB	2231	G
27	23SB	2335	A
27	23SB	2350	A
27	23SB	2437	A
27	23SB	2454	A
27	23SB	2462	G
27	23SB	2496	G
27	23SB	2617	A
27	23SB	2660	G
27	23SB	2704	U
27	23SB	2741	A
27	23SB	2742	U
27	23SB	2748	G
27	23SB	2772	U
27	23SB	2792	A
27	23SB	2806	A
27	23SB	2872	G
28	5SB	13	C
28	5SB	16	U
28	5SB	17	A
28	5SB	26	G
28	5SB	68	A

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

83 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	7MG	16SB	1156	1,59	22,26,27	3.25	7 (31%)	29,39,42	2.82	11 (37%)
1	5MC	16SB	2035	1	18,22,23	3.75	7 (38%)	26,32,35	1.14	2 (7%)
27	OMU	23SA	2567	27,58	19,22,23	2.95	8 (42%)	26,31,34	1.63	4 (15%)
26	5MU	TRNA	54	26	19,22,23	3.92	5 (26%)	28,32,35	3.08	8 (28%)
27	PSU	23SB	1936	27	18,21,22	1.10	1 (5%)	22,30,33	1.61	3 (13%)
1	M2G	16SA	1589	1	20,27,28	3.85	7 (35%)	22,40,43	1.66	4 (18%)
23	MIA	PSIA	37	23	24,31,32	2.39	3 (12%)	26,44,47	3.09	10 (38%)
1	5MC	16SB	2028	1	18,22,23	3.70	7 (38%)	26,32,35	1.36	4 (15%)
1	5MC	16SA	1590	1	18,22,23	3.80	7 (38%)	26,32,35	1.05	1 (3%)
57	PSU	ASIB	32	57	18,21,22	1.06	1 (5%)	22,30,33	1.87	5 (22%)
23	4SU	PSIB	8	23,58	18,21,22	1.68	5 (27%)	26,30,33	2.81	6 (23%)
23	3AU	PSIA	47	23	24,28,29	2.73	8 (33%)	33,40,43	1.65	5 (15%)
57	5MU	ASIB	54	57	19,22,23	3.91	5 (26%)	28,32,35	3.10	8 (28%)
27	PSU	23SB	1942	27	18,21,22	1.13	1 (5%)	22,30,33	1.84	4 (18%)
27	5MC	23SB	1987	59,27	18,22,23	3.88	7 (38%)	26,32,35	0.91	2 (7%)
27	5MU	23SA	1940	27	19,22,23	3.97	5 (26%)	28,32,35	3.23	10 (35%)
23	MIA	PSIB	37	23	24,31,32	2.26	4 (16%)	26,44,47	3.23	9 (34%)
26	PSU	TRNA	39	26	18,21,22	1.11	1 (5%)	22,30,33	1.75	3 (13%)
27	5MC	23SA	1967	27	18,22,23	3.71	7 (38%)	26,32,35	1.29	2 (7%)
27	OMG	23SB	2266	59,23,27	18,26,27	5.15	9 (50%)	19,38,41	3.81	7 (36%)
57	PSU	ASIB	39	57	18,21,22	1.16	1 (5%)	22,30,33	1.72	5 (22%)
1	UR3	16SA	2121	1	19,22,23	2.91	7 (36%)	26,32,35	1.58	2 (7%)
27	OMG	23SA	2266	59,23,27	18,26,27	5.17	9 (50%)	19,38,41	3.70	7 (36%)
27	PSU	23SA	1936	27	18,21,22	1.02	1 (5%)	22,30,33	1.81	4 (18%)
1	MA6	16SA	2142	1	18,26,27	1.00	2 (11%)	19,38,41	2.81	2 (10%)
1	2MG	16SA	1834	1,59	18,26,27	2.80	7 (38%)	16,38,41	1.43	3 (18%)
22	PSU	ASIA	32	22	18,21,22	1.17	1 (5%)	22,30,33	1.58	4 (18%)
27	PSU	23SA	2620	27	18,21,22	1.09	1 (5%)	22,30,33	1.76	4 (18%)
1	4OC	16SB	2030	1,58	20,23,24	2.90	8 (40%)	26,32,35	1.59	3 (11%)
23	PSU	PSIA	55	23	18,21,22	1.18	1 (5%)	22,30,33	1.69	4 (18%)
27	5MU	23SB	1940	27	19,22,23	3.98	5 (26%)	28,32,35	3.49	9 (32%)
27	2MA	23SA	2518	59,27	19,25,26	3.10	5 (26%)	21,37,40	2.09	3 (14%)
24	MIA	ESIA	37	24	24,31,32	2.42	4 (16%)	26,44,47	3.23	9 (34%)
1	2MG	16SB	1834	1	18,26,27	2.80	7 (38%)	16,38,41	1.27	3 (18%)
22	7MG	ASIA	46	22	22,26,27	3.13	6 (27%)	29,39,42	2.82	10 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	3AU	PSIB	47	23	24,28,29	2.83	8 (33%)	33,40,43	2.03	7 (21%)
23	PSU	PSIB	32	23	18,21,22	1.00	1 (5%)	22,30,33	1.88	5 (22%)
23	7MG	PSIB	46	23	22,26,27	3.17	7 (31%)	29,39,42	2.74	10 (34%)
27	5MC	23SB	1967	27	18,22,23	3.80	7 (38%)	26,32,35	1.02	3 (11%)
1	MA6	16SB	2142	1	18,26,27	0.98	1 (5%)	19,38,41	2.86	2 (10%)
27	OMU	23SB	2567	27,58	19,22,23	2.94	8 (42%)	26,31,34	1.76	4 (15%)
1	PSU	16SA	1145	1,59,58	18,21,22	1.11	1 (5%)	22,30,33	2.04	6 (27%)
27	5MU	23SB	1964	59,27	19,22,23	3.91	5 (26%)	28,32,35	3.24	9 (32%)
1	MA6	16SB	2141	1	18,26,27	0.99	2 (11%)	19,38,41	2.61	2 (10%)
26	PSU	TRNA	55	26	18,21,22	1.10	1 (5%)	22,30,33	1.77	3 (13%)
23	PSU	PSIB	39	23	18,21,22	1.13	1 (5%)	22,30,33	1.57	4 (18%)
26	MIA	TRNA	37	26	24,31,32	2.55	4 (16%)	26,44,47	3.65	10 (38%)
1	5MC	16SA	2028	1	18,22,23	3.70	7 (38%)	26,32,35	1.27	2 (7%)
1	5MC	16SB	1590	1	18,22,23	3.91	7 (38%)	26,32,35	1.01	1 (3%)
27	PSU	23SA	1942	27	18,21,22	1.08	1 (5%)	22,30,33	1.69	4 (18%)
12	0TD	S12B	89	12	7,9,10	1.62	2 (28%)	6,11,13	1.99	2 (33%)
22	5MU	ASIA	54	22	19,22,23	3.84	5 (26%)	28,32,35	3.08	9 (32%)
22	MIA	ASIA	37	22	24,31,32	2.42	4 (16%)	26,44,47	3.76	10 (38%)
27	2MA	23SB	2518	59,27,58	19,25,26	3.14	5 (26%)	21,37,40	2.34	4 (19%)
23	PSU	PSIA	39	23	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
1	PSU	16SB	1145	1,58	18,21,22	1.14	1 (5%)	22,30,33	1.68	3 (13%)
1	5MC	16SB	2032	1	18,22,23	3.81	7 (38%)	26,32,35	1.00	2 (7%)
26	PSU	TRNA	32	26	18,21,22	1.13	1 (5%)	22,30,33	1.64	4 (18%)
27	PSU	23SB	2620	27	18,21,22	1.16	1 (5%)	22,30,33	1.75	3 (13%)
1	5MC	16SA	2032	1	18,22,23	3.82	7 (38%)	26,32,35	0.99	1 (3%)
23	4SU	PSIA	8	23	18,21,22	1.83	3 (16%)	26,30,33	2.23	4 (15%)
23	PSU	PSIA	32	23	18,21,22	1.00	1 (5%)	22,30,33	1.52	3 (13%)
22	4SU	ASIA	8	22	18,21,22	1.83	5 (27%)	26,30,33	2.33	5 (19%)
1	7MG	16SA	1156	1,59	22,26,27	3.06	8 (36%)	29,39,42	2.86	11 (37%)
27	OMC	23SA	1945	27	19,22,23	1.84	4 (21%)	26,31,34	1.04	1 (3%)
26	4SU	TRNA	8	26	18,21,22	1.82	3 (16%)	26,30,33	2.23	5 (19%)
1	M2G	16SB	1589	1	20,27,28	3.96	7 (35%)	22,40,43	1.40	4 (18%)
27	5MU	23SA	1964	59,27	19,22,23	3.80	5 (26%)	28,32,35	3.38	11 (39%)
23	5MU	PSIB	54	23	19,22,23	3.91	5 (26%)	28,32,35	2.99	10 (35%)
23	7MG	PSIA	46	23	22,26,27	2.94	6 (27%)	29,39,42	2.82	11 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	PSU	ASIA	39	22	18,21,22	1.12	1 (5%)	22,30,33	1.63	4 (18%)
1	4OC	16SA	2030	1,58	20,23,24	3.15	8 (40%)	26,32,35	0.99	3 (11%)
57	MIA	ASIB	37	57	24,31,32	2.41	4 (16%)	26,44,47	3.31	11 (42%)
23	5MU	PSIA	54	23	19,22,23	3.80	5 (26%)	28,32,35	3.02	7 (25%)
1	5MC	16SA	2035	1	18,22,23	3.68	7 (38%)	26,32,35	1.09	2 (7%)
24	MIA	ESIB	37	24	24,31,32	2.49	4 (16%)	26,44,47	4.26	10 (38%)
23	PSU	PSIB	55	23	18,21,22	1.12	1 (5%)	22,30,33	1.62	3 (13%)
12	0TD	S12A	89	12	7,9,10	1.35	1 (14%)	6,11,13	1.91	1 (16%)
27	OMC	23SB	1945	27	19,22,23	1.87	4 (21%)	26,31,34	0.96	1 (3%)
1	UR3	16SB	2121	1	19,22,23	2.87	8 (42%)	26,32,35	1.44	2 (7%)
22	PSU	ASIA	55	22	18,21,22	1.12	1 (5%)	22,30,33	1.56	4 (18%)
1	MA6	16SA	2141	1	18,26,27	1.01	1 (5%)	19,38,41	2.71	2 (10%)
27	5MC	23SA	1987	59,27	18,22,23	3.81	7 (38%)	26,32,35	0.91	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	7MG	16SB	1156	1,59	-	2/7/37/38	0/3/3/3
1	5MC	16SB	2035	1	-	0/7/25/26	0/2/2/2
27	OMU	23SA	2567	27,58	-	0/9/27/28	0/2/2/2
26	5MU	TRNA	54	26	-	2/7/25/26	0/2/2/2
27	PSU	23SB	1936	27	-	0/7/25/26	0/2/2/2
1	M2G	16SA	1589	1	-	2/7/29/30	0/3/3/3
23	MIA	PSIA	37	23	-	5/11/33/34	0/3/3/3
1	5MC	16SB	2028	1	-	0/7/25/26	0/2/2/2
1	5MC	16SA	1590	1	-	0/7/25/26	0/2/2/2
57	PSU	ASIB	32	57	-	0/7/25/26	0/2/2/2
23	4SU	PSIB	8	23,58	-	2/7/25/26	0/2/2/2
23	3AU	PSIA	47	23	-	7/16/34/35	0/2/2/2
57	5MU	ASIB	54	57	-	2/7/25/26	0/2/2/2
27	PSU	23SB	1942	27	-	0/7/25/26	0/2/2/2
27	5MC	23SB	1987	59,27	-	0/7/25/26	0/2/2/2
27	5MU	23SA	1940	27	-	2/7/25/26	0/2/2/2
23	MIA	PSIB	37	23	-	2/11/33/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PSU	TRNA	39	26	-	0/7/25/26	0/2/2/2
27	5MC	23SA	1967	27	-	0/7/25/26	0/2/2/2
27	OMG	23SB	2266	59,23,27	-	0/5/27/28	0/3/3/3
57	PSU	ASIB	39	57	-	0/7/25/26	0/2/2/2
1	UR3	16SA	2121	1	-	0/7/25/26	0/2/2/2
27	OMG	23SA	2266	59,23,27	-	0/5/27/28	0/3/3/3
27	PSU	23SA	1936	27	-	2/7/25/26	0/2/2/2
1	MA6	16SA	2142	1	-	3/7/29/30	0/3/3/3
1	2MG	16SA	1834	1,59	-	0/5/27/28	0/3/3/3
22	PSU	ASIA	32	22	-	0/7/25/26	0/2/2/2
27	PSU	23SA	2620	27	-	0/7/25/26	0/2/2/2
1	4OC	16SB	2030	1,58	-	2/9/29/30	0/2/2/2
23	PSU	PSIA	55	23	-	3/7/25/26	0/2/2/2
27	5MU	23SB	1940	27	-	0/7/25/26	0/2/2/2
27	2MA	23SA	2518	59,27	-	1/3/25/26	0/3/3/3
24	MIA	ESIA	37	24	-	6/11/33/34	0/3/3/3
1	2MG	16SB	1834	1	-	2/5/27/28	0/3/3/3
22	7MG	ASIA	46	22	-	2/7/37/38	0/3/3/3
23	3AU	PSIB	47	23	-	8/16/34/35	0/2/2/2
23	PSU	PSIB	32	23	-	0/7/25/26	0/2/2/2
23	7MG	PSIB	46	23	-	1/7/37/38	0/3/3/3
27	5MC	23SB	1967	27	-	0/7/25/26	0/2/2/2
1	MA6	16SB	2142	1	-	3/7/29/30	0/3/3/3
27	OMU	23SB	2567	27,58	-	2/9/27/28	0/2/2/2
1	PSU	16SA	1145	1,59,58	-	0/7/25/26	0/2/2/2
27	5MU	23SB	1964	59,27	-	2/7/25/26	0/2/2/2
1	MA6	16SB	2141	1	-	1/7/29/30	0/3/3/3
26	PSU	TRNA	55	26	-	0/7/25/26	0/2/2/2
23	PSU	PSIB	39	23	-	0/7/25/26	0/2/2/2
26	MIA	TRNA	37	26	-	6/11/33/34	0/3/3/3
1	5MC	16SA	2028	1	-	0/7/25/26	0/2/2/2
1	5MC	16SB	1590	1	-	0/7/25/26	0/2/2/2
27	PSU	23SA	1942	27	-	0/7/25/26	0/2/2/2
12	0TD	S12B	89	12	-	3/7/12/14	-
22	5MU	ASIA	54	22	-	0/7/25/26	0/2/2/2
22	MIA	ASIA	37	22	-	4/11/33/34	0/3/3/3
27	2MA	23SB	2518	59,27,58	-	3/3/25/26	0/3/3/3
23	PSU	PSIA	39	23	-	0/7/25/26	0/2/2/2
1	PSU	16SB	1145	1,58	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	16SB	2032	1	-	0/7/25/26	0/2/2/2
26	PSU	TRNA	32	26	-	0/7/25/26	0/2/2/2
27	PSU	23SB	2620	27	-	0/7/25/26	0/2/2/2
1	5MC	16SA	2032	1	-	0/7/25/26	0/2/2/2
23	4SU	PSIA	8	23	-	0/7/25/26	0/2/2/2
23	PSU	PSIA	32	23	-	0/7/25/26	0/2/2/2
22	4SU	ASIA	8	22	-	1/7/25/26	0/2/2/2
1	7MG	16SA	1156	1,59	-	2/7/37/38	0/3/3/3
27	OMC	23SA	1945	27	-	1/9/27/28	0/2/2/2
26	4SU	TRNA	8	26	-	2/7/25/26	0/2/2/2
1	M2G	16SB	1589	1	-	0/7/29/30	0/3/3/3
27	5MU	23SA	1964	59,27	-	2/7/25/26	0/2/2/2
23	5MU	PSIB	54	23	-	2/7/25/26	0/2/2/2
23	7MG	PSIA	46	23	-	2/7/37/38	0/3/3/3
22	PSU	ASIA	39	22	-	0/7/25/26	0/2/2/2
1	4OC	16SA	2030	1,58	-	2/9/29/30	0/2/2/2
57	MIA	ASIB	37	57	-	3/11/33/34	0/3/3/3
23	5MU	PSIA	54	23	-	0/7/25/26	0/2/2/2
1	5MC	16SA	2035	1	-	0/7/25/26	0/2/2/2
24	MIA	ESIB	37	24	-	6/11/33/34	0/3/3/3
23	PSU	PSIB	55	23	-	0/7/25/26	0/2/2/2
12	0TD	S12A	89	12	-	4/7/12/14	-
27	OMC	23SB	1945	27	-	0/9/27/28	0/2/2/2
1	UR3	16SB	2121	1	-	0/7/25/26	0/2/2/2
22	PSU	ASIA	55	22	-	3/7/25/26	0/2/2/2
1	MA6	16SA	2141	1	-	0/7/29/30	0/3/3/3
27	5MC	23SA	1987	59,27	-	0/7/25/26	0/2/2/2

All (364) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	23SB	2266	OMG	C8-N7	-14.81	1.09	1.35
27	23SA	2266	OMG	C8-N7	-14.68	1.10	1.35
1	16SB	1589	M2G	C2-N3	13.12	1.46	1.30
27	23SB	1940	5MU	C2-N1	12.91	1.59	1.38
23	PSIB	54	5MU	C2-N1	12.79	1.59	1.38
27	23SA	1940	5MU	C2-N1	12.78	1.59	1.38
57	ASIB	54	5MU	C2-N1	12.65	1.58	1.38
26	TRNA	54	5MU	C2-N1	12.53	1.58	1.38
27	23SB	1964	5MU	C2-N1	12.53	1.58	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16SA	1589	M2G	C2-N3	12.29	1.45	1.30
23	PSIA	54	5MU	C2-N1	12.19	1.58	1.38
22	ASIA	54	5MU	C2-N1	12.15	1.57	1.38
27	23SA	1964	5MU	C2-N1	11.98	1.57	1.38
27	23SB	2266	OMG	C4-N3	9.82	1.61	1.37
27	23SA	2266	OMG	C4-N3	9.69	1.60	1.37
27	23SB	1987	5MC	C6-C5	9.69	1.50	1.34
1	16SA	1590	5MC	C6-C5	9.58	1.50	1.34
27	23SA	1987	5MC	C6-C5	9.57	1.50	1.34
1	16SB	1590	5MC	C6-C5	9.55	1.50	1.34
1	16SA	2028	5MC	C6-C5	9.46	1.50	1.34
27	23SB	1967	5MC	C6-C5	9.44	1.50	1.34
1	16SB	2035	5MC	C6-C5	9.36	1.50	1.34
1	16SB	2032	5MC	C6-C5	9.25	1.49	1.34
1	16SB	1156	7MG	C5-N7	9.18	1.46	1.35
1	16SB	2028	5MC	C6-C5	9.12	1.49	1.34
27	23SA	1967	5MC	C6-C5	9.12	1.49	1.34
1	16SA	2032	5MC	C6-C5	9.10	1.49	1.34
22	ASIA	46	7MG	C5-N7	9.10	1.46	1.35
1	16SA	2035	5MC	C6-C5	9.04	1.49	1.34
23	PSIB	46	7MG	C5-N7	9.02	1.46	1.35
23	PSIB	47	3AU	C2-N1	8.85	1.51	1.38
27	23SA	2266	OMG	C6-N1	-8.82	1.24	1.37
1	16SA	1156	7MG	C5-N7	8.72	1.45	1.35
27	23SB	2518	2MA	C4-N3	8.61	1.49	1.35
27	23SA	2518	2MA	C4-N3	8.58	1.49	1.35
57	ASIB	37	MIA	C13-C14	8.53	1.56	1.32
23	PSIA	37	MIA	C13-C14	8.47	1.56	1.32
24	ESIB	37	MIA	C13-C14	8.43	1.56	1.32
27	23SB	2266	OMG	C6-N1	-8.40	1.25	1.37
24	ESIA	37	MIA	C13-C14	8.38	1.56	1.32
22	ASIA	37	MIA	C13-C14	8.38	1.56	1.32
1	16SB	1156	7MG	C4-N9	-8.35	1.28	1.37
26	TRNA	37	MIA	C13-C14	8.28	1.56	1.32
23	PSIA	46	7MG	C5-N7	8.25	1.45	1.35
23	PSIB	37	MIA	C13-C14	8.24	1.56	1.32
23	PSIB	46	7MG	C4-N9	-8.21	1.28	1.37
23	PSIA	47	3AU	C2-N1	8.13	1.50	1.38
1	16SA	2121	UR3	C2-N1	7.67	1.49	1.38
1	16SA	2032	5MC	C4-N3	7.64	1.47	1.34
1	16SB	1590	5MC	C4-N3	7.63	1.47	1.34
22	ASIA	46	7MG	C4-N9	-7.52	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16SA	1589	M2G	C2-N2	7.40	1.49	1.35
1	16SB	2032	5MC	C4-N3	7.39	1.46	1.34
1	16SB	2121	UR3	C2-N1	7.37	1.49	1.38
27	23SB	1987	5MC	C4-N3	7.34	1.46	1.34
1	16SB	1589	M2G	C2-N2	7.26	1.49	1.35
27	23SA	1987	5MC	C4-N3	7.15	1.46	1.34
27	23SA	2266	OMG	C5-C4	7.15	1.61	1.43
27	23SB	2266	OMG	C5-C4	7.15	1.61	1.43
27	23SB	1967	5MC	C4-N3	7.04	1.46	1.34
1	16SA	1590	5MC	C4-N3	7.03	1.46	1.34
23	PSIA	46	7MG	C4-N9	-7.02	1.29	1.37
27	23SA	1967	5MC	C4-N3	7.01	1.46	1.34
1	16SA	2030	4OC	C4-N3	6.95	1.44	1.32
1	16SB	2035	5MC	C4-N3	6.95	1.45	1.34
1	16SB	2028	5MC	C4-N3	6.93	1.45	1.34
1	16SA	2028	5MC	C4-N3	6.91	1.45	1.34
1	16SA	2035	5MC	C4-N3	6.90	1.45	1.34
27	23SA	2567	OMU	C2-N1	6.84	1.49	1.38
1	16SA	1156	7MG	C4-N9	-6.76	1.29	1.37
1	16SB	1590	5MC	C2-N3	6.72	1.50	1.36
27	23SB	2567	OMU	C2-N1	6.66	1.49	1.38
27	23SB	1987	5MC	C2-N3	6.62	1.49	1.36
1	16SA	1834	2MG	C2-N2	6.61	1.48	1.33
1	16SB	1834	2MG	C2-N2	6.60	1.48	1.33
27	23SB	1940	5MU	C4-N3	-6.59	1.26	1.38
1	16SB	2032	5MC	C2-N3	6.58	1.49	1.36
27	23SB	1967	5MC	C2-N3	6.52	1.49	1.36
27	23SB	2567	OMU	C2-N3	6.51	1.49	1.38
27	23SA	2567	OMU	C2-N3	6.48	1.49	1.38
1	16SA	2032	5MC	C2-N3	6.48	1.49	1.36
1	16SB	2121	UR3	C6-C5	6.43	1.50	1.35
1	16SA	2121	UR3	C6-C5	6.41	1.50	1.35
23	PSIA	54	5MU	C4-N3	-6.36	1.27	1.38
27	23SA	1964	5MU	C4-N3	-6.34	1.27	1.38
1	16SB	2035	5MC	C2-N3	6.33	1.49	1.36
1	16SA	2035	5MC	C2-N3	6.32	1.49	1.36
27	23SB	1964	5MU	C4-N3	-6.30	1.27	1.38
1	16SB	2028	5MC	C2-N3	6.30	1.49	1.36
27	23SA	1987	5MC	C2-N3	6.30	1.49	1.36
1	16SA	1590	5MC	C2-N3	6.30	1.49	1.36
23	PSIA	47	3AU	C6-C5	6.26	1.49	1.35
1	16SA	2030	4OC	C2-N3	6.24	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	23SA	1967	5MC	C2-N3	6.19	1.48	1.36
23	PSIB	47	3AU	C6-C5	6.18	1.49	1.35
1	16SB	2030	4OC	C4-N3	6.16	1.43	1.32
1	16SA	2028	5MC	C2-N3	6.15	1.48	1.36
1	16SA	2030	4OC	C6-C5	6.15	1.49	1.35
27	23SB	1964	5MU	C2-N3	6.15	1.48	1.38
27	23SB	2518	2MA	C2-N1	6.13	1.44	1.34
57	ASIB	54	5MU	C4-N3	-6.13	1.27	1.38
27	23SA	1940	5MU	C2-N3	6.12	1.48	1.38
23	PSIB	54	5MU	C4-N3	-6.12	1.27	1.38
22	ASIA	54	5MU	C4-N3	-6.12	1.27	1.38
26	TRNA	37	MIA	C6-N6	6.10	1.45	1.34
1	16SA	1156	7MG	C4-N3	6.09	1.48	1.34
26	TRNA	54	5MU	C4-N3	-5.99	1.27	1.38
26	TRNA	54	5MU	C6-N1	5.97	1.48	1.38
26	TRNA	54	5MU	C2-N3	5.97	1.48	1.38
22	ASIA	46	7MG	C4-N3	5.96	1.48	1.34
27	23SA	2518	2MA	C2-N1	5.94	1.44	1.34
1	16SB	2030	4OC	C6-C5	5.93	1.48	1.35
27	23SA	1940	5MU	C4-N3	-5.92	1.27	1.38
27	23SA	1940	5MU	C6-N1	5.87	1.48	1.38
57	ASIB	54	5MU	C6-N1	5.86	1.48	1.38
1	16SB	1589	M2G	C4-N3	5.83	1.51	1.37
22	ASIA	54	5MU	C6-N1	5.81	1.48	1.38
1	16SB	1156	7MG	C4-N3	5.81	1.48	1.34
22	ASIA	54	5MU	C2-N3	5.77	1.48	1.38
27	23SA	1964	5MU	C2-N3	5.75	1.48	1.38
57	ASIB	54	5MU	C2-N3	5.74	1.48	1.38
23	PSIA	46	7MG	C4-N3	5.72	1.47	1.34
24	ESIB	37	MIA	C6-N6	5.72	1.45	1.34
23	PSIB	54	5MU	C2-N3	5.70	1.48	1.38
23	PSIB	54	5MU	C6-N1	5.69	1.47	1.38
23	PSIB	47	3AU	C2-N3	5.68	1.48	1.38
23	PSIA	54	5MU	C6-N1	5.68	1.47	1.38
27	23SB	1940	5MU	C6-N1	5.67	1.47	1.38
27	23SB	2567	OMU	C6-C5	5.62	1.48	1.35
23	PSIA	47	3AU	C2-N3	5.62	1.48	1.38
24	ESIA	37	MIA	C6-N6	5.60	1.44	1.34
27	23SA	2567	OMU	C6-C5	5.60	1.48	1.35
23	PSIB	46	7MG	C4-N3	5.59	1.47	1.34
27	23SB	1964	5MU	C6-N1	5.57	1.47	1.38
57	ASIB	37	MIA	C6-N6	5.54	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	23SB	1940	5MU	C2-N3	5.53	1.47	1.38
27	23SA	2518	2MA	C2-N3	5.51	1.43	1.34
26	TRNA	37	MIA	C2-S10	5.51	1.80	1.75
23	PSIA	54	5MU	C2-N3	5.50	1.47	1.38
1	16SA	1589	M2G	C4-N3	5.39	1.50	1.37
27	23SB	2518	2MA	C2-N3	5.39	1.43	1.34
1	16SA	1834	2MG	C4-N3	5.38	1.50	1.37
1	16SA	2121	UR3	C2-N3	5.37	1.49	1.39
26	TRNA	8	4SU	C5-C4	5.34	1.49	1.42
23	PSIA	8	4SU	C5-C4	5.31	1.49	1.42
1	16SB	1834	2MG	C2-N1	5.28	1.45	1.36
1	16SB	2030	4OC	C2-N3	5.27	1.47	1.36
1	16SB	2121	UR3	C2-N3	5.25	1.49	1.39
27	23SB	2518	2MA	C6-N1	5.25	1.43	1.33
22	ASIA	37	MIA	C6-N6	5.18	1.44	1.34
27	23SA	1964	5MU	C6-N1	5.18	1.46	1.38
22	ASIA	8	4SU	C5-C4	5.16	1.49	1.42
23	PSIB	37	MIA	C6-N6	5.16	1.44	1.34
1	16SB	1834	2MG	C4-N3	5.15	1.49	1.37
22	ASIA	37	MIA	C2-S10	5.14	1.80	1.75
27	23SA	2518	2MA	C6-N1	5.07	1.43	1.33
27	23SA	1964	5MU	C4-C5	5.04	1.53	1.44
1	16SB	1590	5MC	C4-N4	5.03	1.47	1.34
23	PSIA	37	MIA	C6-N6	5.02	1.43	1.34
24	ESIB	37	MIA	C2-S10	4.98	1.79	1.75
23	PSIA	37	MIA	C2-S10	4.98	1.79	1.75
27	23SB	1987	5MC	C4-N4	4.98	1.47	1.34
27	23SA	1987	5MC	C6-N1	4.95	1.46	1.38
1	16SA	2032	5MC	C4-N4	4.93	1.46	1.34
1	16SB	2032	5MC	C4-N4	4.93	1.46	1.34
22	ASIA	54	5MU	C4-C5	4.89	1.52	1.44
27	23SB	1987	5MC	C6-N1	4.88	1.46	1.38
1	16SA	1834	2MG	C2-N1	4.88	1.44	1.36
27	23SB	1967	5MC	C4-N4	4.88	1.46	1.34
27	23SA	1967	5MC	C2-N1	4.87	1.50	1.40
1	16SA	1590	5MC	C4-N4	4.85	1.46	1.34
1	16SB	1590	5MC	C6-N1	4.83	1.46	1.38
1	16SA	1590	5MC	C6-N1	4.83	1.46	1.38
1	16SB	2035	5MC	C4-N4	4.80	1.46	1.34
1	16SA	2032	5MC	C6-N1	4.78	1.46	1.38
27	23SA	1967	5MC	C4-N4	4.77	1.46	1.34
27	23SB	1967	5MC	C6-N1	4.76	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	23SA	1987	5MC	C4-N4	4.75	1.46	1.34
1	16SB	2028	5MC	C4-N4	4.74	1.46	1.34
26	TRNA	54	5MU	C4-C5	4.73	1.52	1.44
1	16SB	2032	5MC	C6-N1	4.73	1.46	1.38
1	16SA	2028	5MC	C4-N4	4.73	1.46	1.34
1	16SA	2035	5MC	C4-N4	4.68	1.46	1.34
27	23SB	1940	5MU	C4-C5	4.68	1.52	1.44
1	16SB	2035	5MC	C6-N1	4.66	1.46	1.38
57	ASIB	54	5MU	C4-C5	4.64	1.52	1.44
24	ESIA	37	MIA	C2-S10	4.62	1.79	1.75
1	16SA	2035	5MC	C6-N1	4.61	1.45	1.38
27	23SA	1940	5MU	C4-C5	4.61	1.52	1.44
27	23SB	1945	OMC	C2-N3	4.60	1.45	1.36
1	16SA	2032	5MC	C2-N1	4.58	1.49	1.40
27	23SA	1987	5MC	C2-N1	4.58	1.49	1.40
1	16SB	2028	5MC	C2-N1	4.54	1.49	1.40
1	16SA	2030	4OC	C2-N1	4.52	1.49	1.40
27	23SB	1967	5MC	C2-N1	4.51	1.49	1.40
1	16SA	2028	5MC	C6-N1	4.51	1.45	1.38
27	23SB	1945	OMC	C4-N4	4.47	1.44	1.33
23	PSIB	8	4SU	C5-C4	4.45	1.48	1.42
57	ASIB	37	MIA	C2-S10	4.45	1.79	1.75
27	23SA	1967	5MC	C6-N1	4.44	1.45	1.38
1	16SB	2030	4OC	C2-N1	4.44	1.49	1.40
1	16SA	2030	4OC	C4-N4	4.43	1.45	1.35
1	16SB	2035	5MC	C2-N1	4.41	1.49	1.40
23	PSIB	46	7MG	C5-C4	-4.41	1.23	1.38
27	23SB	1964	5MU	C4-C5	4.40	1.52	1.44
1	16SB	2028	5MC	C6-N1	4.39	1.45	1.38
1	16SB	1156	7MG	C5-C4	-4.38	1.23	1.38
1	16SA	1590	5MC	C2-N1	4.36	1.49	1.40
1	16SB	1590	5MC	C2-N1	4.36	1.49	1.40
27	23SA	1945	OMC	C4-N4	4.35	1.44	1.33
23	PSIA	54	5MU	C4-C5	4.34	1.52	1.44
22	ASIA	46	7MG	C5-C4	-4.33	1.23	1.38
1	16SB	2032	5MC	C2-N1	4.31	1.49	1.40
1	16SA	1156	7MG	C5-C4	-4.29	1.24	1.38
27	23SA	1945	OMC	C2-N3	4.28	1.45	1.36
23	PSIB	54	5MU	C4-C5	4.28	1.51	1.44
27	23SB	1987	5MC	C2-N1	4.27	1.49	1.40
1	16SA	2035	5MC	C2-N1	4.25	1.49	1.40
23	PSIA	46	7MG	C5-C4	-4.20	1.24	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16SA	1589	M2G	C2-N1	4.19	1.47	1.36
1	16SB	1589	M2G	C2-N1	4.09	1.46	1.36
1	16SA	1589	M2G	C6-N1	4.09	1.44	1.37
1	16SA	1589	M2G	C5-C6	4.07	1.55	1.47
22	ASIA	32	PSU	C6-C5	4.03	1.40	1.35
1	16SA	2028	5MC	C2-N1	4.03	1.48	1.40
1	16SB	2030	4OC	C5-C4	4.03	1.49	1.40
1	16SB	1589	M2G	C5-C6	4.01	1.55	1.47
1	16SB	1834	2MG	C6-N1	3.99	1.43	1.37
27	23SA	2567	OMU	C4-N3	3.98	1.45	1.38
1	16SA	1834	2MG	C6-N1	3.97	1.43	1.37
26	TRNA	8	4SU	C2-N1	3.95	1.44	1.38
27	23SA	2266	OMG	C5-C6	-3.90	1.39	1.47
22	ASIA	8	4SU	C2-N1	3.88	1.44	1.38
1	16SB	1145	PSU	C6-C5	3.85	1.39	1.35
27	23SB	2567	OMU	C4-N3	3.84	1.45	1.38
27	23SA	1945	OMC	C5-C4	3.81	1.51	1.42
23	PSIA	55	PSU	C6-C5	3.80	1.39	1.35
23	PSIB	39	PSU	C6-C5	3.80	1.39	1.35
22	ASIA	39	PSU	C6-C5	3.79	1.39	1.35
27	23SB	2620	PSU	C6-C5	3.79	1.39	1.35
23	PSIA	8	4SU	C2-N1	3.79	1.44	1.38
27	23SB	1945	OMC	C5-C4	3.79	1.51	1.42
22	ASIA	55	PSU	C6-C5	3.78	1.39	1.35
26	TRNA	32	PSU	C6-C5	3.78	1.39	1.35
1	16SA	2030	4OC	C5-C4	3.77	1.48	1.40
26	TRNA	39	PSU	C6-C5	3.76	1.39	1.35
57	ASIB	39	PSU	C6-C5	3.74	1.39	1.35
1	16SB	1589	M2G	C6-N1	3.73	1.43	1.37
23	PSIB	55	PSU	C6-C5	3.72	1.39	1.35
27	23SB	1942	PSU	C6-C5	3.69	1.39	1.35
1	16SA	1145	PSU	C6-C5	3.69	1.39	1.35
23	PSIB	37	MIA	C2-S10	3.59	1.78	1.75
26	TRNA	55	PSU	C6-C5	3.55	1.39	1.35
27	23SA	2620	PSU	C6-C5	3.54	1.39	1.35
27	23SB	1936	PSU	C6-C5	3.53	1.39	1.35
27	23SB	2266	OMG	C5-C6	-3.50	1.40	1.47
27	23SA	1942	PSU	C6-C5	3.46	1.39	1.35
23	PSIB	8	4SU	C2-N1	3.44	1.44	1.38
57	ASIB	32	PSU	C6-C5	3.40	1.39	1.35
1	16SA	2121	UR3	C6-N1	3.39	1.46	1.38
1	16SB	2121	UR3	C6-N1	3.38	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	PSIA	39	PSU	C6-C5	3.28	1.39	1.35
1	16SB	1834	2MG	C5-C6	3.28	1.54	1.47
23	PSIA	32	PSU	C6-C5	3.25	1.39	1.35
23	PSIB	47	3AU	C4-N3	3.22	1.45	1.40
27	23SA	2567	OMU	O4-C4	-3.21	1.18	1.24
1	16SA	1834	2MG	C5-C6	3.20	1.53	1.47
1	16SA	2030	4OC	C6-N1	3.19	1.45	1.38
1	16SA	2035	5MC	O2-C2	-3.19	1.17	1.23
1	16SA	1590	5MC	O2-C2	-3.17	1.17	1.23
1	16SB	2035	5MC	O2-C2	-3.17	1.17	1.23
27	23SA	1936	PSU	C6-C5	3.17	1.39	1.35
1	16SA	2028	5MC	O2-C2	-3.15	1.17	1.23
23	PSIA	47	3AU	C4-N3	3.14	1.45	1.40
1	16SB	2028	5MC	O2-C2	-3.13	1.17	1.23
23	PSIB	32	PSU	C6-C5	3.13	1.39	1.35
27	23SB	2567	OMU	O4-C4	-3.10	1.18	1.24
1	16SB	1156	7MG	C2-N2	3.10	1.41	1.34
1	16SB	2030	4OC	C4-N4	3.08	1.42	1.35
1	16SA	1156	7MG	C2-N2	3.08	1.41	1.34
1	16SB	2030	4OC	C6-N1	3.05	1.45	1.38
27	23SB	1967	5MC	O2-C2	-3.04	1.18	1.23
22	ASIA	46	7MG	C2-N2	3.03	1.41	1.34
24	ESIB	37	MIA	C6-N1	3.00	1.36	1.32
27	23SB	1987	5MC	O2-C2	-2.98	1.18	1.23
1	16SB	2032	5MC	O2-C2	-2.98	1.18	1.23
23	PSIB	46	7MG	C2-N2	2.97	1.41	1.34
23	PSIA	46	7MG	C2-N2	2.97	1.41	1.34
27	23SA	1967	5MC	O2-C2	-2.94	1.18	1.23
1	16SB	1590	5MC	O2-C2	-2.92	1.18	1.23
23	PSIA	47	3AU	C6-N1	2.87	1.44	1.38
23	PSIA	8	4SU	C6-N1	2.84	1.44	1.38
1	16SA	1834	2MG	O6-C6	-2.82	1.17	1.23
27	23SA	2567	OMU	C6-N1	2.81	1.44	1.38
1	16SA	1834	2MG	C5-C4	-2.80	1.35	1.43
27	23SB	2266	OMG	C2-N2	2.77	1.40	1.34
27	23SB	2567	OMU	C6-N1	2.77	1.44	1.38
27	23SA	1987	5MC	O2-C2	-2.74	1.18	1.23
27	23SA	2266	OMG	C2-N2	2.74	1.40	1.34
23	PSIB	47	3AU	C6-N1	2.73	1.44	1.38
22	ASIA	8	4SU	C6-N1	2.71	1.44	1.38
27	23SB	2266	OMG	C2-N3	2.70	1.39	1.33
1	16SA	2032	5MC	O2-C2	-2.70	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	TRNA	37	MIA	C6-N1	2.68	1.36	1.32
1	16SB	2030	4OC	O2-C2	-2.63	1.18	1.23
26	TRNA	8	4SU	C6-N1	2.63	1.44	1.38
1	16SA	2030	4OC	O2-C2	-2.61	1.18	1.23
22	ASIA	37	MIA	C6-N1	2.59	1.36	1.32
1	16SA	1589	M2G	C5-C4	-2.59	1.36	1.43
27	23SA	2266	OMG	O6-C6	-2.57	1.18	1.23
1	16SB	1834	2MG	O6-C6	-2.55	1.18	1.23
27	23SA	2266	OMG	C2-N3	2.55	1.39	1.33
24	ESIA	37	MIA	C6-N1	2.52	1.36	1.32
23	PSIA	46	7MG	C6-N1	-2.51	1.34	1.38
1	16SB	2142	MA6	C5-C4	-2.47	1.34	1.40
27	23SB	2266	OMG	O6-C6	-2.46	1.18	1.23
23	PSIB	8	4SU	C4-N3	2.46	1.40	1.37
1	16SA	2142	MA6	C5-C4	-2.43	1.34	1.40
1	16SB	1834	2MG	C5-C4	-2.43	1.36	1.43
23	PSIA	47	3AU	O4-C4	-2.41	1.18	1.23
27	23SB	2567	OMU	C5-C4	2.41	1.49	1.43
1	16SB	2141	MA6	C5-C4	-2.40	1.34	1.40
1	16SA	2141	MA6	C5-C4	-2.40	1.34	1.40
23	PSIA	47	3AU	C5-C4	2.38	1.49	1.43
27	23SB	2567	OMU	O2-C2	-2.38	1.18	1.23
1	16SA	1156	7MG	C6-N1	-2.37	1.34	1.38
23	PSIB	47	3AU	O4-C4	-2.37	1.18	1.23
27	23SA	1945	OMC	C6-N1	2.31	1.43	1.38
1	16SA	2121	UR3	C5-C4	2.30	1.49	1.43
23	PSIB	8	4SU	C6-N1	2.29	1.43	1.38
23	PSIB	47	3AU	C5-C4	2.29	1.49	1.43
1	16SB	1589	M2G	C5-C4	-2.28	1.37	1.43
12	S12B	89	0TD	OD1-CG	2.27	1.29	1.22
23	PSIA	47	3AU	O2-C2	-2.26	1.18	1.22
23	PSIB	47	3AU	O2-C2	-2.25	1.18	1.22
27	23SA	2567	OMU	C5-C4	2.25	1.48	1.43
1	16SB	2121	UR3	C5-C4	2.24	1.49	1.43
27	23SB	2518	2MA	C6-C5	2.23	1.51	1.43
1	16SA	2121	UR3	O4-C4	-2.22	1.18	1.23
27	23SB	1945	OMC	C6-N1	2.21	1.43	1.38
27	23SA	2518	2MA	C6-C5	2.20	1.51	1.43
1	16SB	2121	UR3	O2-C2	-2.19	1.18	1.22
27	23SA	2266	OMG	C2-N1	-2.18	1.32	1.37
57	ASIB	37	MIA	C6-N1	2.15	1.35	1.32
1	16SA	2142	MA6	C2-N3	2.12	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16SB	2121	UR3	O4-C4	-2.11	1.19	1.23
1	16SA	1156	7MG	C8-N9	2.11	1.47	1.46
27	23SB	2266	OMG	C2-N1	-2.10	1.32	1.37
23	PSIB	8	4SU	C2-N3	2.10	1.41	1.38
27	23SA	2567	OMU	O2-C2	-2.08	1.19	1.23
1	16SA	2121	UR3	O2-C2	-2.08	1.18	1.22
22	ASIA	46	7MG	C6-N1	-2.06	1.35	1.38
23	PSIB	37	MIA	C6-N1	2.06	1.35	1.32
12	S12A	89	0TD	CSB-SB	-2.06	1.75	1.79
22	ASIA	8	4SU	C2-N3	2.05	1.41	1.38
23	PSIB	46	7MG	C5-C6	2.05	1.48	1.43
12	S12B	89	0TD	CB-CG	2.05	1.55	1.52
23	PSIB	46	7MG	C6-N1	-2.05	1.35	1.38
1	16SB	1156	7MG	C8-N9	2.04	1.47	1.46
1	16SB	2141	MA6	C2-N3	2.03	1.35	1.32
1	16SA	1156	7MG	C5-C6	2.02	1.48	1.43
22	ASIA	8	4SU	C4-N3	2.01	1.39	1.37
1	16SB	1156	7MG	C6-N1	-2.01	1.35	1.38
1	16SB	2121	UR3	C4-N3	2.00	1.45	1.40

All (410) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	ESIB	37	MIA	C11-S10-C2	13.00	111.97	102.27
22	ASIA	37	MIA	C11-S10-C2	12.51	111.61	102.27
24	ESIB	37	MIA	C12-C13-C14	-12.37	103.08	127.14
27	23SB	1940	5MU	C5-C4-N3	10.87	124.59	115.31
1	16SB	2142	MA6	N1-C6-N6	-10.65	105.85	117.06
57	ASIB	54	5MU	C5-C4-N3	10.57	124.33	115.31
27	23SA	1940	5MU	C5-C4-N3	10.57	124.33	115.31
24	ESIA	37	MIA	C11-S10-C2	10.56	110.16	102.27
22	ASIA	54	5MU	C5-C4-N3	10.53	124.30	115.31
27	23SA	1964	5MU	C5-C4-N3	10.51	124.28	115.31
1	16SA	2142	MA6	N1-C6-N6	-10.49	106.02	117.06
27	23SB	2266	OMG	C8-N7-C5	10.49	122.97	102.99
26	TRNA	54	5MU	C5-C4-N3	10.38	124.17	115.31
23	PSIB	54	5MU	C5-C4-N3	10.36	124.15	115.31
23	PSIA	54	5MU	C5-C4-N3	10.33	124.12	115.31
57	ASIB	37	MIA	C11-S10-C2	10.09	109.80	102.27
1	16SA	2141	MA6	N1-C6-N6	-10.05	106.48	117.06
26	TRNA	37	MIA	C11-S10-C2	10.00	109.73	102.27
23	PSIB	37	MIA	C12-C13-C14	-9.95	107.78	127.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SA	2266	OMG	C8-N7-C5	9.88	121.81	102.99
27	23SB	1964	5MU	C5-C4-N3	9.67	123.56	115.31
1	16SB	2141	MA6	N1-C6-N6	-9.58	106.97	117.06
22	ASIA	37	MIA	C12-C13-C14	-9.37	108.92	127.14
27	23SB	2266	OMG	C5-C6-N1	9.15	130.11	113.95
57	ASIB	37	MIA	C12-C13-C14	-9.14	109.35	127.14
23	PSIA	37	MIA	C11-S10-C2	9.12	109.08	102.27
27	23SA	2266	OMG	C5-C6-N1	9.08	129.98	113.95
26	TRNA	37	MIA	C12-C13-C14	-8.72	110.17	127.14
23	PSIB	8	4SU	C4-N3-C2	-8.65	118.94	127.34
24	ESIA	37	MIA	C12-C13-C14	-7.89	111.79	127.14
22	ASIA	8	4SU	C4-N3-C2	-7.60	119.95	127.34
26	TRNA	8	4SU	C4-N3-C2	-7.45	120.10	127.34
23	PSIA	8	4SU	C4-N3-C2	-7.31	120.24	127.34
27	23SB	2518	2MA	C2-N3-C4	6.89	121.12	115.52
1	16SB	1156	7MG	C4-C5-N7	6.89	115.09	105.53
27	23SB	1940	5MU	C4-N3-C2	-6.88	118.44	127.35
23	PSIB	37	MIA	C11-S10-C2	6.81	107.35	102.27
23	PSIA	37	MIA	C12-C13-C14	-6.77	113.97	127.14
22	ASIA	46	7MG	C4-C5-N7	6.76	114.92	105.53
23	PSIB	8	4SU	C5-C4-N3	6.75	120.94	114.69
23	PSIA	46	7MG	C4-C5-N7	6.73	114.88	105.53
27	23SA	1964	5MU	C4-N3-C2	-6.67	118.72	127.35
1	16SA	1156	7MG	C4-C5-N7	6.54	114.61	105.53
23	PSIB	8	4SU	C5-C4-S4	-6.41	116.21	124.47
23	PSIB	46	7MG	C4-C5-N7	6.36	114.35	105.53
27	23SA	2518	2MA	C2-N3-C4	6.36	120.69	115.52
27	23SB	1940	5MU	C6-C5-C4	6.33	123.32	118.03
27	23SB	1964	5MU	C6-C5-C4	6.31	123.31	118.03
27	23SA	1940	5MU	O4-C4-C5	-6.31	117.58	124.90
27	23SB	1964	5MU	C4-N3-C2	-6.30	119.19	127.35
26	TRNA	37	MIA	C15-C14-C13	-6.27	104.53	122.65
27	23SA	1940	5MU	C4-N3-C2	-6.26	119.25	127.35
27	23SB	1940	5MU	C5-C6-N1	-6.25	116.91	123.34
27	23SB	2518	2MA	C1'-N9-C4	-6.23	115.70	126.64
27	23SA	1964	5MU	C5-C6-N1	-6.16	117.00	123.34
22	ASIA	46	7MG	CM7-N7-C5	6.14	142.24	126.40
23	PSIB	46	7MG	C5-C4-N9	6.11	114.28	106.35
23	PSIA	8	4SU	C5-C4-N3	6.05	120.30	114.69
1	16SB	1156	7MG	C5-C4-N9	6.03	114.17	106.35
1	16SB	1156	7MG	CM7-N7-C5	6.01	141.90	126.40
1	16SA	1156	7MG	C5-C4-N9	5.98	114.11	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	ASIA	8	4SU	C5-C4-N3	5.97	120.23	114.69
23	PSIA	54	5MU	C5-C6-N1	-5.97	117.20	123.34
26	TRNA	8	4SU	C5-C4-N3	5.94	120.20	114.69
1	16SB	2142	MA6	N3-C2-N1	-5.91	119.44	128.68
23	PSIB	47	3AU	C1'-N1-C2	5.89	126.93	116.99
23	PSIB	47	3AU	O2-C2-N3	-5.86	113.84	121.99
57	ASIB	54	5MU	C4-N3-C2	-5.84	119.78	127.35
22	ASIA	54	5MU	C4-N3-C2	-5.84	119.79	127.35
1	16SA	1156	7MG	CM7-N7-C5	5.83	141.45	126.40
23	PSIA	46	7MG	CM7-N7-C5	5.83	141.44	126.40
27	23SA	1964	5MU	C6-C5-C4	5.80	122.88	118.03
23	PSIB	46	7MG	CM7-N7-C5	5.80	141.37	126.40
26	TRNA	54	5MU	C4-N3-C2	-5.79	119.85	127.35
26	TRNA	37	MIA	C12-N6-C6	5.76	131.07	122.55
1	16SA	2142	MA6	N3-C2-N1	-5.74	119.70	128.68
1	16SA	2141	MA6	N3-C2-N1	-5.72	119.74	128.68
1	16SB	2141	MA6	N3-C2-N1	-5.71	119.76	128.68
24	ESIB	37	MIA	C16-C14-C13	-5.69	106.20	122.65
26	TRNA	37	MIA	C1'-N9-C4	5.68	136.62	126.64
27	23SB	1964	5MU	O4-C4-C5	-5.66	118.34	124.90
27	23SB	2567	OMU	C4-N3-C2	-5.61	119.19	126.58
24	ESIB	37	MIA	C12-N6-C6	-5.58	114.28	122.55
1	16SA	1145	PSU	N1-C2-N3	5.58	121.45	115.13
23	PSIB	54	5MU	O4-C4-C5	-5.54	118.47	124.90
27	23SA	1964	5MU	C5M-C5-C6	-5.48	115.53	122.85
1	16SB	2030	4OC	CM4-N4-C4	-5.45	111.80	122.45
23	PSIA	54	5MU	O4-C4-C5	-5.45	118.59	124.90
22	ASIA	37	MIA	C16-C14-C13	-5.41	107.02	122.65
1	16SA	1156	7MG	C5-C6-N1	5.40	120.52	110.99
23	PSIB	37	MIA	C12-N6-C6	-5.40	114.55	122.55
22	ASIA	46	7MG	C5-C4-N9	5.39	113.35	106.35
23	PSIA	46	7MG	C5-C4-N9	5.38	113.34	106.35
23	PSIA	54	5MU	C4-N3-C2	-5.34	120.43	127.35
27	23SB	1964	5MU	C5-C6-N1	-5.30	117.88	123.34
26	TRNA	54	5MU	O4-C4-C5	-5.28	118.78	124.90
27	23SB	1940	5MU	O4-C4-C5	-5.25	118.81	124.90
23	PSIB	54	5MU	C4-N3-C2	-5.24	120.57	127.35
24	ESIA	37	MIA	C16-C14-C13	-5.23	107.52	122.65
23	PSIA	54	5MU	C6-C5-C4	5.22	122.39	118.03
57	ASIB	54	5MU	O4-C4-C5	-5.21	118.86	124.90
23	PSIA	46	7MG	C6-C5-N7	-5.20	123.74	131.91
27	23SA	1940	5MU	C6-C5-C4	5.16	122.34	118.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16SB	1156	7MG	C5-C6-N1	5.16	120.08	110.99
27	23SA	2567	OMU	C4-N3-C2	-5.14	119.80	126.58
23	PSIB	37	MIA	C15-C14-C13	-5.12	107.85	122.65
22	ASIA	46	7MG	C5-C6-N1	5.10	119.98	110.99
22	ASIA	54	5MU	C5-C6-N1	-5.09	118.10	123.34
23	PSIB	37	MIA	C16-C14-C13	-5.08	107.97	122.65
22	ASIA	54	5MU	O4-C4-C5	-5.07	119.03	124.90
1	16SA	1589	M2G	N1-C2-N2	5.05	122.33	118.04
23	PSIB	32	PSU	N1-C2-N3	5.04	120.84	115.13
57	ASIB	54	5MU	C5-C6-N1	-5.00	118.19	123.34
23	PSIA	37	MIA	C2-N3-C4	4.99	122.20	115.32
27	23SB	2266	OMG	O6-C6-N1	-4.98	114.77	120.65
1	16SA	2028	5MC	C5-C6-N1	-4.94	118.25	123.34
27	23SA	1940	5MU	C5-C6-N1	-4.91	118.29	123.34
23	PSIB	54	5MU	C6-N1-C2	-4.88	116.36	121.30
1	16SA	1156	7MG	C2-N3-C4	4.86	120.95	112.30
26	TRNA	54	5MU	C5-C6-N1	-4.85	118.34	123.34
57	ASIB	32	PSU	N1-C2-N3	4.85	120.63	115.13
57	ASIB	54	5MU	C6-C5-C4	4.85	122.08	118.03
26	TRNA	54	5MU	C6-C5-C4	4.81	122.06	118.03
27	23SA	2266	OMG	O6-C6-N1	-4.81	114.97	120.65
23	PSIA	37	MIA	C12-N6-C6	-4.78	115.47	122.55
27	23SA	2266	OMG	O6-C6-C5	-4.77	115.05	124.37
23	PSIB	46	7MG	C5-C6-N1	4.77	119.40	110.99
1	16SA	2121	UR3	C4-N3-C2	-4.76	120.08	124.56
27	23SB	2266	OMG	O6-C6-C5	-4.74	115.12	124.37
22	ASIA	37	MIA	C2-N3-C4	4.71	121.82	115.32
26	TRNA	55	PSU	C4-N3-C2	-4.68	119.60	126.34
27	23SB	1942	PSU	C4-N3-C2	-4.65	119.64	126.34
27	23SB	2620	PSU	C4-N3-C2	-4.64	119.66	126.34
27	23SA	1936	PSU	C4-N3-C2	-4.63	119.67	126.34
27	23SA	2518	2MA	C1'-N9-C4	-4.61	118.54	126.64
27	23SB	1942	PSU	N1-C2-N3	4.60	120.35	115.13
23	PSIA	46	7MG	C5-C6-N1	4.59	119.08	110.99
57	ASIB	32	PSU	C4-N3-C2	-4.55	119.78	126.34
1	16SA	1145	PSU	C4-N3-C2	-4.55	119.79	126.34
1	16SA	1156	7MG	C5-C4-N3	-4.55	119.47	128.13
23	PSIA	46	7MG	C5-C4-N3	-4.55	119.47	128.13
57	ASIB	37	MIA	C15-C14-C13	-4.53	109.56	122.65
27	23SA	2620	PSU	N1-C2-N3	4.53	120.26	115.13
22	ASIA	54	5MU	C6-C5-C4	4.53	121.81	118.03
27	23SB	1936	PSU	C4-N3-C2	-4.52	119.83	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SB	1964	5MU	C6-N1-C2	-4.52	116.72	121.30
24	ESIB	37	MIA	C15-C14-C13	-4.51	109.62	122.65
23	PSIA	39	PSU	C4-N3-C2	-4.50	119.85	126.34
23	PSIA	39	PSU	N1-C2-N3	4.50	120.23	115.13
22	ASIA	8	4SU	C5-C4-S4	-4.48	118.69	124.47
27	23SA	1964	5MU	O4-C4-C5	-4.48	119.71	124.90
26	TRNA	39	PSU	C4-N3-C2	-4.45	119.92	126.34
27	23SA	2620	PSU	C4-N3-C2	-4.44	119.94	126.34
57	ASIB	39	PSU	C4-N3-C2	-4.43	119.95	126.34
1	16SB	1145	PSU	C4-N3-C2	-4.43	119.96	126.34
27	23SB	2620	PSU	N1-C2-N3	4.42	120.13	115.13
24	ESIB	37	MIA	C2-N3-C4	4.41	121.41	115.32
23	PSIB	55	PSU	C4-N3-C2	-4.37	120.05	126.34
22	ASIA	46	7MG	C2-N3-C4	4.34	120.04	112.30
1	16SB	1145	PSU	N1-C2-N3	4.33	120.04	115.13
23	PSIA	47	3AU	O2-C2-N3	-4.30	116.00	121.99
57	ASIB	39	PSU	N1-C2-N3	4.30	120.00	115.13
23	PSIA	37	MIA	C15-C14-C13	-4.30	110.22	122.65
26	TRNA	39	PSU	N1-C2-N3	4.30	120.00	115.13
27	23SA	1936	PSU	N1-C2-N3	4.29	119.99	115.13
23	PSIB	32	PSU	C4-N3-C2	-4.29	120.16	126.34
1	16SB	1156	7MG	C2-N3-C4	4.28	119.92	112.30
23	PSIA	55	PSU	N1-C2-N3	4.27	119.97	115.13
26	TRNA	55	PSU	N1-C2-N3	4.27	119.96	115.13
26	TRNA	32	PSU	C4-N3-C2	-4.26	120.20	126.34
27	23SA	1967	5MC	C5-C6-N1	-4.24	118.97	123.34
22	ASIA	46	7MG	C6-C5-N7	-4.21	125.29	131.91
1	16SB	2028	5MC	C5-C6-N1	-4.21	119.01	123.34
26	TRNA	37	MIA	C2-N3-C4	4.20	121.11	115.32
26	TRNA	54	5MU	C5M-C5-C6	-4.19	117.26	122.85
23	PSIB	39	PSU	C4-N3-C2	-4.17	120.33	126.34
22	ASIA	32	PSU	N1-C2-N3	4.15	119.83	115.13
22	ASIA	39	PSU	C4-N3-C2	-4.14	120.38	126.34
27	23SA	1942	PSU	N1-C2-N3	4.13	119.81	115.13
23	PSIB	47	3AU	C6-N1-C2	-4.10	118.12	121.79
23	PSIA	32	PSU	C4-N3-C2	-4.09	120.44	126.34
27	23SA	1942	PSU	C4-N3-C2	-4.03	120.53	126.34
22	ASIA	46	7MG	C5-C4-N3	-4.02	120.46	128.13
1	16SA	1156	7MG	C6-C5-N7	-4.02	125.59	131.91
23	PSIB	46	7MG	C2-N3-C4	4.01	119.44	112.30
57	ASIB	54	5MU	C5M-C5-C6	-3.97	117.54	122.85
27	23SA	1940	5MU	C6-N1-C2	-3.97	117.28	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	PSIA	46	7MG	C2-N3-C4	3.96	119.36	112.30
22	ASIA	39	PSU	N1-C2-N3	3.96	119.61	115.13
1	16SB	2121	UR3	C4-N3-C2	-3.95	120.84	124.56
23	PSIA	55	PSU	C4-N3-C2	-3.95	120.65	126.34
27	23SB	1940	5MU	C5M-C5-C6	-3.93	117.60	122.85
1	16SA	2121	UR3	C6-N1-C2	-3.93	118.27	121.79
22	ASIA	54	5MU	C5M-C5-C6	-3.93	117.60	122.85
27	23SA	2567	OMU	C5-C4-N3	3.92	120.70	114.84
23	PSIA	37	MIA	C16-C14-C13	-3.89	111.40	122.65
26	TRNA	32	PSU	N1-C2-N3	3.88	119.53	115.13
24	ESIA	37	MIA	C15-C14-C13	-3.86	111.49	122.65
22	ASIA	37	MIA	C15-C14-C13	-3.86	111.50	122.65
1	16SB	1156	7MG	C6-C5-N7	-3.85	125.86	131.91
23	PSIB	8	4SU	N3-C2-N1	3.85	120.00	114.89
23	PSIB	46	7MG	C6-C5-N7	-3.82	125.90	131.91
23	PSIA	47	3AU	C1'-N1-C2	3.82	123.44	116.99
27	23SB	2567	OMU	C5-C4-N3	3.81	120.55	114.84
27	23SB	1940	5MU	C6-N1-C2	-3.81	117.44	121.30
22	ASIA	32	PSU	C4-N3-C2	-3.80	120.86	126.34
27	23SB	2567	OMU	N3-C2-N1	3.79	119.92	114.89
1	16SB	2121	UR3	C6-N1-C2	-3.78	118.40	121.79
23	PSIA	8	4SU	C5-C4-S4	-3.77	119.61	124.47
23	PSIB	54	5MU	C5M-C5-C6	-3.74	117.85	122.85
22	ASIA	55	PSU	C4-N3-C2	-3.74	120.95	126.34
1	16SB	1589	M2G	C5-C6-N1	3.73	120.54	113.95
24	ESIA	37	MIA	C2-N3-C4	3.73	120.46	115.32
12	S12B	89	0TD	OD2-CG-CB	3.73	121.20	113.15
23	PSIB	55	PSU	N1-C2-N3	3.72	119.35	115.13
22	ASIA	55	PSU	N1-C2-N3	3.72	119.34	115.13
23	PSIB	39	PSU	N1-C2-N3	3.70	119.33	115.13
23	PSIA	32	PSU	N1-C2-N3	3.70	119.32	115.13
27	23SB	1964	5MU	C5M-C5-C6	-3.69	117.93	122.85
57	ASIB	37	MIA	C16-C14-C13	-3.68	112.03	122.65
23	PSIB	46	7MG	C5-C4-N3	-3.66	121.15	128.13
27	23SB	1936	PSU	N1-C2-N3	3.66	119.27	115.13
23	PSIB	37	MIA	C2-N3-C4	3.65	120.35	115.32
27	23SB	2266	OMG	N2-C2-N1	3.62	124.42	116.71
1	16SB	1156	7MG	C5-C4-N3	-3.60	121.28	128.13
22	ASIA	37	MIA	N3-C2-N1	-3.59	120.37	126.98
26	TRNA	54	5MU	C6-N1-C2	-3.59	117.66	121.30
23	PSIB	47	3AU	C4-N3-C2	-3.58	120.14	124.63
57	ASIB	37	MIA	C2-N3-C4	3.58	120.26	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	TRNA	8	4SU	N3-C2-N1	3.56	119.61	114.89
22	ASIA	8	4SU	N3-C2-N1	3.55	119.60	114.89
57	ASIB	54	5MU	C6-N1-C2	-3.53	117.72	121.30
27	23SA	1936	PSU	O2-C2-N1	-3.51	118.93	122.79
26	TRNA	37	MIA	C16-C14-C13	-3.50	112.54	122.65
26	TRNA	8	4SU	C5-C4-S4	-3.49	119.96	124.47
1	16SA	1834	2MG	C5-C6-N1	3.49	120.12	113.95
1	16SA	1589	M2G	C5-C6-N1	3.47	120.08	113.95
23	PSIA	54	5MU	C5M-C5-C6	-3.46	118.23	122.85
1	16SA	1590	5MC	C5-C6-N1	-3.45	119.78	123.34
23	PSIB	54	5MU	C6-C5-C4	3.44	120.91	118.03
23	PSIA	8	4SU	N3-C2-N1	3.41	119.42	114.89
27	23SB	2518	2MA	N3-C2-N1	-3.37	119.57	125.73
23	PSIA	37	MIA	N3-C2-N1	-3.36	120.80	126.98
27	23SB	1964	5MU	N3-C2-N1	3.34	119.33	114.89
23	PSIB	32	PSU	C6-N1-C2	-3.33	119.28	122.68
23	PSIA	47	3AU	C4-N3-C2	-3.32	120.47	124.63
23	PSIB	46	7MG	N9-C8-N7	-3.31	98.64	103.38
27	23SB	1940	5MU	N3-C2-N1	3.30	119.27	114.89
57	ASIB	37	MIA	C1'-N9-C4	3.26	132.37	126.64
1	16SA	1145	PSU	C6-N1-C2	-3.26	119.35	122.68
27	23SA	1940	5MU	C5M-C5-C6	-3.25	118.51	122.85
22	ASIA	37	MIA	C12-N6-C6	-3.25	117.74	122.55
57	ASIB	37	MIA	C5-C6-N1	-3.23	118.12	120.81
27	23SA	1942	PSU	O2-C2-N1	-3.23	119.23	122.79
23	PSIA	39	PSU	O2-C2-N1	-3.23	119.23	122.79
12	S12A	89	0TD	OD2-CG-CB	3.23	120.12	113.15
22	ASIA	54	5MU	C6-N1-C2	-3.21	118.05	121.30
27	23SA	2567	OMU	N3-C2-N1	3.21	119.15	114.89
27	23SA	2266	OMG	N2-C2-N1	3.20	123.54	116.71
23	PSIB	8	4SU	O2-C2-N1	-3.20	118.53	122.79
26	TRNA	37	MIA	C5-C6-N1	-3.19	118.16	120.81
1	16SB	2032	5MC	C5-C6-N1	-3.18	120.06	123.34
1	16SA	2035	5MC	C5-C6-N1	-3.17	120.08	123.34
22	ASIA	46	7MG	O6-C6-C5	-3.16	119.78	127.54
23	PSIA	47	3AU	C6-N1-C2	-3.16	118.96	121.79
24	ESIB	37	MIA	C16-C14-C15	-3.15	107.64	114.60
23	PSIA	55	PSU	O2-C2-N1	-3.14	119.34	122.79
1	16SB	2035	5MC	C5-C6-N1	-3.13	120.12	123.34
23	PSIA	55	PSU	C6-N1-C2	-3.12	119.49	122.68
22	ASIA	46	7MG	N9-C8-N7	-3.12	98.92	103.38
1	16SB	1156	7MG	O6-C6-C5	-3.11	119.92	127.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	TRNA	39	PSU	O2-C2-N1	-3.08	119.40	122.79
27	23SA	2518	2MA	N3-C2-N1	-3.07	120.13	125.73
1	16SB	1834	2MG	C5-C6-N1	3.03	119.30	113.95
23	PSIB	54	5MU	C1'-N1-C2	3.00	123.00	117.57
23	PSIA	46	7MG	C2-N1-C6	-2.99	119.65	125.10
24	ESIA	37	MIA	N3-C2-N1	-2.98	121.49	126.98
27	23SA	1945	OMC	O2-C2-N3	-2.98	117.49	122.33
24	ESIB	37	MIA	N3-C2-N1	-2.98	121.51	126.98
23	PSIA	47	3AU	C5-C4-N3	2.97	119.42	115.50
22	ASIA	39	PSU	O2-C2-N1	-2.97	119.52	122.79
27	23SB	1942	PSU	O2-C2-N1	-2.96	119.53	122.79
1	16SB	1589	M2G	C2-N1-C6	-2.95	118.81	123.71
27	23SA	1964	5MU	O2-C2-N1	-2.95	118.87	122.79
1	16SA	1834	2MG	C8-N7-C5	2.91	108.54	102.99
23	PSIA	46	7MG	N9-C8-N7	-2.91	99.22	103.38
23	PSIB	54	5MU	C5-C6-N1	-2.90	120.36	123.34
26	TRNA	32	PSU	O2-C2-N1	-2.89	119.61	122.79
27	23SA	2266	OMG	C2-N1-C6	2.89	130.41	125.10
1	16SB	2030	4OC	O2-C2-N3	-2.86	117.67	122.33
23	PSIB	46	7MG	C2-N1-C6	-2.86	119.88	125.10
1	16SA	1156	7MG	C2-N1-C6	-2.86	119.89	125.10
23	PSIB	37	MIA	C4-C5-N7	-2.85	106.43	109.40
1	16SA	1156	7MG	N9-C8-N7	-2.85	99.30	103.38
1	16SA	1145	PSU	C6-C5-C4	2.85	120.19	118.20
22	ASIA	55	PSU	O2-C2-N1	-2.83	119.68	122.79
27	23SA	2567	OMU	O4-C4-C5	-2.82	120.20	125.16
1	16SB	2030	4OC	C2'-C1'-N1	-2.82	108.75	114.22
27	23SB	1967	5MC	C5-C6-N1	-2.81	120.45	123.34
27	23SA	1964	5MU	N3-C2-N1	2.80	118.61	114.89
22	ASIA	46	7MG	C2-N1-C6	-2.80	119.99	125.10
22	ASIA	32	PSU	C6-N1-C2	-2.79	119.83	122.68
23	PSIB	47	3AU	C5-C4-N3	2.79	119.17	115.50
1	16SB	1156	7MG	N9-C8-N7	-2.77	99.42	103.38
1	16SA	2032	5MC	C5-C6-N1	-2.77	120.49	123.34
27	23SA	1967	5MC	CM5-C5-C6	-2.76	119.16	122.85
27	23SA	1964	5MU	C6-N1-C2	-2.75	118.51	121.30
26	TRNA	55	PSU	O2-C2-N1	-2.75	119.77	122.79
23	PSIB	46	7MG	O6-C6-C5	-2.75	120.80	127.54
1	16SB	2028	5MC	CM5-C5-C6	-2.74	119.18	122.85
1	16SB	1156	7MG	C2-N1-C6	-2.74	120.10	125.10
23	PSIB	39	PSU	O2-C2-N1	-2.73	119.78	122.79
1	16SA	1156	7MG	O6-C6-C5	-2.73	120.85	127.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SA	1940	5MU	N3-C2-N1	2.72	118.50	114.89
27	23SB	2266	OMG	N1-C2-N3	-2.71	118.25	123.32
23	PSIB	47	3AU	C1'-N1-C6	-2.71	114.94	120.84
27	23SA	1940	5MU	C1'-N1-C2	2.71	122.47	117.57
23	PSIB	8	4SU	S4-C4-N3	2.67	122.84	120.21
57	ASIB	32	PSU	O2-C2-N1	-2.67	119.86	122.79
1	16SB	1834	2MG	C8-N7-C5	2.65	108.04	102.99
22	ASIA	37	MIA	C16-C14-C15	-2.64	108.77	114.60
1	16SA	1589	M2G	C8-N7-C5	2.64	108.02	102.99
22	ASIA	54	5MU	O2-C2-N1	-2.64	119.28	122.79
23	PSIB	55	PSU	O2-C2-N1	-2.63	119.89	122.79
24	ESIA	37	MIA	C2-N1-C6	2.63	121.90	117.19
27	23SB	2518	2MA	CM2-C2-N1	2.63	121.26	117.15
1	16SA	2035	5MC	CM5-C5-C6	-2.61	119.36	122.85
57	ASIB	32	PSU	C6-N1-C2	-2.61	120.02	122.68
22	ASIA	37	MIA	C2-N1-C6	2.60	121.85	117.19
27	23SB	1967	5MC	CM5-C5-C6	-2.60	119.38	122.85
57	ASIB	37	MIA	C16-C14-C15	-2.60	108.86	114.60
27	23SB	2567	OMU	O4-C4-C5	-2.58	120.61	125.16
27	23SB	1964	5MU	O2-C2-N1	-2.58	119.36	122.79
27	23SA	1964	5MU	C5M-C5-C4	2.56	121.59	118.77
27	23SB	1936	PSU	O2-C2-N1	-2.56	119.97	122.79
23	PSIA	46	7MG	O6-C6-C5	-2.56	121.27	127.54
27	23SA	1987	5MC	C5-C6-N1	-2.55	120.71	123.34
27	23SA	2266	OMG	N1-C2-N3	-2.55	118.56	123.32
1	16SA	2028	5MC	CM5-C5-C6	-2.55	119.44	122.85
24	ESIA	37	MIA	C5-C6-N1	-2.52	118.72	120.81
26	TRNA	37	MIA	C16-C14-C15	-2.52	109.04	114.60
1	16SB	1589	M2G	C8-N7-C5	2.50	107.76	102.99
22	ASIA	55	PSU	C6-N1-C2	-2.48	120.14	122.68
27	23SA	2620	PSU	C6-N1-C2	-2.47	120.16	122.68
27	23SA	1942	PSU	C6-N1-C2	-2.46	120.17	122.68
57	ASIB	32	PSU	C6-C5-C4	2.43	119.90	118.20
27	23SB	2266	OMG	C2-N1-C6	2.43	129.56	125.10
1	16SA	1834	2MG	O6-C6-C5	-2.43	119.64	124.37
27	23SB	1942	PSU	C6-C5-C4	2.41	119.89	118.20
23	PSIB	37	MIA	N3-C2-N1	-2.41	122.55	126.98
1	16SB	2028	5MC	C1'-N1-C6	-2.39	117.14	121.12
23	PSIA	32	PSU	O2-C2-N1	-2.39	120.16	122.79
23	PSIA	39	PSU	C6-N1-C2	-2.39	120.24	122.68
1	16SB	1589	M2G	O6-C6-C5	-2.38	119.72	124.37
1	16SB	2032	5MC	CM5-C5-C6	-2.38	119.67	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	ASIB	39	PSU	O2-C2-N1	-2.37	120.18	122.79
1	16SB	2035	5MC	CM5-C5-C6	-2.37	119.69	122.85
27	23SB	1940	5MU	O3'-C3'-C2'	2.36	119.46	111.82
26	TRNA	37	MIA	N3-C2-N1	-2.35	122.65	126.98
27	23SB	1945	OMC	O2-C2-N3	-2.34	118.52	122.33
1	16SA	1145	PSU	O2-C2-N1	-2.34	120.21	122.79
23	PSIA	37	MIA	C2-N1-C6	2.34	121.38	117.19
1	16SA	1589	M2G	C2-N1-C6	-2.34	119.83	123.71
1	16SB	1834	2MG	O6-C6-C5	-2.34	119.81	124.37
57	ASIB	37	MIA	N3-C2-N1	-2.32	122.71	126.98
23	PSIB	37	MIA	C16-C14-C15	-2.32	109.48	114.60
23	PSIB	32	PSU	O2-C2-N1	-2.31	120.25	122.79
27	23SA	1940	5MU	O2-C2-N1	-2.30	119.72	122.79
22	ASIA	54	5MU	N3-C2-N1	2.30	117.94	114.89
12	S12B	89	0TD	OD1-CG-CB	-2.29	117.64	122.44
23	PSIA	54	5MU	C6-N1-C2	-2.29	118.97	121.30
26	TRNA	54	5MU	N3-C2-N1	2.28	117.91	114.89
26	TRNA	8	4SU	C1'-N1-C2	2.26	121.67	117.57
27	23SB	1987	5MC	C5-C6-N1	-2.26	121.01	123.34
57	ASIB	54	5MU	N3-C2-N1	2.25	117.88	114.89
23	PSIB	54	5MU	C5M-C5-C4	2.25	121.24	118.77
22	ASIA	8	4SU	C1'-N1-C2	2.25	121.64	117.57
1	16SB	1590	5MC	CM5-C5-C6	-2.24	119.86	122.85
1	16SA	1145	PSU	O4'-C1'-C2'	2.23	108.29	105.14
27	23SA	2620	PSU	O2-C2-N1	-2.20	120.37	122.79
57	ASIB	37	MIA	C4-C5-N7	-2.20	107.11	109.40
23	PSIB	47	3AU	C10-N3-C4	2.20	121.47	117.14
24	ESIB	37	MIA	C4-C5-N7	-2.18	107.12	109.40
23	PSIA	37	MIA	C4-C5-N7	-2.17	107.14	109.40
22	ASIA	37	MIA	C1'-N9-C4	2.17	130.45	126.64
1	16SA	2030	4OC	C6-C5-C4	2.16	119.61	116.96
57	ASIB	37	MIA	C2-N1-C6	2.16	121.06	117.19
23	PSIB	32	PSU	C6-C5-C4	2.15	119.70	118.20
57	ASIB	39	PSU	C6-N1-C2	-2.15	120.49	122.68
27	23SA	1964	5MU	O4-C4-N3	-2.14	116.01	120.12
27	23SB	1987	5MC	C5-C4-N3	-2.13	119.38	121.67
1	16SA	1156	7MG	N1-C2-N3	-2.12	119.37	123.32
22	ASIA	39	PSU	C6-N1-C2	-2.12	120.52	122.68
1	16SB	1145	PSU	O4'-C1'-C2'	2.11	108.12	105.14
23	PSIA	37	MIA	C16-C14-C15	-2.10	109.97	114.60
24	ESIB	37	MIA	C2-N1-C6	2.10	120.94	117.19
22	ASIA	32	PSU	O2-C2-N1	-2.09	120.49	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	PSIB	39	PSU	C6-N1-C2	-2.09	120.54	122.68
27	23SB	2620	PSU	C6-N1-C2	-2.09	120.55	122.68
27	23SB	1967	5MC	C5-C4-N3	-2.08	119.43	121.67
24	ESIA	37	MIA	C4-C5-N7	-2.07	107.25	109.40
1	16SA	2030	4OC	C5-C4-N3	-2.06	119.27	122.59
23	PSIB	54	5MU	N3-C2-N1	2.06	117.62	114.89
27	23SA	1936	PSU	C6-N1-C2	-2.04	120.60	122.68
1	16SB	2028	5MC	O2-C2-N3	-2.03	119.03	122.33
26	TRNA	32	PSU	C6-N1-C2	-2.03	120.61	122.68
1	16SA	2030	4OC	O2-C2-N3	-2.02	119.04	122.33
23	PSIA	46	7MG	O4'-C1'-N9	-2.02	106.55	109.30
1	16SB	1156	7MG	N1-C2-N3	-2.01	119.56	123.32
57	ASIB	39	PSU	C6-C5-C4	2.01	119.60	118.20

There are no chirality outliers.

All (110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	S12A	89	0TD	SB-CB-CG-OD2
12	S12B	89	0TD	CA-CB-SB-CSB
1	16SA	1156	7MG	O4'-C4'-C5'-O5'
1	16SA	1156	7MG	C3'-C4'-C5'-O5'
1	16SB	1156	7MG	C3'-C4'-C5'-O5'
1	16SB	1834	2MG	O4'-C4'-C5'-O5'
1	16SB	1834	2MG	C3'-C4'-C5'-O5'
1	16SA	2142	MA6	O4'-C4'-C5'-O5'
1	16SA	2142	MA6	C3'-C4'-C5'-O5'
1	16SB	2142	MA6	O4'-C4'-C5'-O5'
22	ASIA	37	MIA	O4'-C4'-C5'-O5'
22	ASIA	37	MIA	C12-C13-C14-C15
22	ASIA	37	MIA	C12-C13-C14-C16
23	PSIA	37	MIA	C3'-C4'-C5'-O5'
23	PSIA	37	MIA	C12-C13-C14-C15
23	PSIB	37	MIA	C12-C13-C14-C15
23	PSIB	37	MIA	C12-C13-C14-C16
23	PSIA	47	3AU	N3-C10-C11-C12
23	PSIA	47	3AU	C10-C11-C12-C13
23	PSIA	47	3AU	C10-C11-C12-N40
23	PSIA	47	3AU	C3'-C4'-C5'-O5'
23	PSIB	47	3AU	C2'-C1'-N1-C2
23	PSIB	54	5MU	C3'-C4'-C5'-O5'
23	PSIB	54	5MU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
24	ESIA	37	MIA	N1-C2-S10-C11
24	ESIA	37	MIA	N3-C2-S10-C11
24	ESIA	37	MIA	C12-C13-C14-C16
24	ESIB	37	MIA	C3'-C4'-C5'-O5'
24	ESIB	37	MIA	N1-C2-S10-C11
24	ESIB	37	MIA	N3-C2-S10-C11
24	ESIB	37	MIA	C12-C13-C14-C16
26	TRNA	8	4SU	C3'-C4'-C5'-O5'
26	TRNA	8	4SU	O4'-C4'-C5'-O5'
26	TRNA	37	MIA	N1-C2-S10-C11
26	TRNA	37	MIA	N3-C2-S10-C11
26	TRNA	37	MIA	C12-C13-C14-C15
26	TRNA	37	MIA	C12-C13-C14-C16
26	TRNA	54	5MU	C3'-C4'-C5'-O5'
26	TRNA	54	5MU	O4'-C4'-C5'-O5'
27	23SB	1964	5MU	O4'-C4'-C5'-O5'
57	ASIB	37	MIA	C12-C13-C14-C15
1	16SB	1156	7MG	O4'-C4'-C5'-O5'
1	16SA	2030	4OC	O4'-C4'-C5'-O5'
1	16SB	2030	4OC	O4'-C4'-C5'-O5'
1	16SB	2030	4OC	C3'-C4'-C5'-O5'
1	16SB	2142	MA6	C3'-C4'-C5'-O5'
22	ASIA	37	MIA	C3'-C4'-C5'-O5'
23	PSIB	8	4SU	C3'-C4'-C5'-O5'
23	PSIB	8	4SU	O4'-C4'-C5'-O5'
23	PSIA	47	3AU	O4'-C4'-C5'-O5'
23	PSIB	47	3AU	C3'-C4'-C5'-O5'
23	PSIB	47	3AU	O4'-C4'-C5'-O5'
23	PSIA	55	PSU	C3'-C4'-C5'-O5'
24	ESIB	37	MIA	O4'-C4'-C5'-O5'
27	23SA	1940	5MU	C3'-C4'-C5'-O5'
27	23SB	1964	5MU	C3'-C4'-C5'-O5'
23	PSIB	47	3AU	C2'-C1'-N1-C6
1	16SA	2030	4OC	C3'-C4'-C5'-O5'
23	PSIA	37	MIA	O4'-C4'-C5'-O5'
27	23SA	1940	5MU	O4'-C4'-C5'-O5'
27	23SB	2567	OMU	C3'-C4'-C5'-O5'
22	ASIA	46	7MG	C3'-C4'-C5'-O5'
22	ASIA	55	PSU	C3'-C4'-C5'-O5'
22	ASIA	55	PSU	O4'-C4'-C5'-O5'
23	PSIA	55	PSU	O4'-C4'-C5'-O5'
27	23SB	2567	OMU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	16SB	2141	MA6	C5-C6-N6-C9
26	TRNA	37	MIA	C4'-C5'-O5'-P
27	23SB	2518	2MA	O4'-C4'-C5'-O5'
23	PSIB	47	3AU	C11-C12-C13-O31
12	S12A	89	0TD	CG-CB-SB-CSB
24	ESIA	37	MIA	C12-C13-C14-C15
23	PSIB	47	3AU	C4'-C5'-O5'-P
23	PSIA	55	PSU	C4'-C5'-O5'-P
12	S12A	89	0TD	SB-CB-CG-OD1
12	S12B	89	0TD	SB-CB-CG-OD1
23	PSIB	47	3AU	C11-C12-C13-O30
24	ESIA	37	MIA	C3'-C4'-C5'-O5'
1	16SB	2142	MA6	C4'-C5'-O5'-P
22	ASIA	46	7MG	O4'-C4'-C5'-O5'
1	16SA	2142	MA6	C4'-C5'-O5'-P
22	ASIA	8	4SU	C4'-C5'-O5'-P
27	23SA	2518	2MA	C4'-C5'-O5'-P
24	ESIA	37	MIA	N6-C12-C13-C14
26	TRNA	37	MIA	N6-C12-C13-C14
57	ASIB	54	5MU	C3'-C4'-C5'-O5'
22	ASIA	55	PSU	O4'-C1'-C5-C4
27	23SA	1936	PSU	O4'-C1'-C5-C4
23	PSIA	47	3AU	C2'-C1'-N1-C2
23	PSIA	47	3AU	C2'-C1'-N1-C6
12	S12A	89	0TD	CA-CB-SB-CSB
27	23SA	1964	5MU	O4'-C4'-C5'-O5'
27	23SB	2518	2MA	C3'-C4'-C5'-O5'
23	PSIA	37	MIA	N1-C2-S10-C11
1	16SA	1589	M2G	O4'-C4'-C5'-O5'
23	PSIA	46	7MG	O4'-C4'-C5'-O5'
57	ASIB	54	5MU	O4'-C4'-C5'-O5'
12	S12B	89	0TD	CG-CB-SB-CSB
27	23SA	1936	PSU	O4'-C1'-C5-C6
24	ESIB	37	MIA	C4'-C5'-O5'-P
23	PSIB	46	7MG	C2'-C1'-N9-C8
23	PSIB	47	3AU	N40-C12-C13-O31
23	PSIA	37	MIA	N3-C2-S10-C11
57	ASIB	37	MIA	N1-C2-S10-C11
57	ASIB	37	MIA	N3-C2-S10-C11
1	16SA	1589	M2G	C3'-C4'-C5'-O5'
23	PSIA	46	7MG	C3'-C4'-C5'-O5'
27	23SA	1964	5MU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
27	23SA	1945	OMC	C2'-C1'-N1-C2
27	23SB	2518	2MA	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1680 ligands modelled in this entry, 1080 are monoatomic - leaving 600 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	$\# Z  > 2$
60	OHX	5SB	208	-	0,6,6	-	-	-		
60	OHX	16SA	2340	-	0,6,6	-	-	-		
60	OHX	23SA	3540	-	0,6,6	-	-	-		
60	OHX	23SA	3483	-	0,6,6	-	-	-		
60	OHX	16SA	2359	-	0,6,6	-	-	-		
60	OHX	23SA	3475	-	0,6,6	-	-	-		
60	OHX	23SB	3449	-	0,6,6	-	-	-		
60	OHX	23SB	3372	-	0,6,6	-	-	-		
60	OHX	23SB	3507	-	0,6,6	-	-	-		
60	OHX	23SA	3442	27	0,6,6	-	-	-		
60	OHX	23SA	3558	-	0,6,6	-	-	-		
60	OHX	23SA	3603	-	0,6,6	-	-	-		
60	OHX	23SB	3500	-	0,6,6	-	-	-		
60	OHX	16SA	2381	-	0,6,6	-	-	-		
60	OHX	23SA	3594	-	0,6,6	-	-	-		
60	OHX	23SA	3437	-	0,6,6	-	-	-		
60	OHX	23SA	3472	-	0,6,6	-	-	-		
60	OHX	23SA	3567	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	OHX	23SB	3468	-	0,6,6	-	-	-		
60	OHX	16SA	2387	-	0,6,6	-	-	-		
60	OHX	23SA	3460	-	0,6,6	-	-	-		
60	OHX	16SA	2400	-	0,6,6	-	-	-		
60	OHX	23SB	3486	-	0,6,6	-	-	-		
60	OHX	23SA	3604	-	0,6,6	-	-	-		
60	OHX	23SA	3531	-	0,6,6	-	-	-		
60	OHX	16SA	2372	-	0,6,6	-	-	-		
60	OHX	16SB	2365	-	0,6,6	-	-	-		
60	OHX	23SA	3563	-	0,6,6	-	-	-		
60	OHX	23SB	3412	-	0,6,6	-	-	-		
60	OHX	23SA	3580	-	0,6,6	-	-	-		
60	OHX	23SA	3609	-	0,6,6	-	-	-		
60	OHX	16SA	2342	-	0,6,6	-	-	-		
60	OHX	16SA	2343	-	0,6,6	-	-	-		
60	OHX	23SA	3612	-	0,6,6	-	-	-		
60	OHX	23SB	3354	-	0,6,6	-	-	-		
60	OHX	23SB	3513	-	0,6,6	-	-	-		
60	OHX	23SA	3476	-	0,6,6	-	-	-		
60	OHX	16SA	2416	1	0,6,6	-	-	-		
60	OHX	23SB	3378	-	0,6,6	-	-	-		
60	OHX	16SB	2383	-	0,6,6	-	-	-		
60	OHX	23SB	3364	-	0,6,6	-	-	-		
60	OHX	23SA	3539	-	0,6,6	-	-	-		
60	OHX	23SA	3454	-	0,6,6	-	-	-		
60	OHX	23SB	3371	27	0,6,6	-	-	-		
60	OHX	S4B	302	4	0,6,6	-	-	-		
60	OHX	23SB	3403	-	0,6,6	-	-	-		
60	OHX	23SB	3385	-	0,6,6	-	-	-		
60	OHX	23SB	3370	-	0,6,6	-	-	-		
60	OHX	16SA	2415	-	0,6,6	-	-	-		
60	OHX	16SA	2377	-	0,6,6	-	-	-		
60	OHX	23SB	3381	-	0,6,6	-	-	-		
60	OHX	23SB	3402	-	0,6,6	-	-	-		
60	OHX	16SB	2328	-	0,6,6	-	-	-		
60	OHX	23SA	3447	-	0,6,6	-	-	-		
60	OHX	23SB	3429	-	0,6,6	-	-	-		
60	OHX	23SB	3473	-	0,6,6	-	-	-		
60	OHX	23SB	3393	-	0,6,6	-	-	-		
60	OHX	16SB	2355	1	0,6,6	-	-	-		
60	OHX	16SB	2361	-	0,6,6	-	-	-		
60	OHX	23SB	3442	-	0,6,6	-	-	-		
60	OHX	5SB	214	-	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	OHX	16SA	2414	-	0,6,6	-	-	-		
60	OHX	23SA	3543	-	0,6,6	-	-	-		
60	OHX	16SB	2358	1	0,6,6	-	-	-		
60	OHX	23SA	3493	-	0,6,6	-	-	-		
60	OHX	23SB	3485	-	0,6,6	-	-	-		
60	OHX	16SA	2403	-	0,6,6	-	-	-		
60	OHX	5SA	212	-	0,6,6	-	-	-		
60	OHX	23SA	3465	-	0,6,6	-	-	-		
60	OHX	23SA	3535	-	0,6,6	-	-	-		
60	OHX	23SA	3479	-	0,6,6	-	-	-		
60	OHX	23SA	3530	-	0,6,6	-	-	-		
60	OHX	L28A	101	-	0,6,6	-	-	-		
60	OHX	23SA	3547	-	0,6,6	-	-	-		
60	OHX	16SA	2358	-	0,6,6	-	-	-		
60	OHX	23SB	3345	-	0,6,6	-	-	-		
60	OHX	23SB	3353	-	0,6,6	-	-	-		
60	OHX	23SB	3331	-	0,6,6	-	-	-		
60	OHX	16SA	2393	-	0,6,6	-	-	-		
60	OHX	23SA	3457	-	0,6,6	-	-	-		
60	OHX	23SA	3599	-	0,6,6	-	-	-		
60	OHX	23SB	3406	-	0,6,6	-	-	-		
60	OHX	16SB	2342	-	0,6,6	-	-	-		
60	OHX	23SB	3430	-	0,6,6	-	-	-		
60	OHX	23SA	3570	27	0,6,6	-	-	-		
60	OHX	23SB	3383	-	0,6,6	-	-	-		
60	OHX	16SB	2396	-	0,6,6	-	-	-		
60	OHX	23SA	3617	-	0,6,6	-	-	-		
60	OHX	23SB	3447	-	0,6,6	-	-	-		
60	OHX	23SA	3586	-	0,6,6	-	-	-		
60	OHX	23SA	3585	-	0,6,6	-	-	-		
60	OHX	23SB	3362	-	0,6,6	-	-	-		
60	OHX	23SB	3343	-	0,6,6	-	-	-		
60	OHX	23SA	3518	-	0,6,6	-	-	-		
60	OHX	23SB	3422	-	0,6,6	-	-	-		
60	OHX	16SB	2343	-	0,6,6	-	-	-		
60	OHX	23SA	3574	-	0,6,6	-	-	-		
60	OHX	23SA	3578	-	0,6,6	-	-	-		
60	OHX	16SA	2345	-	0,6,6	-	-	-		
60	OHX	16SB	2388	-	0,6,6	-	-	-		
60	OHX	16SB	2350	-	0,6,6	-	-	-		
60	OHX	23SB	3358	-	0,6,6	-	-	-		
60	OHX	16SB	2397	-	0,6,6	-	-	-		
60	OHX	23SB	3347	-	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	OHX	23SB	3418	-	0,6,6	-	-	-		
60	OHX	23SA	3516	-	0,6,6	-	-	-		
60	OHX	23SB	3384	-	0,6,6	-	-	-		
60	OHX	23SA	3462	-	0,6,6	-	-	-		
60	OHX	23SA	3584	-	0,6,6	-	-	-		
60	OHX	23SB	3368	-	0,6,6	-	-	-		
60	OHX	23SB	3437	-	0,6,6	-	-	-		
60	OHX	16SB	2368	-	0,6,6	-	-	-		
60	OHX	S8B	201	-	0,6,6	-	-	-		
60	OHX	23SB	3503	-	0,6,6	-	-	-		
60	OHX	23SA	3480	-	0,6,6	-	-	-		
60	OHX	23SA	3602	-	0,6,6	-	-	-		
61	SJH	23SA	3436	-	81,87,87	2.15	18 (22%)	101,128,128	1.73	15 (14%)
60	OHX	23SA	3536	-	0,6,6	-	-	-		
60	OHX	16SA	2350	-	0,6,6	-	-	-		
60	OHX	23SB	3349	-	0,6,6	-	-	-		
60	OHX	23SB	3346	-	0,6,6	-	-	-		
60	OHX	23SA	3452	-	0,6,6	-	-	-		
60	OHX	23SA	3545	-	0,6,6	-	-	-		
60	OHX	23SB	3428	-	0,6,6	-	-	-		
60	OHX	16SA	2384	-	0,6,6	-	-	-		
60	OHX	23SB	3435	-	0,6,6	-	-	-		
60	OHX	23SB	3448	-	0,6,6	-	-	-		
60	OHX	16SA	2355	-	0,6,6	-	-	-		
60	OHX	23SA	3556	-	0,6,6	-	-	-		
60	OHX	23SB	3458	-	0,6,6	-	-	-		
60	OHX	16SB	2386	-	0,6,6	-	-	-		
60	OHX	23SB	3489	-	0,6,6	-	-	-		
60	OHX	23SA	3524	-	0,6,6	-	-	-		
60	OHX	23SB	3495	-	0,6,6	-	-	-		
60	OHX	23SA	3474	-	0,6,6	-	-	-		
60	OHX	16SA	2352	-	0,6,6	-	-	-		
60	OHX	23SA	3582	-	0,6,6	-	-	-		
60	OHX	16SB	2384	-	0,6,6	-	-	-		
60	OHX	23SB	3506	-	0,6,6	-	-	-		
60	OHX	16SB	2379	-	0,6,6	-	-	-		
60	OHX	23SB	3327	27	0,6,6	-	-	-		
60	OHX	23SB	3415	-	0,6,6	-	-	-		
60	OHX	23SA	3499	-	0,6,6	-	-	-		
60	OHX	23SB	3398	-	0,6,6	-	-	-		
60	OHX	23SB	3404	-	0,6,6	-	-	-		
60	OHX	23SA	3466	-	0,6,6	-	-	-		
60	OHX	23SB	3421	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	OHX	23SB	3344	-	0,6,6	-	-	-		
60	OHX	23SB	3365	-	0,6,6	-	-	-		
60	OHX	23SA	3440	-	0,6,6	-	-	-		
60	OHX	23SA	3459	-	0,6,6	-	-	-		
60	OHX	23SA	3520	-	0,6,6	-	-	-		
60	OHX	23SB	3369	-	0,6,6	-	-	-		
60	OHX	L20B	201	-	0,6,6	-	-	-		
60	OHX	16SA	2376	-	0,6,6	-	-	-		
60	OHX	23SB	3452	-	0,6,6	-	-	-		
60	OHX	16SB	2335	1	0,6,6	-	-	-		
60	OHX	23SA	3451	-	0,6,6	-	-	-		
60	OHX	5SA	218	-	0,6,6	-	-	-		
60	OHX	23SB	3376	-	0,6,6	-	-	-		
60	OHX	5SB	211	-	0,6,6	-	-	-		
60	OHX	23SA	3532	-	0,6,6	-	-	-		
60	OHX	PSIB	105	-	0,6,6	-	-	-		
60	OHX	16SA	2390	-	0,6,6	-	-	-		
60	OHX	16SA	2348	-	0,6,6	-	-	-		
60	OHX	23SA	3497	-	0,6,6	-	-	-		
60	OHX	16SB	2376	-	0,6,6	-	-	-		
60	OHX	16SA	2413	-	0,6,6	-	-	-		
60	OHX	16SB	2375	-	0,6,6	-	-	-		
60	OHX	23SB	3508	-	0,6,6	-	-	-		
60	OHX	16SB	2356	-	0,6,6	-	-	-		
60	OHX	16SA	2392	-	0,6,6	-	-	-		
60	OHX	23SB	3427	-	0,6,6	-	-	-		
60	OHX	16SA	2409	-	0,6,6	-	-	-		
60	OHX	16SB	2364	-	0,6,6	-	-	-		
60	OHX	23SB	3375	-	0,6,6	-	-	-		
60	OHX	23SA	3615	-	0,6,6	-	-	-		
60	OHX	23SA	3569	-	0,6,6	-	-	-		
60	OHX	23SB	3492	-	0,6,6	-	-	-		
60	OHX	23SB	3360	-	0,6,6	-	-	-		
60	OHX	16SA	2395	-	0,6,6	-	-	-		
60	OHX	16SA	2337	-	0,6,6	-	-	-		
60	OHX	16SB	2333	-	0,6,6	-	-	-		
60	OHX	23SA	3590	-	0,6,6	-	-	-		
60	OHX	23SA	3523	-	0,6,6	-	-	-		
60	OHX	16SB	2334	-	0,6,6	-	-	-		
60	OHX	16SA	2339	-	0,6,6	-	-	-		
60	OHX	23SA	3495	-	0,6,6	-	-	-		
60	OHX	ASIA	101	-	0,6,6	-	-	-		
60	OHX	23SA	3485	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	OHX	16SB	2347	-	0,6,6	-	-	-		
60	OHX	23SA	3572	-	0,6,6	-	-	-		
60	OHX	23SB	3333	-	0,6,6	-	-	-		
60	OHX	23SA	3562	-	0,6,6	-	-	-		
60	OHX	23SA	3488	-	0,6,6	-	-	-		
60	OHX	L35A	102	56	0,6,6	-	-	-		
60	OHX	16SA	2370	-	0,6,6	-	-	-		
60	OHX	23SB	3431	-	0,6,6	-	-	-		
60	OHX	23SB	3466	-	0,6,6	-	-	-		
60	OHX	16SB	2357	-	0,6,6	-	-	-		
60	OHX	23SB	3361	-	0,6,6	-	-	-		
60	OHX	16SB	2322	-	0,6,6	-	-	-		
60	OHX	23SB	3359	-	0,6,6	-	-	-		
60	OHX	16SA	2410	-	0,6,6	-	-	-		
60	OHX	23SA	3510	-	0,6,6	-	-	-		
60	OHX	ASIA	103	-	0,6,6	-	-	-		
60	OHX	16SB	2394	-	0,6,6	-	-	-		
60	OHX	23SB	3348	-	0,6,6	-	-	-		
60	OHX	23SB	3411	-	0,6,6	-	-	-		
60	OHX	23SB	3388	27	0,6,6	-	-	-		
60	OHX	5SA	216	-	0,6,6	-	-	-		
60	OHX	L27A	103	-	0,6,6	-	-	-		
60	OHX	L15A	203	-	0,6,6	-	-	-		
60	OHX	23SB	3484	-	0,6,6	-	-	-		
60	OHX	23SA	3450	27	0,6,6	-	-	-		
60	OHX	23SA	3593	-	0,6,6	-	-	-		
60	OHX	23SB	3377	-	0,6,6	-	-	-		
60	OHX	23SA	3589	-	0,6,6	-	-	-		
60	OHX	23SA	3468	-	0,6,6	-	-	-		
60	OHX	23SA	3568	-	0,6,6	-	-	-		
60	OHX	23SB	3480	-	0,6,6	-	-	-		
60	OHX	23SA	3526	-	0,6,6	-	-	-		
60	OHX	16SB	2341	-	0,6,6	-	-	-		
60	OHX	23SA	3441	27	0,6,6	-	-	-		
60	OHX	23SB	3488	-	0,6,6	-	-	-		
60	OHX	23SB	3438	-	0,6,6	-	-	-		
60	OHX	23SB	3487	-	0,6,6	-	-	-		
60	OHX	23SB	3499	-	0,6,6	-	-	-		
60	OHX	23SB	3456	-	0,6,6	-	-	-		
60	OHX	16SB	2389	-	0,6,6	-	-	-		
60	OHX	23SB	3459	27	0,6,6	-	-	-		
60	OHX	23SA	3469	-	0,6,6	-	-	-		
60	OHX	16SB	2380	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	OHX	23SA	3600	-	0,6,6	-	-	-		
60	OHX	S14B	101	-	0,6,6	-	-	-		
60	OHX	23SA	3624	-	0,6,6	-	-	-		
60	OHX	23SA	3503	-	0,6,6	-	-	-		
60	OHX	23SA	3554	-	0,6,6	-	-	-		
60	OHX	16SA	2362	-	0,6,6	-	-	-		
60	OHX	23SB	3396	-	0,6,6	-	-	-		
60	OHX	23SA	3565	-	0,6,6	-	-	-		
60	OHX	23SB	3355	-	0,6,6	-	-	-		
60	OHX	23SA	3449	27	0,6,6	-	-	-		
60	OHX	23SA	3537	-	0,6,6	-	-	-		
60	OHX	23SB	3357	-	0,6,6	-	-	-		
60	OHX	16SA	2407	-	0,6,6	-	-	-		
60	OHX	23SB	3505	-	0,6,6	-	-	-		
60	OHX	23SA	3571	-	0,6,6	-	-	-		
60	OHX	23SA	3625	-	0,6,6	-	-	-		
60	OHX	L4A	304	-	0,6,6	-	-	-		
60	OHX	23SA	3611	-	0,6,6	-	-	-		
60	OHX	23SA	3564	-	0,6,6	-	-	-		
60	OHX	16SB	2399	-	0,6,6	-	-	-		
60	OHX	23SB	3444	-	0,6,6	-	-	-		
60	OHX	16SB	2337	-	0,6,6	-	-	-		
60	OHX	23SB	3356	-	0,6,6	-	-	-		
60	OHX	23SB	3330	-	0,6,6	-	-	-		
60	OHX	23SA	3632	-	0,6,6	-	-	-		
60	OHX	16SA	2366	-	0,6,6	-	-	-		
60	OHX	23SB	3446	-	0,6,6	-	-	-		
60	OHX	23SA	3500	-	0,6,6	-	-	-		
60	OHX	16SA	2338	-	0,6,6	-	-	-		
60	OHX	23SA	3573	-	0,6,6	-	-	-		
60	OHX	16SB	2336	-	0,6,6	-	-	-		
60	OHX	23SB	3326	-	0,6,6	-	-	-		
60	OHX	16SB	2352	-	0,6,6	-	-	-		
60	OHX	16SA	2383	-	0,6,6	-	-	-		
60	OHX	16SB	2330	1	0,6,6	-	-	-		
60	OHX	16SA	2398	-	0,6,6	-	-	-		
60	OHX	23SA	3478	-	0,6,6	-	-	-		
60	OHX	23SB	3461	-	0,6,6	-	-	-		
60	OHX	23SB	3425	-	0,6,6	-	-	-		
60	OHX	23SA	3473	-	0,6,6	-	-	-		
60	OHX	23SA	3597	-	0,6,6	-	-	-		
60	OHX	23SA	3626	-	0,6,6	-	-	-		
60	OHX	23SB	3367	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	OHX	23SA	3471	-	0,6,6	-	-	-		
60	OHX	23SB	3409	-	0,6,6	-	-	-		
60	OHX	ESIB	101	-	0,6,6	-	-	-		
60	OHX	23SB	3451	-	0,6,6	-	-	-		
60	OHX	23SA	3601	-	0,6,6	-	-	-		
60	OHX	16SA	2405	-	0,6,6	-	-	-		
60	OHX	23SA	3575	-	0,6,6	-	-	-		
60	OHX	23SA	3519	-	0,6,6	-	-	-		
60	OHX	16SA	2404	-	0,6,6	-	-	-		
60	OHX	23SA	3501	-	0,6,6	-	-	-		
60	OHX	23SB	3340	-	0,6,6	-	-	-		
60	OHX	23SB	3420	-	0,6,6	-	-	-		
60	OHX	23SA	3511	-	0,6,6	-	-	-		
60	OHX	23SA	3548	-	0,6,6	-	-	-		
60	OHX	23SA	3629	-	0,6,6	-	-	-		
60	OHX	23SA	3541	-	0,6,6	-	-	-		
60	OHX	16SB	2329	-	0,6,6	-	-	-		
60	OHX	16SA	2344	-	0,6,6	-	-	-		
60	OHX	16SA	2380	-	0,6,6	-	-	-		
60	OHX	23SA	3546	-	0,6,6	-	-	-		
60	OHX	16SB	2351	-	0,6,6	-	-	-		
60	OHX	5SA	214	-	0,6,6	-	-	-		
60	OHX	23SB	3515	-	0,6,6	-	-	-		
60	OHX	ASIA	102	-	0,6,6	-	-	-		
60	OHX	23SB	3453	-	0,6,6	-	-	-		
60	OHX	23SA	3464	-	0,6,6	-	-	-		
60	OHX	23SA	3477	-	0,6,6	-	-	-		
60	OHX	16SB	2371	-	0,6,6	-	-	-		
60	OHX	16SB	2331	-	0,6,6	-	-	-		
60	OHX	23SA	3517	-	0,6,6	-	-	-		
60	OHX	16SA	2386	-	0,6,6	-	-	-		
60	OHX	23SA	3456	-	0,6,6	-	-	-		
60	OHX	23SA	3608	27	0,6,6	-	-	-		
60	OHX	16SB	2344	-	0,6,6	-	-	-		
60	OHX	16SA	2394	-	0,6,6	-	-	-		
60	OHX	23SA	3502	-	0,6,6	-	-	-		
60	OHX	23SB	3498	-	0,6,6	-	-	-		
60	OHX	16SA	2399	-	0,6,6	-	-	-		
60	OHX	23SA	3576	-	0,6,6	-	-	-		
60	OHX	23SA	3470	-	0,6,6	-	-	-		
60	OHX	23SA	3522	-	0,6,6	-	-	-		
60	OHX	23SA	3619	-	0,6,6	-	-	-		
60	OHX	16SA	2397	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	OHX	16SB	2354	-	0,6,6	-	-	-		
60	OHX	23SA	3552	-	0,6,6	-	-	-		
60	OHX	23SA	3627	-	0,6,6	-	-	-		
60	OHX	23SA	3448	-	0,6,6	-	-	-		
60	OHX	23SB	3394	-	0,6,6	-	-	-		
60	OHX	16SB	2362	-	0,6,6	-	-	-		
60	OHX	16SB	2323	-	0,6,6	-	-	-		
60	OHX	23SB	3490	-	0,6,6	-	-	-		
60	OHX	23SA	3551	-	0,6,6	-	-	-		
60	OHX	23SA	3486	-	0,6,6	-	-	-		
60	OHX	23SB	3493	-	0,6,6	-	-	-		
60	OHX	23SA	3492	-	0,6,6	-	-	-		
60	OHX	TRNA	101	-	0,6,6	-	-	-		
60	OHX	23SA	3512	-	0,6,6	-	-	-		
60	OHX	16SB	2325	-	0,6,6	-	-	-		
60	OHX	23SA	3484	-	0,6,6	-	-	-		
60	OHX	16SA	2365	-	0,6,6	-	-	-		
60	OHX	ASIB	101	-	0,6,6	-	-	-		
60	OHX	16SB	2378	-	0,6,6	-	-	-		
60	OHX	5SA	215	-	0,6,6	-	-	-		
60	OHX	16SA	2368	-	0,6,6	-	-	-		
60	OHX	23SA	3631	-	0,6,6	-	-	-		
60	OHX	23SA	3583	-	0,6,6	-	-	-		
60	OHX	16SA	2408	-	0,6,6	-	-	-		
60	OHX	23SB	3339	27	0,6,6	-	-	-		
60	OHX	23SB	3494	-	0,6,6	-	-	-		
60	OHX	23SA	3534	-	0,6,6	-	-	-		
60	OHX	23SA	3529	-	0,6,6	-	-	-		
60	OHX	L17A	202	-	0,6,6	-	-	-		
60	OHX	23SA	3506	-	0,6,6	-	-	-		
60	OHX	23SB	3439	-	0,6,6	-	-	-		
60	OHX	23SA	3553	-	0,6,6	-	-	-		
60	OHX	16SB	2367	1	0,6,6	-	-	-		
60	OHX	23SA	3507	-	0,6,6	-	-	-		
60	OHX	S19A	101	-	0,6,6	-	-	-		
60	OHX	16SA	2357	-	0,6,6	-	-	-		
60	OHX	23SB	3469	-	0,6,6	-	-	-		
60	OHX	23SB	3436	-	0,6,6	-	-	-		
60	OHX	23SB	3465	-	0,6,6	-	-	-		
60	OHX	23SA	3555	-	0,6,6	-	-	-		
60	OHX	23SA	3622	-	0,6,6	-	-	-		
60	OHX	16SA	2391	-	0,6,6	-	-	-		
60	OHX	23SA	3491	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	OHX	16SA	2412	-	0,6,6	-	-	-		
60	OHX	23SA	3620	-	0,6,6	-	-	-		
60	OHX	23SA	3463	-	0,6,6	-	-	-		
60	OHX	23SA	3525	-	0,6,6	-	-	-		
60	OHX	TRNA	102	-	0,6,6	-	-	-		
60	OHX	23SB	3483	-	0,6,6	-	-	-		
60	OHX	16SA	2382	1	0,6,6	-	-	-		
60	OHX	23SA	3489	-	0,6,6	-	-	-		
60	OHX	23SA	3616	-	0,6,6	-	-	-		
60	OHX	16SB	2369	-	0,6,6	-	-	-		
60	OHX	ASIB	102	-	0,6,6	-	-	-		
60	OHX	16SA	2375	-	0,6,6	-	-	-		
60	OHX	23SB	3334	-	0,6,6	-	-	-		
60	OHX	23SB	3472	-	0,6,6	-	-	-		
60	OHX	23SA	3513	-	0,6,6	-	-	-		
60	OHX	16SB	2339	-	0,6,6	-	-	-		
60	OHX	16SB	2327	-	0,6,6	-	-	-		
60	OHX	16SA	2363	-	0,6,6	-	-	-		
60	OHX	23SB	3417	-	0,6,6	-	-	-		
60	OHX	23SA	3444	-	0,6,6	-	-	-		
60	OHX	5SA	209	-	0,6,6	-	-	-		
60	OHX	16SB	2359	-	0,6,6	-	-	-		
60	OHX	23SA	3595	-	0,6,6	-	-	-		
60	OHX	16SB	2390	-	0,6,6	-	-	-		
60	OHX	23SB	3445	-	0,6,6	-	-	-		
60	OHX	23SA	3596	-	0,6,6	-	-	-		
60	OHX	16SB	2382	-	0,6,6	-	-	-		
60	OHX	23SB	3335	-	0,6,6	-	-	-		
60	OHX	23SB	3511	-	0,6,6	-	-	-		
60	OHX	23SA	3446	-	0,6,6	-	-	-		
60	OHX	23SB	3512	-	0,6,6	-	-	-		
60	OHX	23SB	3328	-	0,6,6	-	-	-		
60	OHX	23SA	3618	-	0,6,6	-	-	-		
60	OHX	16SA	2402	-	0,6,6	-	-	-		
60	OHX	16SA	2373	-	0,6,6	-	-	-		
60	OHX	23SB	3374	-	0,6,6	-	-	-		
60	OHX	23SB	3504	-	0,6,6	-	-	-		
60	OHX	16SA	2356	-	0,6,6	-	-	-		
60	OHX	23SA	3453	-	0,6,6	-	-	-		
60	OHX	23SB	3391	-	0,6,6	-	-	-		
60	OHX	16SB	2381	-	0,6,6	-	-	-		
60	OHX	16SB	2373	-	0,6,6	-	-	-		
60	OHX	23SB	3482	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	OHX	23SA	3527	-	0,6,6	-	-	-		
60	OHX	23SA	3605	-	0,6,6	-	-	-		
60	OHX	23SB	3380	-	0,6,6	-	-	-		
60	OHX	16SB	2370	-	0,6,6	-	-	-		
60	OHX	23SA	3613	-	0,6,6	-	-	-		
60	OHX	23SB	3501	-	0,6,6	-	-	-		
60	OHX	23SB	3502	-	0,6,6	-	-	-		
60	OHX	23SB	3424	-	0,6,6	-	-	-		
60	OHX	23SA	3614	-	0,6,6	-	-	-		
60	OHX	23SA	3579	-	0,6,6	-	-	-		
60	OHX	23SB	3363	-	0,6,6	-	-	-		
60	OHX	5SA	210	-	0,6,6	-	-	-		
60	OHX	23SB	3336	-	0,6,6	-	-	-		
60	OHX	23SA	3544	-	0,6,6	-	-	-		
60	OHX	23SB	3387	62	0,6,6	-	-	-		
60	OHX	23SA	3628	-	0,6,6	-	-	-		
60	OHX	5SB	215	-	0,6,6	-	-	-		
60	OHX	23SB	3405	-	0,6,6	-	-	-		
60	OHX	16SA	2401	-	0,6,6	-	-	-		
60	OHX	16SB	2349	-	0,6,6	-	-	-		
60	OHX	16SB	2366	1	0,6,6	-	-	-		
60	OHX	23SB	3414	-	0,6,6	-	-	-		
60	OHX	16SB	2392	-	0,6,6	-	-	-		
60	OHX	23SB	3440	-	0,6,6	-	-	-		
60	OHX	23SB	3395	-	0,6,6	-	-	-		
60	OHX	16SA	2411	-	0,6,6	-	-	-		
60	OHX	23SB	3408	-	0,6,6	-	-	-		
60	OHX	23SB	3332	-	0,6,6	-	-	-		
60	OHX	16SA	2406	-	0,6,6	-	-	-		
60	OHX	16SB	2374	-	0,6,6	-	-	-		
60	OHX	23SB	3467	-	0,6,6	-	-	-		
60	OHX	16SB	2377	-	0,6,6	-	-	-		
60	OHX	23SB	3457	-	0,6,6	-	-	-		
60	OHX	23SB	3392	-	0,6,6	-	-	-		
60	OHX	16SA	2351	-	0,6,6	-	-	-		
60	OHX	16SB	2338	-	0,6,6	-	-	-		
60	OHX	5SB	206	-	0,6,6	-	-	-		
60	OHX	23SA	3528	-	0,6,6	-	-	-		
60	OHX	23SA	3557	-	0,6,6	-	-	-		
60	OHX	23SB	3382	-	0,6,6	-	-	-		
60	OHX	16SA	2374	-	0,6,6	-	-	-		
60	OHX	5SB	210	-	0,6,6	-	-	-		
60	OHX	16SB	2345	-	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	OHX	23SB	3496	-	0,6,6	-	-	-		
60	OHX	23SA	3514	-	0,6,6	-	-	-		
60	OHX	16SA	2346	-	0,6,6	-	-	-		
60	OHX	23SA	3621	-	0,6,6	-	-	-		
60	OHX	ASIB	103	-	0,6,6	-	-	-		
60	OHX	PSIB	104	-	0,6,6	-	-	-		
60	OHX	23SA	3560	-	0,6,6	-	-	-		
60	OHX	23SB	3463	-	0,6,6	-	-	-		
60	OHX	23SA	3515	-	0,6,6	-	-	-		
61	SJH	23SB	3323	-	81,87,87	2.15	18 (22%)	101,128,128	1.73	15 (14%)
60	OHX	PSIA	105	-	0,6,6	-	-	-		
60	OHX	23SB	3497	-	0,6,6	-	-	-		
60	OHX	16SA	2360	-	0,6,6	-	-	-		
60	OHX	16SA	2389	-	0,6,6	-	-	-		
60	OHX	23SA	3610	-	0,6,6	-	-	-		
60	OHX	16SB	2393	-	0,6,6	-	-	-		
60	OHX	16SB	2326	-	0,6,6	-	-	-		
60	OHX	23SB	3379	-	0,6,6	-	-	-		
60	OHX	23SA	3561	-	0,6,6	-	-	-		
60	OHX	MRNB	101	-	0,6,6	-	-	-		
60	OHX	23SA	3538	-	0,6,6	-	-	-		
60	OHX	23SB	3441	-	0,6,6	-	-	-		
60	OHX	23SA	3498	-	0,6,6	-	-	-		
60	OHX	23SA	3487	-	0,6,6	-	-	-		
60	OHX	23SA	3509	-	0,6,6	-	-	-		
60	OHX	5SB	209	28	0,6,6	-	-	-		
60	OHX	23SB	3460	-	0,6,6	-	-	-		
60	OHX	23SB	3443	-	0,6,6	-	-	-		
60	OHX	16SA	2396	-	0,6,6	-	-	-		
60	OHX	23SA	3439	-	0,6,6	-	-	-		
60	OHX	23SA	3494	-	0,6,6	-	-	-		
60	OHX	MRNA	102	-	0,6,6	-	-	-		
60	OHX	23SA	3550	-	0,6,6	-	-	-		
60	OHX	23SB	3400	-	0,6,6	-	-	-		
60	OHX	23SA	3481	-	0,6,6	-	-	-		
60	OHX	23SA	3623	-	0,6,6	-	-	-		
60	OHX	23SA	3490	-	0,6,6	-	-	-		
60	OHX	23SB	3338	-	0,6,6	-	-	-		
60	OHX	16SA	2371	-	0,6,6	-	-	-		
60	OHX	5SB	212	-	0,6,6	-	-	-		
60	OHX	16SA	2349	-	0,6,6	-	-	-		
60	OHX	23SA	3521	-	0,6,6	-	-	-		
60	OHX	23SB	3342	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	OHX	L17B	201	-	0,6,6	-	-	-		
60	OHX	16SA	2385	-	0,6,6	-	-	-		
60	OHX	23SB	3474	-	0,6,6	-	-	-		
60	OHX	16SB	2360	1	0,6,6	-	-	-		
60	OHX	23SA	3542	-	0,6,6	-	-	-		
60	OHX	23SB	3475	-	0,6,6	-	-	-		
60	OHX	16SB	2385	-	0,6,6	-	-	-		
60	OHX	16SA	2341	-	0,6,6	-	-	-		
60	OHX	23SB	3434	-	0,6,6	-	-	-		
60	OHX	23SB	3509	-	0,6,6	-	-	-		
60	OHX	16SB	2372	-	0,6,6	-	-	-		
60	OHX	23SA	3559	-	0,6,6	-	-	-		
60	OHX	23SB	3397	-	0,6,6	-	-	-		
60	OHX	16SA	2361	-	0,6,6	-	-	-		
60	OHX	23SA	3588	-	0,6,6	-	-	-		
60	OHX	23SA	3566	-	0,6,6	-	-	-		
60	OHX	23SA	3630	-	0,6,6	-	-	-		
60	OHX	23SB	3410	-	0,6,6	-	-	-		
60	OHX	23SA	3504	-	0,6,6	-	-	-		
60	OHX	ESIA	101	-	0,6,6	-	-	-		
60	OHX	23SA	3592	-	0,6,6	-	-	-		
60	OHX	23SA	3549	-	0,6,6	-	-	-		
60	OHX	23SB	3426	-	0,6,6	-	-	-		
60	OHX	16SB	2346	-	0,6,6	-	-	-		
60	OHX	23SB	3476	-	0,6,6	-	-	-		
60	OHX	16SB	2332	-	0,6,6	-	-	-		
60	OHX	5SB	213	-	0,6,6	-	-	-		
60	OHX	23SB	3401	-	0,6,6	-	-	-		
60	OHX	23SA	3508	-	0,6,6	-	-	-		
60	OHX	23SB	3324	-	0,6,6	-	-	-		
60	OHX	23SB	3454	-	0,6,6	-	-	-		
60	OHX	L19A	201	41	0,6,6	-	-	-		
60	OHX	23SA	3505	-	0,6,6	-	-	-		
60	OHX	23SA	3607	-	0,6,6	-	-	-		
60	OHX	23SA	3581	-	0,6,6	-	-	-		
60	OHX	23SB	3450	-	0,6,6	-	-	-		
60	OHX	23SB	3413	-	0,6,6	-	-	-		
60	OHX	23SA	3533	-	0,6,6	-	-	-		
60	OHX	23SB	3514	-	0,6,6	-	-	-		
60	OHX	L27A	104	-	0,6,6	-	-	-		
60	OHX	23SB	3433	-	0,6,6	-	-	-		
60	OHX	16SA	2354	-	0,6,6	-	-	-		
60	OHX	16SB	2348	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	OHX	23SB	3389	-	0,6,6	-	-	-		
60	OHX	16SB	2353	-	0,6,6	-	-	-		
60	OHX	23SB	3481	-	0,6,6	-	-	-		
60	OHX	23SB	3432	-	0,6,6	-	-	-		
60	OHX	23SB	3471	-	0,6,6	-	-	-		
60	OHX	16SB	2340	-	0,6,6	-	-	-		
60	OHX	23SA	3455	-	0,6,6	-	-	-		
60	OHX	23SB	3491	-	0,6,6	-	-	-		
60	OHX	23SA	3591	-	0,6,6	-	-	-		
60	OHX	23SB	3479	-	0,6,6	-	-	-		
60	OHX	23SB	3462	-	0,6,6	-	-	-		
60	OHX	23SB	3352	-	0,6,6	-	-	-		
60	OHX	23SA	3461	-	0,6,6	-	-	-		
60	OHX	23SB	3399	-	0,6,6	-	-	-		
60	OHX	16SA	2353	-	0,6,6	-	-	-		
60	OHX	23SB	3419	-	0,6,6	-	-	-		
60	OHX	23SA	3482	-	0,6,6	-	-	-		
60	OHX	16SB	2398	-	0,6,6	-	-	-		
60	OHX	5SA	211	-	0,6,6	-	-	-		
60	OHX	16SB	2395	-	0,6,6	-	-	-		
60	OHX	23SA	3438	-	0,6,6	-	-	-		
60	OHX	16SA	2379	-	0,6,6	-	-	-		
60	OHX	23SB	3510	-	0,6,6	-	-	-		
60	OHX	23SB	3386	-	0,6,6	-	-	-		
60	OHX	23SA	3443	-	0,6,6	-	-	-		
60	OHX	23SA	3458	-	0,6,6	-	-	-		
60	OHX	23SB	3373	-	0,6,6	-	-	-		
60	OHX	23SB	3478	-	0,6,6	-	-	-		
60	OHX	23SB	3390	-	0,6,6	-	-	-		
60	OHX	23SA	3587	-	0,6,6	-	-	-		
60	OHX	23SB	3407	-	0,6,6	-	-	-		
60	OHX	16SA	2367	-	0,6,6	-	-	-		
60	OHX	16SA	2378	-	0,6,6	-	-	-		
60	OHX	5SA	217	-	0,6,6	-	-	-		
60	OHX	16SB	2391	-	0,6,6	-	-	-		
60	OHX	23SA	3496	-	0,6,6	-	-	-		
60	OHX	23SB	3351	-	0,6,6	-	-	-		
60	OHX	23SB	3423	-	0,6,6	-	-	-		
60	OHX	23SA	3445	-	0,6,6	-	-	-		
60	OHX	23SA	3633	-	0,6,6	-	-	-		
60	OHX	23SA	3598	-	0,6,6	-	-	-		
60	OHX	23SA	3606	-	0,6,6	-	-	-		
60	OHX	23SB	3366	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	OHX	23SB	3455	-	0,6,6	-	-	-		
60	OHX	23SA	3467	-	0,6,6	-	-	-		
60	OHX	23SB	3325	-	0,6,6	-	-	-		
60	OHX	23SB	3337	-	0,6,6	-	-	-		
60	OHX	23SB	3470	-	0,6,6	-	-	-		
60	OHX	16SA	2364	-	0,6,6	-	-	-		
60	OHX	23SA	3577	-	0,6,6	-	-	-		
60	OHX	16SB	2324	-	0,6,6	-	-	-		
60	OHX	PSIB	106	-	0,6,6	-	-	-		
60	OHX	23SB	3477	-	0,6,6	-	-	-		
60	OHX	23SB	3341	-	0,6,6	-	-	-		
60	OHX	16SA	2347	-	0,6,6	-	-	-		
60	OHX	5SB	207	-	0,6,6	-	-	-		
60	OHX	16SB	2363	-	0,6,6	-	-	-		
60	OHX	16SA	2388	-	0,6,6	-	-	-		
60	OHX	23SB	3464	-	0,6,6	-	-	-		
60	OHX	23SB	3329	-	0,6,6	-	-	-		
60	OHX	23SB	3416	-	0,6,6	-	-	-		
60	OHX	16SA	2369	-	0,6,6	-	-	-		
60	OHX	5SA	213	-	0,6,6	-	-	-		
60	OHX	16SB	2387	-	0,6,6	-	-	-		
60	OHX	23SB	3350	-	0,6,6	-	-	-		
60	OHX	L35B	103	-	0,6,6	-	-	-		

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
61	SJH	23SA	3436	-	-	33/93/153/153	0/5/5/5
61	SJH	23SB	3323	-	-	33/93/153/153	0/5/5/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	23SB	3323	SJH	C18-N20	7.10	1.49	1.34
61	23SA	3436	SJH	C18-N20	7.09	1.49	1.34
61	23SA	3436	SJH	C14-C15	6.34	1.64	1.53
61	23SB	3323	SJH	C14-C15	6.33	1.64	1.53
61	23SA	3436	SJH	O47-C48	6.13	1.48	1.34
61	23SB	3323	SJH	O47-C48	6.12	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	23SA	3436	SJH	O17-C18	5.97	1.46	1.34
61	23SB	3323	SJH	O17-C18	5.96	1.46	1.34
61	23SA	3436	SJH	O17-C15	-5.42	1.39	1.46
61	23SB	3323	SJH	O17-C15	-5.41	1.39	1.46
61	23SB	3323	SJH	C25-C24	4.33	1.59	1.49
61	23SB	3323	SJH	C40-C38	4.32	1.59	1.50
61	23SA	3436	SJH	C25-C24	4.31	1.59	1.49
61	23SA	3436	SJH	C40-C38	4.30	1.59	1.50
61	23SB	3323	SJH	O37-C38	3.54	1.44	1.34
61	23SA	3436	SJH	O37-C38	3.53	1.44	1.34
61	23SA	3436	SJH	O71-C70	3.31	1.50	1.41
61	23SB	3323	SJH	O71-C70	3.29	1.50	1.41
61	23SB	3323	SJH	C56-C59	-3.02	1.47	1.53
61	23SA	3436	SJH	C56-C59	-3.01	1.47	1.53
61	23SB	3323	SJH	O69-C68	2.83	1.48	1.43
61	23SA	3436	SJH	O69-C68	2.80	1.48	1.43
61	23SA	3436	SJH	O37-C36	-2.67	1.40	1.44
61	23SB	3323	SJH	O37-C36	-2.63	1.40	1.44
61	23SA	3436	SJH	O30-N29	-2.59	1.18	1.22
61	23SB	3323	SJH	O30-N29	-2.58	1.18	1.22
61	23SA	3436	SJH	O63-C61	2.21	1.49	1.44
61	23SB	3323	SJH	O63-C61	2.20	1.49	1.44
61	23SB	3323	SJH	O10-C11	-2.18	1.38	1.43
61	23SA	3436	SJH	O10-C11	-2.18	1.38	1.43
61	23SA	3436	SJH	C50-C48	2.11	1.56	1.51
61	23SB	3323	SJH	C50-C48	2.08	1.56	1.51
61	23SB	3323	SJH	C14-C12	2.07	1.57	1.54
61	23SA	3436	SJH	C14-C12	2.03	1.56	1.54
61	23SA	3436	SJH	C55-C56	-2.01	1.49	1.53
61	23SB	3323	SJH	C55-C56	-2.01	1.49	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	23SB	3323	SJH	O17-C18-N20	7.26	120.75	109.99
61	23SA	3436	SJH	O17-C18-N20	7.25	120.75	109.99
61	23SB	3323	SJH	C05-C04-N03	-5.79	120.17	126.93
61	23SA	3436	SJH	C05-C04-N03	-5.78	120.19	126.93
61	23SA	3436	SJH	O37-C38-C40	5.34	121.28	111.46
61	23SB	3323	SJH	O37-C38-C40	5.33	121.26	111.46
61	23SA	3436	SJH	O02-N03-C04	4.97	119.30	110.97
61	23SB	3323	SJH	O02-N03-C04	4.95	119.28	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	23SB	3323	SJH	O47-C48-C50	4.06	120.46	111.56
61	23SA	3436	SJH	O47-C48-C50	4.05	120.46	111.56
61	23SA	3436	SJH	O19-C18-N20	-3.99	118.84	124.96
61	23SB	3323	SJH	O19-C18-N20	-3.99	118.84	124.96
61	23SB	3323	SJH	O17-C18-O19	-2.86	120.40	125.62
61	23SA	3436	SJH	O17-C18-O19	-2.86	120.41	125.62
61	23SB	3323	SJH	O39-C38-C40	-2.61	118.97	124.73
61	23SA	3436	SJH	O39-C38-C40	-2.60	118.97	124.73
61	23SA	3436	SJH	C73-C72-C74	-2.42	108.60	113.07
61	23SB	3323	SJH	C73-C72-C74	-2.41	108.62	113.07
61	23SB	3323	SJH	C07-C06-C05	-2.41	108.52	113.22
61	23SA	3436	SJH	C07-C06-C05	-2.41	108.52	113.22
61	23SA	3436	SJH	C62-C61-C59	-2.32	108.61	112.57
61	23SB	3323	SJH	C62-C61-C59	-2.32	108.61	112.57
61	23SA	3436	SJH	O47-C48-O49	-2.19	119.86	123.94
61	23SB	3323	SJH	O47-C48-O49	-2.18	119.87	123.94
61	23SB	3323	SJH	C55-C56-C59	2.09	113.40	107.90
61	23SA	3436	SJH	C55-C56-C59	2.09	113.39	107.90
61	23SA	3436	SJH	C66-C46-C44	-2.08	108.73	114.29
61	23SB	3323	SJH	C66-C46-C44	-2.08	108.73	114.29
61	23SB	3323	SJH	C46-O47-C48	-2.08	114.22	117.78
61	23SA	3436	SJH	C46-O47-C48	-2.07	114.22	117.78

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	23SA	3436	SJH	C12-C14-C15-C16
61	23SA	3436	SJH	C12-C14-C15-O17
61	23SA	3436	SJH	C16-C15-C32-C34
61	23SA	3436	SJH	O17-C15-C32-O33
61	23SA	3436	SJH	O17-C18-N20-C21
61	23SA	3436	SJH	O19-C18-N20-C21
61	23SA	3436	SJH	C05-C04-N03-O02
61	23SA	3436	SJH	C21-C22-N23-C28
61	23SA	3436	SJH	C32-C34-C36-O37
61	23SA	3436	SJH	C35-C34-C36-O37
61	23SA	3436	SJH	C34-C36-C44-C45
61	23SA	3436	SJH	O37-C36-C44-C45
61	23SA	3436	SJH	O37-C36-C44-C46
61	23SA	3436	SJH	C40-C38-O37-C36
61	23SA	3436	SJH	O39-C38-O37-C36

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Mol	Chain	Res	Type	Atoms
61	23SA	3436	SJH	C04-N03-O02-C01
61	23SB	3323	SJH	C12-C14-C15-C16
61	23SB	3323	SJH	C12-C14-C15-O17
61	23SB	3323	SJH	C16-C15-C32-C34
61	23SB	3323	SJH	O17-C15-C32-O33
61	23SB	3323	SJH	O17-C18-N20-C21
61	23SB	3323	SJH	O19-C18-N20-C21
61	23SB	3323	SJH	C05-C04-N03-O02
61	23SB	3323	SJH	C21-C22-N23-C28
61	23SB	3323	SJH	C32-C34-C36-O37
61	23SB	3323	SJH	C35-C34-C36-O37
61	23SB	3323	SJH	C34-C36-C44-C45
61	23SB	3323	SJH	O37-C36-C44-C45
61	23SB	3323	SJH	O37-C36-C44-C46
61	23SB	3323	SJH	C40-C38-O37-C36
61	23SB	3323	SJH	O39-C38-O37-C36
61	23SB	3323	SJH	C04-N03-O02-C01
61	23SA	3436	SJH	N20-C21-C22-N23
61	23SB	3323	SJH	N20-C21-C22-N23
61	23SA	3436	SJH	O10-C11-C64-C52
61	23SB	3323	SJH	O10-C11-C64-C52
61	23SA	3436	SJH	C12-C11-C64-C52
61	23SB	3323	SJH	C12-C11-C64-C52
61	23SA	3436	SJH	C12-C11-C64-C65
61	23SB	3323	SJH	C12-C11-C64-C65
61	23SA	3436	SJH	C74-C76-O77-C78
61	23SB	3323	SJH	C74-C76-O77-C78
61	23SA	3436	SJH	C34-C36-C44-C46
61	23SB	3323	SJH	C34-C36-C44-C46
61	23SA	3436	SJH	C38-C40-C41-C42
61	23SB	3323	SJH	C38-C40-C41-C42
61	23SA	3436	SJH	O10-C11-C64-C65
61	23SB	3323	SJH	O10-C11-C64-C65
61	23SA	3436	SJH	C32-C34-C36-C44
61	23SB	3323	SJH	C32-C34-C36-C44
61	23SA	3436	SJH	C12-C14-C15-C32
61	23SB	3323	SJH	C12-C14-C15-C32
61	23SA	3436	SJH	C14-C15-C32-C34
61	23SB	3323	SJH	C14-C15-C32-C34
61	23SA	3436	SJH	C35-C34-C36-C44
61	23SB	3323	SJH	C35-C34-C36-C44
61	23SA	3436	SJH	O08-C09-O10-C11

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Mol	Chain	Res	Type	Atoms
61	23SB	3323	SJH	O08-C09-O10-C11
61	23SA	3436	SJH	C16-C15-C32-O33
61	23SB	3323	SJH	C16-C15-C32-O33
61	23SA	3436	SJH	O10-C11-C12-C14
61	23SB	3323	SJH	O10-C11-C12-C14
61	23SA	3436	SJH	C82-C09-O10-C11
61	23SB	3323	SJH	C82-C09-O10-C11
61	23SA	3436	SJH	C44-C46-C66-C68
61	23SB	3323	SJH	C44-C46-C66-C68

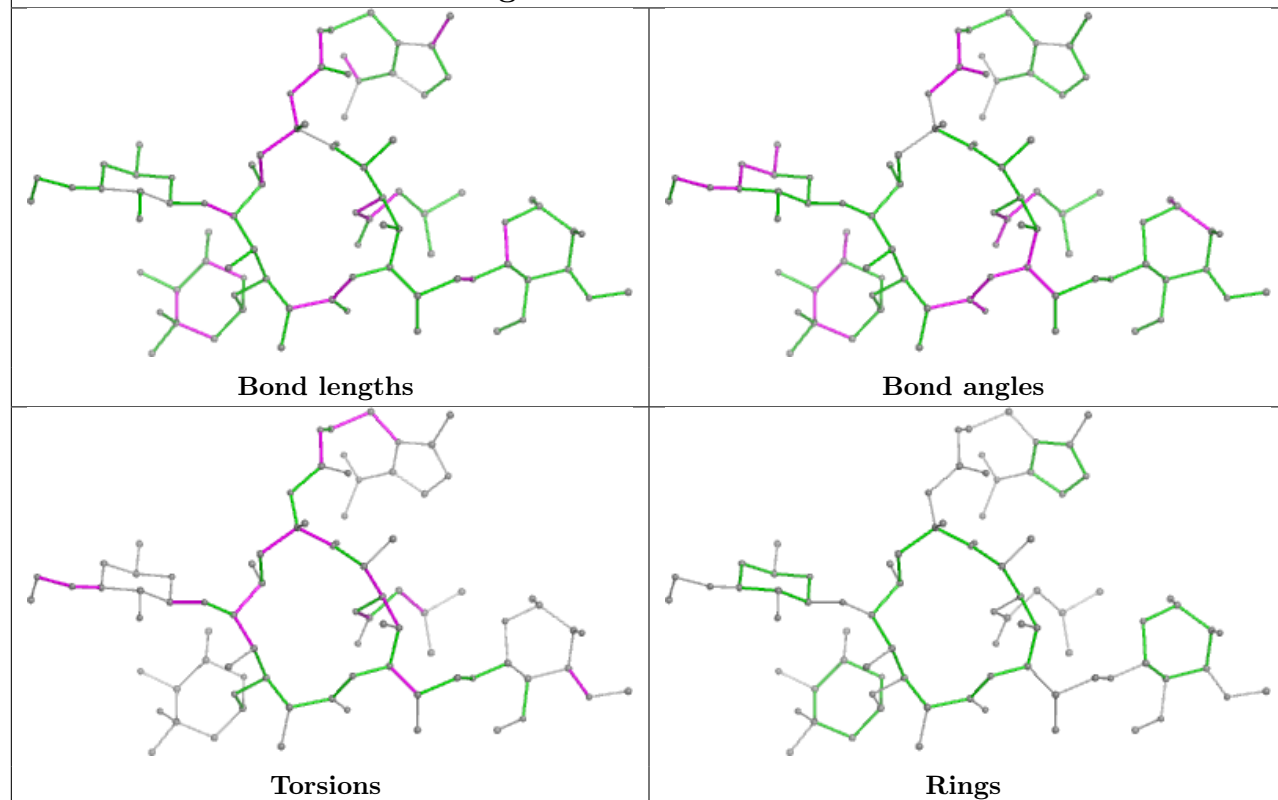
There are no ring outliers.

No monomer is involved in short contacts.

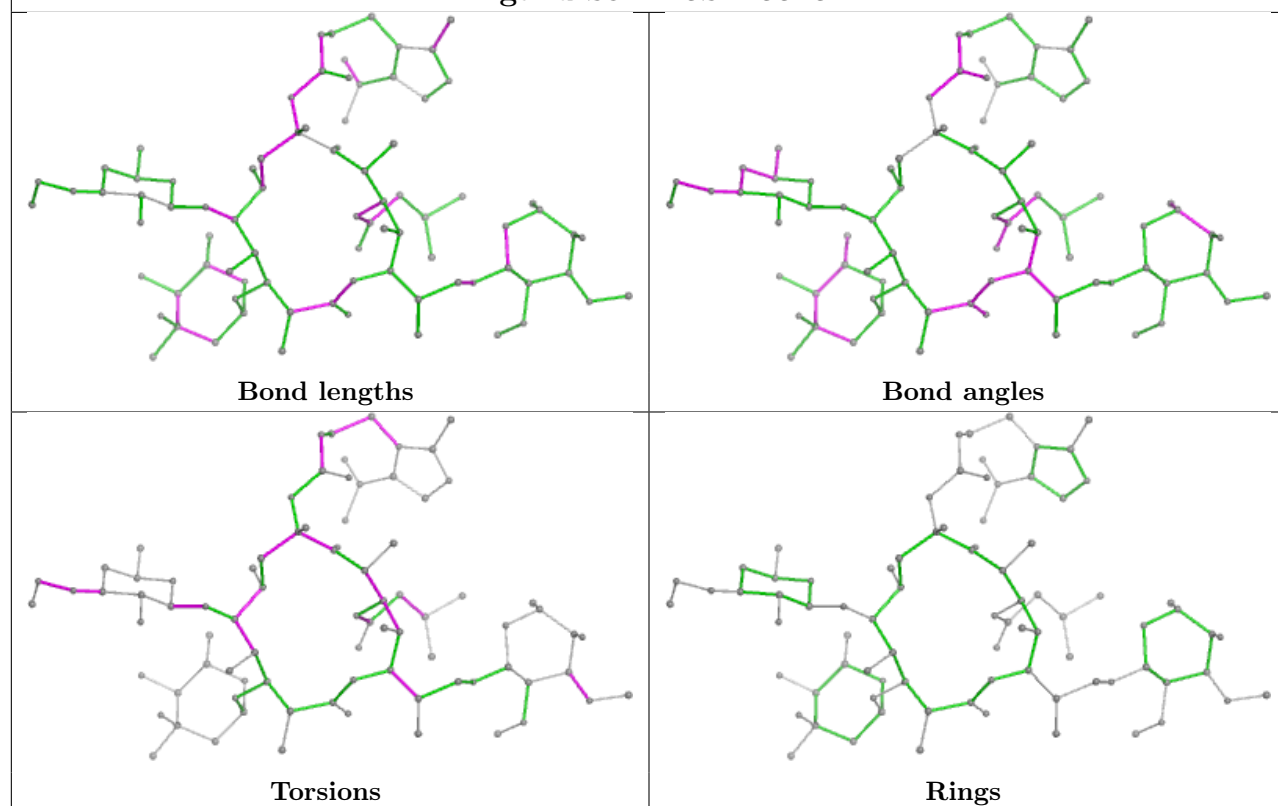
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## Ligand SJH 23SA 3436



## Ligand SJH 23SB 3323



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	S7B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S7B	6:ARG	C	7:ALA	N	3.28

## 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	16SA	1499/1512 (99%)	0.49	40 (2%)	56	36	42, 89, 169, 259	0
1	16SB	1495/1512 (98%)	0.54	20 (1%)	74	58	55, 100, 163, 267	0
2	S2A	237/256 (92%)	1.62	79 (33%)	1	0	90, 125, 163, 177	0
2	S2B	237/256 (92%)	1.76	77 (32%)	1	0	104, 154, 184, 204	0
3	S3A	205/239 (85%)	1.90	81 (39%)	1	0	81, 102, 141, 169	0
3	S3B	206/239 (86%)	1.91	85 (41%)	1	0	104, 129, 156, 162	0
4	S4A	208/209 (99%)	2.40	127 (61%)	0	0	77, 100, 120, 125	0
4	S4B	208/209 (99%)	2.37	126 (60%)	0	0	78, 98, 117, 140	0
5	S5A	151/162 (93%)	1.61	40 (26%)	2	1	66, 88, 109, 135	0
5	S5B	151/162 (93%)	1.67	45 (29%)	1	1	86, 105, 124, 151	0
6	S6A	101/101 (100%)	0.98	2 (1%)	64	45	70, 92, 108, 125	0
6	S6B	101/101 (100%)	1.47	31 (30%)	1	1	72, 93, 110, 132	0
7	S7A	155/156 (99%)	1.24	32 (20%)	3	2	88, 104, 129, 137	0
7	S7B	155/156 (99%)	1.07	27 (17%)	5	3	98, 115, 150, 173	0
8	S8A	138/138 (100%)	1.13	14 (10%)	14	8	77, 92, 105, 112	0
8	S8B	138/138 (100%)	1.50	37 (26%)	2	1	84, 107, 117, 125	0
9	S9A	127/128 (99%)	1.09	18 (14%)	7	4	73, 122, 139, 144	0
9	S9B	127/128 (99%)	0.66	3 (2%)	59	41	97, 136, 153, 155	0
10	S10A	99/105 (94%)	1.43	22 (22%)	3	1	71, 125, 149, 156	0
10	S10B	99/105 (94%)	1.64	30 (30%)	1	1	105, 143, 161, 164	0
11	S11A	116/129 (89%)	1.16	20 (17%)	5	3	58, 89, 112, 143	0
11	S11B	117/129 (90%)	1.49	28 (23%)	2	1	71, 98, 123, 157	0
12	S12A	124/132 (93%)	1.65	38 (30%)	1	1	58, 67, 99, 158	0
12	S12B	124/132 (93%)	1.64	45 (36%)	1	0	69, 87, 114, 167	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	S13A	119/126 (94%)	1.16	19 (15%)	6	3	74, 111, 128, 136	0
13	S13B	121/126 (96%)	0.88	14 (11%)	11	7	98, 138, 149, 159	0
14	S14A	60/61 (98%)	1.33	11 (18%)	4	2	78, 91, 102, 115	0
14	S14B	59/61 (96%)	1.26	12 (20%)	3	2	99, 120, 139, 144	0
15	S15A	88/89 (98%)	0.51	3 (3%)	48	28	62, 83, 108, 117	0
15	S15B	88/89 (98%)	0.83	6 (6%)	25	14	71, 93, 111, 118	0
16	S16A	83/88 (94%)	1.51	18 (21%)	3	1	88, 99, 120, 147	0
16	S16B	84/88 (95%)	1.78	31 (36%)	1	0	78, 89, 108, 143	0
17	S17A	100/105 (95%)	0.79	3 (3%)	52	33	73, 91, 102, 107	0
17	S17B	100/105 (95%)	0.91	9 (9%)	17	10	78, 96, 113, 126	0
18	S18A	71/88 (80%)	1.00	7 (9%)	14	8	70, 86, 121, 148	0
18	S18B	70/88 (79%)	1.59	24 (34%)	1	0	78, 97, 125, 146	0
19	S19A	84/93 (90%)	1.82	30 (35%)	1	0	86, 114, 133, 137	0
19	S19B	86/93 (92%)	0.98	10 (11%)	11	7	127, 150, 175, 187	0
20	S20A	99/106 (93%)	1.33	16 (16%)	5	3	88, 105, 133, 138	0
20	S20B	99/106 (93%)	0.88	9 (9%)	16	9	81, 102, 127, 132	0
21	THXA	24/27 (88%)	0.85	3 (12%)	9	6	88, 100, 111, 129	0
21	THXB	25/27 (92%)	0.37	0	100	100	111, 126, 141, 146	0
22	ASIA	69/76 (90%)	2.81	45 (65%)	0	0	70, 184, 222, 237	0
23	PSIA	68/76 (89%)	0.89	13 (19%)	4	2	60, 86, 105, 153	0
23	PSIB	68/76 (89%)	0.57	3 (4%)	39	23	73, 101, 133, 166	0
24	ESIA	75/76 (98%)	1.68	19 (25%)	2	1	62, 190, 215, 221	0
24	ESIB	75/76 (98%)	1.21	11 (14%)	7	4	71, 195, 220, 233	0
25	MRNA	30/30 (100%)	1.61	8 (26%)	2	1	60, 151, 237, 249	0
25	MRNB	30/30 (100%)	1.02	4 (13%)	8	5	79, 167, 236, 242	0
26	TRNA	67/76 (88%)	1.08	4 (5%)	29	17	106, 174, 201, 215	0
27	23SA	2878/2911 (98%)	-0.34	38 (1%)	74	58	31, 58, 189, 261	0
27	23SB	2864/2911 (98%)	-0.05	46 (1%)	70	52	41, 75, 213, 268	0
28	5SA	122/124 (98%)	-0.32	1 (0%)	82	68	55, 74, 90, 166	0
28	5SB	121/124 (97%)	0.07	4 (3%)	49	30	77, 103, 137, 191	0
29	L2A	272/276 (98%)	0.02	2 (0%)	84	70	30, 50, 67, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
29	L2B	272/276 (98%)	0.34	5 (1%) 67 49	39, 61, 79, 89	0
30	L3A	204/206 (99%)	0.65	14 (6%) 24 14	39, 69, 96, 111	0
30	L3B	204/206 (99%)	1.13	34 (16%) 5 3	52, 86, 116, 127	0
31	L4A	202/210 (96%)	0.13	8 (3%) 43 25	35, 63, 93, 118	0
31	L4B	202/210 (96%)	0.87	24 (11%) 10 6	44, 82, 113, 129	0
32	L5A	181/182 (99%)	0.84	13 (7%) 23 13	68, 84, 115, 128	0
32	L5B	181/182 (99%)	0.73	10 (5%) 32 19	97, 117, 141, 150	0
33	L6A	174/180 (96%)	1.68	57 (32%) 1 0	73, 95, 114, 138	0
33	L6B	173/180 (96%)	2.50	97 (56%) 0 0	154, 199, 241, 259	0
34	L9A	145/148 (97%)	1.73	55 (37%) 1 0	61, 116, 131, 144	0
34	L9B	146/148 (98%)	1.57	47 (32%) 1 0	73, 114, 136, 151	0
35	L13A	138/140 (98%)	0.70	9 (6%) 26 16	50, 68, 100, 111	0
35	L13B	138/140 (98%)	1.83	55 (39%) 1 0	69, 102, 129, 136	0
36	L14A	122/122 (100%)	0.93	17 (13%) 7 4	43, 62, 76, 83	0
36	L14B	122/122 (100%)	1.07	19 (15%) 6 3	59, 81, 101, 114	0
37	L15A	150/150 (100%)	0.25	3 (2%) 64 45	38, 69, 102, 141	0
37	L15B	150/150 (100%)	0.60	7 (4%) 37 22	50, 94, 128, 143	0
38	L16A	141/141 (100%)	0.60	7 (4%) 35 21	43, 64, 90, 122	0
38	L16B	141/141 (100%)	0.55	7 (4%) 35 21	54, 73, 94, 123	0
39	L17A	118/118 (100%)	0.17	1 (0%) 82 68	46, 65, 86, 94	0
39	L17B	118/118 (100%)	0.36	2 (1%) 69 50	55, 74, 94, 111	0
40	L18A	112/112 (100%)	0.54	9 (8%) 20 11	54, 71, 97, 114	0
40	L18B	111/112 (99%)	0.35	4 (3%) 46 27	74, 103, 140, 150	0
41	L19A	137/146 (93%)	1.09	21 (15%) 6 3	57, 74, 125, 158	0
41	L19B	137/146 (93%)	1.00	18 (13%) 8 5	70, 89, 164, 184	0
42	L20A	117/118 (99%)	-0.04	3 (2%) 57 38	39, 57, 85, 115	0
42	L20B	117/118 (99%)	1.43	36 (30%) 1 1	54, 94, 135, 148	0
43	L21A	101/101 (100%)	0.34	1 (0%) 79 64	41, 80, 98, 107	0
43	L21B	101/101 (100%)	2.08	44 (43%) 1 0	55, 113, 129, 141	0
44	L22A	113/113 (100%)	-0.14	1 (0%) 81 66	45, 56, 85, 127	0
44	L22B	113/113 (100%)	0.82	10 (8%) 17 10	51, 66, 112, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
45	L23A	95/96 (98%)	-0.09	0 100 100	41, 56, 76, 95	0
45	L23B	94/96 (97%)	0.23	3 (3%) 50 31	54, 72, 98, 121	0
46	L24A	108/110 (98%)	0.58	7 (6%) 26 16	58, 89, 137, 151	0
46	L24B	106/110 (96%)	1.32	23 (21%) 3 1	67, 97, 146, 152	0
47	L25A	179/206 (86%)	1.22	30 (16%) 5 3	68, 104, 181, 189	0
47	L25B	176/206 (85%)	1.35	36 (20%) 3 2	105, 144, 222, 227	0
48	L27A	84/85 (98%)	0.27	6 (7%) 23 14	43, 57, 84, 105	0
48	L27B	84/85 (98%)	0.33	7 (8%) 19 10	61, 78, 106, 126	0
49	L28A	97/98 (98%)	0.52	9 (9%) 16 9	41, 62, 108, 132	0
49	L28B	97/98 (98%)	0.64	10 (10%) 13 8	51, 73, 116, 132	0
50	L29A	69/72 (95%)	0.43	1 (1%) 73 56	47, 65, 81, 103	0
50	L29B	68/72 (94%)	0.26	1 (1%) 71 54	66, 87, 106, 114	0
51	L30A	59/60 (98%)	0.06	0 100 100	47, 63, 93, 114	0
51	L30B	59/60 (98%)	1.09	10 (16%) 5 3	67, 91, 130, 144	0
52	L31A	71/71 (100%)	1.61	16 (22%) 3 1	88, 134, 169, 174	0
52	L31B	71/71 (100%)	0.72	4 (5%) 31 19	119, 160, 187, 195	0
53	L32A	56/60 (93%)	0.23	3 (5%) 32 19	31, 68, 128, 133	0
53	L32B	56/60 (93%)	1.00	12 (21%) 3 2	51, 79, 138, 149	0
54	L33A	45/54 (83%)	2.14	20 (44%) 1 0	104, 128, 157, 161	0
54	L33B	45/54 (83%)	1.45	10 (22%) 3 1	129, 155, 181, 187	0
55	L34A	48/49 (97%)	-0.35	0 100 100	31, 41, 68, 98	0
55	L34B	49/49 (100%)	-0.04	2 (4%) 42 24	44, 51, 95, 109	0
56	L35A	64/65 (98%)	-0.04	3 (4%) 37 22	39, 53, 68, 94	0
56	L35B	64/65 (98%)	0.41	2 (3%) 51 32	44, 69, 92, 116	0
57	ASIB	72/76 (94%)	1.49	18 (25%) 2 1	100, 215, 252, 257	0
All	All	21114/21740 (97%)	0.63	2361 (11%) 11 7	30, 87, 175, 268	0

All (2361) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	S4A	26	CYS	9.4
4	S4B	26	CYS	9.2
43	L21B	36	PRO	9.0

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Mol	Chain	Res	Type	RSRZ
22	ASIA	1	G	7.7
4	S4B	31	CYS	7.5
22	ASIA	3	C	7.3
34	L9A	140	LEU	7.1
2	S2A	118	LEU	7.1
42	L20B	113	ALA	7.0
33	L6B	38	SER	6.9
4	S4A	32	ALA	6.8
13	S13A	117	VAL	6.8
47	L25A	97	GLU	6.6
4	S4A	115	ARG	6.4
22	ASIA	70	G	6.4
4	S4A	31	CYS	6.4
19	S19A	85	LYS	6.4
2	S2B	218	ALA	6.3
42	L20B	109	LEU	6.3
19	S19A	61	TYR	6.3
22	ASIA	17	C	6.2
4	S4A	89	THR	6.1
4	S4B	158	ILE	6.1
2	S2B	222	ILE	6.1
27	23SB	2911	G	6.0
33	L6B	113	VAL	6.0
30	L3B	57	LYS	6.0
33	L6B	16	SER	6.0
34	L9B	80	PRO	6.0
2	S2B	215	LEU	6.0
4	S4A	9	CYS	5.9
4	S4B	19	LEU	5.9
10	S10B	85	LEU	5.8
33	L6B	72	ILE	5.8
32	L5A	75	LYS	5.8
34	L9B	85	GLU	5.8
52	L31A	33	VAL	5.7
34	L9B	86	THR	5.7
27	23SB	4	C	5.6
22	ASIA	73	A	5.6
27	23SB	2913	C	5.5
28	5SB	90	C	5.5
57	ASIB	1	G	5.5
33	L6B	150	ALA	5.5
4	S4B	128	VAL	5.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	S2B	230	VAL	5.4
2	S2B	186	ALA	5.3
19	S19A	81	ARG	5.3
27	23SB	2912	A	5.3
2	S2B	164	VAL	5.3
33	L6B	174	GLY	5.3
3	S3B	182	ILE	5.3
10	S10B	23	ILE	5.3
22	ASIA	72	C	5.3
43	L21B	45	THR	5.2
4	S4B	32	ALA	5.2
34	L9B	84	GLY	5.2
4	S4A	58	LEU	5.2
33	L6B	103	LEU	5.2
34	L9A	129	THR	5.2
33	L6B	115	VAL	5.2
33	L6B	36	PRO	5.1
3	S3B	205	GLY	5.1
54	L33A	22	ALA	5.1
33	L6B	105	LEU	5.1
33	L6B	35	VAL	5.1
24	ESIA	6	G	5.1
33	L6B	24	VAL	5.1
33	L6B	148	ILE	5.1
4	S4A	178	VAL	5.1
33	L6A	119	GLU	5.1
43	L21B	71	LEU	5.1
4	S4B	86	LYS	5.0
5	S5A	51	VAL	5.0
5	S5B	13	ILE	5.0
4	S4A	86	LYS	5.0
33	L6B	17	VAL	5.0
33	L6B	152	ARG	5.0
33	L6B	26	VAL	4.9
33	L6B	131	VAL	4.9
33	L6B	146	ALA	4.9
3	S3A	193	TYR	4.9
3	S3B	203	PHE	4.8
7	S7A	147	ALA	4.8
4	S4A	114	ARG	4.8
12	S12A	92	GLY	4.8
24	ESIA	14	A	4.8

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Mol	Chain	Res	Type	RSRZ
35	L13A	96	GLU	4.8
43	L21B	35	LEU	4.8
3	S3B	117	ALA	4.8
4	S4B	88	VAL	4.8
12	S12A	117	TYR	4.8
34	L9B	122	GLU	4.8
26	TRNA	73	A	4.8
22	ASIA	71	G	4.8
25	MRNA	53	U	4.8
2	S2B	32	ILE	4.7
2	S2B	214	ILE	4.7
4	S4A	21	LEU	4.7
43	L21B	91	TYR	4.7
27	23SB	1110	G	4.7
4	S4B	110	PHE	4.7
34	L9A	79	ILE	4.7
24	ESIA	1	G	4.7
4	S4B	103	ASN	4.7
4	S4A	110	PHE	4.7
4	S4B	9	CYS	4.7
34	L9A	130	TYR	4.7
33	L6B	114	VAL	4.6
2	S2A	145	LEU	4.6
12	S12A	60	GLY	4.6
42	L20B	88	ILE	4.6
46	L24B	40	GLU	4.6
3	S3B	37	GLN	4.6
22	ASIA	4	C	4.6
33	L6B	37	VAL	4.6
34	L9B	140	LEU	4.6
22	ASIA	49	C	4.6
24	ESIA	12	U	4.5
4	S4B	178	VAL	4.5
3	S3A	80	GLY	4.5
20	S20A	63	ILE	4.5
4	S4B	7	PRO	4.5
35	L13A	134	ARG	4.5
43	L21B	93	GLU	4.5
3	S3B	66	VAL	4.5
36	L14B	91	LEU	4.5
47	L25A	177	PRO	4.5
2	S2A	188	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
3	S3A	167	TRP	4.5
35	L13B	10	GLU	4.4
54	L33A	9	LEU	4.4
2	S2B	162	ILE	4.4
54	L33B	9	LEU	4.4
33	L6B	133	VAL	4.4
39	L17B	69	ASP	4.4
12	S12A	126	ALA	4.4
2	S2A	171	ALA	4.4
3	S3B	157	ILE	4.4
42	L20B	117	GLN	4.3
47	L25A	116	VAL	4.3
2	S2B	47	THR	4.3
12	S12B	82	ILE	4.3
34	L9B	138	ILE	4.3
33	L6A	116	GLU	4.3
34	L9B	92	VAL	4.3
35	L13B	133	GLN	4.3
42	L20B	91	ASP	4.3
30	L3B	53	PRO	4.3
3	S3B	207	VAL	4.3
31	L4B	133	ASN	4.3
10	S10B	82	ILE	4.3
18	S18B	82	THR	4.3
4	S4B	126	ILE	4.3
13	S13A	120	LYS	4.2
47	L25B	176	PRO	4.2
5	S5B	76	ILE	4.2
7	S7A	85	TYR	4.2
22	ASIA	12	U	4.2
3	S3A	94	LEU	4.2
38	L16A	1	MET	4.2
34	L9A	132	PRO	4.2
3	S3B	100	ALA	4.2
5	S5B	125	SER	4.2
4	S4B	101	LEU	4.2
24	ESIA	11	C	4.2
34	L9A	77	LEU	4.2
27	23SB	1139	G	4.2
27	23SA	2913	C	4.2
35	L13B	57	ALA	4.2
2	S2A	162	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
42	L20B	106	PHE	4.2
12	S12B	59	SER	4.2
33	L6A	34	GLU	4.2
31	L4B	12	LEU	4.2
34	L9A	116	LEU	4.2
52	L31A	63	TYR	4.1
4	S4A	88	VAL	4.1
18	S18A	88	LYS	4.1
2	S2B	93	VAL	4.1
12	S12A	59	SER	4.1
22	ASIA	5	G	4.1
6	S6B	45	LEU	4.1
5	S5A	148	VAL	4.1
32	L5A	35	GLU	4.1
33	L6B	34	GLU	4.1
22	ASIA	6	G	4.1
43	L21B	86	GLY	4.1
33	L6B	151	ILE	4.1
2	S2B	145	LEU	4.1
5	S5A	50	GLU	4.1
11	S11B	81	ASP	4.1
4	S4A	126	ILE	4.1
2	S2B	202	PRO	4.1
4	S4A	189	PRO	4.1
18	S18B	26	LEU	4.1
5	S5A	124	GLY	4.0
16	S16B	39	TYR	4.0
7	S7B	86	GLN	4.0
14	S14B	38	GLY	4.0
41	L19B	4	GLY	4.0
4	S4B	12	CYS	4.0
4	S4A	96	LEU	4.0
47	L25B	76	LEU	4.0
33	L6B	121	ILE	4.0
33	L6B	55	PRO	4.0
8	S8A	113	SER	4.0
2	S2B	211	ILE	4.0
4	S4B	150	GLU	4.0
10	S10B	6	ILE	4.0
27	23SB	2910	U	3.9
10	S10A	93	GLY	3.9
33	L6B	48	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
20	S20A	59	ALA	3.9
47	L25A	173	ALA	3.9
5	S5B	28	PHE	3.9
33	L6A	175	LYS	3.9
2	S2B	174	VAL	3.9
20	S20B	63	ILE	3.9
34	L9B	88	ILE	3.9
10	S10B	27	ALA	3.9
4	S4A	152	SER	3.9
27	23SB	2914	C	3.9
5	S5B	124	GLY	3.9
55	L34B	49	ARG	3.9
54	L33A	48	VAL	3.9
2	S2A	61	LEU	3.9
4	S4B	96	LEU	3.9
10	S10A	23	ILE	3.9
33	L6B	85	LYS	3.9
4	S4B	162	LEU	3.9
47	L25B	67	LEU	3.9
36	L14B	37	ASP	3.9
39	L17A	5	LYS	3.9
4	S4A	136	PRO	3.8
33	L6B	15	VAL	3.8
33	L6B	84	SER	3.8
22	ASIA	27	G	3.8
52	L31A	43	TYR	3.8
14	S14A	59	ALA	3.8
44	L22B	113	LYS	3.8
3	S3B	90	GLU	3.8
19	S19B	76	PRO	3.8
3	S3B	64	VAL	3.8
47	L25A	144	LEU	3.8
43	L21B	12	TYR	3.8
13	S13A	119	GLY	3.8
30	L3B	48	GLN	3.8
3	S3B	62	ASP	3.8
2	S2A	71	VAL	3.8
48	L27B	7	LEU	3.8
3	S3A	184	TYR	3.8
4	S4A	146	ILE	3.8
33	L6A	89	ILE	3.8
34	L9B	109	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
54	L33A	23	THR	3.8
3	S3A	203	PHE	3.8
33	L6B	43	VAL	3.8
4	S4B	24	GLU	3.8
20	S20A	84	LEU	3.8
34	L9B	125	GLU	3.8
23	PSIA	1	G	3.8
34	L9A	138	ILE	3.8
12	S12A	64	THR	3.8
4	S4B	91	SER	3.8
27	23SB	5	A	3.8
33	L6B	147	ASN	3.8
30	L3B	47	VAL	3.8
4	S4A	19	LEU	3.8
30	L3B	27	LEU	3.8
47	L25A	59	LEU	3.8
40	L18B	55	ALA	3.8
57	ASIB	70	G	3.7
5	S5A	55	VAL	3.7
35	L13B	7	LYS	3.7
34	L9A	139	GLN	3.7
36	L14A	108	GLU	3.7
3	S3A	128	PHE	3.7
4	S4B	99	SER	3.7
45	L23B	92	LEU	3.7
33	L6B	39	PRO	3.7
3	S3B	171	GLY	3.7
9	S9A	82	ALA	3.7
4	S4B	134	ASP	3.7
35	L13B	93	THR	3.7
26	TRNA	1	G	3.7
27	23SA	931	G	3.7
27	23SA	2911	G	3.7
57	ASIB	6	G	3.7
2	S2B	196	LEU	3.7
4	S4B	92	VAL	3.7
33	L6B	11	VAL	3.7
2	S2B	172	ILE	3.7
3	S3A	161	GLU	3.7
30	L3B	204	ALA	3.7
34	L9B	87	LYS	3.7
35	L13B	32	THR	3.7

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Mol	Chain	Res	Type	RSRZ
47	L25A	107	THR	3.7
4	S4B	170	VAL	3.7
34	L9A	144	VAL	3.7
43	L21B	38	LEU	3.7
46	L24B	49	VAL	3.7
2	S2B	80	ILE	3.7
10	S10B	35	SER	3.7
4	S4B	111	ALA	3.6
7	S7B	147	ALA	3.6
27	23SB	2909	U	3.6
33	L6B	14	GLY	3.6
53	L32B	53	ALA	3.6
30	L3A	52	LEU	3.6
41	L19B	1	MET	3.6
3	S3A	95	THR	3.6
5	S5B	69	VAL	3.6
33	L6A	115	VAL	3.6
14	S14B	52	GLN	3.6
13	S13B	6	GLY	3.6
35	L13B	1	MET	3.6
1	16SA	1063	C	3.6
10	S10B	73	ASP	3.6
9	S9A	115	GLY	3.6
33	L6A	170	ARG	3.6
42	L20B	83	LEU	3.6
22	ASIA	45	U	3.6
33	L6A	168	PRO	3.6
33	L6B	112	PRO	3.6
3	S3B	41	GLY	3.6
12	S12B	16	ARG	3.6
38	L16B	104	PHE	3.6
27	23SA	1121	A	3.6
3	S3A	182	ILE	3.6
12	S12A	44	LYS	3.6
27	23SB	3	U	3.6
46	L24B	101	LYS	3.6
2	S2B	13	ALA	3.6
43	L21B	40	LEU	3.6
10	S10B	75	ILE	3.6
12	S12A	35	THR	3.6
13	S13B	121	LYS	3.6
33	L6B	102	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
8	S8A	39	LEU	3.5
41	L19A	19	LEU	3.5
25	MRNA	55	U	3.5
33	L6B	19	VAL	3.5
34	L9A	92	VAL	3.5
12	S12B	20	LYS	3.5
22	ASIA	11	C	3.5
1	16SA	1054	G	3.5
2	S2A	115	LEU	3.5
3	S3A	87	LEU	3.5
4	S4A	135	LEU	3.5
41	L19A	78	LEU	3.5
48	L27A	85	ALA	3.5
54	L33A	34	LEU	3.5
3	S3A	195	VAL	3.5
3	S3B	75	VAL	3.5
4	S4A	128	VAL	3.5
5	S5B	55	VAL	3.5
19	S19A	45	VAL	3.5
22	ASIA	14	A	3.5
27	23SA	1118	A	3.5
35	L13B	127	ASP	3.5
37	L15B	71	VAL	3.5
13	S13B	84	ILE	3.5
2	S2B	167	PRO	3.5
5	S5B	77	PRO	3.5
33	L6B	96	ALA	3.5
21	THXA	14	TRP	3.5
22	ASIA	62	C	3.5
57	ASIB	74	C	3.5
31	L4B	131	GLY	3.5
3	S3B	138	VAL	3.5
17	S17A	35	VAL	3.5
43	L21B	46	VAL	3.5
11	S11A	67	ASP	3.5
27	23SA	1111	G	3.5
34	L9A	110	ASP	3.5
4	S4A	11	LEU	3.5
4	S4A	87	GLY	3.5
47	L25A	175	VAL	3.5
22	ASIA	2	C	3.5
24	ESIB	11	C	3.5

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Mol	Chain	Res	Type	RSRZ
8	S8B	101	PRO	3.5
8	S8B	112	LEU	3.5
34	L9B	126	TYR	3.5
6	S6B	99	ALA	3.5
19	S19A	79	THR	3.5
22	ASIA	47	U	3.5
16	S16B	80	PHE	3.5
30	L3A	88	GLY	3.5
33	L6A	114	VAL	3.5
47	L25A	174	VAL	3.5
4	S4A	158	ILE	3.5
7	S7A	78	ARG	3.5
3	S3A	44	GLU	3.4
34	L9A	72	LEU	3.4
40	L18A	110	LEU	3.4
57	ASIB	3	C	3.4
33	L6B	56	SER	3.4
4	S4B	133	VAL	3.4
25	MRNA	56	U	3.4
23	PSIB	1	G	3.4
4	S4B	108	LEU	3.4
4	S4B	144	ASP	3.4
34	L9B	135	GLU	3.4
4	S4A	39	PRO	3.4
34	L9A	80	PRO	3.4
44	L22B	111	HIS	3.4
4	S4A	195	ALA	3.4
4	S4A	91	SER	3.4
1	16SA	986	C	3.4
34	L9A	108	THR	3.4
4	S4B	87	GLY	3.4
46	L24B	58	GLY	3.4
3	S3A	134	ILE	3.4
3	S3B	77	ILE	3.4
4	S4B	115	ARG	3.4
43	L21B	99	ILE	3.4
22	ASIA	16	U	3.4
22	ASIA	26	A	3.4
3	S3A	188	LEU	3.4
5	S5A	31	LEU	3.4
24	ESIA	27	G	3.4
24	ESIB	1	G	3.4

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Mol	Chain	Res	Type	RSRZ
27	23SA	2846	G	3.4
2	S2A	159	PRO	3.4
4	S4A	197	PRO	3.4
4	S4B	195	ALA	3.4
16	S16B	46	PRO	3.4
16	S16B	56	ALA	3.4
30	L3B	56	PRO	3.4
33	L6B	118	PRO	3.4
35	L13B	31	ALA	3.4
33	L6B	76	VAL	3.4
31	L4B	175	THR	3.4
38	L16A	21	THR	3.4
4	S4A	12	CYS	3.4
42	L20B	104	GLN	3.4
27	23SA	937	C	3.4
8	S8B	59	LEU	3.4
19	S19A	83	HIS	3.4
22	ASIA	76	A	3.4
33	L6A	86	GLU	3.4
35	L13B	37	LYS	3.4
31	L4B	6	VAL	3.4
53	L32B	51	TYR	3.4
4	S4B	95	GLY	3.4
14	S14A	12	ARG	3.4
2	S2B	42	ILE	3.4
4	S4A	52	SER	3.4
9	S9A	126	SER	3.4
3	S3A	47	LEU	3.4
18	S18A	31	LEU	3.4
54	L33A	36	LEU	3.4
4	S4B	181	MET	3.4
34	L9B	141	LYS	3.4
19	S19B	89	ALA	3.4
13	S13B	8	GLU	3.4
33	L6B	107	VAL	3.4
2	S2A	114	ARG	3.4
7	S7A	82	GLY	3.4
12	S12A	113	SER	3.4
33	L6A	147	ASN	3.3
5	S5A	105	VAL	3.3
33	L6B	21	PRO	3.3
46	L24B	45	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
3	S3A	19	GLU	3.3
4	S4B	34	GLU	3.3
10	S10A	46	ARG	3.3
17	S17B	91	ARG	3.3
19	S19A	82	GLY	3.3
3	S3A	152	ILE	3.3
4	S4B	127	THR	3.3
4	S4A	176	LEU	3.3
34	L9A	68	LEU	3.3
35	L13B	138	LEU	3.3
34	L9A	102	SER	3.3
6	S6B	39	LYS	3.3
35	L13B	90	MET	3.3
2	S2B	184	VAL	3.3
4	S4B	17	VAL	3.3
5	S5B	33	VAL	3.3
7	S7B	150	ALA	3.3
16	S16B	79	VAL	3.3
33	L6B	45	VAL	3.3
4	S4A	172	PRO	3.3
42	L20A	106	PHE	3.3
2	S2B	200	ILE	3.3
10	S10B	67	THR	3.3
12	S12B	41	THR	3.3
4	S4A	85	LYS	3.3
27	23SA	4	C	3.3
10	S10A	59	SER	3.3
49	L28A	86	SER	3.3
2	S2A	186	ALA	3.3
5	S5B	30	ALA	3.3
33	L6A	133	VAL	3.3
34	L9A	94	ALA	3.3
51	L30B	58	VAL	3.3
1	16SA	1053	A	3.3
5	S5A	22	GLY	3.3
19	S19A	84	GLY	3.3
42	L20A	118	GLY	3.3
4	S4B	157	LEU	3.3
8	S8A	133	LEU	3.3
33	L6B	33	LEU	3.3
3	S3A	190	ARG	3.3
11	S11B	77	MET	3.3

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Mol	Chain	Res	Type	RSRZ
23	PSIA	5	G	3.3
2	S2A	15	VAL	3.3
2	S2A	81	VAL	3.3
4	S4B	185	PHE	3.3
9	S9A	52	ALA	3.3
40	L18B	2	ALA	3.3
3	S3B	73	PRO	3.3
3	S3A	78	GLY	3.3
4	S4A	108	LEU	3.3
19	S19A	5	LEU	3.3
24	ESIA	7	A	3.3
40	L18B	56	LEU	3.3
33	L6A	129	THR	3.3
4	S4A	118	ARG	3.3
35	L13B	41	ASP	3.3
37	L15B	18	ARG	3.3
3	S3B	65	ALA	3.3
4	S4A	121	VAL	3.3
34	L9A	115	ALA	3.3
2	S2B	192	SER	3.3
11	S11A	101	SER	3.3
19	S19B	42	PRO	3.3
42	L20B	94	ASN	3.3
20	S20A	55	ILE	3.3
33	L6B	120	GLY	3.3
34	L9A	124	GLY	3.3
4	S4A	150	GLU	3.2
57	ASIB	75	C	3.2
11	S11A	25	TYR	3.2
5	S5A	10	MET	3.2
10	S10A	48	THR	3.2
13	S13B	117	VAL	3.2
32	L5A	80	PHE	3.2
4	S4B	172	PRO	3.2
4	S4A	194	LEU	3.2
32	L5B	127	GLY	3.2
38	L16A	79	LEU	3.2
24	ESIA	13	C	3.2
33	L6A	99	VAL	3.2
4	S4A	48	ALA	3.2
33	L6A	165	ALA	3.2
52	L31A	59	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
2	S2A	110	GLN	3.2
27	23SB	1125	A	3.2
4	S4B	146	ILE	3.2
34	L9B	79	ILE	3.2
41	L19B	88	ILE	3.2
54	L33A	31	PRO	3.2
2	S2A	187	LEU	3.2
3	S3B	196	LEU	3.2
9	S9B	19	LEU	3.2
12	S12A	56	ARG	3.2
43	L21B	15	GLU	3.2
3	S3A	66	VAL	3.2
47	L25B	116	VAL	3.2
3	S3A	121	ALA	3.2
4	S4B	48	ALA	3.2
7	S7A	150	ALA	3.2
1	16SA	1841	C	3.2
5	S5A	49	PRO	3.2
22	ASIA	68	C	3.2
13	S13A	83	ASP	3.2
33	L6B	117	PRO	3.2
22	ASIA	69	G	3.2
27	23SA	1125	A	3.2
33	L6B	80	SER	3.2
17	S17A	101	ARG	3.2
12	S12B	61	TYR	3.2
36	L14B	9	GLU	3.2
47	L25B	161	VAL	3.2
7	S7B	152	ALA	3.2
11	S11B	64	ALA	3.2
12	S12B	65	ALA	3.2
34	L9B	83	ALA	3.2
38	L16B	40	ALA	3.2
47	L25A	7	ALA	3.2
53	L32B	2	ALA	3.2
48	L27B	4	LYS	3.2
2	S2A	222	ILE	3.2
4	S4B	5	ILE	3.2
20	S20B	10	LEU	3.2
8	S8B	54	ASP	3.2
41	L19A	1	MET	3.2
22	ASIA	7	A	3.2

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Mol	Chain	Res	Type	RSRZ
33	L6B	44	VAL	3.2
13	S13B	18	ALA	3.2
35	L13A	18	ALA	3.2
8	S8B	133	LEU	3.2
9	S9A	19	LEU	3.2
47	L25A	146	ILE	3.2
12	S12B	84	GLY	3.1
42	L20B	101	ARG	3.1
8	S8B	113	SER	3.1
30	L3B	55	ASN	3.1
33	L6B	50	VAL	3.1
3	S3B	206	GLU	3.1
2	S2A	152	PHE	3.1
3	S3A	189	ALA	3.1
4	S4A	82	ALA	3.1
22	ASIA	13	C	3.1
27	23SB	2908	C	3.1
45	L23B	91	ALA	3.1
4	S4B	94	LEU	3.1
52	L31A	52	THR	3.1
3	S3A	131	ARG	3.1
8	S8B	72	PRO	3.1
9	S9A	49	PRO	3.1
8	S8B	131	GLY	3.1
27	23SA	929	G	3.1
29	L2A	251	GLY	3.1
40	L18A	108	GLY	3.1
4	S4A	102	ASP	3.1
33	L6B	111	HIS	3.1
3	S3B	141	VAL	3.1
4	S4A	105	VAL	3.1
12	S12B	44	LYS	3.1
38	L16A	20	ALA	3.1
4	S4B	135	LEU	3.1
54	L33B	36	LEU	3.1
8	S8B	45	ILE	3.1
2	S2A	54	THR	3.1
27	23SB	2817	C	3.1
53	L32B	34	PRO	3.1
57	ASIB	2	C	3.1
4	S4A	160	GLN	3.1
22	ASIA	23	A	3.1

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Mol	Chain	Res	Type	RSRZ
27	23SA	2912	A	3.1
3	S3A	135	LYS	3.1
34	L9A	87	LYS	3.1
4	S4B	198	VAL	3.1
4	S4B	203	VAL	3.1
42	L20B	110	VAL	3.1
43	L21B	14	VAL	3.1
48	L27B	3	HIS	3.1
3	S3B	53	ALA	3.1
4	S4B	64	LEU	3.1
4	S4B	97	LEU	3.1
49	L28B	95	LEU	3.1
6	S6B	81	ILE	3.1
12	S12A	30	ARG	3.1
34	L9B	11	ASN	3.1
34	L9A	119	PRO	3.1
31	L4B	207	GLY	3.1
52	L31B	54	GLY	3.1
4	S4A	33	MET	3.1
34	L9A	131	LYS	3.1
2	S2B	15	VAL	3.1
9	S9A	86	VAL	3.1
3	S3A	101	LEU	3.1
3	S3B	94	LEU	3.1
17	S17A	6	LEU	3.1
2	S2B	185	ILE	3.1
3	S3A	48	TYR	3.1
5	S5B	109	ILE	3.1
8	S8A	111	ILE	3.1
3	S3B	80	GLY	3.1
10	S10B	77	PRO	3.1
19	S19A	68	GLY	3.1
24	ESIA	10	G	3.1
34	L9B	78	THR	3.1
3	S3A	103	VAL	3.1
4	S4A	133	VAL	3.1
33	L6B	49	VAL	3.1
4	S4A	206	PHE	3.1
33	L6B	123	PHE	3.1
3	S3B	57	ILE	3.1
8	S8B	111	ILE	3.1
35	L13B	16	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
28	5SA	1	A	3.0
52	L31B	37	SER	3.0
54	L33B	42	TRP	3.0
57	ASIB	73	A	3.0
2	S2B	18	GLY	3.0
5	S5A	23	GLY	3.0
42	L20B	84	LYS	3.0
3	S3B	151	VAL	3.0
4	S4A	162	LEU	3.0
20	S20A	99	LEU	3.0
47	L25A	117	LEU	3.0
4	S4A	49	ARG	3.0
2	S2A	68	ILE	3.0
47	L25B	113	ALA	3.0
53	L32A	53	ALA	3.0
3	S3A	90	GLU	3.0
4	S4A	15	GLU	3.0
44	L22B	30	GLU	3.0
54	L33A	53	LYS	3.0
10	S10B	10	GLY	3.0
33	L6B	129	THR	3.0
8	S8B	26	VAL	3.0
12	S12A	107	VAL	3.0
19	S19A	41	VAL	3.0
2	S2A	149	LEU	3.0
34	L9B	72	LEU	3.0
12	S12B	29	PHE	3.0
2	S2A	173	ALA	3.0
3	S3A	169	ALA	3.0
3	S3B	169	ALA	3.0
3	S3B	202	ILE	3.0
16	S16B	4	ILE	3.0
4	S4B	27	TYR	3.0
33	L6A	81	GLU	3.0
33	L6B	47	GLU	3.0
1	16SB	1115	G	3.0
22	ASIA	10	G	3.0
23	PSIA	70	G	3.0
33	L6B	154	PRO	3.0
4	S4B	165	MET	3.0
12	S12B	19	SER	3.0
12	S12B	52	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
47	L25A	111	VAL	3.0
7	S7A	155	ARG	3.0
8	S8B	119	LEU	3.0
12	S12B	90	LEU	3.0
35	L13B	130	HIS	3.0
4	S4B	4	TYR	3.0
4	S4B	156	GLU	3.0
5	S5A	68	GLU	3.0
5	S5B	68	GLU	3.0
2	S2B	228	GLY	3.0
20	S20A	103	GLY	3.0
31	L4B	147	GLY	3.0
52	L31A	11	PRO	3.0
46	L24A	107	ASP	3.0
4	S4A	199	ASN	3.0
14	S14B	37	PHE	3.0
2	S2A	214	ILE	3.0
10	S10A	26	ALA	3.0
14	S14A	30	ALA	3.0
22	ASIA	24	G	3.0
33	L6B	162	ILE	3.0
34	L9A	120	ILE	3.0
20	S20A	87	LYS	3.0
23	PSIA	17	C	3.0
23	PSIA	67	C	3.0
27	23SA	936	A	3.0
2	S2A	148	TYR	3.0
4	S4B	72	GLU	3.0
8	S8A	66	GLY	3.0
25	MRNB	45	U	3.0
42	L20B	89	GLU	3.0
49	L28A	93	GLU	3.0
3	S3A	198	VAL	3.0
10	S10B	72	VAL	3.0
33	L6B	88	LEU	3.0
47	L25A	179	ASP	3.0
4	S4B	93	PHE	3.0
33	L6A	80	SER	3.0
38	L16B	21	THR	3.0
47	L25B	164	ALA	3.0
7	S7B	153	HIS	2.9
54	L33A	49	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	16SB	1104	G	2.9
8	S8B	27	PRO	2.9
34	L9B	9	LEU	2.9
2	S2A	108	ILE	2.9
2	S2A	182	ILE	2.9
4	S4A	99	SER	2.9
11	S11A	68	ALA	2.9
12	S12B	23	ALA	2.9
18	S18A	20	ALA	2.9
34	L9A	83	ALA	2.9
4	S4B	199	ASN	2.9
42	L20B	66	ASN	2.9
34	L9A	133	HIS	2.9
4	S4B	153	ARG	2.9
47	L25B	79	ARG	2.9
33	L6A	120	GLY	2.9
53	L32A	52	TYR	2.9
12	S12B	80	VAL	2.9
34	L9B	123	LEU	2.9
54	L33A	42	TRP	2.9
34	L9A	117	GLU	2.9
4	S4B	75	PHE	2.9
32	L5B	75	LYS	2.9
34	L9A	141	LYS	2.9
11	S11A	60	ALA	2.9
22	ASIA	63	G	2.9
27	23SA	1221	G	2.9
27	23SA	2166	G	2.9
4	S4A	144	ASP	2.9
12	S12B	30	ARG	2.9
41	L19B	3	ARG	2.9
42	L20B	72	HIS	2.9
2	S2A	136	VAL	2.9
10	S10B	71	LEU	2.9
33	L6A	174	GLY	2.9
33	L6A	126	PRO	2.9
33	L6B	99	VAL	2.9
44	L22B	65	LEU	2.9
54	L33B	34	LEU	2.9
14	S14A	34	TYR	2.9
35	L13B	44	PRO	2.9
5	S5B	50	GLU	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
32	L5A	67	LYS	2.9
36	L14B	113	LYS	2.9
14	S14A	7	ILE	2.9
2	S2B	173	ALA	2.9
4	S4A	111	ALA	2.9
11	S11A	36	ASP	2.9
35	L13B	17	ASP	2.9
3	S3A	132	ARG	2.9
4	S4B	35	ARG	2.9
1	16SB	986	C	2.9
12	S12B	77	HIS	2.9
23	PSIA	4	C	2.9
23	PSIB	67	C	2.9
27	23SB	572	C	2.9
27	23SB	2771	C	2.9
2	S2B	98	LEU	2.9
33	L6A	71	LEU	2.9
33	L6B	64	LEU	2.9
13	S13A	100	GLY	2.9
33	L6A	131	VAL	2.9
4	S4A	106	TYR	2.9
11	S11B	11	LYS	2.9
12	S12A	61	TYR	2.9
16	S16B	66	PRO	2.9
7	S7A	156	TRP	2.9
37	L15A	121	LYS	2.9
10	S10B	96	ILE	2.9
33	L6B	109	PHE	2.9
2	S2B	34	ALA	2.9
6	S6B	101	ALA	2.9
3	S3A	165	THR	2.9
3	S3B	165	THR	2.9
12	S12A	38	ARG	2.9
47	L25B	81	ARG	2.9
3	S3B	49	SER	2.9
4	S4A	137	SER	2.9
4	S4B	152	SER	2.9
40	L18A	1	MET	2.9
53	L32B	30	LEU	2.9
3	S3B	68	VAL	2.9
4	S4B	112	VAL	2.9
4	S4B	161	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
12	S12A	84	GLY	2.9
43	L21B	5	VAL	2.9
54	L33A	29	ASN	2.9
2	S2A	26	PRO	2.9
25	MRNA	54	U	2.9
46	L24A	56	PRO	2.9
22	ASIA	25	C	2.9
35	L13B	60	ILE	2.9
5	S5B	111	GLU	2.8
56	L35B	56	GLU	2.8
2	S2A	85	ALA	2.8
20	S20A	97	ALA	2.8
33	L6B	20	ALA	2.8
47	L25A	172	ALA	2.8
49	L28B	63	ALA	2.8
7	S7A	5	ARG	2.8
34	L9B	35	LEU	2.8
43	L21B	20	LEU	2.8
42	L20A	117	GLN	2.8
12	S12A	17	LYS	2.8
43	L21B	37	VAL	2.8
43	L21B	85	LYS	2.8
44	L22B	112	GLY	2.8
4	S4A	51	PRO	2.8
6	S6B	32	ASN	2.8
12	S12B	45	PRO	2.8
4	S4A	4	TYR	2.8
5	S5A	7	GLU	2.8
5	S5B	86	ALA	2.8
8	S8A	42	GLU	2.8
12	S12B	126	ALA	2.8
16	S16A	7	ALA	2.8
27	23SA	1142	U	2.8
30	L3B	20	ALA	2.8
36	L14A	105	GLU	2.8
35	L13B	12	ARG	2.8
3	S3A	34	LEU	2.8
4	S4B	119	GLN	2.8
4	S4B	148	VAL	2.8
7	S7A	80	VAL	2.8
7	S7B	9	VAL	2.8
7	S7B	87	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
8	S8B	61	VAL	2.8
35	L13B	109	LYS	2.8
51	L30B	20	LYS	2.8
43	L21B	41	GLY	2.8
29	L2B	162	SER	2.8
41	L19B	106	SER	2.8
3	S3B	102	ASN	2.8
8	S8B	35	ILE	2.8
10	S10A	50	ILE	2.8
19	S19A	31	ILE	2.8
33	L6A	123	PHE	2.8
4	S4A	207	TYR	2.8
4	S4B	20	TYR	2.8
13	S13B	87	TYR	2.8
7	S7A	127	ALA	2.8
42	L20B	59	ARG	2.8
42	L20B	111	GLU	2.8
24	ESIB	12	U	2.8
3	S3A	42	LEU	2.8
3	S3A	52	LEU	2.8
4	S4A	101	LEU	2.8
46	L24B	106	LEU	2.8
4	S4B	18	LYS	2.8
23	PSIA	72	C	2.8
57	ASIB	4	C	2.8
5	S5A	72	GLN	2.8
10	S10B	36	GLY	2.8
42	L20B	87	GLY	2.8
2	S2B	159	PRO	2.8
4	S4A	29	PRO	2.8
19	S19A	42	PRO	2.8
33	L6A	128	PRO	2.8
4	S4B	114	ARG	2.8
1	16SA	1065	G	2.8
1	16SB	1817	G	2.8
6	S6B	4	TYR	2.8
19	S19A	3	ARG	2.8
22	ASIA	22	G	2.8
33	L6B	32	GLU	2.8
34	L9A	7	GLU	2.8
51	L30B	60	GLU	2.8
2	S2B	102	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
5	S5B	12	LEU	2.8
10	S10B	90	LEU	2.8
33	L6B	27	LYS	2.8
35	L13A	138	LEU	2.8
46	L24B	34	LYS	2.8
47	L25A	163	LEU	2.8
2	S2A	165	VAL	2.8
2	S2B	165	VAL	2.8
8	S8B	97	VAL	2.8
41	L19B	30	VAL	2.8
2	S2B	6	THR	2.8
3	S3B	124	ILE	2.8
53	L32B	32	PRO	2.8
27	23SB	8	A	2.8
1	16SA	790	C	2.8
23	PSIA	68	C	2.8
2	S2A	218	ALA	2.8
4	S4B	147	ALA	2.8
10	S10B	20	ALA	2.8
40	L18A	2	ALA	2.8
7	S7B	148	ASN	2.8
3	S3B	19	GLU	2.8
3	S3B	43	LEU	2.8
17	S17B	53	LEU	2.8
33	L6A	30	LYS	2.8
33	L6B	18	GLU	2.8
41	L19A	21	GLU	2.8
46	L24A	101	LYS	2.8
48	L27B	5	LYS	2.8
4	S4A	181	MET	2.8
34	L9A	81	VAL	2.8
34	L9A	145	VAL	2.8
43	L21B	51	VAL	2.8
27	23SB	11	G	2.8
2	S2B	190	THR	2.8
3	S3A	81	GLY	2.8
35	L13A	77	GLY	2.8
2	S2A	122	PHE	2.8
7	S7B	43	PHE	2.8
35	L13A	85	ILE	2.8
35	L13B	38	HIS	2.7
47	L25B	25	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
54	L33A	16	CYS	2.7
4	S4B	149	ALA	2.7
5	S5B	54	ALA	2.7
31	L4B	130	ALA	2.7
34	L9A	65	ALA	2.7
34	L9A	95	LYS	2.7
41	L19A	137	LYS	2.7
1	16SB	1053	A	2.7
2	S2A	11	LEU	2.7
10	S10A	90	LEU	2.7
16	S16B	49	LEU	2.7
18	S18B	31	LEU	2.7
35	L13B	87	LEU	2.7
43	L21B	39	LEU	2.7
57	ASIB	76	A	2.7
22	ASIA	74	C	2.7
36	L14B	1	MET	2.7
2	S2A	164	VAL	2.7
4	S4B	105	VAL	2.7
5	S5B	82	VAL	2.7
16	S16B	53	VAL	2.7
33	L6B	169	VAL	2.7
47	L25B	96	VAL	2.7
2	S2A	172	ILE	2.7
4	S4B	171	GLY	2.7
15	S15A	89	GLY	2.7
3	S3A	186	PHE	2.7
4	S4A	209	ARG	2.7
30	L3B	3	GLY	2.7
10	S10B	63	PHE	2.7
4	S4B	189	PRO	2.7
31	L4B	14	PRO	2.7
3	S3A	65	ALA	2.7
16	S16A	56	ALA	2.7
40	L18A	86	ALA	2.7
3	S3B	45	LYS	2.7
3	S3B	184	TYR	2.7
4	S4B	155	LEU	2.7
25	MRNB	56	U	2.7
33	L6A	103	LEU	2.7
33	L6B	98	LEU	2.7
37	L15B	106	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
31	L4A	23	ASP	2.7
12	S12A	15	VAL	2.7
14	S14B	56	VAL	2.7
32	L5A	160	VAL	2.7
1	16SA	1060	C	2.7
4	S4A	14	ARG	2.7
7	S7A	79	ARG	2.7
34	L9A	113	ARG	2.7
3	S3A	5	ILE	2.7
18	S18B	27	GLY	2.7
35	L13B	51	PHE	2.7
16	S16A	41	PRO	2.7
3	S3B	129	ALA	2.7
12	S12B	51	LYS	2.7
18	S18B	84	LYS	2.7
35	L13B	92	ALA	2.7
43	L21B	19	LYS	2.7
2	S2A	155	LEU	2.7
16	S16A	59	TRP	2.7
7	S7A	151	TYR	2.7
4	S4A	170	VAL	2.7
24	ESIA	8	U	2.7
12	S12A	31	ARG	2.7
24	ESIA	15	G	2.7
38	L16A	6	ARG	2.7
2	S2A	42	ILE	2.7
2	S2B	201	ILE	2.7
2	S2B	163	PHE	2.7
4	S4A	167	GLY	2.7
7	S7B	81	GLY	2.7
11	S11A	49	GLY	2.7
12	S12B	67	ILE	2.7
33	L6B	89	ILE	2.7
38	L16A	104	PHE	2.7
47	L25A	115	GLY	2.7
2	S2B	168	THR	2.7
4	S4B	136	PRO	2.7
24	ESIB	36	A	2.7
46	L24B	53	PRO	2.7
5	S5A	21	ALA	2.7
11	S11B	60	ALA	2.7
31	L4A	198	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	S2B	149	LEU	2.7
4	S4A	64	LEU	2.7
6	S6A	43	LEU	2.7
18	S18B	85	LEU	2.7
19	S19A	15	LEU	2.7
3	S3A	75	VAL	2.7
14	S14A	43	CYS	2.7
49	L28A	53	VAL	2.7
3	S3B	183	ASP	2.7
7	S7A	90	GLU	2.7
12	S12A	62	GLU	2.7
16	S16B	47	ASP	2.7
36	L14A	116	SER	2.7
44	L22B	66	GLU	2.7
3	S3A	124	ILE	2.7
8	S8A	45	ILE	2.7
30	L3A	176	ILE	2.7
34	L9B	120	ILE	2.7
48	L27B	12	ASN	2.7
1	16SA	1062	U	2.7
4	S4A	2	GLY	2.7
22	ASIA	51	U	2.7
2	S2A	190	THR	2.7
35	L13B	129	PRO	2.7
3	S3B	101	LEU	2.7
5	S5B	151	LEU	2.7
19	S19A	30	LEU	2.7
19	S19A	71	LEU	2.7
22	ASIA	15	G	2.7
23	PSIA	71	G	2.7
27	23SB	10	G	2.7
27	23SB	2166	G	2.7
30	L3B	49	LEU	2.7
30	L3B	52	LEU	2.7
32	L5B	173	LEU	2.7
34	L9A	128	LEU	2.7
4	S4B	33	MET	2.7
3	S3B	29	TYR	2.7
52	L31A	10	VAL	2.7
1	16SB	1132	C	2.7
3	S3B	30	ARG	2.7
11	S11A	29	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
12	S12B	62	GLU	2.6
33	L6B	9	ILE	2.6
47	L25A	138	GLU	2.6
2	S2A	181	PHE	2.6
3	S3B	186	PHE	2.6
2	S2B	37	ASN	2.6
2	S2B	171	ALA	2.6
3	S3B	189	ALA	2.6
20	S20B	106	ALA	2.6
34	L9B	129	THR	2.6
34	L9B	146	ALA	2.6
47	L25B	117	LEU	2.6
47	L25B	130	PRO	2.6
43	L21B	80	GLN	2.6
3	S3A	21	ARG	2.6
4	S4A	36	ARG	2.6
9	S9A	41	VAL	2.6
13	S13A	98	VAL	2.6
34	L9B	144	VAL	2.6
37	L15A	125	VAL	2.6
43	L21B	72	VAL	2.6
1	16SA	797	G	2.6
27	23SB	2	G	2.6
57	ASIB	71	G	2.6
10	S10A	96	ILE	2.6
35	L13B	84	LYS	2.6
52	L31A	31	ILE	2.6
2	S2A	231	GLU	2.6
2	S2B	9	GLU	2.6
4	S4B	2	GLY	2.6
33	L6B	119	GLU	2.6
43	L21B	28	GLU	2.6
2	S2A	193	ASP	2.6
49	L28B	38	SER	2.6
3	S3B	168	ALA	2.6
4	S4A	129	ASN	2.6
43	L21B	18	LEU	2.6
7	S7A	108	ALA	2.6
11	S11A	64	ALA	2.6
16	S16B	7	ALA	2.6
29	L2B	144	ALA	2.6
34	L9A	98	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
53	L32B	28	PRO	2.6
2	S2A	73	THR	2.6
19	S19B	79	THR	2.6
52	L31B	52	THR	2.6
2	S2B	71	VAL	2.6
4	S4A	119	GLN	2.6
7	S7A	86	GLN	2.6
8	S8A	70	GLN	2.6
17	S17B	101	ARG	2.6
20	S20B	8	ARG	2.6
33	L6A	101	ARG	2.6
22	ASIA	20	U	2.6
27	23SB	2521	U	2.6
7	S7B	85	TYR	2.6
4	S4B	196	LEU	2.6
48	L27A	84	LEU	2.6
4	S4A	164	ALA	2.6
1	16SB	1054	G	2.6
4	S4B	40	PRO	2.6
6	S6B	96	PRO	2.6
7	S7A	83	ALA	2.6
16	S16B	84	ALA	2.6
30	L3B	70	ALA	2.6
34	L9B	94	ALA	2.6
35	L13B	45	ASN	2.6
4	S4B	139	ARG	2.6
27	23SA	1123	C	2.6
34	L9B	133	HIS	2.6
35	L13B	3	THR	2.6
2	S2A	93	VAL	2.6
3	S3B	120	VAL	2.6
41	L19A	15	VAL	2.6
47	L25A	126	VAL	2.6
14	S14A	52	GLN	2.6
4	S4B	85	LYS	2.6
9	S9A	113	LYS	2.6
11	S11B	42	TRP	2.6
12	S12A	123	LYS	2.6
34	L9A	118	LYS	2.6
4	S4A	27	TYR	2.6
34	L9A	109	ILE	2.6
16	S16A	80	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
8	S8A	90	GLY	2.6
32	L5B	111	LEU	2.6
47	L25B	125	LEU	2.6
49	L28B	97	LEU	2.6
5	S5B	70	PRO	2.6
6	S6B	29	ALA	2.6
16	S16B	77	ALA	2.6
4	S4A	193	ASP	2.6
13	S13A	94	ARG	2.6
54	L33A	40	CYS	2.6
2	S2A	7	VAL	2.6
11	S11A	87	THR	2.6
35	L13B	54	VAL	2.6
33	L6B	153	LYS	2.6
54	L33A	27	LYS	2.6
35	L13B	8	GLN	2.6
1	16SA	1699	C	2.6
8	S8B	80	ILE	2.6
22	ASIA	52	G	2.6
24	ESIA	34	G	2.6
57	ASIB	49	C	2.6
3	S3B	128	PHE	2.6
5	S5A	6	PHE	2.6
6	S6B	60	PHE	2.6
9	S9A	37	PHE	2.6
34	L9A	126	TYR	2.6
3	S3B	178	LEU	2.6
4	S4B	58	LEU	2.6
4	S4B	188	LEU	2.6
36	L14B	106	LEU	2.6
24	ESIA	47	U	2.6
25	MRNB	39	U	2.6
2	S2B	141	GLU	2.6
4	S4B	82	ALA	2.6
7	S7A	134	ALA	2.6
33	L6A	96	ALA	2.6
33	L6B	81	GLU	2.6
36	L14B	51	ALA	2.6
42	L20B	108	GLU	2.6
46	L24A	109	GLU	2.6
12	S12B	31	ARG	2.6
30	L3B	74	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
43	L21B	13	ARG	2.6
38	L16B	1	MET	2.6
4	S4A	18	LYS	2.6
5	S5B	105	VAL	2.6
5	S5B	115	VAL	2.6
16	S16A	51	VAL	2.6
34	L9B	91	SER	2.6
3	S3A	67	THR	2.6
5	S5A	98	THR	2.6
11	S11B	87	THR	2.6
11	S11A	42	TRP	2.5
4	S4A	75	PHE	2.5
4	S4A	185	PHE	2.5
3	S3B	87	LEU	2.5
4	S4B	138	TYR	2.5
7	S7B	154	TYR	2.5
10	S10B	65	LEU	2.5
18	S18B	40	LEU	2.5
27	23SA	681	A	2.5
41	L19B	100	TYR	2.5
2	S2A	72	GLY	2.5
3	S3A	41	GLY	2.5
9	S9A	100	GLY	2.5
16	S16B	10	GLY	2.5
33	L6B	108	GLY	2.5
4	S4B	122	ARG	2.5
47	L25A	82	ARG	2.5
53	L32B	55	ARG	2.5
57	ASIB	72	C	2.5
30	L3A	204	ALA	2.5
2	S2B	231	GLU	2.5
12	S12A	45	PRO	2.5
19	S19A	59	PRO	2.5
31	L4B	27	GLU	2.5
34	L9A	111	PRO	2.5
3	S3B	86	VAL	2.5
12	S12B	54	LYS	2.5
14	S14B	58	LYS	2.5
31	L4B	201	VAL	2.5
35	L13B	122	VAL	2.5
43	L21B	47	VAL	2.5
30	L3A	174	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
5	S5B	80	ILE	2.5
33	L6A	92	ILE	2.5
5	S5B	123	LEU	2.5
6	S6B	43	LEU	2.5
16	S16B	73	LEU	2.5
16	S16B	74	LEU	2.5
20	S20A	13	LEU	2.5
54	L33A	10	LEU	2.5
3	S3A	129	ALA	2.5
16	S16A	64	ALA	2.5
4	S4A	22	LYS	2.5
4	S4A	165	MET	2.5
30	L3B	39	PRO	2.5
52	L31A	69	LYS	2.5
3	S3B	103	VAL	2.5
34	L9B	127	VAL	2.5
5	S5B	129	ILE	2.5
46	L24B	44	ILE	2.5
48	L27A	3	HIS	2.5
57	ASIB	55	U	2.5
24	ESIA	44	G	2.5
28	5SB	91	G	2.5
44	L22B	94	ASP	2.5
3	S3A	162	GLN	2.5
4	S4A	77	ASN	2.5
4	S4A	97	LEU	2.5
4	S4B	21	LEU	2.5
6	S6B	19	LEU	2.5
7	S7B	156	TRP	2.5
34	L9A	114	LEU	2.5
46	L24A	106	LEU	2.5
56	L35A	34	TRP	2.5
3	S3A	185	GLY	2.5
4	S4A	66	ARG	2.5
4	S4B	54	TYR	2.5
5	S5B	133	TYR	2.5
35	L13B	36	GLY	2.5
37	L15B	110	TYR	2.5
3	S3A	199	LYS	2.5
5	S5A	48	ALA	2.5
10	S10A	22	LYS	2.5
17	S17B	100	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	S2B	84	GLU	2.5
8	S8B	118	VAL	2.5
30	L3A	175	VAL	2.5
41	L19B	28	VAL	2.5
42	L20B	103	PRO	2.5
30	L3B	73	GLU	2.5
56	L35A	56	GLU	2.5
46	L24B	61	ILE	2.5
2	S2B	118	LEU	2.5
18	S18B	44	LEU	2.5
34	L9B	77	LEU	2.5
41	L19A	45	PHE	2.5
52	L31A	24	THR	2.5
22	ASIA	42	C	2.5
27	23SB	1201	C	2.5
47	L25B	149	SER	2.5
2	S2A	160	ASP	2.5
24	ESIB	47	U	2.5
51	L30B	18	ASP	2.5
2	S2B	204	ASN	2.5
18	S18A	34	TYR	2.5
3	S3A	146	ALA	2.5
4	S4A	147	ALA	2.5
12	S12A	125	ALA	2.5
34	L9B	118	LYS	2.5
36	L14A	109	LYS	2.5
53	L32B	10	LYS	2.5
4	S4A	112	VAL	2.5
4	S4A	198	VAL	2.5
19	S19A	51	VAL	2.5
33	L6A	154	PRO	2.5
36	L14A	52	VAL	2.5
42	L20B	105	VAL	2.5
36	L14B	45	GLU	2.5
41	L19A	109	GLU	2.5
4	S4A	67	ILE	2.5
2	S2B	187	LEU	2.5
2	S2B	213	LEU	2.5
20	S20A	53	LEU	2.5
34	L9A	12	LEU	2.5
47	L25B	150	LEU	2.5
49	L28B	98	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
4	S4B	79	PHE	2.5
33	L6B	97	ARG	2.5
46	L24B	108	THR	2.5
24	ESIB	7	A	2.5
35	L13B	42	TRP	2.5
52	L31A	17	GLY	2.5
52	L31A	66	SER	2.5
56	L35B	34	TRP	2.5
2	S2A	228	GLY	2.5
11	S11B	127	LYS	2.5
36	L14B	12	ASP	2.5
41	L19A	37	GLY	2.5
54	L33A	45	LYS	2.5
13	S13A	2	ALA	2.5
31	L4B	128	ALA	2.5
23	PSIA	45	U	2.5
27	23SB	2167	C	2.5
2	S2A	184	VAL	2.5
3	S3B	198	VAL	2.5
12	S12A	52	VAL	2.5
16	S16B	51	VAL	2.5
18	S18B	86	VAL	2.5
36	L14A	121	VAL	2.5
2	S2A	69	LEU	2.4
14	S14B	53	LEU	2.4
32	L5A	82	LEU	2.4
43	L21B	62	LEU	2.4
8	S8B	44	PHE	2.4
30	L3B	96	PHE	2.4
57	ASIB	5	G	2.4
13	S13A	116	THR	2.4
16	S16B	44	THR	2.4
54	L33B	33	LYS	2.4
2	S2B	97	TRP	2.4
4	S4B	167	GLY	2.4
33	L6A	82	GLY	2.4
34	L9B	124	GLY	2.4
47	L25A	147	GLY	2.4
4	S4A	83	SER	2.4
3	S3A	62	ASP	2.4
3	S3B	56	ASP	2.4
1	16SB	1071	A	2.4

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Mol	Chain	Res	Type	RSRZ
5	S5A	115	VAL	2.4
6	S6B	7	ASN	2.4
6	S6B	63	TYR	2.4
8	S8B	110	ALA	2.4
11	S11B	59	TYR	2.4
40	L18B	74	ALA	2.4
30	L3B	192	ASN	2.4
46	L24B	55	TYR	2.4
35	L13B	9	VAL	2.4
5	S5B	49	PRO	2.4
19	S19A	2	PRO	2.4
51	L30B	2	PRO	2.4
25	MRNA	57	U	2.4
1	16SB	1948	C	2.4
8	S8B	38	ILE	2.4
31	L4B	82	ILE	2.4
3	S3B	16	ARG	2.4
7	S7A	22	LEU	2.4
13	S13A	114	ARG	2.4
20	S20A	104	LEU	2.4
24	ESIB	17	C	2.4
27	23SA	935	C	2.4
30	L3A	195	LEU	2.4
33	L6A	127	GLU	2.4
47	L25A	70	LEU	2.4
54	L33A	12	GLU	2.4
2	S2B	122	PHE	2.4
10	S10A	62	HIS	2.4
19	S19A	32	LYS	2.4
35	L13A	130	HIS	2.4
49	L28B	96	LYS	2.4
3	S3B	67	THR	2.4
18	S18B	25	THR	2.4
3	S3A	158	GLY	2.4
7	S7A	133	GLY	2.4
7	S7A	40	ALA	2.4
11	S11A	99	GLN	2.4
20	S20A	66	ALA	2.4
49	L28A	77	ALA	2.4
2	S2B	136	VAL	2.4
3	S3B	20	SER	2.4
4	S4A	8	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
4	S4A	208	SER	2.4
12	S12B	36	VAL	2.4
21	THXA	21	TYR	2.4
27	23SB	1137	G	2.4
47	L25B	56	VAL	2.4
35	L13B	50	ASP	2.4
41	L19A	18	ASP	2.4
15	S15B	2	PRO	2.4
2	S2A	238	LEU	2.4
2	S2B	108	ILE	2.4
12	S12A	50	ARG	2.4
17	S17B	68	ARG	2.4
19	S19A	20	LEU	2.4
34	L9A	123	LEU	2.4
36	L14A	122	LEU	2.4
36	L14B	49	ARG	2.4
41	L19A	39	ARG	2.4
49	L28A	85	LEU	2.4
4	S4A	60	GLU	2.4
12	S12A	76	GLU	2.4
27	23SB	1225	A	2.4
27	23SB	2644	A	2.4
30	L3B	200	GLU	2.4
33	L6A	167	GLU	2.4
2	S2A	163	PHE	2.4
19	S19A	74	PHE	2.4
54	L33A	17	LYS	2.4
22	ASIA	43	C	2.4
27	23SA	2170	C	2.4
27	23SA	2817	C	2.4
3	S3A	197	GLY	2.4
4	S4A	183	GLY	2.4
6	S6B	20	ALA	2.4
16	S16B	48	TRP	2.4
52	L31A	70	GLY	2.4
5	S5B	67	VAL	2.4
10	S10A	94	VAL	2.4
11	S11A	93	GLN	2.4
33	L6A	143	GLN	2.4
40	L18A	84	GLN	2.4
43	L21A	33	VAL	2.4
2	S2B	33	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
4	S4A	20	TYR	2.4
6	S6B	12	PRO	2.4
8	S8B	57	PRO	2.4
33	L6A	117	PRO	2.4
33	L6B	173	PRO	2.4
34	L9B	111	PRO	2.4
35	L13B	11	PRO	2.4
2	S2A	215	LEU	2.4
4	S4A	186	LEU	2.4
5	S5B	101	ILE	2.4
9	S9A	128	ARG	2.4
19	S19A	12	ASP	2.4
20	S20A	24	LEU	2.4
33	L6A	60	ARG	2.4
35	L13B	97	ARG	2.4
41	L19B	58	ASN	2.4
54	L33B	11	LEU	2.4
54	L33B	26	ASN	2.4
5	S5B	122	GLU	2.4
8	S8B	77	GLU	2.4
22	ASIA	65	G	2.4
24	ESIA	69	G	2.4
27	23SB	557	G	2.4
54	L33B	35	GLU	2.4
22	ASIA	64	A	2.4
12	S12B	11	GLY	2.4
16	S16B	37	GLY	2.4
33	L6B	5	GLY	2.4
3	S3A	50	ALA	2.4
3	S3A	163	ALA	2.4
7	S7A	152	ALA	2.4
10	S10B	87	THR	2.4
12	S12B	64	THR	2.4
32	L5B	57	ALA	2.4
16	S16B	65	GLN	2.4
31	L4A	8	GLN	2.4
1	16SA	1671	C	2.4
28	5SB	93	C	2.4
2	S2B	51	LEU	2.4
3	S3B	91	LEU	2.4
5	S5B	142	LEU	2.4
10	S10B	98	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
13	S13A	9	ILE	2.4
13	S13A	39	ILE	2.4
15	S15B	82	ILE	2.4
31	L4B	10	PRO	2.4
32	L5A	3	LEU	2.4
33	L6A	173	PRO	2.4
16	S16B	11	SER	2.4
42	L20B	95	LEU	2.4
4	S4B	46	LYS	2.4
6	S6B	100	ASN	2.4
10	S10A	12	ASP	2.4
16	S16B	12	LYS	2.4
33	L6A	160	LYS	2.4
35	L13A	127	ASP	2.4
54	L33A	20	ASN	2.4
2	S2A	117	GLU	2.4
13	S13A	8	GLU	2.4
33	L6B	116	GLU	2.4
4	S4A	109	GLY	2.4
7	S7A	81	GLY	2.4
7	S7B	133	GLY	2.4
19	S19A	44	MET	2.4
33	L6B	135	GLY	2.4
41	L19B	37	GLY	2.4
48	L27B	6	GLY	2.4
3	S3B	180	ALA	2.4
15	S15A	30	ALA	2.4
35	L13B	124	ALA	2.4
42	L20B	96	ALA	2.4
16	S16B	20	VAL	2.4
35	L13B	14	VAL	2.4
1	16SA	743	G	2.4
1	16SA	1085	G	2.4
36	L14A	96	THR	2.4
11	S11A	12	ARG	2.4
16	S16B	76	GLN	2.4
27	23SB	6	A	2.4
27	23SB	1074	U	2.4
43	L21B	11	GLN	2.4
46	L24B	50	ARG	2.4
47	L25B	80	ARG	2.4
3	S3B	33	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
5	S5A	43	LEU	2.3
5	S5B	11	ILE	2.3
5	S5B	96	PRO	2.3
18	S18A	78	LEU	2.3
30	L3B	32	PRO	2.3
32	L5B	152	LEU	2.3
41	L19A	88	ILE	2.3
42	L20B	80	ILE	2.3
11	S11B	125	PHE	2.3
14	S14B	43	CYS	2.3
43	L21B	98	GLU	2.3
3	S3A	141	VAL	2.3
3	S3B	200	ALA	2.3
4	S4B	8	VAL	2.3
6	S6B	65	VAL	2.3
7	S7A	2	ALA	2.3
3	S3B	167	TRP	2.3
10	S10B	81	THR	2.3
12	S12A	16	ARG	2.3
12	S12A	58	THR	2.3
43	L21B	21	ARG	2.3
2	S2A	10	LEU	2.3
6	S6B	61	LEU	2.3
4	S4B	160	GLN	2.3
9	S9A	81	ILE	2.3
9	S9A	127	LYS	2.3
10	S10A	65	LEU	2.3
35	L13B	99	LEU	2.3
44	L22B	51	LEU	2.3
31	L4B	28	ILE	2.3
34	L9B	139	GLN	2.3
4	S4A	54	TYR	2.3
4	S4B	29	PRO	2.3
38	L16B	68	ILE	2.3
1	16SA	727	U	2.3
4	S4A	79	PHE	2.3
23	PSIA	69	G	2.3
24	ESIB	69	G	2.3
17	S17B	39	SER	2.3
47	L25B	66	SER	2.3
8	S8B	121	ASP	2.3
11	S11B	38	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
36	L14A	29	ASN	2.3
4	S4B	60	GLU	2.3
47	L25B	168	GLU	2.3
2	S2B	66	GLY	2.3
3	S3A	2	GLY	2.3
2	S2A	153	ARG	2.3
5	S5A	14	ARG	2.3
7	S7B	80	VAL	2.3
10	S10B	101	VAL	2.3
11	S11B	68	ALA	2.3
15	S15B	86	GLY	2.3
27	23SA	1124	C	2.3
27	23SA	2171	C	2.3
27	23SA	2492	C	2.3
27	23SA	2810	C	2.3
27	23SB	1148	C	2.3
33	L6B	145	ALA	2.3
35	L13B	49	GLY	2.3
15	S15B	88	ARG	2.3
30	L3B	199	ARG	2.3
33	L6A	95	ARG	2.3
42	L20B	100	VAL	2.3
2	S2B	44	LEU	2.3
3	S3A	18	TRP	2.3
3	S3A	91	LEU	2.3
3	S3B	47	LEU	2.3
4	S4A	196	LEU	2.3
5	S5B	98	THR	2.3
5	S5B	139	LEU	2.3
11	S11B	51	LYS	2.3
18	S18A	85	LEU	2.3
35	L13B	29	LYS	2.3
41	L19A	82	LEU	2.3
2	S2B	58	ILE	2.3
4	S4A	5	ILE	2.3
33	L6B	92	ILE	2.3
47	L25B	120	ILE	2.3
4	S4A	40	PRO	2.3
33	L6B	29	PRO	2.3
5	S5A	133	TYR	2.3
8	S8B	62	TYR	2.3
34	L9B	130	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
2	S2B	28	PHE	2.3
46	L24B	60	PHE	2.3
22	ASIA	50	U	2.3
4	S4B	145	GLU	2.3
7	S7B	73	MET	2.3
27	23SB	2823	A	2.3
19	S19A	78	ARG	2.3
29	L2B	28	GLU	2.3
35	L13B	39	ARG	2.3
37	L15B	74	GLU	2.3
2	S2A	99	GLY	2.3
3	S3A	171	GLY	2.3
3	S3B	195	VAL	2.3
4	S4A	149	ALA	2.3
6	S6B	49	ALA	2.3
7	S7B	39	ALA	2.3
8	S8B	28	ALA	2.3
12	S12A	63	VAL	2.3
12	S12B	87	VAL	2.3
30	L3A	193	GLY	2.3
31	L4B	22	ALA	2.3
49	L28B	53	VAL	2.3
2	S2A	169	LYS	2.3
4	S4A	166	LYS	2.3
19	S19A	14	HIS	2.3
19	S19B	88	LYS	2.3
22	ASIA	44	G	2.3
24	ESIA	5	G	2.3
29	L2B	38	LYS	2.3
30	L3A	97	LYS	2.3
34	L9B	112	LYS	2.3
35	L13B	121	LYS	2.3
36	L14B	59	LYS	2.3
54	L33B	25	LYS	2.3
2	S2A	58	ILE	2.3
18	S18B	75	ILE	2.3
4	S4B	89	THR	2.3
27	23SB	2165	C	2.3
6	S6B	94	GLN	2.3
30	L3B	54	GLN	2.3
30	L3B	62	PRO	2.3
47	L25B	134	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
10	S10A	11	PHE	2.3
12	S12B	66	TYR	2.3
31	L4B	7	TYR	2.3
7	S7A	149	ARG	2.3
3	S3A	99	VAL	2.3
3	S3B	113	ALA	2.3
4	S4A	80	GLU	2.3
5	S5B	34	VAL	2.3
6	S6B	37	VAL	2.3
10	S10B	59	SER	2.3
18	S18B	39	VAL	2.3
33	L6A	169	VAL	2.3
34	L9A	91	SER	2.3
4	S4B	22	LYS	2.3
9	S9A	110	GLU	2.3
12	S12B	60	GLY	2.3
16	S16B	50	LYS	2.3
16	S16B	63	GLY	2.3
52	L31A	50	VAL	2.3
4	S4A	125	HIS	2.3
4	S4B	11	LEU	2.3
13	S13B	90	LEU	2.3
35	L13B	128	HIS	2.3
38	L16B	79	LEU	2.3
43	L21B	25	LEU	2.3
4	S4B	173	TRP	2.3
8	S8B	138	TRP	2.3
14	S14A	27	CYS	2.3
16	S16A	48	TRP	2.3
13	S13B	103	THR	2.3
4	S4A	62	GLN	2.3
1	16SA	1105	G	2.3
1	16SA	1121	G	2.3
1	16SB	1064	G	2.3
27	23SA	1122	G	2.3
27	23SB	1199	C	2.3
27	23SB	2813	C	2.3
4	S4A	47	ARG	2.3
8	S8A	1	MET	2.3
3	S3B	116	VAL	2.3
4	S4B	56	VAL	2.3
19	S19B	45	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
31	L4A	126	VAL	2.3
34	L9B	121	LYS	2.3
41	L19A	33	LYS	2.3
7	S7B	83	ALA	2.3
19	S19B	82	GLY	2.3
33	L6A	156	ALA	2.3
33	L6B	75	ALA	2.3
36	L14A	103	ALA	2.3
42	L20B	116	ALA	2.3
52	L31B	33	VAL	2.3
16	S16A	37	GLY	2.3
33	L6B	82	GLY	2.3
45	L23B	94	GLY	2.3
49	L28A	84	GLY	2.3
2	S2A	84	GLU	2.3
2	S2B	69	LEU	2.3
4	S4A	94	LEU	2.3
8	S8B	107	LEU	2.3
18	S18B	38	GLU	2.3
20	S20B	104	LEU	2.3
32	L5B	60	LEU	2.3
34	L9A	58	LEU	2.3
37	L15B	148	LEU	2.3
52	L31A	37	SER	2.3
2	S2A	5	ILE	2.2
2	S2A	80	ILE	2.2
4	S4A	103	ASN	2.2
4	S4A	154	ASN	2.2
4	S4B	102	ASP	2.2
7	S7B	103	TRP	2.2
23	PSIA	20	U	2.2
9	S9A	64	THR	2.2
36	L14A	65	THR	2.2
47	L25B	83	PRO	2.2
11	S11B	25	TYR	2.2
33	L6B	83	TYR	2.2
5	S5A	25	ARG	2.2
6	S6B	77	ARG	2.2
13	S13A	11	ARG	2.2
33	L6B	23	ARG	2.2
56	L35A	46	ARG	2.2
30	L3A	1	MET	2.2

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Mol	Chain	Res	Type	RSRZ
33	L6A	41	MET	2.2
53	L32B	37	LYS	2.2
3	S3B	130	VAL	2.2
4	S4A	148	VAL	2.2
5	S5A	41	VAL	2.2
5	S5A	67	VAL	2.2
11	S11B	14	VAL	2.2
34	L9B	142	VAL	2.2
35	L13B	53	VAL	2.2
3	S3A	12	LEU	2.2
4	S4B	176	LEU	2.2
4	S4B	186	LEU	2.2
5	S5B	43	LEU	2.2
8	S8B	2	LEU	2.2
11	S11B	86	GLY	2.2
14	S14B	44	LEU	2.2
17	S17B	22	LEU	2.2
18	S18B	73	ALA	2.2
32	L5A	43	LEU	2.2
32	L5A	139	LEU	2.2
27	23SB	2816	G	2.2
46	L24A	110	GLU	2.2
10	S10B	13	HIS	2.2
42	L20B	62	ILE	2.2
2	S2B	24	TRP	2.2
42	L20B	97	ASP	2.2
2	S2B	17	PHE	2.2
4	S4B	39	PRO	2.2
3	S3A	118	GLN	2.2
4	S4A	35	ARG	2.2
6	S6B	86	ARG	2.2
7	S7A	154	TYR	2.2
7	S7B	136	LYS	2.2
11	S11A	70	LYS	2.2
13	S13A	87	TYR	2.2
27	23SA	2169	U	2.2
33	L6A	85	LYS	2.2
46	L24B	54	LYS	2.2
47	L25B	28	MET	2.2
3	S3A	173	VAL	2.2
19	S19B	41	VAL	2.2
19	S19B	60	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
42	L20B	63	VAL	2.2
1	16SA	696	A	2.2
1	16SA	791	A	2.2
1	16SA	1854	A	2.2
18	S18B	79	LEU	2.2
27	23SB	1094	A	2.2
33	L6A	105	LEU	2.2
51	L30B	8	LEU	2.2
4	S4B	143	GLY	2.2
11	S11B	52	GLY	2.2
18	S18A	77	GLY	2.2
40	L18A	109	GLY	2.2
46	L24B	104	GLY	2.2
5	S5A	118	ILE	2.2
31	L4A	206	ILE	2.2
6	S6B	42	GLU	2.2
43	L21B	23	GLU	2.2
3	S3A	69	HIS	2.2
2	S2A	235	SER	2.2
47	L25B	153	SER	2.2
2	S2A	195	ASP	2.2
3	S3B	63	ASN	2.2
4	S4A	7	PRO	2.2
5	S5A	96	PRO	2.2
5	S5B	65	ASN	2.2
7	S7A	93	PRO	2.2
27	23SA	698	C	2.2
43	L21B	16	PRO	2.2
43	L21B	29	PRO	2.2
1	16SB	652	G	2.2
1	16SB	1660	G	2.2
4	S4B	169	LYS	2.2
5	S5A	47	LYS	2.2
32	L5A	182	LYS	2.2
33	L6B	77	LYS	2.2
35	L13B	137	LYS	2.2
57	ASIB	69	G	2.2
4	S4B	207	TYR	2.2
16	S16A	39	TYR	2.2
43	L21B	81	TYR	2.2
54	L33B	13	CYS	2.2
3	S3B	55	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
4	S4A	17	VAL	2.2
6	S6B	90	VAL	2.2
12	S12B	40	VAL	2.2
16	S16A	79	VAL	2.2
31	L4B	126	VAL	2.2
33	L6B	79	VAL	2.2
36	L14A	58	VAL	2.2
4	S4B	194	LEU	2.2
31	L4B	20	LEU	2.2
33	L6A	98	LEU	2.2
34	L9A	6	LEU	2.2
34	L9B	116	LEU	2.2
42	L20B	98	LEU	2.2
3	S3A	53	ALA	2.2
11	S11B	74	ALA	2.2
13	S13A	42	ALA	2.2
25	MRNA	39	U	2.2
31	L4B	21	ALA	2.2
37	L15A	150	ALA	2.2
42	L20B	86	ALA	2.2
47	L25A	113	ALA	2.2
3	S3B	96	GLY	2.2
7	S7B	82	GLY	2.2
2	S2B	182	ILE	2.2
5	S5A	109	ILE	2.2
16	S16B	36	ILE	2.2
17	S17B	59	ILE	2.2
36	L14B	87	ILE	2.2
1	16SA	701	A	2.2
1	16SA	811	A	2.2
1	16SA	1049	A	2.2
2	S2A	12	GLU	2.2
3	S3B	166	GLU	2.2
4	S4B	200	GLU	2.2
15	S15B	26	GLU	2.2
47	L25A	119	GLU	2.2
2	S2A	144	ARG	2.2
3	S3A	10	PHE	2.2
10	S10B	19	SER	2.2
11	S11B	101	SER	2.2
29	L2A	262	ARG	2.2
33	L6B	155	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	S2A	179	LYS	2.2
16	S16B	3	LYS	2.2
33	L6A	29	PRO	2.2
34	L9B	119	PRO	2.2
36	L14B	48	PRO	2.2
47	L25B	78	LYS	2.2
47	L25B	158	PRO	2.2
36	L14B	13	ASN	2.2
1	16SB	1082	C	2.2
2	S2A	240	GLN	2.2
3	S3A	64	VAL	2.2
3	S3B	175	LEU	2.2
4	S4A	92	VAL	2.2
4	S4B	121	VAL	2.2
9	S9B	4	TYR	2.2
10	S10B	34	VAL	2.2
14	S14B	39	LEU	2.2
22	ASIA	67	C	2.2
32	L5B	138	GLN	2.2
47	L25B	165	VAL	2.2
2	S2A	13	ALA	2.2
2	S2B	29	ALA	2.2
5	S5B	94	ALA	2.2
4	S4B	183	GLY	2.2
35	L13B	125	GLY	2.2
47	L25A	143	GLY	2.2
27	23SB	1221	G	2.2
57	ASIB	65	G	2.2
1	16SA	984	U	2.2
4	S4B	98	GLU	2.2
6	S6B	66	GLU	2.2
5	S5A	9	LYS	2.2
5	S5A	26	PHE	2.2
10	S10A	45	ARG	2.2
11	S11B	54	ARG	2.2
42	L20B	112	ARG	2.2
49	L28B	93	GLU	2.2
12	S12A	14	LYS	2.2
18	S18B	88	LYS	2.2
42	L20B	114	LYS	2.2
35	L13B	13	TRP	2.2
1	16SA	2026	A	2.2

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Mol	Chain	Res	Type	RSRZ
24	ESIB	35	A	2.2
27	23SA	944	A	2.2
2	S2B	48	MET	2.2
2	S2B	107	THR	2.2
3	S3A	55	VAL	2.2
3	S3A	130	VAL	2.2
3	S3B	34	LEU	2.2
4	S4A	120	LEU	2.2
4	S4B	177	ASP	2.2
6	S6B	6	VAL	2.2
18	S18B	22	VAL	2.2
18	S18B	78	LEU	2.2
30	L3B	182	LEU	2.2
30	L3B	198	VAL	2.2
36	L14B	14	THR	2.2
41	L19B	78	LEU	2.2
43	L21B	32	THR	2.2
47	L25B	41	LEU	2.2
6	S6A	101	ALA	2.1
6	S6B	64	GLN	2.2
20	S20A	52	ALA	2.1
30	L3A	48	GLN	2.2
33	L6A	164	TYR	2.2
35	L13B	132	ALA	2.1
13	S13B	119	GLY	2.1
33	L6A	100	GLY	2.1
36	L14A	55	GLY	2.1
46	L24A	104	GLY	2.1
33	L6B	136	ILE	2.1
34	L9A	88	ILE	2.1
41	L19B	83	ILE	2.1
53	L32B	33	CYS	2.1
1	16SA	1058	C	2.1
33	L6A	97	ARG	2.1
35	L13B	134	ARG	2.1
5	S5A	57	LYS	2.1
13	S13B	120	LYS	2.1
46	L24B	46	LYS	2.1
47	L25A	88	PHE	2.1
47	L25B	156	LYS	2.1
3	S3A	166	GLU	2.1
5	S5A	8	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
36	L14B	54	GLU	2.1
1	16SA	1782	G	2.1
2	S2A	97	TRP	2.1
4	S4B	197	PRO	2.1
7	S7A	88	PRO	2.1
27	23SB	12	U	2.1
27	23SA	641	G	2.1
27	23SB	571	G	2.1
2	S2A	112	VAL	2.1
5	S5B	53	LEU	2.1
10	S10A	8	LEU	2.1
10	S10A	88	LEU	2.1
12	S12B	24	LEU	2.1
13	S13B	19	LEU	2.1
16	S16A	73	LEU	2.1
30	L3A	27	LEU	2.1
47	L25A	165	VAL	2.1
2	S2B	25	ASN	2.1
11	S11A	117	ASN	2.1
30	L3B	92	THR	2.1
50	L29B	47	ASN	2.1
2	S2A	60	ASP	2.1
2	S2B	177	ALA	2.1
3	S3B	50	ALA	2.1
1	16SA	1072	A	2.1
7	S7A	110	GLN	2.1
11	S11B	100	ALA	2.1
12	S12A	23	ALA	2.1
12	S12B	117	TYR	2.1
14	S14B	59	ALA	2.1
30	L3B	89	ASP	2.1
31	L4A	128	ALA	2.1
41	L19A	135	ALA	2.1
42	L20B	76	TYR	2.1
28	5SB	92	A	2.1
2	S2B	203	GLY	2.1
10	S10B	74	ILE	2.1
13	S13B	78	ILE	2.1
16	S16A	10	GLY	2.1
41	L19B	50	ILE	2.1
43	L21B	4	ILE	2.1
16	S16B	8	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
4	S4A	184	LYS	2.1
9	S9A	116	LYS	2.1
18	S18B	68	LYS	2.1
20	S20A	21	LYS	2.1
30	L3B	69	LYS	2.1
36	L14B	109	LYS	2.1
44	L22B	110	LYS	2.1
48	L27A	5	LYS	2.1
54	L33A	33	LYS	2.1
41	L19B	45	PHE	2.1
3	S3B	69	HIS	2.1
34	L9A	85	GLU	2.1
36	L14A	45	GLU	2.1
40	L18A	111	GLU	2.1
1	16SA	1076	C	2.1
3	S3A	7	PRO	2.1
11	S11B	113	PRO	2.1
16	S16B	15	PRO	2.1
23	PSIB	17	C	2.1
27	23SA	933	C	2.1
27	23SB	2759	C	2.1
33	L6A	118	PRO	2.1
46	L24B	56	PRO	2.1
7	S7B	22	LEU	2.1
8	S8A	112	LEU	2.1
31	L4B	140	LEU	2.1
33	L6B	71	LEU	2.1
47	L25B	144	LEU	2.1
49	L28A	94	LEU	2.1
4	S4A	140	VAL	2.1
5	S5A	32	VAL	2.1
12	S12A	33	VAL	2.1
53	L32A	57	VAL	2.1
24	ESIA	33	U	2.1
25	MRNA	44	U	2.1
27	23SA	2909	U	2.1
34	L9B	143	SER	2.1
20	S20B	52	ALA	2.1
33	L6B	106	THR	2.1
34	L9B	108	THR	2.1
41	L19B	5	ALA	2.1
43	L21B	7	THR	2.1

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Mol	Chain	Res	Type	RSRZ
4	S4B	129	ASN	2.1
6	S6B	13	ASN	2.1
4	S4A	42	GLN	2.1
5	S5A	56	GLN	2.1
1	16SA	1050	G	2.1
1	16SA	1106	G	2.1
1	16SB	687	G	2.1
6	S6B	83	ASP	2.1
11	S11A	110	ASP	2.1
30	L3B	26	ILE	2.1
27	23SA	932	G	2.1
30	L3B	83	ASP	2.1
31	L4B	55	GLY	2.1
41	L19A	7	ILE	2.1
43	L21B	70	ILE	2.1
43	L21B	101	GLY	2.1
50	L29A	50	ILE	2.1
4	S4A	57	ARG	2.1
7	S7A	137	LYS	2.1
12	S12B	56	ARG	2.1
20	S20B	38	LYS	2.1
21	THXA	25	LYS	2.1
29	L2B	5	LYS	2.1
33	L6A	77	LYS	2.1
37	L15B	46	LYS	2.1
3	S3B	10	PHE	2.1
5	S5B	84	PHE	2.1
24	ESIA	35	A	2.1
35	L13B	117	PHE	2.1
57	ASIB	7	A	2.1
2	S2B	12	GLU	2.1
3	S3B	44	GLU	2.1
4	S4A	179	GLU	2.1
5	S5A	155	GLU	2.1
5	S5A	12	LEU	2.1
5	S5B	93	PRO	2.1
11	S11A	98	LEU	2.1
11	S11B	39	PRO	2.1
36	L14A	112	MET	2.1
39	L17B	82	GLU	2.1
46	L24B	68	HIS	2.1
46	L24B	91	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
52	L31A	3	GLU	2.1
3	S3B	76	VAL	2.1
5	S5A	34	VAL	2.1
12	S12A	37	VAL	2.1
12	S12B	63	VAL	2.1
43	L21B	61	VAL	2.1
55	L34B	46	VAL	2.1
10	S10A	32	ALA	2.1
42	L20B	99	ALA	2.1
4	S4A	28	SER	2.1
4	S4B	175	SER	2.1
8	S8B	13	ILE	2.1
12	S12A	82	ILE	2.1
41	L19A	40	THR	2.1
41	L19B	62	THR	2.1
48	L27A	9	SER	2.1
1	16SA	810	U	2.1
2	S2B	99	GLY	2.1
3	S3B	48	TYR	2.1
3	S3B	185	GLY	2.1
2	S2B	110	GLN	2.1
3	S3A	110	ASN	2.1
15	S15A	48	LYS	2.1
18	S18B	41	LYS	2.1
24	ESIB	16	U	2.1
47	L25B	48	PHE	2.1
2	S2A	138	LEU	2.1
2	S2A	202	PRO	2.1
4	S4B	37	PRO	2.1
8	S8A	72	PRO	2.1
8	S8B	63	LEU	2.1
10	S10A	85	LEU	2.1
12	S12B	22	PRO	2.1
13	S13B	10	PRO	2.1
14	S14A	6	LEU	2.1
27	23SB	2648	G	2.1
27	23SB	2903	G	2.1
30	L3B	181	LEU	2.1
30	L3B	34	VAL	2.1
32	L5B	35	GLU	2.1
33	L6A	111	HIS	2.1
35	L13B	86	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	16SA	1071	A	2.1
34	L9A	142	VAL	2.1
35	L13B	96	GLU	2.1
36	L14B	52	VAL	2.1
41	L19A	11	GLU	2.1
47	L25B	119	GLU	2.1
2	S2A	34	ALA	2.1
3	S3A	113	ALA	2.1
3	S3A	84	ILE	2.1
4	S4A	65	ARG	2.1
4	S4B	166	LYS	2.1
7	S7B	53	LYS	2.1
7	S7B	137	LYS	2.1
10	S10A	6	ILE	2.1
18	S18B	19	LYS	2.1
19	S19A	7	LYS	2.1
20	S20B	80	ARG	2.1
30	L3B	58	ARG	2.1
32	L5A	83	ARG	2.1
33	L6A	4	ILE	2.1
33	L6A	72	ILE	2.1
41	L19A	50	ILE	2.1
41	L19A	83	ILE	2.1
3	S3B	9	GLY	2.1
5	S5A	114	GLY	2.1
5	S5B	39	GLY	2.1
5	S5B	103	GLY	2.1
7	S7B	151	TYR	2.1
8	S8B	94	TYR	2.1
8	S8B	106	GLY	2.1
16	S16A	38	TYR	2.1
31	L4A	131	GLY	2.1
46	L24B	59	GLY	2.1
51	L30B	27	GLY	2.1
19	S19A	35	SER	2.1
43	L21B	73	SER	2.1
12	S12B	75	GLN	2.1
33	L6B	74	ASN	2.1
41	L19B	38	ASN	2.1
7	S7A	26	PHE	2.1
26	TRNA	11	C	2.1
26	TRNA	43	C	2.1

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Mol	Chain	Res	Type	RSRZ
25	MRNA	42	U	2.1
25	MRNB	57	U	2.1
30	L3A	89	ASP	2.1
31	L4B	197	ASP	2.1
33	L6A	171	LEU	2.1
2	S2A	230	VAL	2.1
2	S2B	219	VAL	2.1
9	S9A	44	VAL	2.1
10	S10B	94	VAL	2.1
12	S12B	15	VAL	2.1
13	S13A	113	PRO	2.1
33	L6A	35	VAL	2.1
51	L30B	56	VAL	2.1
7	S7A	103	TRP	2.0
14	S14A	24	CYS	2.1
30	L3A	40	GLU	2.1
34	L9A	135	GLU	2.1
4	S4A	59	ARG	2.0
4	S4B	3	ARG	2.0
4	S4B	63	LYS	2.0
4	S4B	168	ARG	2.0
8	S8A	134	ILE	2.0
11	S11B	97	ALA	2.0
12	S12B	17	LYS	2.0
12	S12B	43	LYS	2.0
12	S12B	97	ILE	2.0
13	S13A	75	ALA	2.0
33	L6B	25	LYS	2.0
34	L9A	82	ARG	2.0
34	L9A	97	ILE	2.0
46	L24B	75	ILE	2.0
47	L25A	120	ILE	2.0
49	L28A	92	LYS	2.0
1	16SA	1001	A	2.0
1	16SA	798	G	2.0
1	16SA	1051	G	2.0
1	16SB	1105	G	2.0
1	16SB	1509	G	2.0
4	S4A	95	GLY	2.0
4	S4B	109	GLY	2.0
18	S18B	48	GLY	2.0
19	S19B	84	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
27	23SA	939	A	2.0
27	23SA	2491	A	2.0
27	23SB	574	A	2.0
24	ESIA	65	G	2.0
27	23SA	928	G	2.0
27	23SB	576	G	2.0
53	L32B	52	TYR	2.0
2	S2A	95	GLN	2.0
4	S4B	83	SER	2.0
16	S16A	76	GLN	2.0
42	L20B	79	PHE	2.0
2	S2A	204	ASN	2.0
12	S12B	5	ASN	2.0
18	S18B	36	ASN	2.0
5	S5B	5	ASP	2.0
10	S10B	8	LEU	2.0
32	L5A	111	LEU	2.0
40	L18A	80	LEU	2.0
49	L28B	80	LEU	2.0
3	S3A	106	VAL	2.0
3	S3A	120	VAL	2.0
3	S3B	153	VAL	2.0
5	S5A	69	VAL	2.0
8	S8A	53	VAL	2.0
8	S8B	129	VAL	2.0
9	S9B	26	VAL	2.0
11	S11A	47	VAL	2.0
12	S12B	79	VAL	2.0
16	S16A	53	VAL	2.0
19	S19A	76	PRO	2.0
27	23SA	2165	C	2.0
30	L3B	98	PRO	2.0
36	L14A	115	VAL	2.0
47	L25B	58	VAL	2.0
47	L25B	128	VAL	2.0
51	L30B	36	VAL	2.0
1	16SA	2025	C	2.0
1	16SB	1731	C	2.0
11	S11B	22	HIS	2.0
12	S12A	96	HIS	2.0
2	S2B	179	LYS	2.0
3	S3B	38	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
7	S7A	32	ARG	2.0
12	S12A	20	LYS	2.0
12	S12A	43	LYS	2.0
12	S12A	110	ARG	2.0
12	S12B	38	ARG	2.0
18	S18B	55	ARG	2.0
31	L4B	127	GLU	2.0
33	L6B	13	LYS	2.0
33	L6B	101	ARG	2.0
46	L24B	4	LYS	2.0
3	S3A	100	ALA	2.0
3	S3B	146	ALA	2.0
4	S4B	164	ALA	2.0
8	S8B	135	CYS	2.0
10	S10A	98	ILE	2.0
11	S11A	61	ALA	2.0
11	S11B	19	ALA	2.0
14	S14A	40	CYS	2.0
33	L6A	121	ILE	2.0
48	L27A	2	ALA	2.0
32	L5B	134	GLY	2.0
3	S3A	201	TYR	2.0
3	S3B	201	TYR	2.0
8	S8B	48	TYR	2.0
34	L9A	78	THR	2.0
2	S2A	76	GLN	2.0
4	S4B	45	GLN	2.0
16	S16A	9	PHE	2.0
1	16SA	1052	A	2.0
2	S2A	192	SER	2.0
12	S12A	19	SER	2.0
22	ASIA	9	A	2.0
27	23SB	2814	A	2.0
34	L9A	5	LEU	2.0
34	L9B	128	LEU	2.0
41	L19A	31	SER	2.0
49	L28A	82	LEU	2.0
49	L28B	17	SER	2.0
32	L5A	40	ASN	2.0
34	L9A	74	ASN	2.0
47	L25A	1	MET	2.0
1	16SA	1120	G	2.0

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Mol	Chain	Res	Type	RSRZ
1	16SB	857	G	2.0
2	S2A	174	VAL	2.0
3	S3A	68	VAL	2.0
4	S4A	53	ASP	2.0
12	S12B	107	VAL	2.0
23	PSIA	6	G	2.0
24	ESIB	63	G	2.0
27	23SA	2811	G	2.0
31	L4A	6	VAL	2.0
33	L6B	52	VAL	2.0
34	L9B	145	VAL	2.0
44	L22B	50	VAL	2.0
47	L25A	96	VAL	2.0
51	L30B	59	VAL	2.0
20	S20A	98	PRO	2.0
38	L16B	39	PRO	2.0
4	S4B	25	ARG	2.0
15	S15B	68	ARG	2.0
33	L6B	51	ARG	2.0
35	L13B	21	LYS	2.0
2	S2B	170	GLU	2.0
3	S3A	35	GLU	2.0
4	S4A	145	GLU	2.0
4	S4A	163	GLU	2.0
7	S7B	74	GLU	2.0
7	S7B	139	GLU	2.0
1	16SA	726	U	2.0
1	16SB	1070	U	2.0
11	S11B	15	ALA	2.0
11	S11B	21	ILE	2.0
13	S13A	4	ILE	2.0
14	S14B	10	ALA	2.0
17	S17B	58	GLU	2.0
20	S20B	59	ALA	2.0
34	L9B	97	ILE	2.0
35	L13A	16	ILE	2.0
36	L14A	118	ALA	2.0
36	L14B	46	ALA	2.0
38	L16A	105	GLU	2.0
41	L19B	86	ILE	2.0
48	L27B	2	ALA	2.0
1	16SB	1728	C	2.0

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Mol	Chain	Res	Type	RSRZ
4	S4A	171	GLY	2.0
8	S8B	130	GLY	2.0
14	S14B	40	CYS	2.0
16	S16A	30	GLY	2.0
44	L22A	112	GLY	2.0
47	L25B	160	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
22	4SU	ASIA	8	20/21	0.49	0.18	200,201,209,209	0
26	PSU	TRNA	39	20/21	0.53	0.15	141,167,176,177	0
26	PSU	TRNA	55	20/21	0.53	0.12	140,149,172,173	0
22	PSU	ASIA	55	20/21	0.55	0.21	148,161,170,173	0
24	MIA	ESIB	37	29/30	0.55	0.24	133,151,155,159	0
26	PSU	TRNA	32	20/21	0.57	0.12	180,186,193,193	0
57	5MU	ASIB	54	21/22	0.60	0.16	149,182,188,190	0
23	3AU	PSIB	47	27/28	0.61	0.16	125,144,154,157	0
26	MIA	TRNA	37	29/30	0.63	0.21	115,137,156,159	0
26	5MU	TRNA	54	21/22	0.64	0.13	150,157,163,165	0
23	PSU	PSIB	55	20/21	0.68	0.14	93,105,114,116	0
26	4SU	TRNA	8	20/21	0.70	0.14	169,173,178,179	0
23	5MU	PSIB	54	21/22	0.73	0.16	99,107,116,124	0
22	5MU	ASIA	54	21/22	0.75	0.23	116,137,145,147	0
1	2MG	16SB	1834	24/25	0.77	0.12	112,121,124,134	0
12	0TD	S12B	89	10/11	0.78	0.17	80,85,98,103	0
24	MIA	ESIA	37	29/30	0.78	0.19	119,144,147,154	0
22	7MG	ASIA	46	24/25	0.79	0.18	199,203,213,220	0
57	PSU	ASIB	39	20/21	0.80	0.14	100,119,125,126	0
23	7MG	PSIB	46	24/25	0.80	0.11	110,121,137,139	0
1	5MC	16SB	1590	21/22	0.82	0.13	78,90,100,102	0
23	PSU	PSIA	55	20/21	0.83	0.11	82,88,107,108	0
23	3AU	PSIA	47	27/28	0.83	0.19	93,118,131,133	0
1	7MG	16SB	1156	24/25	0.84	0.15	72,84,99,102	0
1	M2G	16SB	1589	25/26	0.84	0.13	80,89,97,102	0
27	5MU	23SB	1940	21/22	0.84	0.13	76,89,106,108	0
23	PSU	PSIB	32	20/21	0.84	0.12	81,89,102,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	7MG	PSIA	46	24/25	0.84	0.14	79,89,111,120	0
23	4SU	PSIB	8	20/21	0.85	0.09	97,105,114,118	0
1	PSU	16SB	1145	20/21	0.85	0.11	81,88,98,101	0
57	PSU	ASIB	32	20/21	0.86	0.09	111,122,129,131	0
1	PSU	16SA	1145	20/21	0.86	0.16	63,74,87,89	0
23	5MU	PSIA	54	21/22	0.86	0.13	84,91,100,102	0
1	2MG	16SA	1834	24/25	0.87	0.12	77,82,89,99	0
27	PSU	23SB	1942	20/21	0.87	0.13	75,81,94,96	0
12	0TD	S12A	89	10/11	0.87	0.17	62,66,74,84	0
1	5MC	16SB	2028	21/22	0.87	0.12	77,87,91,96	0
23	PSU	PSIB	39	20/21	0.87	0.12	77,85,90,93	0
22	PSU	ASIA	32	20/21	0.88	0.17	84,89,99,100	0
23	MIA	PSIB	37	29/30	0.88	0.14	78,86,101,106	0
23	PSU	PSIA	32	20/21	0.89	0.12	61,71,78,79	0
22	PSU	ASIA	39	20/21	0.90	0.15	75,89,94,96	0
1	5MC	16SB	2032	21/22	0.90	0.11	56,69,76,84	0
57	MIA	ASIB	37	29/30	0.91	0.12	90,101,110,111	0
1	4OC	16SB	2030	22/23	0.91	0.11	62,74,89,92	0
1	7MG	16SA	1156	24/25	0.91	0.16	49,65,74,86	0
27	PSU	23SB	1936	20/21	0.92	0.10	61,78,82,83	0
23	PSU	PSIA	39	20/21	0.92	0.12	59,63,73,76	0
1	UR3	16SB	2121	21/22	0.92	0.12	53,64,72,79	0
22	MIA	ASIA	37	29/30	0.92	0.15	55,69,76,81	0
1	5MC	16SB	2035	21/22	0.92	0.10	62,70,74,76	0
23	MIA	PSIA	37	29/30	0.92	0.15	58,65,82,85	0
23	4SU	PSIA	8	20/21	0.92	0.10	70,77,82,84	0
27	PSU	23SA	1936	20/21	0.93	0.13	52,56,64,70	0
27	OMC	23SB	1945	21/22	0.93	0.09	64,75,83,85	0
27	5MC	23SB	1987	21/22	0.93	0.10	54,62,74,81	0
1	5MC	16SA	1590	21/22	0.93	0.12	59,67,77,79	0
27	5MU	23SA	1940	21/22	0.93	0.13	54,67,75,85	0
1	5MC	16SA	2028	21/22	0.93	0.12	47,64,70,72	0
27	PSU	23SA	1942	20/21	0.93	0.14	55,63,77,83	0
27	OMG	23SB	2266	24/25	0.94	0.09	51,57,61,63	0
27	OMU	23SB	2567	21/22	0.94	0.12	51,62,71,79	0
1	M2G	16SA	1589	25/26	0.94	0.12	56,63,73,79	0
1	MA6	16SB	2141	24/25	0.94	0.10	61,71,81,82	0
27	5MC	23SA	1967	21/22	0.94	0.11	41,53,60,70	0
1	MA6	16SB	2142	24/25	0.94	0.10	57,70,78,87	0
27	OMC	23SA	1945	21/22	0.95	0.10	44,54,60,64	0
1	5MC	16SA	2032	21/22	0.95	0.12	46,52,59,63	0
27	PSU	23SB	2620	20/21	0.95	0.10	42,49,60,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
27	5MU	23SA	1964	21/22	0.95	0.09	33,41,49,56	0
1	UR3	16SA	2121	21/22	0.95	0.13	39,52,60,61	0
27	5MC	23SB	1967	21/22	0.95	0.10	56,70,78,86	0
1	5MC	16SA	2035	21/22	0.95	0.11	44,49,56,62	0
27	2MA	23SA	2518	23/24	0.96	0.09	32,39,49,56	0
27	2MA	23SB	2518	23/24	0.96	0.10	40,46,52,55	0
27	OMU	23SA	2567	21/22	0.96	0.10	41,47,53,68	0
1	MA6	16SA	2142	24/25	0.96	0.10	36,48,58,66	0
1	MA6	16SA	2141	24/25	0.96	0.10	41,48,53,58	0
27	5MC	23SA	1987	21/22	0.96	0.10	42,47,54,66	0
1	4OC	16SA	2030	22/23	0.96	0.11	49,57,64,71	0
27	OMG	23SA	2266	24/25	0.96	0.09	35,42,51,53	0
27	5MU	23SB	1964	21/22	0.96	0.08	48,56,63,67	0
27	PSU	23SA	2620	20/21	0.97	0.07	34,41,48,53	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	23SB	3121	1/1	0.11	0.22	105,105,105,105	0
59	K	23SA	3390	1/1	0.22	0.47	129,129,129,129	0
58	MG	23SB	3114	1/1	0.29	0.29	95,95,95,95	0
59	K	16SA	2319	1/1	0.30	0.24	109,109,109,109	0
58	MG	23SB	3111	1/1	0.35	0.22	97,97,97,97	0
58	MG	16SB	2235	1/1	0.36	0.18	142,142,142,142	0
59	K	16SA	2299	1/1	0.37	0.12	136,136,136,136	0
58	MG	16SB	2225[B]	1/1	0.38	0.38	67,67,67,67	1
58	MG	16SB	2225[A]	1/1	0.38	0.38	73,73,73,73	1
58	MG	16SB	2247	1/1	0.39	0.32	96,96,96,96	0
59	K	16SB	2297	1/1	0.39	0.17	125,125,125,125	0
58	MG	23SA	3034	1/1	0.43	0.20	79,79,79,79	0
59	K	23SB	3321	1/1	0.43	0.17	116,116,116,116	0
58	MG	16SB	2246	1/1	0.44	0.18	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	MG	16SA	2250	1/1	0.48	0.26	97,97,97,97	0
59	K	16SB	2286	1/1	0.48	0.17	135,135,135,135	0
59	K	16SA	2311	1/1	0.48	0.21	107,107,107,107	0
58	MG	16SA	2237	1/1	0.48	0.13	121,121,121,121	0
59	K	23SB	3300	1/1	0.49	0.14	122,122,122,122	0
59	K	23SB	3315	1/1	0.50	0.16	130,130,130,130	0
58	MG	16SB	2265	1/1	0.51	0.18	153,153,153,153	0
59	K	16SB	2316	1/1	0.52	0.18	105,105,105,105	0
58	MG	16SB	2240	1/1	0.53	0.35	90,90,90,90	0
58	MG	23SB	3219	1/1	0.53	0.25	110,110,110,110	0
59	K	23SB	3319	1/1	0.53	0.30	116,116,116,116	0
58	MG	23SA	3104	1/1	0.53	0.18	86,86,86,86	0
58	MG	16SA	2253	1/1	0.54	0.22	91,91,91,91	0
58	MG	23SB	3063[A]	1/1	0.54	0.38	57,57,57,57	1
58	MG	23SB	3063[B]	1/1	0.54	0.38	61,61,61,61	1
59	K	23SA	3434	1/1	0.56	0.13	120,120,120,120	0
58	MG	16SA	2217	1/1	0.57	0.42	80,80,80,80	0
58	MG	23SB	3013	1/1	0.57	0.20	90,90,90,90	0
58	MG	16SA	2243	1/1	0.57	0.33	84,84,84,84	0
58	MG	23SA	3116	1/1	0.57	0.20	87,87,87,87	0
58	MG	16SA	2222	1/1	0.58	0.19	94,94,94,94	0
58	MG	23SA	3102	1/1	0.58	0.32	84,84,84,84	0
59	K	23SB	3280	1/1	0.59	0.17	108,108,108,108	0
58	MG	23SA	3097	1/1	0.59	0.18	71,71,71,71	0
59	K	16SB	2292	1/1	0.59	0.16	126,126,126,126	0
59	K	16SA	2300	1/1	0.59	0.18	100,100,100,100	0
58	MG	16SA	2248	1/1	0.59	0.14	115,115,115,115	0
59	K	16SA	2336	1/1	0.60	0.14	120,120,120,120	0
58	MG	23SA	3117	1/1	0.60	0.35	72,72,72,72	0
58	MG	16SB	2270	1/1	0.61	0.19	68,68,68,68	0
58	MG	16SB	2204	1/1	0.61	0.33	101,101,101,101	0
59	K	23SB	3268	1/1	0.62	0.24	118,118,118,118	0
58	MG	16SB	2220	1/1	0.62	0.26	82,82,82,82	0
59	K	23SB	3242	1/1	0.63	0.15	124,124,124,124	0
58	MG	5SA	201	1/1	0.63	0.16	66,66,66,66	0
58	MG	23SA	3093	1/1	0.63	0.15	59,59,59,59	0
58	MG	16SA	2239	1/1	0.63	0.21	75,75,75,75	0
59	K	23SA	3341	1/1	0.63	0.13	111,111,111,111	0
58	MG	23SA	3138	1/1	0.63	0.12	76,76,76,76	0
59	K	16SB	2318	1/1	0.63	0.20	110,110,110,110	0
58	MG	16SB	2237	1/1	0.64	0.22	94,94,94,94	0
59	K	23SA	3421	1/1	0.64	0.14	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	MG	5SA	202	1/1	0.64	0.12	66,66,66,66	0
59	K	S20A	201	1/1	0.64	0.12	125,125,125,125	0
58	MG	16SB	2254	1/1	0.64	0.17	90,90,90,90	0
58	MG	16SB	2209	1/1	0.65	0.31	91,91,91,91	0
58	MG	23SA	3149	1/1	0.65	0.09	87,87,87,87	0
59	K	16SB	2302	1/1	0.65	0.16	129,129,129,129	0
58	MG	PSIB	102	1/1	0.65	0.36	93,93,93,93	0
58	MG	16SA	2231	1/1	0.66	0.31	65,65,65,65	0
58	MG	16SA	2244	1/1	0.66	0.15	99,99,99,99	0
58	MG	23SB	3110	1/1	0.66	0.29	81,81,81,81	0
58	MG	23SA	3241	1/1	0.66	0.17	49,49,49,49	0
58	MG	16SA	2240	1/1	0.66	0.18	88,88,88,88	0
58	MG	23SA	3162	1/1	0.67	0.10	93,93,93,93	0
58	MG	16SB	2233	1/1	0.67	0.29	90,90,90,90	0
58	MG	16SA	2269	1/1	0.67	0.12	144,144,144,144	0
58	MG	16SB	2283	1/1	0.68	0.16	127,127,127,127	0
58	MG	16SA	2235	1/1	0.68	0.13	98,98,98,98	0
58	MG	16SB	2212	1/1	0.68	0.22	95,95,95,95	0
59	K	23SB	3322	1/1	0.68	0.15	122,122,122,122	0
58	MG	16SB	2202	1/1	0.69	0.12	74,74,74,74	0
58	MG	23SB	3128	1/1	0.69	0.37	95,95,95,95	0
58	MG	23SB	3116	1/1	0.69	0.29	103,103,103,103	0
59	K	16SA	2302	1/1	0.70	0.15	111,111,111,111	0
58	MG	16SA	2212	1/1	0.70	0.34	85,85,85,85	0
58	MG	23SA	3172	1/1	0.70	0.14	60,60,60,60	0
58	MG	23SA	3178	1/1	0.70	0.20	88,88,88,88	0
58	MG	23SA	3121	1/1	0.70	0.26	85,85,85,85	0
58	MG	16SA	2233	1/1	0.70	0.24	92,92,92,92	0
59	K	23SA	3350	1/1	0.70	0.10	100,100,100,100	0
58	MG	23SB	3132	1/1	0.70	0.24	80,80,80,80	0
59	K	23SA	3409	1/1	0.70	0.16	100,100,100,100	0
58	MG	23SA	3144	1/1	0.70	0.14	86,86,86,86	0
58	MG	23SB	3068	1/1	0.70	0.26	84,84,84,84	0
58	MG	16SA	2228	1/1	0.70	0.30	71,71,71,71	0
59	K	16SB	2288	1/1	0.70	0.16	92,92,92,92	0
58	MG	23SB	3109	1/1	0.71	0.28	79,79,79,79	0
58	MG	16SB	2210	1/1	0.71	0.28	80,80,80,80	0
59	K	16SA	2331	1/1	0.71	0.14	98,98,98,98	0
58	MG	23SA	3157	1/1	0.71	0.15	83,83,83,83	0
58	MG	16SB	2282	1/1	0.71	0.13	114,114,114,114	0
58	MG	16SB	2238	1/1	0.71	0.27	85,85,85,85	0
58	MG	MRNA	101	1/1	0.71	0.14	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	MG	16SB	2244	1/1	0.71	0.12	99,99,99,99	0
58	MG	16SA	2220	1/1	0.71	0.29	66,66,66,66	0
58	MG	23SA	3148	1/1	0.71	0.18	79,79,79,79	0
58	MG	16SA	2241	1/1	0.71	0.13	102,102,102,102	0
58	MG	23SB	3077	1/1	0.71	0.32	77,77,77,77	0
58	MG	23SB	3084	1/1	0.71	0.39	77,77,77,77	0
59	K	L4B	301	1/1	0.71	0.14	118,118,118,118	0
58	MG	23SA	3163	1/1	0.72	0.24	80,80,80,80	0
59	K	23SA	3393	1/1	0.72	0.21	101,101,101,101	0
58	MG	23SA	3063	1/1	0.72	0.23	70,70,70,70	0
58	MG	16SA	2208	1/1	0.72	0.14	67,67,67,67	0
58	MG	L4A	301	1/1	0.72	0.11	60,60,60,60	0
58	MG	16SB	2226	1/1	0.72	0.34	77,77,77,77	0
58	MG	23SB	3053	1/1	0.72	0.21	80,80,80,80	0
58	MG	16SB	2216	1/1	0.73	0.16	86,86,86,86	0
59	K	16SA	2312	1/1	0.73	0.10	114,114,114,114	0
58	MG	16SB	2249	1/1	0.73	0.21	91,91,91,91	0
59	K	16SA	2320	1/1	0.73	0.19	123,123,123,123	0
59	K	23SB	3275	1/1	0.73	0.18	104,104,104,104	0
58	MG	23SA	3168	1/1	0.73	0.22	85,85,85,85	0
59	K	16SA	2292	1/1	0.73	0.17	103,103,103,103	0
58	MG	23SA	3015	1/1	0.73	0.42	85,85,85,85	0
59	K	16SB	2289	1/1	0.73	0.25	109,109,109,109	0
58	MG	23SA	3112	1/1	0.73	0.25	74,74,74,74	0
59	K	23SA	3342	1/1	0.73	0.14	95,95,95,95	0
58	MG	23SB	3087	1/1	0.73	0.41	77,77,77,77	0
59	K	L16B	201	1/1	0.73	0.11	108,108,108,108	0
60	OHX	23SB	3497	7/7	0.73	0.14	159,164,168,271	0
58	MG	23SB	3041	1/1	0.74	0.25	64,64,64,64	0
58	MG	23SB	3108	1/1	0.74	0.14	76,76,76,76	0
58	MG	16SA	2261	1/1	0.74	0.15	97,97,97,97	0
58	MG	23SB	3059	1/1	0.74	0.18	74,74,74,74	0
59	K	23SB	3317	1/1	0.74	0.10	102,102,102,102	0
58	MG	16SB	2248	1/1	0.74	0.44	79,79,79,79	0
58	MG	16SB	2243	1/1	0.74	0.30	73,73,73,73	0
58	MG	23SB	3064	1/1	0.74	0.34	57,57,57,57	0
58	MG	S5B	202	1/1	0.74	0.17	93,93,93,93	0
58	MG	23SA	3324	1/1	0.74	0.28	111,111,111,111	0
60	OHX	23SB	3388	7/7	0.74	0.19	91,102,118,203	0
58	MG	16SB	2214	1/1	0.74	0.37	67,67,67,67	0
59	K	16SA	2321	1/1	0.75	0.18	105,105,105,105	0
59	K	23SA	3427	1/1	0.75	0.15	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	K	23SA	3428	1/1	0.75	0.12	114,114,114,114	0
58	MG	16SA	2234	1/1	0.75	0.26	75,75,75,75	0
59	K	S13B	201	1/1	0.75	0.11	137,137,137,137	0
59	K	S20B	201	1/1	0.75	0.13	119,119,119,119	0
59	K	23SA	3351	1/1	0.75	0.17	86,86,86,86	0
58	MG	16SA	2256	1/1	0.75	0.21	93,93,93,93	0
60	OHX	16SA	2407	7/7	0.75	0.12	136,147,163,250	0
60	OHX	16SB	2383	7/7	0.75	0.12	141,154,160,266	0
58	MG	23SA	3130	1/1	0.75	0.13	62,62,62,62	0
58	MG	23SA	3080	1/1	0.75	0.16	87,87,87,87	0
58	MG	5SB	201	1/1	0.76	0.15	89,89,89,89	0
58	MG	16SA	2247	1/1	0.76	0.27	74,74,74,74	0
58	MG	S4A	301	1/1	0.76	0.12	109,109,109,109	0
59	K	23SB	3303	1/1	0.76	0.14	95,95,95,95	0
58	MG	23SA	3139	1/1	0.76	0.13	59,59,59,59	0
58	MG	16SB	2217	1/1	0.76	0.36	71,71,71,71	0
58	MG	16SA	2255	1/1	0.76	0.28	65,65,65,65	0
59	K	16SB	2305	1/1	0.76	0.11	93,93,93,93	0
58	MG	23SA	3100	1/1	0.76	0.17	93,93,93,93	0
58	MG	23SB	3117	1/1	0.76	0.18	75,75,75,75	0
58	MG	23SA	3175	1/1	0.76	0.18	74,74,74,74	0
58	MG	23SA	3065	1/1	0.76	0.19	72,72,72,72	0
58	MG	23SA	3150	1/1	0.76	0.31	74,74,74,74	0
59	K	23SB	3247	1/1	0.76	0.10	108,108,108,108	0
58	MG	23SB	3038	1/1	0.76	0.30	81,81,81,81	0
58	MG	23SA	3110	1/1	0.77	0.23	64,64,64,64	0
59	K	23SA	3360	1/1	0.77	0.12	90,90,90,90	0
58	MG	23SA	3153	1/1	0.77	0.32	79,79,79,79	0
59	K	23SB	3311	1/1	0.77	0.33	108,108,108,108	0
58	MG	23SB	3058	1/1	0.77	0.21	64,64,64,64	0
58	MG	23SA	3311	1/1	0.77	0.14	104,104,104,104	0
58	MG	16SB	2203	1/1	0.77	0.25	70,70,70,70	0
59	K	S4B	301	1/1	0.77	0.25	101,101,101,101	0
58	MG	23SA	3111	1/1	0.77	0.24	111,111,111,111	0
58	MG	16SB	2206	1/1	0.77	0.17	81,81,81,81	0
59	K	L5B	202	1/1	0.77	0.11	127,127,127,127	0
59	K	23SB	3241	1/1	0.77	0.12	96,96,96,96	0
58	MG	16SB	2252	1/1	0.77	0.13	98,98,98,98	0
58	MG	23SA	3050	1/1	0.77	0.23	64,64,64,64	0
59	K	23SA	3345	1/1	0.77	0.15	104,104,104,104	0
60	OHX	23SB	3448	7/7	0.77	0.14	108,113,129,237	0
58	MG	23SB	3120	1/1	0.77	0.15	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
59	K	23SA	3346	1/1	0.78	0.16	108,108,108,108	0
58	MG	5SA	203	1/1	0.78	0.29	82,82,82,82	0
58	MG	23SA	3328	1/1	0.78	0.09	110,110,110,110	0
59	K	23SA	3352	1/1	0.78	0.20	80,80,80,80	0
58	MG	16SB	2201	1/1	0.78	0.25	69,69,69,69	0
58	MG	16SB	2236	1/1	0.78	0.31	82,82,82,82	0
58	MG	23SA	3166	1/1	0.78	0.33	67,67,67,67	0
58	MG	16SB	2211	1/1	0.78	0.18	87,87,87,87	0
60	OHX	23SA	3560	7/7	0.78	0.14	60,91,113,235	0
60	OHX	23SA	3600	7/7	0.78	0.12	122,125,155,245	0
58	MG	23SB	3099	1/1	0.78	0.15	81,81,81,81	0
58	MG	23SB	3105	1/1	0.78	0.13	76,76,76,76	0
59	K	16SB	2321	1/1	0.78	0.11	101,101,101,101	0
58	MG	23SA	3072	1/1	0.78	0.26	91,91,91,91	0
58	MG	23SA	3089	1/1	0.79	0.10	60,60,60,60	0
59	K	23SA	3413	1/1	0.79	0.21	97,97,97,97	0
59	K	23SB	3274	1/1	0.79	0.12	114,114,114,114	0
58	MG	16SB	2266	1/1	0.79	0.13	113,113,113,113	0
58	MG	16SA	2252	1/1	0.79	0.35	72,72,72,72	0
58	MG	16SB	2273	1/1	0.79	0.12	70,70,70,70	0
59	K	16SA	2322	1/1	0.79	0.15	92,92,92,92	0
59	K	23SB	3304	1/1	0.79	0.12	98,98,98,98	0
58	MG	23SA	3096	1/1	0.79	0.19	66,66,66,66	0
59	K	23SB	3313	1/1	0.79	0.12	126,126,126,126	0
58	MG	16SB	2219	1/1	0.79	0.23	81,81,81,81	0
58	MG	23SA	3017	1/1	0.79	0.15	90,90,90,90	0
58	MG	23SB	3169	1/1	0.79	0.12	57,57,57,57	0
58	MG	23SA	3031	1/1	0.79	0.25	65,65,65,65	0
58	MG	23SB	3003	1/1	0.79	0.29	71,71,71,71	0
58	MG	L5B	201	1/1	0.79	0.12	123,123,123,123	0
59	K	16SB	2311	1/1	0.79	0.14	107,107,107,107	0
58	MG	23SA	3124	1/1	0.79	0.21	78,78,78,78	0
58	MG	23SA	3128	1/1	0.79	0.25	98,98,98,98	0
58	MG	16SA	2245	1/1	0.79	0.22	70,70,70,70	0
59	K	23SA	3357	1/1	0.79	0.11	94,94,94,94	0
60	OHX	23SA	3603	7/7	0.79	0.13	141,147,166,236	0
60	OHX	16SB	2359	7/7	0.79	0.13	119,129,145,253	0
58	MG	23SA	3037	1/1	0.79	0.22	89,89,89,89	0
59	K	16SA	2307	1/1	0.79	0.15	75,75,75,75	0
58	MG	23SA	3087	1/1	0.79	0.10	73,73,73,73	0
59	K	23SA	3404	1/1	0.79	0.10	73,73,73,73	0
58	MG	23SA	3020	1/1	0.80	0.23	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
59	K	23SB	3282	1/1	0.80	0.20	81,81,81,81	0
59	K	23SB	3295	1/1	0.80	0.17	98,98,98,98	0
59	K	PSIA	104	1/1	0.80	0.16	98,98,98,98	0
59	K	23SB	3301	1/1	0.80	0.11	88,88,88,88	0
59	K	L5A	302	1/1	0.80	0.14	102,102,102,102	0
59	K	23SA	3336	1/1	0.80	0.11	120,120,120,120	0
58	MG	16SB	2245	1/1	0.80	0.15	93,93,93,93	0
59	K	16SA	2293	1/1	0.80	0.11	102,102,102,102	0
59	K	23SB	3314	1/1	0.80	0.13	75,75,75,75	0
59	K	16SA	2295	1/1	0.80	0.14	108,108,108,108	0
58	MG	16SB	2269	1/1	0.80	0.11	105,105,105,105	0
59	K	23SA	3349	1/1	0.80	0.31	103,103,103,103	0
58	MG	23SB	3080	1/1	0.80	0.24	85,85,85,85	0
58	MG	23SA	3217	1/1	0.80	0.14	66,66,66,66	0
58	MG	23SB	3119	1/1	0.80	0.28	91,91,91,91	0
58	MG	23SA	3107	1/1	0.80	0.34	85,85,85,85	0
58	MG	23SA	3280	1/1	0.80	0.13	84,84,84,84	0
59	K	23SA	3381	1/1	0.80	0.10	94,94,94,94	0
60	OHX	23SA	3512	7/7	0.80	0.14	128,135,145,228	0
59	K	23SA	3387	1/1	0.80	0.13	64,64,64,64	0
58	MG	23SB	3103	1/1	0.80	0.22	75,75,75,75	0
58	MG	23SB	3104	1/1	0.80	0.32	89,89,89,89	0
58	MG	23SA	3098	1/1	0.80	0.31	65,65,65,65	0
58	MG	23SA	3085	1/1	0.80	0.07	77,77,77,77	0
58	MG	23SB	3220	1/1	0.80	0.20	45,45,45,45	0
59	K	16SA	2334	1/1	0.80	0.23	97,97,97,97	0
58	MG	23SA	3007	1/1	0.80	0.27	67,67,67,67	0
58	MG	L17A	201	1/1	0.81	0.22	89,89,89,89	0
58	MG	16SA	2287	1/1	0.81	0.11	100,100,100,100	0
58	MG	23SA	3052	1/1	0.81	0.31	62,62,62,62	0
58	MG	16SB	2255	1/1	0.81	0.18	73,73,73,73	0
58	MG	23SA	3074	1/1	0.81	0.26	52,52,52,52	0
59	K	16SA	2330	1/1	0.81	0.12	100,100,100,100	0
59	K	16SB	2287	1/1	0.81	0.13	127,127,127,127	0
59	K	23SA	3356	1/1	0.81	0.21	89,89,89,89	0
58	MG	16SB	2231	1/1	0.81	0.22	87,87,87,87	0
59	K	23SA	3359	1/1	0.81	0.07	101,101,101,101	0
59	K	16SA	2333	1/1	0.81	0.25	99,99,99,99	0
58	MG	23SA	3060	1/1	0.81	0.23	80,80,80,80	0
58	MG	23SB	3046	1/1	0.81	0.27	50,50,50,50	0
60	OHX	23SA	3633	7/7	0.81	0.10	87,94,101,243	0
58	MG	16SB	2234	1/1	0.81	0.19	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
59	K	16SA	2301	1/1	0.81	0.20	115,115,115,115	0
60	OHX	16SB	2392	7/7	0.81	0.12	157,166,172,266	0
58	MG	23SA	3131	1/1	0.81	0.18	81,81,81,81	0
58	MG	16SB	2279	1/1	0.81	0.12	103,103,103,103	0
60	OHX	23SB	3485	7/7	0.81	0.12	145,151,159,232	0
58	MG	16SA	2219	1/1	0.81	0.25	65,65,65,65	0
59	K	23SB	3306	1/1	0.82	0.13	88,88,88,88	0
58	MG	16SA	2232	1/1	0.82	0.25	74,74,74,74	0
58	MG	16SB	2261	1/1	0.82	0.07	133,133,133,133	0
58	MG	23SA	3137	1/1	0.82	0.15	75,75,75,75	0
58	MG	23SB	3224	1/1	0.82	0.13	79,79,79,79	0
58	MG	16SB	2222	1/1	0.82	0.21	68,68,68,68	0
59	K	16SA	2332	1/1	0.82	0.18	94,94,94,94	0
58	MG	L2B	301	1/1	0.82	0.31	78,78,78,78	0
58	MG	16SB	2242	1/1	0.82	0.29	61,61,61,61	0
58	MG	23SA	3090	1/1	0.82	0.20	77,77,77,77	0
58	MG	23SA	3109	1/1	0.82	0.24	60,60,60,60	0
59	K	23SA	3407	1/1	0.82	0.09	112,112,112,112	0
60	OHX	16SA	2391	7/7	0.82	0.15	88,112,122,226	0
58	MG	23SA	3167	1/1	0.82	0.22	42,42,42,42	0
58	MG	16SB	2227	1/1	0.82	0.21	61,61,61,61	0
58	MG	23SA	3278	1/1	0.82	0.15	67,67,67,67	0
58	MG	16SB	2284	1/1	0.82	0.10	112,112,112,112	0
59	K	23SA	3343	1/1	0.82	0.40	110,110,110,110	0
60	OHX	23SA	3604	7/7	0.82	0.12	122,137,150,246	0
59	K	23SA	3430	1/1	0.82	0.17	112,112,112,112	0
58	MG	23SA	3143	1/1	0.82	0.21	44,44,44,44	0
60	OHX	16SB	2368	7/7	0.82	0.13	101,107,114,229	0
59	K	L3A	303	1/1	0.82	0.10	87,87,87,87	0
58	MG	L23A	101	1/1	0.82	0.12	57,57,57,57	0
60	OHX	S8B	201	7/7	0.82	0.10	133,155,169,246	0
59	K	23SA	3348	1/1	0.82	0.08	85,85,85,85	0
58	MG	23SB	3124	1/1	0.82	0.22	68,68,68,68	0
58	MG	23SA	3170	1/1	0.82	0.26	77,77,77,77	0
58	MG	23SA	3312	1/1	0.82	0.10	86,86,86,86	0
60	OHX	23SB	3508	7/7	0.82	0.11	163,169,177,258	0
60	OHX	23SB	3509	7/7	0.82	0.11	135,148,161,244	0
60	OHX	23SB	3510	7/7	0.82	0.10	144,156,172,247	0
58	MG	23SA	3127	1/1	0.83	0.16	67,67,67,67	0
58	MG	16SA	2279	1/1	0.83	0.14	84,84,84,84	0
59	K	16SB	2298	1/1	0.83	0.08	104,104,104,104	0
58	MG	16SB	2263	1/1	0.83	0.11	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
59	K	16SB	2304	1/1	0.83	0.10	96,96,96,96	0
58	MG	23SB	3147	1/1	0.83	0.16	56,56,56,56	0
58	MG	23SB	3094	1/1	0.83	0.31	62,62,62,62	0
59	K	16SA	2328	1/1	0.83	0.17	103,103,103,103	0
58	MG	23SB	3188	1/1	0.83	0.14	37,37,37,37	0
58	MG	23SB	3020	1/1	0.83	0.20	51,51,51,51	0
58	MG	23SB	3033	1/1	0.83	0.23	68,68,68,68	0
58	MG	16SA	2238	1/1	0.83	0.34	75,75,75,75	0
58	MG	23SB	3237	1/1	0.83	0.31	91,91,91,91	0
58	MG	16SA	2246	1/1	0.83	0.27	73,73,73,73	0
58	MG	16SA	2257	1/1	0.83	0.30	55,55,55,55	0
58	MG	23SA	3270	1/1	0.83	0.11	63,63,63,63	0
59	K	23SB	3252	1/1	0.83	0.18	84,84,84,84	0
58	MG	23SB	3054	1/1	0.83	0.09	71,71,71,71	0
58	MG	16SA	2249	1/1	0.83	0.35	72,72,72,72	0
59	K	16SA	2294	1/1	0.83	0.14	89,89,89,89	0
59	K	23SA	3432	1/1	0.83	0.12	93,93,93,93	0
60	OHX	16SB	2379	7/7	0.83	0.11	150,159,165,251	0
58	MG	23SA	3013	1/1	0.83	0.38	69,69,69,69	0
60	OHX	16SB	2385	7/7	0.83	0.12	160,164,166,249	0
59	K	23SB	3283	1/1	0.83	0.12	101,101,101,101	0
59	K	23SB	3291	1/1	0.83	0.10	76,76,76,76	0
59	K	23SB	3294	1/1	0.83	0.11	131,131,131,131	0
58	MG	23SB	3115	1/1	0.83	0.11	53,53,53,53	0
58	MG	16SA	2254	1/1	0.83	0.14	70,70,70,70	0
58	MG	16SA	2276	1/1	0.83	0.13	87,87,87,87	0
58	MG	16SB	2253	1/1	0.83	0.35	71,71,71,71	0
58	MG	S5B	201	1/1	0.83	0.28	69,69,69,69	0
58	MG	23SA	3126	1/1	0.83	0.14	61,61,61,61	0
60	OHX	5SB	214	7/7	0.83	0.12	126,136,154,239	0
59	K	23SB	3273	1/1	0.84	0.17	83,83,83,83	0
60	OHX	16SA	2376	7/7	0.84	0.13	99,103,107,223	0
58	MG	16SA	2201	1/1	0.84	0.26	72,72,72,72	0
58	MG	16SB	2230	1/1	0.84	0.24	68,68,68,68	0
58	MG	23SB	3081	1/1	0.84	0.14	54,54,54,54	0
58	MG	23SB	3045	1/1	0.84	0.27	45,45,45,45	0
60	OHX	23SA	3598	7/7	0.84	0.11	123,128,144,226	0
58	MG	16SA	2213	1/1	0.84	0.17	60,60,60,60	0
58	MG	23SA	3103	1/1	0.84	0.33	60,60,60,60	0
58	MG	PSIB	103	1/1	0.84	0.23	66,66,66,66	0
58	MG	23SB	3056	1/1	0.84	0.23	59,59,59,59	0
60	OHX	L28A	101	7/7	0.84	0.10	82,89,94,243	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	MG	23SA	3257	1/1	0.84	0.17	37,37,37,37	0
58	MG	23SB	3160	1/1	0.84	0.11	111,111,111,111	0
59	K	16SB	2315	1/1	0.84	0.15	122,122,122,122	0
58	MG	23SB	3006	1/1	0.84	0.34	54,54,54,54	0
59	K	23SA	3344	1/1	0.84	0.09	86,86,86,86	0
59	K	23SA	3422	1/1	0.84	0.09	75,75,75,75	0
58	MG	23SB	3177	1/1	0.84	0.13	57,57,57,57	0
58	MG	23SB	3062	1/1	0.84	0.17	67,67,67,67	0
58	MG	23SB	3199	1/1	0.84	0.19	79,79,79,79	0
60	OHX	23SB	3470	7/7	0.84	0.13	106,129,148,206	0
58	MG	16SA	2226	1/1	0.84	0.21	66,66,66,66	0
58	MG	23SA	3066	1/1	0.84	0.14	60,60,60,60	0
58	MG	23SB	3027	1/1	0.84	0.18	63,63,63,63	0
58	MG	16SA	2236	1/1	0.84	0.36	61,61,61,61	0
58	MG	23SB	3076	1/1	0.84	0.23	62,62,62,62	0
59	K	23SB	3272	1/1	0.84	0.15	111,111,111,111	0
59	K	23SA	3419	1/1	0.85	0.09	78,78,78,78	0
59	K	16SA	2296	1/1	0.85	0.12	93,93,93,93	0
59	K	23SA	3338	1/1	0.85	0.18	105,105,105,105	0
59	K	23SB	3245	1/1	0.85	0.13	81,81,81,81	0
59	K	16SA	2298	1/1	0.85	0.13	90,90,90,90	0
58	MG	23SB	3057	1/1	0.85	0.21	59,59,59,59	0
59	K	23SB	3254	1/1	0.85	0.12	65,65,65,65	0
58	MG	23SB	3133	1/1	0.85	0.20	83,83,83,83	0
60	OHX	23SA	3539	7/7	0.85	0.10	81,91,100,236	0
58	MG	23SA	3155	1/1	0.85	0.29	67,67,67,67	0
58	MG	23SA	3012	1/1	0.85	0.10	98,98,98,98	0
58	MG	23SA	3140	1/1	0.85	0.18	77,77,77,77	0
58	MG	16SA	2225	1/1	0.85	0.13	83,83,83,83	0
58	MG	L5A	301	1/1	0.85	0.25	71,71,71,71	0
58	MG	23SA	3114	1/1	0.85	0.23	65,65,65,65	0
58	MG	16SA	2202	1/1	0.85	0.24	64,64,64,64	0
59	K	23SB	3286	1/1	0.85	0.14	92,92,92,92	0
58	MG	23SB	3112	1/1	0.85	0.22	57,57,57,57	0
58	MG	23SB	3223	1/1	0.85	0.11	80,80,80,80	0
60	OHX	16SB	2382	7/7	0.85	0.12	143,150,162,242	0
59	K	16SB	2293	1/1	0.85	0.08	102,102,102,102	0
58	MG	23SB	3040	1/1	0.85	0.27	53,53,53,53	0
60	OHX	16SB	2388	7/7	0.85	0.12	111,113,150,236	0
59	K	23SA	3358	1/1	0.85	0.12	83,83,83,83	0
58	MG	23SA	3002	1/1	0.85	0.31	54,54,54,54	0
58	MG	23SA	3088	1/1	0.85	0.23	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	MG	16SA	2211	1/1	0.85	0.17	52,52,52,52	0
60	OHX	23SB	3461	7/7	0.85	0.09	112,118,121,252	0
58	MG	23SB	3082	1/1	0.85	0.23	77,77,77,77	0
58	MG	16SB	2239	1/1	0.85	0.13	97,97,97,97	0
59	K	16SA	2335	1/1	0.85	0.08	108,108,108,108	0
58	MG	23SB	3086	1/1	0.85	0.28	77,77,77,77	0
58	MG	23SA	3174	1/1	0.85	0.12	60,60,60,60	0
59	K	PSIA	103	1/1	0.85	0.10	84,84,84,84	0
60	OHX	23SB	3512	7/7	0.85	0.10	154,161,175,244	0
58	MG	23SA	3154	1/1	0.85	0.26	76,76,76,76	0
61	SJH	23SB	3323	83/83	0.85	0.19	50,50,50,50	0
58	MG	23SA	3129	1/1	0.86	0.17	54,54,54,54	0
59	K	23SB	3318	1/1	0.86	0.15	73,73,73,73	0
58	MG	23SA	3177	1/1	0.86	0.33	65,65,65,65	0
58	MG	23SB	3070	1/1	0.86	0.27	56,56,56,56	0
58	MG	23SB	3073	1/1	0.86	0.34	75,75,75,75	0
58	MG	16SB	2223	1/1	0.86	0.29	68,68,68,68	0
58	MG	23SA	3152	1/1	0.86	0.12	65,65,65,65	0
59	K	16SB	2319	1/1	0.86	0.23	84,84,84,84	0
59	K	23SA	3384	1/1	0.86	0.07	89,89,89,89	0
58	MG	23SA	3214	1/1	0.86	0.09	43,43,43,43	0
60	OHX	16SA	2399	7/7	0.86	0.11	162,172,178,247	0
59	K	16SA	2327	1/1	0.86	0.29	82,82,82,82	0
60	OHX	23SA	3511	7/7	0.86	0.12	129,155,160,239	0
59	K	23SA	3391	1/1	0.86	0.12	72,72,72,72	0
58	MG	16SB	2251	1/1	0.86	0.09	54,54,54,54	0
60	OHX	23SA	3559	7/7	0.86	0.09	106,114,120,233	0
58	MG	23SB	3016	1/1	0.86	0.25	42,42,42,42	0
58	MG	23SA	3070	1/1	0.86	0.21	72,72,72,72	0
58	MG	23SA	3230	1/1	0.86	0.14	114,114,114,114	0
58	MG	23SB	3031	1/1	0.86	0.28	69,69,69,69	0
59	K	23SA	3418	1/1	0.86	0.09	62,62,62,62	0
60	OHX	23SA	3613	7/7	0.86	0.12	100,119,125,217	0
60	OHX	23SA	3614	7/7	0.86	0.09	109,128,161,248	0
60	OHX	23SA	3628	7/7	0.86	0.10	149,156,162,258	0
59	K	23SB	3259	1/1	0.86	0.10	69,69,69,69	0
58	MG	16SB	2228	1/1	0.86	0.32	66,66,66,66	0
58	MG	23SA	3003	1/1	0.86	0.16	62,62,62,62	0
58	MG	23SB	3101	1/1	0.86	0.20	74,74,74,74	0
60	OHX	16SB	2372	7/7	0.86	0.11	94,114,129,214	0
60	OHX	16SB	2378	7/7	0.86	0.12	125,127,138,207	0
58	MG	23SA	3135	1/1	0.86	0.12	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	MG	16SB	2262	1/1	0.86	0.12	77,77,77,77	0
59	K	23SB	3278	1/1	0.86	0.25	82,82,82,82	0
58	MG	5SB	203	1/1	0.86	0.29	55,55,55,55	0
58	MG	16SA	2258	1/1	0.86	0.10	88,88,88,88	0
58	MG	16SB	2205	1/1	0.86	0.24	55,55,55,55	0
60	OHX	16SB	2396	7/7	0.86	0.11	118,139,162,230	0
59	K	23SA	3435	1/1	0.86	0.11	78,78,78,78	0
60	OHX	MRNB	101	7/7	0.86	0.11	140,145,154,244	0
58	MG	23SB	3052	1/1	0.86	0.34	56,56,56,56	0
58	MG	23SA	3009	1/1	0.86	0.21	51,51,51,51	0
58	MG	16SA	2286	1/1	0.86	0.10	98,98,98,98	0
58	MG	23SA	3300	1/1	0.86	0.09	65,65,65,65	0
58	MG	16SA	2204	1/1	0.86	0.20	56,56,56,56	0
58	MG	23SA	3141	1/1	0.86	0.22	69,69,69,69	0
58	MG	16SA	2229	1/1	0.86	0.18	48,48,48,48	0
58	MG	16SA	2272	1/1	0.86	0.12	56,56,56,56	0
58	MG	16SA	2223	1/1	0.86	0.18	69,69,69,69	0
58	MG	23SA	3024	1/1	0.86	0.16	53,53,53,53	0
60	OHX	23SB	3515	7/7	0.86	0.10	98,102,106,258	0
59	K	16SB	2299	1/1	0.86	0.10	84,84,84,84	0
59	K	16SA	2303	1/1	0.86	0.14	111,111,111,111	0
58	MG	23SB	3097	1/1	0.87	0.18	75,75,75,75	0
60	OHX	16SA	2400	7/7	0.87	0.10	131,143,159,239	0
60	OHX	16SA	2406	7/7	0.87	0.11	130,144,148,254	0
58	MG	23SA	3160	1/1	0.87	0.12	75,75,75,75	0
60	OHX	ASIA	102	7/7	0.87	0.12	99,122,129,226	0
59	K	23SB	3243	1/1	0.87	0.14	110,110,110,110	0
59	K	23SA	3415	1/1	0.87	0.09	91,91,91,91	0
58	MG	23SA	3033	1/1	0.87	0.15	78,78,78,78	0
58	MG	23SA	3263	1/1	0.87	0.10	45,45,45,45	0
58	MG	23SB	3229	1/1	0.87	0.15	94,94,94,94	0
58	MG	16SA	2267	1/1	0.87	0.11	102,102,102,102	0
58	MG	16SA	2210	1/1	0.87	0.36	53,53,53,53	0
58	MG	5SB	202	1/1	0.87	0.09	77,77,77,77	0
58	MG	23SA	3044	1/1	0.87	0.17	69,69,69,69	0
59	K	23SA	3431	1/1	0.87	0.07	70,70,70,70	0
58	MG	23SA	3283	1/1	0.87	0.12	39,39,39,39	0
58	MG	23SA	3285	1/1	0.87	0.14	42,42,42,42	0
58	MG	23SA	3291	1/1	0.87	0.11	60,60,60,60	0
58	MG	23SA	3077	1/1	0.87	0.23	57,57,57,57	0
58	MG	16SA	2227	1/1	0.87	0.32	67,67,67,67	0
58	MG	23SA	3171	1/1	0.87	0.08	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	K	23SB	3288	1/1	0.87	0.09	88,88,88,88	0
60	OHX	16SB	2375	7/7	0.87	0.12	112,129,142,222	0
58	MG	23SA	3081	1/1	0.87	0.14	59,59,59,59	0
58	MG	23SB	3065	1/1	0.87	0.14	59,59,59,59	0
60	OHX	16SB	2381	7/7	0.87	0.10	141,152,160,225	0
58	MG	23SA	3008	1/1	0.87	0.08	84,84,84,84	0
59	K	16SB	2291	1/1	0.87	0.23	85,85,85,85	0
58	MG	23SB	3069	1/1	0.87	0.21	67,67,67,67	0
58	MG	23SA	3055	1/1	0.87	0.30	62,62,62,62	0
58	MG	16SA	2275	1/1	0.87	0.13	58,58,58,58	0
60	OHX	16SB	2393	7/7	0.87	0.10	134,138,165,251	0
58	MG	23SB	3127	1/1	0.87	0.09	63,63,63,63	0
60	OHX	16SB	2398	7/7	0.87	0.09	93,103,110,241	0
59	K	23SB	3310	1/1	0.87	0.14	74,74,74,74	0
58	MG	23SA	3061	1/1	0.87	0.24	67,67,67,67	0
60	OHX	23SB	3358	7/7	0.87	0.15	54,81,112,155	0
58	MG	23SA	3029	1/1	0.87	0.17	45,45,45,45	0
58	MG	16SA	2230	1/1	0.87	0.20	68,68,68,68	0
60	OHX	23SB	3456	7/7	0.87	0.11	83,92,104,232	0
58	MG	23SA	3223	1/1	0.87	0.12	47,47,47,47	0
58	MG	23SB	3150	1/1	0.87	0.12	65,65,65,65	0
58	MG	23SA	3159	1/1	0.87	0.32	63,63,63,63	0
58	MG	23SB	3035	1/1	0.87	0.24	60,60,60,60	0
60	OHX	23SB	3506	7/7	0.87	0.10	150,165,174,249	0
59	K	16SA	2324	1/1	0.87	0.20	79,79,79,79	0
58	MG	L32A	101	1/1	0.87	0.14	68,68,68,68	0
58	MG	23SA	3239	1/1	0.87	0.15	35,35,35,35	0
60	OHX	23SB	3511	7/7	0.87	0.10	185,187,188,263	0
59	K	23SA	3399	1/1	0.87	0.15	79,79,79,79	0
59	K	S6B	201	1/1	0.87	0.16	97,97,97,97	0
58	MG	23SB	3192	1/1	0.87	0.13	59,59,59,59	0
58	MG	16SB	2232	1/1	0.87	0.31	69,69,69,69	0
58	MG	16SB	2285	1/1	0.88	0.10	91,91,91,91	0
59	K	23SA	3372	1/1	0.88	0.14	69,69,69,69	0
58	MG	23SB	3236	1/1	0.88	0.10	106,106,106,106	0
58	MG	16SB	2224	1/1	0.88	0.23	70,70,70,70	0
60	OHX	23SA	3608	7/7	0.88	0.10	152,160,170,242	0
58	MG	23SB	3051	1/1	0.88	0.25	46,46,46,46	0
58	MG	23SA	3123	1/1	0.88	0.24	78,78,78,78	0
60	OHX	23SA	3625	7/7	0.88	0.11	125,130,156,230	0
58	MG	16SB	2260	1/1	0.88	0.10	96,96,96,96	0
60	OHX	23SA	3631	7/7	0.88	0.10	97,104,111,227	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	MG	23SB	3123	1/1	0.88	0.31	61,61,61,61	0
60	OHX	5SA	213	7/7	0.88	0.11	75,92,112,197	0
59	K	16SB	2306	1/1	0.88	0.12	81,81,81,81	0
59	K	23SB	3302	1/1	0.88	0.10	91,91,91,91	0
60	OHX	16SB	2365	7/7	0.88	0.10	94,104,122,243	0
59	K	16SB	2308	1/1	0.88	0.10	105,105,105,105	0
59	K	23SA	3398	1/1	0.88	0.08	65,65,65,65	0
58	MG	16SA	2218	1/1	0.88	0.14	71,71,71,71	0
58	MG	23SA	3054	1/1	0.88	0.23	42,42,42,42	0
59	K	S13A	201	1/1	0.88	0.10	90,90,90,90	0
58	MG	23SA	3006	1/1	0.88	0.28	54,54,54,54	0
58	MG	23SB	3130	1/1	0.88	0.27	56,56,56,56	0
58	MG	23SA	3293	1/1	0.88	0.08	67,67,67,67	0
58	MG	23SA	3295	1/1	0.88	0.17	62,62,62,62	0
58	MG	23SB	3100	1/1	0.88	0.21	81,81,81,81	0
59	K	23SA	3339	1/1	0.88	0.12	113,113,113,113	0
58	MG	23SA	3169	1/1	0.88	0.22	87,87,87,87	0
58	MG	23SB	3158	1/1	0.88	0.10	72,72,72,72	0
58	MG	23SB	3022	1/1	0.88	0.14	46,46,46,46	0
58	MG	23SB	3164	1/1	0.88	0.13	63,63,63,63	0
58	MG	23SA	3189	1/1	0.88	0.13	51,51,51,51	0
58	MG	L35A	101	1/1	0.88	0.23	68,68,68,68	0
59	K	16SA	2310	1/1	0.88	0.07	79,79,79,79	0
60	OHX	23SB	3417	7/7	0.88	0.10	84,93,104,216	0
60	OHX	23SB	3441	7/7	0.88	0.11	80,90,114,205	0
58	MG	16SB	2276	1/1	0.88	0.09	104,104,104,104	0
60	OHX	23SB	3453	7/7	0.88	0.09	108,109,124,237	0
59	K	23SB	3264	1/1	0.88	0.12	84,84,84,84	0
60	OHX	23SB	3459	7/7	0.88	0.11	142,161,168,231	0
60	OHX	16SA	2404	7/7	0.88	0.11	156,159,166,251	0
60	OHX	23SB	3465	7/7	0.88	0.08	106,109,117,246	0
58	MG	23SA	3142	1/1	0.88	0.27	61,61,61,61	0
59	K	23SB	3271	1/1	0.88	0.22	85,85,85,85	0
59	K	16SA	2316	1/1	0.88	0.10	92,92,92,92	0
60	OHX	23SB	3498	7/7	0.88	0.11	110,121,148,223	0
60	OHX	23SB	3499	7/7	0.88	0.10	117,142,151,221	0
58	MG	23SA	3273	1/1	0.88	0.12	100,100,100,100	0
58	MG	23SA	3325	1/1	0.88	0.12	42,42,42,42	0
58	MG	23SB	3072	1/1	0.88	0.21	56,56,56,56	0
60	OHX	23SA	3552	7/7	0.88	0.10	94,98,103,214	0
60	OHX	23SA	3555	7/7	0.88	0.10	109,119,127,236	0
58	MG	23SA	3101	1/1	0.88	0.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	MG	23SB	3044	1/1	0.88	0.36	45,45,45,45	0
60	OHX	23SA	3564	7/7	0.88	0.10	75,83,93,207	0
60	OHX	23SA	3597	7/7	0.88	0.10	136,148,161,225	0
58	MG	23SA	3161	1/1	0.89	0.15	48,48,48,48	0
58	MG	23SB	3028	1/1	0.89	0.09	70,70,70,70	0
60	OHX	23SA	3622	7/7	0.89	0.10	128,144,153,225	0
58	MG	23SA	3334	1/1	0.89	0.11	65,65,65,65	0
58	MG	23SA	3113	1/1	0.89	0.08	59,59,59,59	0
58	MG	16SA	2221	1/1	0.89	0.26	59,59,59,59	0
59	K	16SB	2313	1/1	0.89	0.12	91,91,91,91	0
58	MG	16SB	2271	1/1	0.89	0.11	97,97,97,97	0
58	MG	23SA	3115	1/1	0.89	0.10	62,62,62,62	0
60	OHX	16SB	2348	7/7	0.89	0.10	112,114,120,229	0
60	OHX	16SB	2349	7/7	0.89	0.11	89,98,117,198	0
59	K	23SB	3312	1/1	0.89	0.07	89,89,89,89	0
59	K	23SA	3402	1/1	0.89	0.09	61,61,61,61	0
58	MG	16SA	2207	1/1	0.89	0.14	79,79,79,79	0
59	K	S6A	201	1/1	0.89	0.26	98,98,98,98	0
58	MG	16SA	2282	1/1	0.89	0.07	105,105,105,105	0
58	MG	23SB	3083	1/1	0.89	0.21	75,75,75,75	0
58	MG	16SA	2285	1/1	0.89	0.09	118,118,118,118	0
59	K	23SB	3320	1/1	0.89	0.14	82,82,82,82	0
58	MG	23SB	3129	1/1	0.89	0.22	56,56,56,56	0
58	MG	23SA	3005	1/1	0.89	0.20	57,57,57,57	0
59	K	L3B	303	1/1	0.89	0.11	98,98,98,98	0
59	K	23SA	3337	1/1	0.89	0.18	88,88,88,88	0
58	MG	23SA	3035	1/1	0.89	0.19	63,63,63,63	0
59	K	16SA	2297	1/1	0.89	0.19	95,95,95,95	0
60	OHX	16SB	2395	7/7	0.89	0.10	132,140,148,232	0
58	MG	L33A	101	1/1	0.89	0.26	87,87,87,87	0
60	OHX	16SA	2390	7/7	0.89	0.09	109,122,132,247	0
58	MG	23SB	3095	1/1	0.89	0.14	66,66,66,66	0
58	MG	23SA	3083	1/1	0.89	0.15	58,58,58,58	0
59	K	23SB	3258	1/1	0.89	0.07	58,58,58,58	0
58	MG	23SA	3084	1/1	0.89	0.16	46,46,46,46	0
60	OHX	23SB	3411	7/7	0.89	0.09	103,109,121,218	0
58	MG	23SA	3062	1/1	0.89	0.10	78,78,78,78	0
60	OHX	23SB	3421	7/7	0.89	0.09	93,96,114,233	0
60	OHX	23SB	3433	7/7	0.89	0.11	94,104,115,211	0
58	MG	16SA	2260	1/1	0.89	0.09	93,93,93,93	0
60	OHX	16SA	2409	7/7	0.89	0.10	123,137,158,221	0
58	MG	23SB	3165	1/1	0.89	0.10	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	23SB	3166	1/1	0.89	0.15	41,41,41,41	0
58	MG	23SA	3043	1/1	0.89	0.26	73,73,73,73	0
58	MG	23SB	3004	1/1	0.89	0.23	47,47,47,47	0
60	OHX	23SB	3462	7/7	0.89	0.09	100,106,116,237	0
60	OHX	23SA	3546	7/7	0.89	0.12	117,124,152,208	0
60	OHX	23SA	3550	7/7	0.89	0.09	97,104,114,218	0
60	OHX	23SB	3483	7/7	0.89	0.09	127,135,150,240	0
58	MG	23SA	3187	1/1	0.89	0.11	39,39,39,39	0
60	OHX	23SB	3493	7/7	0.89	0.09	123,130,149,234	0
59	K	23SA	3355	1/1	0.89	0.12	65,65,65,65	0
59	K	16SB	2290	1/1	0.89	0.07	112,112,112,112	0
58	MG	16SA	2205	1/1	0.89	0.28	54,54,54,54	0
60	OHX	23SB	3501	7/7	0.89	0.09	152,156,161,252	0
60	OHX	23SB	3503	7/7	0.89	0.09	126,131,152,227	0
58	MG	23SB	3193	1/1	0.89	0.10	70,70,70,70	0
60	OHX	23SA	3588	7/7	0.89	0.11	115,116,136,199	0
58	MG	23SA	3132	1/1	0.89	0.14	62,62,62,62	0
58	MG	23SA	3069	1/1	0.89	0.12	65,65,65,65	0
59	K	16SA	2323	1/1	0.89	0.08	75,75,75,75	0
58	MG	23SA	3091	1/1	0.89	0.18	53,53,53,53	0
58	MG	23SB	3025	1/1	0.89	0.17	61,61,61,61	0
60	OHX	23SA	3607	7/7	0.89	0.10	108,129,141,206	0
61	SJH	23SA	3436	83/83	0.89	0.14	50,50,50,50	0
59	K	23SB	3298	1/1	0.89	0.06	89,89,89,89	0
58	MG	16SB	2258	1/1	0.90	0.08	95,95,95,95	0
60	OHX	23SA	3616	7/7	0.90	0.10	180,184,189,253	0
58	MG	23SB	3010	1/1	0.90	0.34	52,52,52,52	0
58	MG	23SA	3125	1/1	0.90	0.11	59,59,59,59	0
58	MG	16SB	2208	1/1	0.90	0.14	74,74,74,74	0
58	MG	23SA	3036	1/1	0.90	0.18	64,64,64,64	0
58	MG	23SA	3218	1/1	0.90	0.14	59,59,59,59	0
58	MG	23SB	3023	1/1	0.90	0.26	66,66,66,66	0
58	MG	23SA	3092	1/1	0.90	0.18	61,61,61,61	0
59	K	16SB	2317	1/1	0.90	0.15	82,82,82,82	0
58	MG	23SA	3023	1/1	0.90	0.19	70,70,70,70	0
58	MG	23SA	3146	1/1	0.90	0.07	69,69,69,69	0
59	K	23SA	3408	1/1	0.90	0.07	76,76,76,76	0
58	MG	23SA	3041	1/1	0.90	0.16	60,60,60,60	0
58	MG	16SA	2288	1/1	0.90	0.10	88,88,88,88	0
59	K	23SA	3414	1/1	0.90	0.08	70,70,70,70	0
60	OHX	16SB	2376	7/7	0.90	0.12	99,115,127,194	0
58	MG	23SB	3034	1/1	0.90	0.22	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	K	23SB	3240	1/1	0.90	0.10	87,87,87,87	0
59	K	5SB	205	1/1	0.90	0.06	102,102,102,102	0
59	K	23SA	3416	1/1	0.90	0.07	79,79,79,79	0
58	MG	16SA	2214	1/1	0.90	0.40	54,54,54,54	0
60	OHX	16SB	2384	7/7	0.90	0.09	159,166,170,246	0
58	MG	23SB	3036	1/1	0.90	0.28	53,53,53,53	0
58	MG	23SA	3151	1/1	0.90	0.19	72,72,72,72	0
60	OHX	16SA	2356	7/7	0.90	0.11	115,120,125,207	0
59	K	23SB	3246	1/1	0.90	0.26	91,91,91,91	0
58	MG	16SB	2277	1/1	0.90	0.08	98,98,98,98	0
58	MG	23SB	3131	1/1	0.90	0.26	59,59,59,59	0
60	OHX	16SA	2392	7/7	0.90	0.10	110,128,151,224	0
58	MG	16SA	2251	1/1	0.90	0.35	59,59,59,59	0
60	OHX	ASIB	103	7/7	0.90	0.09	123,125,144,231	0
60	OHX	PSIB	105	7/7	0.90	0.09	144,155,165,240	0
60	OHX	PSIB	106	7/7	0.90	0.09	133,142,147,228	0
59	K	23SB	3256	1/1	0.90	0.12	69,69,69,69	0
60	OHX	16SA	2401	7/7	0.90	0.09	128,136,164,243	0
60	OHX	16SA	2402	7/7	0.90	0.10	138,140,154,213	0
58	MG	16SA	2273	1/1	0.90	0.09	69,69,69,69	0
60	OHX	16SA	2405	7/7	0.90	0.09	153,161,170,238	0
58	MG	23SB	3088	1/1	0.90	0.15	64,64,64,64	0
60	OHX	23SB	3426	7/7	0.90	0.08	106,114,129,238	0
60	OHX	23SB	3432	7/7	0.90	0.08	100,106,118,232	0
58	MG	23SA	3136	1/1	0.90	0.16	61,61,61,61	0
60	OHX	16SA	2408	7/7	0.90	0.08	162,169,175,253	0
58	MG	23SA	3019	1/1	0.90	0.12	38,38,38,38	0
60	OHX	16SA	2410	7/7	0.90	0.09	109,114,126,227	0
60	OHX	16SA	2414	7/7	0.90	0.09	101,104,112,212	0
59	K	23SB	3270	1/1	0.90	0.13	68,68,68,68	0
60	OHX	23SA	3478	7/7	0.90	0.11	68,79,105,167	0
58	MG	23SA	3071	1/1	0.90	0.26	74,74,74,74	0
59	K	16SA	2305	1/1	0.90	0.22	78,78,78,78	0
60	OHX	23SB	3469	7/7	0.90	0.12	114,120,138,183	0
60	OHX	23SA	3527	7/7	0.90	0.08	76,87,107,193	0
58	MG	23SB	3161	1/1	0.90	0.12	51,51,51,51	0
60	OHX	23SB	3484	7/7	0.90	0.10	122,131,158,229	0
59	K	L16A	201	1/1	0.90	0.14	89,89,89,89	0
58	MG	23SB	3098	1/1	0.90	0.20	67,67,67,67	0
60	OHX	23SB	3496	7/7	0.90	0.09	104,118,141,241	0
58	MG	16SA	2280	1/1	0.90	0.10	87,87,87,87	0
58	MG	23SA	3073	1/1	0.90	0.12	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	MG	PSIB	101	1/1	0.90	0.18	66,66,66,66	0
58	MG	23SB	3173	1/1	0.90	0.10	34,34,34,34	0
58	MG	23SB	3102	1/1	0.90	0.38	65,65,65,65	0
60	OHX	23SB	3504	7/7	0.90	0.08	137,145,154,245	0
60	OHX	23SB	3505	7/7	0.90	0.09	136,158,167,230	0
58	MG	23SA	3191	1/1	0.90	0.11	42,42,42,42	0
59	K	23SB	3289	1/1	0.90	0.07	79,79,79,79	0
59	K	23SB	3290	1/1	0.90	0.08	81,81,81,81	0
58	MG	16SB	2229	1/1	0.90	0.30	55,55,55,55	0
58	MG	23SA	3198	1/1	0.90	0.12	46,46,46,46	0
59	K	23SA	3367	1/1	0.90	0.10	57,57,57,57	0
60	OHX	23SB	3513	7/7	0.90	0.08	98,102,105,234	0
60	OHX	23SA	3605	7/7	0.90	0.12	111,117,144,211	0
59	K	23SB	3296	1/1	0.90	0.15	103,103,103,103	0
58	MG	23SA	3210	1/1	0.90	0.07	38,38,38,38	0
59	K	16SA	2326	1/1	0.90	0.06	80,80,80,80	0
59	K	23SB	3250	1/1	0.91	0.08	65,65,65,65	0
58	MG	23SB	3186	1/1	0.91	0.07	87,87,87,87	0
58	MG	23SB	3085	1/1	0.91	0.33	61,61,61,61	0
60	OHX	16SA	2361	7/7	0.91	0.10	116,140,162,226	0
60	OHX	16SA	2366	7/7	0.91	0.11	79,89,113,211	0
60	OHX	16SA	2368	7/7	0.91	0.10	76,97,115,198	0
60	OHX	16SB	2373	7/7	0.91	0.10	122,126,140,219	0
60	OHX	16SA	2369	7/7	0.91	0.11	92,97,108,196	0
58	MG	23SB	3002	1/1	0.91	0.23	65,65,65,65	0
60	OHX	16SA	2383	7/7	0.91	0.09	102,107,121,224	0
60	OHX	16SA	2385	7/7	0.91	0.10	122,136,150,215	0
58	MG	23SB	3118	1/1	0.91	0.19	80,80,80,80	0
59	K	16SA	2315	1/1	0.91	0.10	76,76,76,76	0
58	MG	23SA	3216	1/1	0.91	0.09	63,63,63,63	0
60	OHX	16SA	2397	7/7	0.91	0.09	154,160,167,245	0
59	K	5SA	208	1/1	0.91	0.08	81,81,81,81	0
59	K	23SB	3269	1/1	0.91	0.09	100,100,100,100	0
60	OHX	16SB	2391	7/7	0.91	0.09	122,127,148,225	0
59	K	16SA	2318	1/1	0.91	0.13	97,97,97,97	0
58	MG	16SB	2218	1/1	0.91	0.21	64,64,64,64	0
58	MG	23SB	3091	1/1	0.91	0.35	58,58,58,58	0
58	MG	23SB	3222	1/1	0.91	0.10	77,77,77,77	0
58	MG	23SB	3093	1/1	0.91	0.14	67,67,67,67	0
58	MG	23SA	3248	1/1	0.91	0.15	51,51,51,51	0
59	K	23SB	3276	1/1	0.91	0.07	65,65,65,65	0
58	MG	23SB	3008	1/1	0.91	0.11	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
59	K	23SA	3361	1/1	0.91	0.18	79,79,79,79	0
58	MG	23SB	3230	1/1	0.91	0.12	67,67,67,67	0
60	OHX	16SA	2415	7/7	0.91	0.09	125,133,149,248	0
58	MG	23SB	3235	1/1	0.91	0.11	109,109,109,109	0
58	MG	16SB	2280	1/1	0.91	0.07	104,104,104,104	0
60	OHX	23SA	3495	7/7	0.91	0.10	85,95,107,177	0
59	K	16SB	2294	1/1	0.91	0.06	109,109,109,109	0
58	MG	23SB	3066	1/1	0.91	0.27	57,57,57,57	0
60	OHX	23SA	3513	7/7	0.91	0.08	75,97,110,190	0
59	K	23SA	3385	1/1	0.91	0.23	74,74,74,74	0
60	OHX	23SB	3440	7/7	0.91	0.09	109,113,121,229	0
60	OHX	23SA	3529	7/7	0.91	0.09	81,94,113,196	0
60	OHX	23SA	3530	7/7	0.91	0.10	87,108,124,202	0
58	MG	23SA	3014	1/1	0.91	0.38	65,65,65,65	0
58	MG	23SB	3042	1/1	0.91	0.15	53,53,53,53	0
58	MG	23SB	3014	1/1	0.91	0.21	49,49,49,49	0
58	MG	23SA	3261	1/1	0.91	0.10	37,37,37,37	0
58	MG	L3B	302	1/1	0.91	0.10	45,45,45,45	0
60	OHX	23SB	3464	7/7	0.91	0.09	97,102,112,211	0
59	K	23SB	3299	1/1	0.91	0.10	56,56,56,56	0
58	MG	23SB	3018	1/1	0.91	0.08	47,47,47,47	0
59	K	23SA	3401	1/1	0.91	0.07	77,77,77,77	0
60	OHX	23SB	3472	7/7	0.91	0.09	132,136,154,230	0
60	OHX	23SB	3477	7/7	0.91	0.11	113,132,148,190	0
60	OHX	23SA	3576	7/7	0.91	0.09	75,83,109,209	0
58	MG	23SB	3075	1/1	0.91	0.33	63,63,63,63	0
58	MG	23SA	3156	1/1	0.91	0.21	59,59,59,59	0
58	MG	23SB	3106	1/1	0.91	0.15	87,87,87,87	0
58	MG	23SA	3027	1/1	0.91	0.14	38,38,38,38	0
58	MG	23SB	3079	1/1	0.91	0.17	51,51,51,51	0
58	MG	16SA	2224	1/1	0.91	0.20	36,36,36,36	0
58	MG	16SB	2213	1/1	0.91	0.21	72,72,72,72	0
60	OHX	23SA	3606	7/7	0.91	0.08	118,126,147,227	0
58	MG	23SA	3048	1/1	0.91	0.24	62,62,62,62	0
58	MG	16SB	2215	1/1	0.91	0.17	42,42,42,42	0
59	K	23SA	3340	1/1	0.91	0.09	84,84,84,84	0
58	MG	23SA	3279	1/1	0.91	0.06	99,99,99,99	0
58	MG	23SB	3181	1/1	0.91	0.09	53,53,53,53	0
58	MG	23SB	3183	1/1	0.91	0.09	65,65,65,65	0
59	K	23SA	3423	1/1	0.91	0.12	72,72,72,72	0
59	K	23SA	3424	1/1	0.91	0.22	100,100,100,100	0
59	K	23SB	3244	1/1	0.91	0.12	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
60	OHX	23SA	3632	7/7	0.91	0.08	79,85,98,239	0
59	K	23SA	3425	1/1	0.91	0.06	65,65,65,65	0
60	OHX	5SB	212	7/7	0.91	0.09	89,113,122,208	0
60	OHX	5SB	213	7/7	0.91	0.09	110,122,136,226	0
59	K	23SA	3426	1/1	0.91	0.12	102,102,102,102	0
60	OHX	5SA	218	7/7	0.91	0.08	138,150,160,226	0
58	MG	23SB	3184	1/1	0.91	0.08	71,71,71,71	0
58	MG	23SA	3158	1/1	0.92	0.20	39,39,39,39	0
60	OHX	16SB	2353	7/7	0.92	0.09	112,131,139,226	0
60	OHX	16SB	2355	7/7	0.92	0.09	110,116,123,197	0
58	MG	23SB	3055	1/1	0.92	0.27	56,56,56,56	0
60	OHX	16SB	2360	7/7	0.92	0.09	106,120,137,211	0
58	MG	16SA	2271	1/1	0.92	0.10	49,49,49,49	0
58	MG	23SB	3125	1/1	0.92	0.15	52,52,52,52	0
60	OHX	16SB	2371	7/7	0.92	0.08	95,106,111,208	0
58	MG	23SB	3092	1/1	0.92	0.15	83,83,83,83	0
59	K	23SA	3365	1/1	0.92	0.07	67,67,67,67	0
59	K	23SA	3366	1/1	0.92	0.07	48,48,48,48	0
58	MG	23SB	3227	1/1	0.92	0.17	63,63,63,63	0
58	MG	23SA	3079	1/1	0.92	0.34	66,66,66,66	0
60	OHX	16SA	2403	7/7	0.92	0.08	145,149,153,234	0
59	K	23SB	3277	1/1	0.92	0.10	78,78,78,78	0
58	MG	23SA	3067	1/1	0.92	0.28	71,71,71,71	0
59	K	23SA	3382	1/1	0.92	0.11	69,69,69,69	0
58	MG	23SA	3220	1/1	0.92	0.12	32,32,32,32	0
58	MG	23SA	3176	1/1	0.92	0.10	61,61,61,61	0
58	MG	16SB	2281	1/1	0.92	0.10	85,85,85,85	0
60	OHX	16SB	2389	7/7	0.92	0.09	118,137,157,208	0
60	OHX	16SB	2390	7/7	0.92	0.09	147,151,155,217	0
58	MG	16SB	2250	1/1	0.92	0.10	58,58,58,58	0
60	OHX	16SA	2411	7/7	0.92	0.08	196,200,203,282	0
58	MG	23SB	3138	1/1	0.92	0.10	41,41,41,41	0
60	OHX	16SB	2394	7/7	0.92	0.08	131,145,156,224	0
58	MG	23SA	3010	1/1	0.92	0.19	41,41,41,41	0
58	MG	L15A	202	1/1	0.92	0.08	62,62,62,62	0
60	OHX	16SB	2397	7/7	0.92	0.08	132,141,150,237	0
60	OHX	MRNA	102	7/7	0.92	0.11	105,114,119,213	0
60	OHX	16SB	2399	7/7	0.92	0.08	107,114,120,238	0
60	OHX	23SA	3470	7/7	0.92	0.13	46,51,99,161	0
58	MG	L3B	301	1/1	0.92	0.24	47,47,47,47	0
58	MG	23SA	3046	1/1	0.92	0.22	56,56,56,56	0
59	K	16SB	2307	1/1	0.92	0.09	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
59	K	23SB	3297	1/1	0.92	0.08	79,79,79,79	0
58	MG	23SA	3047	1/1	0.92	0.15	59,59,59,59	0
60	OHX	23SB	3385	7/7	0.92	0.10	87,99,111,177	0
59	K	16SB	2309	1/1	0.92	0.11	89,89,89,89	0
59	K	16SB	2310	1/1	0.92	0.26	96,96,96,96	0
59	K	23SA	3403	1/1	0.92	0.07	61,61,61,61	0
58	MG	L35B	102	1/1	0.92	0.21	89,89,89,89	0
59	K	16SA	2291	1/1	0.92	0.07	95,95,95,95	0
58	MG	23SA	3026	1/1	0.92	0.22	57,57,57,57	0
58	MG	23SA	3307	1/1	0.92	0.07	37,37,37,37	0
60	OHX	23SB	3438	7/7	0.92	0.10	118,134,139,208	0
59	K	23SB	3307	1/1	0.92	0.13	88,88,88,88	0
59	K	23SB	3309	1/1	0.92	0.08	71,71,71,71	0
60	OHX	23SB	3442	7/7	0.92	0.09	89,106,113,212	0
59	K	23SA	3410	1/1	0.92	0.07	73,73,73,73	0
59	K	23SA	3411	1/1	0.92	0.09	81,81,81,81	0
60	OHX	23SA	3570	7/7	0.92	0.09	133,152,161,233	0
58	MG	L34A	101	1/1	0.92	0.30	63,63,63,63	0
58	MG	23SB	3039	1/1	0.92	0.24	44,44,44,44	0
60	OHX	23SA	3590	7/7	0.92	0.08	141,152,157,234	0
60	OHX	23SB	3463	7/7	0.92	0.07	134,143,146,248	0
60	OHX	23SA	3591	7/7	0.92	0.08	99,119,144,202	0
60	OHX	23SA	3595	7/7	0.92	0.10	91,115,138,225	0
60	OHX	23SB	3466	7/7	0.92	0.09	104,123,142,206	0
58	MG	23SA	3190	1/1	0.92	0.12	89,89,89,89	0
58	MG	23SB	3001	1/1	0.92	0.21	42,42,42,42	0
58	MG	23SA	3040	1/1	0.92	0.12	53,53,53,53	0
60	OHX	23SB	3474	7/7	0.92	0.09	126,129,149,216	0
60	OHX	23SA	3602	7/7	0.92	0.08	113,120,138,213	0
60	OHX	23SB	3479	7/7	0.92	0.10	118,134,146,193	0
60	OHX	23SB	3481	7/7	0.92	0.07	143,153,167,246	0
58	MG	16SB	2221	1/1	0.92	0.23	42,42,42,42	0
58	MG	16SB	2264	1/1	0.92	0.08	98,98,98,98	0
58	MG	16SA	2290	1/1	0.92	0.20	71,71,71,71	0
60	OHX	23SB	3488	7/7	0.92	0.09	129,138,150,229	0
60	OHX	23SB	3490	7/7	0.92	0.09	135,138,156,200	0
58	MG	23SB	3047	1/1	0.92	0.32	59,59,59,59	0
60	OHX	23SB	3494	7/7	0.92	0.09	135,141,158,212	0
58	MG	23SB	3049	1/1	0.92	0.35	56,56,56,56	0
58	MG	23SB	3191	1/1	0.92	0.09	80,80,80,80	0
60	OHX	23SA	3612	7/7	0.92	0.08	91,119,133,210	0
58	MG	16SB	2241	1/1	0.92	0.23	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	MG	23SA	3147	1/1	0.92	0.25	41,41,41,41	0
58	MG	23SB	3197	1/1	0.92	0.09	66,66,66,66	0
60	OHX	23SA	3618	7/7	0.92	0.09	127,141,163,218	0
60	OHX	23SA	3619	7/7	0.92	0.09	114,133,137,209	0
58	MG	23SA	3327	1/1	0.92	0.10	75,75,75,75	0
59	K	16SA	2314	1/1	0.92	0.09	65,65,65,65	0
60	OHX	23SA	3627	7/7	0.92	0.09	123,131,152,228	0
60	OHX	16SA	2358	7/7	0.92	0.09	105,106,129,192	0
59	K	23SA	3353	1/1	0.92	0.09	64,64,64,64	0
58	MG	23SB	3208	1/1	0.92	0.17	53,53,53,53	0
58	MG	23SB	3216	1/1	0.92	0.08	88,88,88,88	0
59	K	23SB	3261	1/1	0.92	0.10	59,59,59,59	0
60	OHX	5SB	209	7/7	0.92	0.09	112,121,129,202	0
60	OHX	5SB	210	7/7	0.92	0.07	111,121,129,222	0
59	K	23SB	3263	1/1	0.92	0.25	93,93,93,93	0
60	OHX	L27A	103	7/7	0.92	0.09	88,92,103,211	0
60	OHX	16SA	2380	7/7	0.92	0.10	75,91,104,201	0
60	OHX	5SB	215	7/7	0.92	0.09	137,146,158,239	0
60	OHX	16SB	2338	7/7	0.92	0.12	82,95,114,179	0
59	K	5SA	207	1/1	0.92	0.09	70,70,70,70	0
58	MG	23SB	3195	1/1	0.93	0.10	46,46,46,46	0
60	OHX	23SA	3514	7/7	0.93	0.09	79,100,109,186	0
60	OHX	23SA	3515	7/7	0.93	0.15	73,81,96,166	0
60	OHX	23SA	3521	7/7	0.93	0.20	82,84,100,161	0
58	MG	23SB	3005	1/1	0.93	0.26	53,53,53,53	0
58	MG	23SB	3198	1/1	0.93	0.08	54,54,54,54	0
60	OHX	16SB	2386	7/7	0.93	0.10	116,126,138,198	0
60	OHX	16SB	2387	7/7	0.93	0.08	139,144,150,218	0
58	MG	23SA	3086	1/1	0.93	0.20	62,62,62,62	0
58	MG	23SB	3202	1/1	0.93	0.09	45,45,45,45	0
60	OHX	23SA	3543	7/7	0.93	0.08	76,92,101,198	0
58	MG	23SB	3048	1/1	0.93	0.10	43,43,43,43	0
59	K	23SA	3354	1/1	0.93	0.13	92,92,92,92	0
58	MG	16SA	2274	1/1	0.93	0.10	57,57,57,57	0
60	OHX	23SA	3554	7/7	0.93	0.07	98,107,109,231	0
58	MG	16SA	2206	1/1	0.93	0.32	31,31,31,31	0
60	OHX	23SA	3558	7/7	0.93	0.08	94,112,120,185	0
58	MG	23SA	3268	1/1	0.93	0.12	31,31,31,31	0
58	MG	16SA	2289	1/1	0.93	0.11	102,102,102,102	0
60	OHX	23SA	3561	7/7	0.93	0.10	79,83,104,176	0
60	OHX	23SA	3562	7/7	0.93	0.07	94,100,111,223	0
58	MG	23SA	3272	1/1	0.93	0.07	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
60	OHX	23SA	3567	7/7	0.93	0.07	97,99,113,230	0
58	MG	23SB	3017	1/1	0.93	0.10	38,38,38,38	0
60	OHX	23SA	3575	7/7	0.93	0.09	76,80,105,188	0
58	MG	16SA	2284	1/1	0.93	0.08	95,95,95,95	0
59	K	23SA	3364	1/1	0.93	0.09	46,46,46,46	0
58	MG	16SA	2259	1/1	0.93	0.08	77,77,77,77	0
60	OHX	23SB	3407	7/7	0.93	0.08	92,104,113,194	0
58	MG	23SA	3038	1/1	0.93	0.24	58,58,58,58	0
60	OHX	23SB	3415	7/7	0.93	0.09	89,94,111,191	0
60	OHX	23SA	3592	7/7	0.93	0.09	142,146,163,235	0
60	OHX	23SA	3593	7/7	0.93	0.08	117,129,149,224	0
59	K	23SB	3262	1/1	0.93	0.08	61,61,61,61	0
60	OHX	16SA	2348	7/7	0.93	0.11	77,89,99,143	0
58	MG	23SB	3134	1/1	0.93	0.13	53,53,53,53	0
60	OHX	23SB	3436	7/7	0.93	0.08	92,97,106,198	0
58	MG	23SA	3039	1/1	0.93	0.17	29,29,29,29	0
60	OHX	23SB	3439	7/7	0.93	0.08	79,91,98,201	0
59	K	23SB	3266	1/1	0.93	0.16	82,82,82,82	0
59	K	23SA	3375	1/1	0.93	0.07	52,52,52,52	0
59	K	23SA	3378	1/1	0.93	0.08	70,70,70,70	0
60	OHX	23SB	3444	7/7	0.93	0.08	89,96,108,221	0
59	K	23SA	3380	1/1	0.93	0.08	78,78,78,78	0
60	OHX	16SA	2371	7/7	0.93	0.10	89,93,120,170	0
60	OHX	16SA	2375	7/7	0.93	0.10	98,106,121,189	0
58	MG	23SB	3024	1/1	0.93	0.15	76,76,76,76	0
60	OHX	23SA	3609	7/7	0.93	0.07	128,133,141,224	0
60	OHX	23SA	3611	7/7	0.93	0.09	97,100,101,213	0
60	OHX	16SA	2379	7/7	0.93	0.08	107,116,125,210	0
58	MG	23SA	3056	1/1	0.93	0.23	57,57,57,57	0
59	K	23SA	3383	1/1	0.93	0.11	75,75,75,75	0
60	OHX	23SA	3615	7/7	0.93	0.08	94,104,121,185	0
58	MG	23SA	3203	1/1	0.93	0.10	45,45,45,45	0
60	OHX	16SA	2388	7/7	0.93	0.09	88,100,107,202	0
58	MG	23SA	3058	1/1	0.93	0.16	49,49,49,49	0
60	OHX	23SA	3620	7/7	0.93	0.08	122,127,151,215	0
60	OHX	23SB	3476	7/7	0.93	0.08	123,129,146,201	0
59	K	23SA	3386	1/1	0.93	0.06	64,64,64,64	0
60	OHX	23SB	3478	7/7	0.93	0.10	99,109,121,194	0
60	OHX	23SA	3624	7/7	0.93	0.08	94,112,133,228	0
58	MG	23SB	3030	1/1	0.93	0.30	54,54,54,54	0
60	OHX	16SA	2395	7/7	0.93	0.08	130,134,147,229	0
58	MG	23SB	3162	1/1	0.93	0.08	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
60	OHX	23SA	3630	7/7	0.93	0.08	102,118,137,188	0
60	OHX	23SB	3487	7/7	0.93	0.08	124,135,141,225	0
58	MG	23SA	3078	1/1	0.93	0.20	54,54,54,54	0
58	MG	23SA	3165	1/1	0.93	0.26	64,64,64,64	0
59	K	23SA	3397	1/1	0.93	0.07	52,52,52,52	0
58	MG	23SA	3145	1/1	0.93	0.20	53,53,53,53	0
60	OHX	5SA	217	7/7	0.93	0.09	114,124,140,203	0
59	K	23SB	3287	1/1	0.93	0.10	80,80,80,80	0
58	MG	23SA	3028	1/1	0.93	0.26	41,41,41,41	0
58	MG	23SB	3172	1/1	0.93	0.08	46,46,46,46	0
60	OHX	23SB	3500	7/7	0.93	0.08	188,188,201,242	0
58	MG	16SA	2203	1/1	0.93	0.32	62,62,62,62	0
60	OHX	23SB	3502	7/7	0.93	0.08	111,132,143,216	0
60	OHX	16SB	2343	7/7	0.93	0.10	98,100,125,168	0
60	OHX	16SB	2345	7/7	0.93	0.09	92,101,115,193	0
58	MG	23SA	3042	1/1	0.93	0.11	40,40,40,40	0
58	MG	23SB	3178	1/1	0.93	0.09	57,57,57,57	0
60	OHX	23SB	3507	7/7	0.93	0.09	110,119,128,207	0
58	MG	16SB	2256	1/1	0.93	0.09	72,72,72,72	0
59	K	16SB	2312	1/1	0.93	0.07	82,82,82,82	0
58	MG	23SA	3082	1/1	0.93	0.16	40,40,40,40	0
59	K	16SB	2314	1/1	0.93	0.10	102,102,102,102	0
60	OHX	16SB	2363	7/7	0.93	0.09	139,140,164,204	0
58	MG	23SA	3001	1/1	0.93	0.22	41,41,41,41	0
58	MG	23SB	3078	1/1	0.93	0.11	48,48,48,48	0
60	OHX	16SB	2369	7/7	0.93	0.09	88,99,116,191	0
58	MG	23SA	3064	1/1	0.93	0.21	57,57,57,57	0
58	MG	23SB	3190	1/1	0.93	0.12	51,51,51,51	0
58	MG	23SB	3043	1/1	0.93	0.23	34,34,34,34	0
58	MG	23SA	3032	1/1	0.93	0.13	61,61,61,61	0
58	MG	23SA	3249	1/1	0.93	0.08	35,35,35,35	0
60	OHX	L35B	103	7/7	0.93	0.10	121,122,130,188	0
60	OHX	16SB	2377	7/7	0.93	0.08	138,140,149,221	0
59	K	23SA	3347	1/1	0.93	0.07	72,72,72,72	0
58	MG	23SB	3170	1/1	0.94	0.09	57,57,57,57	0
59	K	23SB	3248	1/1	0.94	0.24	100,100,100,100	0
59	K	23SB	3249	1/1	0.94	0.07	66,66,66,66	0
58	MG	23SA	3120	1/1	0.94	0.08	70,70,70,70	0
60	OHX	23SA	3563	7/7	0.94	0.06	93,103,112,234	0
59	K	23SB	3251	1/1	0.94	0.06	56,56,56,56	0
58	MG	23SA	3018	1/1	0.94	0.20	34,34,34,34	0
60	OHX	23SA	3569	7/7	0.94	0.07	99,109,119,234	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	MG	23SB	3174	1/1	0.94	0.12	54,54,54,54	0
60	OHX	16SA	2355	7/7	0.94	0.08	90,108,124,164	0
58	MG	23SB	3060	1/1	0.94	0.30	44,44,44,44	0
60	OHX	23SA	3578	7/7	0.94	0.07	138,140,158,239	0
59	K	23SA	3433	1/1	0.94	0.10	57,57,57,57	0
60	OHX	S4B	302	7/7	0.94	0.08	112,116,130,195	0
58	MG	16SB	2274	1/1	0.94	0.07	80,80,80,80	0
58	MG	23SA	3264	1/1	0.94	0.12	45,45,45,45	0
58	MG	23SA	3122	1/1	0.94	0.25	49,49,49,49	0
58	MG	23SB	3107	1/1	0.94	0.30	75,75,75,75	0
60	OHX	ESIB	101	7/7	0.94	0.08	152,164,172,232	0
58	MG	23SA	3211	1/1	0.94	0.08	61,61,61,61	0
59	K	23SB	3265	1/1	0.94	0.07	51,51,51,51	0
60	OHX	23SB	3359	7/7	0.94	0.09	110,120,133,166	0
60	OHX	23SB	3366	7/7	0.94	0.10	68,87,109,158	0
60	OHX	23SB	3372	7/7	0.94	0.08	91,97,114,160	0
58	MG	23SA	3105	1/1	0.94	0.10	73,73,73,73	0
60	OHX	23SA	3599	7/7	0.94	0.08	140,146,155,214	0
60	OHX	23SB	3389	7/7	0.94	0.08	61,98,105,173	0
58	MG	23SB	3029	1/1	0.94	0.27	44,44,44,44	0
60	OHX	23SB	3410	7/7	0.94	0.09	113,115,120,199	0
60	OHX	23SA	3601	7/7	0.94	0.07	119,135,151,211	0
58	MG	16SA	2277	1/1	0.94	0.07	63,63,63,63	0
60	OHX	16SA	2381	7/7	0.94	0.08	134,138,146,225	0
58	MG	23SA	3274	1/1	0.94	0.09	47,47,47,47	0
60	OHX	23SB	3424	7/7	0.94	0.07	102,113,118,190	0
60	OHX	16SA	2384	7/7	0.94	0.07	104,120,127,210	0
60	OHX	23SB	3428	7/7	0.94	0.11	92,112,132,177	0
58	MG	23SB	3032	1/1	0.94	0.15	55,55,55,55	0
60	OHX	16SA	2387	7/7	0.94	0.09	100,103,114,193	0
60	OHX	23SB	3434	7/7	0.94	0.08	98,99,117,181	0
60	OHX	23SB	3435	7/7	0.94	0.07	111,113,124,228	0
58	MG	23SB	3071	1/1	0.94	0.28	53,53,53,53	0
58	MG	23SA	3275	1/1	0.94	0.10	71,71,71,71	0
60	OHX	23SA	3610	7/7	0.94	0.07	132,141,164,238	0
58	MG	23SA	3051	1/1	0.94	0.19	69,69,69,69	0
58	MG	23SB	3074	1/1	0.94	0.37	58,58,58,58	0
60	OHX	16SA	2394	7/7	0.94	0.07	114,116,133,196	0
58	MG	23SA	3094	1/1	0.94	0.06	77,77,77,77	0
58	MG	16SA	2216	1/1	0.94	0.13	36,36,36,36	0
60	OHX	23SB	3450	7/7	0.94	0.07	105,107,114,220	0
59	K	16SB	2296	1/1	0.94	0.08	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	MG	23SB	3037	1/1	0.94	0.36	56,56,56,56	0
58	MG	23SB	3217	1/1	0.94	0.05	88,88,88,88	0
60	OHX	23SB	3460	7/7	0.94	0.07	88,91,110,224	0
58	MG	23SB	3218	1/1	0.94	0.06	42,42,42,42	0
59	K	16SB	2300	1/1	0.94	0.06	72,72,72,72	0
60	OHX	23SA	3623	7/7	0.94	0.08	106,117,141,204	0
58	MG	23SA	3022	1/1	0.94	0.21	49,49,49,49	0
59	K	16SA	2329	1/1	0.94	0.09	94,94,94,94	0
58	MG	23SA	3076	1/1	0.94	0.33	62,62,62,62	0
58	MG	23SA	3286	1/1	0.94	0.09	42,42,42,42	0
58	MG	23SA	3237	1/1	0.94	0.07	46,46,46,46	0
60	OHX	23SB	3471	7/7	0.94	0.07	134,141,156,215	0
58	MG	23SA	3030	1/1	0.94	0.22	54,54,54,54	0
60	OHX	23SB	3473	7/7	0.94	0.08	106,109,130,178	0
58	MG	23SB	3225	1/1	0.94	0.11	85,85,85,85	0
58	MG	23SA	3294	1/1	0.94	0.08	44,44,44,44	0
60	OHX	16SA	2412	7/7	0.94	0.09	99,106,111,207	0
60	OHX	5SA	216	7/7	0.94	0.08	84,97,113,216	0
58	MG	23SA	3240	1/1	0.94	0.12	28,28,28,28	0
58	MG	23SA	3296	1/1	0.94	0.10	48,48,48,48	0
60	OHX	23SB	3482	7/7	0.94	0.07	129,137,145,231	0
58	MG	23SB	3233	1/1	0.94	0.09	102,102,102,102	0
58	MG	23SA	3016	1/1	0.94	0.15	66,66,66,66	0
60	OHX	16SB	2328	7/7	0.94	0.10	83,93,105,146	0
60	OHX	TRNA	102	7/7	0.94	0.07	118,122,143,229	0
58	MG	23SA	3303	1/1	0.94	0.09	54,54,54,54	0
58	MG	PSIA	102	1/1	0.94	0.09	84,84,84,84	0
60	OHX	23SA	3479	7/7	0.94	0.09	92,105,110,166	0
58	MG	23SB	3238	1/1	0.94	0.07	40,40,40,40	0
60	OHX	16SB	2350	7/7	0.94	0.07	101,111,113,186	0
58	MG	23SB	3137	1/1	0.94	0.07	60,60,60,60	0
60	OHX	16SB	2354	7/7	0.94	0.08	87,94,105,178	0
59	K	23SB	3305	1/1	0.94	0.12	69,69,69,69	0
60	OHX	16SB	2356	7/7	0.94	0.09	96,103,117,193	0
58	MG	23SB	3089	1/1	0.94	0.16	72,72,72,72	0
59	K	16SB	2320	1/1	0.94	0.10	97,97,97,97	0
59	K	23SB	3308	1/1	0.94	0.07	85,85,85,85	0
60	OHX	16SB	2364	7/7	0.94	0.09	109,111,126,185	0
60	OHX	23SA	3519	7/7	0.94	0.07	93,100,111,208	0
58	MG	23SB	3009	1/1	0.94	0.21	40,40,40,40	0
60	OHX	23SA	3523	7/7	0.94	0.20	71,90,93,140	0
60	OHX	16SB	2370	7/7	0.94	0.07	123,128,137,241	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
60	OHX	23SA	3524	7/7	0.94	0.18	82,85,101,153	0
60	OHX	23SA	3525	7/7	0.94	0.08	107,110,130,195	0
58	MG	23SB	3050	1/1	0.94	0.16	55,55,55,55	0
60	OHX	16SB	2374	7/7	0.94	0.09	105,117,136,182	0
58	MG	23SB	3156	1/1	0.94	0.07	48,48,48,48	0
60	OHX	23SB	3514	7/7	0.94	0.06	102,108,117,230	0
58	MG	23SB	3157	1/1	0.94	0.08	42,42,42,42	0
60	OHX	5SB	206	7/7	0.94	0.09	90,101,122,161	0
58	MG	16SB	2207	1/1	0.94	0.11	61,61,61,61	0
60	OHX	23SA	3541	7/7	0.94	0.16	69,83,95,155	0
58	MG	23SA	3134	1/1	0.94	0.10	60,60,60,60	0
58	MG	23SA	3059	1/1	0.94	0.08	61,61,61,61	0
58	MG	23SB	3096	1/1	0.94	0.53	80,80,80,80	0
58	MG	23SB	3015	1/1	0.94	0.17	44,44,44,44	0
60	OHX	L20B	201	7/7	0.94	0.08	88,98,107,189	0
58	MG	16SB	2267	1/1	0.94	0.07	72,72,72,72	0
58	MG	23SA	3314	1/1	0.94	0.17	57,57,57,57	0
58	MG	23SA	3321	1/1	0.94	0.08	43,43,43,43	0
60	OHX	23SA	3577	7/7	0.95	0.07	80,96,102,220	0
58	MG	L3A	301	1/1	0.95	0.14	54,54,54,54	0
60	OHX	23SA	3579	7/7	0.95	0.06	92,103,109,213	0
60	OHX	23SA	3582	7/7	0.95	0.07	109,116,130,206	0
58	MG	23SB	3136	1/1	0.95	0.09	47,47,47,47	0
60	OHX	16SA	2382	7/7	0.95	0.07	101,104,120,187	0
60	OHX	ASIB	102	7/7	0.95	0.09	150,170,188,213	0
59	K	23SA	3369	1/1	0.95	0.05	50,50,50,50	0
58	MG	23SA	3236	1/1	0.95	0.17	102,102,102,102	0
59	K	23SA	3374	1/1	0.95	0.09	69,69,69,69	0
60	OHX	23SA	3594	7/7	0.95	0.07	86,92,102,199	0
60	OHX	16SA	2386	7/7	0.95	0.08	101,109,118,167	0
58	MG	23SA	3119	1/1	0.95	0.15	59,59,59,59	0
58	MG	23SB	3144	1/1	0.95	0.09	58,58,58,58	0
60	OHX	16SA	2389	7/7	0.95	0.08	108,111,117,198	0
59	K	23SA	3379	1/1	0.95	0.12	60,60,60,60	0
60	OHX	23SB	3383	7/7	0.95	0.08	95,102,112,175	0
58	MG	23SB	3145	1/1	0.95	0.08	60,60,60,60	0
58	MG	L15A	201	1/1	0.95	0.10	52,52,52,52	0
60	OHX	16SA	2393	7/7	0.95	0.08	108,114,137,185	0
60	OHX	23SB	3395	7/7	0.95	0.09	86,95,112,173	0
60	OHX	23SB	3399	7/7	0.95	0.10	89,90,102,150	0
60	OHX	23SB	3406	7/7	0.95	0.07	90,98,104,195	0
59	K	16SB	2295	1/1	0.95	0.09	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
60	OHX	23SB	3409	7/7	0.95	0.08	84,92,100,160	0
58	MG	23SB	3148	1/1	0.95	0.07	69,69,69,69	0
60	OHX	16SA	2396	7/7	0.95	0.10	99,106,128,172	0
58	MG	16SA	2242	1/1	0.95	0.33	63,63,63,63	0
58	MG	16SA	2283	1/1	0.95	0.12	85,85,85,85	0
58	MG	23SA	3133	1/1	0.95	0.13	58,58,58,58	0
60	OHX	23SB	3423	7/7	0.95	0.08	96,107,117,182	0
58	MG	L27A	101	1/1	0.95	0.19	40,40,40,40	0
58	MG	23SB	3231	1/1	0.95	0.07	111,111,111,111	0
59	K	23SA	3388	1/1	0.95	0.08	74,74,74,74	0
60	OHX	23SB	3431	7/7	0.95	0.06	113,115,123,203	0
58	MG	23SB	3232	1/1	0.95	0.07	50,50,50,50	0
59	K	23SB	3292	1/1	0.95	0.06	80,80,80,80	0
58	MG	23SB	3159	1/1	0.95	0.07	56,56,56,56	0
58	MG	L30A	101	1/1	0.95	0.09	54,54,54,54	0
60	OHX	23SA	3617	7/7	0.95	0.07	93,106,124,185	0
59	K	23SA	3395	1/1	0.95	0.08	61,61,61,61	0
58	MG	23SA	3245	1/1	0.95	0.07	51,51,51,51	0
58	MG	23SA	3045	1/1	0.95	0.17	33,33,33,33	0
58	MG	23SA	3207	1/1	0.95	0.13	40,40,40,40	0
59	K	23SA	3400	1/1	0.95	0.12	56,56,56,56	0
60	OHX	16SA	2413	7/7	0.95	0.08	87,97,103,201	0
60	OHX	23SB	3447	7/7	0.95	0.08	86,91,103,193	0
58	MG	23SA	3025	1/1	0.95	0.25	58,58,58,58	0
58	MG	23SA	3301	1/1	0.95	0.10	37,37,37,37	0
60	OHX	23SB	3451	7/7	0.95	0.07	96,110,128,184	0
60	OHX	23SB	3452	7/7	0.95	0.07	105,116,122,211	0
60	OHX	S19A	101	7/7	0.95	0.09	105,123,131,174	0
58	MG	23SA	3258	1/1	0.95	0.06	42,42,42,42	0
60	OHX	23SB	3457	7/7	0.95	0.10	90,92,116,167	0
60	OHX	23SB	3458	7/7	0.95	0.07	98,102,111,227	0
60	OHX	ESIA	101	7/7	0.95	0.07	143,154,174,216	0
58	MG	23SA	3173	1/1	0.95	0.26	46,46,46,46	0
58	MG	23SB	3113	1/1	0.95	0.08	52,52,52,52	0
60	OHX	23SA	3465	7/7	0.95	0.11	73,76,89,133	0
58	MG	23SA	3213	1/1	0.95	0.09	49,49,49,49	0
58	MG	23SB	3007	1/1	0.95	0.28	34,34,34,34	0
58	MG	23SB	3175	1/1	0.95	0.08	62,62,62,62	0
60	OHX	23SA	3492	7/7	0.95	0.15	69,79,89,131	0
60	OHX	23SB	3468	7/7	0.95	0.08	110,122,131,185	0
60	OHX	L27A	104	7/7	0.95	0.08	111,116,145,172	0
58	MG	23SA	3075	1/1	0.95	0.06	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
60	OHX	L35A	102	7/7	0.95	0.09	98,107,111,169	0
60	OHX	23SA	3497	7/7	0.95	0.11	62,85,98,140	0
60	OHX	16SB	2334	7/7	0.95	0.09	118,127,134,170	0
60	OHX	16SB	2336	7/7	0.95	0.10	68,90,111,131	0
60	OHX	23SA	3508	7/7	0.95	0.08	73,82,110,156	0
60	OHX	16SB	2341	7/7	0.95	0.07	96,100,117,187	0
59	K	23SA	3412	1/1	0.95	0.07	40,40,40,40	0
58	MG	23SA	3068	1/1	0.95	0.38	60,60,60,60	0
58	MG	23SA	3315	1/1	0.95	0.07	101,101,101,101	0
58	MG	23SB	3011	1/1	0.95	0.31	43,43,43,43	0
58	MG	16SA	2281	1/1	0.95	0.07	40,40,40,40	0
60	OHX	23SA	3516	7/7	0.95	0.13	70,77,90,165	0
58	MG	16SB	2268	1/1	0.95	0.06	86,86,86,86	0
60	OHX	23SB	3486	7/7	0.95	0.07	96,100,116,205	0
58	MG	23SB	3122	1/1	0.95	0.15	38,38,38,38	0
59	K	23SA	3420	1/1	0.95	0.07	71,71,71,71	0
60	OHX	16SB	2357	7/7	0.95	0.07	103,106,112,188	0
60	OHX	23SB	3491	7/7	0.95	0.07	132,134,135,208	0
60	OHX	23SB	3492	7/7	0.95	0.07	97,109,131,185	0
58	MG	23SB	3189	1/1	0.95	0.08	52,52,52,52	0
58	MG	23SA	3004	1/1	0.95	0.29	40,40,40,40	0
60	OHX	23SB	3495	7/7	0.95	0.07	143,146,157,198	0
58	MG	23SA	3095	1/1	0.95	0.24	51,51,51,51	0
58	MG	23SA	3180	1/1	0.95	0.14	37,37,37,37	0
58	MG	23SA	3224	1/1	0.95	0.06	69,69,69,69	0
60	OHX	16SB	2367	7/7	0.95	0.08	191,194,215,295	0
60	OHX	23SA	3532	7/7	0.95	0.11	60,78,105,175	0
58	MG	23SA	3226	1/1	0.95	0.06	76,76,76,76	0
60	OHX	23SA	3540	7/7	0.95	0.06	77,94,109,196	0
58	MG	23SB	3196	1/1	0.95	0.10	53,53,53,53	0
60	OHX	23SA	3542	7/7	0.95	0.08	90,100,107,188	0
58	MG	16SB	2275	1/1	0.95	0.11	80,80,80,80	0
59	K	23SA	3429	1/1	0.95	0.17	76,76,76,76	0
59	K	16SA	2308	1/1	0.95	0.06	78,78,78,78	0
60	OHX	16SA	2351	7/7	0.95	0.09	85,94,107,150	0
60	OHX	23SA	3553	7/7	0.95	0.08	71,80,96,181	0
59	K	16SA	2309	1/1	0.95	0.08	85,85,85,85	0
58	MG	23SA	3106	1/1	0.95	0.23	63,63,63,63	0
58	MG	23SA	3233	1/1	0.95	0.16	70,70,70,70	0
60	OHX	16SA	2360	7/7	0.95	0.07	92,94,119,193	0
58	MG	23SA	3281	1/1	0.95	0.07	39,39,39,39	0
60	OHX	16SA	2364	7/7	0.95	0.08	72,94,101,159	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	K	16SA	2313	1/1	0.95	0.07	62,62,62,62	0
58	MG	23SB	3204	1/1	0.95	0.08	34,34,34,34	0
59	K	23SA	3362	1/1	0.95	0.05	39,39,39,39	0
60	OHX	5SB	211	7/7	0.95	0.07	107,114,125,191	0
58	MG	23SB	3206	1/1	0.95	0.14	63,63,63,63	0
60	OHX	23SA	3568	7/7	0.95	0.08	84,98,111,175	0
59	K	L4A	303	1/1	0.95	0.06	80,80,80,80	0
59	K	23SB	3267	1/1	0.95	0.13	65,65,65,65	0
60	OHX	23SA	3572	7/7	0.95	0.07	89,101,111,205	0
60	OHX	23SA	3573	7/7	0.95	0.07	77,83,98,186	0
60	OHX	16SA	2378	7/7	0.95	0.08	104,108,111,178	0
58	MG	23SB	3026	1/1	0.95	0.16	47,47,47,47	0
60	OHX	23SB	3396	7/7	0.96	0.07	86,89,98,176	0
60	OHX	23SB	3397	7/7	0.96	0.06	82,86,94,166	0
60	OHX	23SB	3398	7/7	0.96	0.06	102,110,115,193	0
59	K	16SA	2304	1/1	0.96	0.23	77,77,77,77	0
60	OHX	23SB	3400	7/7	0.96	0.07	110,122,130,188	0
60	OHX	23SB	3403	7/7	0.96	0.08	89,99,119,158	0
60	OHX	5SA	210	7/7	0.96	0.08	68,97,110,132	0
60	OHX	5SA	212	7/7	0.96	0.08	83,95,112,163	0
60	OHX	23SB	3408	7/7	0.96	0.08	78,89,99,156	0
59	K	23SB	3316	1/1	0.96	0.27	89,89,89,89	0
60	OHX	23SA	3548	7/7	0.96	0.12	66,73,104,175	0
60	OHX	23SA	3549	7/7	0.96	0.07	82,94,102,158	0
60	OHX	23SB	3413	7/7	0.96	0.08	79,83,95,170	0
60	OHX	23SB	3414	7/7	0.96	0.11	76,79,91,152	0
60	OHX	16SA	2398	7/7	0.96	0.07	120,122,129,185	0
60	OHX	23SB	3416	7/7	0.96	0.08	94,107,122,167	0
60	OHX	L15A	203	7/7	0.96	0.14	76,83,97,140	0
58	MG	23SA	3185	1/1	0.96	0.07	35,35,35,35	0
58	MG	23SA	3186	1/1	0.96	0.06	23,23,23,23	0
58	MG	23SA	3259	1/1	0.96	0.07	64,64,64,64	0
60	OHX	23SB	3425	7/7	0.96	0.08	74,89,96,169	0
58	MG	23SB	3185	1/1	0.96	0.06	77,77,77,77	0
60	OHX	23SA	3556	7/7	0.96	0.07	87,91,98,175	0
60	OHX	23SB	3429	7/7	0.96	0.07	105,111,115,204	0
60	OHX	23SB	3430	7/7	0.96	0.07	96,102,106,185	0
60	OHX	23SA	3557	7/7	0.96	0.06	94,104,119,199	0
60	OHX	16SB	2335	7/7	0.96	0.08	110,123,134,166	0
58	MG	23SB	3141	1/1	0.96	0.06	44,44,44,44	0
58	MG	23SA	3316	1/1	0.96	0.12	86,86,86,86	0
58	MG	23SB	3234	1/1	0.96	0.06	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
59	K	L2B	302	1/1	0.96	0.07	65,65,65,65	0
58	MG	23SB	3061	1/1	0.96	0.34	59,59,59,59	0
60	OHX	16SB	2346	7/7	0.96	0.07	84,98,106,161	0
60	OHX	16SB	2347	7/7	0.96	0.07	113,116,121,183	0
58	MG	16SB	2278	1/1	0.96	0.08	73,73,73,73	0
58	MG	23SA	3319	1/1	0.96	0.05	68,68,68,68	0
60	OHX	23SB	3443	7/7	0.96	0.07	90,95,107,189	0
60	OHX	23SA	3566	7/7	0.96	0.06	95,99,108,197	0
60	OHX	23SB	3445	7/7	0.96	0.07	97,105,117,180	0
60	OHX	23SB	3446	7/7	0.96	0.06	83,97,99,203	0
60	OHX	16SB	2352	7/7	0.96	0.07	85,96,108,177	0
59	K	23SA	3389	1/1	0.96	0.05	68,68,68,68	0
60	OHX	23SB	3449	7/7	0.96	0.06	102,106,109,189	0
59	K	23SB	3281	1/1	0.96	0.07	75,75,75,75	0
58	MG	16SA	2263	1/1	0.96	0.07	70,70,70,70	0
59	K	16SA	2317	1/1	0.96	0.04	50,50,50,50	0
60	OHX	23SA	3571	7/7	0.96	0.13	70,83,95,178	0
60	OHX	23SB	3454	7/7	0.96	0.07	91,102,107,180	0
59	K	23SB	3285	1/1	0.96	0.05	70,70,70,70	0
60	OHX	16SA	2357	7/7	0.96	0.07	93,100,111,175	0
60	OHX	16SB	2361	7/7	0.96	0.07	120,121,125,206	0
60	OHX	23SA	3574	7/7	0.96	0.06	84,98,110,186	0
60	OHX	16SA	2416	7/7	0.96	0.08	96,107,111,178	0
58	MG	23SB	3153	1/1	0.96	0.08	52,52,52,52	0
60	OHX	16SB	2366	7/7	0.96	0.07	98,106,112,182	0
58	MG	23SB	3090	1/1	0.96	0.13	65,65,65,65	0
60	OHX	ASIA	103	7/7	0.96	0.10	138,148,166,192	0
58	MG	16SB	2257	1/1	0.96	0.07	64,64,64,64	0
58	MG	23SA	3322	1/1	0.96	0.07	43,43,43,43	0
60	OHX	23SA	3585	7/7	0.96	0.07	95,99,129,168	0
60	OHX	23SA	3586	7/7	0.96	0.07	101,106,128,162	0
58	MG	16SB	2259	1/1	0.96	0.06	96,96,96,96	0
60	OHX	23SA	3589	7/7	0.96	0.08	112,126,132,194	0
60	OHX	23SA	3459	7/7	0.96	0.12	55,83,96,117	0
58	MG	23SA	3323	1/1	0.96	0.07	25,25,25,25	0
58	MG	PSIA	101	1/1	0.96	0.30	56,56,56,56	0
60	OHX	23SB	3475	7/7	0.96	0.08	166,169,173,226	0
60	OHX	16SA	2370	7/7	0.96	0.08	85,94,98,186	0
59	K	16SA	2325	1/1	0.96	0.07	80,80,80,80	0
60	OHX	16SB	2380	7/7	0.96	0.07	141,148,159,212	0
60	OHX	23SA	3480	7/7	0.96	0.09	74,80,103,129	0
60	OHX	23SB	3480	7/7	0.96	0.06	121,142,146,213	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	OHX	23SA	3486	7/7	0.96	0.10	55,72,99,142	0
60	OHX	16SA	2372	7/7	0.96	0.08	73,90,105,162	0
60	OHX	16SA	2373	7/7	0.96	0.06	113,116,123,191	0
58	MG	L35B	101	1/1	0.96	0.09	91,91,91,91	0
60	OHX	23SA	3498	7/7	0.96	0.19	62,67,77,108	0
60	OHX	23SA	3501	7/7	0.96	0.08	86,95,99,151	0
58	MG	23SB	3021	1/1	0.96	0.05	66,66,66,66	0
60	OHX	23SA	3510	7/7	0.96	0.13	73,82,88,134	0
60	OHX	16SA	2377	7/7	0.96	0.07	104,109,116,184	0
58	MG	23SB	3205	1/1	0.96	0.08	54,54,54,54	0
58	MG	23SA	3099	1/1	0.96	0.07	54,54,54,54	0
58	MG	23SA	3265	1/1	0.96	0.07	41,41,41,41	0
58	MG	23SB	3212	1/1	0.96	0.06	56,56,56,56	0
58	MG	23SA	3011	1/1	0.96	0.28	43,43,43,43	0
60	OHX	23SA	3517	7/7	0.96	0.07	75,89,104,170	0
59	K	23SA	3363	1/1	0.96	0.06	53,53,53,53	0
58	MG	23SA	3197	1/1	0.96	0.07	52,52,52,52	0
58	MG	16SA	2262	1/1	0.96	0.08	70,70,70,70	0
59	K	23SB	3257	1/1	0.96	0.04	77,77,77,77	0
58	MG	23SA	3243	1/1	0.96	0.06	36,36,36,36	0
60	OHX	S14B	101	7/7	0.96	0.08	102,124,132,165	0
58	MG	23SA	3202	1/1	0.96	0.07	74,74,74,74	0
60	OHX	23SA	3528	7/7	0.96	0.07	87,90,100,182	0
59	K	16SB	2301	1/1	0.96	0.07	92,92,92,92	0
59	K	23SA	3417	1/1	0.96	0.06	68,68,68,68	0
60	OHX	23SA	3621	7/7	0.96	0.08	96,102,123,180	0
58	MG	23SA	3118	1/1	0.96	0.10	52,52,52,52	0
60	OHX	23SB	3357	7/7	0.96	0.07	81,94,106,158	0
60	OHX	23SA	3533	7/7	0.96	0.06	85,91,99,178	0
60	OHX	23SA	3534	7/7	0.96	0.08	75,93,110,174	0
60	OHX	23SB	3361	7/7	0.96	0.08	76,89,106,161	0
60	OHX	23SB	3364	7/7	0.96	0.11	77,86,99,142	0
60	OHX	23SA	3537	7/7	0.96	0.06	98,104,109,202	0
60	OHX	23SA	3626	7/7	0.96	0.07	106,109,123,185	0
60	OHX	23SB	3373	7/7	0.96	0.15	72,84,91,148	0
60	OHX	5SB	208	7/7	0.96	0.07	99,101,116,175	0
60	OHX	23SB	3378	7/7	0.96	0.10	71,85,90,156	0
60	OHX	23SB	3381	7/7	0.96	0.08	82,98,103,149	0
60	OHX	23SB	3382	7/7	0.96	0.07	92,100,102,184	0
60	OHX	23SA	3538	7/7	0.96	0.07	95,114,124,179	0
60	OHX	23SB	3384	7/7	0.96	0.07	90,103,109,158	0
58	MG	23SA	3306	1/1	0.96	0.10	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
59	K	23SA	3373	1/1	0.96	0.04	37,37,37,37	0
58	MG	23SA	3206	1/1	0.96	0.07	55,55,55,55	0
60	OHX	23SB	3392	7/7	0.96	0.12	67,88,95,140	0
60	OHX	23SB	3393	7/7	0.96	0.08	79,88,96,165	0
58	MG	23SA	3252	1/1	0.96	0.07	50,50,50,50	0
60	OHX	TRNA	101	7/7	0.97	0.07	126,128,151,181	0
60	OHX	16SA	2362	7/7	0.97	0.06	68,86,95,171	0
60	OHX	23SA	3454	7/7	0.97	0.11	62,77,97,102	0
60	OHX	16SA	2363	7/7	0.97	0.07	87,99,108,136	0
60	OHX	16SB	2351	7/7	0.97	0.06	116,129,145,187	0
58	MG	23SB	3207	1/1	0.97	0.14	51,51,51,51	0
60	OHX	23SB	3418	7/7	0.97	0.07	122,132,139,198	0
60	OHX	23SB	3420	7/7	0.97	0.07	99,102,107,176	0
60	OHX	23SA	3466	7/7	0.97	0.10	53,79,99,128	0
60	OHX	23SA	3468	7/7	0.97	0.08	51,67,97,150	0
60	OHX	16SA	2365	7/7	0.97	0.07	82,95,103,153	0
60	OHX	23SA	3477	7/7	0.97	0.08	71,87,97,132	0
58	MG	23SA	3282	1/1	0.97	0.05	30,30,30,30	0
60	OHX	16SB	2358	7/7	0.97	0.06	104,114,122,205	0
58	MG	23SA	3318	1/1	0.97	0.06	64,64,64,64	0
59	K	23SA	3335	1/1	0.97	0.05	70,70,70,70	0
60	OHX	23SA	3481	7/7	0.97	0.07	81,94,105,138	0
60	OHX	23SA	3483	7/7	0.97	0.10	68,75,84,124	0
60	OHX	23SA	3580	7/7	0.97	0.06	90,92,101,178	0
58	MG	23SB	3213	1/1	0.97	0.08	42,42,42,42	0
60	OHX	23SA	3584	7/7	0.97	0.05	92,105,118,200	0
60	OHX	23SA	3487	7/7	0.97	0.14	68,87,98,133	0
60	OHX	23SA	3489	7/7	0.97	0.10	83,85,99,126	0
60	OHX	23SA	3587	7/7	0.97	0.09	81,88,96,150	0
58	MG	23SB	3215	1/1	0.97	0.06	42,42,42,42	0
58	MG	23SA	3234	1/1	0.97	0.07	93,93,93,93	0
60	OHX	23SA	3496	7/7	0.97	0.11	72,80,86,150	0
58	MG	23SA	3320	1/1	0.97	0.07	93,93,93,93	0
58	MG	16SA	2266	1/1	0.97	0.06	86,86,86,86	0
60	OHX	23SA	3499	7/7	0.97	0.08	68,88,99,163	0
58	MG	16SA	2215	1/1	0.97	0.21	40,40,40,40	0
60	OHX	23SA	3503	7/7	0.97	0.14	80,89,99,149	0
60	OHX	23SA	3596	7/7	0.97	0.07	95,124,136,188	0
60	OHX	23SA	3504	7/7	0.97	0.13	87,89,95,142	0
60	OHX	23SA	3505	7/7	0.97	0.12	79,87,103,142	0
60	OHX	23SA	3506	7/7	0.97	0.10	58,69,82,144	0
58	MG	23SA	3287	1/1	0.97	0.04	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
60	OHX	23SA	3509	7/7	0.97	0.07	103,106,119,151	0
59	K	L2A	301	1/1	0.97	0.07	52,52,52,52	0
60	OHX	23SB	3455	7/7	0.97	0.06	80,87,94,174	0
58	MG	23SB	3221	1/1	0.97	0.04	94,94,94,94	0
58	MG	23SA	3289	1/1	0.97	0.06	33,33,33,33	0
58	MG	23SA	3179	1/1	0.97	0.08	31,31,31,31	0
59	K	23SA	3394	1/1	0.97	0.08	59,59,59,59	0
58	MG	23SB	3126	1/1	0.97	0.07	59,59,59,59	0
59	K	23SA	3396	1/1	0.97	0.06	68,68,68,68	0
58	MG	16SA	2265	1/1	0.97	0.09	73,73,73,73	0
58	MG	23SA	3049	1/1	0.97	0.10	40,40,40,40	0
60	OHX	23SA	3520	7/7	0.97	0.08	81,88,104,156	0
58	MG	23SA	3331	1/1	0.97	0.15	42,42,42,42	0
59	K	23SB	3253	1/1	0.97	0.06	54,54,54,54	0
60	OHX	23SB	3467	7/7	0.97	0.07	94,109,115,181	0
58	MG	23SB	3179	1/1	0.97	0.06	47,47,47,47	0
58	MG	23SA	3332	1/1	0.97	0.10	32,32,32,32	0
58	MG	23SB	3182	1/1	0.97	0.05	62,62,62,62	0
58	MG	23SA	3333	1/1	0.97	0.07	95,95,95,95	0
58	MG	23SB	3067	1/1	0.97	0.13	36,36,36,36	0
59	K	23SB	3260	1/1	0.97	0.06	53,53,53,53	0
59	K	23SA	3405	1/1	0.97	0.07	72,72,72,72	0
60	OHX	ASIB	101	7/7	0.97	0.07	107,120,125,167	0
58	MG	23SA	3221	1/1	0.97	0.07	60,60,60,60	0
58	MG	23SA	3271	1/1	0.97	0.10	67,67,67,67	0
60	OHX	23SA	3535	7/7	0.97	0.05	90,95,110,191	0
58	MG	23SA	3108	1/1	0.97	0.14	51,51,51,51	0
58	MG	23SA	3247	1/1	0.97	0.05	26,26,26,26	0
58	MG	23SA	3302	1/1	0.97	0.06	39,39,39,39	0
60	OHX	23SB	3326	7/7	0.97	0.16	56,72,101,137	0
60	OHX	23SB	3335	7/7	0.97	0.16	60,83,91,162	0
60	OHX	23SB	3342	7/7	0.97	0.09	47,60,90,114	0
60	OHX	23SB	3344	7/7	0.97	0.08	80,88,104,133	0
60	OHX	23SB	3346	7/7	0.97	0.09	85,96,101,143	0
60	OHX	23SB	3349	7/7	0.97	0.11	84,92,100,127	0
60	OHX	23SB	3352	7/7	0.97	0.08	69,81,101,121	0
60	OHX	23SB	3489	7/7	0.97	0.06	111,122,129,189	0
60	OHX	23SB	3355	7/7	0.97	0.08	89,92,104,140	0
58	MG	16SB	2272	1/1	0.97	0.07	90,90,90,90	0
59	K	16SB	2303	1/1	0.97	0.06	74,74,74,74	0
60	OHX	23SA	3629	7/7	0.97	0.06	87,91,106,176	0
58	MG	23SB	3012	1/1	0.97	0.05	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	MG	16SA	2278	1/1	0.97	0.15	93,93,93,93	0
60	OHX	23SA	3544	7/7	0.97	0.12	64,81,89,161	0
60	OHX	23SB	3369	7/7	0.97	0.09	60,77,90,136	0
60	OHX	23SB	3371	7/7	0.97	0.08	104,112,125,154	0
60	OHX	23SA	3545	7/7	0.97	0.06	77,91,112,179	0
58	MG	23SA	3188	1/1	0.97	0.05	50,50,50,50	0
60	OHX	23SB	3374	7/7	0.97	0.09	82,95,101,131	0
60	OHX	23SB	3375	7/7	0.97	0.07	82,94,101,135	0
60	OHX	5SA	211	7/7	0.97	0.06	90,102,112,165	0
60	OHX	23SA	3547	7/7	0.97	0.08	69,73,100,135	0
58	MG	23SA	3277	1/1	0.97	0.08	59,59,59,59	0
58	MG	23SA	3308	1/1	0.97	0.12	38,38,38,38	0
58	MG	23SA	3310	1/1	0.97	0.15	57,57,57,57	0
60	OHX	23SA	3551	7/7	0.97	0.06	90,96,108,182	0
58	MG	16SA	2270	1/1	0.97	0.06	73,73,73,73	0
60	OHX	16SA	2342	7/7	0.97	0.09	98,105,114,137	0
60	OHX	23SB	3390	7/7	0.97	0.06	82,92,101,166	0
60	OHX	23SB	3391	7/7	0.97	0.08	92,101,112,165	0
60	OHX	16SA	2347	7/7	0.97	0.08	107,109,124,145	0
58	MG	23SB	3200	1/1	0.97	0.08	82,82,82,82	0
58	MG	23SB	3201	1/1	0.97	0.07	73,73,73,73	0
60	OHX	16SA	2353	7/7	0.97	0.07	89,94,102,156	0
58	MG	23SB	3019	1/1	0.97	0.10	51,51,51,51	0
59	K	23SB	3279	1/1	0.97	0.04	52,52,52,52	0
58	MG	23SA	3256	1/1	0.97	0.07	34,34,34,34	0
58	MG	23SA	3232	1/1	0.97	0.07	82,82,82,82	0
60	OHX	23SB	3402	7/7	0.97	0.06	96,103,111,160	0
60	OHX	16SB	2340	7/7	0.97	0.07	95,106,110,161	0
60	OHX	23SB	3405	7/7	0.97	0.07	100,109,116,160	0
60	OHX	16SA	2359	7/7	0.97	0.13	75,86,97,154	0
60	OHX	16SB	2342	7/7	0.97	0.06	98,111,117,180	0
59	K	23SA	3376	1/1	0.97	0.06	59,59,59,59	0
58	MG	23SA	3021	1/1	0.97	0.17	43,43,43,43	0
60	OHX	23SA	3565	7/7	0.97	0.09	67,68,89,172	0
60	OHX	23SB	3387	7/7	0.98	0.06	80,92,108,123	0
60	OHX	23SA	3536	7/7	0.98	0.06	72,84,94,136	0
59	K	23SA	3370	1/1	0.98	0.03	61,61,61,61	0
59	K	23SA	3371	1/1	0.98	0.03	41,41,41,41	0
58	MG	23SA	3284	1/1	0.98	0.05	42,42,42,42	0
58	MG	23SA	3164	1/1	0.98	0.09	33,33,33,33	0
58	MG	23SB	3226	1/1	0.98	0.08	76,76,76,76	0
60	OHX	23SB	3394	7/7	0.98	0.07	72,84,101,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	MG	23SA	3262	1/1	0.98	0.04	63,63,63,63	0
60	OHX	16SB	2325	7/7	0.98	0.09	84,96,101,124	0
58	MG	23SB	3228	1/1	0.98	0.05	91,91,91,91	0
60	OHX	16SB	2330	7/7	0.98	0.07	85,93,109,126	0
60	OHX	16SB	2331	7/7	0.98	0.06	97,100,108,156	0
60	OHX	16SB	2332	7/7	0.98	0.08	99,104,117,138	0
60	OHX	23SB	3401	7/7	0.98	0.05	87,94,107,156	0
59	K	23SA	3377	1/1	0.98	0.06	38,38,38,38	0
58	MG	23SA	3205	1/1	0.98	0.06	39,39,39,39	0
60	OHX	23SB	3404	7/7	0.98	0.06	70,80,97,130	0
58	MG	23SA	3288	1/1	0.98	0.04	44,44,44,44	0
60	OHX	16SB	2337	7/7	0.98	0.05	90,94,105,154	0
58	MG	23SA	3053	1/1	0.98	0.30	36,36,36,36	0
60	OHX	16SB	2339	7/7	0.98	0.05	88,95,111,154	0
58	MG	23SA	3290	1/1	0.98	0.05	50,50,50,50	0
58	MG	23SA	3181	1/1	0.98	0.05	42,42,42,42	0
58	MG	23SA	3292	1/1	0.98	0.08	55,55,55,55	0
60	OHX	23SB	3412	7/7	0.98	0.06	104,109,121,169	0
60	OHX	16SA	2343	7/7	0.98	0.08	81,94,106,121	0
60	OHX	16SB	2344	7/7	0.98	0.05	101,109,122,168	0
60	OHX	16SA	2346	7/7	0.98	0.07	78,80,100,113	0
58	MG	23SA	3267	1/1	0.98	0.04	43,43,43,43	0
58	MG	23SA	3329	1/1	0.98	0.09	49,49,49,49	0
60	OHX	16SA	2349	7/7	0.98	0.07	90,104,118,118	0
60	OHX	23SB	3419	7/7	0.98	0.08	79,86,91,139	0
60	OHX	16SA	2350	7/7	0.98	0.06	100,101,107,154	0
58	MG	23SA	3222	1/1	0.98	0.05	32,32,32,32	0
60	OHX	23SB	3422	7/7	0.98	0.05	81,92,100,148	0
60	OHX	23SA	3437	7/7	0.98	0.17	54,56,72,138	0
60	OHX	23SA	3440	7/7	0.98	0.14	43,67,70,125	0
60	OHX	23SA	3441	7/7	0.98	0.12	78,81,98,141	0
60	OHX	23SA	3453	7/7	0.98	0.09	63,75,88,98	0
60	OHX	23SB	3427	7/7	0.98	0.06	78,91,105,136	0
60	OHX	16SA	2352	7/7	0.98	0.07	78,83,104,130	0
60	OHX	23SA	3457	7/7	0.98	0.07	50,69,94,96	0
60	OHX	23SA	3458	7/7	0.98	0.06	60,71,82,107	0
58	MG	23SA	3269	1/1	0.98	0.04	52,52,52,52	0
60	OHX	23SA	3460	7/7	0.98	0.06	66,80,100,111	0
60	OHX	23SA	3461	7/7	0.98	0.06	70,73,97,117	0
60	OHX	23SA	3463	7/7	0.98	0.09	35,55,79,103	0
60	OHX	16SB	2362	7/7	0.98	0.06	94,96,112,155	0
60	OHX	23SA	3464	7/7	0.98	0.08	70,74,94,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
60	OHX	23SB	3437	7/7	0.98	0.05	93,101,104,163	0
60	OHX	16SA	2354	7/7	0.98	0.06	84,96,105,152	0
58	MG	23SB	3239	1/1	0.98	0.07	85,85,85,85	0
58	MG	23SA	3242	1/1	0.98	0.04	38,38,38,38	0
60	OHX	23SA	3469	7/7	0.98	0.09	60,67,79,108	0
58	MG	23SB	3187	1/1	0.98	0.09	54,54,54,54	0
60	OHX	23SA	3471	7/7	0.98	0.07	72,75,95,114	0
60	OHX	23SA	3472	7/7	0.98	0.07	57,69,75,136	0
60	OHX	23SA	3474	7/7	0.98	0.05	85,92,102,143	0
60	OHX	23SA	3475	7/7	0.98	0.08	69,79,97,138	0
60	OHX	23SA	3476	7/7	0.98	0.06	76,91,98,125	0
58	MG	23SB	3135	1/1	0.98	0.06	62,62,62,62	0
60	OHX	23SA	3581	7/7	0.98	0.06	83,96,108,158	0
59	K	23SA	3392	1/1	0.98	0.03	47,47,47,47	0
60	OHX	23SA	3583	7/7	0.98	0.05	86,90,110,172	0
58	MG	5SB	204	1/1	0.98	0.04	81,81,81,81	0
58	MG	23SA	3297	1/1	0.98	0.06	59,59,59,59	0
58	MG	23SA	3298	1/1	0.98	0.05	32,32,32,32	0
60	OHX	23SA	3482	7/7	0.98	0.12	64,70,94,116	0
58	MG	23SA	3209	1/1	0.98	0.06	48,48,48,48	0
60	OHX	23SA	3485	7/7	0.98	0.06	80,92,101,147	0
58	MG	23SB	3140	1/1	0.98	0.04	44,44,44,44	0
58	MG	L27B	101	1/1	0.98	0.11	63,63,63,63	0
60	OHX	23SA	3488	7/7	0.98	0.07	76,78,90,125	0
58	MG	23SA	3244	1/1	0.98	0.06	20,20,20,20	0
60	OHX	23SA	3490	7/7	0.98	0.06	86,96,102,157	0
60	OHX	23SA	3491	7/7	0.98	0.07	74,84,104,130	0
58	MG	23SB	3194	1/1	0.98	0.04	71,71,71,71	0
60	OHX	23SA	3493	7/7	0.98	0.07	78,81,99,132	0
58	MG	23SB	3142	1/1	0.98	0.06	50,50,50,50	0
59	K	23SB	3284	1/1	0.98	0.03	64,64,64,64	0
58	MG	5SA	206	1/1	0.98	0.10	75,75,75,75	0
58	MG	23SA	3183	1/1	0.98	0.06	50,50,50,50	0
58	MG	23SA	3057	1/1	0.98	0.06	45,45,45,45	0
60	OHX	23SA	3500	7/7	0.98	0.08	76,80,87,134	0
60	OHX	16SA	2374	7/7	0.98	0.08	78,87,97,143	0
60	OHX	23SA	3502	7/7	0.98	0.07	74,89,108,136	0
58	MG	23SA	3304	1/1	0.98	0.04	39,39,39,39	0
59	K	23SA	3406	1/1	0.98	0.09	60,60,60,60	0
58	MG	23SA	3305	1/1	0.98	0.08	48,48,48,48	0
58	MG	23SB	3151	1/1	0.98	0.11	33,33,33,33	0
60	OHX	23SA	3507	7/7	0.98	0.06	91,98,112,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	MG	23SB	3152	1/1	0.98	0.06	53,53,53,53	0
60	OHX	PSIB	104	7/7	0.98	0.07	100,109,114,132	0
59	K	23SB	3293	1/1	0.98	0.06	67,67,67,67	0
58	MG	23SB	3203	1/1	0.98	0.06	53,53,53,53	0
58	MG	23SA	3228	1/1	0.98	0.04	56,56,56,56	0
58	MG	23SB	3154	1/1	0.98	0.04	55,55,55,55	0
58	MG	23SB	3155	1/1	0.98	0.06	73,73,73,73	0
60	OHX	23SB	3332	7/7	0.98	0.07	75,95,101,131	0
58	MG	23SA	3276	1/1	0.98	0.06	74,74,74,74	0
58	MG	23SA	3212	1/1	0.98	0.05	56,56,56,56	0
60	OHX	23SB	3343	7/7	0.98	0.07	65,75,88,109	0
58	MG	23SB	3209	1/1	0.98	0.05	59,59,59,59	0
60	OHX	23SB	3345	7/7	0.98	0.09	66,76,89,118	0
59	K	16SA	2306	1/1	0.98	0.09	69,69,69,69	0
60	OHX	23SB	3348	7/7	0.98	0.12	64,74,82,129	0
60	OHX	23SA	3518	7/7	0.98	0.07	60,64,93,123	0
60	OHX	23SB	3350	7/7	0.98	0.08	78,81,103,108	0
58	MG	23SB	3211	1/1	0.98	0.04	41,41,41,41	0
60	OHX	23SB	3353	7/7	0.98	0.06	86,93,106,141	0
58	MG	23SA	3309	1/1	0.98	0.04	71,71,71,71	0
60	OHX	23SB	3356	7/7	0.98	0.07	75,88,102,144	0
58	MG	L27A	102	1/1	0.98	0.05	63,63,63,63	0
60	OHX	23SA	3522	7/7	0.98	0.05	88,94,101,161	0
58	MG	23SB	3214	1/1	0.98	0.06	69,69,69,69	0
60	OHX	23SB	3360	7/7	0.98	0.06	90,95,105,131	0
58	MG	23SA	3231	1/1	0.98	0.06	78,78,78,78	0
60	OHX	23SB	3362	7/7	0.98	0.05	91,96,101,157	0
60	OHX	23SB	3363	7/7	0.98	0.07	67,75,85,121	0
58	MG	23SA	3253	1/1	0.98	0.09	29,29,29,29	0
60	OHX	23SA	3526	7/7	0.98	0.06	68,76,93,135	0
60	OHX	23SB	3367	7/7	0.98	0.10	68,73,95,125	0
60	OHX	23SB	3368	7/7	0.98	0.07	79,91,110,135	0
58	MG	16SA	2209	1/1	0.98	0.10	62,62,62,62	0
60	OHX	23SB	3370	7/7	0.98	0.10	69,86,96,123	0
58	MG	23SA	3313	1/1	0.98	0.12	86,86,86,86	0
58	MG	23SA	3199	1/1	0.98	0.07	36,36,36,36	0
58	MG	16SA	2268	1/1	0.98	0.05	50,50,50,50	0
60	OHX	5SA	209	7/7	0.98	0.08	73,79,90,91	0
60	OHX	5SB	207	7/7	0.98	0.08	80,94,115,116	0
60	OHX	23SA	3531	7/7	0.98	0.05	86,94,101,174	0
60	OHX	23SB	3376	7/7	0.98	0.07	89,92,107,148	0
60	OHX	23SB	3377	7/7	0.98	0.06	76,93,102,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	MG	23SB	3167	1/1	0.98	0.07	50,50,50,50	0
60	OHX	23SB	3379	7/7	0.98	0.06	92,100,107,135	0
60	OHX	23SB	3380	7/7	0.98	0.07	86,93,108,134	0
58	MG	23SB	3168	1/1	0.98	0.04	45,45,45,45	0
59	K	23SA	3368	1/1	0.98	0.04	39,39,39,39	0
60	OHX	5SA	214	7/7	0.98	0.06	71,90,101,152	0
60	OHX	5SA	215	7/7	0.98	0.04	98,108,110,190	0
58	MG	23SA	3235	1/1	0.98	0.06	38,38,38,38	0
60	OHX	23SB	3386	7/7	0.98	0.09	58,74,95,127	0
58	MG	23SA	3227	1/1	0.99	0.04	68,68,68,68	0
60	OHX	23SB	3351	7/7	0.99	0.08	68,84,98,103	0
58	MG	23SA	3299	1/1	0.99	0.03	58,58,58,58	0
58	MG	23SA	3192	1/1	0.99	0.09	40,40,40,40	0
60	OHX	23SB	3354	7/7	0.99	0.07	83,92,96,126	0
58	MG	23SA	3260	1/1	0.99	0.05	44,44,44,44	0
58	MG	23SA	3229	1/1	0.99	0.05	69,69,69,69	0
58	MG	23SA	3201	1/1	0.99	0.04	36,36,36,36	0
58	MG	23SB	3139	1/1	0.99	0.03	42,42,42,42	0
58	MG	23SB	3171	1/1	0.99	0.05	42,42,42,42	0
58	MG	23SA	3326	1/1	0.99	0.06	60,60,60,60	0
60	OHX	23SA	3484	7/7	0.99	0.06	68,80,83,121	0
58	MG	23SA	3219	1/1	0.99	0.05	46,46,46,46	0
58	MG	23SA	3193	1/1	0.99	0.06	46,46,46,46	0
60	OHX	16SA	2367	7/7	0.99	0.06	88,96,101,142	0
60	OHX	23SB	3365	7/7	0.99	0.05	102,104,111,148	0
58	MG	23SB	3143	1/1	0.99	0.06	46,46,46,46	0
58	MG	23SB	3210	1/1	0.99	0.09	73,73,73,73	0
58	MG	23SB	3176	1/1	0.99	0.03	44,44,44,44	0
58	MG	23SA	3246	1/1	0.99	0.04	41,41,41,41	0
58	MG	23SA	3330	1/1	0.99	0.03	47,47,47,47	0
58	MG	23SB	3146	1/1	0.99	0.09	61,61,61,61	0
60	OHX	23SA	3494	7/7	0.99	0.06	48,58,79,112	0
60	OHX	ASIA	101	7/7	0.99	0.06	94,101,119,138	0
58	MG	23SB	3180	1/1	0.99	0.06	42,42,42,42	0
58	MG	23SA	3266	1/1	0.99	0.09	45,45,45,45	0
60	OHX	PSIA	105	7/7	0.99	0.06	84,94,100,118	0
58	MG	23SA	3195	1/1	0.99	0.05	33,33,33,33	0
58	MG	23SB	3149	1/1	0.99	0.11	64,64,64,64	0
58	MG	23SA	3196	1/1	0.99	0.09	65,65,65,65	0
59	K	23SB	3255	1/1	0.99	0.04	51,51,51,51	0
58	MG	23SA	3184	1/1	0.99	0.04	23,23,23,23	0
60	OHX	23SA	3438	7/7	0.99	0.10	37,46,60,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
60	OHX	16SA	2337	7/7	0.99	0.09	67,67,82,96	0
60	OHX	16SA	2338	7/7	0.99	0.10	64,86,90,90	0
60	OHX	23SA	3442	7/7	0.99	0.10	56,63,82,104	0
60	OHX	23SA	3443	7/7	0.99	0.09	44,56,64,99	0
60	OHX	23SA	3444	7/7	0.99	0.07	59,69,82,94	0
60	OHX	23SA	3446	7/7	0.99	0.06	56,65,79,90	0
60	OHX	23SA	3447	7/7	0.99	0.11	49,60,75,116	0
60	OHX	23SA	3448	7/7	0.99	0.06	60,70,78,91	0
60	OHX	23SA	3449	7/7	0.99	0.08	69,80,87,90	0
60	OHX	23SA	3450	7/7	0.99	0.07	77,87,96,98	0
60	OHX	23SA	3451	7/7	0.99	0.08	63,74,84,95	0
60	OHX	L4A	304	7/7	0.99	0.20	33,37,51,146	0
60	OHX	23SA	3452	7/7	0.99	0.07	54,64,86,94	0
60	OHX	L17A	202	7/7	0.99	0.08	61,71,78,89	0
60	OHX	L19A	201	7/7	0.99	0.06	79,85,96,119	0
60	OHX	16SA	2339	7/7	0.99	0.09	60,69,87,91	0
60	OHX	16SA	2340	7/7	0.99	0.07	74,81,92,100	0
60	OHX	23SA	3455	7/7	0.99	0.08	56,72,90,98	0
60	OHX	23SA	3456	7/7	0.99	0.07	69,75,93,104	0
60	OHX	16SB	2322	7/7	0.99	0.08	72,83,93,94	0
60	OHX	16SB	2323	7/7	0.99	0.08	77,87,98,102	0
60	OHX	16SB	2324	7/7	0.99	0.07	86,88,100,108	0
60	OHX	16SA	2341	7/7	0.99	0.06	82,101,107,124	0
60	OHX	16SB	2326	7/7	0.99	0.06	96,105,113,125	0
60	OHX	16SB	2327	7/7	0.99	0.06	87,94,111,120	0
58	MG	23SA	3250	1/1	0.99	0.06	49,49,49,49	0
60	OHX	16SB	2329	7/7	0.99	0.06	67,78,92,96	0
58	MG	23SA	3251	1/1	0.99	0.10	39,39,39,39	0
60	OHX	16SA	2344	7/7	0.99	0.06	78,92,99,110	0
60	OHX	16SA	2345	7/7	0.99	0.06	85,99,115,130	0
60	OHX	16SB	2333	7/7	0.99	0.05	92,96,103,121	0
60	OHX	23SA	3462	7/7	0.99	0.06	61,68,88,100	0
58	MG	23SA	3215	1/1	0.99	0.04	47,47,47,47	0
58	MG	5SA	204	1/1	0.99	0.03	60,60,60,60	0
60	OHX	23SB	3324	7/7	0.99	0.14	37,44,75,112	0
58	MG	5SA	205	1/1	0.99	0.04	54,54,54,54	0
60	OHX	23SB	3328	7/7	0.99	0.10	53,62,75,105	0
60	OHX	23SB	3329	7/7	0.99	0.08	65,75,94,96	0
60	OHX	23SB	3330	7/7	0.99	0.05	58,71,85,87	0
60	OHX	23SB	3331	7/7	0.99	0.07	83,87,102,104	0
58	MG	23SA	3225	1/1	0.99	0.07	60,60,60,60	0
60	OHX	23SB	3334	7/7	0.99	0.08	72,79,82,102	0

*Continued on next page...*



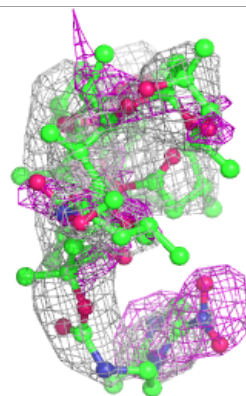
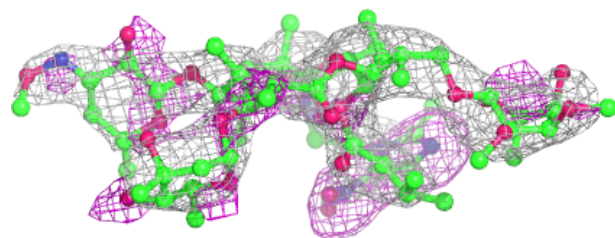
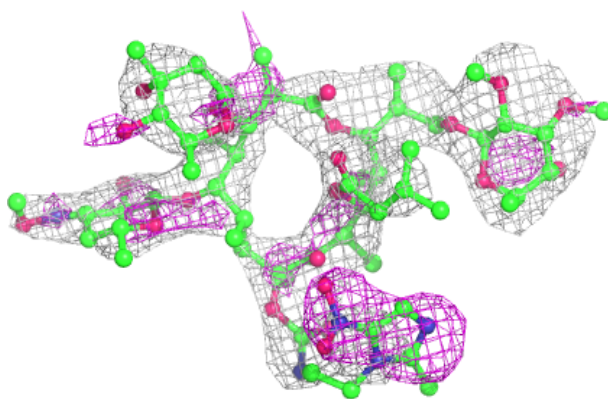
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	OHX	23SA	3467	7/7	0.99	0.06	67,87,98,117	0
60	OHX	23SB	3336	7/7	0.99	0.06	58,76,89,104	0
60	OHX	23SB	3337	7/7	0.99	0.06	79,83,95,96	0
60	OHX	23SB	3338	7/7	0.99	0.07	74,84,95,113	0
60	OHX	23SB	3339	7/7	0.99	0.08	95,104,111,114	0
60	OHX	23SB	3340	7/7	0.99	0.07	79,82,103,105	0
60	OHX	23SB	3341	7/7	0.99	0.06	72,88,98,114	0
58	MG	23SA	3254	1/1	0.99	0.03	46,46,46,46	0
58	MG	23SA	3255	1/1	0.99	0.04	72,72,72,72	0
58	MG	L4A	302	1/1	0.99	0.04	72,72,72,72	0
58	MG	23SA	3238	1/1	0.99	0.04	33,33,33,33	0
60	OHX	L17B	201	7/7	0.99	0.10	67,75,89,93	0
58	MG	16SA	2264	1/1	0.99	0.03	45,45,45,45	0
60	OHX	23SB	3347	7/7	0.99	0.06	72,78,92,131	0
60	OHX	23SA	3473	7/7	0.99	0.05	72,78,93,118	0
58	MG	23SB	3163	1/1	0.99	0.06	45,45,45,45	0
60	OHX	23SB	3327	7/7	1.00	0.08	67,73,94,97	0
58	MG	23SA	3317	1/1	1.00	0.03	52,52,52,52	0
58	MG	L3A	302	1/1	1.00	0.01	29,29,29,29	0
60	OHX	23SA	3439	7/7	1.00	0.06	65,75,79,85	0
58	MG	23SA	3200	1/1	1.00	0.08	39,39,39,39	0
58	MG	23SA	3208	1/1	1.00	0.07	33,33,33,33	0
60	OHX	23SB	3333	7/7	1.00	0.05	67,70,73,93	0
58	MG	23SA	3204	1/1	1.00	0.02	32,32,32,32	0
58	MG	23SA	3194	1/1	1.00	0.04	33,33,33,33	0
58	MG	23SA	3182	1/1	1.00	0.07	46,46,46,46	0
60	OHX	23SB	3325	7/7	1.00	0.10	57,58,71,96	0
60	OHX	23SA	3445	7/7	1.00	0.06	58,63,73,86	0

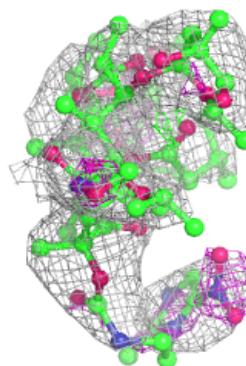
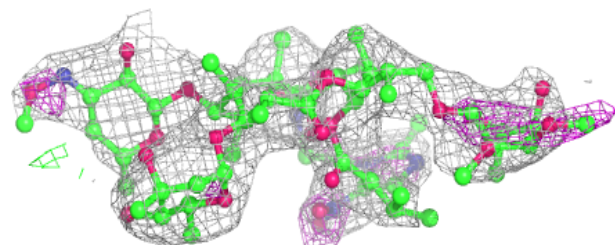
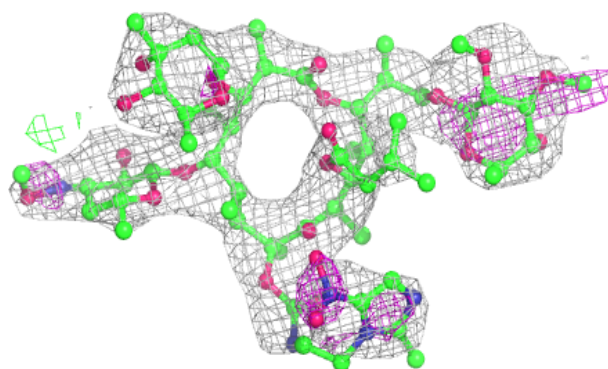
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around SJH 23SB 3323:**

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

**Electron density around SJH 23SA 3436:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.