



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 11, 2025 – 07:47 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

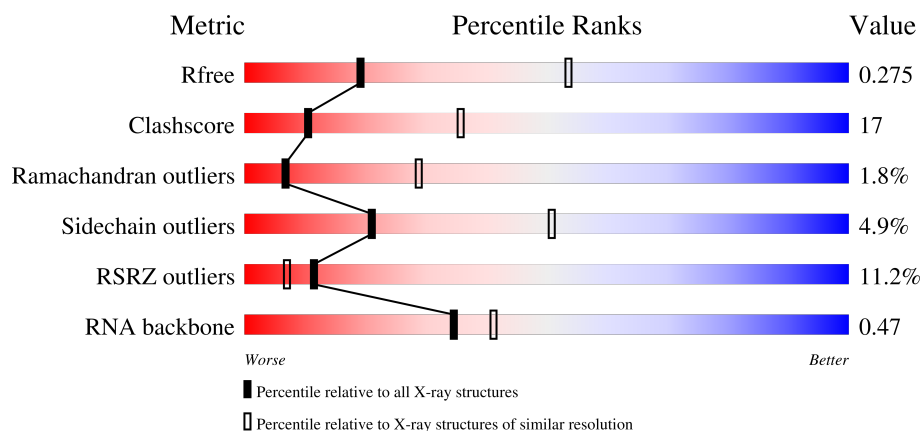
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	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 ≥ 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>71%</div> <div>24%</div> <div>.</div> </div>
1	16SB	1512	<div> <div>%</div> <div>71%</div> <div>25%</div> <div>.</div> </div>
2	S2A	256	<div> <div>31%</div> <div>53%</div> <div>35%</div> <div>5%</div> <div>7%</div> </div>
2	S2B	256	<div> <div>30%</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	






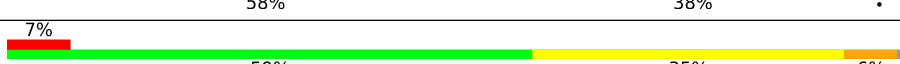
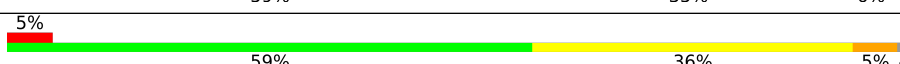
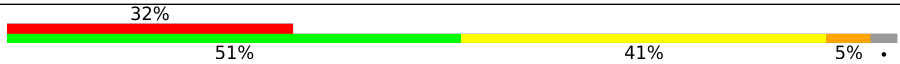

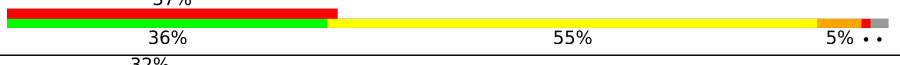
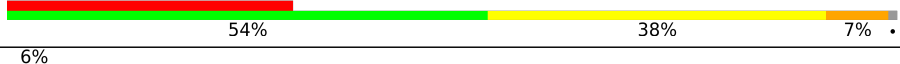
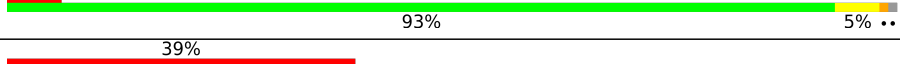
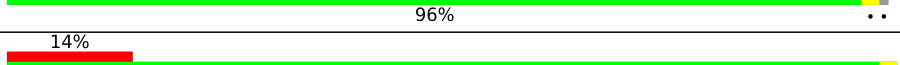
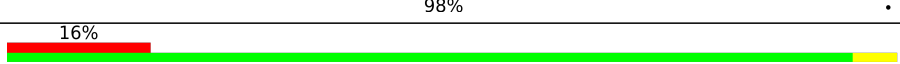
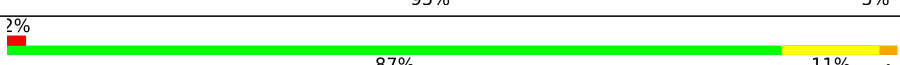
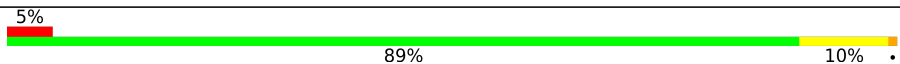
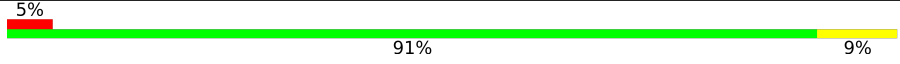
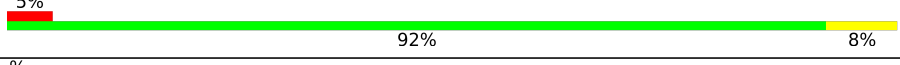
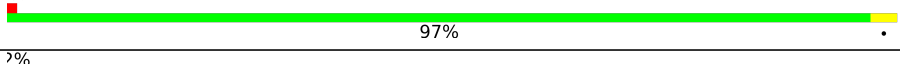
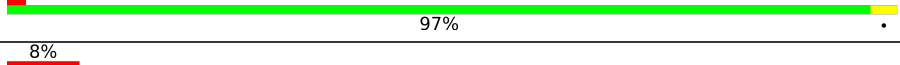
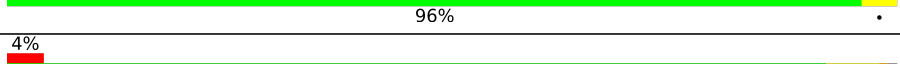
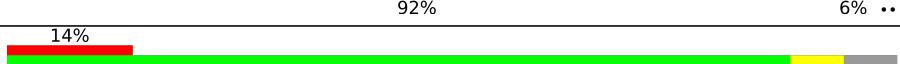



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Mol	Chain	Length	Quality of chain
15	S15B	89	
16	S16A	88	
16	S16B	88	
17	S17A	105	
17	S17B	105	
18	S18A	88	
18	S18B	88	
19	S19A	93	
19	S19B	93	
20	S20A	106	
20	S20B	106	
21	THXA	27	
21	THXB	27	
22	ASIA	76	
23	PSIA	76	
23	PSIB	76	
24	ESIA	76	
24	ESIB	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).

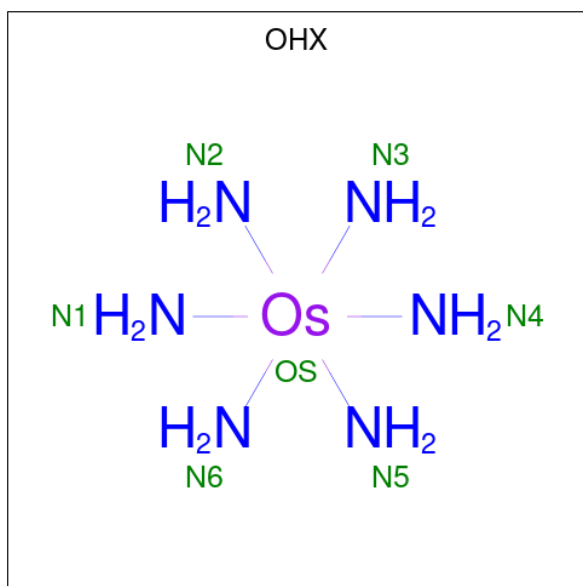
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	16SA	46	Total 46	K 46	0	0
59	S6A	1	Total 1	K 1	0	0
59	S13A	1	Total 1	K 1	0	0
59	S20A	1	Total 1	K 1	0	0
59	PSIA	2	Total 2	K 2	0	0
59	23SA	101	Total 101	K 101	0	0
59	5SA	2	Total 2	K 2	0	0
59	L2A	1	Total 1	K 1	0	0
59	L3A	1	Total 1	K 1	0	0
59	L4A	1	Total 1	K 1	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		

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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		

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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
			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
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60	23SA	1	Total	N	Os	0	0
			7	6	1		
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60	23SA	1	Total	N	Os	0	0
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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
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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	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
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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		
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			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		
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
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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		
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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		
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			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
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			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
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60	23SA	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	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
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60	23SA	1	Total	N	Os	0	0
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60	23SA	1	Total	N	Os	0	0
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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		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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
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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
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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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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
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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		
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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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		
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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		
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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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			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
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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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			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
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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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			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		
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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		
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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		
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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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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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		
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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		
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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		
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			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
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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		
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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		
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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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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		
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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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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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		
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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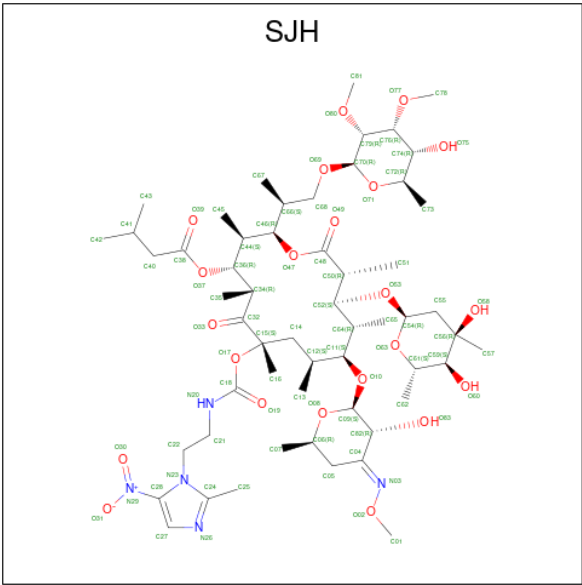
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	23SB	1	Total	N	Os	0	0
			7	6	1		
60	5SB	1	Total	N	Os	0	0
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60	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
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	L17B	1	Total	N	Os	0	0
			7	6	1		
60	L20B	1	Total	N	Os	0	0
			7	6	1		
60	L35B	1	Total	N	Os	0	0
			7	6	1		

- 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: C₅₆H₉₃N₅O₂₂).



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

- Molecule 62 is water.

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

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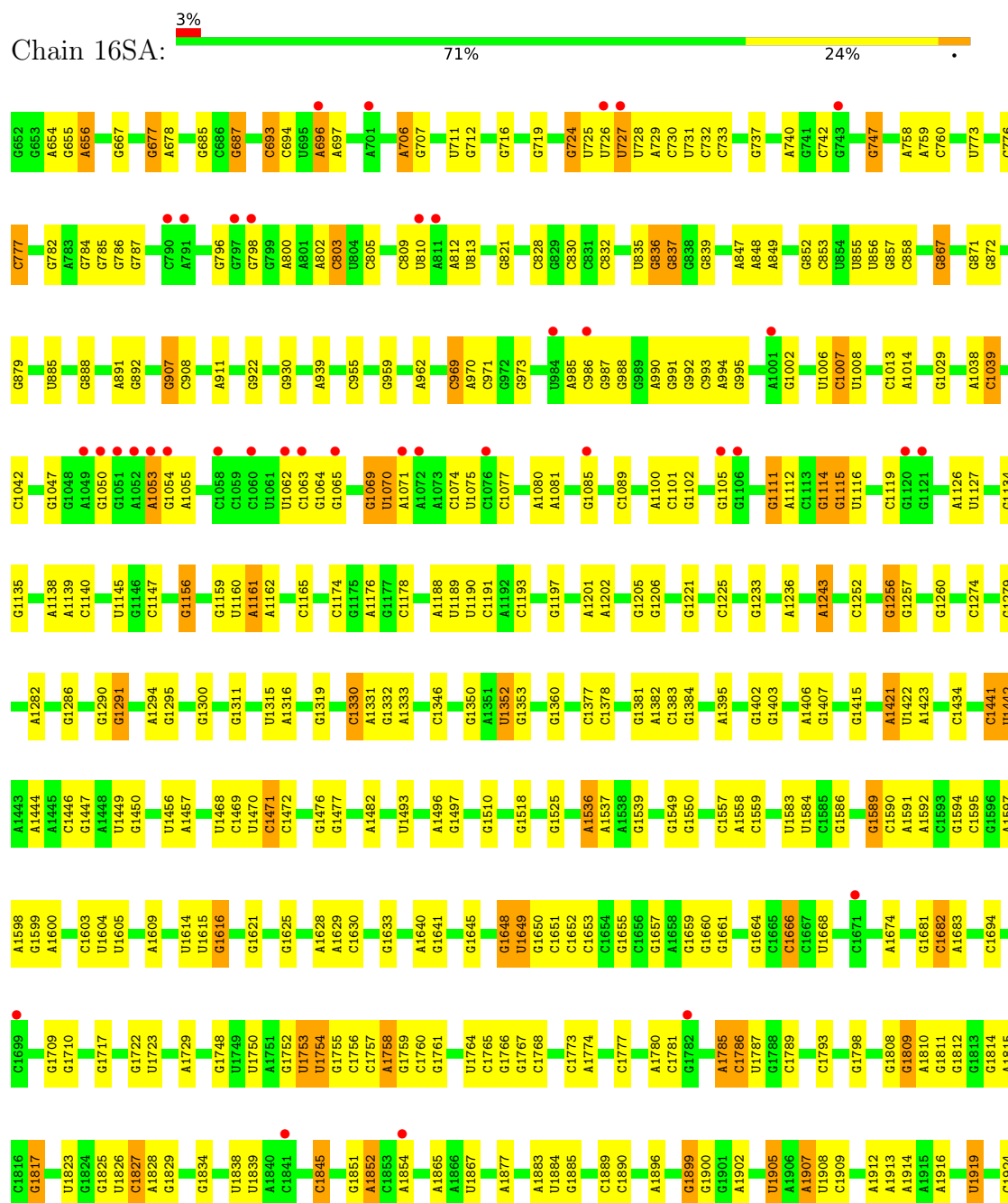
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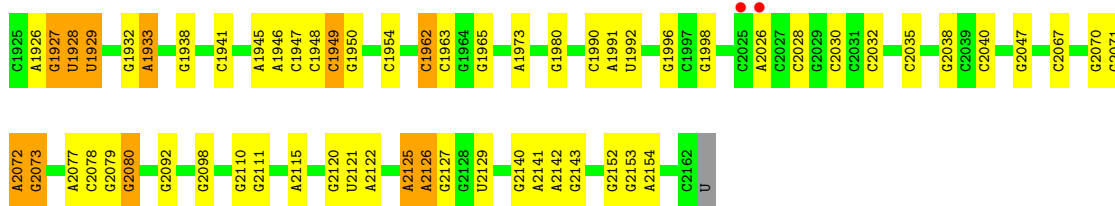
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	L30A	1	Total 1	O 1	0	0
62	L34A	1	Total 1	O 1	0	0
62	L35A	1	Total 1	O 1	0	0
62	16SB	158	Total 158	O 158	0	0
62	S4B	1	Total 1	O 1	0	0
62	S5B	1	Total 1	O 1	0	0
62	S9B	1	Total 1	O 1	0	0
62	S12B	2	Total 2	O 2	0	0
62	S14B	2	Total 2	O 2	0	0
62	23SB	518	Total 518	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

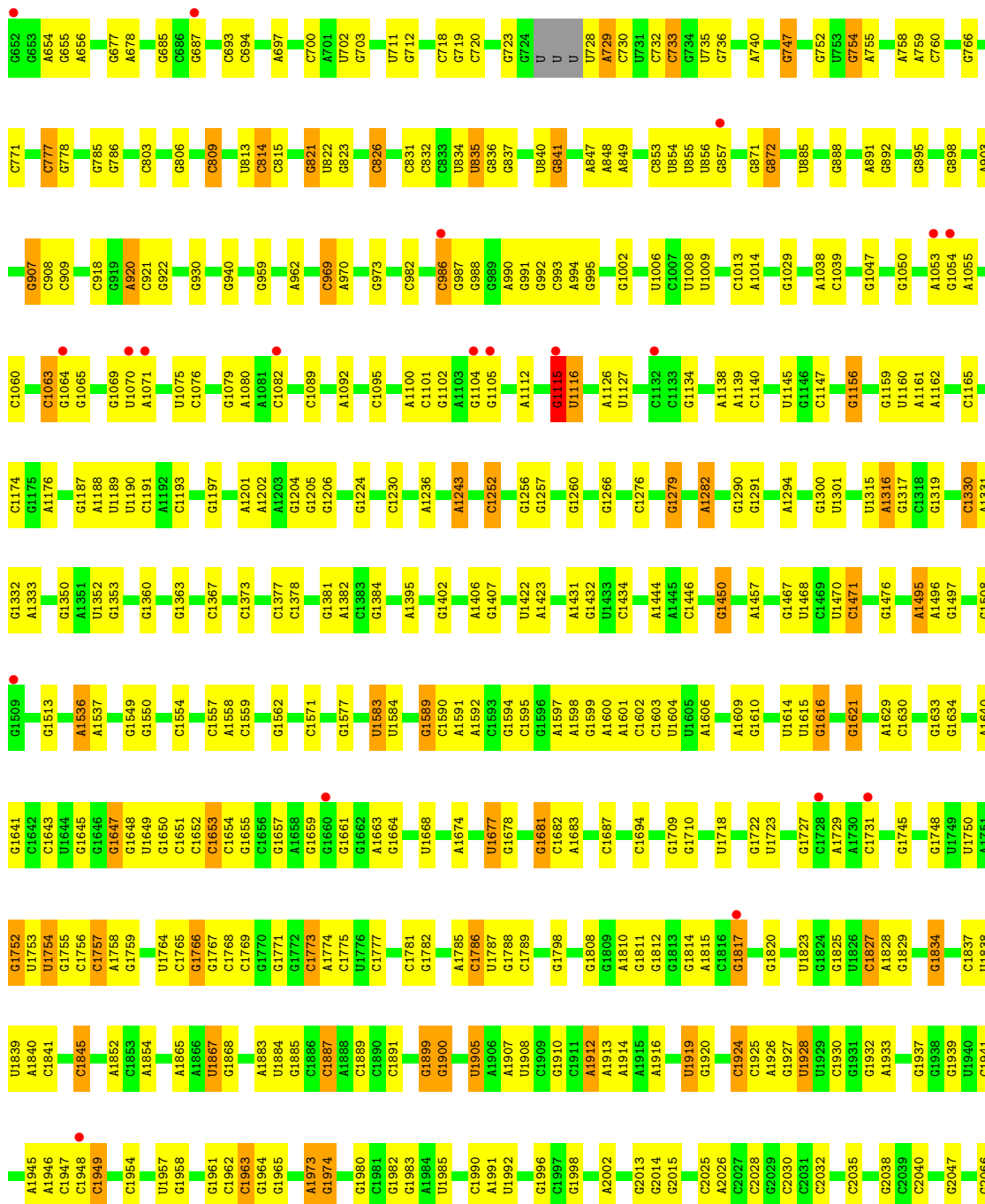
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

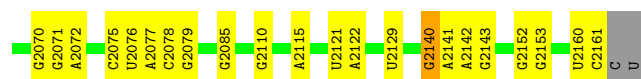
• Molecule 1: 16S rRNA



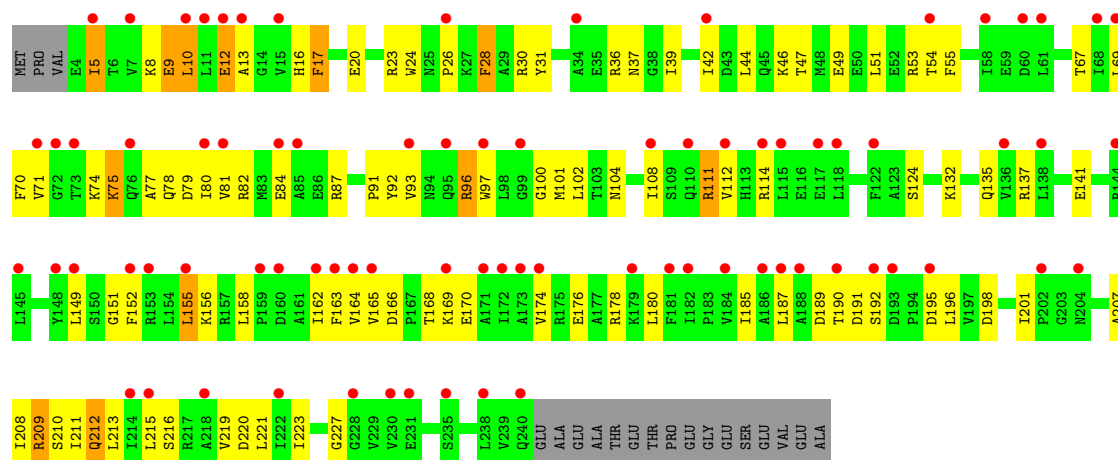


• Molecule 1: 16S rRNA

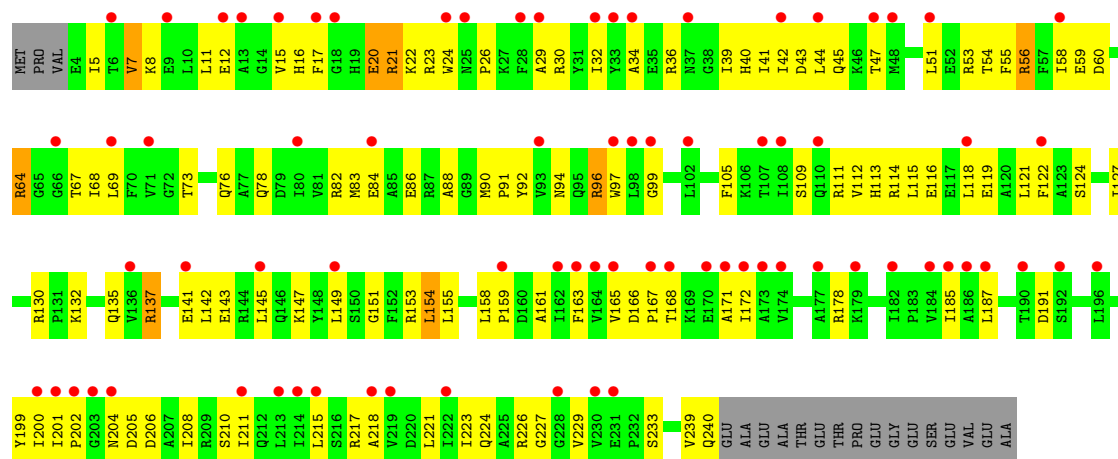




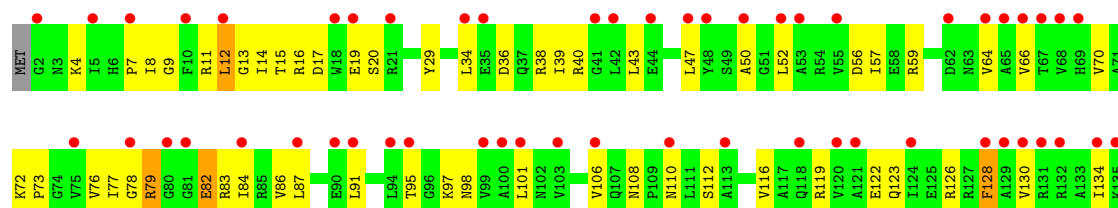
• Molecule 2: 30S ribosomal protein S2

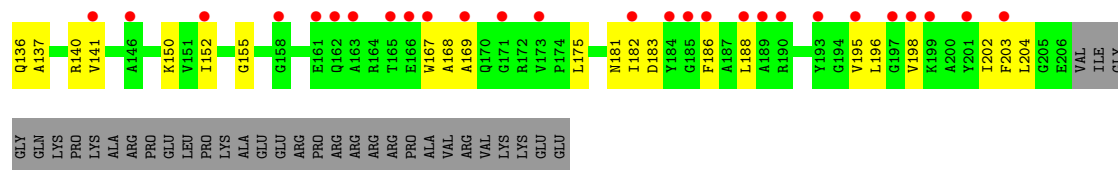


• Molecule 2: 30S ribosomal protein S2

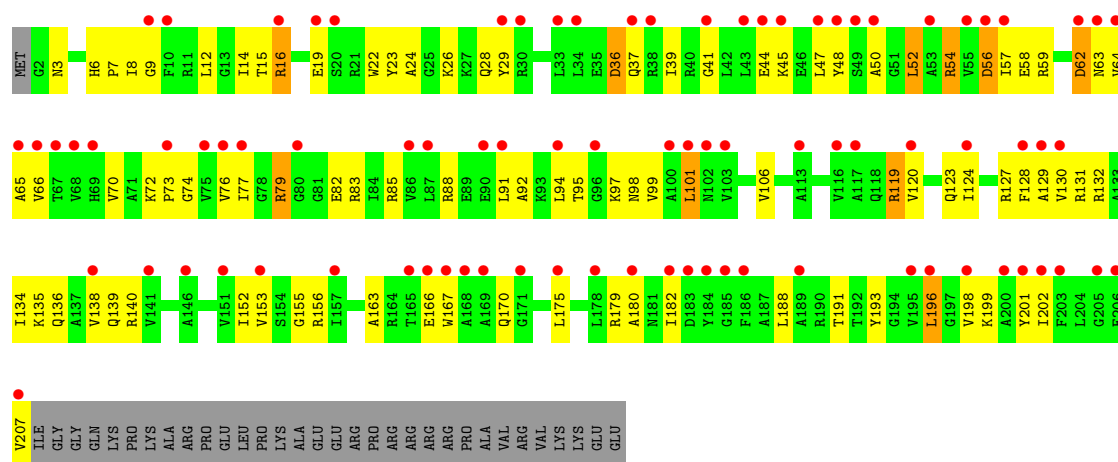


• Molecule 3: 30S ribosomal protein S3

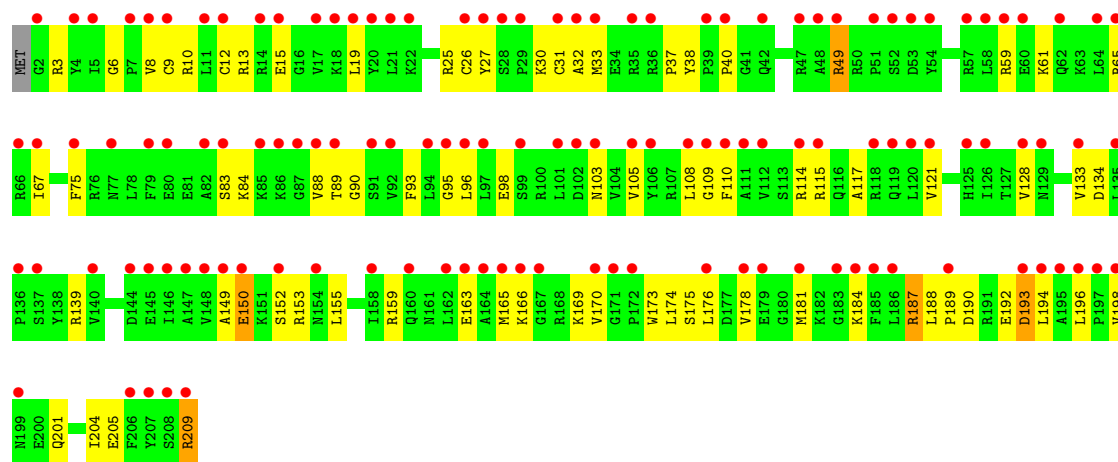




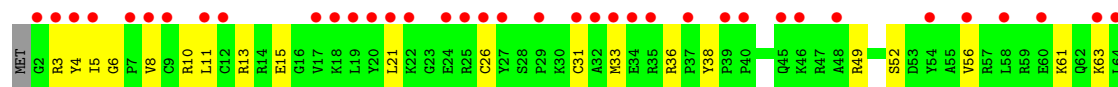
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

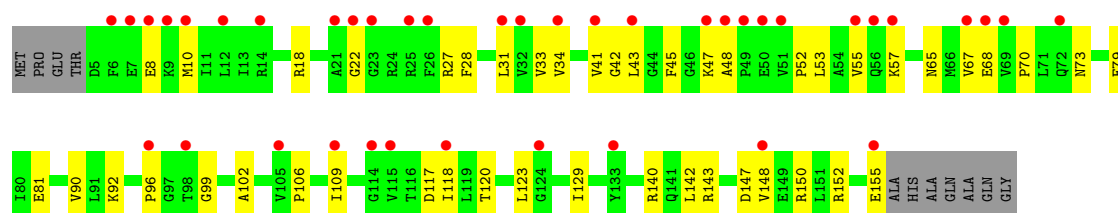


• Molecule 4: 30S ribosomal protein S4

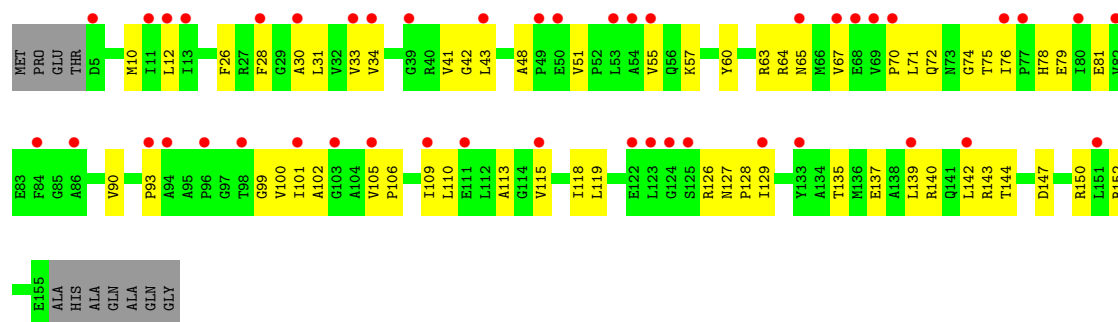




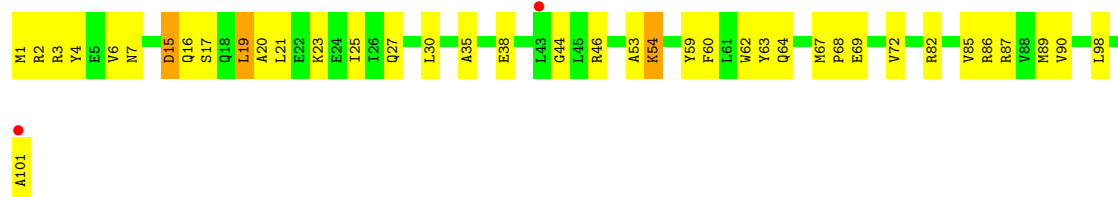
• Molecule 5: 30S ribosomal protein S5



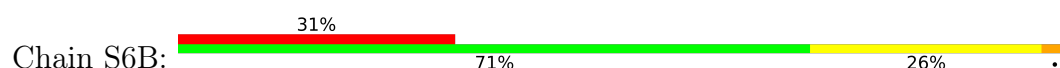
• Molecule 5: 30S ribosomal protein S5

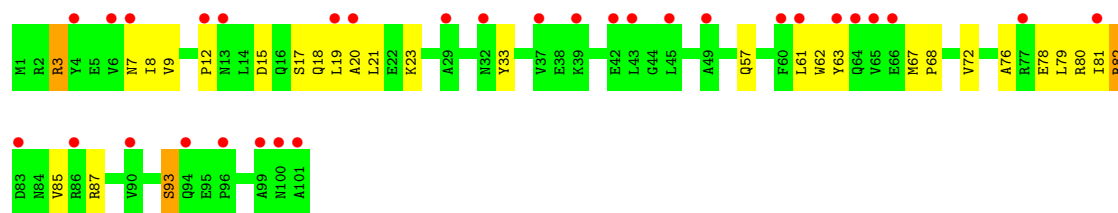


• Molecule 6: 30S ribosomal protein S6

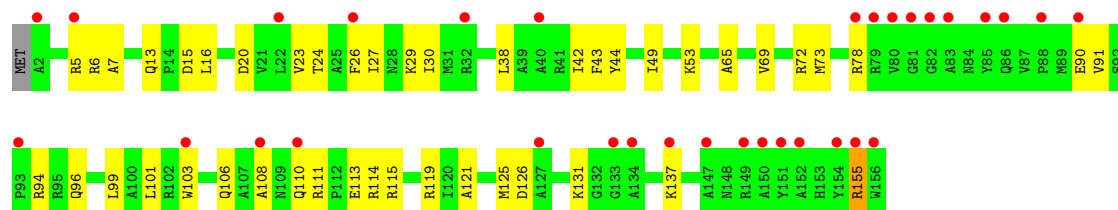
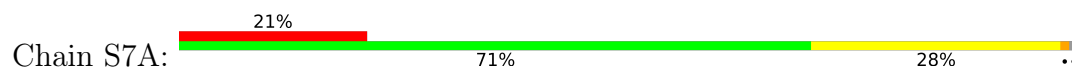


• Molecule 6: 30S ribosomal protein S6

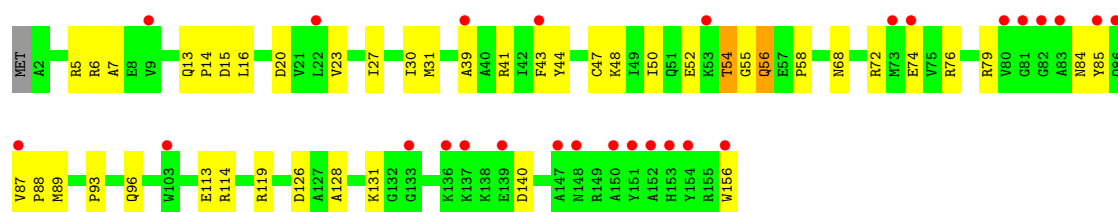
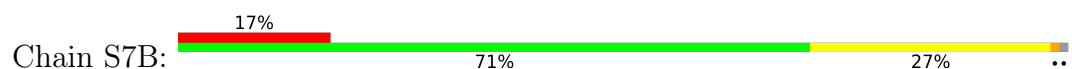




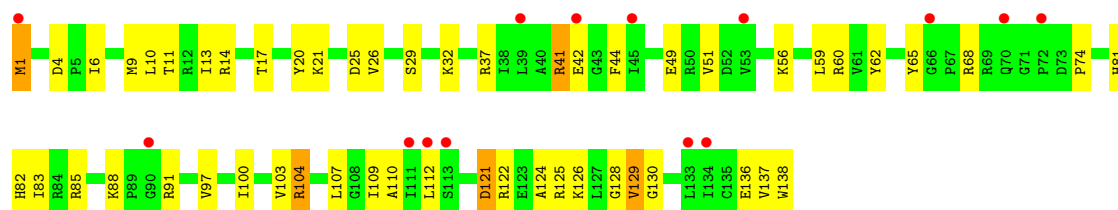
• Molecule 7: 30S ribosomal protein S7



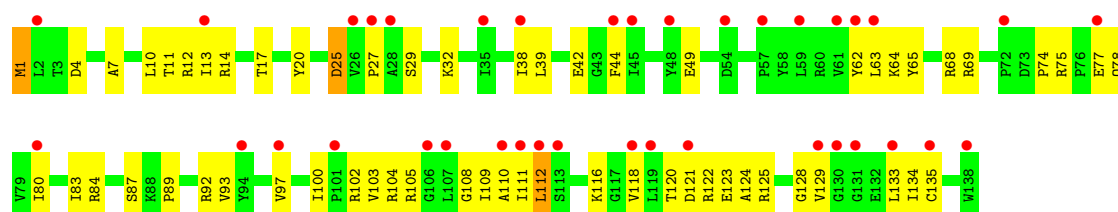
• Molecule 7: 30S ribosomal protein S7



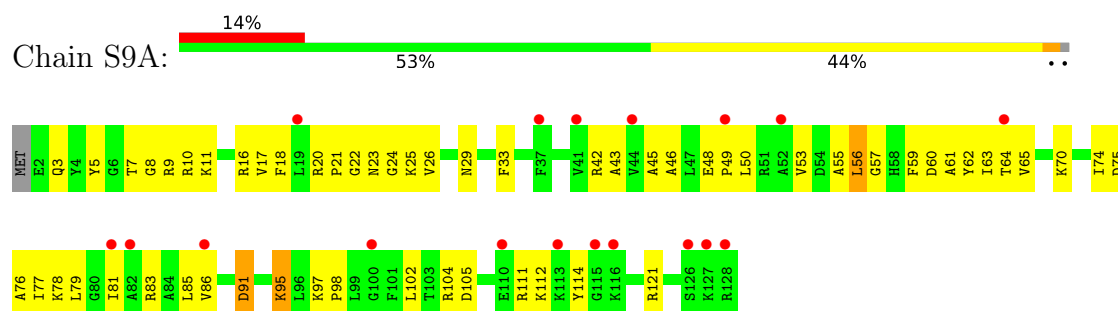
• Molecule 8: 30S ribosomal protein S8



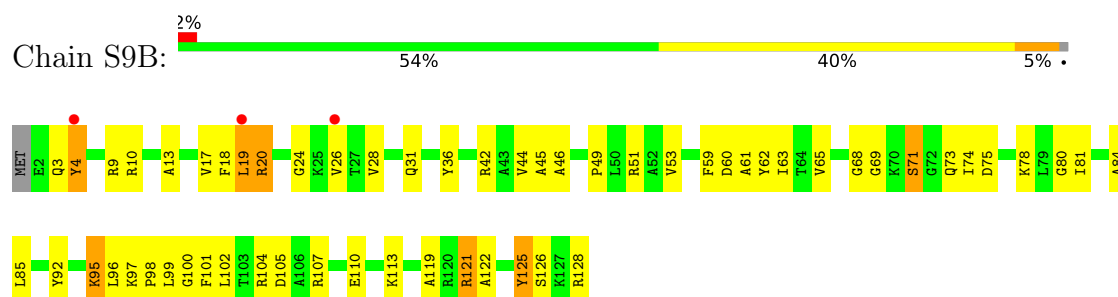
• Molecule 8: 30S ribosomal protein S8



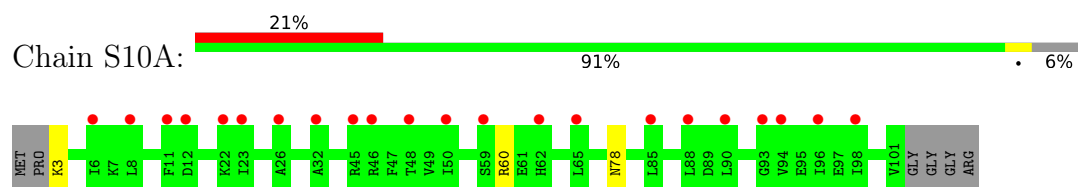
- Molecule 9: 30S ribosomal protein S9



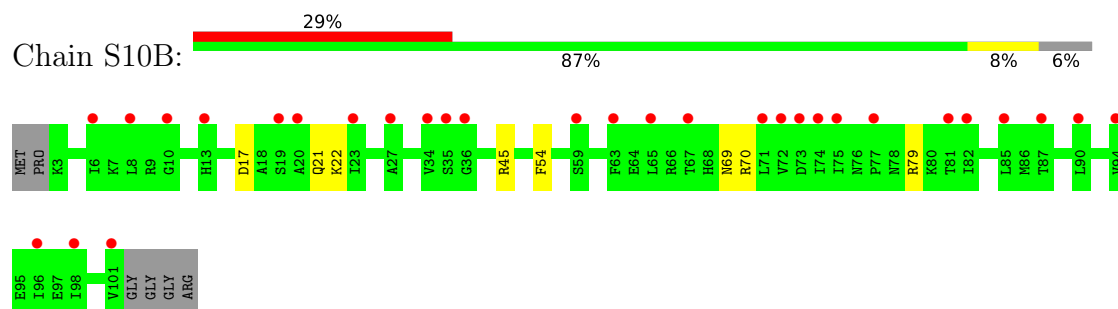
- Molecule 9: 30S ribosomal protein S9



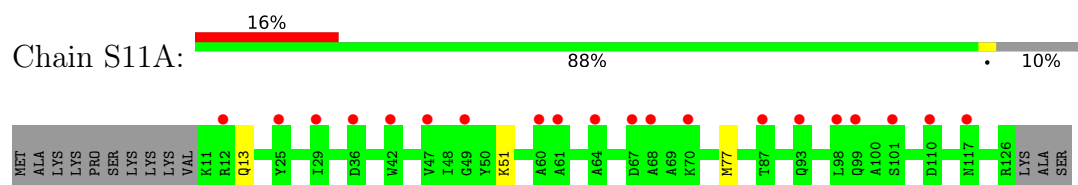
- Molecule 10: 30S ribosomal protein S10



- Molecule 10: 30S ribosomal protein S10

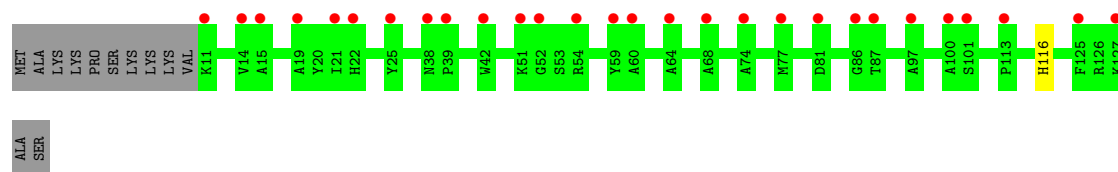


- Molecule 11: 30S ribosomal protein S11

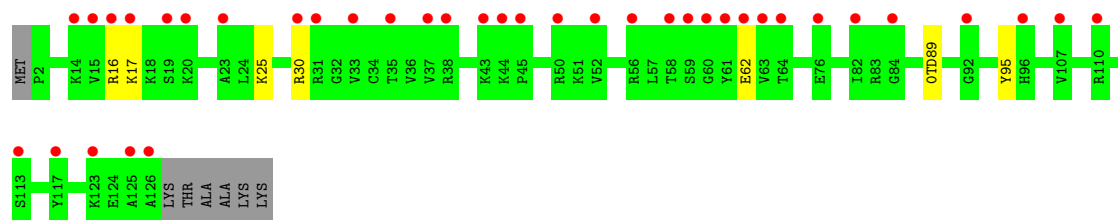


- Molecule 11: 30S ribosomal protein S11

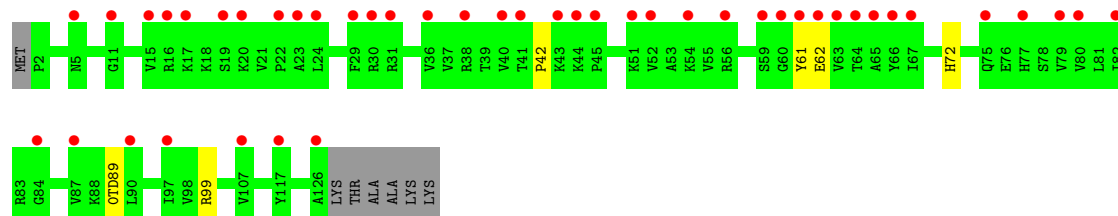




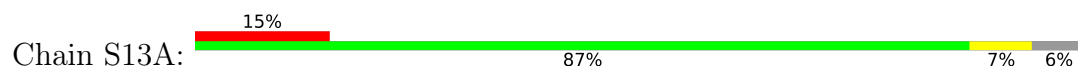
- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12



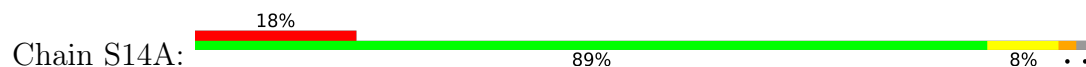
- Molecule 13: 30S ribosomal protein S13



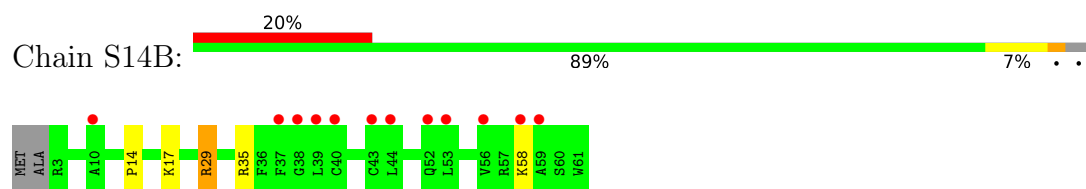
- Molecule 13: 30S ribosomal protein S13



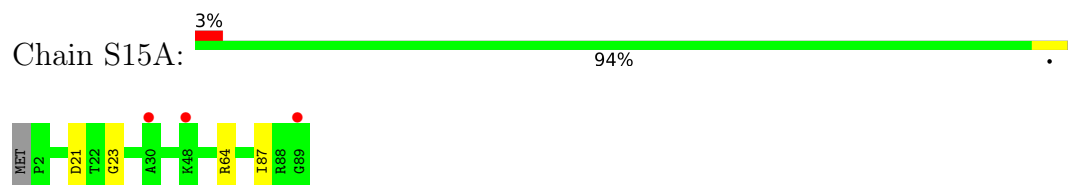
- Molecule 14: 30S ribosomal protein S14 type Z



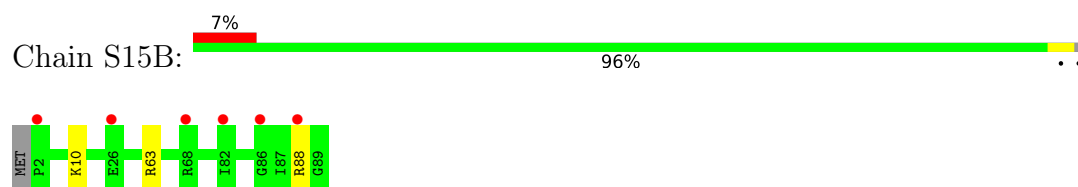
- Molecule 14: 30S ribosomal protein S14 type Z



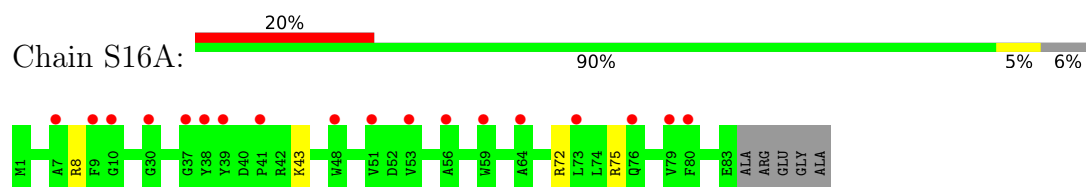
- Molecule 15: 30S ribosomal protein S15



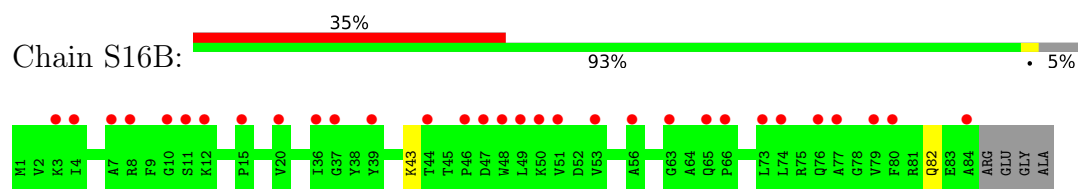
- Molecule 15: 30S ribosomal protein S15



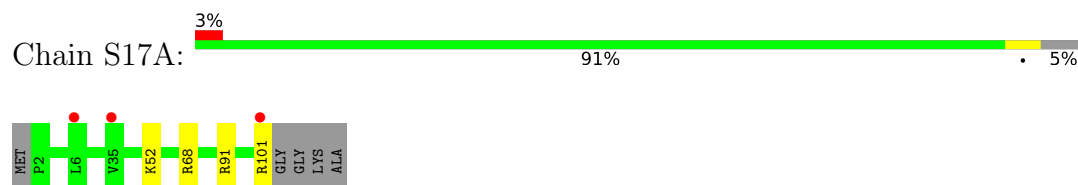
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16

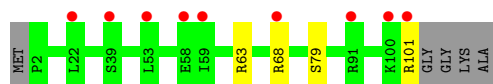


- Molecule 17: 30S ribosomal protein S17

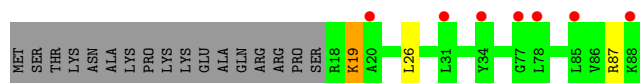
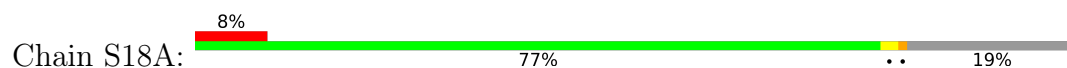


- Molecule 17: 30S ribosomal protein S17

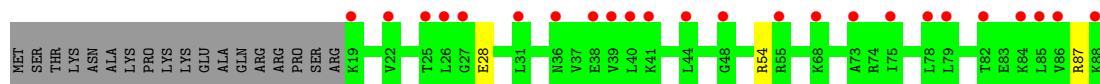
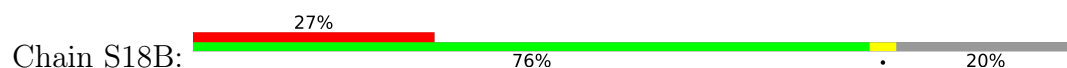




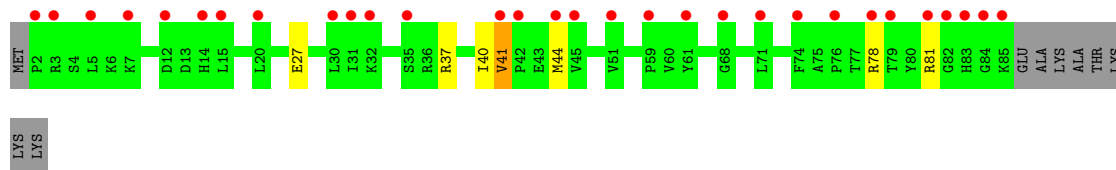
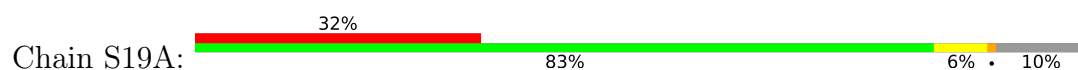
- Molecule 18: 30S ribosomal protein S18



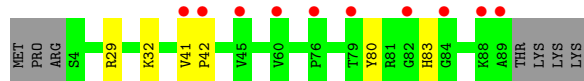
- Molecule 18: 30S ribosomal protein S18



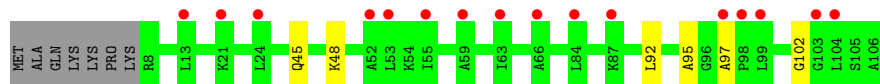
- Molecule 19: 30S ribosomal protein S19



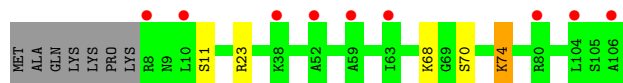
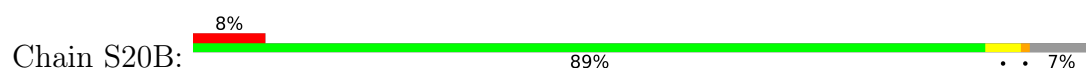
- Molecule 19: 30S ribosomal protein S19



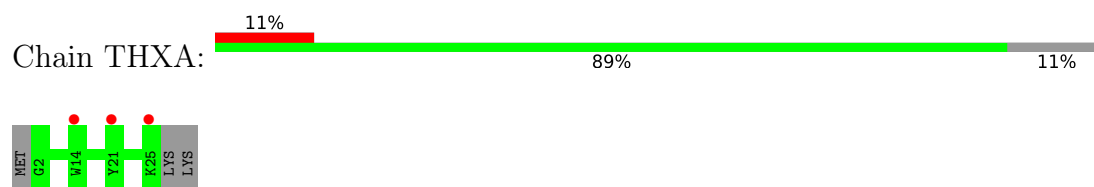
- Molecule 20: 30S ribosomal protein S20



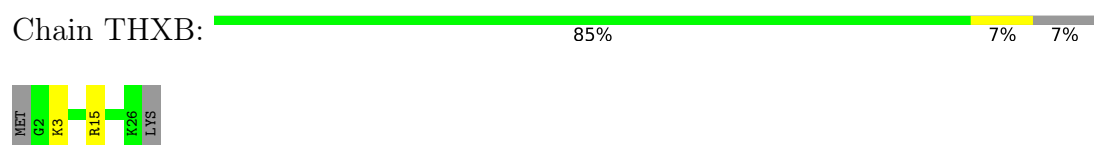
- Molecule 20: 30S ribosomal protein S20



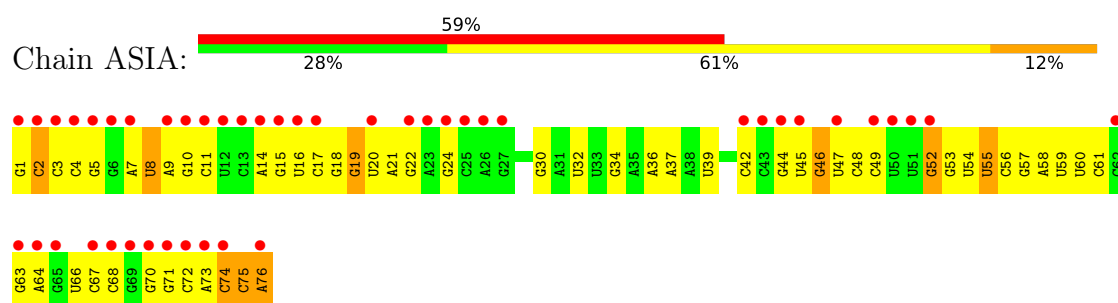
- Molecule 21: 30S ribosomal protein Thx



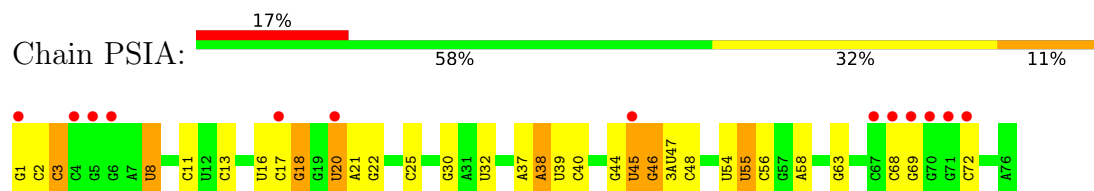
- Molecule 21: 30S ribosomal protein Thx



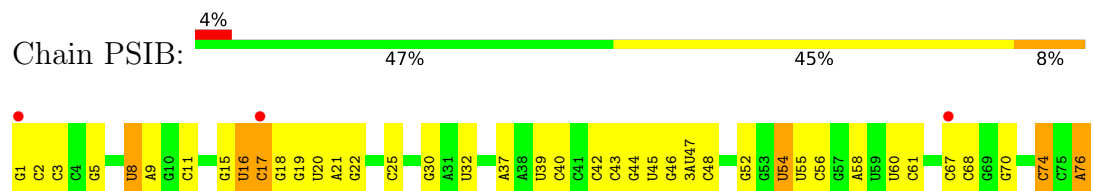
- Molecule 22: Phe-tRNA



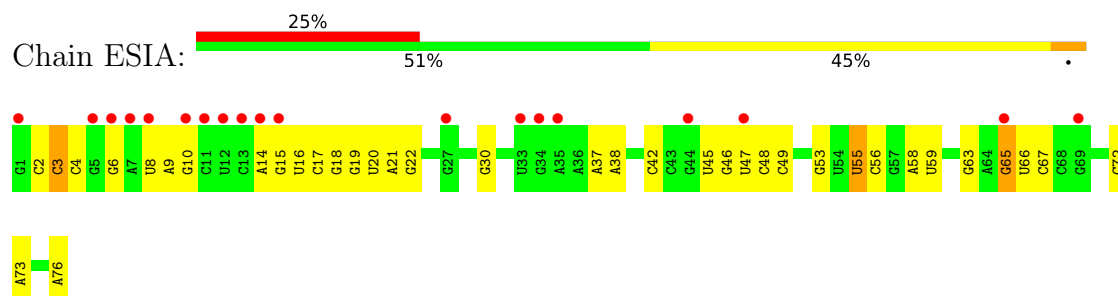
- Molecule 23: Phe-tRNA



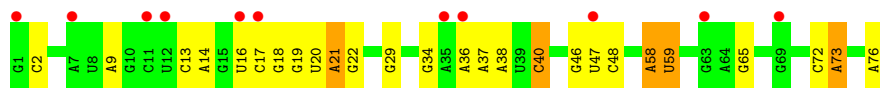
- Molecule 23: Phe-tRNA



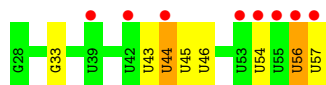
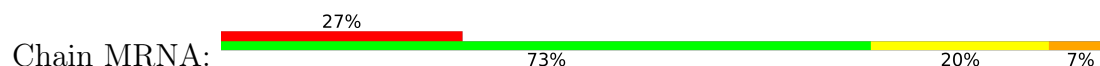
- Molecule 24: Phe-tRNA



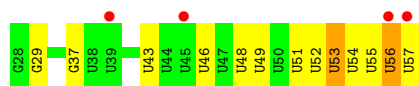
- Molecule 24: Phe-tRNA



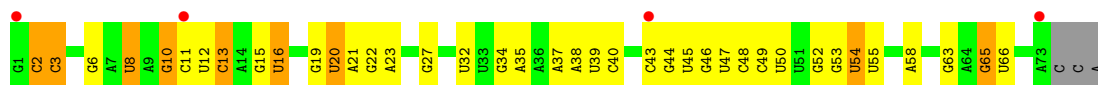
- Molecule 25: mRNA



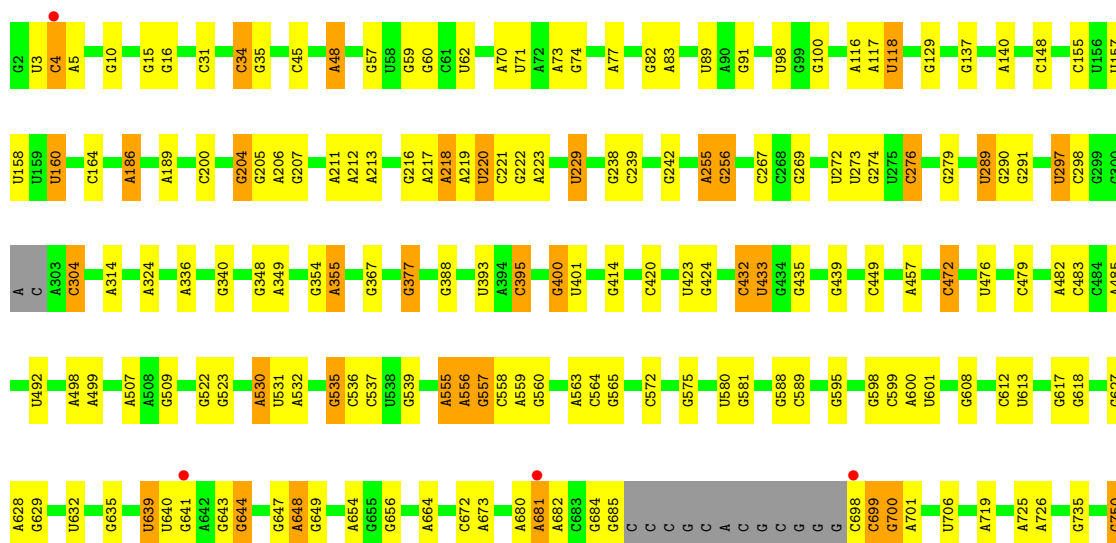
- Molecule 25: mRNA



- Molecule 26: Phe-tRNA

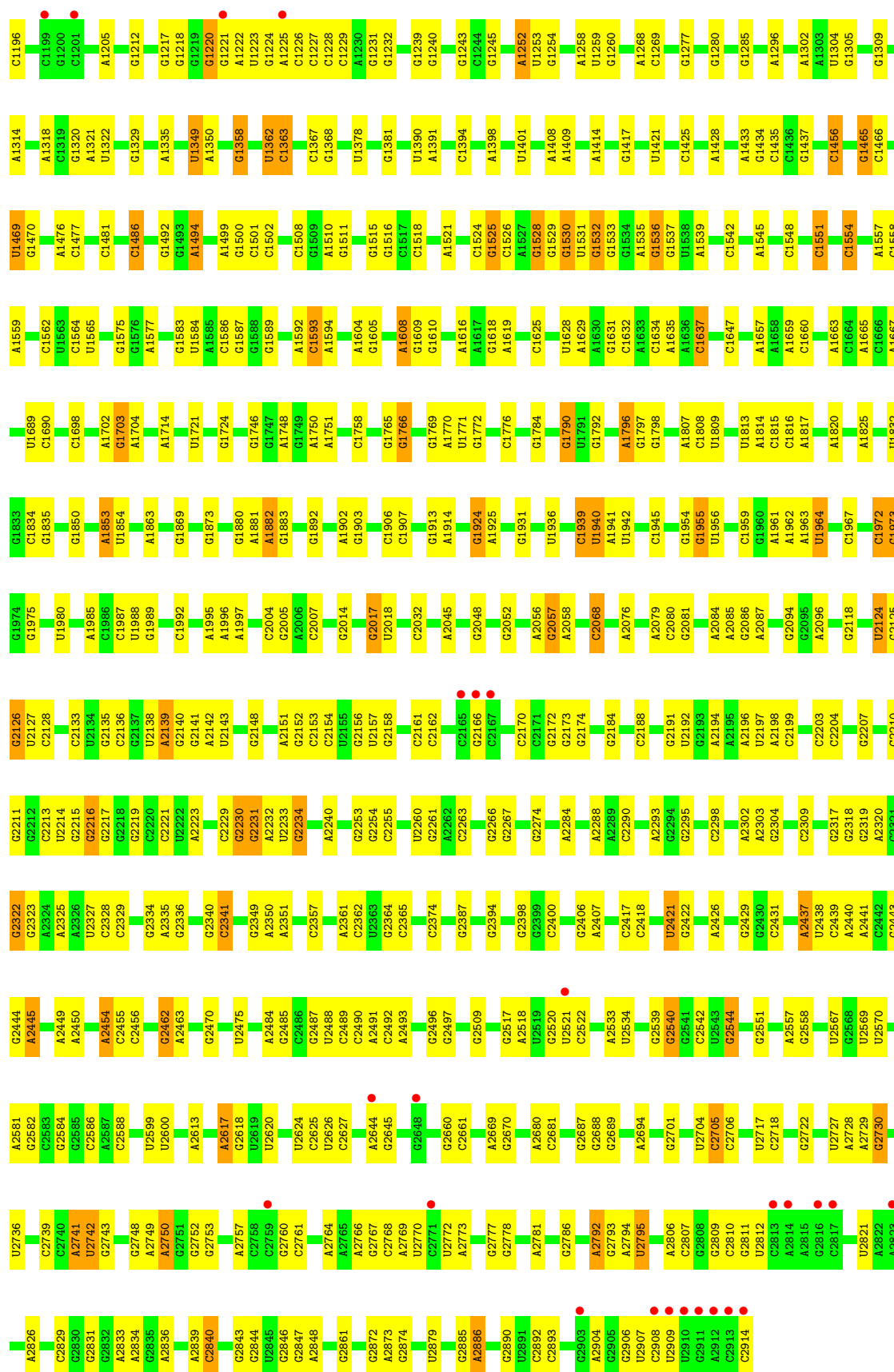


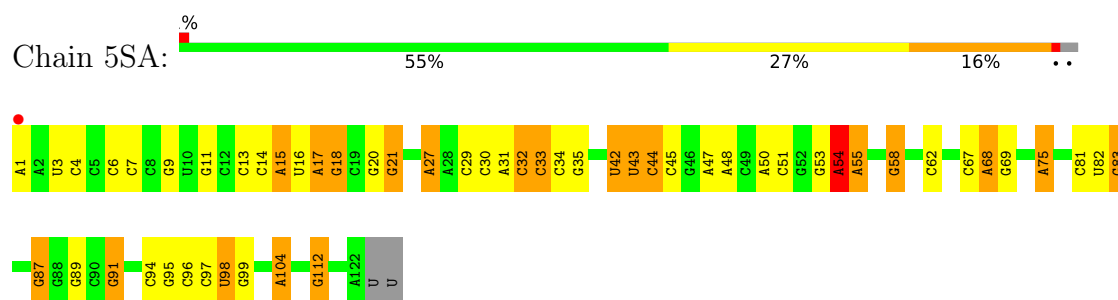
- Molecule 27: 23S rRNA



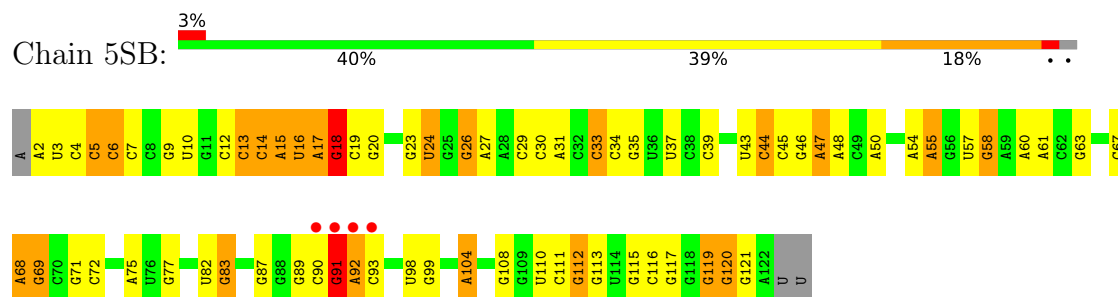
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A2302	A2303	G2304	G2319	A2320	C2321	G2322	G2323	A2326	G2327	C2328	C2329	G2333	G2334	A2335	G2336	G2340	C2341	G2349	A2350	A2351	A2361	C2362	C2365	G2394	C2395	G2398	G2399	C2400	G2406	A2407	C2417	G2420	U2421	G2422	G2425	A2426	C2435	G2436	A2437	U2438	G2439	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	C2290	G2291	A2292	A2293	G2294	G2295	C2298	C2299	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	G2158	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	G1892	A1893	G1894	G1899	A1902	G1903	C1907	G1913	A1914	G1924	A1925	A1926	C1927	G1928	G1929	C1930	G1931	U1936	C1939	U1940	A1941	U1942	C1945									
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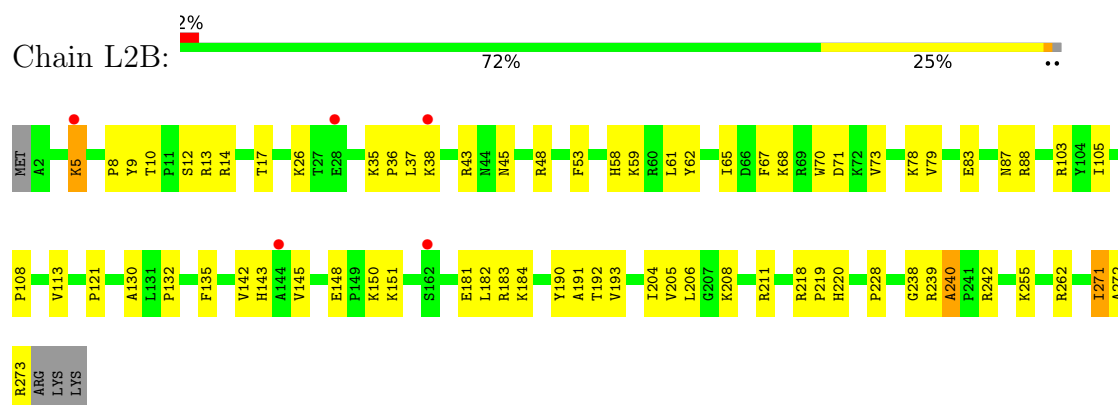
• Molecule 28: 5S rRNA



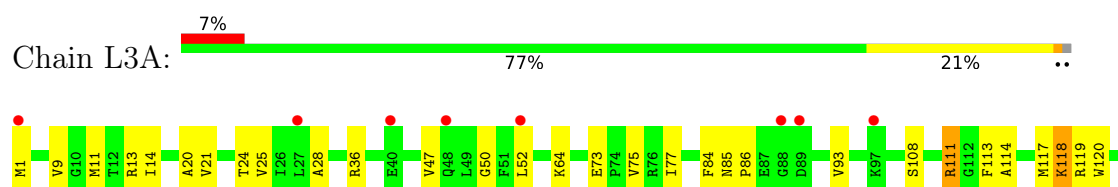
• Molecule 29: 50S ribosomal protein L2

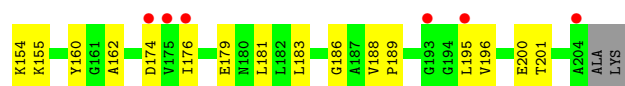


• Molecule 29: 50S ribosomal protein L2

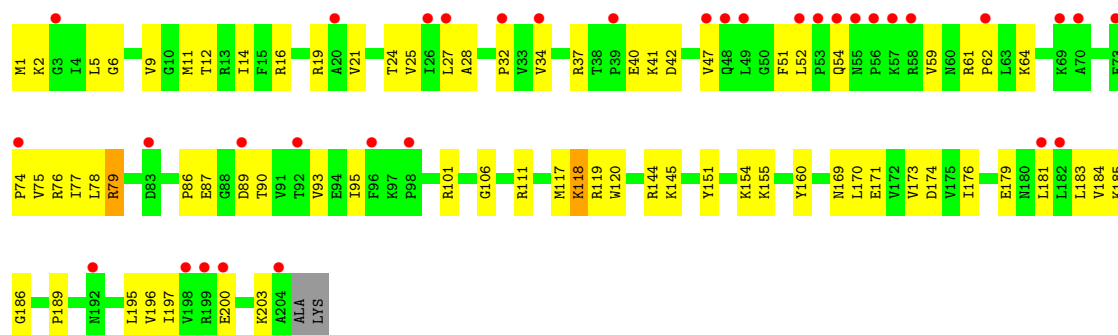


• Molecule 30: 50S ribosomal protein L3

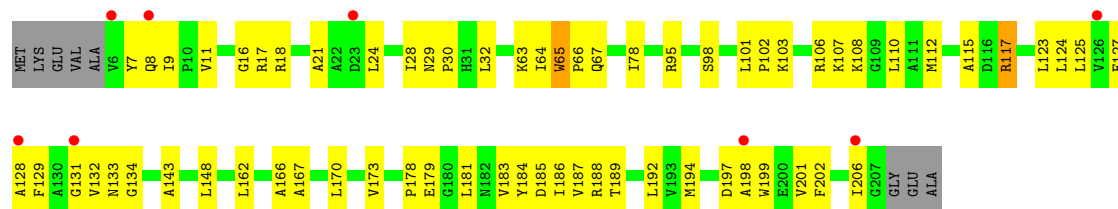




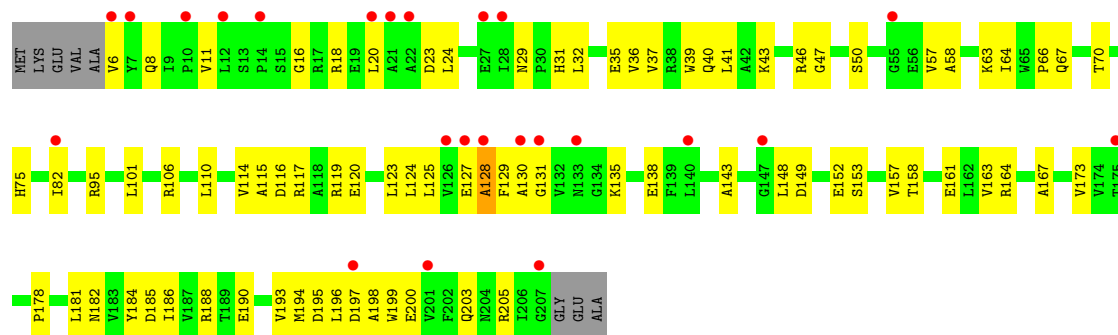
- Molecule 30: 50S ribosomal protein L3



- Molecule 31: 50S ribosomal protein L4

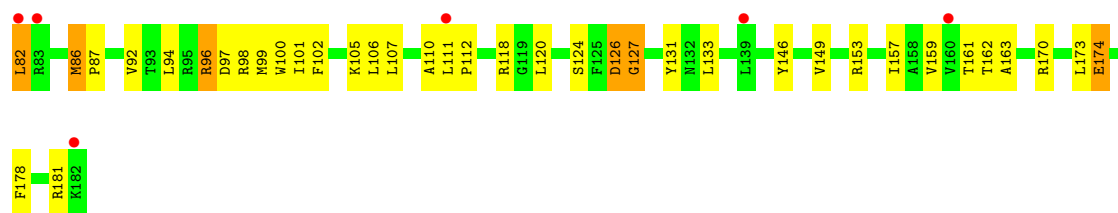


- Molecule 31: 50S ribosomal protein L4

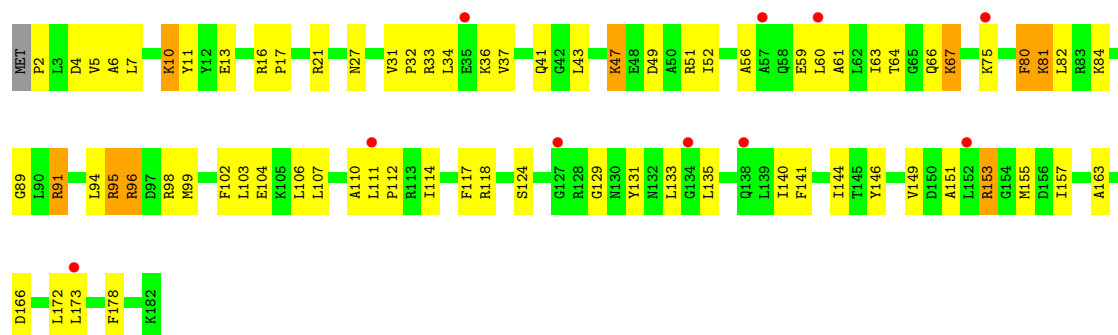


- Molecule 32: 50S ribosomal protein L5

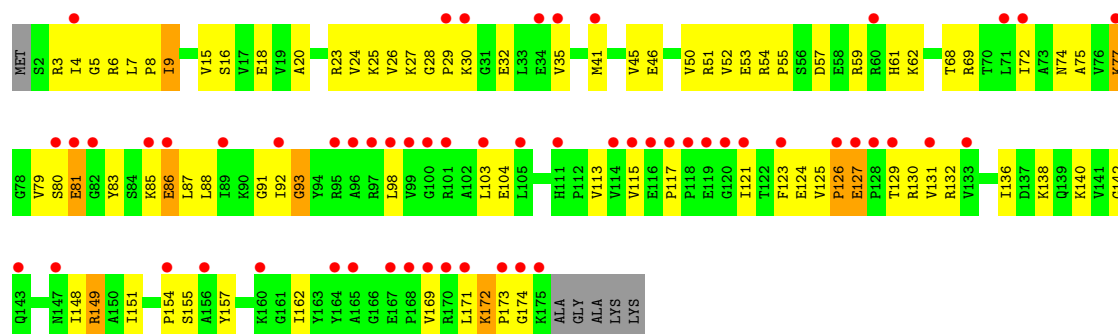




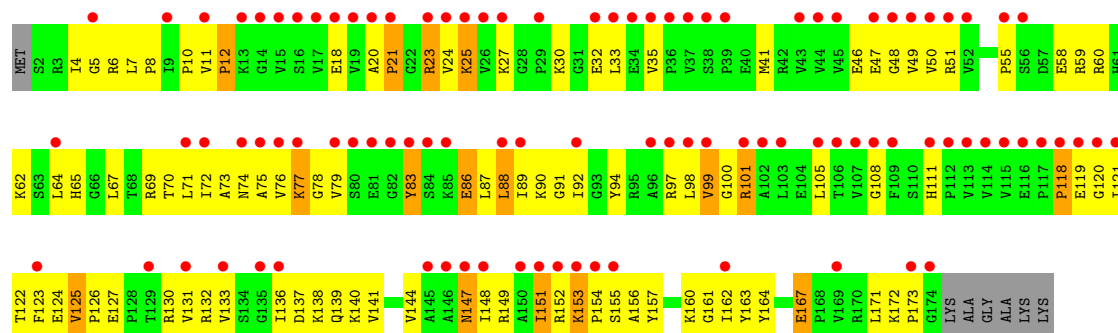
• Molecule 32: 50S ribosomal protein L5



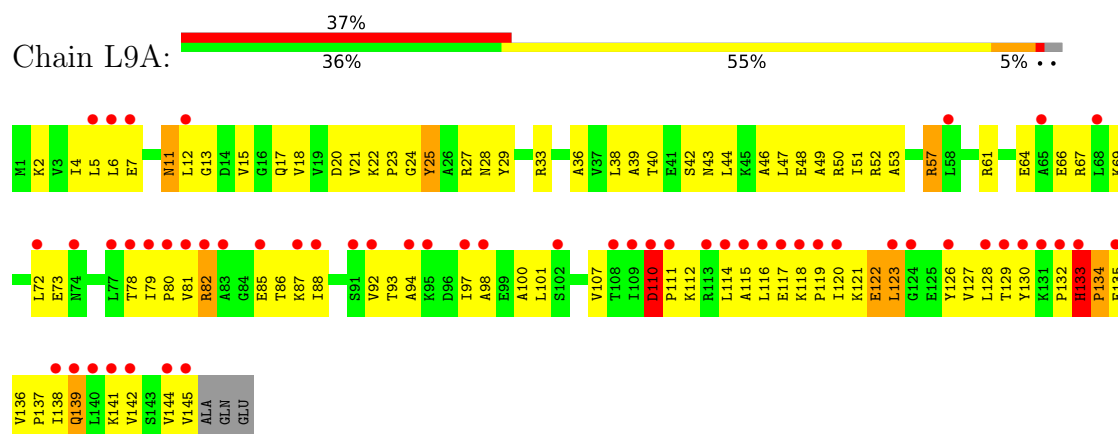
• Molecule 33: 50S ribosomal protein L6



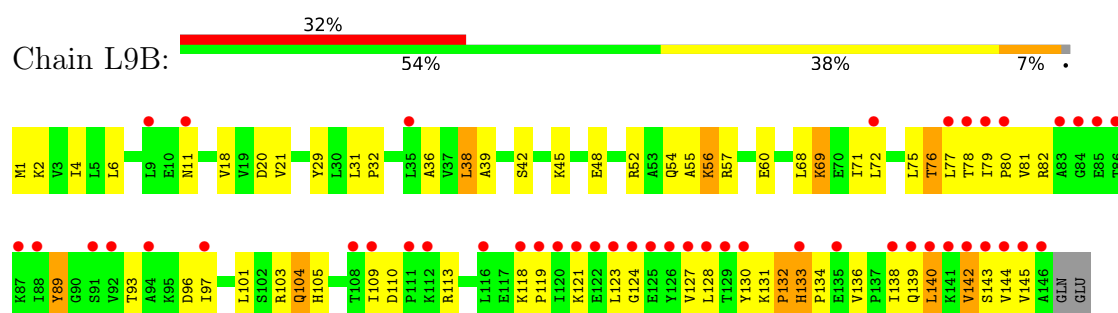
• Molecule 33: 50S ribosomal protein L6



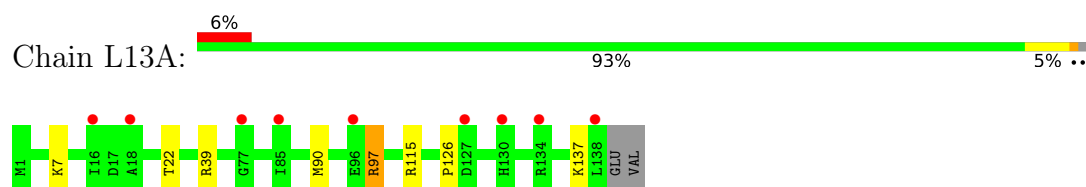
- Molecule 34: 50S ribosomal protein L9



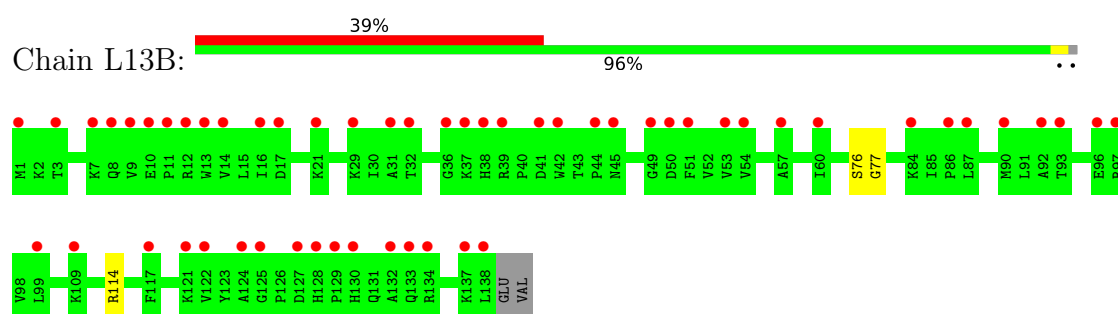
- Molecule 34: 50S ribosomal protein L9



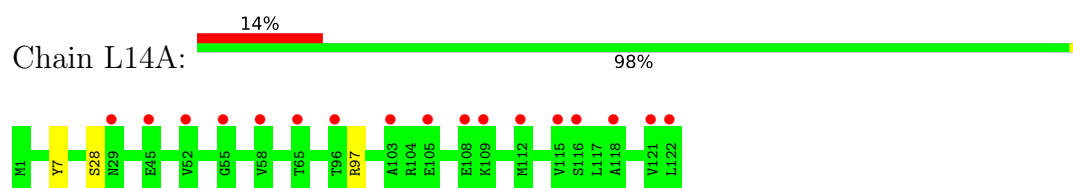
- Molecule 35: 50S ribosomal protein L13



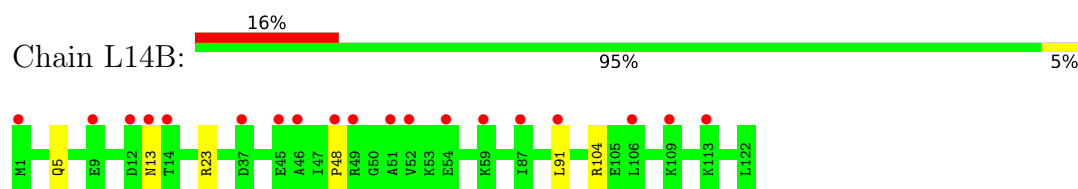
- Molecule 35: 50S ribosomal protein L13



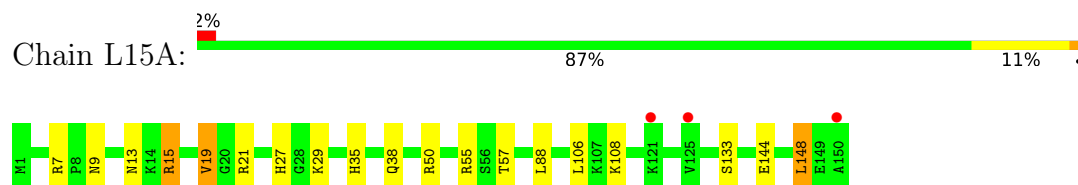
- Molecule 36: 50S ribosomal protein L14



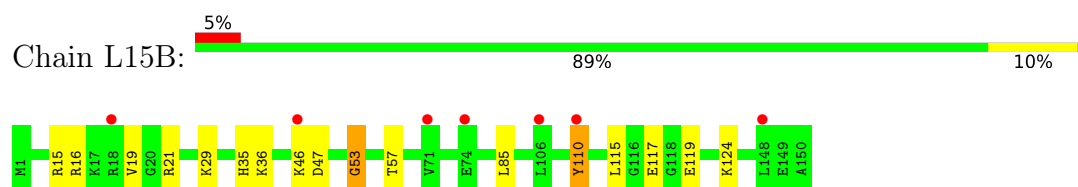
• Molecule 36: 50S ribosomal protein L14



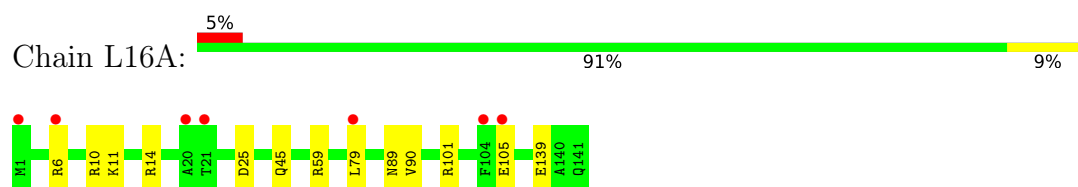
• Molecule 37: 50S ribosomal protein L15



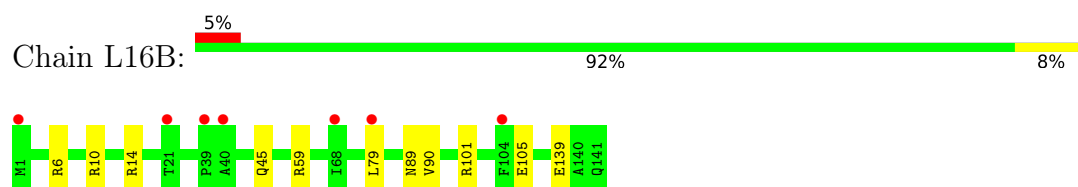
• Molecule 37: 50S ribosomal protein L15



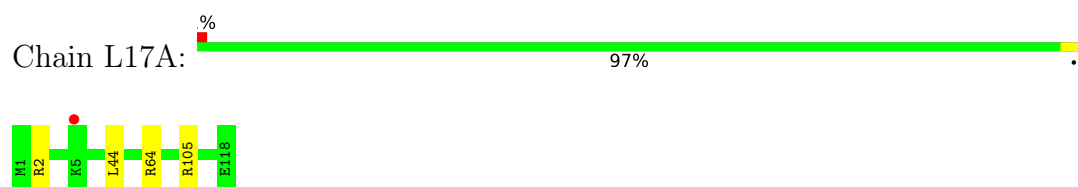
• Molecule 38: 50S ribosomal protein L16



• Molecule 38: 50S ribosomal protein L16



• Molecule 39: 50S ribosomal protein L17

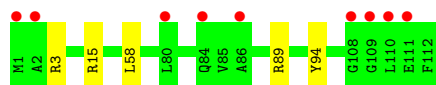


• Molecule 39: 50S ribosomal protein L17

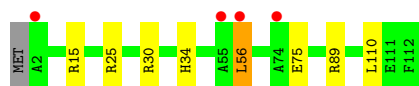




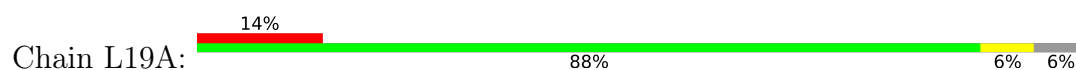
- Molecule 40: 50S ribosomal protein L18



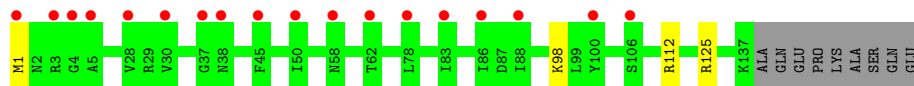
- Molecule 40: 50S ribosomal protein L18



- Molecule 41: 50S ribosomal protein L19



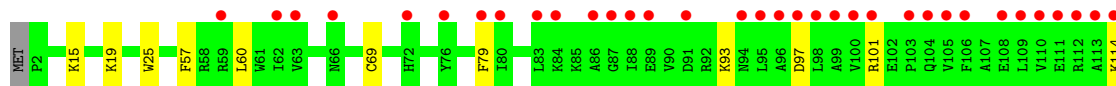
- Molecule 41: 50S ribosomal protein L19



- Molecule 42: 50S ribosomal protein L20

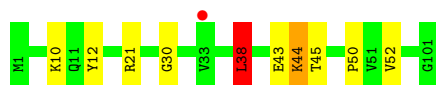


- Molecule 42: 50S ribosomal protein L20

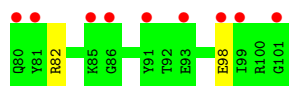
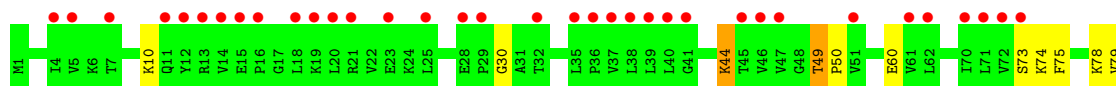
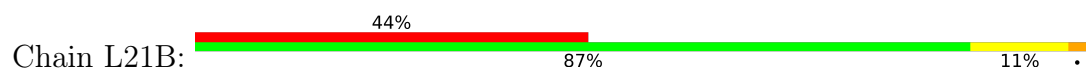




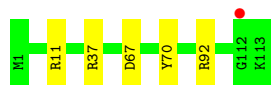
- Molecule 43: 50S ribosomal protein L21



- Molecule 43: 50S ribosomal protein L21



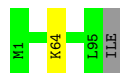
- Molecule 44: 50S ribosomal protein L22



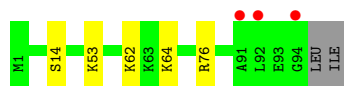
- Molecule 44: 50S ribosomal protein L22



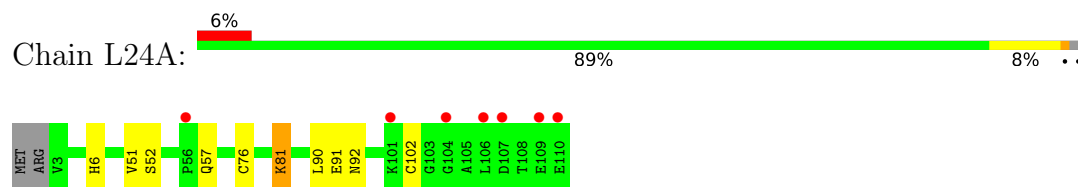
- Molecule 45: 50S ribosomal protein L23



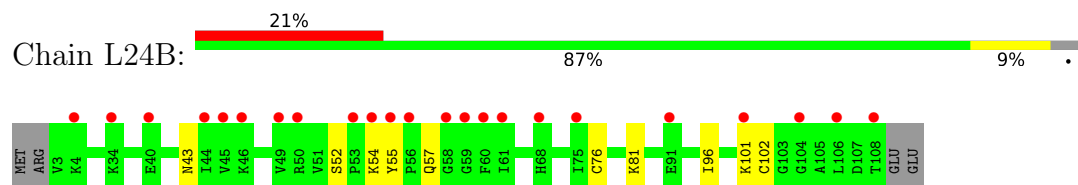
- Molecule 45: 50S ribosomal protein L23



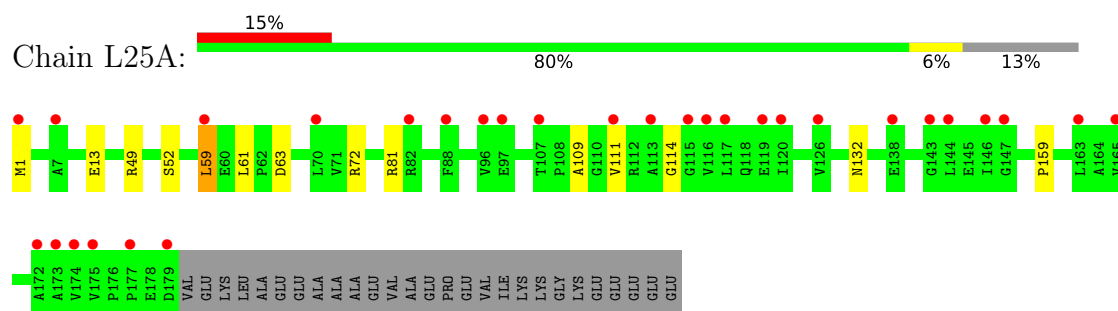
- Molecule 46: 50S ribosomal protein L24



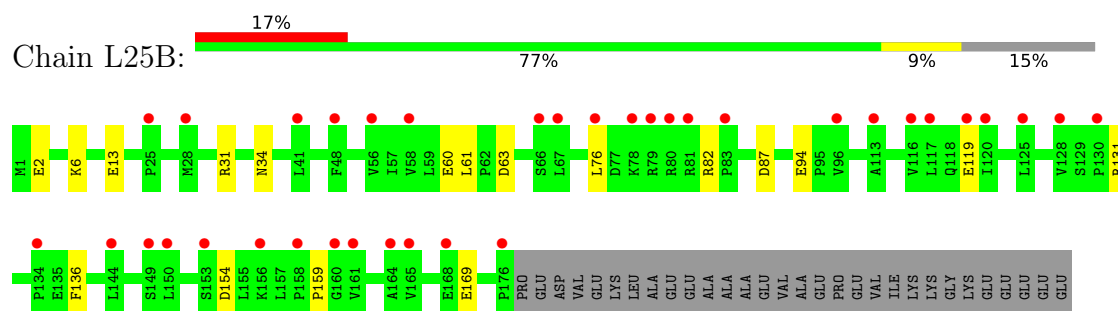
- Molecule 46: 50S ribosomal protein L24



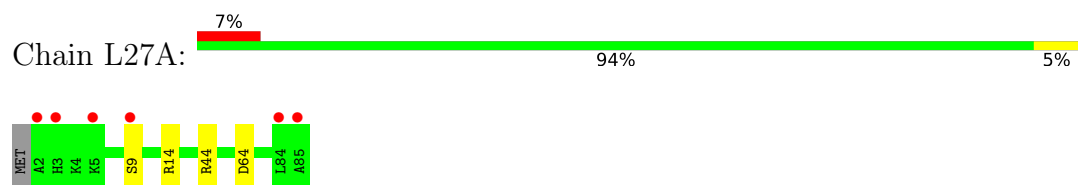
- Molecule 47: 50S ribosomal protein L25



- Molecule 47: 50S ribosomal protein L25

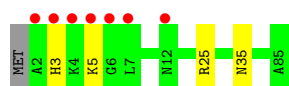


- Molecule 48: 50S ribosomal protein L27

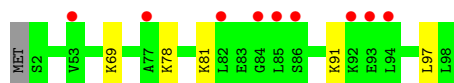


- Molecule 48: 50S ribosomal protein L27





- Molecule 49: 50S ribosomal protein L28



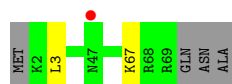
- Molecule 49: 50S ribosomal protein L28



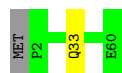
- Molecule 50: 50S ribosomal protein L29



- Molecule 50: 50S ribosomal protein L29



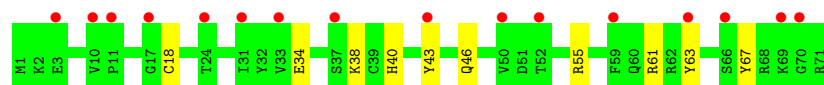
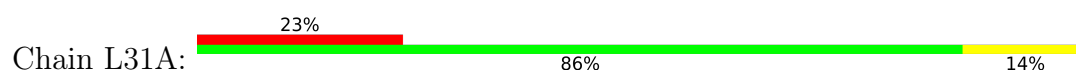
- Molecule 51: 50S ribosomal protein L30



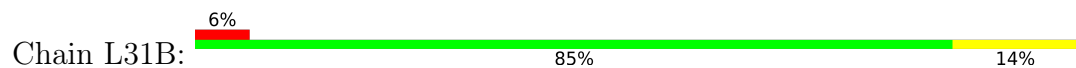
- Molecule 51: 50S ribosomal protein L30



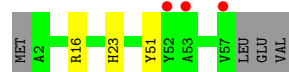
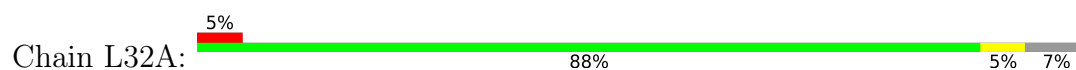
- Molecule 52: 50S ribosomal protein L31



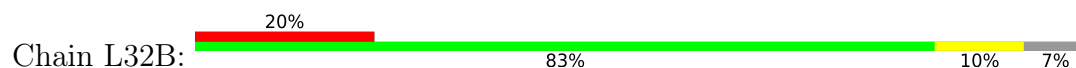
- Molecule 52: 50S ribosomal protein L31



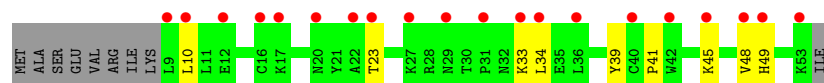
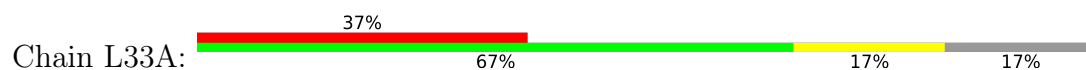
- Molecule 53: 50S ribosomal protein L32



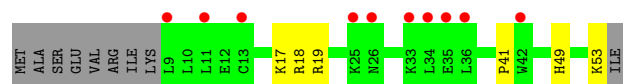
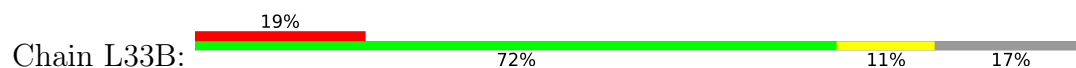
- Molecule 53: 50S ribosomal protein L32



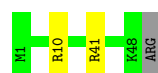
- Molecule 54: 50S ribosomal protein L33



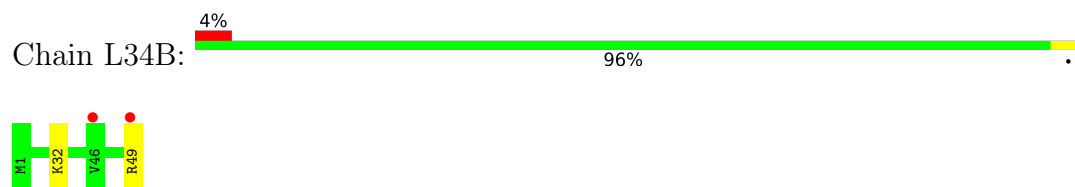
- Molecule 54: 50S ribosomal protein L33



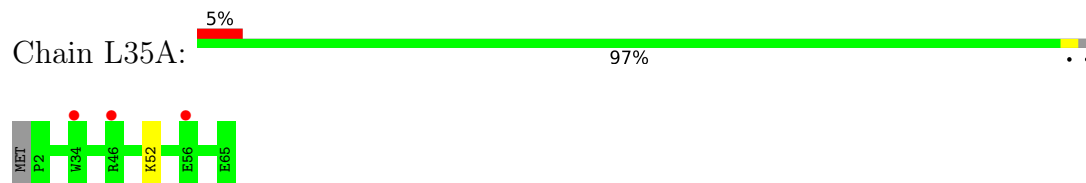
- Molecule 55: 50S ribosomal protein L34



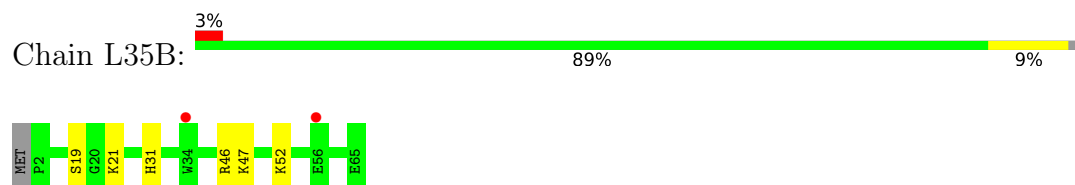
- Molecule 55: 50S ribosomal protein L34



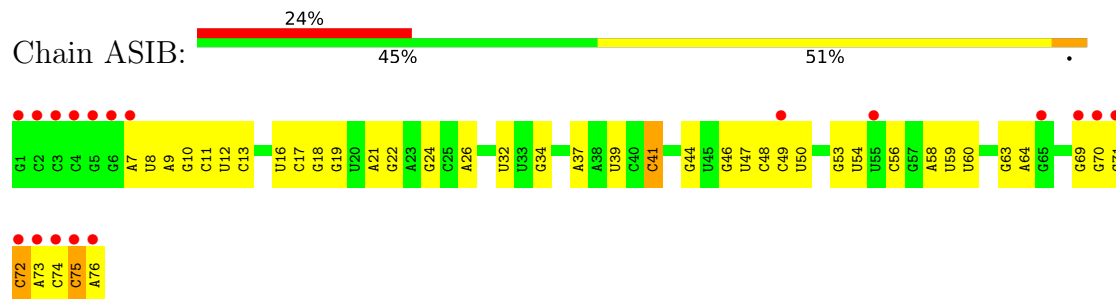
- Molecule 56: 50S ribosomal protein L35



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	79.5	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	L2A	45	ASN	Peptide
31	L4A	132	VAL	Peptide

Continued on next page...

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Mol	Chain	Res	Type	Group
31	L4A	65	TRP	Peptide
13	S13A	105	THR	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

The worst 5 of 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

The worst 5 of 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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

5 of 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

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 468 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	S3B	52	LEU
50	L29B	67	LYS
12	S12B	72	HIS
48	L27B	5	LYS
42	L20B	69	CYS

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%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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%)

5 of 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

5 of 258 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	23SB	2017	G
27	23SB	2350	A
27	23SA	1703	G
27	23SA	1657	A
27	23SB	2617	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 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'

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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-	-	-		
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

The worst 5 of 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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

The worst 5 of 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

There are no chirality outliers.

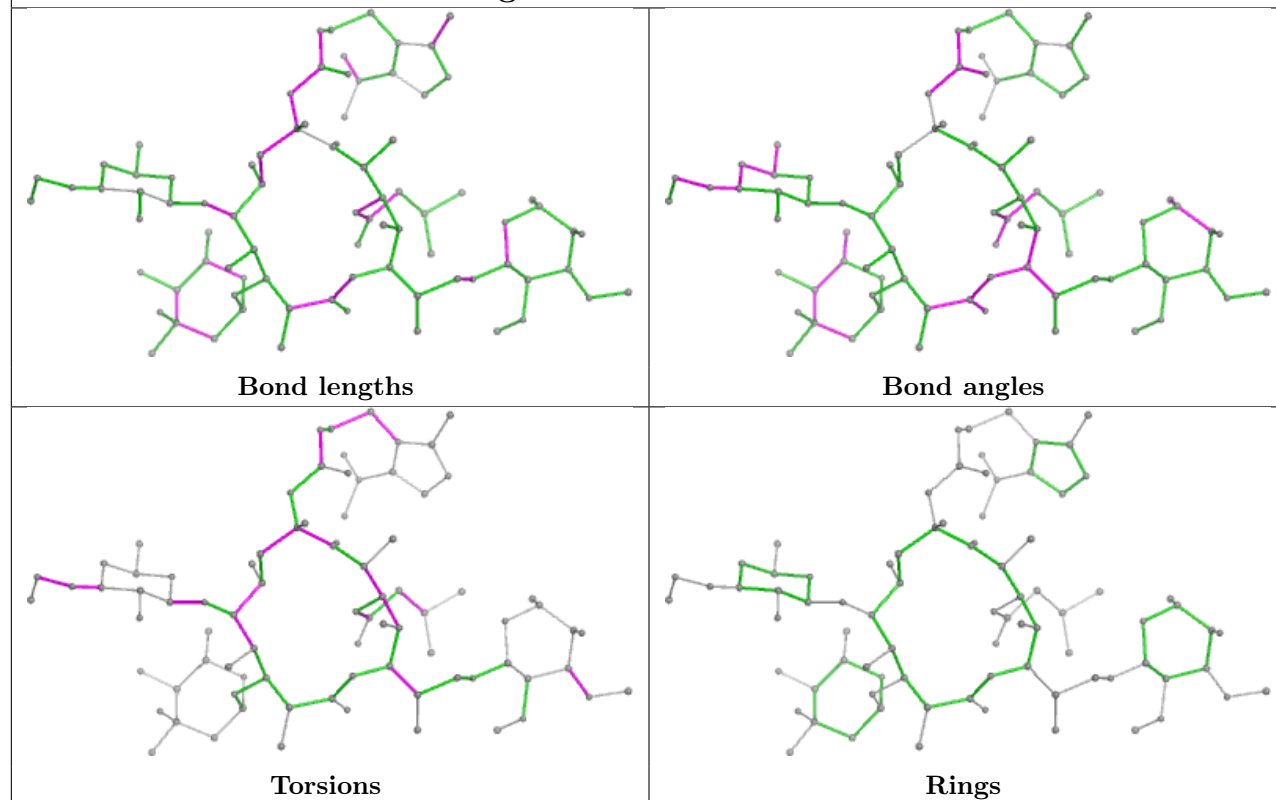
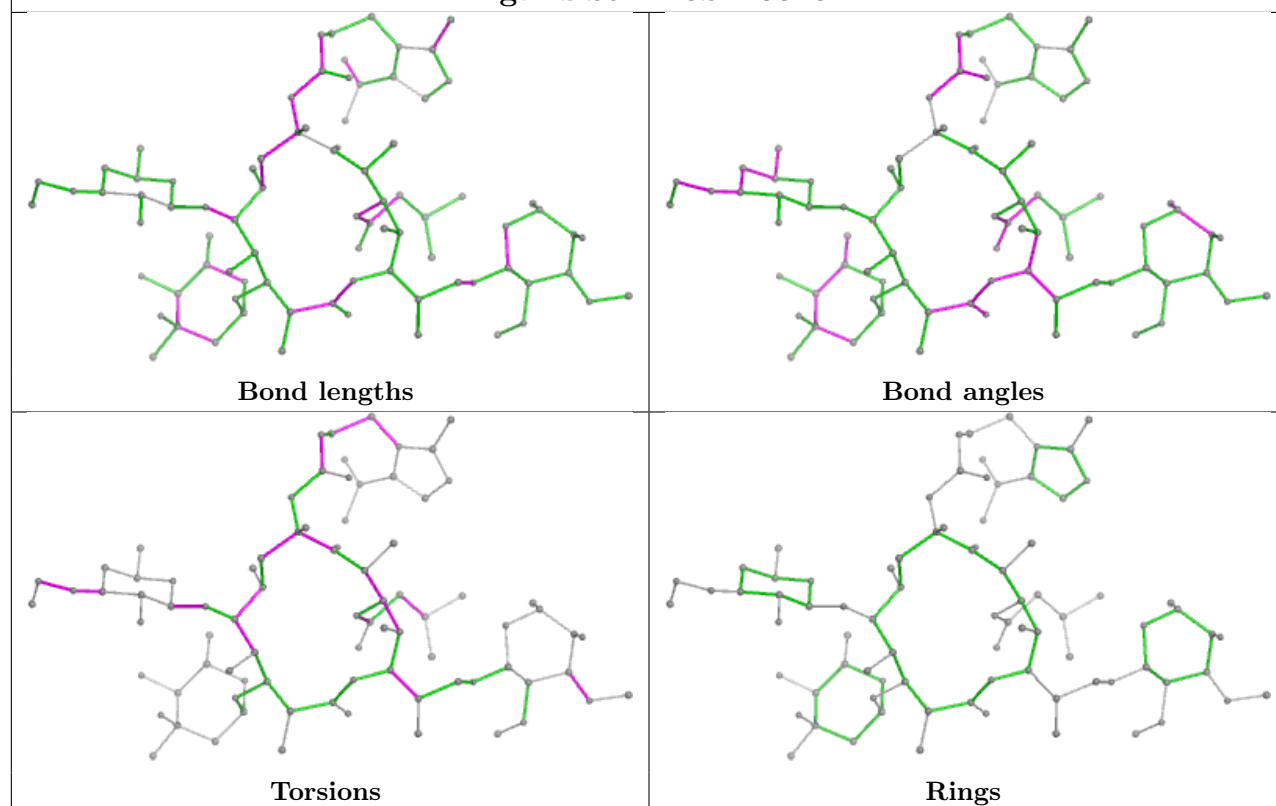
5 of 66 torsion outliers are listed below:

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

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	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 ²)	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 ²)	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 ²)	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

The worst 5 of 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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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
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

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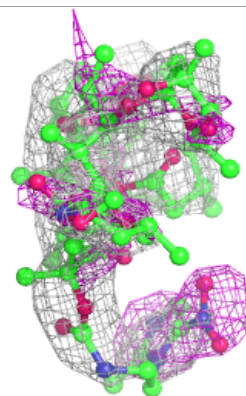
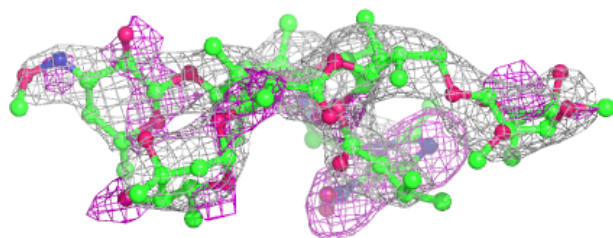
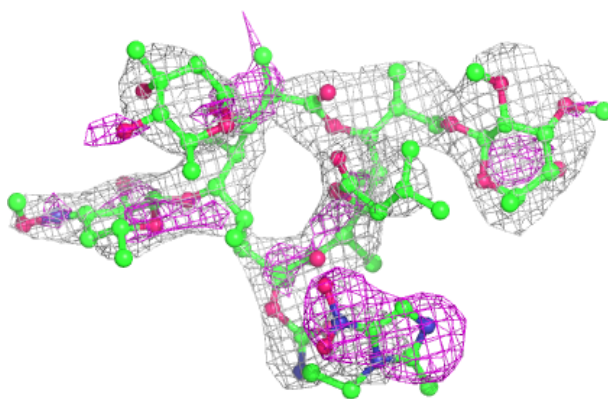
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	OHX	23SB	3339	7/7	0.99	0.08	95,104,111,114	0
60	OHX	23SB	3340	7/7	0.99	0.07	79,82,103,105	0
60	OHX	23SB	3341	7/7	0.99	0.06	72,88,98,114	0
58	MG	23SA	3254	1/1	0.99	0.03	46,46,46,46	0
58	MG	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

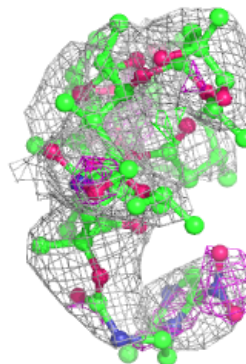
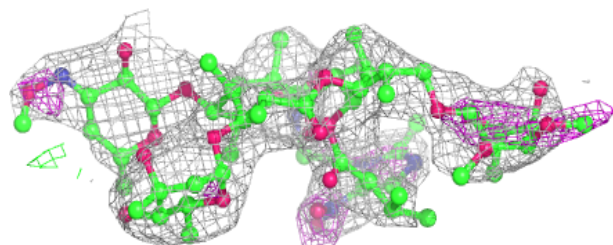
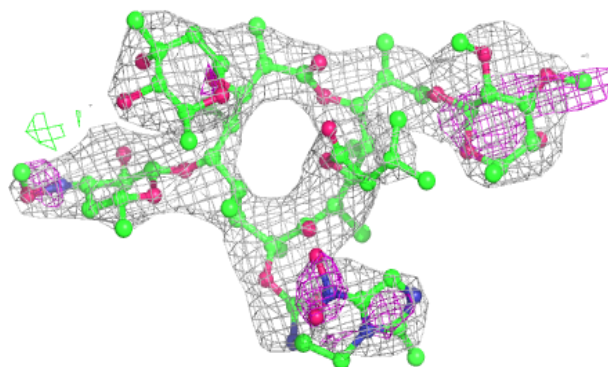
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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