



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 11, 2025 – 07:12 pm GMT

PDB ID : 7AZO
Title : 70S thermus thermophilus ribosome with bound antibiotic lead SEQ-977
Authors : Jenner, L.B.; Yusupov, M.; Yusupova, G.
Deposited on : 2020-11-17
Resolution : 3.30 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

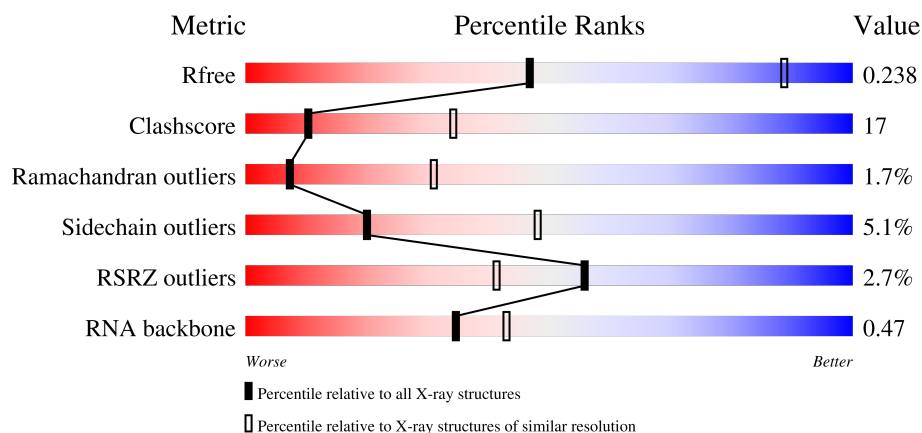
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



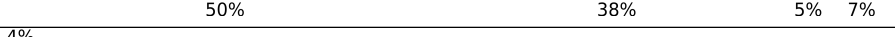
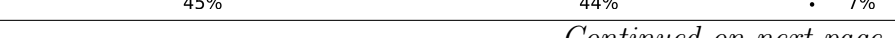
The reported resolution of this entry is 3.30 Å.

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	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)
RNA backbone	3690	1014 (3.64-2.96)

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	 72% 24% .
1	16SB	1512	 71% 25% .
2	S2A	256	 3% 50% 38% 5% 7%
2	S2B	256	 4% 45% 44% . 7%

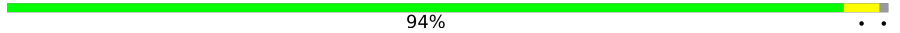

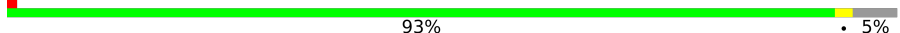






















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Mol	Chain	Length	Quality of chain
3	S3A	239	
3	S3B	239	
4	S4A	209	
4	S4B	209	
5	S5A	162	
5	S5B	162	
6	S6A	101	
6	S6B	101	
7	S7A	156	
7	S7B	156	
8	S8A	138	
8	S8B	138	
9	S9A	128	
9	S9B	128	
10	S10A	105	
10	S10B	105	
11	S11A	129	
11	S11B	129	
12	S12A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
















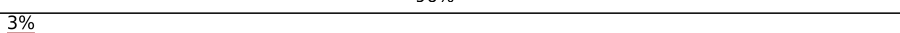
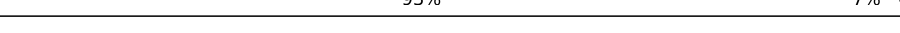




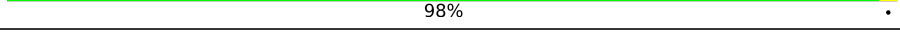
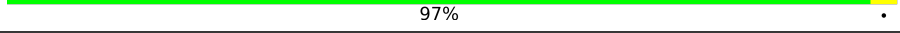
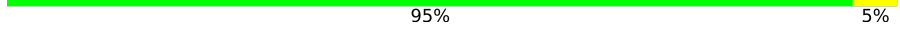

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Mol	Chain	Length	Quality of chain
15	S15B	89	
16	S16A	88	
16	S16B	88	
17	S17A	105	
17	S17B	105	
18	S18A	88	
18	S18B	88	
19	S19A	93	
19	S19B	93	
20	S20A	106	
20	S20B	106	
21	THXA	27	
21	THXB	27	
22	ASIA	76	
23	PSIA	76	
23	PSIB	76	
24	ESIA	76	
24	ESIB	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	 73% 24% ..
29	L2B	276	 71% 26% ..
30	L3A	206	 75% 23% ..
30	L3B	206	 68% 29% ..
31	L4A	210	 60% 35% . .
31	L4B	210	 58% 38% .
32	L5A	182	 63% 32% . .
32	L5B	182	 59% 35% 6% .
33	L6A	180	 50% 42% . 5%
33	L6B	180	 46% 46% 5% .
34	L9A	148	 47% 43% 8% ..
34	L9B	148	 52% 41% 6% .
35	L13A	140	 94% ..
35	L13B	140	 96% ..
36	L14A	122	 96% .
36	L14B	122	 93% 7% .
37	L15A	150	 87% 11% .
37	L15B	150	 88% 11% .
38	L16A	141	 91% 9%
38	L16B	141	 91% 9%
39	L17A	118	 98% .
39	L17B	118	 97% .
40	L18A	112	 95% 5%
40	L18B	112	 91% 7% ..
41	L19A	146	 88% 5% 6%

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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	16SB	2304[A]	-	-	-	X
58	MG	16SB	2304[B]	-	-	-	X
58	MG	23SA	3015	-	-	-	X
59	OHX	S4A	301	-	-	X	-

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 306403 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	1512	Total	C	N	O	P	0	0	0
			32509	14478	6016	10503	1512			
1	16SB	1508	Total	C	N	O	P	0	0	0
			32429	14442	6008	10471	1508			

- 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 RNA (30-MER).

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	2873	Total	C	N	O	P	0	0	0
			61886	27548	11574	19891	2873			

- 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	171	Total	C	N	O	S	0	0	0
			1316	835	247	233	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	93	Total	C	N	O	S	0	0	0
			738	480	133	124	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	71	Total	C	N	O	S	0	0	0
			590	367	119	103	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).

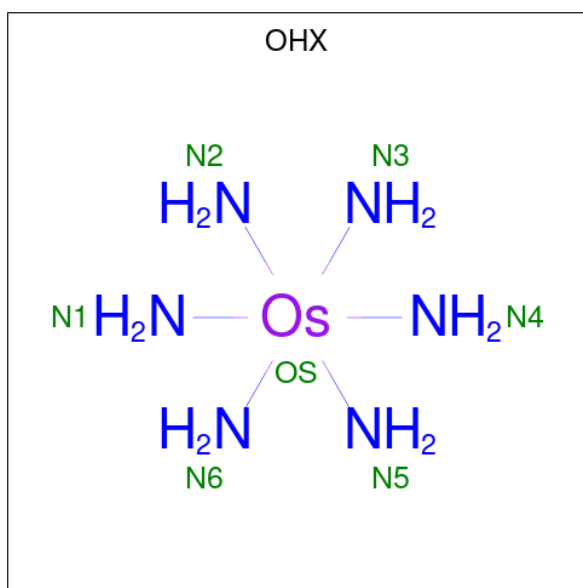
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	16SA	92	Total	Mg	0	0
			92	92		
58	S4A	1	Total	Mg	0	0
			1	1		
58	PSIA	2	Total	Mg	0	0
			2	2		
58	23SA	332	Total	Mg	0	0
			332	332		
58	5SA	6	Total	Mg	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	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	1	Total 1	Mg 1	0	0
58	PSIB	3	Total 3	Mg 3	0	0
58	23SB	240	Total 241	Mg 241	0	1
58	5SB	4	Total 4	Mg 4	0	0
58	L3B	2	Total 2	Mg 2	0	0
58	L4B	1	Total 1	Mg 1	0	0
58	L5B	1	Total 1	Mg 1	0	0
58	L15B	1	Total 1	Mg 1	0	0
58	L35B	2	Total 2	Mg 2	0	0

- Molecule 59 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	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		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	16SA	1	Total	N	Os	0	0
			7	6	1		
59	S4A	1	Total	N	Os	0	0
			7	6	1		
59	S10A	1	Total	N	Os	0	0
			7	6	1		
59	S19A	1	Total	N	Os	0	0
			7	6	1		
59	ASIA	1	Total	N	Os	0	0
			7	6	1		
59	ASIA	1	Total	N	Os	0	0
			7	6	1		
59	ASIA	1	Total	N	Os	0	0
			7	6	1		
59	PSIA	1	Total	N	Os	0	0
			7	6	1		
59	ESIA	1	Total	N	Os	0	0
			7	6	1		
59	MRNA	1	Total	N	Os	0	0
			7	6	1		
59	TRNA	1	Total	N	Os	0	0
			7	6	1		
59	TRNA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
59	23SA	1	Total	N	Os	0	0
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59	23SA	1	Total	N	Os	0	0
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59	23SA	1	Total	N	Os	0	0
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59	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		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
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59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
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59	23SA	1	Total	N	Os	0	0
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			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
59	23SA	1	Total	N	Os	0	0
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			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
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59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
			7	6	1		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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59	23SA	1	Total	N	Os	0	0
			7	6	1		
59	23SA	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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59	5SA	1	Total	N	Os	0	0
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59	5SA	1	Total	N	Os	0	0
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59	5SA	1	Total	N	Os	0	0
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59	5SA	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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59	L15A	1	Total	N	Os	0	0
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59	L17A	1	Total	N	Os	0	0
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59	L19A	1	Total	N	Os	0	0
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59	L20A	1	Total	N	Os	0	0
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59	L27A	1	Total	N	Os	0	0
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59	L27A	1	Total	N	Os	0	0
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59	L28A	1	Total	N	Os	0	0
			7	6	1		
59	L35A	1	Total	N	Os	0	0
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59	16SB	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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59	16SB	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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59	16SB	1	Total	N	Os	0	0
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59	S4B	1	Total	N	Os	0	0
			7	6	1		
59	S14B	1	Total	N	Os	0	0
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59	ASIB	1	Total	N	Os	0	0
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59	ASIB	1	Total	N	Os	0	0
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59	PSIB	1	Total	N	Os	0	0
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59	PSIB	1	Total	N	Os	0	0
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59	ESIB	1	Total	N	Os	0	0
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59	MRNB	1	Total	N	Os	0	0
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59	23SB	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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59	23SB	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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59	23SB	1	Total	N	Os	0	0
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			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	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		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	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		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	23SB	1	Total	N	Os	0	0
			7	6	1		
59	5SB	1	Total	N	Os	0	0
			7	6	1		
59	5SB	1	Total	N	Os	0	0
			7	6	1		
59	5SB	1	Total	N	Os	0	0
			7	6	1		
59	5SB	1	Total	N	Os	0	0
			7	6	1		
59	5SB	1	Total	N	Os	0	0
			7	6	1		
59	5SB	1	Total	N	Os	0	0
			7	6	1		
59	5SB	1	Total	N	Os	0	0
			7	6	1		
59	5SB	1	Total	N	Os	0	0
			7	6	1		
59	5SB	1	Total	N	Os	0	0
			7	6	1		
59	L4B	1	Total	N	Os	0	0
			7	6	1		
59	L17B	1	Total	N	Os	0	0
			7	6	1		
59	L20B	1	Total	N	Os	0	0
			7	6	1		
59	L35B	1	Total	N	Os	0	0
			7	6	1		

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	16SA	46	Total	K	0	0
			46	46		

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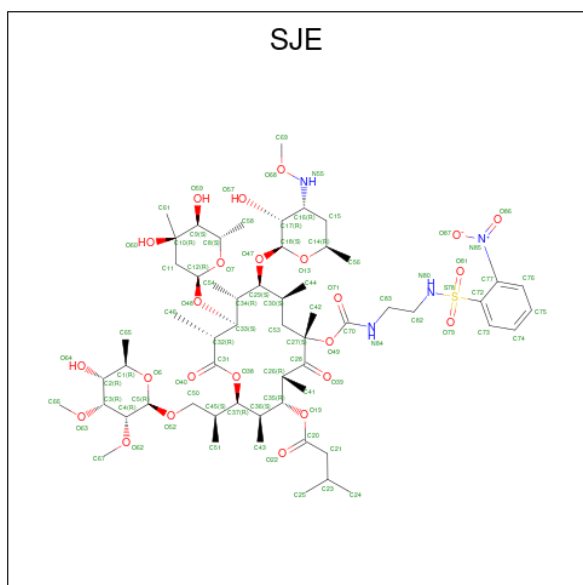
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	S6A	1	Total 1	K 1	0	0
60	S13A	1	Total 1	K 1	0	0
60	S20A	1	Total 1	K 1	0	0
60	PSIA	2	Total 2	K 2	0	0
60	23SA	102	Total 102	K 102	0	0
60	5SA	2	Total 2	K 2	0	0
60	L2A	1	Total 1	K 1	0	0
60	L3A	1	Total 1	K 1	0	0
60	L4A	1	Total 1	K 1	0	0
60	L5A	1	Total 1	K 1	0	0
60	16SB	35	Total 35	K 35	0	0
60	S4B	1	Total 1	K 1	0	0
60	S6B	1	Total 1	K 1	0	0
60	S13B	1	Total 1	K 1	0	0
60	S14B	1	Total 1	K 1	0	0
60	S20B	1	Total 1	K 1	0	0
60	23SB	81	Total 81	K 81	0	0
60	5SB	1	Total 1	K 1	0	0
60	L2B	1	Total 1	K 1	0	0
60	L3B	1	Total 1	K 1	0	0
60	L4B	1	Total 1	K 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	L5B	1	Total	K	0	0
			1	1		
60	L15B	1	Total	K	0	0
			1	1		
60	L16B	1	Total	K	0	0
			1	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,4R,6R)-3-hydroxy-4-(methoxyamino)-6-methyltetrahydro-2H-pyran-2-yl)oxy)-3,5,7,9,11,13-hexamethyl-7-((2-((2-nitrophenyl)sulfonamido)ethyl)carbamoyl)oxy)-6,14-dioxooxacyclotetradecan-4-yl 3-methylbutanoate (three-letter code: SJE) (formula: C₅₈H₉₆N₄O₂₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	23SA	1	Total	C	N	O	S	0	0
			87	58	4	24	1		
61	23SB	1	Total	C	N	O	S	0	0
			87	58	4	24	1		

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	16SA	172	Total	O	0	0
			172	172		
62	S4A	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	S5A	1	Total 1	O 1	0	0
62	S12A	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	THXA	3	Total 3	O 3	0	0
62	PSIA	7	Total 7	O 7	0	0
62	ESIA	1	Total 1	O 1	0	0
62	23SA	788	Total 788	O 788	0	0
62	5SA	14	Total 14	O 14	0	0
62	L2A	10	Total 10	O 10	0	0
62	L3A	7	Total 7	O 7	0	0
62	L4A	6	Total 6	O 6	0	0
62	L15A	9	Total 9	O 9	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
62	L30A	1	Total 1	O 1	0	0

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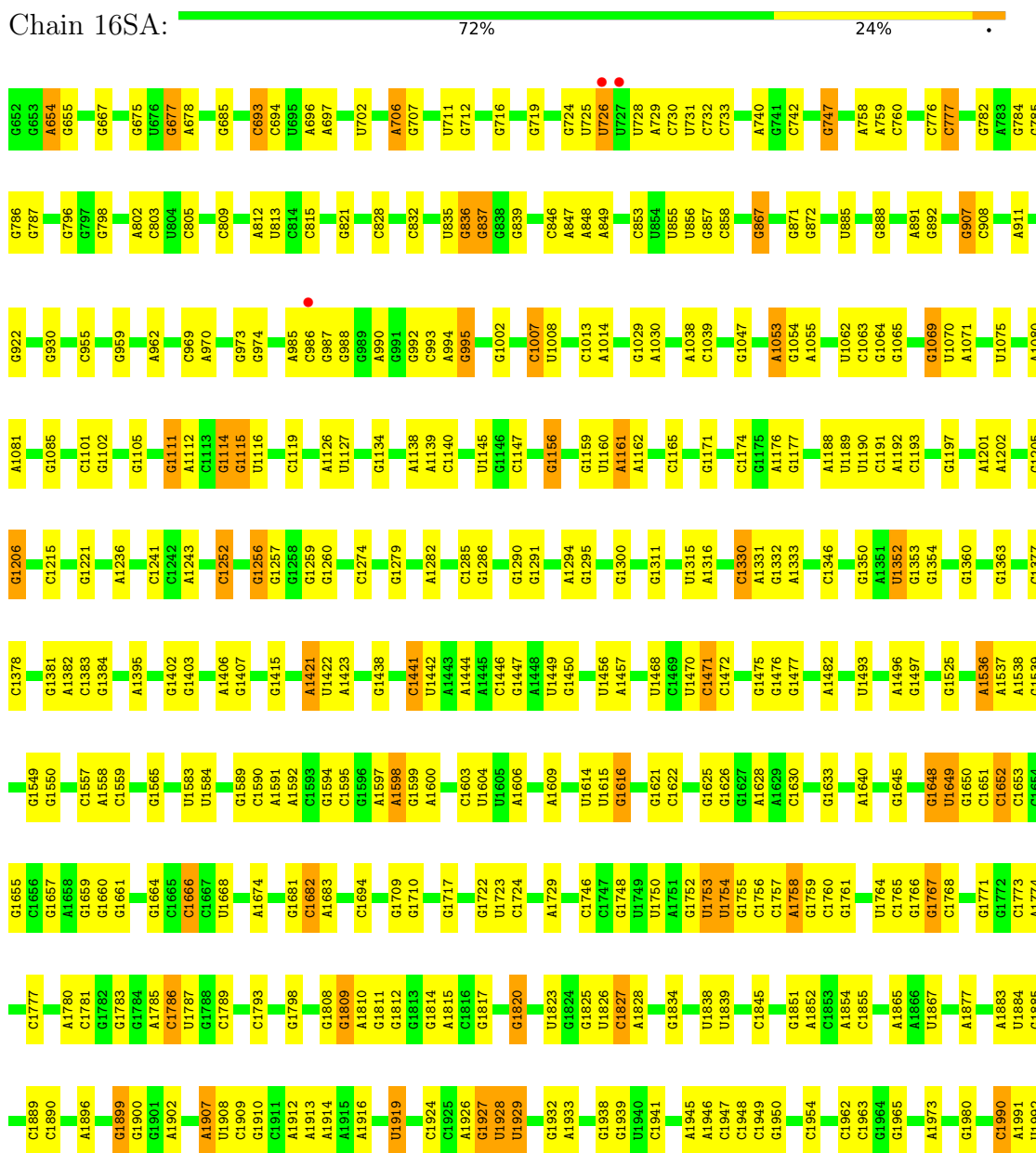
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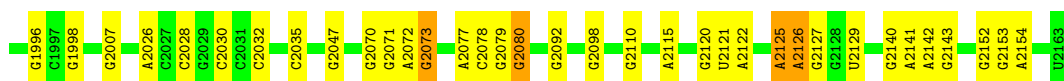
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	L34A	1	Total 1	O 1	0	0
62	L35A	1	Total 1	O 1	0	0
62	16SB	157	Total 157	O 157	0	0
62	S4B	2	Total 2	O 2	0	0
62	S5B	1	Total 1	O 1	0	0
62	S9B	1	Total 1	O 1	0	0
62	S12B	2	Total 2	O 2	0	0
62	S14B	2	Total 2	O 2	0	0
62	23SB	519	Total 519	O 519	0	0
62	5SB	5	Total 5	O 5	0	0
62	L2B	12	Total 12	O 12	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	L19B	1	Total 1	O 1	0	0
62	L27B	2	Total 2	O 2	0	0
62	L28B	1	Total 1	O 1	0	0
62	L30B	1	Total 1	O 1	0	0
62	L35B	6	Total 6	O 6	0	0

3 Residue-property plots [i](#)

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.

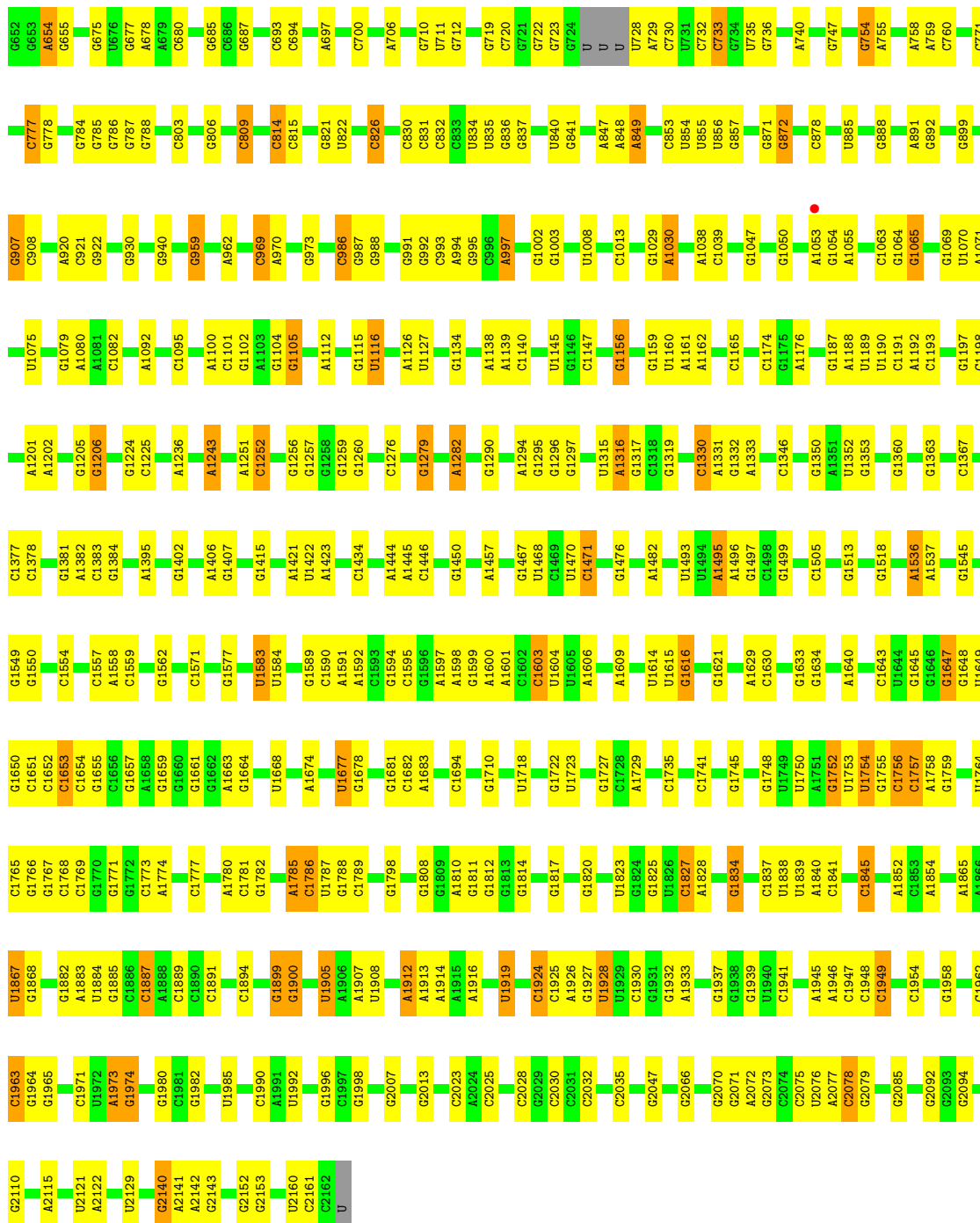
• Molecule 1: 16S rRNA





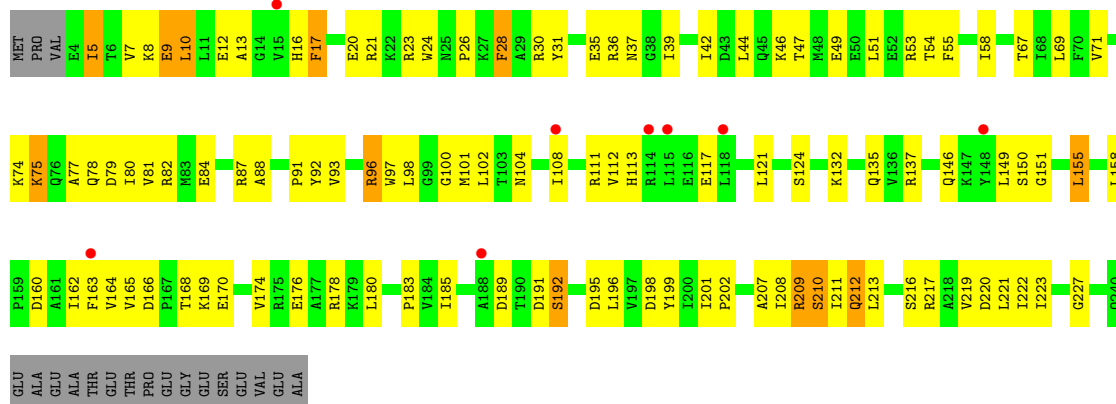
• Molecule 1: 16S rRNA

Chain 16SB: 71% 25%



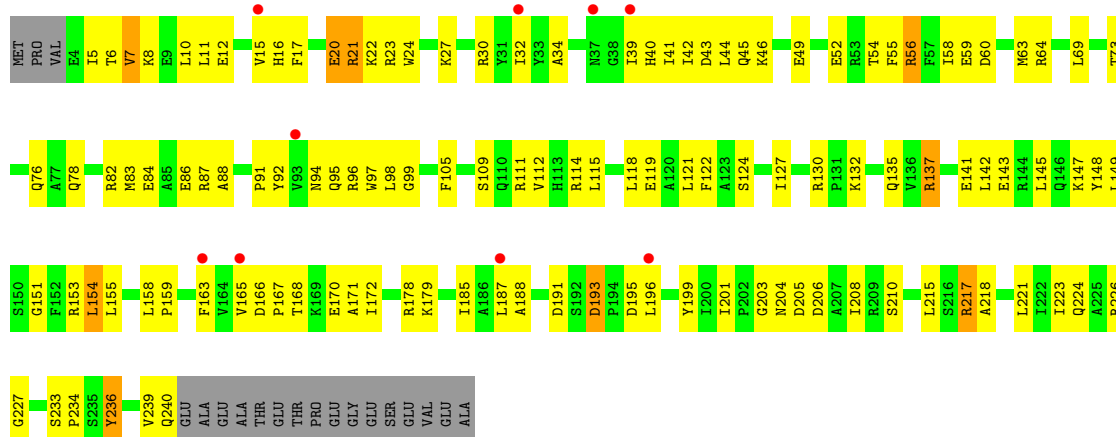
• Molecule 2: 30S ribosomal protein S2

Chain S2A: 



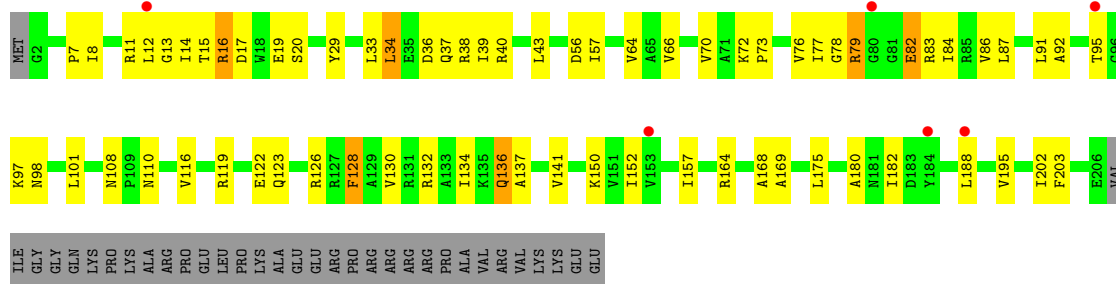
• Molecule 2: 30S ribosomal protein S2

Chain S2B: 



• Molecule 3: 30S ribosomal protein S3

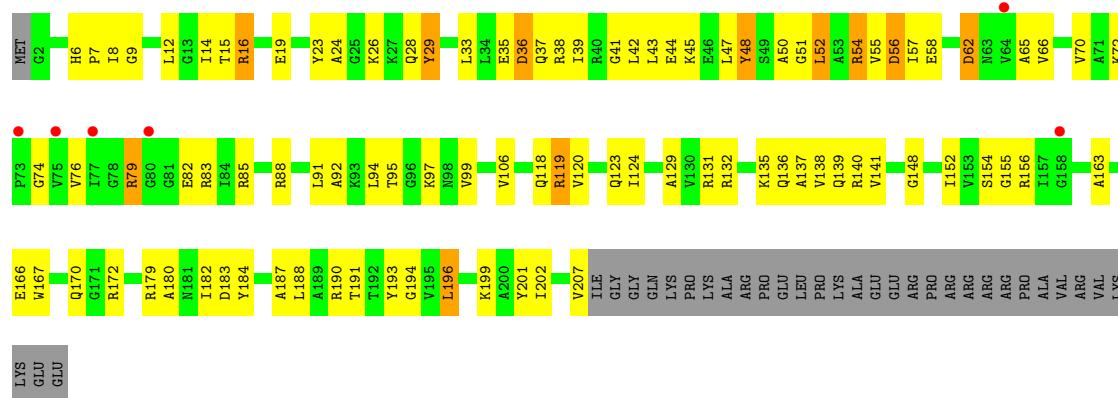
Chain S3A: 



• Molecule 3: 30S ribosomal protein S3

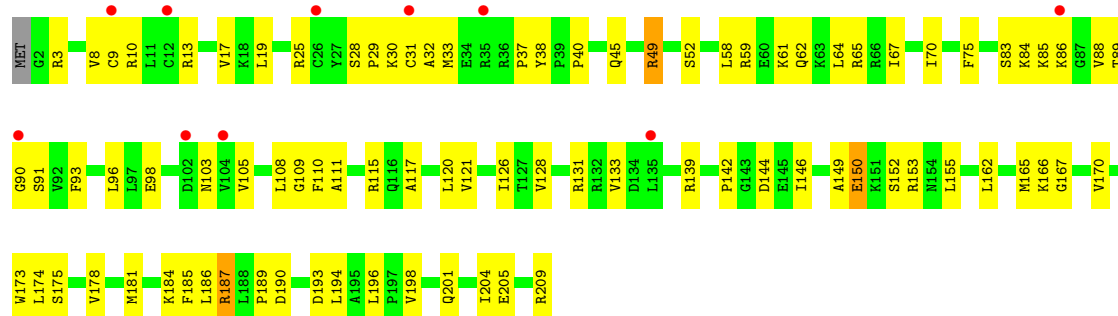
Chain S3B: 





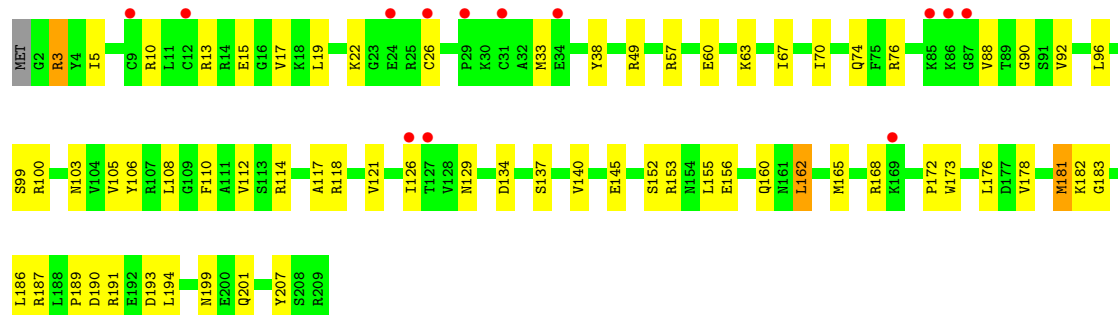
• Molecule 4: 30S ribosomal protein S4

Chain S4A: 5% 58% 40% .



• Molecule 4: 30S ribosomal protein S4

Chain S4B: 6% 68% 30% .



• Molecule 5: 30S ribosomal protein S5

Chain S5A: % 65% 28% 7%

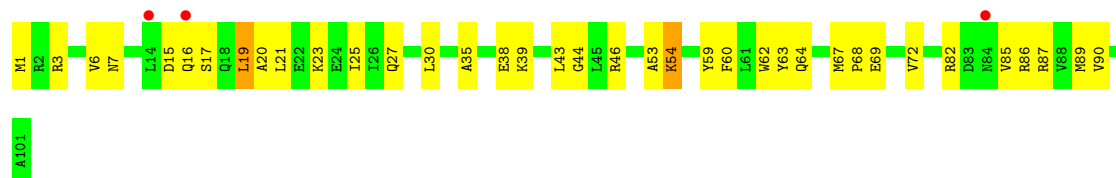




• Molecule 5: 30S ribosomal protein S5



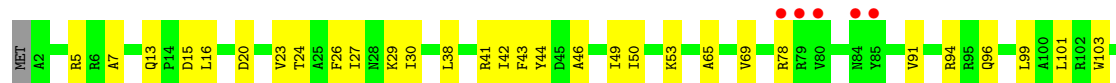
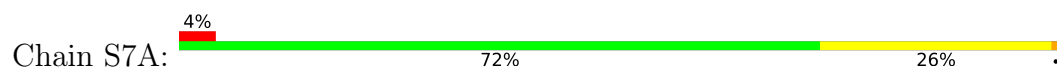
• Molecule 6: 30S ribosomal protein S6



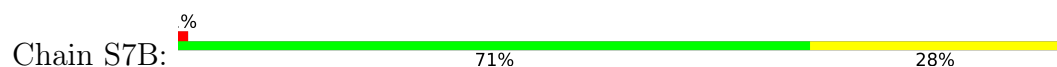
• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7



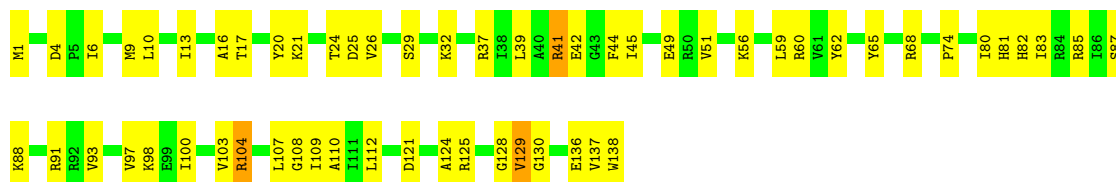
• Molecule 7: 30S ribosomal protein S7





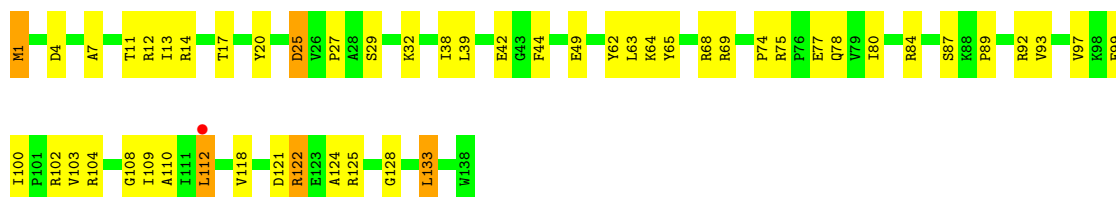
- Molecule 8: 30S ribosomal protein S8

Chain S8A: 58% 40%



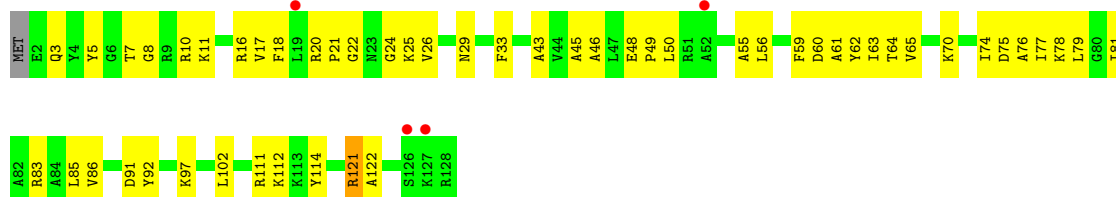
- Molecule 8: 30S ribosomal protein S8

Chain S8B: 63% 33%



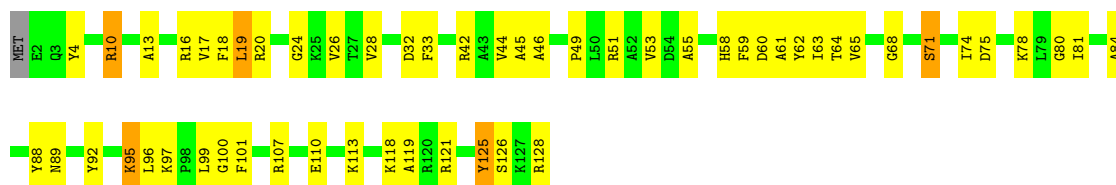
- Molecule 9: 30S ribosomal protein S9

Chain S9A: 3% 59% 40%



- Molecule 9: 30S ribosomal protein S9

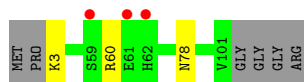
Chain S9B: 56% 39%



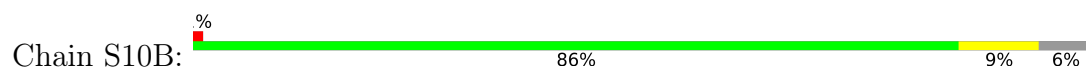
- Molecule 10: 30S ribosomal protein S10

Chain S10A: 3% 91% 6%

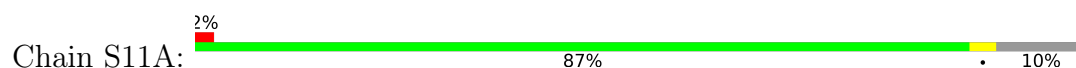




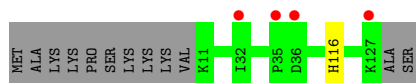
- Molecule 10: 30S ribosomal protein S10



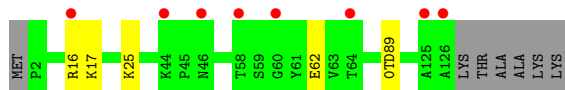
- Molecule 11: 30S ribosomal protein S11



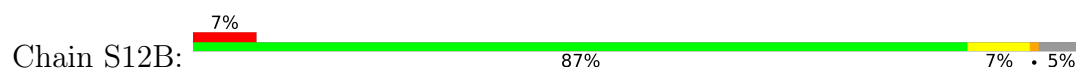
- Molecule 11: 30S ribosomal protein S11



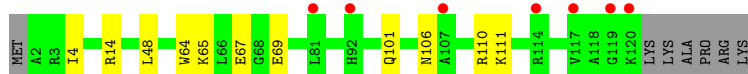
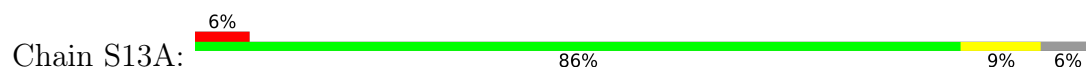
- Molecule 12: 30S ribosomal protein S12



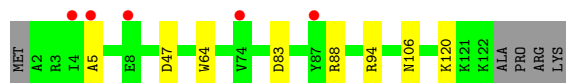
- Molecule 12: 30S ribosomal protein S12



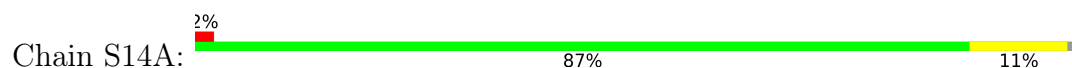
- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S14 type Z



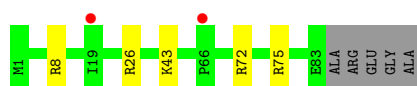
- Molecule 15: 30S ribosomal protein S15



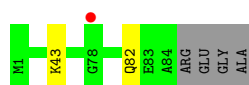
- Molecule 15: 30S ribosomal protein S15



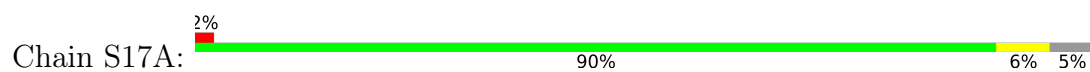
- Molecule 16: 30S ribosomal protein S16



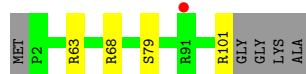
- Molecule 16: 30S ribosomal protein S16



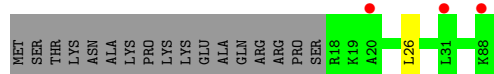
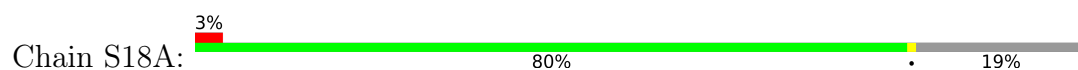
- Molecule 17: 30S ribosomal protein S17



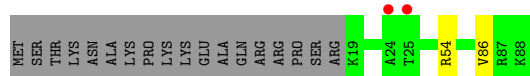
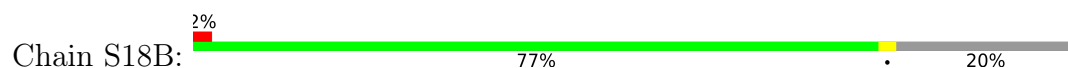
- Molecule 17: 30S ribosomal protein S17



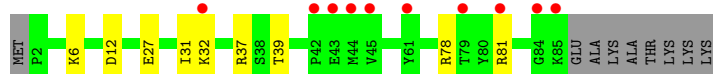
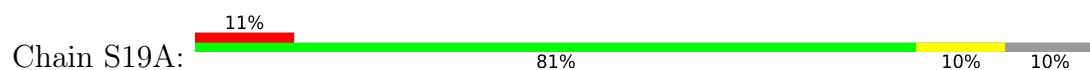
- Molecule 18: 30S ribosomal protein S18



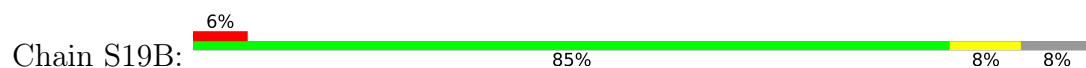
- Molecule 18: 30S ribosomal protein S18



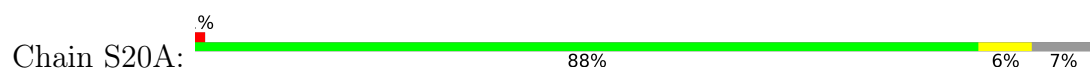
- Molecule 19: 30S ribosomal protein S19



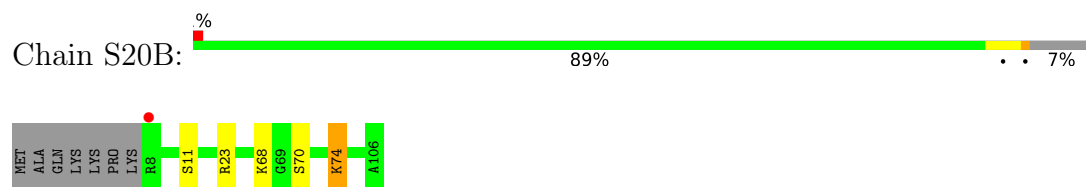
- Molecule 19: 30S ribosomal protein S19



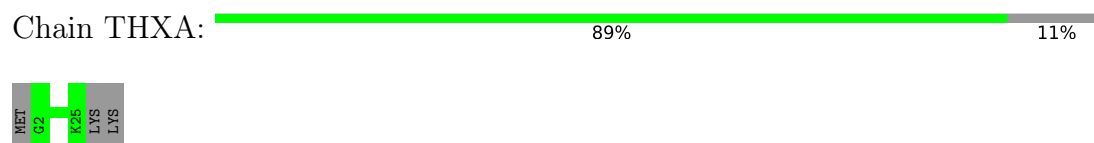
- Molecule 20: 30S ribosomal protein S20



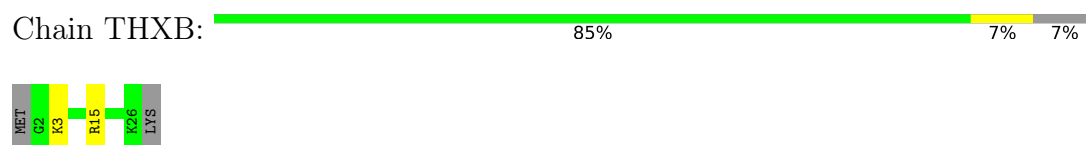
- Molecule 20: 30S ribosomal protein S20



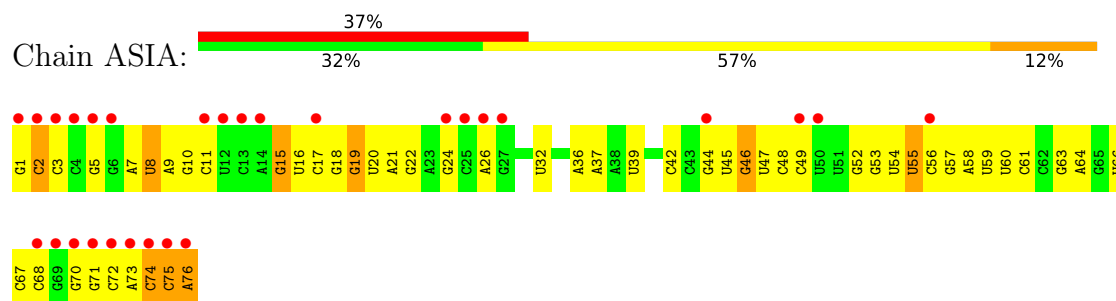
- Molecule 21: 30S ribosomal protein Thx



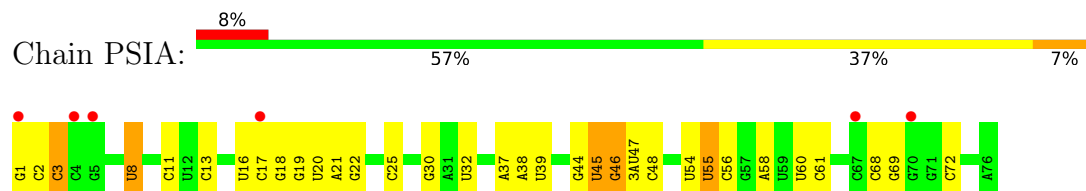
- Molecule 21: 30S ribosomal protein Thx



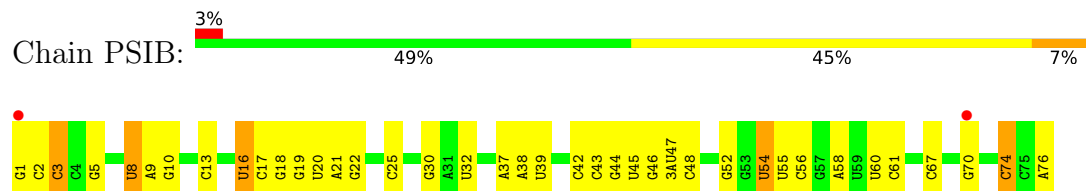
- Molecule 22: Phe-tRNA



- Molecule 23: Phe-tRNA

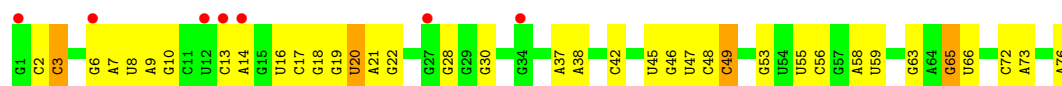


- Molecule 23: Phe-tRNA



- Molecule 24: Phe-tRNA

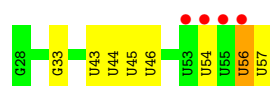
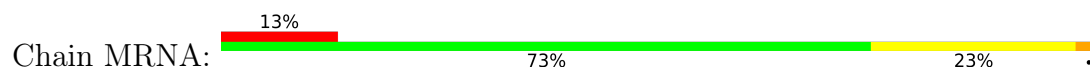




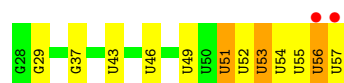
• Molecule 24: Phe-tRNA



• Molecule 25: RNA (30-MER)



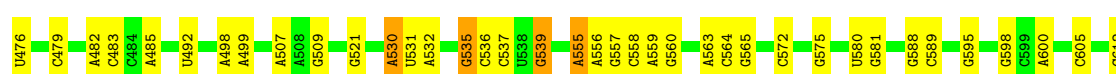
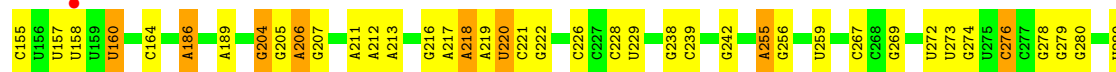
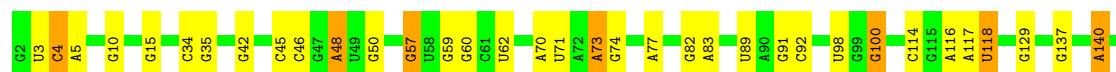
• Molecule 25: RNA (30-MER)



• Molecule 26: Phe-tRNA



• Molecule 27: 23S rRNA





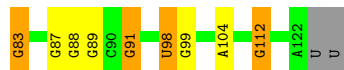
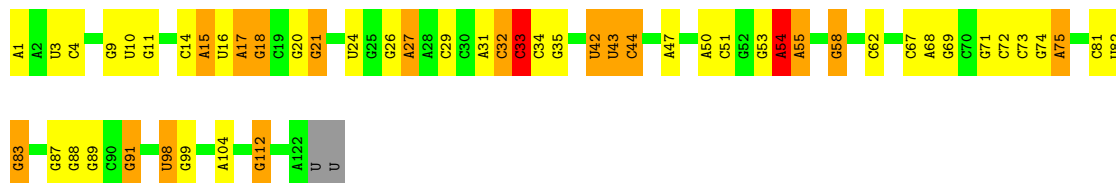


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G1137	G1243	A1391	C1517	G1609	G1769	C1907	U2018	G2158	G2261	G2365	G2497	C2661	G2793
U1138	G1244	C1394	C1518	G1610	U1770	G1913	C2021	C2161	G2266	G2387	G2509	A2669	A2794
G1139	G1245	U1394	A1521	A1616	U1771	A1914	A2045	C2162	G2267	G2394	G2517	G2670	U2795
C					G1772								
G													
U													
A	A1252	A1398	C1524	A1619	C1776	G1924	G2048	C2170	C2278	G2398	G2518	A2680	A2806
U	G1254	U1401	G1525	A1628	G1784	A1925		G2171	A2282	G2399	U2519	C2681	C2807
A			A1527	U1628				G2172		C2400	G2520	G2687	C2810
U			G1528	A1629				G2174		G2406	U2521	G2688	G2811
A	A1258	A1408	G1529	A1630						A2407	C2522		U2812
G	U1259	A1409	G1530	A1631	G1790	U1936	A2056	G2184	A2288		G2523		
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			G1532	C1634	G1792	C1939	A2058	C2188	A2293	C2417	G2538		
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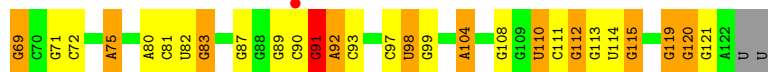
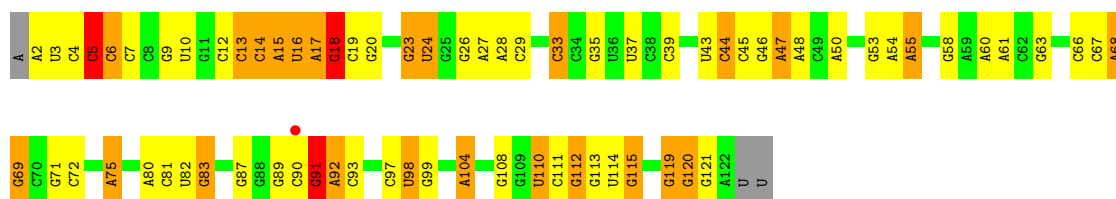
- Molecule 28: 5S rRNA

Chain 5SA: 56% 27% 13% ..



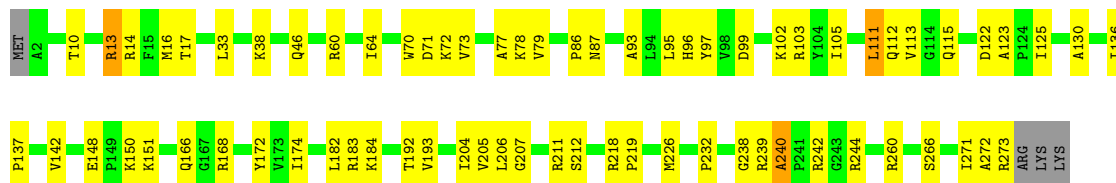
- Molecule 28: 5S rRNA

Chain 5SB: 40% 36% 19% ..



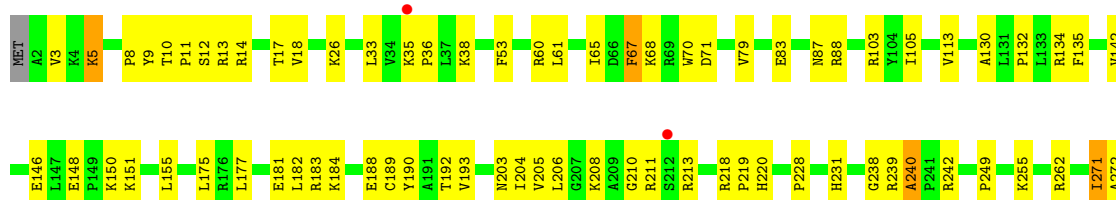
- Molecule 29: 50S ribosomal protein L2

Chain L2A: 73% 24% ..

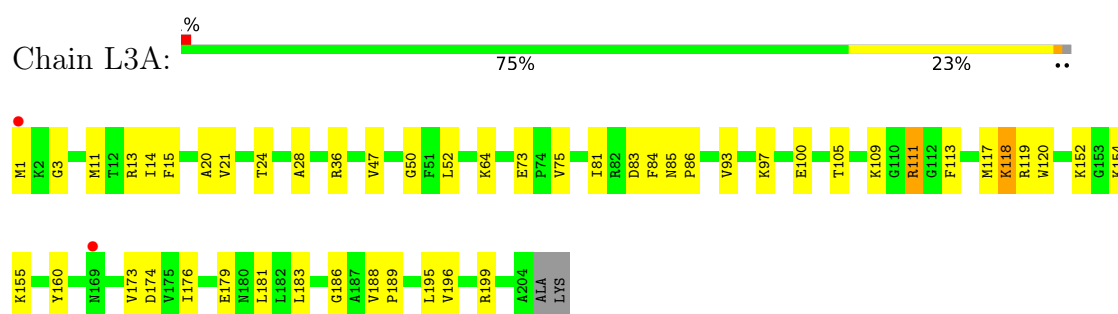


- Molecule 29: 50S ribosomal protein L2

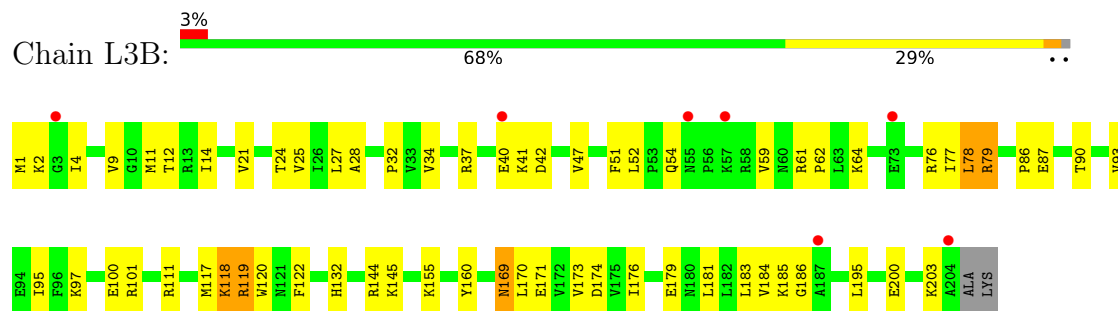
Chain L2B: 71% 26% ..



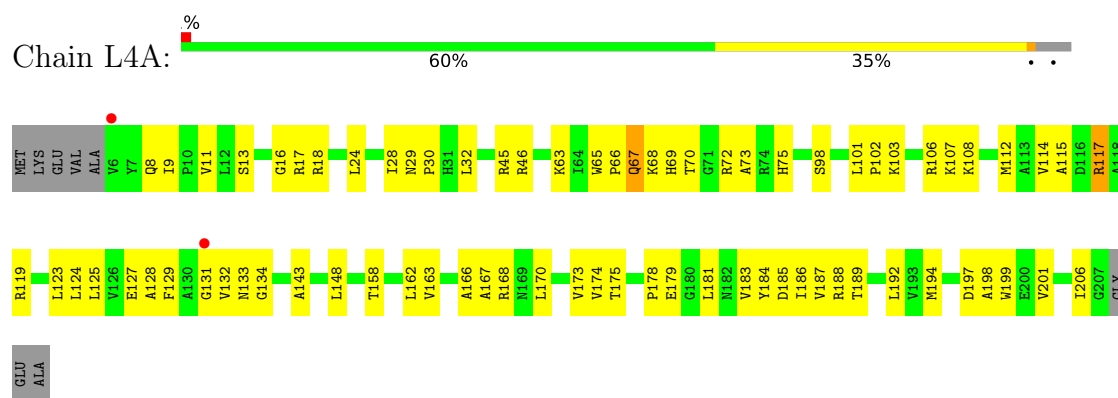
- Molecule 30: 50S ribosomal protein L3



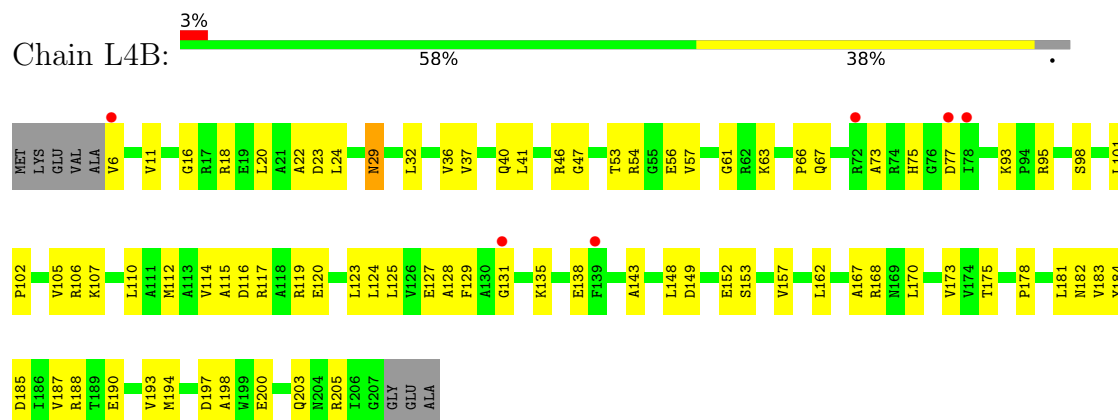
- Molecule 30: 50S ribosomal protein L3



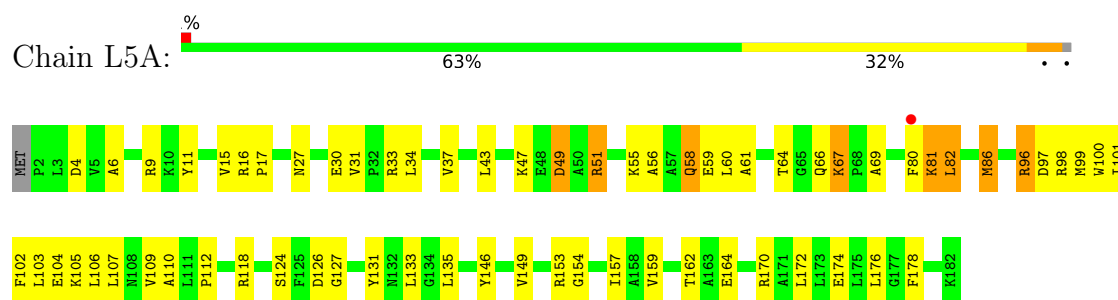
- Molecule 31: 50S ribosomal protein L4



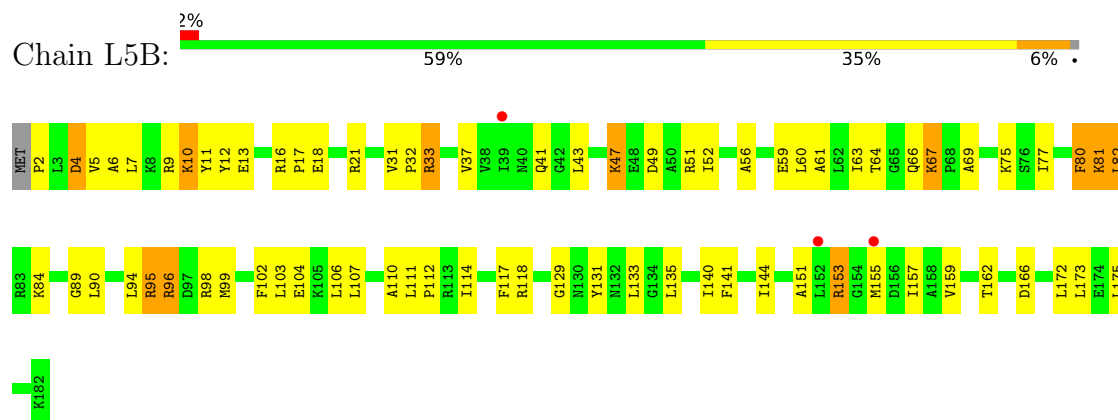
- Molecule 31: 50S ribosomal protein L4



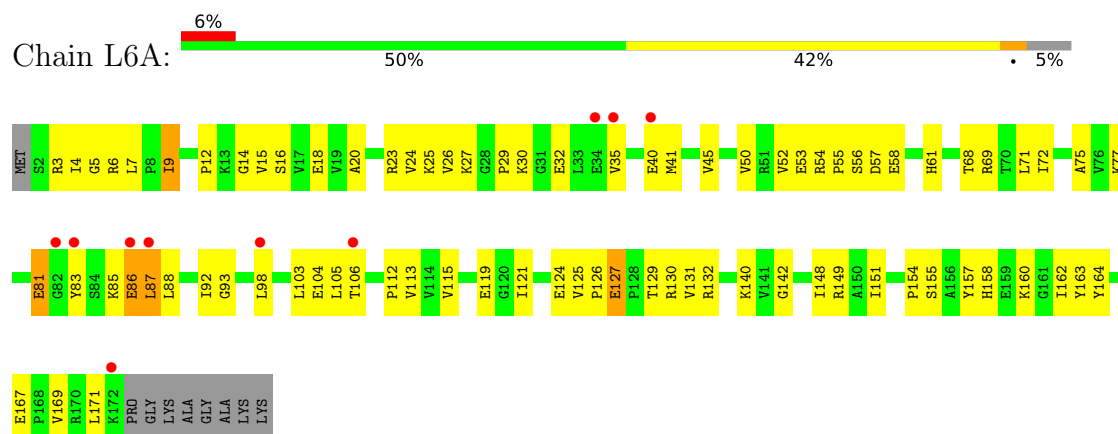
- Molecule 32: 50S ribosomal protein L5



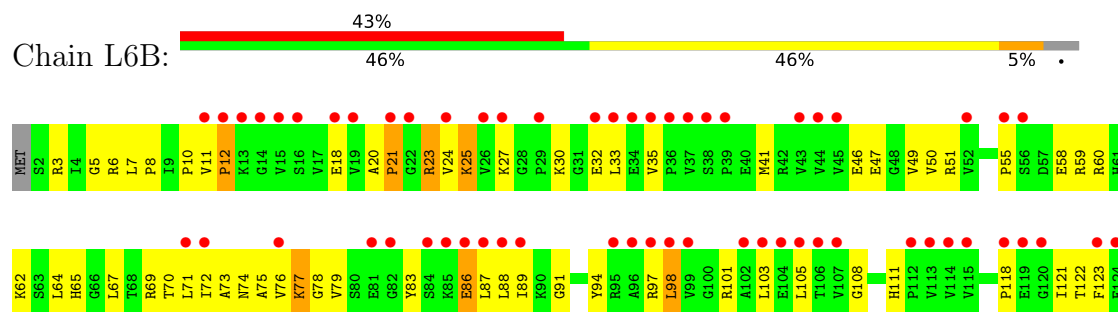
• Molecule 32: 50S ribosomal protein L5



• Molecule 33: 50S ribosomal protein L6

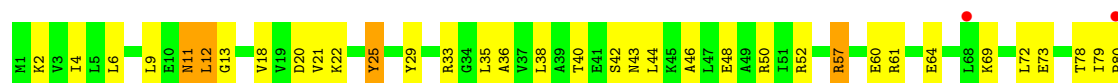


• Molecule 33: 50S ribosomal protein L6





- Molecule 34: 50S ribosomal protein L9



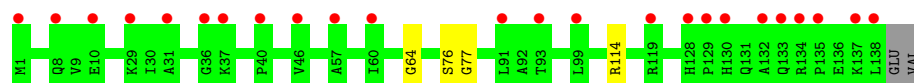
- Molecule 34: 50S ribosomal protein L9



- Molecule 35: 50S ribosomal protein L13



- Molecule 35: 50S ribosomal protein L13



- Molecule 36: 50S ribosomal protein L14



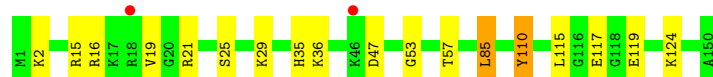
- Molecule 36: 50S ribosomal protein L14



- Molecule 37: 50S ribosomal protein L15



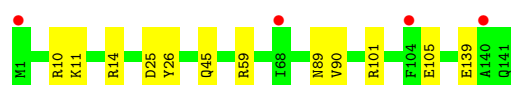
- Molecule 37: 50S ribosomal protein L15



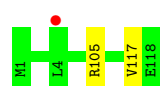
- Molecule 38: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L16



- Molecule 39: 50S ribosomal protein L17



- Molecule 39: 50S ribosomal protein L17



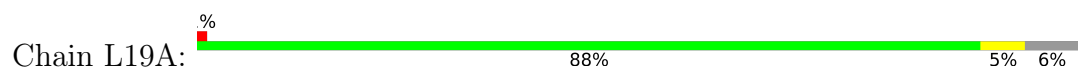
- Molecule 40: 50S ribosomal protein L18



- Molecule 40: 50S ribosomal protein L18



- Molecule 41: 50S ribosomal protein L19



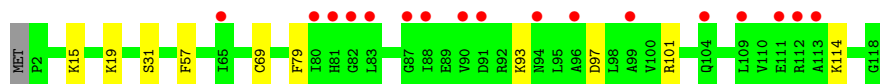
- Molecule 41: 50S ribosomal protein L19



- Molecule 42: 50S ribosomal protein L20



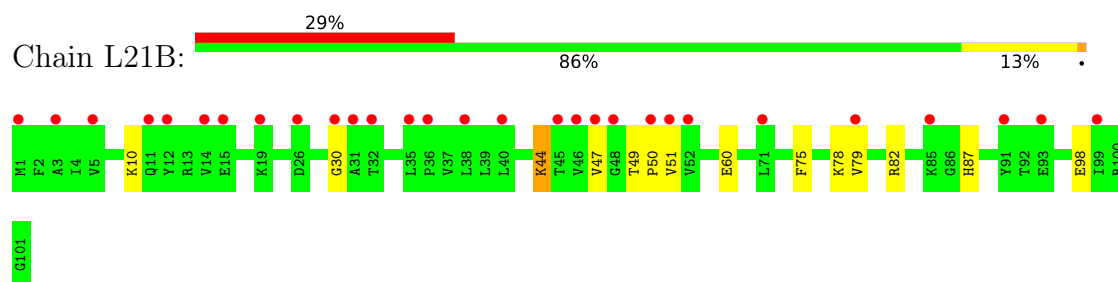
- Molecule 42: 50S ribosomal protein L20



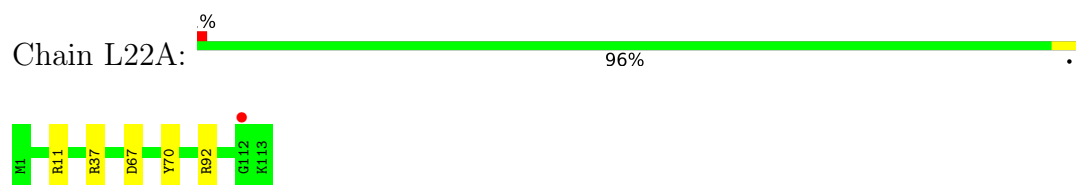
- Molecule 43: 50S ribosomal protein L21



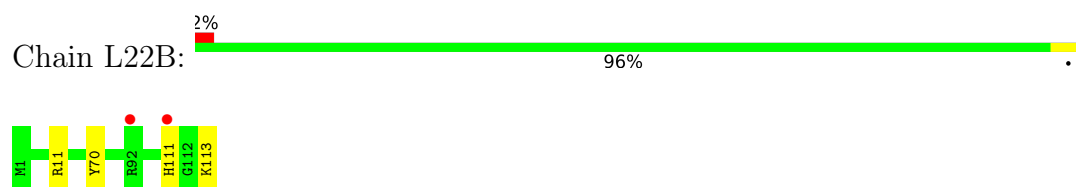
- Molecule 43: 50S ribosomal protein L21



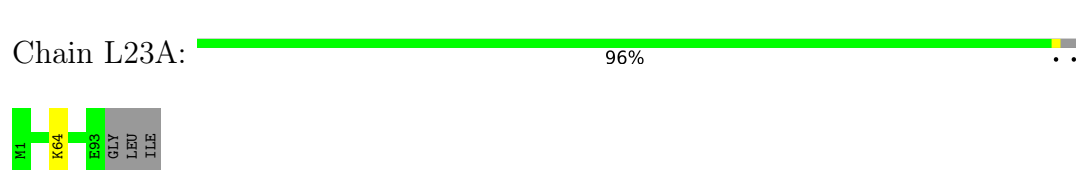
- Molecule 44: 50S ribosomal protein L22



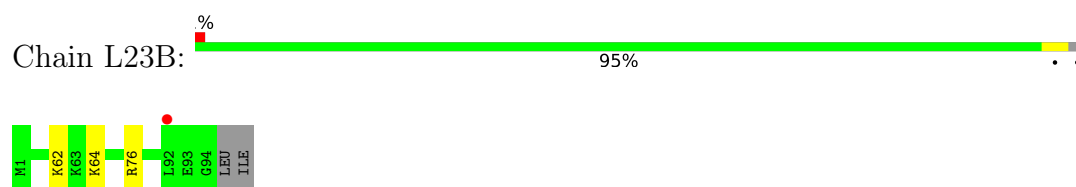
- Molecule 44: 50S ribosomal protein L22



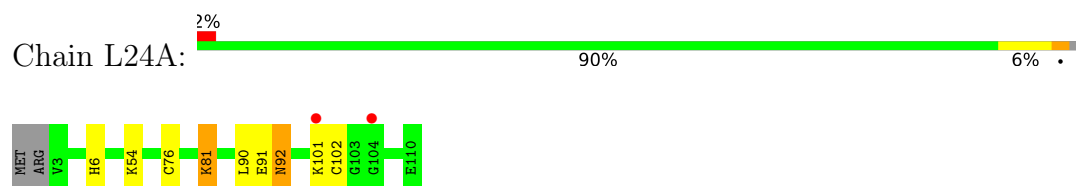
- Molecule 45: 50S ribosomal protein L23



- Molecule 45: 50S ribosomal protein L23



- Molecule 46: 50S ribosomal protein L24

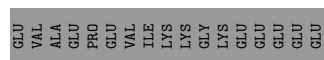
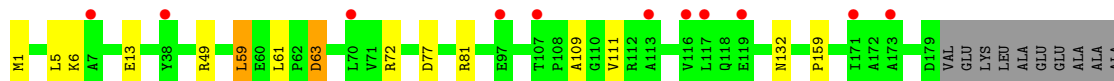
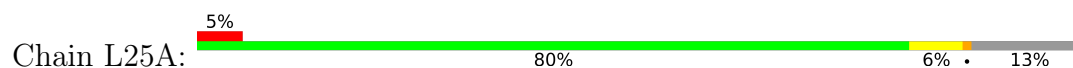


- Molecule 46: 50S ribosomal protein L24

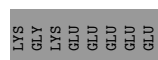
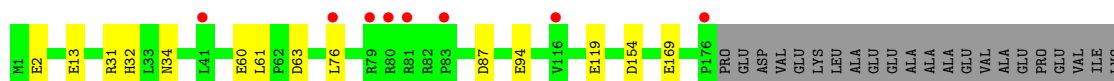
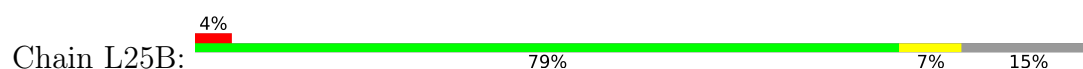




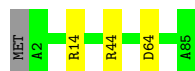
- Molecule 47: 50S ribosomal protein L25



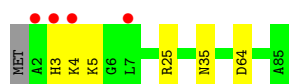
- Molecule 47: 50S ribosomal protein L25



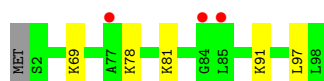
- Molecule 48: 50S ribosomal protein L27



- Molecule 48: 50S ribosomal protein L27

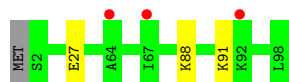


- Molecule 49: 50S ribosomal protein L28



- Molecule 49: 50S ribosomal protein L28





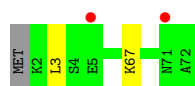
- Molecule 50: 50S ribosomal protein L29

Chain L29A: 92% . .



- Molecule 50: 50S ribosomal protein L29

Chain L29B: 96% . .



- Molecule 51: 50S ribosomal protein L30

Chain L30A: 95% . .



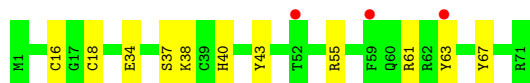
- Molecule 51: 50S ribosomal protein L30

Chain L30B: 95% . .



- Molecule 52: 50S ribosomal protein L31

Chain L31A: 85% 15%



- Molecule 52: 50S ribosomal protein L31

Chain L31B: 89% 10% .

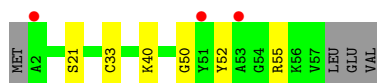
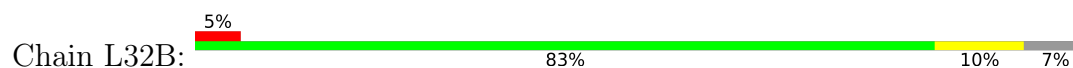


- Molecule 53: 50S ribosomal protein L32

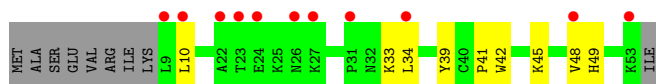
Chain L32A: 88% 5% 7%



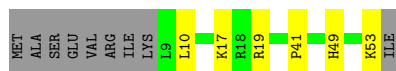
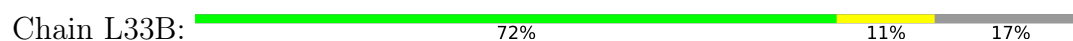
- Molecule 53: 50S ribosomal protein L32



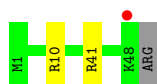
- Molecule 54: 50S ribosomal protein L33



- Molecule 54: 50S ribosomal protein L33



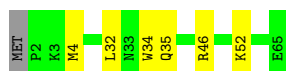
- Molecule 55: 50S ribosomal protein L34



- Molecule 55: 50S ribosomal protein L34



- Molecule 56: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L35

Chain L35B:

94%

5% •



● Molecule 57: Phe-tRNA

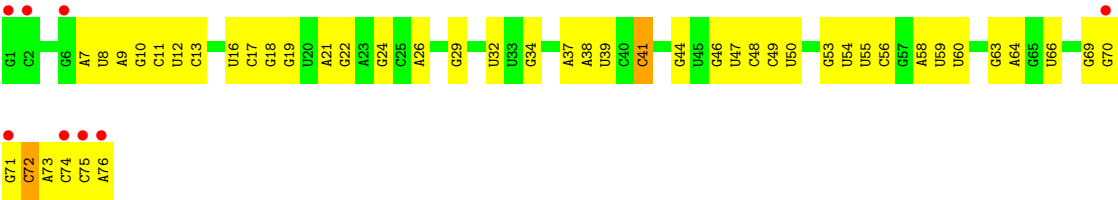
Chain ASIB:

11%

39%

58%

•



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.77Å 446.87Å 616.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	253.87 – 3.30 253.87 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (253.87-3.30) 100.0 (253.87-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.214 , 0.238 0.214 , 0.238	Depositor DCC
R_{free} test set	834928 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	93.1	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	306403	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% 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: 0TD, MG, G7M, OHX, OMU, H2U, SJE, 4SU, MIA, M2G, K, 2MG, 3AU, UR3, OMG, 5MC, MA6, OMC, 4OC, 5MU, PSU, 2MA

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	0.48	2/36088 (0.0%)	1.19	254/56320 (0.5%)
1	16SB	0.46	0/35999	1.19	261/56180 (0.5%)
2	S2A	0.34	0/1959	0.68	0/2642
2	S2B	0.31	0/1959	0.66	0/2642
3	S3A	0.33	0/1629	0.70	0/2195
3	S3B	0.30	0/1636	0.68	1/2205 (0.0%)
4	S4A	0.35	0/1732	0.71	0/2318
4	S4B	0.32	0/1732	0.66	0/2318
5	S5A	0.34	0/1171	0.69	0/1576
5	S5B	0.32	0/1171	0.66	0/1576
6	S6A	0.32	0/855	0.67	0/1154
6	S6B	0.33	0/855	0.63	0/1154
7	S7A	0.35	0/1275	0.67	0/1709
7	S7B	0.31	0/1275	0.62	0/1709
8	S8A	0.32	0/1135	0.69	0/1527
8	S8B	0.29	0/1135	0.65	0/1527
9	S9A	0.35	0/1028	0.71	1/1379 (0.1%)
9	S9B	0.34	0/1028	0.75	2/1379 (0.1%)
10	S10A	0.32	0/814	0.66	0/1095
10	S10B	0.31	0/814	0.70	0/1095
11	S11A	0.31	0/879	0.59	0/1187
11	S11B	0.29	0/888	0.60	0/1198
12	S12A	0.35	0/982	0.72	0/1313
12	S12B	0.32	0/982	0.68	1/1313 (0.1%)
13	S13A	0.31	0/956	0.71	0/1281
13	S13B	0.28	0/974	0.66	0/1303
14	S14A	0.41	0/500	0.76	1/664 (0.2%)
14	S14B	0.35	0/495	0.72	0/657
15	S15A	0.31	0/744	0.65	0/992
15	S15B	0.28	0/744	0.60	0/992
16	S16A	0.32	0/716	0.70	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	S16B	0.32	0/721	0.65	0/970
17	S17A	0.33	0/847	0.68	0/1131
17	S17B	0.30	0/847	0.63	0/1131
18	S18A	0.32	0/589	0.74	0/782
18	S18B	0.31	0/578	0.71	0/768
19	S19A	0.33	0/689	0.81	1/926 (0.1%)
19	S19B	0.32	0/698	0.69	0/938
20	S20A	0.35	0/764	0.74	0/1007
20	S20B	0.29	0/764	0.65	0/1007
21	THXA	0.30	0/212	0.76	0/277
21	THXB	0.29	0/221	0.75	0/288
22	ASIA	0.52	0/1647	1.44	33/2565 (1.3%)
23	PSIA	0.53	0/1602	1.27	6/2493 (0.2%)
23	PSIB	0.52	0/1602	1.21	13/2493 (0.5%)
24	ESIA	0.50	0/1783	1.20	15/2776 (0.5%)
24	ESIB	0.45	0/1783	1.14	8/2776 (0.3%)
25	MRNA	0.38	0/689	1.04	3/1069 (0.3%)
25	MRNB	0.41	0/689	1.15	8/1069 (0.7%)
26	TRNA	0.44	0/1560	1.16	6/2431 (0.2%)
27	23SA	0.53	3/69430 (0.0%)	1.20	471/108380 (0.4%)
27	23SB	0.52	10/69052 (0.0%)	1.20	514/107791 (0.5%)
28	5SA	0.51	1/2928 (0.0%)	1.21	19/4568 (0.4%)
28	5SB	0.53	0/2906	1.32	36/4533 (0.8%)
29	L2A	0.36	0/2165	0.72	1/2919 (0.0%)
29	L2B	0.36	0/2165	0.70	0/2919
30	L3A	0.34	0/1596	0.64	0/2153
30	L3B	0.33	0/1596	0.63	1/2153 (0.0%)
31	L4A	0.41	0/1620	0.69	0/2194
31	L4B	0.33	0/1620	0.67	0/2194
32	L5A	0.32	0/1498	0.67	0/2016
32	L5B	0.31	0/1498	0.65	0/2016
33	L6A	0.35	0/1341	0.73	1/1813 (0.1%)
33	L6B	0.31	0/1353	0.72	1/1830 (0.1%)
34	L9A	0.32	0/1146	0.78	1/1551 (0.1%)
34	L9B	0.32	0/1151	0.68	1/1558 (0.1%)
35	L13A	0.34	0/1131	0.70	0/1525
35	L13B	0.29	0/1131	0.65	0/1525
36	L14A	0.37	0/942	0.69	0/1269
36	L14B	0.37	0/942	0.67	1/1269 (0.1%)
37	L15A	0.39	0/1161	0.87	2/1544 (0.1%)
37	L15B	0.36	0/1161	0.81	1/1544 (0.1%)
38	L16A	0.34	0/1142	0.67	0/1527
38	L16B	0.34	0/1142	0.67	0/1527

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L17A	0.31	0/981	0.72	0/1312
39	L17B	0.34	0/981	0.69	0/1312
40	L18A	0.32	0/899	0.82	0/1197
40	L18B	0.33	0/891	0.74	1/1187 (0.1%)
41	L19A	0.35	0/1155	0.72	0/1542
41	L19B	0.32	0/1155	0.70	0/1542
42	L20A	0.36	0/981	0.71	1/1306 (0.1%)
42	L20B	0.32	0/981	0.67	0/1306
43	L21A	0.36	0/789	0.82	2/1057 (0.2%)
43	L21B	0.39	0/789	0.76	0/1057
44	L22A	0.36	0/910	0.67	0/1220
44	L22B	0.34	0/910	0.65	0/1220
45	L23A	0.39	0/752	0.67	0/1009
45	L23B	0.35	0/756	0.61	0/1014
46	L24A	0.35	0/837	0.70	0/1118
46	L24B	0.33	0/787	0.66	0/1056
47	L25A	0.33	0/1460	0.72	2/1982 (0.1%)
47	L25B	0.30	0/1435	0.70	0/1947
48	L27A	0.38	0/670	0.73	0/892
48	L27B	0.36	0/670	0.69	0/892
49	L28A	0.36	0/769	0.68	0/1022
49	L28B	0.37	0/769	0.76	0/1022
50	L29A	0.31	0/585	0.68	0/773
50	L29B	0.31	0/592	0.65	0/784
51	L30A	0.33	0/473	0.69	0/635
51	L30B	0.32	0/473	0.71	1/635 (0.2%)
52	L31A	0.35	0/593	0.72	0/795
52	L31B	0.33	0/593	0.70	0/795
53	L32A	0.39	0/448	0.67	0/606
53	L32B	0.33	0/448	0.68	0/606
54	L33A	0.37	0/396	0.91	1/529 (0.2%)
54	L33B	0.44	0/396	0.97	1/529 (0.2%)
55	L34A	0.35	0/426	0.77	0/561
55	L34B	0.36	0/437	0.78	0/575
56	L35A	0.31	0/524	0.64	0/691
56	L35B	0.30	0/524	0.66	0/691
57	ASIB	0.45	0/1717	1.24	11/2674 (0.4%)
All	All	0.46	16/323204 (0.0%)	1.09	1684/483869 (0.3%)

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
34	L9A	0	2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	23SA	2086	G	O3'-P	-11.54	1.47	1.61
1	16SA	1717	G	C6-N1	7.25	1.44	1.39
27	23SB	2127	U	C2-N3	7.24	1.42	1.37
27	23SB	2087	A	O3'-P	-7.19	1.52	1.61
27	23SB	44	G	C6-N1	7.04	1.44	1.39

The worst 5 of 1684 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	23SB	1291	A	N1-C2-N3	-30.14	114.23	129.30
27	23SB	1291	A	C2-N3-C4	19.13	120.17	110.60
27	23SA	1924	G	N3-C4-N9	-14.88	117.07	126.00
1	16SA	1717	G	C5-C6-O6	-14.08	120.15	128.60
1	16SA	1717	G	N3-C2-N2	-14.08	110.05	119.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	L9A	110	ASP	Peptide
34	L9A	131	LYS	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	32509	0	0	0	10
1	16SB	32429	0	0	0	0
2	S2A	1924	0	1975	82	0
2	S2B	1924	0	1975	101	0
3	S3A	1605	0	1668	47	0
3	S3B	1612	0	1677	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S4A	1702	0	1767	69	0
4	S4B	1702	0	1764	43	0
5	S5A	1155	0	1213	27	0
5	S5B	1155	0	1212	31	0
6	S6A	842	0	857	26	0
6	S6B	842	0	857	22	0
7	S7A	1256	0	1296	28	0
7	S7B	1256	0	1296	26	0
8	S8A	1115	0	1177	42	0
8	S8B	1115	0	1177	42	0
9	S9A	1009	0	1037	40	0
9	S9B	1009	0	1037	49	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	MRNB	621	0	0	0	0
26	TRNA	1565	0	0	0	4
27	23SA	62225	0	0	0	1
27	23SB	61886	0	0	0	2
28	5SA	2617	0	1327	33	0
28	5SB	2598	0	1316	45	0
29	L2A	2115	0	2195	48	0
29	L2B	2115	0	2195	50	0
30	L3A	1563	0	1629	29	0
30	L3B	1563	0	1629	51	0
31	L4A	1585	0	1632	57	0
31	L4B	1585	0	1632	55	0
32	L5A	1473	0	1535	46	0
32	L5B	1473	0	1535	56	0
33	L6A	1316	0	1395	71	0
33	L6B	1327	0	1405	67	10
34	L9A	1131	0	1218	100	0
34	L9B	1136	0	1223	50	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	2
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	2
42	L20B	963	0	0	0	0
43	L21A	778	0	0	0	1
43	L21B	778	0	0	0	0
44	L22A	899	0	0	0	0
44	L22B	899	0	0	0	0
45	L23A	738	0	0	0	0
45	L23B	742	0	0	0	0
46	L24A	824	0	0	0	0
46	L24B	775	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	590	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	92	0	0	0	0
58	16SB	86	0	0	0	0
58	23SA	332	0	0	0	0
58	23SB	241	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	L15B	1	0	0	0	0
58	L23A	1	0	0	0	0
58	L27A	2	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	L4B	1	0	0	0	0
58	L5A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	L5B	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	1	0	0	0	0
59	16SA	574	0	0	0	0
59	16SB	546	0	0	0	0
59	23SA	1435	0	0	0	2
59	23SB	1393	0	0	0	0
59	5SA	77	0	0	0	0
59	5SB	77	0	0	0	0
59	ASIA	21	0	0	0	0
59	ASIB	21	0	0	0	0
59	ESIA	7	0	0	0	0
59	ESIB	7	0	0	0	0
59	L15A	7	0	0	0	0
59	L17A	7	0	0	0	0
59	L17B	7	0	0	0	0
59	L19A	7	0	0	0	0
59	L20A	7	0	0	0	0
59	L20B	7	0	0	0	0
59	L27A	14	0	0	0	0
59	L28A	7	0	0	0	0
59	L35A	7	0	0	0	0
59	L35B	7	0	0	0	0
59	L4A	7	0	0	0	0
59	L4B	7	0	0	0	0
59	MRNA	7	0	0	0	0
59	MRNB	7	0	0	0	0
59	PSIA	7	0	0	0	0
59	PSIB	14	0	0	0	0
59	S10A	7	0	0	0	0
59	S14B	7	0	0	0	0
59	S19A	7	0	0	0	0
59	S4A	7	0	0	5	0
59	S4B	7	0	0	0	0
59	TRNA	14	0	0	0	0
60	16SA	46	0	0	0	0
60	16SB	35	0	0	0	0
60	23SA	102	0	0	0	0
60	23SB	81	0	0	0	0
60	5SA	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	5SB	1	0	0	0	0
60	L15B	1	0	0	0	0
60	L16B	1	0	0	0	0
60	L2A	1	0	0	0	0
60	L2B	1	0	0	0	0
60	L3A	1	0	0	0	0
60	L3B	1	0	0	0	0
60	L4A	1	0	0	0	0
60	L4B	1	0	0	0	0
60	L5A	1	0	0	0	0
60	L5B	1	0	0	0	0
60	PSIA	2	0	0	0	0
60	S13A	1	0	0	0	0
60	S13B	1	0	0	0	0
60	S14B	1	0	0	0	0
60	S20A	1	0	0	0	0
60	S20B	1	0	0	0	0
60	S4B	1	0	0	0	0
60	S6A	1	0	0	0	0
60	S6B	1	0	0	0	0
61	23SA	87	0	0	0	0
61	23SB	87	0	0	0	0
62	16SA	172	0	0	0	0
62	16SB	157	0	0	0	0
62	23SA	788	0	0	0	0
62	23SB	519	0	0	0	0
62	5SA	14	0	0	3	0
62	5SB	5	0	0	2	0
62	ESIA	1	0	0	0	0
62	L15A	9	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	L19B	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	10	0	0	3	0
62	L2B	12	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	L30A	1	0	0	0	0
62	L30B	1	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	1	0
62	L4A	6	0	0	0	0
62	L4B	1	0	0	0	0
62	PSIA	7	0	0	0	0
62	S12A	1	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	S4A	3	0	0	0	0
62	S4B	2	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	306403	0	43851	1471	17

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 1471 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:114:LEU:CD1	34:L9A:130:TYR:HD1	1.38	1.37
9:S9B:58:HIS:O	9:S9B:59:PHE:CD1	1.79	1.36
34:L9A:69:LYS:HG3	34:L9A:136:VAL:CG2	1.61	1.28
34:L9A:114:LEU:CD1	34:L9A:130:TYR:CD1	2.19	1.24
34:L9A:73:GLU:HG3	34:L9A:136:VAL:CG2	1.68	1.23

The worst 5 of 17 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)
1:16SA:726:U:C5	33:L6B:129:THR:N[3_555]	1.30	0.90
42:L20A:118:GLY:N	59:23SA:3304:OHX:N2[4_465]	1.35	0.85
26:TRNA:37:MIA:C12	37:L15B:2:LYS:NZ[2_464]	1.43	0.77
1:16SA:726:U:C4	33:L6B:130:ARG:N[3_555]	1.52	0.68
1:16SA:726:U:O4	33:L6B:130:ARG:CB[3_555]	1.64	0.56

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%)	196 (83%)	35 (15%)	4 (2%)	7	31
2	S2B	235/256 (92%)	193 (82%)	36 (15%)	6 (3%)	4	23
3	S3A	203/239 (85%)	177 (87%)	24 (12%)	2 (1%)	13	42
3	S3B	204/239 (85%)	181 (89%)	23 (11%)	0	100	100
4	S4A	206/209 (99%)	186 (90%)	20 (10%)	0	100	100
4	S4B	206/209 (99%)	189 (92%)	17 (8%)	0	100	100
5	S5A	149/162 (92%)	141 (95%)	8 (5%)	0	100	100
5	S5B	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
6	S6A	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	S6B	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
7	S7A	153/156 (98%)	142 (93%)	11 (7%)	0	100	100
7	S7B	153/156 (98%)	141 (92%)	11 (7%)	1 (1%)	19	50
8	S8A	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	19	50
8	S8B	136/138 (99%)	126 (93%)	9 (7%)	1 (1%)	19	50
9	S9A	125/128 (98%)	108 (86%)	16 (13%)	1 (1%)	16	46
9	S9B	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
10	S10A	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
10	S10B	97/105 (92%)	83 (86%)	12 (12%)	2 (2%)	5	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	S11A	114/129 (88%)	106 (93%)	8 (7%)	0	100	100
11	S11B	115/129 (89%)	105 (91%)	10 (9%)	0	100	100
12	S12A	122/132 (92%)	106 (87%)	15 (12%)	1 (1%)	16	46
12	S12B	122/132 (92%)	108 (88%)	12 (10%)	2 (2%)	8	32
13	S13A	117/126 (93%)	97 (83%)	16 (14%)	4 (3%)	3	19
13	S13B	119/126 (94%)	95 (80%)	20 (17%)	4 (3%)	3	19
14	S14A	58/61 (95%)	50 (86%)	5 (9%)	3 (5%)	1	11
14	S14B	57/61 (93%)	47 (82%)	7 (12%)	3 (5%)	1	10
15	S15A	86/89 (97%)	81 (94%)	3 (4%)	2 (2%)	5	26
15	S15B	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	11	38
16	S16A	81/88 (92%)	78 (96%)	3 (4%)	0	100	100
16	S16B	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	S17A	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
17	S17B	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
18	S18A	69/88 (78%)	62 (90%)	7 (10%)	0	100	100
18	S18B	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	8	33
19	S19A	82/93 (88%)	64 (78%)	18 (22%)	0	100	100
19	S19B	84/93 (90%)	65 (77%)	17 (20%)	2 (2%)	5	25
20	S20A	97/106 (92%)	84 (87%)	9 (9%)	4 (4%)	2	15
20	S20B	97/106 (92%)	81 (84%)	13 (13%)	3 (3%)	3	21
21	THXA	22/27 (82%)	20 (91%)	2 (9%)	0	100	100
21	THXB	23/27 (85%)	20 (87%)	2 (9%)	1 (4%)	2	14
29	L2A	270/276 (98%)	244 (90%)	22 (8%)	4 (2%)	8	33
29	L2B	270/276 (98%)	244 (90%)	23 (8%)	3 (1%)	12	40
30	L3A	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	13	42
30	L3B	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	13	42
31	L4A	200/210 (95%)	183 (92%)	15 (8%)	2 (1%)	13	42
31	L4B	200/210 (95%)	182 (91%)	17 (8%)	1 (0%)	25	56
32	L5A	179/182 (98%)	153 (86%)	20 (11%)	6 (3%)	3	19
32	L5B	179/182 (98%)	154 (86%)	20 (11%)	5 (3%)	4	22
33	L6A	169/180 (94%)	140 (83%)	24 (14%)	5 (3%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	L6B	171/180 (95%)	133 (78%)	31 (18%)	7 (4%)	2	15
34	L9A	143/148 (97%)	117 (82%)	19 (13%)	7 (5%)	2	12
34	L9B	144/148 (97%)	119 (83%)	22 (15%)	3 (2%)	5	27
35	L13A	136/140 (97%)	116 (85%)	16 (12%)	4 (3%)	3	22
35	L13B	136/140 (97%)	119 (88%)	15 (11%)	2 (2%)	8	33
36	L14A	120/122 (98%)	112 (93%)	5 (4%)	3 (2%)	4	24
36	L14B	120/122 (98%)	107 (89%)	11 (9%)	2 (2%)	7	31
37	L15A	148/150 (99%)	119 (80%)	21 (14%)	8 (5%)	1	10
37	L15B	148/150 (99%)	113 (76%)	25 (17%)	10 (7%)	1	7
38	L16A	139/141 (99%)	116 (84%)	19 (14%)	4 (3%)	3	22
38	L16B	139/141 (99%)	113 (81%)	22 (16%)	4 (3%)	3	22
39	L17A	116/118 (98%)	103 (89%)	12 (10%)	1 (1%)	14	44
39	L17B	116/118 (98%)	105 (90%)	11 (10%)	0	100	100
40	L18A	110/112 (98%)	89 (81%)	19 (17%)	2 (2%)	7	30
40	L18B	109/112 (97%)	89 (82%)	20 (18%)	0	100	100
41	L19A	135/146 (92%)	119 (88%)	15 (11%)	1 (1%)	19	50
41	L19B	135/146 (92%)	118 (87%)	17 (13%)	0	100	100
42	L20A	115/118 (98%)	107 (93%)	8 (7%)	0	100	100
42	L20B	115/118 (98%)	104 (90%)	9 (8%)	2 (2%)	7	31
43	L21A	99/101 (98%)	86 (87%)	9 (9%)	4 (4%)	2	16
43	L21B	99/101 (98%)	78 (79%)	15 (15%)	6 (6%)	1	9
44	L22A	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
44	L22B	111/113 (98%)	100 (90%)	11 (10%)	0	100	100
45	L23A	91/96 (95%)	86 (94%)	5 (6%)	0	100	100
45	L23B	92/96 (96%)	86 (94%)	6 (6%)	0	100	100
46	L24A	106/110 (96%)	85 (80%)	15 (14%)	6 (6%)	1	9
46	L24B	104/110 (94%)	83 (80%)	15 (14%)	6 (6%)	1	9
47	L25A	177/206 (86%)	137 (77%)	33 (19%)	7 (4%)	2	16
47	L25B	174/206 (84%)	135 (78%)	35 (20%)	4 (2%)	5	26
48	L27A	82/85 (96%)	73 (89%)	9 (11%)	0	100	100
48	L27B	82/85 (96%)	70 (85%)	11 (13%)	1 (1%)	11	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	L28A	95/98 (97%)	84 (88%)	9 (10%)	2 (2%)	5	27
49	L28B	95/98 (97%)	81 (85%)	13 (14%)	1 (1%)	12	40
50	L29A	67/72 (93%)	61 (91%)	6 (9%)	0	100	100
50	L29B	69/72 (96%)	64 (93%)	5 (7%)	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%)	45 (65%)	20 (29%)	4 (6%)	1	9
52	L31B	69/71 (97%)	44 (64%)	21 (30%)	4 (6%)	1	9
53	L32A	54/60 (90%)	45 (83%)	9 (17%)	0	100	100
53	L32B	54/60 (90%)	50 (93%)	3 (6%)	1 (2%)	6	29
54	L33A	43/54 (80%)	27 (63%)	12 (28%)	4 (9%)	0	3
54	L33B	43/54 (80%)	31 (72%)	8 (19%)	4 (9%)	0	3
55	L34A	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
55	L34B	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
56	L35A	62/65 (95%)	57 (92%)	4 (6%)	1 (2%)	8	32
56	L35B	62/65 (95%)	56 (90%)	6 (10%)	0	100	100
All	All	11387/12054 (94%)	9944 (87%)	1249 (11%)	194 (2%)	7	31

5 of 194 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S2A	10	LEU
3	S3A	12	LEU
12	S12A	62	GLU
13	S13A	67	GLU
13	S13A	101	GLN

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	28
2	S2B	205/220 (93%)	198 (97%)	7 (3%)	32	59
3	S3A	159/188 (85%)	151 (95%)	8 (5%)	20	48
3	S3B	160/188 (85%)	143 (89%)	17 (11%)	5	21
4	S4A	180/181 (99%)	170 (94%)	10 (6%)	17	45
4	S4B	180/181 (99%)	172 (96%)	8 (4%)	24	52
5	S5A	116/123 (94%)	113 (97%)	3 (3%)	41	66
5	S5B	116/123 (94%)	111 (96%)	5 (4%)	25	53
6	S6A	90/90 (100%)	87 (97%)	3 (3%)	33	60
6	S6B	90/90 (100%)	88 (98%)	2 (2%)	47	69
7	S7A	126/127 (99%)	121 (96%)	5 (4%)	27	55
7	S7B	126/127 (99%)	119 (94%)	7 (6%)	17	45
8	S8A	119/119 (100%)	112 (94%)	7 (6%)	16	43
8	S8B	119/119 (100%)	112 (94%)	7 (6%)	16	43
9	S9A	98/99 (99%)	94 (96%)	4 (4%)	26	54
9	S9B	98/99 (99%)	88 (90%)	10 (10%)	6	23
10	S10A	89/92 (97%)	86 (97%)	3 (3%)	32	59
10	S10B	89/92 (97%)	82 (92%)	7 (8%)	10	32
11	S11A	88/99 (89%)	84 (96%)	4 (4%)	23	52
11	S11B	89/99 (90%)	88 (99%)	1 (1%)	70	82
12	S12A	103/108 (95%)	100 (97%)	3 (3%)	37	63
12	S12B	103/108 (95%)	96 (93%)	7 (7%)	13	38
13	S13A	95/101 (94%)	88 (93%)	7 (7%)	11	34
13	S13B	97/101 (96%)	93 (96%)	4 (4%)	26	54
14	S14A	49/50 (98%)	46 (94%)	3 (6%)	15	42
14	S14B	49/50 (98%)	48 (98%)	1 (2%)	50	71
15	S15A	79/80 (99%)	78 (99%)	1 (1%)	65	79
15	S15B	79/80 (99%)	76 (96%)	3 (4%)	28	56
16	S16A	72/74 (97%)	67 (93%)	5 (7%)	13	38
16	S16B	72/74 (97%)	70 (97%)	2 (3%)	38	64
17	S17A	95/97 (98%)	89 (94%)	6 (6%)	15	41
17	S17B	95/97 (98%)	91 (96%)	4 (4%)	25	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	S18A	62/77 (80%)	61 (98%)	1 (2%)	58	76
18	S18B	61/77 (79%)	60 (98%)	1 (2%)	58	76
19	S19A	73/80 (91%)	65 (89%)	8 (11%)	5	20
19	S19B	73/80 (91%)	68 (93%)	5 (7%)	13	38
20	S20A	76/82 (93%)	74 (97%)	2 (3%)	41	66
20	S20B	76/82 (93%)	73 (96%)	3 (4%)	27	55
21	THXA	19/22 (86%)	19 (100%)	0	100	100
21	THXB	20/22 (91%)	19 (95%)	1 (5%)	20	48
29	L2A	214/218 (98%)	209 (98%)	5 (2%)	45	68
29	L2B	214/218 (98%)	207 (97%)	7 (3%)	33	60
30	L3A	165/166 (99%)	159 (96%)	6 (4%)	30	57
30	L3B	165/166 (99%)	161 (98%)	4 (2%)	44	68
31	L4A	161/166 (97%)	153 (95%)	8 (5%)	20	48
31	L4B	161/166 (97%)	159 (99%)	2 (1%)	67	80
32	L5A	155/156 (99%)	150 (97%)	5 (3%)	34	61
32	L5B	155/156 (99%)	144 (93%)	11 (7%)	12	37
33	L6A	143/148 (97%)	138 (96%)	5 (4%)	31	58
33	L6B	144/148 (97%)	129 (90%)	15 (10%)	5	22
34	L9A	122/124 (98%)	113 (93%)	9 (7%)	11	34
34	L9B	122/124 (98%)	114 (93%)	8 (7%)	14	40
35	L13A	117/119 (98%)	113 (97%)	4 (3%)	32	59
35	L13B	117/119 (98%)	115 (98%)	2 (2%)	56	74
36	L14A	100/100 (100%)	98 (98%)	2 (2%)	50	71
36	L14B	100/100 (100%)	93 (93%)	7 (7%)	12	37
37	L15A	116/116 (100%)	105 (90%)	11 (10%)	7	25
37	L15B	116/116 (100%)	108 (93%)	8 (7%)	13	38
38	L16A	111/111 (100%)	102 (92%)	9 (8%)	9	31
38	L16B	111/111 (100%)	103 (93%)	8 (7%)	12	36
39	L17A	101/101 (100%)	100 (99%)	1 (1%)	73	84
39	L17B	101/101 (100%)	97 (96%)	4 (4%)	27	55
40	L18A	88/88 (100%)	84 (96%)	4 (4%)	23	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	L18B	87/88 (99%)	78 (90%)	9 (10%)	6	22
41	L19A	120/127 (94%)	113 (94%)	7 (6%)	17	44
41	L19B	120/127 (94%)	114 (95%)	6 (5%)	20	48
42	L20A	93/94 (99%)	90 (97%)	3 (3%)	34	61
42	L20B	93/94 (99%)	85 (91%)	8 (9%)	8	30
43	L21A	82/82 (100%)	78 (95%)	4 (5%)	21	49
43	L21B	82/82 (100%)	73 (89%)	9 (11%)	5	20
44	L22A	92/92 (100%)	87 (95%)	5 (5%)	18	46
44	L22B	92/92 (100%)	88 (96%)	4 (4%)	25	53
45	L23A	76/78 (97%)	75 (99%)	1 (1%)	65	79
45	L23B	76/78 (97%)	73 (96%)	3 (4%)	27	55
46	L24A	89/91 (98%)	84 (94%)	5 (6%)	17	45
46	L24B	79/91 (87%)	76 (96%)	3 (4%)	28	56
47	L25A	158/179 (88%)	150 (95%)	8 (5%)	20	48
47	L25B	155/179 (87%)	145 (94%)	10 (6%)	14	40
48	L27A	66/67 (98%)	63 (96%)	3 (4%)	23	52
48	L27B	66/67 (98%)	61 (92%)	5 (8%)	11	34
49	L28A	82/83 (99%)	79 (96%)	3 (4%)	29	56
49	L28B	82/83 (99%)	80 (98%)	2 (2%)	44	68
50	L29A	65/67 (97%)	62 (95%)	3 (5%)	23	52
50	L29B	64/67 (96%)	62 (97%)	2 (3%)	35	61
51	L30A	51/52 (98%)	49 (96%)	2 (4%)	27	55
51	L30B	51/52 (98%)	50 (98%)	1 (2%)	50	71
52	L31A	63/63 (100%)	56 (89%)	7 (11%)	5	19
52	L31B	63/63 (100%)	58 (92%)	5 (8%)	10	32
53	L32A	48/52 (92%)	45 (94%)	3 (6%)	15	41
53	L32B	48/52 (92%)	43 (90%)	5 (10%)	5	22
54	L33A	44/52 (85%)	40 (91%)	4 (9%)	7	27
54	L33B	44/52 (85%)	43 (98%)	1 (2%)	45	68
55	L34A	41/42 (98%)	39 (95%)	2 (5%)	21	49
55	L34B	42/42 (100%)	39 (93%)	3 (7%)	12	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
56	L35A	54/55 (98%)	49 (91%)	5 (9%)	7 26
56	L35B	54/55 (98%)	51 (94%)	3 (6%)	17 45
All	All	9611/9996 (96%)	9119 (95%)	492 (5%)	20 48

5 of 492 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
56	L35A	34	TRP
43	L21B	82	ARG
8	S8B	112	LEU
43	L21B	49	THR
50	L29B	67	LYS

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16SA	1508/1512 (99%)	317 (21%)	47 (3%)
1	16SB	1504/1512 (99%)	336 (22%)	46 (3%)
22	ASIA	74/76 (97%)	42 (56%)	1 (1%)
23	PSIA	73/76 (96%)	24 (32%)	2 (2%)
23	PSIB	73/76 (96%)	29 (39%)	2 (2%)
24	ESIA	74/76 (97%)	34 (45%)	2 (2%)
24	ESIB	74/76 (97%)	23 (31%)	2 (2%)
25	MRNA	29/30 (96%)	7 (24%)	2 (6%)
25	MRNB	29/30 (96%)	11 (37%)	2 (6%)
26	TRNA	71/76 (93%)	34 (47%)	3 (4%)
27	23SA	2883/2911 (99%)	632 (21%)	70 (2%)
27	23SB	2867/2911 (98%)	658 (22%)	64 (2%)
28	5SA	121/124 (97%)	27 (22%)	1 (0%)
28	5SB	120/124 (96%)	34 (28%)	4 (3%)
57	ASIB	74/76 (97%)	38 (51%)	2 (2%)
All	All	9574/9686 (98%)	2246 (23%)	250 (2%)

5 of 2246 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16SA	654	A

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Mol	Chain	Res	Type
1	16SA	655	G
1	16SA	678	A
1	16SA	685	G
1	16SA	693	C

5 of 250 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	23SA	2496	G
27	23SB	1940	5MU
1	16SB	1315	U
27	23SB	1880	G
27	23SB	2617	A

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

87 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	MA6	16SA	2142	1	18,26,27	1.01	2 (11%)	19,38,41	2.85	2 (10%)
23	G7M	PSIB	46	23	20,26,27	4.78	5 (25%)	17,39,42	1.13	1 (5%)
26	MIA	TRNA	37	26,27	24,31,32	2.59	5 (20%)	26,44,47	3.55	8 (30%)
26	PSU	TRNA	55	26	18,21,22	1.09	1 (5%)	22,30,33	1.77	4 (18%)
1	MA6	16SB	2142	1	18,26,27	0.99	2 (11%)	19,38,41	2.80	2 (10%)
23	4SU	PSIB	8	23,58	18,21,22	1.87	5 (27%)	26,30,33	2.91	6 (23%)
27	2MA	23SB	2518	60,58,27	19,25,26	3.00	5 (26%)	21,37,40	2.04	4 (19%)
26	H2U	TRNA	16	26	18,21,22	2.02	4 (22%)	21,30,33	2.07	5 (23%)
27	PSU	23SA	2620	27	18,21,22	1.14	1 (5%)	22,30,33	1.82	4 (18%)
24	MIA	ESIB	37	24	24,31,32	2.43	4 (16%)	26,44,47	4.25	11 (42%)
27	PSU	23SA	1942	27	18,21,22	1.03	1 (5%)	22,30,33	1.79	4 (18%)
22	4SU	ASIA	8	22	18,21,22	1.81	4 (22%)	26,30,33	2.36	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	16SA	1834	60,1	18,26,27	2.63	7 (38%)	16,38,41	1.33	3 (18%)
1	5MC	16SB	2032	1	18,22,23	3.87	7 (38%)	26,32,35	0.94	2 (7%)
23	3AU	PSIA	47	23	24,28,29	2.80	8 (33%)	33,40,43	1.54	6 (18%)
1	5MC	16SA	2032	1	18,22,23	3.82	7 (38%)	26,32,35	0.89	2 (7%)
27	PSU	23SB	2620	27	18,21,22	1.18	1 (5%)	22,30,33	1.76	3 (13%)
23	PSU	PSIB	32	23	18,21,22	1.03	1 (5%)	22,30,33	1.69	4 (18%)
27	OMU	23SA	2567	58,27	19,22,23	2.93	8 (42%)	26,31,34	1.85	5 (19%)
27	OMG	23SA	2266	60,23,27	18,26,27	5.17	9 (50%)	19,38,41	3.73	7 (36%)
26	PSU	TRNA	39	26	18,21,22	1.14	1 (5%)	22,30,33	1.80	5 (22%)
27	OMU	23SB	2567	58,27	19,22,23	2.98	8 (42%)	26,31,34	1.83	5 (19%)
23	PSU	PSIA	55	23	18,21,22	1.21	1 (5%)	22,30,33	1.65	4 (18%)
1	5MC	16SA	2028	1	18,22,23	3.81	7 (38%)	26,32,35	1.09	1 (3%)
26	PSU	TRNA	32	26	18,21,22	1.14	1 (5%)	22,30,33	1.72	4 (18%)
57	PSU	ASIB	39	57	18,21,22	1.11	1 (5%)	22,30,33	1.68	4 (18%)
26	H2U	TRNA	20	28,26	18,21,22	2.27	4 (22%)	21,30,33	1.84	5 (23%)
22	G7M	ASIA	46	22	20,26,27	4.73	5 (25%)	17,39,42	1.06	1 (5%)
27	OMC	23SA	1945	60,27	19,22,23	1.73	4 (21%)	26,31,34	0.82	0
1	5MC	16SA	1590	1	18,22,23	3.74	7 (38%)	26,32,35	1.07	1 (3%)
27	PSU	23SB	1936	27	18,21,22	1.14	1 (5%)	22,30,33	1.52	3 (13%)
27	5MC	23SB	1987	60,27	18,22,23	3.79	7 (38%)	26,32,35	0.92	1 (3%)
23	MIA	PSIB	37	23	24,31,32	2.33	4 (16%)	26,44,47	2.83	11 (42%)
22	PSU	ASIA	32	22	18,21,22	1.11	1 (5%)	22,30,33	1.53	4 (18%)
22	5MU	ASIA	54	22	19,22,23	3.84	5 (26%)	28,32,35	3.25	10 (35%)
27	OMG	23SB	2266	60,23,27	18,26,27	5.25	9 (50%)	19,38,41	3.80	7 (36%)
1	G7M	16SA	1156	60,1	20,26,27	4.72	6 (30%)	17,39,42	1.05	1 (5%)
1	M2G	16SB	1589	1	20,27,28	3.92	7 (35%)	22,40,43	1.24	4 (18%)
1	G7M	16SB	1156	60,1	20,26,27	4.73	5 (25%)	17,39,42	1.07	1 (5%)
23	PSU	PSIA	39	23	18,21,22	1.06	1 (5%)	22,30,33	1.65	3 (13%)
27	5MC	23SB	1967	27	18,22,23	3.81	7 (38%)	26,32,35	1.06	3 (11%)
1	2MG	16SB	1834	1	18,26,27	2.71	7 (38%)	16,38,41	1.35	4 (25%)
1	UR3	16SB	2121	1	19,22,23	2.86	7 (36%)	26,32,35	1.46	3 (11%)
12	0TD	S12A	89	12	7,9,10	1.48	1 (14%)	6,11,13	1.87	1 (16%)
23	5MU	PSIB	54	23	19,22,23	3.90	5 (26%)	28,32,35	3.07	9 (32%)
57	PSU	ASIB	32	57	18,21,22	1.02	1 (5%)	22,30,33	1.68	4 (18%)
1	4OC	16SB	2030	1,58	20,23,24	2.85	8 (40%)	26,32,35	1.41	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	16SB	2028	1	18,22,23	3.80	7 (38%)	26,32,35	1.21	3 (11%)
1	4OC	16SA	2030	1	20,23,24	3.10	8 (40%)	26,32,35	0.88	1 (3%)
24	MIA	ESIA	37	24	24,31,32	2.42	4 (16%)	26,44,47	3.21	9 (34%)
57	MIA	ASIB	37	57	24,31,32	2.32	4 (16%)	26,44,47	3.06	10 (38%)
1	5MC	16SB	2035	1	18,22,23	3.86	7 (38%)	26,32,35	1.10	3 (11%)
27	OMC	23SB	1945	27	19,22,23	1.80	4 (21%)	26,31,34	0.92	1 (3%)
1	5MC	16SB	1590	1	18,22,23	3.84	7 (38%)	26,32,35	1.00	1 (3%)
57	5MU	ASIB	54	57	19,22,23	3.89	5 (26%)	28,32,35	3.16	8 (28%)
23	MIA	PSIA	37	23	24,31,32	2.32	3 (12%)	26,44,47	2.51	10 (38%)
22	PSU	ASIA	55	22	18,21,22	1.04	1 (5%)	22,30,33	1.71	4 (18%)
22	MIA	ASIA	37	22	24,31,32	2.30	4 (16%)	26,44,47	3.21	11 (42%)
27	2MA	23SA	2518	60,27	19,25,26	2.98	5 (26%)	21,37,40	1.88	4 (19%)
23	5MU	PSIA	54	23	19,22,23	3.79	5 (26%)	28,32,35	3.16	7 (25%)
26	4SU	TRNA	8	26	18,21,22	1.79	3 (16%)	26,30,33	2.40	5 (19%)
23	H2U	PSIB	16	23	18,21,22	2.05	4 (22%)	21,30,33	1.86	5 (23%)
27	5MU	23SA	1964	60,27	19,22,23	3.78	5 (26%)	28,32,35	3.39	10 (35%)
27	5MU	23SB	1964	60,27	19,22,23	3.81	5 (26%)	28,32,35	3.29	9 (32%)
1	PSU	16SB	1145	1,58	18,21,22	1.11	1 (5%)	22,30,33	1.67	3 (13%)
27	5MC	23SA	1967	27	18,22,23	3.74	7 (38%)	26,32,35	1.17	1 (3%)
12	0TD	S12B	89	12	7,9,10	1.56	1 (14%)	6,11,13	1.99	2 (33%)
1	PSU	16SA	1145	1,58	18,21,22	1.14	1 (5%)	22,30,33	1.70	4 (18%)
23	G7M	PSIA	46	23	20,26,27	4.69	5 (25%)	17,39,42	1.13	1 (5%)
23	4SU	PSIA	8	23	18,21,22	1.77	3 (16%)	26,30,33	2.51	5 (19%)
26	5MU	TRNA	54	26	19,22,23	3.92	5 (26%)	28,32,35	3.20	9 (32%)
23	3AU	PSIB	47	23	24,28,29	2.84	8 (33%)	33,40,43	1.96	8 (24%)
1	5MC	16SA	2035	1	18,22,23	3.73	7 (38%)	26,32,35	1.07	1 (3%)
27	5MC	23SA	1987	60,27	18,22,23	3.71	7 (38%)	26,32,35	0.96	1 (3%)
23	PSU	PSIA	32	23	18,21,22	1.03	1 (5%)	22,30,33	1.59	3 (13%)
23	H2U	PSIA	16	23	18,21,22	2.01	4 (22%)	21,30,33	2.06	5 (23%)
27	5MU	23SA	1940	27	19,22,23	4.11	5 (26%)	28,32,35	3.47	10 (35%)
27	5MU	23SB	1940	27	19,22,23	3.98	5 (26%)	28,32,35	3.32	9 (32%)
23	PSU	PSIB	39	23	18,21,22	1.11	1 (5%)	22,30,33	1.63	4 (18%)
1	MA6	16SB	2141	1	18,26,27	1.00	1 (5%)	19,38,41	2.40	2 (10%)
22	PSU	ASIA	39	22	18,21,22	1.13	1 (5%)	22,30,33	1.58	3 (13%)
1	MA6	16SA	2141	1	18,26,27	1.01	2 (11%)	19,38,41	2.67	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PSU	PSIB	55	23	18,21,22	1.11	1 (5%)	22,30,33	1.67	3 (13%)
27	PSU	23SA	1936	27	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)
1	UR3	16SA	2121	1	19,22,23	2.81	8 (42%)	26,32,35	1.52	3 (11%)
1	M2G	16SA	1589	1	20,27,28	3.74	7 (35%)	22,40,43	1.55	4 (18%)
27	PSU	23SB	1942	27	18,21,22	1.13	1 (5%)	22,30,33	1.64	4 (18%)

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	MA6	16SA	2142	1	-	3/7/29/30	0/3/3/3
23	G7M	PSIB	46	23	-	0/3/25/26	0/3/3/3
26	MIA	TRNA	37	26,27	-	5/11/33/34	0/3/3/3
26	PSU	TRNA	55	26	-	0/7/25/26	0/2/2/2
1	MA6	16SB	2142	1	-	3/7/29/30	0/3/3/3
23	4SU	PSIB	8	23,58	-	2/7/25/26	0/2/2/2
27	2MA	23SB	2518	60,58,27	-	3/3/25/26	0/3/3/3
26	H2U	TRNA	16	26	-	3/7/38/39	0/2/2/2
27	PSU	23SA	2620	27	-	0/7/25/26	0/2/2/2
24	MIA	ESIB	37	24	-	6/11/33/34	0/3/3/3
27	PSU	23SA	1942	27	-	0/7/25/26	0/2/2/2
22	4SU	ASIA	8	22	-	1/7/25/26	0/2/2/2
1	2MG	16SA	1834	60,1	-	0/5/27/28	0/3/3/3
1	5MC	16SB	2032	1	-	0/7/25/26	0/2/2/2
23	3AU	PSIA	47	23	-	7/16/34/35	0/2/2/2
1	5MC	16SA	2032	1	-	0/7/25/26	0/2/2/2
27	PSU	23SB	2620	27	-	0/7/25/26	0/2/2/2
23	PSU	PSIB	32	23	-	0/7/25/26	0/2/2/2
27	OMU	23SA	2567	58,27	-	0/9/27/28	0/2/2/2
27	OMG	23SA	2266	60,23,27	-	1/5/27/28	0/3/3/3
26	PSU	TRNA	39	26	-	0/7/25/26	0/2/2/2
27	OMU	23SB	2567	58,27	-	2/9/27/28	0/2/2/2
23	PSU	PSIA	55	23	-	3/7/25/26	0/2/2/2
1	5MC	16SA	2028	1	-	0/7/25/26	0/2/2/2
26	PSU	TRNA	32	26	-	0/7/25/26	0/2/2/2
57	PSU	ASIB	39	57	-	0/7/25/26	0/2/2/2
26	H2U	TRNA	20	28,26	-	5/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	G7M	ASIA	46	22	-	2/3/25/26	0/3/3/3
27	OMC	23SA	1945	60,27	-	1/9/27/28	0/2/2/2
1	5MC	16SA	1590	1	-	0/7/25/26	0/2/2/2
27	PSU	23SB	1936	27	-	0/7/25/26	0/2/2/2
27	5MC	23SB	1987	60,27	-	0/7/25/26	0/2/2/2
23	MIA	PSIB	37	23	-	6/11/33/34	0/3/3/3
22	PSU	ASIA	32	22	-	0/7/25/26	0/2/2/2
22	5MU	ASIA	54	22	-	0/7/25/26	0/2/2/2
27	OMG	23SB	2266	60,23,27	-	1/5/27/28	0/3/3/3
1	G7M	16SA	1156	60,1	-	2/3/25/26	0/3/3/3
1	M2G	16SB	1589	1	-	0/7/29/30	0/3/3/3
1	G7M	16SB	1156	60,1	-	2/3/25/26	0/3/3/3
23	PSU	PSIA	39	23	-	0/7/25/26	0/2/2/2
27	5MC	23SB	1967	27	-	0/7/25/26	0/2/2/2
1	2MG	16SB	1834	1	-	2/5/27/28	0/3/3/3
1	UR3	16SB	2121	1	-	0/7/25/26	0/2/2/2
12	0TD	S12A	89	12	-	2/7/12/14	-
23	5MU	PSIB	54	23	-	2/7/25/26	0/2/2/2
57	PSU	ASIB	32	57	-	0/7/25/26	0/2/2/2
1	4OC	16SB	2030	1,58	-	2/9/29/30	0/2/2/2
1	5MC	16SB	2028	1	-	0/7/25/26	0/2/2/2
1	4OC	16SA	2030	1	-	2/9/29/30	0/2/2/2
24	MIA	ESIA	37	24	-	7/11/33/34	0/3/3/3
57	MIA	ASIB	37	57	-	3/11/33/34	0/3/3/3
1	5MC	16SB	2035	1	-	0/7/25/26	0/2/2/2
27	OMC	23SB	1945	27	-	1/9/27/28	0/2/2/2
1	5MC	16SB	1590	1	-	0/7/25/26	0/2/2/2
57	5MU	ASIB	54	57	-	0/7/25/26	0/2/2/2
23	MIA	PSIA	37	23	-	5/11/33/34	0/3/3/3
22	PSU	ASIA	55	22	-	3/7/25/26	0/2/2/2
22	MIA	ASIA	37	22	-	6/11/33/34	0/3/3/3
27	2MA	23SA	2518	60,27	-	1/3/25/26	0/3/3/3
23	5MU	PSIA	54	23	-	0/7/25/26	0/2/2/2
26	4SU	TRNA	8	26	-	2/7/25/26	0/2/2/2
23	H2U	PSIB	16	23	-	0/7/38/39	0/2/2/2
27	5MU	23SA	1964	60,27	-	2/7/25/26	0/2/2/2
27	5MU	23SB	1964	60,27	-	2/7/25/26	0/2/2/2
1	PSU	16SB	1145	1,58	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	5MC	23SA	1967	27	-	0/7/25/26	0/2/2/2
12	0TD	S12B	89	12	-	3/7/12/14	-
1	PSU	16SA	1145	1,58	-	0/7/25/26	0/2/2/2
23	G7M	PSIA	46	23	-	2/3/25/26	0/3/3/3
23	4SU	PSIA	8	23	-	0/7/25/26	0/2/2/2
26	5MU	TRNA	54	26	-	2/7/25/26	0/2/2/2
23	3AU	PSIB	47	23	-	7/16/34/35	0/2/2/2
1	5MC	16SA	2035	1	-	0/7/25/26	0/2/2/2
27	5MC	23SA	1987	60,27	-	0/7/25/26	0/2/2/2
23	PSU	PSIA	32	23	-	0/7/25/26	0/2/2/2
23	H2U	PSIA	16	23	-	0/7/38/39	0/2/2/2
27	5MU	23SA	1940	27	-	3/7/25/26	0/2/2/2
27	5MU	23SB	1940	27	-	0/7/25/26	0/2/2/2
23	PSU	PSIB	39	23	-	0/7/25/26	0/2/2/2
1	MA6	16SB	2141	1	-	0/7/29/30	0/3/3/3
22	PSU	ASIA	39	22	-	0/7/25/26	0/2/2/2
1	MA6	16SA	2141	1	-	0/7/29/30	0/3/3/3
23	PSU	PSIB	55	23	-	0/7/25/26	0/2/2/2
27	PSU	23SA	1936	27	-	0/7/25/26	0/2/2/2
1	UR3	16SA	2121	1	-	0/7/25/26	0/2/2/2
1	M2G	16SA	1589	1	-	0/7/29/30	0/3/3/3
27	PSU	23SB	1942	27	-	0/7/25/26	0/2/2/2

The worst 5 of 372 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	PSIB	46	G7M	C8-N7	17.49	1.65	1.33
22	ASIA	46	G7M	C8-N7	17.30	1.64	1.33
1	16SB	1156	G7M	C8-N7	17.25	1.64	1.33
23	PSIA	46	G7M	C8-N7	17.15	1.64	1.33
1	16SA	1156	G7M	C8-N7	17.09	1.64	1.33

The worst 5 of 383 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	ESIB	37	MIA	C11-S10-C2	15.35	113.73	102.27
27	23SA	1940	5MU	C5-C4-N3	11.38	125.02	115.31
24	ESIB	37	MIA	C12-C13-C14	-10.88	105.97	127.14
23	PSIA	54	5MU	C5-C4-N3	10.88	124.59	115.31
27	23SA	1964	5MU	C5-C4-N3	10.87	124.58	115.31

There are no chirality outliers.

5 of 117 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16SA	1156	G7M	O4'-C4'-C5'-O5'
1	16SA	1156	G7M	C3'-C4'-C5'-O5'
1	16SA	2142	MA6	O4'-C4'-C5'-O5'
12	S12A	89	0TD	CG-CB-SB-CSB
22	ASIA	37	MIA	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	TRNA	37	MIA	0	4

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1698 ligands modelled in this entry, 1077 are monoatomic - leaving 621 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	$\# Z > 2$
59	OHX	23SA	3327	-	0,6,6	-	-	-		
59	OHX	23SA	3286	-	0,6,6	-	-	-		
59	OHX	16SA	2340	-	0,6,6	-	-	-		
59	OHX	5SB	210	-	0,6,6	-	-	-		
59	OHX	23SB	3047	-	0,6,6	-	-	-		
59	OHX	23SB	3086	-	0,6,6	-	-	-		
59	OHX	23SA	3309	-	0,6,6	-	-	-		
59	OHX	16SB	2216	-	0,6,6	-	-	-		
59	OHX	16SA	2331	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	OHX	23SB	3133	-	0,6,6	-	-	-		
59	OHX	16SA	2308	-	0,6,6	-	-	-		
59	OHX	16SA	2314	-	0,6,6	-	-	-		
59	OHX	23SB	3156	-	0,6,6	-	-	-		
59	OHX	23SB	3192	-	0,6,6	-	-	-		
59	OHX	23SA	3375	-	0,6,6	-	-	-		
59	OHX	23SA	3202	-	0,6,6	-	-	-		
59	OHX	L27A	103	-	0,6,6	-	-	-		
59	OHX	16SB	2204	-	0,6,6	-	-	-		
59	OHX	23SB	3002	-	0,6,6	-	-	-		
59	OHX	23SA	3200	-	0,6,6	-	-	-		
59	OHX	23SA	3350	-	0,6,6	-	-	-		
59	OHX	23SA	3225	-	0,6,6	-	-	-		
59	OHX	23SA	3259	-	0,6,6	-	-	-		
59	OHX	23SA	3357	27	0,6,6	-	-	-		
59	OHX	23SA	3268	-	0,6,6	-	-	-		
59	OHX	16SB	2219	-	0,6,6	-	-	-		
59	OHX	23SA	3361	-	0,6,6	-	-	-		
59	OHX	23SA	3297	-	0,6,6	-	-	-		
59	OHX	23SA	3369	-	0,6,6	-	-	-		
59	OHX	23SB	3168	-	0,6,6	-	-	-		
59	OHX	23SA	3322	-	0,6,6	-	-	-		
59	OHX	5SA	206	-	0,6,6	-	-	-		
59	OHX	5SA	211	-	0,6,6	-	-	-		
59	OHX	23SB	3088	-	0,6,6	-	-	-		
59	OHX	23SB	3097	-	0,6,6	-	-	-		
59	OHX	16SA	2339	-	0,6,6	-	-	-		
59	OHX	23SB	3067	-	0,6,6	-	-	-		
59	OHX	23SA	3329	-	0,6,6	-	-	-		
59	OHX	16SA	2260	-	0,6,6	-	-	-		
59	OHX	23SB	3172	-	0,6,6	-	-	-		
59	OHX	23SB	3008	-	0,6,6	-	-	-		
59	OHX	23SB	3195	-	0,6,6	-	-	-		
59	OHX	5SB	207	-	0,6,6	-	-	-		
59	OHX	MRNA	101	-	0,6,6	-	-	-		
59	OHX	23SB	3041	-	0,6,6	-	-	-		
59	OHX	23SB	3122	-	0,6,6	-	-	-		
59	OHX	23SB	3129	-	0,6,6	-	-	-		
59	OHX	16SB	2261	-	0,6,6	-	-	-		
59	OHX	16SA	2276	-	0,6,6	-	-	-		
59	OHX	23SA	3241	-	0,6,6	-	-	-		
59	OHX	16SA	2333	-	0,6,6	-	-	-		
59	OHX	23SA	3276	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	OHX	16SB	2201	1	0,6,6	-	-	-		
59	OHX	5SA	208	-	0,6,6	-	-	-		
59	OHX	23SB	3072	-	0,6,6	-	-	-		
59	OHX	23SA	3198	-	0,6,6	-	-	-		
59	OHX	23SA	3287	-	0,6,6	-	-	-		
59	OHX	S19A	101	-	0,6,6	-	-	-		
59	OHX	16SA	2326	-	0,6,6	-	-	-		
59	OHX	23SB	3031	-	0,6,6	-	-	-		
59	OHX	23SA	3232	-	0,6,6	-	-	-		
59	OHX	23SA	3238	-	0,6,6	-	-	-		
59	OHX	23SA	3288	-	0,6,6	-	-	-		
59	OHX	23SA	3354	-	0,6,6	-	-	-		
59	OHX	23SA	3239	-	0,6,6	-	-	-		
59	OHX	23SA	3285	-	0,6,6	-	-	-		
59	OHX	23SB	3080	-	0,6,6	-	-	-		
59	OHX	23SB	3091	-	0,6,6	-	-	-		
59	OHX	23SB	3134	-	0,6,6	-	-	-		
59	OHX	23SA	3362	-	0,6,6	-	-	-		
59	OHX	23SB	3150	-	0,6,6	-	-	-		
59	OHX	23SA	3333	-	0,6,6	-	-	-		
59	OHX	23SB	3118	-	0,6,6	-	-	-		
59	OHX	23SB	3139	-	0,6,6	-	-	-		
59	OHX	23SA	3184	-	0,6,6	-	-	-		
59	OHX	23SA	3307	-	0,6,6	-	-	-		
59	OHX	23SA	3204	-	0,6,6	-	-	-		
59	OHX	23SA	3320	-	0,6,6	-	-	-		
59	OHX	23SB	3176	-	0,6,6	-	-	-		
59	OHX	23SB	3015	27	0,6,6	-	-	-		
59	OHX	23SA	3317	-	0,6,6	-	-	-		
59	OHX	23SB	3022	-	0,6,6	-	-	-		
59	OHX	23SB	3089	-	0,6,6	-	-	-		
59	OHX	23SA	3247	-	0,6,6	-	-	-		
59	OHX	16SB	2239	1	0,6,6	-	-	-		
59	OHX	23SB	3153	-	0,6,6	-	-	-		
59	OHX	23SB	3104	-	0,6,6	-	-	-		
59	OHX	23SB	3186	-	0,6,6	-	-	-		
59	OHX	23SB	3135	-	0,6,6	-	-	-		
59	OHX	23SB	3038	-	0,6,6	-	-	-		
59	OHX	23SB	3098	-	0,6,6	-	-	-		
59	OHX	23SA	3243	-	0,6,6	-	-	-		
59	OHX	16SA	2270	-	0,6,6	-	-	-		
59	OHX	23SB	3010	-	0,6,6	-	-	-		
59	OHX	16SB	2215	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	OHX	23SB	3193	-	0,6,6	-	-	-		
59	OHX	23SA	3312	-	0,6,6	-	-	-		
59	OHX	16SB	2217	-	0,6,6	-	-	-		
59	OHX	23SB	3187	-	0,6,6	-	-	-		
59	OHX	16SB	2272	-	0,6,6	-	-	-		
59	OHX	23SA	3237	-	0,6,6	-	-	-		
59	OHX	23SA	3335	-	0,6,6	-	-	-		
59	OHX	23SB	3105	-	0,6,6	-	-	-		
59	OHX	23SB	3049	-	0,6,6	-	-	-		
59	OHX	16SA	2275	-	0,6,6	-	-	-		
59	OHX	23SA	3339	-	0,6,6	-	-	-		
59	OHX	16SB	2232	-	0,6,6	-	-	-		
59	OHX	23SB	3005	-	0,6,6	-	-	-		
59	OHX	23SA	3310	-	0,6,6	-	-	-		
59	OHX	23SA	3334	-	0,6,6	-	-	-		
59	OHX	23SB	3073	-	0,6,6	-	-	-		
59	OHX	23SB	3037	-	0,6,6	-	-	-		
59	OHX	16SB	2277	-	0,6,6	-	-	-		
59	OHX	23SB	3066	-	0,6,6	-	-	-		
59	OHX	16SA	2321	-	0,6,6	-	-	-		
59	OHX	23SA	3186	-	0,6,6	-	-	-		
59	OHX	23SA	3214	-	0,6,6	-	-	-		
59	OHX	L27A	102	-	0,6,6	-	-	-		
59	OHX	23SB	3029	-	0,6,6	-	-	-		
59	OHX	16SB	2253	-	0,6,6	-	-	-		
59	OHX	16SA	2272	-	0,6,6	-	-	-		
59	OHX	16SA	2335	-	0,6,6	-	-	-		
59	OHX	23SB	3001	-	0,6,6	-	-	-		
59	OHX	23SA	3179	-	0,6,6	-	-	-		
59	OHX	ASIA	102	-	0,6,6	-	-	-		
59	OHX	TRNA	102	-	0,6,6	-	-	-		
59	OHX	23SB	3119	-	0,6,6	-	-	-		
59	OHX	23SB	3199	-	0,6,6	-	-	-		
59	OHX	L28A	101	-	0,6,6	-	-	-		
59	OHX	16SB	2263	-	0,6,6	-	-	-		
59	OHX	23SA	3328	-	0,6,6	-	-	-		
59	OHX	23SA	3203	-	0,6,6	-	-	-		
59	OHX	23SB	3004	-	0,6,6	-	-	-		
59	OHX	23SB	3171	-	0,6,6	-	-	-		
59	OHX	S10A	201	1	0,6,6	-	-	-		
59	OHX	23SA	3205	-	0,6,6	-	-	-		
59	OHX	23SB	3079	-	0,6,6	-	-	-		
59	OHX	23SB	3030	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	OHX	16SB	2213	-	0,6,6	-	-	-		
59	OHX	23SB	3197	-	0,6,6	-	-	-		
59	OHX	23SA	3191	27	0,6,6	-	-	-		
59	OHX	23SA	3234	-	0,6,6	-	-	-		
59	OHX	23SA	3277	-	0,6,6	-	-	-		
59	OHX	16SB	2237	1	0,6,6	-	-	-		
59	OHX	16SB	2226	-	0,6,6	-	-	-		
59	OHX	16SB	2257	-	0,6,6	-	-	-		
59	OHX	23SA	3208	-	0,6,6	-	-	-		
59	OHX	23SA	3323	-	0,6,6	-	-	-		
59	OHX	16SA	2306	1	0,6,6	-	-	-		
59	OHX	23SA	3315	-	0,6,6	-	-	-		
59	OHX	16SA	2271	-	0,6,6	-	-	-		
59	OHX	23SA	3308	-	0,6,6	-	-	-		
59	OHX	23SA	3381	-	0,6,6	-	-	-		
59	OHX	23SA	3219	-	0,6,6	-	-	-		
59	OHX	16SA	2297	-	0,6,6	-	-	-		
59	OHX	16SA	2274	-	0,6,6	-	-	-		
59	OHX	23SA	3343	-	0,6,6	-	-	-		
59	OHX	23SA	3265	-	0,6,6	-	-	-		
59	OHX	23SA	3269	-	0,6,6	-	-	-		
59	OHX	23SA	3365	-	0,6,6	-	-	-		
59	OHX	23SB	3110	-	0,6,6	-	-	-		
59	OHX	23SB	3183	-	0,6,6	-	-	-		
59	OHX	23SA	3236	-	0,6,6	-	-	-		
59	OHX	23SB	3145	-	0,6,6	-	-	-		
59	OHX	16SB	2227	-	0,6,6	-	-	-		
59	OHX	23SB	3107	-	0,6,6	-	-	-		
59	OHX	23SA	3178	-	0,6,6	-	-	-		
59	OHX	16SB	2207	-	0,6,6	-	-	-		
59	OHX	23SB	3093	-	0,6,6	-	-	-		
59	OHX	23SA	3197	-	0,6,6	-	-	-		
59	OHX	16SA	2317	-	0,6,6	-	-	-		
59	OHX	5SB	209	-	0,6,6	-	-	-		
59	OHX	23SB	3012	-	0,6,6	-	-	-		
59	OHX	23SB	3051	-	0,6,6	-	-	-		
59	OHX	23SB	3019	-	0,6,6	-	-	-		
59	OHX	23SA	3262	-	0,6,6	-	-	-		
59	OHX	16SB	2270	-	0,6,6	-	-	-		
59	OHX	23SA	3319	-	0,6,6	-	-	-		
59	OHX	16SA	2301	-	0,6,6	-	-	-		
59	OHX	16SB	2210	-	0,6,6	-	-	-		
59	OHX	16SA	2261	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	OHX	23SA	3273	-	0,6,6	-	-	-		
59	OHX	23SA	3183	27	0,6,6	-	-	-		
59	OHX	16SA	2278	-	0,6,6	-	-	-		
59	OHX	16SA	2323	-	0,6,6	-	-	-		
59	OHX	23SA	3340	-	0,6,6	-	-	-		
59	OHX	16SA	2279	-	0,6,6	-	-	-		
59	OHX	16SA	2281	-	0,6,6	-	-	-		
59	OHX	16SA	2322	-	0,6,6	-	-	-		
59	OHX	23SB	3149	-	0,6,6	-	-	-		
59	OHX	16SB	2248	-	0,6,6	-	-	-		
59	OHX	23SA	3348	-	0,6,6	-	-	-		
59	OHX	23SB	3063	-	0,6,6	-	-	-		
59	OHX	23SA	3233	-	0,6,6	-	-	-		
59	OHX	16SB	2262	-	0,6,6	-	-	-		
59	OHX	23SB	3017	-	0,6,6	-	-	-		
59	OHX	16SB	2233	-	0,6,6	-	-	-		
59	OHX	23SB	3189	-	0,6,6	-	-	-		
59	OHX	23SB	3112	-	0,6,6	-	-	-		
59	OHX	23SB	3116	27	0,6,6	-	-	-		
59	OHX	16SA	2313	-	0,6,6	-	-	-		
59	OHX	23SA	3366	-	0,6,6	-	-	-		
59	OHX	23SA	3336	-	0,6,6	-	-	-		
59	OHX	16SA	2318	-	0,6,6	-	-	-		
59	OHX	23SA	3299	-	0,6,6	-	-	-		
59	OHX	23SA	3379	-	0,6,6	-	-	-		
59	OHX	23SA	3209	-	0,6,6	-	-	-		
59	OHX	23SA	3294	-	0,6,6	-	-	-		
59	OHX	23SB	3115	-	0,6,6	-	-	-		
59	OHX	23SB	3007	-	0,6,6	-	-	-		
59	OHX	5SA	204	-	0,6,6	-	-	-		
59	OHX	23SA	3345	-	0,6,6	-	-	-		
59	OHX	23SB	3198	-	0,6,6	-	-	-		
59	OHX	23SA	3229	-	0,6,6	-	-	-		
59	OHX	23SB	3103	-	0,6,6	-	-	-		
59	OHX	16SB	2256	-	0,6,6	-	-	-		
59	OHX	23SB	3054	-	0,6,6	-	-	-		
59	OHX	16SA	2282	-	0,6,6	-	-	-		
59	OHX	16SA	2293	-	0,6,6	-	-	-		
59	OHX	23SB	3125	-	0,6,6	-	-	-		
59	OHX	23SA	3324	-	0,6,6	-	-	-		
59	OHX	23SB	3111	-	0,6,6	-	-	-		
59	OHX	L35A	102	-	0,6,6	-	-	-		
59	OHX	16SB	2209	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	OHX	23SB	3138	27	0,6,6	-	-	-		
59	OHX	23SB	3143	-	0,6,6	-	-	-		
59	OHX	16SA	2269	-	0,6,6	-	-	-		
59	OHX	16SB	2203	-	0,6,6	-	-	-		
61	SJE	23SB	3521	-	87,91,91	4.10	23 (26%)	117,134,134	1.99	22 (18%)
59	OHX	16SA	2334	-	0,6,6	-	-	-		
59	OHX	23SA	3351	-	0,6,6	-	-	-		
59	OHX	23SB	3069	-	0,6,6	-	-	-		
59	OHX	L4A	302	-	0,6,6	-	-	-		
59	OHX	S14B	101	-	0,6,6	-	-	-		
59	OHX	16SB	2205	-	0,6,6	-	-	-		
59	OHX	23SB	3175	-	0,6,6	-	-	-		
59	OHX	23SB	3056	-	0,6,6	-	-	-		
59	OHX	ASIA	101	-	0,6,6	-	-	-		
59	OHX	23SA	3325	-	0,6,6	-	-	-		
59	OHX	ESIB	101	-	0,6,6	-	-	-		
59	OHX	23SB	3159	-	0,6,6	-	-	-		
59	OHX	23SB	3123	-	0,6,6	-	-	-		
59	OHX	23SA	3192	-	0,6,6	-	-	-		
59	OHX	23SA	3275	-	0,6,6	-	-	-		
59	OHX	23SA	3372	-	0,6,6	-	-	-		
59	OHX	16SA	2316	-	0,6,6	-	-	-		
59	OHX	23SA	3220	-	0,6,6	-	-	-		
59	OHX	23SA	3303	-	0,6,6	-	-	-		
59	OHX	16SA	2330	-	0,6,6	-	-	-		
59	OHX	16SB	2234	1	0,6,6	-	-	-		
59	OHX	23SB	3023	-	0,6,6	-	-	-		
59	OHX	5SA	210	-	0,6,6	-	-	-		
59	OHX	23SB	3027	-	0,6,6	-	-	-		
59	OHX	23SA	3181	-	0,6,6	-	-	-		
59	OHX	23SB	3127	-	0,6,6	-	-	-		
59	OHX	5SB	202	-	0,6,6	-	-	-		
59	OHX	5SB	205	28	0,6,6	-	-	-		
59	OHX	23SB	3120	-	0,6,6	-	-	-		
59	OHX	16SB	2259	-	0,6,6	-	-	-		
59	OHX	23SA	3359	-	0,6,6	-	-	-		
59	OHX	5SA	207	-	0,6,6	-	-	-		
59	OHX	16SB	2278	-	0,6,6	-	-	-		
59	OHX	23SA	3254	-	0,6,6	-	-	-		
59	OHX	16SB	2206	-	0,6,6	-	-	-		
59	OHX	16SA	2329	-	0,6,6	-	-	-		
59	OHX	23SA	3301	-	0,6,6	-	-	-		
59	OHX	16SB	2235	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	OHX	23SB	3141	-	0,6,6	-	-	-		
59	OHX	23SA	3182	27	0,6,6	-	-	-		
59	OHX	16SA	2294	-	0,6,6	-	-	-		
59	OHX	16SB	2267	-	0,6,6	-	-	-		
59	OHX	23SA	3188	-	0,6,6	-	-	-		
59	OHX	16SA	2295	-	0,6,6	-	-	-		
59	OHX	23SB	3194	-	0,6,6	-	-	-		
59	OHX	23SA	3274	-	0,6,6	-	-	-		
59	OHX	23SA	3253	-	0,6,6	-	-	-		
59	OHX	5SB	201	-	0,6,6	-	-	-		
59	OHX	5SA	213	-	0,6,6	-	-	-		
59	OHX	16SB	2220	-	0,6,6	-	-	-		
59	OHX	16SB	2223	-	0,6,6	-	-	-		
59	OHX	16SB	2221	-	0,6,6	-	-	-		
59	OHX	16SB	2240	-	0,6,6	-	-	-		
59	OHX	23SA	3337	-	0,6,6	-	-	-		
59	OHX	23SB	3083	-	0,6,6	-	-	-		
59	OHX	23SB	3131	-	0,6,6	-	-	-		
59	OHX	23SB	3130	-	0,6,6	-	-	-		
59	OHX	23SA	3321	-	0,6,6	-	-	-		
59	OHX	23SB	3157	-	0,6,6	-	-	-		
59	OHX	16SB	2247	-	0,6,6	-	-	-		
59	OHX	S4B	301	-	0,6,6	-	-	-		
59	OHX	23SA	3228	-	0,6,6	-	-	-		
59	OHX	23SA	3249	-	0,6,6	-	-	-		
59	OHX	23SA	3284	-	0,6,6	-	-	-		
59	OHX	23SB	3055	-	0,6,6	-	-	-		
59	OHX	23SA	3316	-	0,6,6	-	-	-		
59	OHX	23SB	3184	-	0,6,6	-	-	-		
59	OHX	23SA	3213	-	0,6,6	-	-	-		
59	OHX	23SB	3084	-	0,6,6	-	-	-		
59	OHX	23SA	3370	-	0,6,6	-	-	-		
59	OHX	23SA	3270	-	0,6,6	-	-	-		
59	OHX	23SA	3302	-	0,6,6	-	-	-		
59	OHX	23SA	3291	27	0,6,6	-	-	-		
59	OHX	23SA	3280	-	0,6,6	-	-	-		
59	OHX	23SB	3169	-	0,6,6	-	-	-		
59	OHX	23SA	3378	-	0,6,6	-	-	-		
59	OHX	23SB	3048	-	0,6,6	-	-	-		
59	OHX	23SB	3142	-	0,6,6	-	-	-		
59	OHX	16SA	2268	-	0,6,6	-	-	-		
59	OHX	TRNA	101	-	0,6,6	-	-	-		
59	OHX	ASIB	101	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	OHX	16SB	2273	-	0,6,6	-	-	-		
59	OHX	L35B	101	-	0,6,6	-	-	-		
59	OHX	23SB	3165	-	0,6,6	-	-	-		
59	OHX	23SB	3033	-	0,6,6	-	-	-		
59	OHX	23SB	3132	-	0,6,6	-	-	-		
59	OHX	23SA	3363	-	0,6,6	-	-	-		
59	OHX	23SB	3167	-	0,6,6	-	-	-		
59	OHX	23SA	3207	-	0,6,6	-	-	-		
59	OHX	23SA	3353	-	0,6,6	-	-	-		
59	OHX	PSIA	102	23	0,6,6	-	-	-		
59	OHX	23SA	3223	-	0,6,6	-	-	-		
59	OHX	16SB	2202	-	0,6,6	-	-	-		
59	OHX	16SA	2320	-	0,6,6	-	-	-		
59	OHX	16SB	2269	-	0,6,6	-	-	-		
59	OHX	23SA	3300	-	0,6,6	-	-	-		
59	OHX	23SA	3235	-	0,6,6	-	-	-		
59	OHX	23SA	3360	-	0,6,6	-	-	-		
59	OHX	23SB	3191	-	0,6,6	-	-	-		
59	OHX	23SA	3374	-	0,6,6	-	-	-		
59	OHX	23SA	3261	-	0,6,6	-	-	-		
59	OHX	16SA	2296	-	0,6,6	-	-	-		
59	OHX	23SA	3211	-	0,6,6	-	-	-		
59	OHX	16SA	2309	1	0,6,6	-	-	-		
59	OHX	16SB	2260	-	0,6,6	-	-	-		
59	OHX	5SB	211	-	0,6,6	-	-	-		
59	OHX	23SB	3173	-	0,6,6	-	-	-		
59	OHX	16SA	2277	-	0,6,6	-	-	-		
59	OHX	23SB	3059	-	0,6,6	-	-	-		
59	OHX	23SB	3164	-	0,6,6	-	-	-		
59	OHX	23SB	3071	-	0,6,6	-	-	-		
59	OHX	23SB	3166	-	0,6,6	-	-	-		
59	OHX	23SA	3222	-	0,6,6	-	-	-		
59	OHX	23SB	3092	-	0,6,6	-	-	-		
59	OHX	23SA	3364	-	0,6,6	-	-	-		
59	OHX	23SB	3052	-	0,6,6	-	-	-		
59	OHX	23SB	3108	-	0,6,6	-	-	-		
59	OHX	23SA	3278	-	0,6,6	-	-	-		
59	OHX	23SA	3272	-	0,6,6	-	-	-		
59	OHX	16SB	2225	-	0,6,6	-	-	-		
59	OHX	23SA	3314	-	0,6,6	-	-	-		
59	OHX	23SB	3160	-	0,6,6	-	-	-		
59	OHX	23SA	3264	-	0,6,6	-	-	-		
59	OHX	16SB	2244	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	OHX	23SB	3065	62	0,6,6	-	-	-		
59	OHX	23SB	3053	-	0,6,6	-	-	-		
59	OHX	16SB	2236	-	0,6,6	-	-	-		
59	OHX	23SB	3018	-	0,6,6	-	-	-		
59	OHX	16SA	2288	-	0,6,6	-	-	-		
59	OHX	23SA	3257	-	0,6,6	-	-	-		
59	OHX	23SA	3377	-	0,6,6	-	-	-		
59	OHX	16SA	2262	-	0,6,6	-	-	-		
59	OHX	23SB	3085	-	0,6,6	-	-	-		
59	OHX	23SB	3021	-	0,6,6	-	-	-		
59	OHX	23SB	3036	-	0,6,6	-	-	-		
59	OHX	23SA	3224	-	0,6,6	-	-	-		
59	OHX	23SB	3121	-	0,6,6	-	-	-		
59	OHX	23SA	3295	-	0,6,6	-	-	-		
59	OHX	23SB	3136	-	0,6,6	-	-	-		
59	OHX	23SA	3267	-	0,6,6	-	-	-		
59	OHX	16SA	2304	-	0,6,6	-	-	-		
59	OHX	16SA	2325	-	0,6,6	-	-	-		
59	OHX	23SB	3117	-	0,6,6	-	-	-		
59	OHX	23SA	3231	-	0,6,6	-	-	-		
59	OHX	23SB	3161	-	0,6,6	-	-	-		
59	OHX	16SB	2258	-	0,6,6	-	-	-		
59	OHX	16SA	2263	-	0,6,6	-	-	-		
59	OHX	23SA	3250	-	0,6,6	-	-	-		
59	OHX	23SA	3338	-	0,6,6	-	-	-		
59	OHX	16SA	2307	-	0,6,6	-	-	-		
59	OHX	16SA	2299	-	0,6,6	-	-	-		
59	OHX	16SA	2337	-	0,6,6	-	-	-		
59	OHX	23SA	3266	-	0,6,6	-	-	-		
59	OHX	23SA	3376	-	0,6,6	-	-	-		
59	OHX	23SB	3011	-	0,6,6	-	-	-		
59	OHX	23SB	3057	-	0,6,6	-	-	-		
59	OHX	23SA	3230	-	0,6,6	-	-	-		
59	OHX	16SB	2271	-	0,6,6	-	-	-		
59	OHX	16SB	2276	-	0,6,6	-	-	-		
59	OHX	23SB	3064	-	0,6,6	-	-	-		
59	OHX	23SB	3046	-	0,6,6	-	-	-		
59	OHX	23SA	3196	-	0,6,6	-	-	-		
59	OHX	23SB	3137	-	0,6,6	-	-	-		
59	OHX	23SB	3077	-	0,6,6	-	-	-		
59	OHX	23SA	3185	-	0,6,6	-	-	-		
59	OHX	23SA	3298	-	0,6,6	-	-	-		
59	OHX	23SB	3040	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	OHX	16SB	2268	-	0,6,6	-	-	-		
59	OHX	23SA	3260	-	0,6,6	-	-	-		
59	OHX	23SA	3248	-	0,6,6	-	-	-		
59	OHX	23SA	3194	-	0,6,6	-	-	-		
59	OHX	16SA	2280	-	0,6,6	-	-	-		
59	OHX	16SA	2341	-	0,6,6	-	-	-		
59	OHX	23SA	3279	-	0,6,6	-	-	-		
59	OHX	23SA	3227	-	0,6,6	-	-	-		
59	OHX	23SB	3006	-	0,6,6	-	-	-		
59	OHX	16SA	2266	1	0,6,6	-	-	-		
59	OHX	23SA	3330	-	0,6,6	-	-	-		
59	OHX	23SA	3344	-	0,6,6	-	-	-		
59	OHX	ESIA	101	-	0,6,6	-	-	-		
59	OHX	ASIB	102	-	0,6,6	-	-	-		
59	OHX	16SB	2274	-	0,6,6	-	-	-		
59	OHX	16SB	2212	-	0,6,6	-	-	-		
59	OHX	5SB	206	-	0,6,6	-	-	-		
59	OHX	23SA	3240	-	0,6,6	-	-	-		
59	OHX	16SA	2291	-	0,6,6	-	-	-		
59	OHX	23SA	3180	-	0,6,6	-	-	-		
59	OHX	23SB	3148	-	0,6,6	-	-	-		
59	OHX	23SB	3013	-	0,6,6	-	-	-		
59	OHX	23SA	3346	-	0,6,6	-	-	-		
59	OHX	16SB	2249	-	0,6,6	-	-	-		
59	OHX	23SA	3281	-	0,6,6	-	-	-		
59	OHX	16SB	2214	-	0,6,6	-	-	-		
59	OHX	23SB	3039	-	0,6,6	-	-	-		
59	OHX	23SB	3174	-	0,6,6	-	-	-		
59	OHX	23SB	3152	-	0,6,6	-	-	-		
59	OHX	16SA	2284	-	0,6,6	-	-	-		
59	OHX	16SB	2245	1	0,6,6	-	-	-		
59	OHX	23SA	3226	-	0,6,6	-	-	-		
59	OHX	23SB	3100	-	0,6,6	-	-	-		
59	OHX	L20B	201	-	0,6,6	-	-	-		
59	OHX	23SA	3216	-	0,6,6	-	-	-		
59	OHX	23SA	3352	-	0,6,6	-	-	-		
59	OHX	23SB	3025	-	0,6,6	-	-	-		
59	OHX	23SA	3368	-	0,6,6	-	-	-		
59	OHX	S4A	301	-	0,6,6	-	-	-		
59	OHX	23SB	3181	-	0,6,6	-	-	-		
59	OHX	23SA	3258	-	0,6,6	-	-	-		
59	OHX	5SA	209	-	0,6,6	-	-	-		
59	OHX	16SA	2285	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	OHX	16SB	2254	-	0,6,6	-	-	-		
59	OHX	23SB	3058	-	0,6,6	-	-	-		
59	OHX	23SA	3292	-	0,6,6	-	-	-		
59	OHX	23SA	3221	-	0,6,6	-	-	-		
59	OHX	23SA	3255	-	0,6,6	-	-	-		
59	OHX	23SA	3217	-	0,6,6	-	-	-		
59	OHX	23SB	3177	-	0,6,6	-	-	-		
59	OHX	16SB	2222	-	0,6,6	-	-	-		
59	OHX	23SB	3190	-	0,6,6	-	-	-		
59	OHX	16SB	2230	-	0,6,6	-	-	-		
59	OHX	16SA	2303	-	0,6,6	-	-	-		
59	OHX	23SB	3016	-	0,6,6	-	-	-		
59	OHX	23SB	3082	-	0,6,6	-	-	-		
59	OHX	23SA	3290	-	0,6,6	-	-	-		
59	OHX	16SA	2265	-	0,6,6	-	-	-		
59	OHX	16SB	2218	-	0,6,6	-	-	-		
59	OHX	23SA	3263	-	0,6,6	-	-	-		
59	OHX	23SA	3311	-	0,6,6	-	-	-		
59	OHX	L15A	201	-	0,6,6	-	-	-		
59	OHX	16SA	2287	-	0,6,6	-	-	-		
59	OHX	23SA	3283	-	0,6,6	-	-	-		
59	OHX	23SA	3206	-	0,6,6	-	-	-		
59	OHX	ASIB	103	-	0,6,6	-	-	-		
59	OHX	23SB	3060	-	0,6,6	-	-	-		
59	OHX	23SA	3282	-	0,6,6	-	-	-		
59	OHX	23SA	3355	-	0,6,6	-	-	-		
59	OHX	5SA	212	-	0,6,6	-	-	-		
59	OHX	23SA	3371	-	0,6,6	-	-	-		
59	OHX	23SA	3373	-	0,6,6	-	-	-		
59	OHX	23SB	3061	-	0,6,6	-	-	-		
59	OHX	23SB	3124	-	0,6,6	-	-	-		
59	OHX	23SA	3305	-	0,6,6	-	-	-		
59	OHX	23SA	3342	-	0,6,6	-	-	-		
59	OHX	23SA	3215	-	0,6,6	-	-	-		
59	OHX	23SA	3349	-	0,6,6	-	-	-		
59	OHX	16SA	2327	-	0,6,6	-	-	-		
59	OHX	23SB	3126	-	0,6,6	-	-	-		
59	OHX	23SA	3304	-	0,6,6	-	-	-		
59	OHX	23SB	3068	-	0,6,6	-	-	-		
59	OHX	ASIA	103	-	0,6,6	-	-	-		
59	OHX	16SA	2267	-	0,6,6	-	-	-		
59	OHX	23SA	3251	-	0,6,6	-	-	-		
59	OHX	16SA	2290	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	OHX	23SA	3271	-	0,6,6	-	-	-		
59	OHX	23SB	3024	-	0,6,6	-	-	-		
59	OHX	16SA	2292	-	0,6,6	-	-	-		
59	OHX	16SA	2328	-	0,6,6	-	-	-		
59	OHX	23SB	3003	27	0,6,6	-	-	-		
59	OHX	23SB	3020	-	0,6,6	-	-	-		
59	OHX	23SB	3087	-	0,6,6	-	-	-		
59	OHX	23SB	3182	27	0,6,6	-	-	-		
59	OHX	23SB	3188	-	0,6,6	-	-	-		
59	OHX	23SB	3095	-	0,6,6	-	-	-		
59	OHX	16SB	2228	-	0,6,6	-	-	-		
59	OHX	23SB	3140	-	0,6,6	-	-	-		
59	OHX	23SA	3195	-	0,6,6	-	-	-		
59	OHX	16SA	2286	-	0,6,6	-	-	-		
59	OHX	5SB	203	-	0,6,6	-	-	-		
59	OHX	23SB	3144	-	0,6,6	-	-	-		
59	OHX	16SB	2243	-	0,6,6	-	-	-		
59	OHX	5SA	205	-	0,6,6	-	-	-		
59	OHX	16SB	2229	-	0,6,6	-	-	-		
59	OHX	23SB	3076	-	0,6,6	-	-	-		
59	OHX	23SB	3075	-	0,6,6	-	-	-		
59	OHX	16SB	2266	-	0,6,6	-	-	-		
59	OHX	16SA	2310	-	0,6,6	-	-	-		
59	OHX	23SB	3109	-	0,6,6	-	-	-		
59	OHX	23SA	3193	-	0,6,6	-	-	-		
59	OHX	16SB	2238	-	0,6,6	-	-	-		
59	OHX	23SB	3155	-	0,6,6	-	-	-		
59	OHX	PSIB	101	-	0,6,6	-	-	-		
59	OHX	23SB	3081	-	0,6,6	-	-	-		
59	OHX	16SB	2224	-	0,6,6	-	-	-		
59	OHX	23SA	3331	-	0,6,6	-	-	-		
59	OHX	23SA	3380	-	0,6,6	-	-	-		
59	OHX	16SB	2255	-	0,6,6	-	-	-		
59	OHX	16SA	2302	-	0,6,6	-	-	-		
59	OHX	16SB	2275	-	0,6,6	-	-	-		
59	OHX	23SA	3210	-	0,6,6	-	-	-		
59	OHX	23SA	3313	-	0,6,6	-	-	-		
59	OHX	23SA	3244	-	0,6,6	-	-	-		
59	OHX	23SA	3356	-	0,6,6	-	-	-		
59	OHX	23SB	3035	-	0,6,6	-	-	-		
59	OHX	5SA	214	-	0,6,6	-	-	-		
59	OHX	23SB	3042	-	0,6,6	-	-	-		
59	OHX	23SA	3347	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	OHX	16SA	2298	-	0,6,6	-	-	-		
59	OHX	16SA	2300	-	0,6,6	-	-	-		
59	OHX	23SB	3094	-	0,6,6	-	-	-		
59	OHX	L17B	201	-	0,6,6	-	-	-		
59	OHX	16SB	2250	-	0,6,6	-	-	-		
59	OHX	16SB	2241	-	0,6,6	-	-	-		
59	OHX	23SB	3179	-	0,6,6	-	-	-		
59	OHX	23SB	3044	-	0,6,6	-	-	-		
59	OHX	MRNB	101	-	0,6,6	-	-	-		
59	OHX	23SB	3154	27	0,6,6	-	-	-		
59	OHX	16SB	2246	-	0,6,6	-	-	-		
59	OHX	23SA	3256	-	0,6,6	-	-	-		
59	OHX	23SB	3113	-	0,6,6	-	-	-		
59	OHX	16SB	2252	-	0,6,6	-	-	-		
59	OHX	23SB	3096	-	0,6,6	-	-	-		
59	OHX	23SB	3185	-	0,6,6	-	-	-		
59	OHX	16SB	2251	-	0,6,6	-	-	-		
59	OHX	23SB	3062	-	0,6,6	-	-	-		
59	OHX	16SA	2289	-	0,6,6	-	-	-		
59	OHX	23SA	3201	-	0,6,6	-	-	-		
59	OHX	16SA	2305	-	0,6,6	-	-	-		
59	OHX	23SB	3128	-	0,6,6	-	-	-		
59	OHX	16SB	2231	-	0,6,6	-	-	-		
59	OHX	23SA	3382	-	0,6,6	-	-	-		
59	OHX	23SA	3187	-	0,6,6	-	-	-		
59	OHX	23SB	3146	-	0,6,6	-	-	-		
59	OHX	16SA	2312	-	0,6,6	-	-	-		
59	OHX	L19A	201	41	0,6,6	-	-	-		
59	OHX	5SB	208	-	0,6,6	-	-	-		
59	OHX	23SA	3246	-	0,6,6	-	-	-		
59	OHX	16SA	2319	-	0,6,6	-	-	-		
59	OHX	16SA	2324	-	0,6,6	-	-	-		
59	OHX	23SA	3242	-	0,6,6	-	-	-		
59	OHX	23SB	3114	-	0,6,6	-	-	-		
59	OHX	16SA	2315	-	0,6,6	-	-	-		
59	OHX	23SA	3367	-	0,6,6	-	-	-		
59	OHX	23SB	3026	-	0,6,6	-	-	-		
59	OHX	23SB	3151	-	0,6,6	-	-	-		
59	OHX	16SA	2264	-	0,6,6	-	-	-		
59	OHX	23SA	3318	27	0,6,6	-	-	-		
59	OHX	23SB	3014	-	0,6,6	-	-	-		
59	OHX	23SA	3306	-	0,6,6	-	-	-		
59	OHX	23SA	3358	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	OHX	23SB	3043	-	0,6,6	-	-	-		
59	OHX	23SB	3180	-	0,6,6	-	-	-		
59	OHX	23SB	3106	-	0,6,6	-	-	-		
59	OHX	23SB	3028	-	0,6,6	-	-	-		
59	OHX	23SB	3170	-	0,6,6	-	-	-		
59	OHX	23SB	3045	-	0,6,6	-	-	-		
59	OHX	23SA	3218	-	0,6,6	-	-	-		
59	OHX	23SA	3245	-	0,6,6	-	-	-		
59	OHX	23SB	3158	-	0,6,6	-	-	-		
59	OHX	23SA	3199	-	0,6,6	-	-	-		
59	OHX	16SB	2208	-	0,6,6	-	-	-		
59	OHX	L4B	301	-	0,6,6	-	-	-		
59	OHX	16SA	2311	-	0,6,6	-	-	-		
59	OHX	16SA	2332	-	0,6,6	-	-	-		
59	OHX	23SB	3196	-	0,6,6	-	-	-		
59	OHX	23SA	3293	-	0,6,6	-	-	-		
59	OHX	23SB	3032	-	0,6,6	-	-	-		
59	OHX	16SB	2242	-	0,6,6	-	-	-		
59	OHX	23SB	3178	-	0,6,6	-	-	-		
59	OHX	23SB	3102	-	0,6,6	-	-	-		
59	OHX	16SA	2338	-	0,6,6	-	-	-		
61	SJE	23SA	3640	-	87,91,91	4.12	25 (28%)	117,134,134	2.02	28 (23%)
59	OHX	23SA	3190	27	0,6,6	-	-	-		
59	OHX	23SA	3212	-	0,6,6	-	-	-		
59	OHX	16SB	2265	-	0,6,6	-	-	-		
59	OHX	PSIB	102	-	0,6,6	-	-	-		
59	OHX	23SB	3101	-	0,6,6	-	-	-		
59	OHX	L20A	201	-	0,6,6	-	-	-		
59	OHX	23SA	3296	-	0,6,6	-	-	-		
59	OHX	23SB	3147	-	0,6,6	-	-	-		
59	OHX	23SB	3099	-	0,6,6	-	-	-		
59	OHX	23SB	3078	-	0,6,6	-	-	-		
59	OHX	16SA	2336	-	0,6,6	-	-	-		
59	OHX	16SB	2264	-	0,6,6	-	-	-		
59	OHX	23SB	3162	-	0,6,6	-	-	-		
59	OHX	23SB	3074	-	0,6,6	-	-	-		
59	OHX	23SB	3009	-	0,6,6	-	-	-		
59	OHX	23SB	3070	-	0,6,6	-	-	-		
59	OHX	23SA	3332	-	0,6,6	-	-	-		
59	OHX	16SB	2211	-	0,6,6	-	-	-		
59	OHX	16SA	2273	-	0,6,6	-	-	-		
59	OHX	23SA	3326	27	0,6,6	-	-	-		
59	OHX	23SB	3034	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	OHX	23SB	3163	-	0,6,6	-	-	-		
59	OHX	23SA	3289	-	0,6,6	-	-	-		
59	OHX	23SA	3341	-	0,6,6	-	-	-		
59	OHX	23SA	3189	-	0,6,6	-	-	-		
59	OHX	23SB	3050	-	0,6,6	-	-	-		
59	OHX	5SB	204	-	0,6,6	-	-	-		
59	OHX	23SA	3252	-	0,6,6	-	-	-		
59	OHX	23SB	3090	-	0,6,6	-	-	-		
59	OHX	L17A	201	-	0,6,6	-	-	-		
59	OHX	16SA	2283	-	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	SJE	23SA	3640	-	-	40/101/161/161	0/5/5/5
61	SJE	23SB	3521	-	-	41/101/161/161	0/5/5/5

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	23SA	3640	SJE	O81-S78	20.69	1.67	1.43
61	23SB	3521	SJE	O79-S78	20.54	1.66	1.43
61	23SB	3521	SJE	O81-S78	20.44	1.66	1.43
61	23SA	3640	SJE	O79-S78	20.23	1.66	1.43
61	23SB	3521	SJE	O86-N85	11.19	1.41	1.22

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	23SA	3640	SJE	O81-S78-O79	-10.60	106.52	119.55
61	23SB	3521	SJE	O81-S78-O79	-9.38	108.02	119.55
61	23SA	3640	SJE	O49-C70-N84	6.47	119.59	109.99
61	23SB	3521	SJE	C18-C17-C16	6.16	119.28	109.19
61	23SB	3521	SJE	O49-C70-N84	6.05	118.97	109.99

There are no chirality outliers.

5 of 81 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	23SA	3640	SJE	C21-C20-O19-C35
61	23SA	3640	SJE	O22-C20-O19-C35
61	23SA	3640	SJE	C28-C26-C35-O19
61	23SA	3640	SJE	C41-C26-C35-O19
61	23SA	3640	SJE	C42-C27-C28-C26

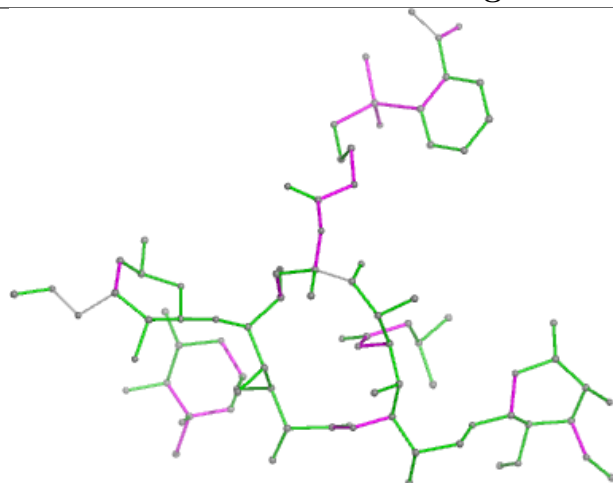
There are no ring outliers.

2 monomers are involved in 7 short contacts:

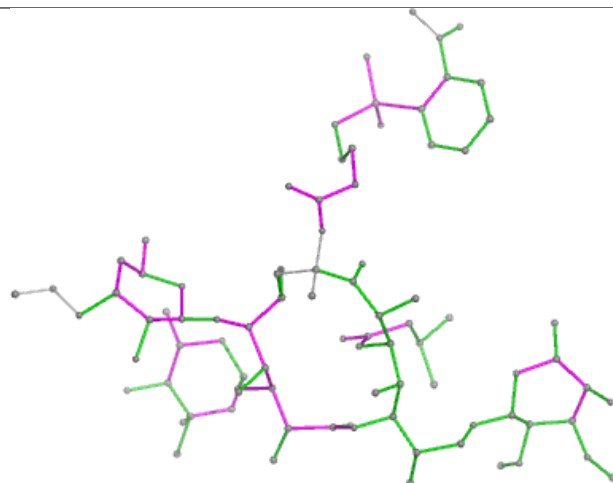
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	S4A	301	OHX	5	0
59	23SA	3304	OHX	0	2

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.

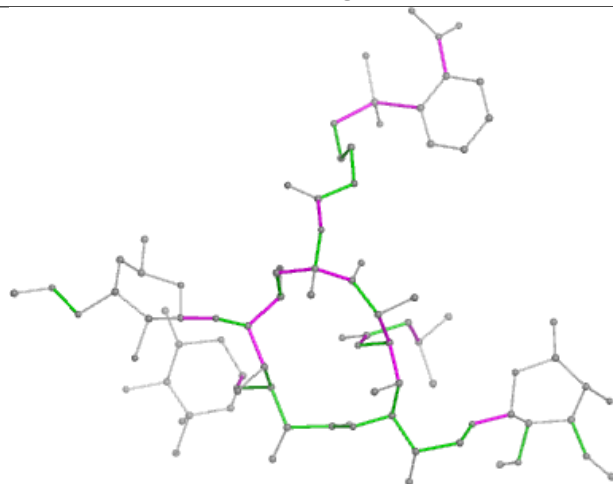
Ligand SJE 23SB 3521



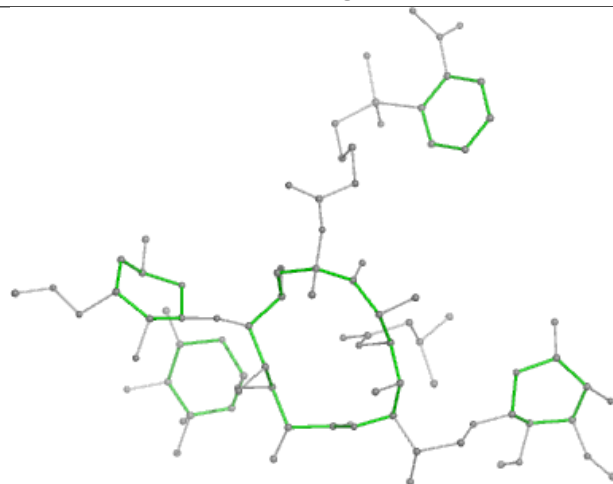
Bond lengths



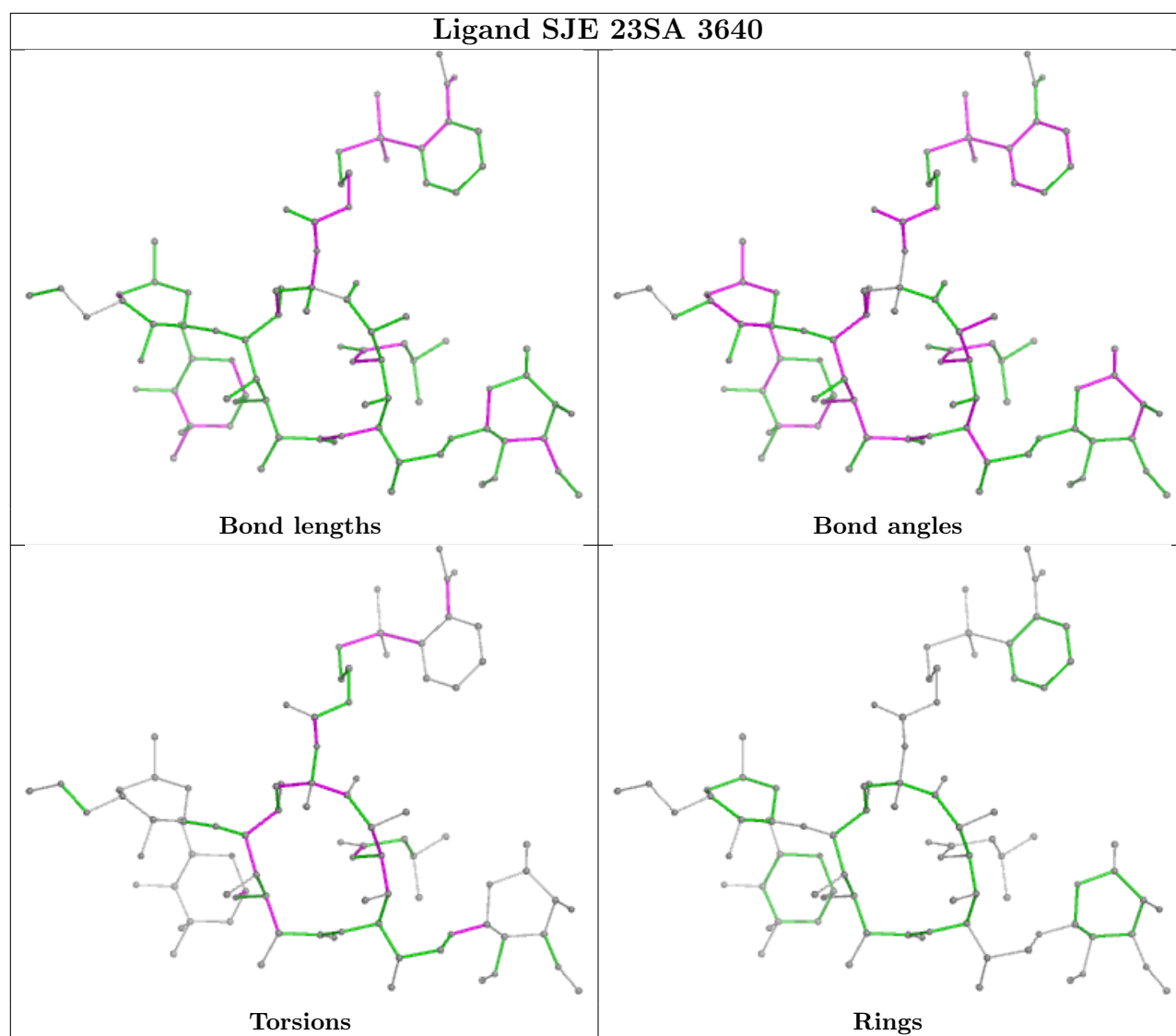
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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	1500/1512 (99%)	-0.48	3 (0%) 92 88	45, 89, 170, 260	0
1	16SB	1496/1512 (98%)	-0.65	1 (0%) 92 91	57, 100, 164, 267	0
2	S2A	237/256 (92%)	0.43	8 (3%) 48 35	91, 125, 164, 178	0
2	S2B	237/256 (92%)	0.59	9 (3%) 44 33	105, 153, 186, 205	0
3	S3A	205/239 (85%)	0.44	6 (2%) 54 40	80, 100, 141, 168	0
3	S3B	206/239 (86%)	0.35	6 (2%) 54 40	104, 128, 157, 161	0
4	S4A	208/209 (99%)	0.45	10 (4%) 36 28	75, 97, 119, 128	0
4	S4B	208/209 (99%)	0.57	13 (6%) 27 22	79, 96, 117, 138	0
5	S5A	151/162 (93%)	0.32	2 (1%) 74 61	65, 87, 108, 132	0
5	S5B	151/162 (93%)	0.25	3 (1%) 64 50	86, 105, 123, 151	0
6	S6A	101/101 (100%)	0.38	3 (2%) 52 39	70, 91, 107, 124	0
6	S6B	101/101 (100%)	0.43	4 (3%) 43 32	73, 94, 109, 132	0
7	S7A	155/156 (99%)	0.16	7 (4%) 39 29	90, 105, 129, 138	0
7	S7B	155/156 (99%)	0.07	1 (0%) 85 78	30, 115, 151, 175	0
8	S8A	138/138 (100%)	0.01	0 100 100	75, 92, 104, 114	0
8	S8B	138/138 (100%)	-0.20	1 (0%) 84 75	83, 104, 115, 125	0
9	S9A	127/128 (99%)	0.08	4 (3%) 51 38	72, 121, 140, 144	0
9	S9B	127/128 (99%)	-0.28	0 100 100	77, 136, 152, 156	0
10	S10A	99/105 (94%)	0.14	3 (3%) 52 39	72, 124, 151, 154	0
10	S10B	99/105 (94%)	0.06	1 (1%) 79 68	104, 144, 159, 166	0
11	S11A	116/129 (89%)	0.26	2 (1%) 69 55	63, 90, 113, 142	0
11	S11B	117/129 (90%)	0.14	4 (3%) 48 35	76, 97, 122, 156	0
12	S12A	124/132 (93%)	0.41	8 (6%) 26 21	57, 66, 98, 162	0
12	S12B	124/132 (93%)	0.46	9 (7%) 22 19	69, 86, 112, 167	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	S13A	119/126 (94%)	0.23	7 (5%) 29 24	77, 113, 129, 138	0
13	S13B	121/126 (96%)	0.06	5 (4%) 42 31	100, 138, 150, 159	0
14	S14A	60/61 (98%)	0.07	1 (1%) 69 55	78, 90, 103, 117	0
14	S14B	59/61 (96%)	-0.04	1 (1%) 69 55	106, 119, 143, 146	0
15	S15A	88/89 (98%)	-0.01	0 100 100	65, 84, 108, 115	0
15	S15B	88/89 (98%)	-0.24	0 100 100	73, 96, 112, 119	0
16	S16A	83/88 (94%)	0.17	2 (2%) 59 44	86, 98, 118, 146	0
16	S16B	84/88 (95%)	0.05	1 (1%) 76 64	79, 88, 106, 144	0
17	S17A	100/105 (95%)	0.02	2 (2%) 64 50	74, 90, 101, 104	0
17	S17B	100/105 (95%)	-0.05	1 (1%) 79 68	80, 97, 114, 126	0
18	S18A	71/88 (80%)	0.35	3 (4%) 41 31	72, 88, 121, 148	0
18	S18B	70/88 (79%)	0.40	2 (2%) 54 40	80, 97, 125, 148	0
19	S19A	84/93 (90%)	0.62	10 (11%) 10 10	30, 114, 133, 139	0
19	S19B	86/93 (92%)	0.29	6 (6%) 24 20	125, 151, 177, 188	0
20	S20A	99/106 (93%)	0.13	1 (1%) 79 68	58, 105, 133, 139	0
20	S20B	99/106 (93%)	-0.17	1 (1%) 79 68	60, 103, 127, 133	0
21	THXA	24/27 (88%)	-0.33	0 100 100	92, 102, 114, 129	0
21	THXB	25/27 (92%)	-0.24	0 100 100	113, 127, 143, 148	0
22	ASIA	69/76 (90%)	1.78	28 (40%) 1 0	71, 185, 223, 237	0
23	PSIA	67/76 (88%)	0.21	6 (8%) 17 15	62, 86, 106, 154	0
23	PSIB	67/76 (88%)	-0.05	2 (2%) 52 39	73, 103, 134, 167	0
24	ESIA	75/76 (98%)	0.70	7 (9%) 16 15	61, 191, 216, 221	0
24	ESIB	75/76 (98%)	0.19	0 100 100	72, 196, 221, 233	0
25	MRNA	30/30 (100%)	0.89	4 (13%) 8 8	60, 150, 238, 250	0
25	MRNB	30/30 (100%)	0.19	2 (6%) 25 20	79, 168, 237, 243	0
26	TRNA	65/76 (85%)	0.31	3 (4%) 38 29	106, 176, 202, 216	0
27	23SA	2878/2911 (98%)	-0.76	12 (0%) 89 83	33, 60, 190, 262	0
27	23SB	2862/2911 (98%)	-0.54	20 (0%) 84 75	40, 76, 213, 270	0
28	5SA	122/124 (98%)	-0.81	0 100 100	57, 76, 92, 167	0
28	5SB	121/124 (97%)	-0.49	1 (0%) 82 72	80, 105, 137, 192	0
29	L2A	272/276 (98%)	-0.21	0 100 100	35, 52, 68, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	L2B	272/276 (98%)	-0.25	2 (0%) 84 75	41, 62, 81, 92	0
30	L3A	204/206 (99%)	-0.09	2 (0%) 79 68	41, 68, 95, 114	0
30	L3B	204/206 (99%)	0.40	7 (3%) 48 35	49, 86, 115, 128	0
31	L4A	202/210 (96%)	-0.33	2 (0%) 79 68	35, 64, 94, 117	0
31	L4B	202/210 (96%)	0.13	6 (2%) 52 39	48, 85, 113, 129	0
32	L5A	181/182 (99%)	0.03	1 (0%) 85 78	70, 87, 114, 130	0
32	L5B	181/182 (99%)	0.12	3 (1%) 69 55	100, 119, 142, 152	0
33	L6A	171/180 (95%)	0.68	10 (5%) 30 24	30, 94, 113, 136	0
33	L6B	173/180 (96%)	1.92	78 (45%) 1 0	154, 201, 242, 260	0
34	L9A	145/148 (97%)	0.85	19 (13%) 8 8	61, 116, 131, 146	0
34	L9B	146/148 (98%)	0.92	30 (20%) 3 3	75, 116, 137, 150	0
35	L13A	138/140 (98%)	0.00	3 (2%) 62 47	51, 70, 102, 112	0
35	L13B	138/140 (98%)	1.07	24 (17%) 5 4	68, 101, 130, 136	0
36	L14A	122/122 (100%)	0.10	3 (2%) 58 43	44, 62, 75, 84	0
36	L14B	122/122 (100%)	0.46	4 (3%) 49 36	62, 81, 101, 112	0
37	L15A	150/150 (100%)	-0.22	0 100 100	38, 69, 99, 141	0
37	L15B	150/150 (100%)	-0.09	2 (1%) 74 61	49, 95, 127, 145	0
38	L16A	141/141 (100%)	0.11	6 (4%) 40 30	48, 66, 89, 120	0
38	L16B	141/141 (100%)	0.25	4 (2%) 55 40	58, 73, 93, 123	0
39	L17A	118/118 (100%)	-0.34	1 (0%) 82 72	49, 66, 85, 94	0
39	L17B	118/118 (100%)	-0.15	0 100 100	57, 75, 94, 111	0
40	L18A	112/112 (100%)	-0.02	1 (0%) 81 70	57, 72, 99, 115	0
40	L18B	111/112 (99%)	-0.12	0 100 100	73, 104, 141, 150	0
41	L19A	137/146 (93%)	0.14	2 (1%) 71 58	56, 73, 129, 158	0
41	L19B	137/146 (93%)	0.34	3 (2%) 62 47	72, 90, 167, 185	0
42	L20A	117/118 (99%)	-0.43	1 (0%) 81 70	43, 60, 88, 115	0
42	L20B	117/118 (99%)	0.66	17 (14%) 7 7	57, 94, 136, 149	0
43	L21A	101/101 (100%)	-0.10	1 (0%) 79 68	44, 81, 98, 110	0
43	L21B	101/101 (100%)	1.44	29 (28%) 1 1	58, 112, 128, 142	0
44	L22A	113/113 (100%)	-0.47	1 (0%) 81 70	43, 57, 88, 128	0
44	L22B	113/113 (100%)	0.19	2 (1%) 67 53	52, 65, 114, 147	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
45	L23A	93/96 (96%)	-0.35	0	100	100	44, 57, 75, 98	0
45	L23B	94/96 (97%)	-0.07	1 (1%)	77	66	58, 73, 98, 121	0
46	L24A	108/110 (98%)	0.02	2 (1%)	66	51	61, 87, 135, 151	0
46	L24B	106/110 (96%)	0.87	13 (12%)	9	9	66, 99, 145, 153	0
47	L25A	179/206 (86%)	0.39	11 (6%)	28	23	70, 104, 181, 189	0
47	L25B	176/206 (85%)	0.71	8 (4%)	39	29	107, 145, 224, 228	0
48	L27A	84/85 (98%)	-0.23	0	100	100	45, 59, 84, 104	0
48	L27B	84/85 (98%)	-0.12	4 (4%)	36	28	63, 79, 100, 128	0
49	L28A	97/98 (98%)	0.11	3 (3%)	51	38	43, 63, 110, 132	0
49	L28B	97/98 (98%)	0.14	3 (3%)	51	38	52, 75, 118, 132	0
50	L29A	69/72 (95%)	-0.01	0	100	100	50, 66, 81, 105	0
50	L29B	71/72 (98%)	0.03	2 (2%)	55	40	70, 89, 109, 138	0
51	L30A	59/60 (98%)	-0.30	0	100	100	48, 66, 96, 115	0
51	L30B	59/60 (98%)	0.40	2 (3%)	48	35	69, 90, 130, 146	0
52	L31A	71/71 (100%)	0.46	3 (4%)	41	31	95, 137, 172, 175	0
52	L31B	71/71 (100%)	0.12	0	100	100	123, 160, 188, 194	0
53	L32A	56/60 (93%)	-0.28	1 (1%)	67	53	38, 70, 126, 133	0
53	L32B	56/60 (93%)	0.46	3 (5%)	32	26	47, 78, 139, 150	0
54	L33A	45/54 (83%)	1.38	11 (24%)	2	1	106, 130, 157, 160	0
54	L33B	45/54 (83%)	0.40	0	100	100	129, 157, 182, 188	0
55	L34A	48/49 (97%)	-0.57	1 (2%)	63	48	37, 42, 57, 78	0
55	L34B	49/49 (100%)	-0.35	1 (2%)	64	50	42, 51, 97, 109	0
56	L35A	64/65 (98%)	-0.50	0	100	100	38, 54, 71, 93	0
56	L35B	64/65 (98%)	-0.12	0	100	100	30, 70, 91, 116	0
57	ASIB	72/76 (94%)	0.71	8 (11%)	12	11	98, 216, 254, 258	0
All	All	21108/21740 (97%)	-0.14	577 (2%)	56	41	30, 88, 176, 270	0

The worst 5 of 577 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	L6B	72	ILE	7.3
4	S4A	9	CYS	6.2
34	L9A	129	THR	6.2

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Mol	Chain	Res	Type	RSRZ
22	ASIA	1	G	6.0
12	S12A	44	LYS	5.9

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
26	H2U	TRNA	16	20/21	0.50	0.12	145,157,174,175	0
23	H2U	PSIB	16	20/21	0.60	0.12	109,134,154,162	0
26	PSU	TRNA	32	20/21	0.63	0.11	182,188,194,195	0
26	H2U	TRNA	20	20/21	0.63	0.10	145,163,173,181	0
22	PSU	ASIA	55	20/21	0.67	0.12	146,160,172,173	0
26	PSU	TRNA	55	20/21	0.67	0.09	143,151,170,173	0
26	4SU	TRNA	8	20/21	0.67	0.12	169,174,178,181	0
26	PSU	TRNA	39	20/21	0.68	0.10	134,167,176,179	0
57	5MU	ASIB	54	21/22	0.68	0.13	145,183,189,193	0
23	3AU	PSIB	47	27/28	0.69	0.13	127,146,156,158	0
23	5MU	PSIB	54	21/22	0.71	0.11	102,108,115,117	0
26	5MU	TRNA	54	21/22	0.73	0.09	151,158,162,164	0
22	4SU	ASIA	8	20/21	0.74	0.14	200,203,207,208	0
23	PSU	PSIB	55	20/21	0.76	0.10	100,105,112,112	0
24	MIA	ESIB	37	29/30	0.78	0.18	130,151,154,154	0
26	MIA	TRNA	37	29/30	0.79	0.17	115,135,154,162	0
23	G7M	PSIB	46	24/25	0.81	0.10	109,119,139,142	0
23	4SU	PSIB	8	20/21	0.81	0.10	101,106,116,120	0
22	G7M	ASIA	46	24/25	0.82	0.15	201,205,216,222	0
23	PSU	PSIA	55	20/21	0.84	0.09	84,89,100,103	0
23	3AU	PSIA	47	27/28	0.84	0.14	94,118,133,135	0
22	5MU	ASIA	54	21/22	0.85	0.12	113,137,147,148	0
1	2MG	16SB	1834	24/25	0.86	0.09	111,120,124,126	0
27	5MU	23SB	1940	21/22	0.87	0.10	85,92,102,106	0
57	PSU	ASIB	32	20/21	0.87	0.08	111,121,129,135	0
24	MIA	ESIA	37	29/30	0.87	0.14	120,144,148,150	0
12	0TD	S12B	89	10/11	0.88	0.14	82,85,91,98	0
12	0TD	S12A	89	10/11	0.89	0.17	59,65,68,72	0
57	PSU	ASIB	39	20/21	0.89	0.09	102,120,127,130	0
22	PSU	ASIA	39	20/21	0.89	0.14	77,88,95,99	0
23	5MU	PSIA	54	21/22	0.90	0.09	88,91,100,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	M2G	16SB	1589	25/26	0.90	0.09	81,91,96,102	0
23	G7M	PSIA	46	24/25	0.91	0.11	77,88,112,114	0
23	H2U	PSIA	16	20/21	0.91	0.10	91,111,134,148	0
1	PSU	16SB	1145	20/21	0.92	0.07	85,90,95,97	0
1	4OC	16SB	2030	22/23	0.92	0.09	68,75,81,95	0
27	5MC	23SB	1987	21/22	0.92	0.11	57,67,74,81	0
1	G7M	16SB	1156	24/25	0.92	0.10	78,83,90,91	0
1	PSU	16SA	1145	20/21	0.92	0.11	69,74,79,81	0
1	5MC	16SB	1590	21/22	0.92	0.08	83,90,96,102	0
22	PSU	ASIA	32	20/21	0.93	0.11	82,90,97,98	0
23	PSU	PSIA	32	20/21	0.93	0.08	67,71,75,79	0
27	OMU	23SB	2567	21/22	0.93	0.11	57,64,67,71	0
1	5MC	16SB	2028	21/22	0.93	0.09	78,84,87,90	0
27	PSU	23SB	1936	20/21	0.93	0.07	72,79,83,85	0
27	5MU	23SA	1940	21/22	0.93	0.11	60,67,75,81	0
27	PSU	23SB	1942	20/21	0.94	0.07	76,81,86,87	0
22	MIA	ASIA	37	29/30	0.94	0.12	64,70,77,79	0
27	PSU	23SA	1936	20/21	0.94	0.11	57,59,62,70	0
23	PSU	PSIB	32	20/21	0.94	0.08	86,91,97,102	0
57	MIA	ASIB	37	29/30	0.94	0.08	83,96,107,111	0
23	PSU	PSIB	39	20/21	0.94	0.06	80,86,90,93	0
1	5MC	16SA	1590	21/22	0.94	0.09	65,69,73,81	0
27	5MC	23SA	1967	21/22	0.95	0.10	51,55,61,69	0
1	5MC	16SA	2032	21/22	0.95	0.13	51,53,60,61	0
27	OMG	23SB	2266	24/25	0.95	0.09	53,58,63,65	0
23	4SU	PSIA	8	20/21	0.95	0.07	72,75,81,83	0
27	PSU	23SB	2620	20/21	0.95	0.09	48,54,60,64	0
1	G7M	16SA	1156	24/25	0.95	0.12	58,67,71,77	0
23	MIA	PSIB	37	29/30	0.95	0.09	82,87,100,103	0
1	2MG	16SA	1834	24/25	0.95	0.07	77,83,87,89	0
27	5MU	23SA	1964	21/22	0.95	0.09	38,44,49,54	0
27	OMC	23SB	1945	21/22	0.96	0.07	69,77,79,81	0
1	UR3	16SA	2121	21/22	0.96	0.11	51,54,60,68	0
27	5MU	23SB	1964	21/22	0.96	0.08	55,59,67,70	0
23	PSU	PSIA	39	20/21	0.96	0.07	59,66,69,69	0
27	5MC	23SB	1967	21/22	0.96	0.07	66,73,78,88	0
27	5MC	23SA	1987	21/22	0.96	0.10	46,50,55,59	0
1	5MC	16SA	2028	21/22	0.96	0.09	54,65,68,71	0
1	M2G	16SA	1589	25/26	0.96	0.07	59,65,72,74	0
27	2MA	23SA	2518	23/24	0.96	0.09	34,40,44,50	0
1	5MC	16SB	2032	21/22	0.96	0.07	63,69,74,76	0
1	UR3	16SB	2121	21/22	0.96	0.09	59,66,70,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	MA6	16SB	2141	24/25	0.96	0.08	68,74,77,79	0
1	MA6	16SB	2142	24/25	0.96	0.09	65,71,74,77	0
23	MIA	PSIA	37	29/30	0.96	0.09	57,65,80,85	0
27	OMC	23SA	1945	21/22	0.96	0.09	53,55,58,61	0
27	2MA	23SB	2518	23/24	0.97	0.09	45,48,52,53	0
27	OMU	23SA	2567	21/22	0.97	0.09	42,48,52,58	0
1	4OC	16SA	2030	22/23	0.97	0.10	56,60,64,67	0
27	PSU	23SA	2620	20/21	0.97	0.06	44,47,53,57	0
1	MA6	16SA	2142	24/25	0.97	0.09	49,52,54,59	0
1	5MC	16SB	2035	21/22	0.97	0.07	64,69,73,76	0
27	OMG	23SA	2266	24/25	0.97	0.07	40,45,49,51	0
27	PSU	23SA	1942	20/21	0.97	0.11	57,63,68,68	0
1	5MC	16SA	2035	21/22	0.97	0.12	45,54,59,62	0
1	MA6	16SA	2141	24/25	0.98	0.08	49,52,55,56	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	3320	1/1	-0.17	0.15	112,112,112,112	0
58	MG	16SA	2250	1/1	0.29	0.14	114,114,114,114	0
58	MG	23SB	3328	1/1	0.30	0.37	102,102,102,102	0
60	K	23SA	3594	1/1	0.31	0.30	127,127,127,127	0
58	MG	16SB	2304[B]	1/1	0.35	0.46	56,56,56,56	1
58	MG	16SB	2304[A]	1/1	0.35	0.46	59,59,59,59	1
58	MG	23SA	3152	1/1	0.39	0.27	95,95,95,95	0
60	K	S4B	302	1/1	0.47	0.21	115,115,115,115	0
58	MG	16SB	2313	1/1	0.48	0.19	142,142,142,142	0
58	MG	16SA	2213	1/1	0.50	0.29	103,103,103,103	0
60	K	23SB	3492	1/1	0.51	0.09	146,146,146,146	0
58	MG	23SB	3314	1/1	0.52	0.17	89,89,89,89	0
60	K	16SA	2383	1/1	0.53	0.14	123,123,123,123	0
58	MG	16SA	2245	1/1	0.54	0.29	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	23SB	3262[B]	1/1	0.56	0.38	59,59,59,59	1
58	MG	23SB	3262[A]	1/1	0.56	0.38	55,55,55,55	1
58	MG	23SB	3212	1/1	0.57	0.23	83,83,83,83	0
58	MG	16SB	2343	1/1	0.57	0.12	148,148,148,148	0
58	MG	23SB	3318	1/1	0.58	0.17	88,88,88,88	0
60	K	16SA	2403	1/1	0.58	0.15	84,84,84,84	0
60	K	23SA	3539	1/1	0.58	0.10	125,125,125,125	0
58	MG	16SA	2242	1/1	0.59	0.14	93,93,93,93	0
60	K	23SB	3519	1/1	0.59	0.15	119,119,119,119	0
58	MG	23SA	3110	1/1	0.60	0.28	109,109,109,109	0
60	K	S20B	201	1/1	0.61	0.10	121,121,121,121	0
58	MG	16SA	2246	1/1	0.61	0.08	100,100,100,100	0
58	MG	23SA	3177	1/1	0.61	0.14	91,91,91,91	0
58	MG	23SA	3127	1/1	0.62	0.18	107,107,107,107	0
60	K	23SA	3634	1/1	0.62	0.15	104,104,104,104	0
58	MG	23SA	3137	1/1	0.62	0.12	89,89,89,89	0
58	MG	23SB	3311	1/1	0.63	0.23	75,75,75,75	0
58	MG	23SB	3293	1/1	0.63	0.33	71,71,71,71	0
60	K	23SA	3548	1/1	0.64	0.20	100,100,100,100	0
60	K	23SA	3549	1/1	0.64	0.10	104,104,104,104	0
58	MG	23SB	3285	1/1	0.64	0.29	77,77,77,77	0
58	MG	23SA	3103	1/1	0.64	0.15	85,85,85,85	0
58	MG	16SA	2241	1/1	0.65	0.28	81,81,81,81	0
60	K	L15B	202	1/1	0.65	0.14	96,96,96,96	0
60	K	16SB	2364	1/1	0.66	0.10	132,132,132,132	0
60	K	16SA	2376	1/1	0.66	0.13	106,106,106,106	0
58	MG	16SA	2223	1/1	0.66	0.15	102,102,102,102	0
58	MG	16SB	2323	1/1	0.67	0.15	92,92,92,92	0
58	MG	16SA	2255	1/1	0.67	0.25	82,82,82,82	0
58	MG	16SB	2322	1/1	0.67	0.16	99,99,99,99	0
60	K	23SA	3563	1/1	0.67	0.13	83,83,83,83	0
60	K	16SA	2395	1/1	0.68	0.14	105,105,105,105	0
58	MG	23SA	3013	1/1	0.68	0.31	69,69,69,69	0
58	MG	16SB	2317	1/1	0.69	0.19	98,98,98,98	0
58	MG	16SB	2314	1/1	0.70	0.22	99,99,99,99	0
58	MG	16SA	2238	1/1	0.70	0.18	118,118,118,118	0
58	MG	PSIB	105	1/1	0.70	0.24	78,78,78,78	0
58	MG	16SA	2258	1/1	0.70	0.26	95,95,95,95	0
60	K	16SB	2395	1/1	0.70	0.12	103,103,103,103	0
60	K	23SA	3575	1/1	0.71	0.12	68,68,68,68	0
60	K	L3B	303	1/1	0.71	0.13	98,98,98,98	0
60	K	23SA	3545	1/1	0.71	0.16	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	16SA	2237	1/1	0.72	0.32	62,62,62,62	0
58	MG	23SB	3286	1/1	0.72	0.26	65,65,65,65	0
58	MG	16SB	2309	1/1	0.72	0.27	77,77,77,77	0
58	MG	23SA	3015	1/1	0.72	0.46	91,91,91,91	0
60	K	23SB	3515	1/1	0.72	0.08	88,88,88,88	0
58	MG	23SA	3100	1/1	0.72	0.15	66,66,66,66	0
58	MG	16SA	2234	1/1	0.72	0.27	83,83,83,83	0
58	MG	16SA	2249	1/1	0.72	0.25	77,77,77,77	0
58	MG	5SB	213	1/1	0.73	0.12	79,79,79,79	0
58	MG	23SA	3154	1/1	0.73	0.20	59,59,59,59	0
60	K	23SA	3611	1/1	0.73	0.12	118,118,118,118	0
58	MG	S5B	201	1/1	0.73	0.19	96,96,96,96	0
58	MG	23SA	3034	1/1	0.73	0.13	60,60,60,60	0
60	K	16SB	2370	1/1	0.73	0.09	135,135,135,135	0
58	MG	23SB	3276	1/1	0.73	0.30	82,82,82,82	0
60	K	23SB	3442	1/1	0.74	0.15	112,112,112,112	0
60	K	23SB	3481	1/1	0.74	0.13	105,105,105,105	0
58	MG	23SA	3159	1/1	0.74	0.16	83,83,83,83	0
58	MG	23SA	3099	1/1	0.74	0.11	80,80,80,80	0
58	MG	23SB	3309	1/1	0.74	0.33	77,77,77,77	0
60	K	16SA	2384	1/1	0.74	0.17	106,106,106,106	0
58	MG	16SA	2224	1/1	0.74	0.17	73,73,73,73	0
60	K	16SA	2408	1/1	0.75	0.17	89,89,89,89	0
58	MG	16SB	2294	1/1	0.75	0.20	77,77,77,77	0
58	MG	16SB	2324	1/1	0.75	0.17	86,86,86,86	0
60	K	23SA	3638	1/1	0.75	0.11	104,104,104,104	0
60	K	23SB	3513	1/1	0.75	0.08	127,127,127,127	0
58	MG	23SA	3088	1/1	0.75	0.15	72,72,72,72	0
58	MG	16SB	2315	1/1	0.75	0.25	85,85,85,85	0
58	MG	23SA	3142	1/1	0.75	0.28	36,36,36,36	0
58	MG	16SB	2284	1/1	0.75	0.20	84,84,84,84	0
60	K	23SA	3542	1/1	0.76	0.10	105,105,105,105	0
58	MG	16SA	2239	1/1	0.76	0.15	84,84,84,84	0
58	MG	23SB	3419	1/1	0.76	0.15	99,99,99,99	0
58	MG	23SB	3315	1/1	0.76	0.09	58,58,58,58	0
60	K	23SA	3560	1/1	0.76	0.08	89,89,89,89	0
58	MG	PSIB	104	1/1	0.76	0.30	79,79,79,79	0
60	K	16SA	2415	1/1	0.76	0.09	89,89,89,89	0
58	MG	23SA	3095	1/1	0.76	0.13	67,67,67,67	0
58	MG	16SA	2232	1/1	0.77	0.33	66,66,66,66	0
60	K	23SB	3493	1/1	0.77	0.16	98,98,98,98	0
58	MG	23SA	3059	1/1	0.77	0.20	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	K	16SA	2404	1/1	0.77	0.10	114,114,114,114	0
58	MG	16SA	2252	1/1	0.77	0.21	86,86,86,86	0
58	MG	23SB	3268	1/1	0.77	0.14	66,66,66,66	0
58	MG	L30A	101	1/1	0.77	0.16	54,54,54,54	0
59	OHX	23SB	3192	7/7	0.78	0.10	169,174,178,271	0
60	K	16SB	2388	1/1	0.78	0.08	119,119,119,119	0
60	K	16SB	2393	1/1	0.78	0.09	96,96,96,96	0
59	OHX	23SB	3193	7/7	0.78	0.11	132,147,161,243	0
60	K	16SB	2396	1/1	0.78	0.15	92,92,92,92	0
58	MG	23SA	3130	1/1	0.78	0.15	61,61,61,61	0
60	K	S14B	102	1/1	0.78	0.08	116,116,116,116	0
58	MG	16SB	2295	1/1	0.78	0.27	66,66,66,66	0
58	MG	23SB	3239	1/1	0.78	0.27	50,50,50,50	0
60	K	16SA	2386	1/1	0.78	0.15	117,117,117,117	0
58	MG	23SB	3310	1/1	0.78	0.31	79,79,79,79	0
58	MG	23SB	3283	1/1	0.78	0.34	72,72,72,72	0
60	K	23SB	3511	1/1	0.78	0.09	119,119,119,119	0
58	MG	16SB	2287	1/1	0.78	0.19	103,103,103,103	0
60	K	23SA	3632	1/1	0.78	0.11	116,116,116,116	0
59	OHX	16SA	2315	7/7	0.78	0.11	101,111,120,229	0
59	OHX	23SA	3308	7/7	0.78	0.12	78,95,108,232	0
59	OHX	23SA	3352	7/7	0.78	0.12	140,147,169,246	0
58	MG	16SA	2211	1/1	0.79	0.28	70,70,70,70	0
59	OHX	23SB	3163	7/7	0.79	0.11	127,143,150,243	0
58	MG	23SA	3023	1/1	0.79	0.20	77,77,77,77	0
58	MG	23SB	3281	1/1	0.79	0.20	77,77,77,77	0
58	MG	16SA	2230	1/1	0.79	0.30	60,60,60,60	0
58	MG	23SA	3037	1/1	0.79	0.15	88,88,88,88	0
58	MG	23SB	3322	1/1	0.79	0.18	72,72,72,72	0
58	MG	16SA	2254	1/1	0.79	0.31	67,67,67,67	0
58	MG	23SB	3332	1/1	0.79	0.26	67,67,67,67	0
58	MG	23SB	3253	1/1	0.79	0.10	78,78,78,78	0
60	K	23SB	3501	1/1	0.79	0.12	84,84,84,84	0
60	K	23SB	3509	1/1	0.79	0.28	102,102,102,102	0
58	MG	23SB	3300	1/1	0.79	0.16	67,67,67,67	0
58	MG	16SB	2333	1/1	0.79	0.27	88,88,88,88	0
58	MG	23SA	3065	1/1	0.79	0.21	56,56,56,56	0
60	K	16SA	2416	1/1	0.79	0.13	86,86,86,86	0
60	K	16SA	2418	1/1	0.79	0.18	97,97,97,97	0
60	K	L5B	202	1/1	0.79	0.09	110,110,110,110	0
60	K	S20A	201	1/1	0.79	0.08	123,123,123,123	0
58	MG	16SA	2218	1/1	0.80	0.40	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	16SB	2326	1/1	0.80	0.39	78,78,78,78	0
58	MG	23SB	3301	1/1	0.80	0.16	75,75,75,75	0
58	MG	16SB	2281	1/1	0.80	0.23	81,81,81,81	0
59	OHX	16SB	2261	7/7	0.80	0.10	136,151,159,251	0
58	MG	23SB	3284	1/1	0.80	0.32	69,69,69,69	0
58	MG	23SB	3209	1/1	0.80	0.33	63,63,63,63	0
60	K	23SA	3547	1/1	0.80	0.11	72,72,72,72	0
60	K	16SA	2405	1/1	0.80	0.10	115,115,115,115	0
58	MG	23SA	3101	1/1	0.80	0.34	73,73,73,73	0
60	K	23SA	3554	1/1	0.81	0.14	87,87,87,87	0
58	MG	23SA	3532	1/1	0.81	0.08	100,100,100,100	0
58	MG	23SA	3086	1/1	0.81	0.19	71,71,71,71	0
58	MG	23SB	3201	1/1	0.81	0.22	72,72,72,72	0
60	K	23SB	3467	1/1	0.81	0.24	106,106,106,106	0
59	OHX	23SA	3362	7/7	0.81	0.12	102,109,127,232	0
60	K	23SA	3595	1/1	0.81	0.13	71,71,71,71	0
58	MG	16SA	2221	1/1	0.81	0.28	62,62,62,62	0
58	MG	16SA	2236	1/1	0.81	0.16	99,99,99,99	0
59	OHX	23SB	3177	7/7	0.81	0.12	117,128,145,232	0
58	MG	16SB	2325	1/1	0.81	0.23	92,92,92,92	0
58	MG	23SA	3067	1/1	0.81	0.33	71,71,71,71	0
58	MG	23SB	3297	1/1	0.81	0.25	68,68,68,68	0
58	MG	16SB	2290	1/1	0.81	0.20	79,79,79,79	0
58	MG	23SB	3399	1/1	0.81	0.11	88,88,88,88	0
58	MG	23SA	3427	1/1	0.81	0.12	53,53,53,53	0
58	MG	16SB	2316	1/1	0.81	0.21	80,80,80,80	0
58	MG	23SB	3319	1/1	0.82	0.12	83,83,83,83	0
60	K	23SA	3544	1/1	0.82	0.08	91,91,91,91	0
58	MG	16SB	2327	1/1	0.82	0.20	93,93,93,93	0
60	K	16SB	2398	1/1	0.82	0.09	101,101,101,101	0
58	MG	23SA	3089	1/1	0.82	0.17	77,77,77,77	0
58	MG	23SB	3257	1/1	0.82	0.26	62,62,62,62	0
58	MG	23SB	3258	1/1	0.82	0.18	72,72,72,72	0
58	MG	16SA	2235	1/1	0.82	0.31	80,80,80,80	0
60	K	23SB	3462	1/1	0.82	0.13	102,102,102,102	0
58	MG	5SA	201	1/1	0.82	0.16	67,67,67,67	0
58	MG	23SB	3303	1/1	0.82	0.15	66,66,66,66	0
58	MG	23SB	3267	1/1	0.82	0.16	63,63,63,63	0
59	OHX	16SA	2333	7/7	0.82	0.10	128,146,168,234	0
58	MG	23SA	3055	1/1	0.82	0.19	51,51,51,51	0
60	K	23SA	3608	1/1	0.82	0.09	80,80,80,80	0
58	MG	16SA	2243	1/1	0.82	0.23	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	OHX	23SA	3353	7/7	0.82	0.11	128,135,151,244	0
58	MG	23SA	3176	1/1	0.82	0.34	63,63,63,63	0
59	OHX	23SA	3382	7/7	0.82	0.10	86,97,101,238	0
58	MG	23SA	3060	1/1	0.82	0.22	63,63,63,63	0
60	K	PSIA	105	1/1	0.82	0.11	100,100,100,100	0
58	MG	16SB	2288	1/1	0.82	0.28	70,70,70,70	0
58	MG	23SA	3109	1/1	0.83	0.18	55,55,55,55	0
58	MG	23SB	3295	1/1	0.83	0.19	57,57,57,57	0
58	MG	23SA	3148	1/1	0.83	0.06	64,64,64,64	0
58	MG	23SB	3360	1/1	0.83	0.18	111,111,111,111	0
58	MG	23SB	3299	1/1	0.83	0.16	68,68,68,68	0
58	MG	23SB	3263	1/1	0.83	0.34	56,56,56,56	0
58	MG	5SB	212	1/1	0.83	0.13	103,103,103,103	0
60	K	16SB	2365	1/1	0.83	0.10	126,126,126,126	0
58	MG	16SA	2222	1/1	0.83	0.33	74,74,74,74	0
58	MG	L15B	201	1/1	0.83	0.15	58,58,58,58	0
59	OHX	16SA	2300	7/7	0.83	0.12	104,105,114,228	0
58	MG	16SB	2301	1/1	0.83	0.28	68,68,68,68	0
59	OHX	16SA	2325	7/7	0.83	0.10	137,144,157,243	0
58	MG	23SB	3307	1/1	0.83	0.19	71,71,71,71	0
59	OHX	23SA	3304	7/7	0.83	0.10	109,115,118,229	0
60	K	16SA	2419	1/1	0.83	0.13	95,95,95,95	0
58	MG	23SB	3272	1/1	0.83	0.26	57,57,57,57	0
58	MG	23SA	3124	1/1	0.83	0.15	72,72,72,72	0
58	MG	23SB	3280	1/1	0.83	0.17	59,59,59,59	0
58	MG	L33A	101	1/1	0.83	0.27	95,95,95,95	0
59	OHX	23SA	3363	7/7	0.83	0.10	109,126,158,239	0
59	OHX	23SA	3369	7/7	0.83	0.10	125,136,152,237	0
59	OHX	23SA	3381	7/7	0.83	0.24	74,88,105,228	0
60	K	23SB	3494	1/1	0.83	0.12	109,109,109,109	0
58	MG	23SA	3017	1/1	0.83	0.15	73,73,73,73	0
59	OHX	L28A	101	7/7	0.83	0.10	84,89,95,234	0
59	OHX	16SB	2257	7/7	0.83	0.10	149,153,169,230	0
58	MG	23SA	3161	1/1	0.83	0.07	88,88,88,88	0
58	MG	23SA	3106	1/1	0.83	0.24	60,60,60,60	0
58	MG	23SA	3108	1/1	0.83	0.23	46,46,46,46	0
60	K	23SB	3520	1/1	0.83	0.10	107,107,107,107	0
60	K	23SA	3586	1/1	0.83	0.09	73,73,73,73	0
60	K	23SA	3588	1/1	0.83	0.27	70,70,70,70	0
59	OHX	23SB	3185	7/7	0.83	0.10	130,138,151,236	0
58	MG	23SA	3445	1/1	0.84	0.12	43,43,43,43	0
58	MG	16SB	2307	1/1	0.84	0.41	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	K	16SB	2367	1/1	0.84	0.11	115,115,115,115	0
58	MG	16SA	2247	1/1	0.84	0.25	66,66,66,66	0
60	K	16SB	2387	1/1	0.84	0.17	93,93,93,93	0
58	MG	23SA	3537	1/1	0.84	0.15	72,72,72,72	0
58	MG	23SA	3147	1/1	0.84	0.12	76,76,76,76	0
58	MG	16SB	2344	1/1	0.84	0.09	107,107,107,107	0
58	MG	23SB	3265	1/1	0.84	0.24	57,57,57,57	0
59	OHX	23SB	3140	7/7	0.84	0.10	108,117,123,240	0
58	MG	L5B	201	1/1	0.84	0.08	122,122,122,122	0
58	MG	16SB	2291	1/1	0.84	0.20	73,73,73,73	0
59	OHX	23SB	3180	7/7	0.84	0.11	104,121,149,231	0
58	MG	16SB	2292	1/1	0.84	0.35	59,59,59,59	0
59	OHX	23SB	3186	7/7	0.84	0.11	122,128,152,228	0
58	MG	5SA	202	1/1	0.84	0.07	67,67,67,67	0
58	MG	16SB	2321	1/1	0.84	0.28	73,73,73,73	0
58	MG	23SA	3128	1/1	0.84	0.17	62,62,62,62	0
60	K	16SA	2377	1/1	0.84	0.09	101,101,101,101	0
60	K	23SA	3584	1/1	0.84	0.07	85,85,85,85	0
60	K	23SB	3498	1/1	0.84	0.07	108,108,108,108	0
60	K	16SA	2380	1/1	0.84	0.14	91,91,91,91	0
60	K	23SB	3502	1/1	0.84	0.10	97,97,97,97	0
59	OHX	23SA	3257	7/7	0.84	0.11	134,139,144,224	0
58	MG	23SB	3210	1/1	0.84	0.28	60,60,60,60	0
58	MG	23SA	3116	1/1	0.84	0.20	62,62,62,62	0
59	OHX	23SA	3346	7/7	0.84	0.10	143,147,162,241	0
60	K	23SB	3517	1/1	0.84	0.24	103,103,103,103	0
58	MG	23SB	3218	1/1	0.84	0.21	56,56,56,56	0
60	K	23SA	3625	1/1	0.84	0.08	83,83,83,83	0
58	MG	23SB	3230	1/1	0.84	0.24	66,66,66,66	0
59	OHX	23SA	3354	7/7	0.84	0.13	110,114,141,218	0
58	MG	23SA	3002	1/1	0.84	0.25	58,58,58,58	0
60	K	L3A	303	1/1	0.85	0.10	88,88,88,88	0
60	K	16SA	2398	1/1	0.85	0.12	67,67,67,67	0
58	MG	23SB	3234	1/1	0.85	0.24	55,55,55,55	0
58	MG	23SA	3092	1/1	0.85	0.07	60,60,60,60	0
58	MG	23SA	3006	1/1	0.85	0.24	50,50,50,50	0
59	OHX	23SA	3374	7/7	0.85	0.11	123,128,153,223	0
59	OHX	23SA	3380	7/7	0.85	0.10	101,108,113,232	0
58	MG	23SA	3118	1/1	0.85	0.14	59,59,59,59	0
58	MG	16SB	2330	1/1	0.85	0.15	93,93,93,93	0
59	OHX	5SA	213	7/7	0.85	0.10	118,123,145,229	0
58	MG	23SA	3156	1/1	0.85	0.10	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	16SB	2279	1/1	0.85	0.20	68,68,68,68	0
60	K	S13B	201	1/1	0.85	0.08	139,139,139,139	0
58	MG	L4B	302	1/1	0.85	0.27	94,94,94,94	0
59	OHX	16SB	2272	7/7	0.85	0.10	140,141,165,247	0
58	MG	16SB	2312	1/1	0.85	0.13	71,71,71,71	0
60	K	23SB	3448	1/1	0.85	0.17	104,104,104,104	0
59	OHX	23SB	3161	7/7	0.85	0.09	142,150,169,244	0
58	MG	23SB	3304	1/1	0.85	0.21	68,68,68,68	0
60	K	23SB	3478	1/1	0.85	0.13	94,94,94,94	0
59	OHX	23SB	3165	7/7	0.85	0.09	146,151,160,234	0
59	OHX	23SB	3172	7/7	0.85	0.10	120,133,146,238	0
58	MG	23SA	3063	1/1	0.85	0.18	66,66,66,66	0
59	OHX	23SB	3179	7/7	0.85	0.11	154,162,169,245	0
58	MG	23SA	3008	1/1	0.85	0.09	73,73,73,73	0
58	MG	23SA	3036	1/1	0.85	0.18	53,53,53,53	0
59	OHX	16SA	2328	7/7	0.85	0.11	143,155,166,234	0
58	MG	23SA	3069	1/1	0.85	0.19	70,70,70,70	0
59	OHX	TRNA	102	7/7	0.85	0.09	125,127,144,247	0
59	OHX	23SB	3199	7/7	0.85	0.10	100,103,106,239	0
58	MG	23SB	3207	1/1	0.85	0.18	47,47,47,47	0
58	MG	23SA	3422	1/1	0.85	0.13	63,63,63,63	0
58	MG	23SB	3316	1/1	0.85	0.15	62,62,62,62	0
58	MG	16SA	2229	1/1	0.85	0.22	71,71,71,71	0
58	MG	16SA	2248	1/1	0.85	0.26	83,83,83,83	0
58	MG	23SA	3143	1/1	0.85	0.19	69,69,69,69	0
58	MG	16SA	2226	1/1	0.85	0.12	78,78,78,78	0
58	MG	5SA	203	1/1	0.86	0.25	79,79,79,79	0
58	MG	23SB	3220	1/1	0.86	0.08	72,72,72,72	0
58	MG	L23A	101	1/1	0.86	0.10	60,60,60,60	0
58	MG	23SA	3171	1/1	0.86	0.12	49,49,49,49	0
58	MG	L32A	101	1/1	0.86	0.13	67,67,67,67	0
60	K	L5A	302	1/1	0.86	0.12	83,83,83,83	0
58	MG	23SB	3240	1/1	0.86	0.22	54,54,54,54	0
58	MG	23SA	3094	1/1	0.86	0.19	55,55,55,55	0
60	K	16SB	2366	1/1	0.86	0.10	88,88,88,88	0
60	K	16SA	2391	1/1	0.86	0.12	86,86,86,86	0
58	MG	16SB	2332	1/1	0.86	0.15	92,92,92,92	0
60	K	16SB	2375	1/1	0.86	0.08	106,106,106,106	0
60	K	16SB	2381	1/1	0.86	0.09	100,100,100,100	0
58	MG	23SA	3083	1/1	0.86	0.17	41,41,41,41	0
58	MG	16SA	2220	1/1	0.86	0.20	47,47,47,47	0
60	K	16SB	2390	1/1	0.86	0.12	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	23SA	3051	1/1	0.86	0.30	53,53,53,53	0
58	MG	16SB	2363	1/1	0.86	0.10	89,89,89,89	0
59	OHX	16SB	2264	7/7	0.86	0.09	140,157,163,237	0
58	MG	23SA	3131	1/1	0.86	0.12	63,63,63,63	0
59	OHX	16SB	2277	7/7	0.86	0.09	99,106,111,245	0
59	OHX	23SB	3110	7/7	0.86	0.09	104,110,117,225	0
59	OHX	23SB	3119	7/7	0.86	0.10	86,94,113,210	0
59	OHX	23SB	3126	7/7	0.86	0.10	110,115,124,217	0
59	OHX	23SB	3135	7/7	0.86	0.11	81,95,103,232	0
58	MG	23SA	3499	1/1	0.86	0.14	56,56,56,56	0
59	OHX	23SB	3148	7/7	0.86	0.10	111,126,143,215	0
59	OHX	23SB	3157	7/7	0.86	0.10	120,135,155,223	0
58	MG	16SB	2289	1/1	0.86	0.13	89,89,89,89	0
59	OHX	ASIA	102	7/7	0.86	0.11	113,120,131,219	0
58	MG	23SA	3136	1/1	0.86	0.10	77,77,77,77	0
58	MG	23SB	3273	1/1	0.86	0.37	51,51,51,51	0
60	K	23SA	3550	1/1	0.86	0.18	81,81,81,81	0
59	OHX	23SB	3174	7/7	0.86	0.10	128,128,151,234	0
58	MG	16SB	2318	1/1	0.86	0.30	65,65,65,65	0
58	MG	23SB	3279	1/1	0.86	0.23	82,82,82,82	0
59	OHX	23SA	3312	7/7	0.86	0.23	74,87,95,219	0
59	OHX	23SB	3181	7/7	0.86	0.09	118,141,152,230	0
58	MG	16SA	2257	1/1	0.86	0.24	54,54,54,54	0
59	OHX	23SA	3347	7/7	0.86	0.10	126,132,144,218	0
58	MG	23SA	3080	1/1	0.86	0.18	57,57,57,57	0
58	MG	23SA	3170	1/1	0.86	0.08	69,69,69,69	0
60	K	23SA	3597	1/1	0.86	0.12	87,87,87,87	0
59	OHX	23SB	3194	7/7	0.86	0.09	133,151,170,230	0
59	OHX	23SB	3196	7/7	0.86	0.10	157,162,174,238	0
60	K	23SA	3617	1/1	0.86	0.10	74,74,74,74	0
58	MG	23SB	3372	1/1	0.87	0.10	50,50,50,50	0
58	MG	23SB	3388	1/1	0.87	0.12	38,38,38,38	0
58	MG	16SB	2302	1/1	0.87	0.35	66,66,66,66	0
60	K	16SA	2379	1/1	0.87	0.07	111,111,111,111	0
58	MG	23SA	3081	1/1	0.87	0.20	50,50,50,50	0
58	MG	16SA	2219	1/1	0.87	0.14	74,74,74,74	0
58	MG	23SA	3005	1/1	0.87	0.17	54,54,54,54	0
60	K	16SA	2385	1/1	0.87	0.17	107,107,107,107	0
58	MG	16SA	2209	1/1	0.87	0.08	86,86,86,86	0
60	K	16SA	2387	1/1	0.87	0.10	93,93,93,93	0
58	MG	16SB	2311	1/1	0.87	0.33	84,84,84,84	0
59	OHX	16SB	2246	7/7	0.87	0.10	104,108,114,227	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	K	16SB	2379	1/1	0.87	0.11	121,121,121,121	0
58	MG	23SA	3026	1/1	0.87	0.18	52,52,52,52	0
58	MG	23SB	3261	1/1	0.87	0.19	52,52,52,52	0
58	MG	16SB	2361	1/1	0.87	0.08	122,122,122,122	0
58	MG	23SA	3007	1/1	0.87	0.26	61,61,61,61	0
60	K	16SB	2392	1/1	0.87	0.08	117,117,117,117	0
59	OHX	16SA	2326	7/7	0.87	0.10	127,136,164,238	0
58	MG	23SA	3117	1/1	0.87	0.11	81,81,81,81	0
58	MG	16SA	2204	1/1	0.87	0.23	52,52,52,52	0
59	OHX	23SB	3122	7/7	0.87	0.11	93,97,102,223	0
58	MG	23SA	3516	1/1	0.87	0.09	84,84,84,84	0
60	K	16SA	2420	1/1	0.87	0.10	99,99,99,99	0
59	OHX	23SB	3127	7/7	0.87	0.09	109,115,122,246	0
58	MG	16SA	2259	1/1	0.87	0.22	47,47,47,47	0
58	MG	23SB	3202	1/1	0.87	0.29	51,51,51,51	0
59	OHX	23SB	3144	7/7	0.87	0.08	103,111,118,233	0
59	OHX	23SA	3258	7/7	0.87	0.09	90,100,113,211	0
59	OHX	23SB	3151	7/7	0.87	0.09	135,140,158,248	0
60	K	23SB	3475	1/1	0.87	0.10	90,90,90,90	0
59	OHX	23SA	3272	7/7	0.87	0.10	84,96,103,208	0
60	K	23SB	3479	1/1	0.87	0.09	76,76,76,76	0
59	OHX	23SA	3288	7/7	0.87	0.18	82,88,106,207	0
59	OHX	23SA	3295	7/7	0.87	0.08	103,109,114,228	0
59	OHX	23SA	3298	7/7	0.87	0.09	95,100,108,219	0
60	K	23SA	3553	1/1	0.87	0.13	92,92,92,92	0
58	MG	23SB	3204	1/1	0.87	0.29	54,54,54,54	0
58	MG	23SA	3045	1/1	0.87	0.27	44,44,44,44	0
58	MG	23SA	3071	1/1	0.87	0.19	77,77,77,77	0
59	OHX	23SA	3336	7/7	0.87	0.10	112,116,141,218	0
58	MG	23SA	3049	1/1	0.87	0.23	57,57,57,57	0
58	MG	23SA	3163	1/1	0.87	0.18	45,45,45,45	0
59	OHX	23SA	3349	7/7	0.87	0.09	115,126,155,229	0
58	MG	23SB	3327	1/1	0.87	0.09	59,59,59,59	0
59	OHX	23SB	3189	7/7	0.87	0.10	147,159,176,238	0
58	MG	16SB	2296	1/1	0.87	0.20	71,71,71,71	0
58	MG	23SA	3168	1/1	0.87	0.17	89,89,89,89	0
59	OHX	23SA	3361	7/7	0.87	0.10	86,117,130,220	0
58	MG	23SB	3223	1/1	0.87	0.17	79,79,79,79	0
59	OHX	16SA	2332	7/7	0.88	0.10	133,137,152,236	0
58	MG	23SA	3102	1/1	0.88	0.26	45,45,45,45	0
59	OHX	23SA	3373	7/7	0.88	0.10	92,109,134,230	0
59	OHX	16SA	2335	7/7	0.88	0.09	127,136,156,226	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	23SA	3020	1/1	0.88	0.24	32,32,32,32	0
58	MG	23SB	3329	1/1	0.88	0.25	64,64,64,64	0
58	MG	16SA	2201	1/1	0.88	0.24	73,73,73,73	0
59	OHX	5SA	209	7/7	0.88	0.10	81,100,111,199	0
58	MG	23SA	3402	1/1	0.88	0.13	49,49,49,49	0
58	MG	23SA	3097	1/1	0.88	0.25	50,50,50,50	0
58	MG	L3A	301	1/1	0.88	0.21	57,57,57,57	0
60	K	S6B	201	1/1	0.88	0.09	85,85,85,85	0
59	OHX	16SB	2249	7/7	0.88	0.09	102,104,116,221	0
58	MG	23SA	3078	1/1	0.88	0.23	50,50,50,50	0
58	MG	23SB	3232	1/1	0.88	0.22	60,60,60,60	0
60	K	23SB	3441	1/1	0.88	0.12	88,88,88,88	0
60	K	23SA	3562	1/1	0.88	0.05	80,80,80,80	0
58	MG	23SA	3019	1/1	0.88	0.11	35,35,35,35	0
59	OHX	23SA	3307	7/7	0.88	0.09	108,113,123,223	0
59	OHX	16SB	2273	7/7	0.88	0.09	129,146,161,233	0
59	OHX	16SB	2275	7/7	0.88	0.10	115,137,163,225	0
60	K	23SB	3476	1/1	0.88	0.22	77,77,77,77	0
60	K	16SA	2378	1/1	0.88	0.09	93,93,93,93	0
58	MG	23SB	3236	1/1	0.88	0.28	58,58,58,58	0
59	OHX	MRNB	101	7/7	0.88	0.09	144,148,154,235	0
58	MG	23SA	3484	1/1	0.88	0.12	84,84,84,84	0
59	OHX	23SB	3114	7/7	0.88	0.08	96,100,108,207	0
58	MG	23SA	3489	1/1	0.88	0.11	36,36,36,36	0
59	OHX	23SA	3339	7/7	0.88	0.09	99,120,146,218	0
60	K	23SB	3499	1/1	0.88	0.09	85,85,85,85	0
59	OHX	23SA	3345	7/7	0.88	0.10	107,120,136,224	0
58	MG	23SA	3495	1/1	0.88	0.09	67,67,67,67	0
59	OHX	23SB	3132	7/7	0.88	0.09	105,111,127,226	0
59	OHX	16SA	2290	7/7	0.88	0.18	82,92,113,204	0
60	K	23SB	3512	1/1	0.88	0.11	79,79,79,79	0
59	OHX	16SA	2292	7/7	0.88	0.11	88,100,116,196	0
59	OHX	23SB	3143	7/7	0.88	0.09	101,107,113,221	0
58	MG	23SA	3169	1/1	0.88	0.21	82,82,82,82	0
58	MG	16SB	2282	1/1	0.88	0.35	83,83,83,83	0
59	OHX	23SB	3149	7/7	0.88	0.09	111,128,143,208	0
58	MG	23SA	3068	1/1	0.88	0.09	64,64,64,64	0
58	MG	16SB	2308	1/1	0.88	0.30	59,59,59,59	0
58	MG	23SB	3324	1/1	0.88	0.13	58,58,58,58	0
59	OHX	23SA	3311	7/7	0.89	0.09	99,101,117,228	0
58	MG	23SA	3421	1/1	0.89	0.10	63,63,63,63	0
58	MG	23SA	3079	1/1	0.89	0.11	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	23SA	3144	1/1	0.89	0.20	52,52,52,52	0
60	K	23SA	3635	1/1	0.89	0.04	69,69,69,69	0
60	K	23SA	3636	1/1	0.89	0.08	85,85,85,85	0
59	OHX	23SA	3341	7/7	0.89	0.10	113,122,146,225	0
60	K	16SA	2382	1/1	0.89	0.10	88,88,88,88	0
59	OHX	23SB	3035	7/7	0.89	0.14	65,93,108,150	0
58	MG	23SA	3166	1/1	0.89	0.19	38,38,38,38	0
58	MG	L5A	301	1/1	0.89	0.25	67,67,67,67	0
58	MG	23SB	3255	1/1	0.89	0.29	50,50,50,50	0
59	OHX	16SA	2316	7/7	0.89	0.08	114,126,153,236	0
60	K	16SA	2389	1/1	0.89	0.13	82,82,82,82	0
59	OHX	23SA	3350	7/7	0.89	0.08	121,138,153,230	0
59	OHX	16SA	2318	7/7	0.89	0.08	113,116,137,211	0
60	K	16SA	2396	1/1	0.89	0.07	103,103,103,103	0
60	K	16SB	2382	1/1	0.89	0.10	94,94,94,94	0
60	K	16SB	2384	1/1	0.89	0.08	98,98,98,98	0
58	MG	16SA	2240	1/1	0.89	0.33	70,70,70,70	0
58	MG	16SA	2205	1/1	0.89	0.27	51,51,51,51	0
59	OHX	23SA	3358	7/7	0.89	0.08	129,130,145,238	0
58	MG	23SB	3323	1/1	0.89	0.27	45,45,45,45	0
58	MG	23SB	3259	1/1	0.89	0.34	35,35,35,35	0
58	MG	23SB	3260	1/1	0.89	0.35	63,63,63,63	0
59	OHX	23SA	3365	7/7	0.89	0.08	184,185,193,269	0
58	MG	23SB	3296	1/1	0.89	0.43	72,72,72,72	0
59	OHX	23SA	3370	7/7	0.89	0.11	94,101,133,213	0
59	OHX	23SB	3159	7/7	0.89	0.09	124,131,146,207	0
59	OHX	23SA	3371	7/7	0.89	0.09	130,141,155,222	0
58	MG	23SA	3121	1/1	0.89	0.18	54,54,54,54	0
58	MG	23SA	3057	1/1	0.89	0.16	44,44,44,44	0
60	K	23SA	3540	1/1	0.89	0.07	79,79,79,79	0
59	OHX	23SB	3170	7/7	0.89	0.08	132,138,158,216	0
60	K	23SB	3445	1/1	0.89	0.09	66,66,66,66	0
58	MG	23SA	3140	1/1	0.89	0.12	61,61,61,61	0
58	MG	23SB	3366	1/1	0.89	0.15	39,39,39,39	0
60	K	23SA	3546	1/1	0.89	0.23	94,94,94,94	0
60	K	23SB	3471	1/1	0.89	0.14	106,106,106,106	0
59	OHX	23SB	3176	7/7	0.89	0.09	143,147,163,222	0
58	MG	23SA	3524	1/1	0.89	0.08	113,113,113,113	0
59	OHX	23SB	3178	7/7	0.89	0.10	103,113,139,232	0
59	OHX	23SA	3274	7/7	0.89	0.08	95,102,117,215	0
60	K	23SB	3480	1/1	0.89	0.13	80,80,80,80	0
59	OHX	23SA	3286	7/7	0.89	0.24	75,84,102,179	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	K	23SB	3490	1/1	0.89	0.07	84,84,84,84	0
59	OHX	5SA	214	7/7	0.89	0.08	138,149,161,234	0
58	MG	23SB	3222	1/1	0.89	0.19	64,64,64,64	0
58	MG	23SA	3158	1/1	0.89	0.32	77,77,77,77	0
59	OHX	23SB	3188	7/7	0.89	0.08	134,155,164,228	0
58	MG	23SB	3224	1/1	0.89	0.18	68,68,68,68	0
60	K	23SA	3581	1/1	0.89	0.10	72,72,72,72	0
59	OHX	23SB	3190	7/7	0.89	0.09	112,126,151,218	0
59	OHX	16SB	2250	7/7	0.89	0.09	110,121,130,223	0
59	OHX	16SB	2253	7/7	0.89	0.09	122,127,146,233	0
60	K	23SA	3591	1/1	0.89	0.10	66,66,66,66	0
60	K	23SA	3592	1/1	0.89	0.09	67,67,67,67	0
58	MG	23SB	3308	1/1	0.89	0.14	73,73,73,73	0
59	OHX	23SB	3195	7/7	0.89	0.09	182,185,190,255	0
58	MG	16SA	2225	1/1	0.89	0.24	50,50,50,50	0
60	K	23SA	3599	1/1	0.89	0.07	66,66,66,66	0
58	MG	PSIB	103	1/1	0.89	0.23	52,52,52,52	0
59	OHX	5SB	210	7/7	0.89	0.09	125,130,151,226	0
60	K	23SA	3613	1/1	0.89	0.11	91,91,91,91	0
61	SJE	23SA	3640	87/87	0.89	0.14	44,53,86,93	0
58	MG	23SA	3115	1/1	0.90	0.21	91,91,91,91	0
58	MG	23SB	3244	1/1	0.90	0.24	43,43,43,43	0
58	MG	23SB	3245	1/1	0.90	0.22	45,45,45,45	0
58	MG	23SB	3250	1/1	0.90	0.25	41,41,41,41	0
58	MG	16SB	2306	1/1	0.90	0.19	56,56,56,56	0
59	OHX	23SB	3183	7/7	0.90	0.08	148,155,160,237	0
58	MG	23SB	3292	1/1	0.90	0.17	57,57,57,57	0
58	MG	23SA	3014	1/1	0.90	0.28	70,70,70,70	0
58	MG	23SA	3483	1/1	0.90	0.07	92,92,92,92	0
59	OHX	5SA	208	7/7	0.90	0.08	98,106,114,218	0
59	OHX	23SA	3252	7/7	0.90	0.16	83,84,115,187	0
59	OHX	23SB	3191	7/7	0.90	0.09	112,116,127,213	0
58	MG	16SA	2227	1/1	0.90	0.18	56,56,56,56	0
58	MG	23SB	3336	1/1	0.90	0.08	64,64,64,64	0
58	MG	23SB	3346	1/1	0.90	0.11	56,56,56,56	0
59	OHX	16SB	2217	7/7	0.90	0.10	95,102,111,201	0
58	MG	23SA	3075	1/1	0.90	0.31	61,61,61,61	0
59	OHX	23SB	3197	7/7	0.90	0.09	100,101,110,231	0
59	OHX	23SB	3198	7/7	0.90	0.08	107,108,121,238	0
59	OHX	23SA	3284	7/7	0.90	0.17	84,87,97,215	0
59	OHX	5SB	208	7/7	0.90	0.10	98,111,123,206	0
58	MG	23SA	3139	1/1	0.90	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	16SB	2293	1/1	0.90	0.22	48,48,48,48	0
59	OHX	16SB	2256	7/7	0.90	0.08	125,127,138,219	0
58	MG	23SB	3219	1/1	0.90	0.17	61,61,61,61	0
60	K	16SB	2374	1/1	0.90	0.07	94,94,94,94	0
58	MG	23SB	3389	1/1	0.90	0.09	54,54,54,54	0
59	OHX	16SB	2262	7/7	0.90	0.08	158,164,176,252	0
60	K	16SA	2381	1/1	0.90	0.09	109,109,109,109	0
59	OHX	23SA	3302	7/7	0.90	0.13	83,91,106,208	0
58	MG	23SA	3172	1/1	0.90	0.30	58,58,58,58	0
60	K	16SB	2386	1/1	0.90	0.08	94,94,94,94	0
58	MG	23SA	3016	1/1	0.90	0.12	59,59,59,59	0
58	MG	23SB	3420	1/1	0.90	0.12	62,62,62,62	0
59	OHX	23SA	3310	7/7	0.90	0.07	99,106,111,224	0
59	OHX	ASIB	103	7/7	0.90	0.08	124,130,147,238	0
58	MG	23SB	3431	1/1	0.90	0.08	113,113,113,113	0
58	MG	23SB	3264	1/1	0.90	0.08	55,55,55,55	0
59	OHX	23SB	3063	7/7	0.90	0.10	90,104,112,182	0
59	OHX	23SB	3095	7/7	0.90	0.09	94,97,104,213	0
59	OHX	23SB	3099	7/7	0.90	0.08	87,101,111,219	0
60	K	16SA	2402	1/1	0.90	0.18	89,89,89,89	0
59	OHX	23SA	3317	7/7	0.90	0.08	107,109,120,235	0
59	OHX	23SA	3318	7/7	0.90	0.09	138,157,165,234	0
59	OHX	23SB	3117	7/7	0.90	0.22	88,92,98,197	0
59	OHX	23SB	3118	7/7	0.90	0.08	114,118,121,225	0
60	K	16SA	2411	1/1	0.90	0.25	82,82,82,82	0
58	MG	16SA	2214	1/1	0.90	0.16	76,76,76,76	0
60	K	23SB	3446	1/1	0.90	0.13	85,85,85,85	0
60	K	23SB	3447	1/1	0.90	0.08	97,97,97,97	0
58	MG	5SB	214	1/1	0.90	0.31	56,56,56,56	0
60	K	23SB	3449	1/1	0.90	0.08	63,63,63,63	0
60	K	23SB	3454	1/1	0.90	0.08	74,74,74,74	0
60	K	16SA	2417	1/1	0.90	0.09	81,81,81,81	0
58	MG	16SB	2298	1/1	0.90	0.31	72,72,72,72	0
60	K	23SB	3468	1/1	0.90	0.06	97,97,97,97	0
59	OHX	23SA	3342	7/7	0.90	0.27	87,93,102,203	0
60	K	23SB	3473	1/1	0.90	0.11	108,108,108,108	0
59	OHX	23SB	3131	7/7	0.90	0.08	114,116,124,216	0
60	K	S13A	201	1/1	0.90	0.07	108,108,108,108	0
59	OHX	23SA	3343	7/7	0.90	0.10	93,117,131,217	0
60	K	PSIA	104	1/1	0.90	0.12	80,80,80,80	0
58	MG	23SB	3227	1/1	0.90	0.09	76,76,76,76	0
58	MG	23SA	3047	1/1	0.90	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	K	23SB	3487	1/1	0.90	0.06	65,65,65,65	0
59	OHX	23SB	3141	7/7	0.90	0.08	98,103,118,228	0
59	OHX	16SA	2281	7/7	0.90	0.09	106,115,123,199	0
58	MG	23SB	3312	1/1	0.90	0.18	41,41,41,41	0
58	MG	16SB	2319	1/1	0.90	0.33	57,57,57,57	0
58	MG	23SA	3162	1/1	0.90	0.25	62,62,62,62	0
59	OHX	16SA	2307	7/7	0.90	0.09	106,110,119,215	0
59	OHX	16SA	2310	7/7	0.90	0.10	109,114,122,197	0
59	OHX	23SA	3355	7/7	0.90	0.08	117,125,148,217	0
60	K	23SB	3507	1/1	0.90	0.10	72,72,72,72	0
60	K	23SB	3508	1/1	0.90	0.14	76,76,76,76	0
59	OHX	16SA	2314	7/7	0.90	0.08	119,126,128,235	0
60	K	23SA	3552	1/1	0.90	0.14	83,83,83,83	0
59	OHX	23SA	3360	7/7	0.90	0.10	90,94,110,208	0
58	MG	23SA	3112	1/1	0.90	0.06	60,60,60,60	0
60	K	23SB	3514	1/1	0.90	0.23	95,95,95,95	0
60	K	23SA	3556	1/1	0.90	0.07	60,60,60,60	0
60	K	23SB	3516	1/1	0.90	0.15	77,77,77,77	0
59	OHX	23SB	3168	7/7	0.90	0.10	123,133,154,222	0
60	K	23SB	3518	1/1	0.90	0.11	86,86,86,86	0
58	MG	23SB	3317	1/1	0.90	0.11	78,78,78,78	0
59	OHX	23SB	3171	7/7	0.90	0.09	129,131,134,212	0
60	K	23SA	3564	1/1	0.90	0.09	72,72,72,72	0
58	MG	23SB	3200	1/1	0.90	0.25	39,39,39,39	0
59	OHX	16SA	2323	7/7	0.90	0.08	162,167,181,233	0
59	OHX	23SA	3368	7/7	0.90	0.10	115,130,133,209	0
59	OHX	23SA	3348	7/7	0.91	0.09	138,148,158,224	0
59	OHX	16SB	2263	7/7	0.91	0.08	157,159,167,234	0
58	MG	23SB	3361	1/1	0.91	0.11	51,51,51,51	0
58	MG	16SA	2203	1/1	0.91	0.34	60,60,60,60	0
58	MG	23SA	3175	1/1	0.91	0.09	52,52,52,52	0
58	MG	23SB	3205	1/1	0.91	0.24	54,54,54,54	0
58	MG	16SB	2320	1/1	0.91	0.22	62,62,62,62	0
59	OHX	23SA	3221	7/7	0.91	0.10	73,86,105,162	0
59	OHX	PSIB	102	7/7	0.91	0.08	143,157,164,248	0
59	OHX	23SA	3356	7/7	0.91	0.08	111,129,143,223	0
59	OHX	23SA	3357	7/7	0.91	0.09	156,158,169,238	0
58	MG	23SB	3398	1/1	0.91	0.13	46,46,46,46	0
59	OHX	23SB	3087	7/7	0.91	0.17	86,94,99,175	0
59	OHX	23SB	3089	7/7	0.91	0.07	106,112,116,216	0
59	OHX	23SA	3359	7/7	0.91	0.08	128,136,163,233	0
58	MG	23SA	3123	1/1	0.91	0.12	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	23SA	3150	1/1	0.91	0.20	60,60,60,60	0
58	MG	16SA	2215	1/1	0.91	0.40	58,58,58,58	0
58	MG	23SA	3091	1/1	0.91	0.15	66,66,66,66	0
59	OHX	5SB	207	7/7	0.91	0.08	115,121,127,222	0
58	MG	16SB	2299	1/1	0.91	0.20	50,50,50,50	0
60	K	23SA	3568	1/1	0.91	0.05	58,58,58,58	0
59	OHX	23SA	3367	7/7	0.91	0.08	122,139,164,218	0
58	MG	L15A	202	1/1	0.91	0.16	59,59,59,59	0
58	MG	16SA	2231	1/1	0.91	0.20	57,57,57,57	0
58	MG	23SA	3044	1/1	0.91	0.12	65,65,65,65	0
60	K	23SA	3587	1/1	0.91	0.07	91,91,91,91	0
58	MG	23SA	3018	1/1	0.91	0.23	30,30,30,30	0
58	MG	23SB	3226	1/1	0.91	0.16	60,60,60,60	0
58	MG	23SA	3482	1/1	0.91	0.11	66,66,66,66	0
59	OHX	23SB	3136	7/7	0.91	0.09	97,102,117,216	0
59	OHX	23SB	3138	7/7	0.91	0.09	150,164,170,228	0
59	OHX	23SA	3377	7/7	0.91	0.08	145,154,161,239	0
60	K	23SB	3485	1/1	0.91	0.10	72,72,72,72	0
59	OHX	16SA	2286	7/7	0.91	0.24	75,88,94,169	0
58	MG	16SB	2339	1/1	0.91	0.06	124,124,124,124	0
58	MG	23SA	3111	1/1	0.91	0.17	56,56,56,56	0
58	MG	23SA	3096	1/1	0.91	0.09	70,70,70,70	0
58	MG	23SA	3033	1/1	0.91	0.18	74,74,74,74	0
59	OHX	23SB	3150	7/7	0.91	0.08	134,143,159,230	0
60	K	23SA	3631	1/1	0.91	0.10	78,78,78,78	0
60	K	23SB	3500	1/1	0.91	0.06	80,80,80,80	0
58	MG	16SB	2283	1/1	0.91	0.18	48,48,48,48	0
59	OHX	23SB	3153	7/7	0.91	0.08	123,135,155,235	0
60	K	23SB	3505	1/1	0.91	0.12	75,75,75,75	0
59	OHX	23SB	3155	7/7	0.91	0.08	136,149,154,230	0
58	MG	23SA	3084	1/1	0.91	0.05	64,64,64,64	0
59	OHX	23SA	3324	7/7	0.91	0.09	85,91,107,225	0
58	MG	23SA	3497	1/1	0.91	0.07	81,81,81,81	0
60	K	16SA	2406	1/1	0.91	0.07	87,87,87,87	0
59	OHX	16SB	2222	7/7	0.91	0.10	108,112,124,190	0
60	K	16SA	2409	1/1	0.91	0.11	81,81,81,81	0
59	OHX	16SB	2227	7/7	0.91	0.07	115,116,122,221	0
58	MG	23SB	3288	1/1	0.91	0.14	72,72,72,72	0
58	MG	23SA	3141	1/1	0.91	0.24	60,60,60,60	0
59	OHX	16SA	2319	7/7	0.91	0.07	131,143,148,232	0
58	MG	23SA	3073	1/1	0.91	0.11	42,42,42,42	0
58	MG	23SA	3087	1/1	0.91	0.19	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	K	16SB	2380	1/1	0.91	0.07	91,91,91,91	0
60	K	L4B	303	1/1	0.91	0.07	98,98,98,98	0
58	MG	23SA	3120	1/1	0.91	0.09	67,67,67,67	0
60	K	S6A	201	1/1	0.91	0.11	82,82,82,82	0
58	MG	23SB	3256	1/1	0.91	0.18	47,47,47,47	0
58	MG	23SB	3291	1/1	0.92	0.15	79,79,79,79	0
58	MG	23SB	3237	1/1	0.92	0.22	73,73,73,73	0
60	K	23SA	3614	1/1	0.92	0.10	65,65,65,65	0
58	MG	16SA	2244	1/1	0.92	0.29	62,62,62,62	0
59	OHX	16SB	2267	7/7	0.92	0.08	109,115,145,208	0
60	K	23SA	3626	1/1	0.92	0.06	69,69,69,69	0
58	MG	23SB	3429	1/1	0.92	0.16	93,93,93,93	0
58	MG	23SB	3294	1/1	0.92	0.08	55,55,55,55	0
59	OHX	5SB	206	7/7	0.92	0.08	120,123,129,223	0
58	MG	23SA	3384	1/1	0.92	0.11	43,43,43,43	0
59	OHX	23SA	3333	7/7	0.92	0.08	101,104,130,208	0
58	MG	23SA	3393	1/1	0.92	0.09	54,54,54,54	0
60	K	5SA	219	1/1	0.92	0.05	72,72,72,72	0
59	OHX	5SB	211	7/7	0.92	0.08	134,145,159,239	0
59	OHX	L20B	201	7/7	0.92	0.16	88,95,110,186	0
58	MG	16SA	2208	1/1	0.92	0.17	77,77,77,77	0
58	MG	L3B	301	1/1	0.92	0.18	40,40,40,40	0
58	MG	L3B	302	1/1	0.92	0.11	50,50,50,50	0
58	MG	23SB	3298	1/1	0.92	0.26	55,55,55,55	0
58	MG	23SB	3248	1/1	0.92	0.35	44,44,44,44	0
58	MG	23SA	3157	1/1	0.92	0.20	39,39,39,39	0
59	OHX	23SB	3093	7/7	0.92	0.08	93,100,110,208	0
58	MG	L35B	103	1/1	0.92	0.18	82,82,82,82	0
58	MG	23SB	3252	1/1	0.92	0.08	68,68,68,68	0
59	OHX	23SB	3104	7/7	0.92	0.08	111,116,130,225	0
58	MG	L27A	101	1/1	0.92	0.17	35,35,35,35	0
58	MG	23SA	3046	1/1	0.92	0.19	52,52,52,52	0
58	MG	23SA	3424	1/1	0.92	0.12	36,36,36,36	0
59	OHX	16SA	2295	7/7	0.92	0.08	97,101,119,212	0
59	OHX	16SA	2299	7/7	0.92	0.08	107,114,116,211	0
59	OHX	23SB	3120	7/7	0.92	0.07	94,104,115,226	0
60	K	16SB	2391	1/1	0.92	0.07	87,87,87,87	0
59	OHX	23SB	3121	7/7	0.92	0.08	95,102,110,221	0
58	MG	16SB	2310	1/1	0.92	0.39	75,75,75,75	0
60	K	16SB	2394	1/1	0.92	0.09	92,92,92,92	0
58	MG	16SA	2233	1/1	0.92	0.10	71,71,71,71	0
58	MG	L34A	101	1/1	0.92	0.23	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	OHX	23SB	3129	7/7	0.92	0.07	103,109,115,227	0
59	OHX	23SB	3130	7/7	0.92	0.08	106,117,124,209	0
59	OHX	16SA	2312	7/7	0.92	0.23	92,98,105,188	0
58	MG	23SA	3437	1/1	0.92	0.23	67,67,67,67	0
58	MG	23SB	3203	1/1	0.92	0.29	40,40,40,40	0
60	K	16SA	2412	1/1	0.92	0.14	92,92,92,92	0
58	MG	23SA	3011	1/1	0.92	0.19	42,42,42,42	0
58	MG	23SA	3461	1/1	0.92	0.11	44,44,44,44	0
59	OHX	23SB	3139	7/7	0.92	0.08	90,97,109,222	0
58	MG	23SA	3072	1/1	0.92	0.14	68,68,68,68	0
59	OHX	23SA	3364	7/7	0.92	0.08	96,103,122,203	0
59	OHX	23SB	3142	7/7	0.92	0.08	136,146,149,236	0
58	MG	16SA	2367	1/1	0.92	0.16	83,83,83,83	0
59	OHX	16SA	2324	7/7	0.92	0.08	131,145,160,226	0
58	MG	16SB	2286	1/1	0.92	0.17	77,77,77,77	0
58	MG	23SA	3164	1/1	0.92	0.29	61,61,61,61	0
58	MG	23SA	3165	1/1	0.92	0.29	62,62,62,62	0
58	MG	23SA	3031	1/1	0.92	0.12	58,58,58,58	0
58	MG	23SA	3167	1/1	0.92	0.20	77,77,77,77	0
60	K	23SB	3474	1/1	0.92	0.09	63,63,63,63	0
60	K	23SA	3541	1/1	0.92	0.09	102,102,102,102	0
58	MG	23SB	3275	1/1	0.92	0.23	65,65,65,65	0
59	OHX	16SA	2340	7/7	0.92	0.08	102,105,115,209	0
59	OHX	23SA	3378	7/7	0.92	0.23	81,87,102,184	0
58	MG	23SA	3077	1/1	0.92	0.19	48,48,48,48	0
59	OHX	23SB	3162	7/7	0.92	0.07	129,137,145,231	0
58	MG	23SB	3277	1/1	0.92	0.12	41,41,41,41	0
59	OHX	23SB	3164	7/7	0.92	0.08	124,135,157,228	0
58	MG	23SB	3278	1/1	0.92	0.16	45,45,45,45	0
59	OHX	5SA	206	7/7	0.92	0.15	91,97,113,184	0
59	OHX	23SA	3239	7/7	0.92	0.08	95,99,109,191	0
58	MG	23SA	3500	1/1	0.92	0.12	49,49,49,49	0
60	K	23SA	3555	1/1	0.92	0.17	71,71,71,71	0
58	MG	16SA	2374	1/1	0.92	0.14	73,73,73,73	0
60	K	23SA	3557	1/1	0.92	0.07	84,84,84,84	0
60	K	23SA	3559	1/1	0.92	0.20	82,82,82,82	0
58	MG	PSIA	101	1/1	0.92	0.30	54,54,54,54	0
59	OHX	L15A	201	7/7	0.92	0.19	84,91,102,193	0
59	OHX	L27A	103	7/7	0.92	0.08	108,119,145,199	0
58	MG	23SB	3282	1/1	0.92	0.23	64,64,64,64	0
58	MG	16SA	2216	1/1	0.92	0.28	46,46,46,46	0
58	MG	23SA	3061	1/1	0.92	0.09	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	16SB	2331	1/1	0.92	0.30	55,55,55,55	0
59	OHX	23SB	3182	7/7	0.92	0.08	190,192,204,241	0
59	OHX	16SB	2228	7/7	0.92	0.08	99,100,112,192	0
59	OHX	23SB	3184	7/7	0.92	0.08	116,132,141,221	0
59	OHX	16SB	2244	7/7	0.92	0.07	99,108,114,225	0
58	MG	23SB	3378	1/1	0.92	0.09	70,70,70,70	0
58	MG	23SB	3381	1/1	0.92	0.11	49,49,49,49	0
58	MG	23SB	3384	1/1	0.92	0.09	70,70,70,70	0
58	MG	16SA	2212	1/1	0.92	0.17	55,55,55,55	0
58	MG	23SA	3064	1/1	0.92	0.18	55,55,55,55	0
58	MG	23SB	3396	1/1	0.92	0.08	55,55,55,55	0
60	K	23SA	3603	1/1	0.92	0.09	83,83,83,83	0
60	K	23SA	3604	1/1	0.92	0.08	58,58,58,58	0
58	MG	23SB	3289	1/1	0.92	0.18	72,72,72,72	0
58	MG	23SA	3032	1/1	0.93	0.16	49,49,49,49	0
58	MG	16SB	2305	1/1	0.93	0.27	67,67,67,67	0
59	OHX	23SB	3167	7/7	0.93	0.08	121,136,143,203	0
59	OHX	S4A	301	7/7	0.93	0.09	118,122,140,210	0
58	MG	16SB	2348	1/1	0.93	0.08	56,56,56,56	0
58	MG	23SB	3241	1/1	0.93	0.13	50,50,50,50	0
60	K	23SA	3593	1/1	0.93	0.05	69,69,69,69	0
58	MG	16SB	2354	1/1	0.93	0.06	102,102,102,102	0
59	OHX	23SB	3173	7/7	0.93	0.07	97,115,128,200	0
59	OHX	23SA	3224	7/7	0.93	0.17	86,94,104,168	0
58	MG	23SB	3386	1/1	0.93	0.07	91,91,91,91	0
60	K	23SA	3601	1/1	0.93	0.08	55,55,55,55	0
58	MG	23SA	3467	1/1	0.93	0.08	41,41,41,41	0
59	OHX	5SA	212	7/7	0.93	0.07	89,95,109,210	0
58	MG	23SB	3246	1/1	0.93	0.34	57,57,57,57	0
60	K	23SA	3610	1/1	0.93	0.07	62,62,62,62	0
58	MG	23SB	3391	1/1	0.93	0.07	71,71,71,71	0
59	OHX	23SA	3261	7/7	0.93	0.18	78,81,93,181	0
59	OHX	23SA	3262	7/7	0.93	0.17	81,85,101,178	0
59	OHX	23SA	3266	7/7	0.93	0.23	81,85,97,177	0
60	K	23SA	3618	1/1	0.93	0.05	62,62,62,62	0
60	K	23SA	3620	1/1	0.93	0.08	70,70,70,70	0
60	K	23SA	3623	1/1	0.93	0.06	80,80,80,80	0
59	OHX	23SA	3270	7/7	0.93	0.08	109,117,127,194	0
58	MG	23SB	3393	1/1	0.93	0.08	70,70,70,70	0
60	K	23SA	3627	1/1	0.93	0.06	67,67,67,67	0
58	MG	23SA	3472	1/1	0.93	0.13	39,39,39,39	0
58	MG	23SA	3149	1/1	0.93	0.25	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	OHX	16SB	2234	7/7	0.93	0.07	117,118,120,196	0
59	OHX	16SB	2242	7/7	0.93	0.09	140,145,168,211	0
59	OHX	23SA	3285	7/7	0.93	0.07	90,99,105,205	0
58	MG	23SB	3251	1/1	0.93	0.29	54,54,54,54	0
60	K	23SA	3639	1/1	0.93	0.07	80,80,80,80	0
58	MG	L35A	101	1/1	0.93	0.15	51,51,51,51	0
59	OHX	23SA	3293	7/7	0.93	0.20	70,76,97,195	0
59	OHX	16SB	2252	7/7	0.93	0.08	109,120,138,208	0
58	MG	23SA	3114	1/1	0.93	0.09	55,55,55,55	0
58	MG	23SB	3428	1/1	0.93	0.08	84,84,84,84	0
59	OHX	23SA	3301	7/7	0.93	0.07	121,123,127,230	0
59	OHX	16SB	2259	7/7	0.93	0.07	145,150,156,224	0
59	OHX	5SB	205	7/7	0.93	0.07	120,123,130,211	0
58	MG	16SA	2253	1/1	0.93	0.28	50,50,50,50	0
58	MG	23SA	3487	1/1	0.93	0.11	40,40,40,40	0
59	OHX	23SA	3306	7/7	0.93	0.07	100,113,126,199	0
59	OHX	5SB	209	7/7	0.93	0.08	121,127,134,216	0
58	MG	23SB	3437	1/1	0.93	0.29	86,86,86,86	0
58	MG	16SA	2256	1/1	0.93	0.14	72,72,72,72	0
59	OHX	16SB	2268	7/7	0.93	0.07	123,133,154,220	0
60	K	16SA	2375	1/1	0.93	0.07	101,101,101,101	0
59	OHX	16SB	2271	7/7	0.93	0.07	156,167,170,247	0
59	OHX	23SA	3309	7/7	0.93	0.14	85,88,102,183	0
58	MG	23SA	3173	1/1	0.93	0.07	59,59,59,59	0
58	MG	16SB	2285	1/1	0.93	0.13	65,65,65,65	0
59	OHX	16SB	2276	7/7	0.93	0.07	131,137,146,224	0
58	MG	23SB	3306	1/1	0.93	0.16	65,65,65,65	0
59	OHX	23SA	3314	7/7	0.93	0.07	95,99,111,204	0
58	MG	16SA	2363	1/1	0.93	0.07	72,72,72,72	0
58	MG	23SA	3138	1/1	0.93	0.09	46,46,46,46	0
59	OHX	23SA	3319	7/7	0.93	0.19	82,85,93,207	0
59	OHX	23SB	3051	7/7	0.93	0.15	94,102,104,171	0
59	OHX	23SB	3052	7/7	0.93	0.21	91,95,101,175	0
59	OHX	23SA	3320	7/7	0.93	0.07	94,95,109,191	0
59	OHX	23SB	3067	7/7	0.93	0.09	79,95,108,174	0
59	OHX	23SA	3323	7/7	0.93	0.12	84,89,105,197	0
60	K	23SB	3440	1/1	0.93	0.07	94,94,94,94	0
58	MG	23SB	3206	1/1	0.93	0.24	34,34,34,34	0
59	OHX	23SA	3331	7/7	0.93	0.07	91,98,108,201	0
58	MG	23SA	3054	1/1	0.93	0.24	51,51,51,51	0
59	OHX	23SA	3334	7/7	0.93	0.07	99,115,137,214	0
58	MG	23SA	3505	1/1	0.93	0.11	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	OHX	23SA	3337	7/7	0.93	0.07	109,123,134,204	0
59	OHX	23SB	3111	7/7	0.93	0.08	103,108,114,205	0
59	OHX	23SB	3112	7/7	0.93	0.07	104,112,119,206	0
59	OHX	23SB	3113	7/7	0.93	0.07	112,115,125,216	0
60	K	23SB	3465	1/1	0.93	0.13	75,75,75,75	0
59	OHX	23SA	3338	7/7	0.93	0.07	138,150,158,232	0
58	MG	23SA	3003	1/1	0.93	0.15	60,60,60,60	0
60	K	23SB	3470	1/1	0.93	0.14	78,78,78,78	0
60	K	16SA	2414	1/1	0.93	0.07	100,100,100,100	0
59	OHX	23SA	3340	7/7	0.93	0.08	133,146,163,217	0
58	MG	23SA	3160	1/1	0.93	0.15	55,55,55,55	0
58	MG	23SB	3266	1/1	0.93	0.17	38,38,38,38	0
58	MG	23SB	3213	1/1	0.93	0.16	40,40,40,40	0
59	OHX	23SA	3344	7/7	0.93	0.07	95,121,141,216	0
59	OHX	23SB	3124	7/7	0.93	0.08	83,94,106,213	0
58	MG	23SB	3214	1/1	0.93	0.20	48,48,48,48	0
59	OHX	16SA	2296	7/7	0.93	0.08	87,99,108,193	0
58	MG	23SB	3269	1/1	0.93	0.26	50,50,50,50	0
60	K	23SB	3486	1/1	0.93	0.09	73,73,73,73	0
58	MG	23SB	3270	1/1	0.93	0.22	43,43,43,43	0
60	K	23SB	3488	1/1	0.93	0.08	85,85,85,85	0
60	K	23SB	3489	1/1	0.93	0.05	65,65,65,65	0
59	OHX	16SA	2304	7/7	0.93	0.20	88,96,98,193	0
59	OHX	16SA	2306	7/7	0.93	0.08	109,111,118,204	0
58	MG	23SA	3040	1/1	0.93	0.21	55,55,55,55	0
59	OHX	16SA	2309	7/7	0.93	0.08	132,139,149,214	0
58	MG	23SA	3411	1/1	0.93	0.11	43,43,43,43	0
60	K	23SA	3543	1/1	0.93	0.10	86,86,86,86	0
58	MG	23SA	3122	1/1	0.93	0.10	57,57,57,57	0
58	MG	23SA	3082	1/1	0.93	0.16	50,50,50,50	0
58	MG	23SB	3325	1/1	0.93	0.16	47,47,47,47	0
60	K	23SB	3504	1/1	0.93	0.09	87,87,87,87	0
58	MG	23SA	3027	1/1	0.93	0.14	45,45,45,45	0
58	MG	16SB	2297	1/1	0.93	0.30	64,64,64,64	0
58	MG	23SA	3145	1/1	0.93	0.07	70,70,70,70	0
59	OHX	23SB	3145	7/7	0.93	0.08	106,124,142,220	0
59	OHX	16SA	2321	7/7	0.93	0.07	157,159,162,233	0
59	OHX	16SA	2322	7/7	0.93	0.07	118,126,134,205	0
58	MG	23SA	3146	1/1	0.93	0.23	48,48,48,48	0
58	MG	23SB	3333	1/1	0.93	0.10	42,42,42,42	0
59	OHX	23SB	3152	7/7	0.93	0.08	103,105,129,194	0
58	MG	23SA	3443	1/1	0.93	0.16	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	16SA	2228	1/1	0.93	0.29	64,64,64,64	0
59	OHX	23SB	3156	7/7	0.93	0.06	125,130,147,212	0
59	OHX	16SA	2327	7/7	0.93	0.07	134,143,149,217	0
59	OHX	23SB	3158	7/7	0.93	0.08	105,107,121,203	0
58	MG	16SB	2336	1/1	0.93	0.08	105,105,105,105	0
59	OHX	16SA	2331	7/7	0.93	0.07	155,162,169,236	0
58	MG	23SA	3452	1/1	0.93	0.11	40,40,40,40	0
60	K	23SA	3578	1/1	0.93	0.05	54,54,54,54	0
58	MG	23SB	3364	1/1	0.93	0.09	65,65,65,65	0
61	SJE	23SB	3521	87/87	0.93	0.14	48,59,87,95	0
59	OHX	23SA	3259	7/7	0.94	0.07	90,96,110,189	0
59	OHX	23SA	3260	7/7	0.94	0.19	71,90,98,175	0
60	K	23SA	3589	1/1	0.94	0.09	85,85,85,85	0
58	MG	23SA	3465	1/1	0.94	0.09	53,53,53,53	0
58	MG	23SB	3434	1/1	0.94	0.06	96,96,96,96	0
58	MG	23SB	3436	1/1	0.94	0.10	94,94,94,94	0
59	OHX	23SB	3166	7/7	0.94	0.08	91,100,114,205	0
59	OHX	23SA	3267	7/7	0.94	0.18	91,99,103,186	0
59	OHX	23SA	3269	7/7	0.94	0.22	86,89,103,177	0
58	MG	23SB	3313	1/1	0.94	0.05	48,48,48,48	0
58	MG	23SB	3439	1/1	0.94	0.08	87,87,87,87	0
58	MG	16SB	2341	1/1	0.94	0.07	130,130,130,130	0
59	OHX	23SA	3275	7/7	0.94	0.07	100,110,119,213	0
60	K	23SA	3606	1/1	0.94	0.05	57,57,57,57	0
59	OHX	23SA	3277	7/7	0.94	0.19	76,84,101,204	0
60	K	23SA	3609	1/1	0.94	0.06	71,71,71,71	0
59	OHX	23SB	3175	7/7	0.94	0.07	138,142,159,216	0
59	OHX	23SA	3278	7/7	0.94	0.07	85,98,101,210	0
60	K	23SA	3612	1/1	0.94	0.04	73,73,73,73	0
58	MG	16SA	2210	1/1	0.94	0.15	46,46,46,46	0
59	OHX	16SB	2233	7/7	0.94	0.07	93,102,105,189	0
58	MG	23SB	3231	1/1	0.94	0.12	51,51,51,51	0
59	OHX	16SB	2236	7/7	0.94	0.07	104,107,118,194	0
60	K	23SA	3619	1/1	0.94	0.04	81,81,81,81	0
59	OHX	16SB	2238	7/7	0.94	0.06	124,131,141,228	0
60	K	23SA	3622	1/1	0.94	0.07	61,61,61,61	0
59	OHX	16SB	2239	7/7	0.94	0.07	116,122,133,205	0
58	MG	23SA	3009	1/1	0.94	0.22	40,40,40,40	0
58	MG	23SA	3477	1/1	0.94	0.12	90,90,90,90	0
59	OHX	23SA	3292	7/7	0.94	0.11	68,81,98,170	0
60	K	23SA	3628	1/1	0.94	0.15	83,83,83,83	0
59	OHX	16SB	2247	7/7	0.94	0.08	100,103,110,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	OHX	23SB	3187	7/7	0.94	0.06	134,143,152,229	0
58	MG	23SA	3478	1/1	0.94	0.08	50,50,50,50	0
58	MG	23SA	3010	1/1	0.94	0.17	39,39,39,39	0
58	MG	23SA	3043	1/1	0.94	0.18	57,57,57,57	0
59	OHX	23SA	3299	7/7	0.94	0.11	69,80,102,183	0
59	OHX	23SA	3300	7/7	0.94	0.06	99,105,112,220	0
58	MG	16SA	2353	1/1	0.94	0.05	138,138,138,138	0
59	OHX	16SA	2271	7/7	0.94	0.10	80,94,97,147	0
59	OHX	16SA	2274	7/7	0.94	0.14	93,97,105,164	0
59	OHX	16SA	2279	7/7	0.94	0.08	118,121,129,197	0
58	MG	23SA	3024	1/1	0.94	0.14	45,45,45,45	0
58	MG	23SB	3243	1/1	0.94	0.23	30,30,30,30	0
59	OHX	16SB	2266	7/7	0.94	0.07	135,142,152,217	0
59	OHX	5SB	204	7/7	0.94	0.07	98,106,120,191	0
59	OHX	16SA	2288	7/7	0.94	0.07	90,100,106,201	0
58	MG	23SA	3012	1/1	0.94	0.06	91,91,91,91	0
60	K	16SB	2376	1/1	0.94	0.05	75,75,75,75	0
60	K	16SB	2377	1/1	0.94	0.06	82,82,82,82	0
59	OHX	16SB	2270	7/7	0.94	0.08	116,127,150,209	0
58	MG	23SA	3151	1/1	0.94	0.12	59,59,59,59	0
59	OHX	16SA	2293	7/7	0.94	0.09	92,98,111,198	0
58	MG	23SA	3085	1/1	0.94	0.15	52,52,52,52	0
59	OHX	16SB	2274	7/7	0.94	0.07	131,136,142,211	0
59	OHX	23SA	3315	7/7	0.94	0.07	98,100,118,232	0
58	MG	23SB	3330	1/1	0.94	0.26	54,54,54,54	0
59	OHX	16SA	2297	7/7	0.94	0.07	114,122,131,209	0
59	OHX	16SB	2278	7/7	0.94	0.07	112,116,120,223	0
59	OHX	16SA	2298	7/7	0.94	0.19	80,87,106,181	0
58	MG	23SA	3107	1/1	0.94	0.18	37,37,37,37	0
58	MG	23SB	3287	1/1	0.94	0.15	61,61,61,61	0
59	OHX	16SA	2301	7/7	0.94	0.07	107,112,121,213	0
59	OHX	23SA	3325	7/7	0.94	0.06	89,95,103,220	0
59	OHX	23SA	3327	7/7	0.94	0.07	88,96,114,211	0
59	OHX	23SB	3054	7/7	0.94	0.18	89,95,100,168	0
59	OHX	23SB	3058	7/7	0.94	0.15	80,87,94,165	0
59	OHX	23SB	3059	7/7	0.94	0.12	91,101,107,175	0
58	MG	23SB	3335	1/1	0.94	0.08	51,51,51,51	0
60	K	16SA	2388	1/1	0.94	0.26	79,79,79,79	0
59	OHX	16SA	2305	7/7	0.94	0.07	133,141,150,228	0
59	OHX	23SB	3074	7/7	0.94	0.21	82,94,96,173	0
59	OHX	23SB	3079	7/7	0.94	0.12	94,98,106,173	0
59	OHX	23SB	3081	7/7	0.94	0.07	100,106,119,201	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	K	23SB	3443	1/1	0.94	0.14	110,110,110,110	0
58	MG	23SB	3249	1/1	0.94	0.14	56,56,56,56	0
60	K	16SA	2401	1/1	0.94	0.08	63,63,63,63	0
58	MG	16SA	2359	1/1	0.94	0.11	62,62,62,62	0
58	MG	23SB	3349	1/1	0.94	0.08	71,71,71,71	0
58	MG	23SB	3356	1/1	0.94	0.08	39,39,39,39	0
60	K	23SB	3450	1/1	0.94	0.07	72,72,72,72	0
60	K	23SB	3451	1/1	0.94	0.06	67,67,67,67	0
58	MG	23SA	3132	1/1	0.94	0.05	57,57,57,57	0
59	OHX	23SB	3103	7/7	0.94	0.18	67,90,98,176	0
60	K	16SA	2407	1/1	0.94	0.05	75,75,75,75	0
59	OHX	16SA	2313	7/7	0.94	0.07	110,116,122,207	0
59	OHX	23SB	3105	7/7	0.94	0.17	88,96,107,174	0
59	OHX	23SB	3107	7/7	0.94	0.07	102,114,119,205	0
58	MG	23SA	3513	1/1	0.94	0.08	84,84,84,84	0
60	K	23SB	3472	1/1	0.94	0.17	77,77,77,77	0
58	MG	23SA	3133	1/1	0.94	0.11	48,48,48,48	0
58	MG	23SB	3254	1/1	0.94	0.27	46,46,46,46	0
59	OHX	16SA	2317	7/7	0.94	0.09	112,120,138,202	0
58	MG	23SB	3369	1/1	0.94	0.07	46,46,46,46	0
58	MG	23SA	3420	1/1	0.94	0.09	57,57,57,57	0
58	MG	23SB	3373	1/1	0.94	0.08	48,48,48,48	0
58	MG	23SA	3134	1/1	0.94	0.11	74,74,74,74	0
58	MG	16SA	2360	1/1	0.94	0.10	72,72,72,72	0
58	MG	23SB	3383	1/1	0.94	0.07	77,77,77,77	0
59	OHX	23SA	3351	7/7	0.94	0.07	116,125,140,218	0
58	MG	23SA	3050	1/1	0.94	0.17	58,58,58,58	0
58	MG	23SB	3385	1/1	0.94	0.07	82,82,82,82	0
58	MG	16SA	2251	1/1	0.94	0.28	60,60,60,60	0
58	MG	23SA	3053	1/1	0.94	0.18	33,33,33,33	0
59	OHX	16SA	2330	7/7	0.94	0.07	153,156,163,230	0
58	MG	5SA	216	1/1	0.94	0.08	67,67,67,67	0
58	MG	23SB	3390	1/1	0.94	0.10	44,44,44,44	0
58	MG	23SB	3302	1/1	0.94	0.17	49,49,49,49	0
58	MG	23SB	3215	1/1	0.94	0.19	37,37,37,37	0
58	MG	23SB	3216	1/1	0.94	0.11	42,42,42,42	0
59	OHX	16SA	2341	7/7	0.94	0.07	135,136,149,239	0
58	MG	16SA	2217	1/1	0.94	0.14	40,40,40,40	0
59	OHX	S10A	201	7/7	0.94	0.08	106,108,115,206	0
58	MG	23SA	3093	1/1	0.94	0.06	77,77,77,77	0
59	OHX	23SA	3366	7/7	0.94	0.07	99,105,125,207	0
58	MG	23SB	3407	1/1	0.94	0.10	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	OHX	23SA	3195	7/7	0.94	0.11	71,86,93,123	0
59	OHX	23SB	3146	7/7	0.94	0.07	98,108,114,209	0
59	OHX	23SA	3212	7/7	0.94	0.11	51,57,86,140	0
58	MG	23SB	3417	1/1	0.94	0.06	84,84,84,84	0
60	K	23SA	3558	1/1	0.94	0.10	55,55,55,55	0
58	MG	16SB	2300	1/1	0.94	0.31	48,48,48,48	0
59	OHX	23SA	3372	7/7	0.94	0.08	103,116,140,217	0
58	MG	16SA	2368	1/1	0.94	0.06	91,91,91,91	0
58	MG	23SA	3056	1/1	0.94	0.14	48,48,48,48	0
59	OHX	23SB	3154	7/7	0.94	0.09	165,172,176,225	0
59	OHX	23SA	3376	7/7	0.94	0.08	121,128,151,229	0
59	OHX	23SA	3255	7/7	0.94	0.08	131,151,160,208	0
59	OHX	23SA	3256	7/7	0.94	0.21	72,85,91,147	0
60	K	23SA	3580	1/1	0.94	0.11	39,39,39,39	0
58	MG	16SB	2303	1/1	0.94	0.17	61,61,61,61	0
58	MG	23SB	3430	1/1	0.94	0.09	70,70,70,70	0
59	OHX	23SB	3160	7/7	0.94	0.07	120,142,146,214	0
59	OHX	16SA	2276	7/7	0.95	0.12	93,96,108,169	0
58	MG	23SA	3504	1/1	0.95	0.06	67,67,67,67	0
59	OHX	16SA	2280	7/7	0.95	0.07	100,102,112,186	0
59	OHX	23SA	3226	7/7	0.95	0.18	71,76,95,148	0
59	OHX	23SA	3227	7/7	0.95	0.17	77,84,88,170	0
59	OHX	S4B	301	7/7	0.95	0.08	116,119,128,186	0
59	OHX	ASIB	102	7/7	0.95	0.07	152,174,187,224	0
59	OHX	23SA	3231	7/7	0.95	0.16	79,87,94,150	0
59	OHX	23SA	3233	7/7	0.95	0.11	83,89,99,153	0
59	OHX	23SA	3236	7/7	0.95	0.18	76,86,90,178	0
59	OHX	23SB	3032	7/7	0.95	0.11	86,101,105,158	0
58	MG	PSIA	103	1/1	0.95	0.08	83,83,83,83	0
59	OHX	23SB	3036	7/7	0.95	0.08	113,117,131,172	0
59	OHX	23SB	3041	7/7	0.95	0.14	82,86,98,151	0
59	OHX	23SB	3050	7/7	0.95	0.17	74,79,98,166	0
59	OHX	5SB	203	7/7	0.95	0.07	102,107,119,182	0
59	OHX	23SA	3241	7/7	0.95	0.15	65,85,97,158	0
60	K	23SA	3629	1/1	0.95	0.06	65,65,65,65	0
59	OHX	23SA	3247	7/7	0.95	0.18	85,87,97,160	0
59	OHX	16SA	2283	7/7	0.95	0.06	101,107,114,179	0
60	K	23SA	3633	1/1	0.95	0.15	77,77,77,77	0
59	OHX	23SA	3254	7/7	0.95	0.14	74,86,94,175	0
59	OHX	16SA	2284	7/7	0.95	0.07	132,148,162,222	0
59	OHX	23SB	3061	7/7	0.95	0.07	100,105,115,190	0
59	OHX	23SB	3062	7/7	0.95	0.06	100,103,111,185	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	23SA	3511	1/1	0.95	0.05	36,36,36,36	0
59	OHX	23SB	3066	7/7	0.95	0.08	94,102,114,188	0
59	OHX	L35B	101	7/7	0.95	0.09	120,126,131,191	0
60	K	L4A	304	1/1	0.95	0.07	77,77,77,77	0
58	MG	23SB	3370	1/1	0.95	0.09	49,49,49,49	0
59	OHX	23SB	3073	7/7	0.95	0.07	89,100,113,186	0
59	OHX	16SA	2289	7/7	0.95	0.11	89,94,104,178	0
59	OHX	23SB	3075	7/7	0.95	0.13	84,93,98,173	0
59	OHX	23SB	3076	7/7	0.95	0.06	109,111,118,213	0
60	K	16SB	2368	1/1	0.95	0.04	103,103,103,103	0
60	K	16SB	2369	1/1	0.95	0.15	82,82,82,82	0
58	MG	23SA	3512	1/1	0.95	0.13	45,45,45,45	0
58	MG	23SA	3434	1/1	0.95	0.12	102,102,102,102	0
58	MG	23SB	3377	1/1	0.95	0.08	47,47,47,47	0
59	OHX	23SB	3088	7/7	0.95	0.08	110,117,123,193	0
59	OHX	16SA	2294	7/7	0.95	0.07	89,94,99,207	0
59	OHX	23SB	3092	7/7	0.95	0.16	78,84,94,180	0
58	MG	23SA	3515	1/1	0.95	0.06	101,101,101,101	0
58	MG	23SA	3001	1/1	0.95	0.30	34,34,34,34	0
59	OHX	23SA	3268	7/7	0.95	0.18	80,89,92,148	0
59	OHX	23SB	3102	7/7	0.95	0.06	108,115,119,215	0
58	MG	23SA	3519	1/1	0.95	0.08	94,94,94,94	0
58	MG	23SA	3523	1/1	0.95	0.09	70,70,70,70	0
58	MG	23SA	3155	1/1	0.95	0.18	55,55,55,55	0
60	K	16SB	2389	1/1	0.95	0.04	82,82,82,82	0
59	OHX	23SB	3106	7/7	0.95	0.08	100,119,134,193	0
59	OHX	23SA	3273	7/7	0.95	0.16	85,96,99,180	0
58	MG	23SA	3528	1/1	0.95	0.07	42,42,42,42	0
58	MG	23SA	3529	1/1	0.95	0.09	42,42,42,42	0
59	OHX	16SA	2303	7/7	0.95	0.06	117,118,127,222	0
59	OHX	23SA	3375	7/7	0.95	0.06	102,110,125,192	0
58	MG	16SB	2329	1/1	0.95	0.11	63,63,63,63	0
59	OHX	23SB	3116	7/7	0.95	0.07	126,131,140,206	0
59	OHX	23SA	3280	7/7	0.95	0.06	90,100,112,211	0
58	MG	23SA	3531	1/1	0.95	0.11	69,69,69,69	0
59	OHX	23SA	3379	7/7	0.95	0.06	102,114,136,186	0
58	MG	23SA	3022	1/1	0.95	0.22	40,40,40,40	0
60	K	16SA	2413	1/1	0.95	0.07	84,84,84,84	0
58	MG	23SA	3535	1/1	0.95	0.14	59,59,59,59	0
59	OHX	16SA	2308	7/7	0.95	0.06	110,118,129,200	0
59	OHX	23SB	3123	7/7	0.95	0.06	105,108,120,206	0
59	OHX	23SA	3291	7/7	0.95	0.07	126,133,145,190	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	K	23SB	3444	1/1	0.95	0.07	84,84,84,84	0
58	MG	16SA	2355	1/1	0.95	0.09	51,51,51,51	0
58	MG	23SA	3174	1/1	0.95	0.11	53,53,53,53	0
59	OHX	16SA	2311	7/7	0.95	0.07	102,108,117,196	0
58	MG	23SB	3271	1/1	0.95	0.21	46,46,46,46	0
58	MG	23SB	3228	1/1	0.95	0.28	43,43,43,43	0
58	MG	23SB	3408	1/1	0.95	0.14	51,51,51,51	0
59	OHX	L20A	201	7/7	0.95	0.10	80,91,102,185	0
60	K	23SB	3452	1/1	0.95	0.08	84,84,84,84	0
59	OHX	L27A	102	7/7	0.95	0.18	86,89,102,190	0
60	K	23SB	3458	1/1	0.95	0.07	72,72,72,72	0
60	K	23SB	3461	1/1	0.95	0.06	67,67,67,67	0
58	MG	23SA	3125	1/1	0.95	0.14	62,62,62,62	0
60	K	23SB	3463	1/1	0.95	0.05	83,83,83,83	0
60	K	23SB	3464	1/1	0.95	0.07	53,53,53,53	0
58	MG	23SA	3126	1/1	0.95	0.09	62,62,62,62	0
60	K	23SB	3466	1/1	0.95	0.07	68,68,68,68	0
59	OHX	L35A	102	7/7	0.95	0.09	94,106,113,166	0
59	OHX	16SB	2215	7/7	0.95	0.10	92,100,110,164	0
60	K	23SB	3469	1/1	0.95	0.07	64,64,64,64	0
59	OHX	16SB	2216	7/7	0.95	0.12	98,101,113,179	0
58	MG	16SA	2357	1/1	0.95	0.07	63,63,63,63	0
59	OHX	16SB	2218	7/7	0.95	0.12	95,98,107,169	0
59	OHX	16SB	2220	7/7	0.95	0.07	98,104,110,191	0
58	MG	23SB	3422	1/1	0.95	0.07	72,72,72,72	0
59	OHX	16SB	2224	7/7	0.95	0.06	97,105,114,200	0
58	MG	23SB	3424	1/1	0.95	0.09	71,71,71,71	0
59	OHX	16SA	2320	7/7	0.95	0.08	99,106,126,191	0
59	OHX	16SB	2229	7/7	0.95	0.06	111,112,116,211	0
58	MG	23SB	3233	1/1	0.95	0.21	41,41,41,41	0
58	MG	16SA	2207	1/1	0.95	0.17	42,42,42,42	0
59	OHX	16SB	2235	7/7	0.95	0.06	105,111,120,212	0
58	MG	23SA	3391	1/1	0.95	0.10	37,37,37,37	0
58	MG	16SB	2351	1/1	0.95	0.07	68,68,68,68	0
58	MG	23SB	3238	1/1	0.95	0.17	46,46,46,46	0
58	MG	23SA	3479	1/1	0.95	0.11	76,76,76,76	0
59	OHX	23SA	3316	7/7	0.95	0.06	90,97,113,204	0
58	MG	16SB	2358	1/1	0.95	0.06	105,105,105,105	0
58	MG	23SA	3392	1/1	0.95	0.08	52,52,52,52	0
59	OHX	16SA	2329	7/7	0.95	0.06	144,149,154,226	0
60	K	23SB	3495	1/1	0.95	0.05	73,73,73,73	0
60	K	23SB	3496	1/1	0.95	0.08	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	K	23SA	3565	1/1	0.95	0.07	46,46,46,46	0
58	MG	16SA	2369	1/1	0.95	0.05	120,120,120,120	0
60	K	23SA	3570	1/1	0.95	0.07	51,51,51,51	0
59	OHX	16SB	2251	7/7	0.95	0.07	125,131,136,216	0
58	MG	16SA	2371	1/1	0.95	0.05	100,100,100,100	0
60	K	23SB	3503	1/1	0.95	0.12	72,72,72,72	0
60	K	23SA	3579	1/1	0.95	0.04	60,60,60,60	0
58	MG	23SA	3486	1/1	0.95	0.08	42,42,42,42	0
59	OHX	16SB	2254	7/7	0.95	0.07	100,105,128,186	0
58	MG	16SA	2202	1/1	0.95	0.20	57,57,57,57	0
59	OHX	23SA	3326	7/7	0.95	0.07	138,143,162,229	0
60	K	23SB	3510	1/1	0.95	0.04	75,75,75,75	0
58	MG	23SA	3414	1/1	0.95	0.06	50,50,50,50	0
59	OHX	16SB	2260	7/7	0.95	0.07	145,153,160,239	0
59	OHX	16SA	2336	7/7	0.95	0.07	106,114,119,210	0
59	OHX	16SA	2337	7/7	0.95	0.07	197,199,204,249	0
59	OHX	16SA	2339	7/7	0.95	0.08	93,98,102,201	0
58	MG	23SA	3076	1/1	0.95	0.18	57,57,57,57	0
59	OHX	16SB	2265	7/7	0.95	0.07	110,127,139,201	0
58	MG	23SA	3048	1/1	0.95	0.14	33,33,33,33	0
58	MG	16SB	2280	1/1	0.95	0.11	59,59,59,59	0
58	MG	L35B	102	1/1	0.95	0.11	91,91,91,91	0
58	MG	23SB	3357	1/1	0.95	0.10	65,65,65,65	0
60	K	23SA	3602	1/1	0.95	0.06	67,67,67,67	0
59	OHX	MRNA	101	7/7	0.95	0.07	109,113,121,212	0
58	MG	23SA	3135	1/1	0.95	0.11	55,55,55,55	0
60	K	23SA	3605	1/1	0.95	0.05	74,74,74,74	0
58	MG	16SA	2362	1/1	0.95	0.12	93,93,93,93	0
59	OHX	16SA	2334	7/7	0.96	0.06	161,169,178,239	0
58	MG	23SB	3274	1/1	0.96	0.31	57,57,57,57	0
58	MG	23SA	3442	1/1	0.96	0.06	48,48,48,48	0
59	OHX	23SA	3321	7/7	0.96	0.13	77,81,92,196	0
59	OHX	23SA	3322	7/7	0.96	0.06	88,102,106,193	0
59	OHX	16SB	2255	7/7	0.96	0.06	133,135,154,207	0
58	MG	23SB	3326	1/1	0.96	0.08	58,58,58,58	0
59	OHX	23SB	3169	7/7	0.96	0.06	104,124,127,192	0
59	OHX	16SA	2338	7/7	0.96	0.07	96,105,108,199	0
58	MG	16SA	2366	1/1	0.96	0.06	107,107,107,107	0
58	MG	23SB	3229	1/1	0.96	0.29	44,44,44,44	0
58	MG	23SA	3526	1/1	0.96	0.12	76,76,76,76	0
59	OHX	23SA	3328	7/7	0.96	0.12	93,96,104,189	0
59	OHX	23SA	3329	7/7	0.96	0.14	90,93,105,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	23SA	3070	1/1	0.96	0.25	58,58,58,58	0
59	OHX	23SA	3332	7/7	0.96	0.06	98,103,115,190	0
58	MG	23SB	3331	1/1	0.96	0.19	58,58,58,58	0
58	MG	23SA	3129	1/1	0.96	0.06	54,54,54,54	0
59	OHX	23SA	3335	7/7	0.96	0.13	83,87,102,172	0
59	OHX	ESIA	101	7/7	0.96	0.07	144,159,173,194	0
58	MG	16SA	2347	1/1	0.96	0.07	78,78,78,78	0
58	MG	23SA	3462	1/1	0.96	0.07	51,51,51,51	0
58	MG	16SB	2347	1/1	0.96	0.10	92,92,92,92	0
59	OHX	23SA	3205	7/7	0.96	0.12	38,59,83,130	0
59	OHX	23SA	3208	7/7	0.96	0.12	72,79,94,145	0
58	MG	23SA	3463	1/1	0.96	0.07	60,60,60,60	0
58	MG	23SB	3347	1/1	0.96	0.08	65,65,65,65	0
58	MG	23SA	3035	1/1	0.96	0.14	52,52,52,52	0
59	OHX	23SA	3225	7/7	0.96	0.06	96,99,104,174	0
60	K	23SA	3637	1/1	0.96	0.14	60,60,60,60	0
59	OHX	16SA	2275	7/7	0.96	0.09	80,83,104,161	0
58	MG	23SB	3355	1/1	0.96	0.07	65,65,65,65	0
59	OHX	23SA	3230	7/7	0.96	0.09	67,77,97,168	0
59	OHX	16SA	2278	7/7	0.96	0.06	100,115,119,183	0
59	OHX	23SB	3030	7/7	0.96	0.14	80,86,109,145	0
58	MG	16SB	2352	1/1	0.96	0.07	73,73,73,73	0
59	OHX	23SB	3034	7/7	0.96	0.12	90,91,105,156	0
58	MG	23SA	3153	1/1	0.96	0.13	51,51,51,51	0
59	OHX	23SA	3237	7/7	0.96	0.11	79,89,105,162	0
58	MG	23SB	3358	1/1	0.96	0.06	47,47,47,47	0
59	OHX	23SB	3048	7/7	0.96	0.08	111,117,132,161	0
59	OHX	23SB	3049	7/7	0.96	0.06	92,103,111,173	0
59	OHX	23SA	3240	7/7	0.96	0.11	69,78,93,170	0
60	K	16SB	2373	1/1	0.96	0.13	93,93,93,93	0
58	MG	16SB	2357	1/1	0.96	0.06	96,96,96,96	0
59	OHX	23SA	3243	7/7	0.96	0.10	79,89,95,159	0
59	OHX	23SA	3245	7/7	0.96	0.13	86,96,104,177	0
59	OHX	23SB	3055	7/7	0.96	0.14	65,81,87,153	0
60	K	16SB	2378	1/1	0.96	0.07	94,94,94,94	0
58	MG	23SB	3242	1/1	0.96	0.19	39,39,39,39	0
59	OHX	23SA	3250	7/7	0.96	0.13	58,64,77,149	0
59	OHX	23SB	3060	7/7	0.96	0.10	95,99,105,180	0
58	MG	23SB	3362	1/1	0.96	0.07	49,49,49,49	0
60	K	16SB	2383	1/1	0.96	0.05	92,92,92,92	0
58	MG	23SA	3021	1/1	0.96	0.17	40,40,40,40	0
58	MG	16SB	2360	1/1	0.96	0.05	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	OHX	23SB	3064	7/7	0.96	0.18	77,82,98,167	0
58	MG	23SB	3367	1/1	0.96	0.09	49,49,49,49	0
59	OHX	16SA	2291	7/7	0.96	0.12	91,96,102,165	0
59	OHX	23SB	3068	7/7	0.96	0.17	87,92,101,181	0
59	OHX	23SB	3069	7/7	0.96	0.07	98,105,118,189	0
59	OHX	23SB	3070	7/7	0.96	0.14	81,89,95,163	0
59	OHX	23SB	3071	7/7	0.96	0.12	85,94,100,182	0
58	MG	23SA	3474	1/1	0.96	0.07	59,59,59,59	0
58	MG	23SA	3476	1/1	0.96	0.08	51,51,51,51	0
58	MG	5SA	217	1/1	0.96	0.12	85,85,85,85	0
60	K	16SB	2397	1/1	0.96	0.04	97,97,97,97	0
58	MG	16SA	2342	1/1	0.96	0.07	85,85,85,85	0
58	MG	23SB	3374	1/1	0.96	0.11	48,48,48,48	0
59	OHX	23SA	3264	7/7	0.96	0.05	98,101,114,196	0
59	OHX	23SB	3082	7/7	0.96	0.12	79,84,97,168	0
59	OHX	23SB	3084	7/7	0.96	0.09	94,97,110,191	0
59	OHX	23SB	3085	7/7	0.96	0.06	105,109,112,199	0
59	OHX	23SA	3265	7/7	0.96	0.07	83,93,109,192	0
58	MG	23SB	3375	1/1	0.96	0.07	66,66,66,66	0
58	MG	23SA	3039	1/1	0.96	0.14	30,30,30,30	0
59	OHX	23SB	3091	7/7	0.96	0.12	81,89,94,189	0
58	MG	23SA	3390	1/1	0.96	0.06	38,38,38,38	0
58	MG	23SA	3113	1/1	0.96	0.23	52,52,52,52	0
59	OHX	23SB	3094	7/7	0.96	0.06	107,111,129,187	0
58	MG	23SA	3004	1/1	0.96	0.24	35,35,35,35	0
59	OHX	23SB	3096	7/7	0.96	0.06	128,134,148,208	0
59	OHX	23SB	3097	7/7	0.96	0.16	82,88,95,172	0
59	OHX	23SB	3098	7/7	0.96	0.10	97,101,109,177	0
59	OHX	16SA	2302	7/7	0.96	0.07	105,107,113,183	0
59	OHX	23SB	3101	7/7	0.96	0.07	104,111,115,185	0
60	K	23SB	3453	1/1	0.96	0.05	59,59,59,59	0
58	MG	L27A	104	1/1	0.96	0.09	65,65,65,65	0
60	K	23SB	3456	1/1	0.96	0.04	75,75,75,75	0
60	K	23SB	3457	1/1	0.96	0.05	63,63,63,63	0
58	MG	23SA	3042	1/1	0.96	0.14	47,47,47,47	0
60	K	23SB	3460	1/1	0.96	0.06	61,61,61,61	0
58	MG	23SA	3396	1/1	0.96	0.06	34,34,34,34	0
59	OHX	23SA	3276	7/7	0.96	0.06	87,98,104,204	0
58	MG	23SA	3399	1/1	0.96	0.06	37,37,37,37	0
58	MG	23SB	3305	1/1	0.96	0.09	65,65,65,65	0
59	OHX	23SB	3108	7/7	0.96	0.06	95,101,104,191	0
59	OHX	23SB	3109	7/7	0.96	0.05	118,119,125,207	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	OHX	5SA	207	7/7	0.96	0.06	97,103,109,176	0
59	OHX	23SA	3279	7/7	0.96	0.06	92,97,106,198	0
58	MG	23SA	3401	1/1	0.96	0.06	63,63,63,63	0
59	OHX	5SA	210	7/7	0.96	0.17	81,88,100,168	0
59	OHX	5SA	211	7/7	0.96	0.06	101,107,113,190	0
59	OHX	23SB	3115	7/7	0.96	0.05	98,104,112,200	0
59	OHX	23SA	3282	7/7	0.96	0.06	101,104,113,206	0
58	MG	16SA	2361	1/1	0.96	0.06	75,75,75,75	0
58	MG	23SB	3392	1/1	0.96	0.09	52,52,52,52	0
58	MG	23SA	3025	1/1	0.96	0.29	64,64,64,64	0
59	OHX	23SA	3287	7/7	0.96	0.07	97,100,105,189	0
58	MG	23SA	3413	1/1	0.96	0.07	55,55,55,55	0
58	MG	23SA	3098	1/1	0.96	0.06	54,54,54,54	0
58	MG	23SA	3501	1/1	0.96	0.09	66,66,66,66	0
60	K	23SB	3482	1/1	0.96	0.05	66,66,66,66	0
58	MG	23SB	3406	1/1	0.96	0.16	68,68,68,68	0
59	OHX	23SB	3125	7/7	0.96	0.07	90,93,105,217	0
59	OHX	16SB	2207	7/7	0.96	0.07	89,95,104,159	0
59	OHX	16SB	2213	7/7	0.96	0.07	123,129,137,180	0
59	OHX	16SB	2214	7/7	0.96	0.08	116,119,134,169	0
59	OHX	23SA	3294	7/7	0.96	0.10	85,97,105,191	0
58	MG	16SA	2344	1/1	0.96	0.06	82,82,82,82	0
59	OHX	23SA	3296	7/7	0.96	0.06	94,97,113,192	0
58	MG	16SA	2345	1/1	0.96	0.06	89,89,89,89	0
58	MG	23SB	3413	1/1	0.96	0.07	42,42,42,42	0
59	OHX	23SB	3137	7/7	0.96	0.05	99,103,110,209	0
59	OHX	16SB	2221	7/7	0.96	0.05	108,115,121,190	0
58	MG	23SB	3414	1/1	0.96	0.06	83,83,83,83	0
58	MG	23SB	3416	1/1	0.96	0.07	98,98,98,98	0
60	K	23SA	3566	1/1	0.96	0.04	51,51,51,51	0
58	MG	23SA	3510	1/1	0.96	0.12	75,75,75,75	0
58	MG	23SB	3418	1/1	0.96	0.07	51,51,51,51	0
60	K	23SA	3574	1/1	0.96	0.04	52,52,52,52	0
59	OHX	23SA	3305	7/7	0.96	0.05	97,104,122,196	0
59	OHX	16SB	2231	7/7	0.96	0.06	94,98,110,186	0
59	OHX	16SB	2232	7/7	0.96	0.05	126,132,138,218	0
58	MG	23SB	3217	1/1	0.96	0.10	48,48,48,48	0
58	MG	23SA	3029	1/1	0.96	0.16	37,37,37,37	0
60	K	23SA	3582	1/1	0.96	0.06	53,53,53,53	0
60	K	23SA	3583	1/1	0.96	0.10	65,65,65,65	0
58	MG	16SA	2364	1/1	0.96	0.07	86,86,86,86	0
58	MG	16SA	2365	1/1	0.96	0.09	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	23SB	3425	1/1	0.96	0.18	84,84,84,84	0
58	MG	23SA	3431	1/1	0.96	0.05	79,79,79,79	0
59	OHX	16SB	2240	7/7	0.96	0.06	120,126,130,218	0
58	MG	23SA	3104	1/1	0.96	0.07	63,63,63,63	0
59	OHX	16SB	2243	7/7	0.96	0.06	115,117,121,193	0
58	MG	23SB	3321	1/1	0.96	0.15	39,39,39,39	0
59	OHX	16SB	2245	7/7	0.96	0.06	100,107,114,181	0
58	MG	23SA	3518	1/1	0.96	0.14	61,61,61,61	0
58	MG	23SB	3433	1/1	0.96	0.06	106,106,106,106	0
59	OHX	16SB	2248	7/7	0.96	0.05	123,130,136,226	0
60	K	L16B	201	1/1	0.96	0.05	92,92,92,92	0
60	K	23SA	3600	1/1	0.96	0.07	68,68,68,68	0
58	MG	23SA	3105	1/1	0.96	0.20	59,59,59,59	0
59	OHX	23SB	3083	7/7	0.97	0.05	110,114,121,181	0
59	OHX	23SA	3234	7/7	0.97	0.08	91,94,101,156	0
58	MG	23SB	3337	1/1	0.97	0.06	48,48,48,48	0
60	K	23SA	3630	1/1	0.97	0.07	80,80,80,80	0
59	OHX	23SB	3086	7/7	0.97	0.10	85,86,104,167	0
59	OHX	16SB	2225	7/7	0.97	0.10	94,95,103,163	0
59	OHX	16SB	2226	7/7	0.97	0.05	117,119,123,191	0
58	MG	23SB	3343	1/1	0.97	0.09	65,65,65,65	0
58	MG	23SB	3344	1/1	0.97	0.06	50,50,50,50	0
58	MG	23SA	3456	1/1	0.97	0.06	50,50,50,50	0
59	OHX	16SB	2230	7/7	0.97	0.04	126,136,146,203	0
58	MG	23SA	3458	1/1	0.97	0.07	55,55,55,55	0
59	OHX	23SA	3242	7/7	0.97	0.17	54,62,72,135	0
60	K	5SA	218	1/1	0.97	0.04	79,79,79,79	0
59	OHX	23SA	3330	7/7	0.97	0.06	112,118,131,203	0
60	K	L2A	301	1/1	0.97	0.05	47,47,47,47	0
58	MG	23SB	3423	1/1	0.97	0.05	73,73,73,73	0
59	OHX	23SA	3244	7/7	0.97	0.10	76,82,89,144	0
58	MG	23SA	3460	1/1	0.97	0.09	38,38,38,38	0
59	OHX	23SB	3100	7/7	0.97	0.11	90,93,100,175	0
59	OHX	16SB	2237	7/7	0.97	0.06	109,114,118,214	0
59	OHX	23SA	3246	7/7	0.97	0.08	88,94,111,180	0
58	MG	23SB	3352	1/1	0.97	0.06	47,47,47,47	0
59	OHX	23SA	3248	7/7	0.97	0.11	84,89,103,166	0
59	OHX	16SB	2241	7/7	0.97	0.06	97,104,110,191	0
59	OHX	23SA	3249	7/7	0.97	0.13	81,94,100,157	0
60	K	16SB	2371	1/1	0.97	0.05	99,99,99,99	0
60	K	16SB	2372	1/1	0.97	0.04	105,105,105,105	0
58	MG	23SB	3427	1/1	0.97	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	23SA	3119	1/1	0.97	0.05	61,61,61,61	0
60	K	16SA	2397	1/1	0.97	0.07	62,62,62,62	0
59	OHX	23SA	3253	7/7	0.97	0.05	106,111,120,187	0
60	K	16SA	2400	1/1	0.97	0.04	89,89,89,89	0
58	MG	16SB	2345	1/1	0.97	0.07	64,64,64,64	0
58	MG	16SA	2372	1/1	0.97	0.05	92,92,92,92	0
58	MG	16SA	2373	1/1	0.97	0.12	98,98,98,98	0
58	MG	23SB	3221	1/1	0.97	0.14	47,47,47,47	0
58	MG	16SB	2349	1/1	0.97	0.17	90,90,90,90	0
58	MG	16SB	2350	1/1	0.97	0.08	99,99,99,99	0
58	MG	16SA	2351	1/1	0.97	0.08	103,103,103,103	0
58	MG	S4A	302	1/1	0.97	0.06	98,98,98,98	0
58	MG	16SA	2206	1/1	0.97	0.36	40,40,40,40	0
60	K	16SA	2410	1/1	0.97	0.04	77,77,77,77	0
58	MG	23SA	3415	1/1	0.97	0.05	67,67,67,67	0
58	MG	23SA	3417	1/1	0.97	0.10	58,58,58,58	0
58	MG	16SB	2359	1/1	0.97	0.06	103,103,103,103	0
59	OHX	16SB	2258	7/7	0.97	0.05	144,147,157,204	0
58	MG	23SA	3028	1/1	0.97	0.23	41,41,41,41	0
58	MG	23SA	3038	1/1	0.97	0.17	45,45,45,45	0
58	MG	16SB	2362	1/1	0.97	0.09	113,113,113,113	0
58	MG	23SA	3385	1/1	0.97	0.06	41,41,41,41	0
58	MG	23SB	3235	1/1	0.97	0.21	59,59,59,59	0
59	OHX	23SB	3128	7/7	0.97	0.05	108,110,117,202	0
58	MG	23SA	3387	1/1	0.97	0.06	55,55,55,55	0
59	OHX	16SA	2265	7/7	0.97	0.07	104,105,123,150	0
59	OHX	16SA	2269	7/7	0.97	0.08	81,87,100,141	0
58	MG	23SA	3389	1/1	0.97	0.06	41,41,41,41	0
59	OHX	23SB	3133	7/7	0.97	0.05	96,99,110,198	0
59	OHX	16SA	2273	7/7	0.97	0.09	96,101,112,163	0
58	MG	23SA	3430	1/1	0.97	0.05	74,74,74,74	0
58	MG	16SA	2370	1/1	0.97	0.05	102,102,102,102	0
58	MG	23SA	3433	1/1	0.97	0.05	77,77,77,77	0
59	OHX	23SA	3281	7/7	0.97	0.11	76,91,95,177	0
58	MG	23SA	3030	1/1	0.97	0.28	51,51,51,51	0
59	OHX	23SA	3283	7/7	0.97	0.05	106,113,119,187	0
58	MG	23SA	3493	1/1	0.97	0.05	44,44,44,44	0
58	MG	23SA	3066	1/1	0.97	0.20	59,59,59,59	0
58	MG	23SA	3438	1/1	0.97	0.05	88,88,88,88	0
59	OHX	16SA	2282	7/7	0.97	0.12	84,85,91,155	0
58	MG	23SA	3041	1/1	0.97	0.07	32,32,32,32	0
60	K	23SA	3551	1/1	0.97	0.04	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	OHX	23SB	3147	7/7	0.97	0.05	109,122,129,186	0
59	OHX	23SA	3289	7/7	0.97	0.14	72,79,86,180	0
60	K	23SB	3455	1/1	0.97	0.11	61,61,61,61	0
59	OHX	PSIB	101	7/7	0.97	0.08	104,107,121,137	0
59	OHX	23SA	3290	7/7	0.97	0.12	83,93,105,198	0
59	OHX	ESIB	101	7/7	0.97	0.06	150,166,173,207	0
58	MG	23SA	3394	1/1	0.97	0.08	71,71,71,71	0
59	OHX	23SB	3020	7/7	0.97	0.07	89,94,103,130	0
59	OHX	23SB	3022	7/7	0.97	0.08	92,97,106,138	0
59	OHX	23SB	3023	7/7	0.97	0.08	75,79,88,131	0
60	K	23SA	3561	1/1	0.97	0.06	75,75,75,75	0
59	OHX	23SB	3025	7/7	0.97	0.11	87,93,101,135	0
59	OHX	23SB	3026	7/7	0.97	0.12	83,92,104,131	0
59	OHX	S19A	101	7/7	0.97	0.06	115,125,129,181	0
58	MG	23SB	3395	1/1	0.97	0.12	43,43,43,43	0
59	OHX	ASIA	103	7/7	0.97	0.07	142,155,169,215	0
60	K	23SA	3567	1/1	0.97	0.06	46,46,46,46	0
59	OHX	16SA	2287	7/7	0.97	0.08	96,103,109,167	0
58	MG	23SB	3247	1/1	0.97	0.06	45,45,45,45	0
60	K	23SA	3572	1/1	0.97	0.05	51,51,51,51	0
59	OHX	23SB	3038	7/7	0.97	0.09	82,91,105,153	0
59	OHX	23SB	3039	7/7	0.97	0.07	92,95,103,158	0
59	OHX	23SA	3297	7/7	0.97	0.09	97,99,109,183	0
60	K	23SB	3477	1/1	0.97	0.03	60,60,60,60	0
59	OHX	23SB	3043	7/7	0.97	0.08	81,88,108,166	0
59	OHX	23SB	3044	7/7	0.97	0.15	69,77,95,151	0
59	OHX	23SB	3045	7/7	0.97	0.08	84,95,110,160	0
59	OHX	23SB	3046	7/7	0.97	0.09	64,76,84,147	0
59	OHX	23SB	3047	7/7	0.97	0.11	74,90,94,149	0
60	K	23SB	3483	1/1	0.97	0.06	69,69,69,69	0
60	K	23SB	3484	1/1	0.97	0.07	80,80,80,80	0
59	OHX	5SA	205	7/7	0.97	0.09	75,95,106,138	0
60	K	23SA	3585	1/1	0.97	0.08	54,54,54,54	0
59	OHX	TRNA	101	7/7	0.97	0.06	135,137,154,191	0
58	MG	L15A	203	1/1	0.97	0.11	65,65,65,65	0
58	MG	23SB	3208	1/1	0.97	0.30	52,52,52,52	0
59	OHX	23SA	3200	7/7	0.97	0.11	62,89,92,138	0
60	K	23SB	3491	1/1	0.97	0.08	68,68,68,68	0
60	K	23SA	3590	1/1	0.97	0.09	67,67,67,67	0
58	MG	23SB	3403	1/1	0.97	0.06	52,52,52,52	0
59	OHX	23SA	3303	7/7	0.97	0.10	91,92,104,183	0
59	OHX	23SB	3057	7/7	0.97	0.10	96,99,115,167	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	OHX	23SA	3207	7/7	0.97	0.11	73,78,88,136	0
60	K	23SB	3497	1/1	0.97	0.06	48,48,48,48	0
58	MG	23SB	3404	1/1	0.97	0.08	37,37,37,37	0
60	K	23SA	3596	1/1	0.97	0.03	59,59,59,59	0
59	OHX	23SA	3209	7/7	0.97	0.08	76,90,103,134	0
60	K	23SA	3598	1/1	0.97	0.11	58,58,58,58	0
59	OHX	23SA	3210	7/7	0.97	0.11	57,67,87,122	0
59	OHX	23SA	3211	7/7	0.97	0.11	61,66,83,132	0
58	MG	23SA	3444	1/1	0.97	0.11	29,29,29,29	0
59	OHX	23SA	3220	7/7	0.97	0.07	85,86,101,146	0
60	K	23SB	3506	1/1	0.97	0.06	75,75,75,75	0
59	OHX	23SB	3065	7/7	0.97	0.10	86,93,109,147	0
58	MG	23SB	3290	1/1	0.97	0.31	47,47,47,47	0
59	OHX	23SA	3222	7/7	0.97	0.06	99,103,115,175	0
58	MG	23SA	3395	1/1	0.97	0.07	34,34,34,34	0
60	K	23SA	3607	1/1	0.97	0.04	59,59,59,59	0
59	OHX	16SB	2210	7/7	0.97	0.10	96,101,107,163	0
59	OHX	16SB	2211	7/7	0.97	0.07	101,114,117,162	0
58	MG	23SB	3411	1/1	0.97	0.06	41,41,41,41	0
59	OHX	23SB	3072	7/7	0.97	0.08	81,88,103,161	0
58	MG	23SB	3412	1/1	0.97	0.06	56,56,56,56	0
58	MG	23SB	3211	1/1	0.97	0.05	52,52,52,52	0
59	OHX	23SA	3228	7/7	0.97	0.09	70,82,89,143	0
60	K	23SA	3616	1/1	0.97	0.05	42,42,42,42	0
58	MG	16SA	2358	1/1	0.97	0.10	48,48,48,48	0
60	K	5SB	216	1/1	0.97	0.03	101,101,101,101	0
60	K	L2B	301	1/1	0.97	0.05	62,62,62,62	0
59	OHX	23SB	3077	7/7	0.97	0.10	87,95,105,161	0
59	OHX	23SB	3078	7/7	0.97	0.05	115,122,131,189	0
59	OHX	5SB	201	7/7	0.97	0.07	103,112,120,159	0
58	MG	23SB	3415	1/1	0.97	0.07	46,46,46,46	0
59	OHX	23SB	3080	7/7	0.97	0.06	95,105,112,179	0
59	OHX	23SA	3232	7/7	0.97	0.07	78,84,95,161	0
58	MG	23SA	3507	1/1	0.97	0.07	55,55,55,55	0
58	MG	23SA	3457	1/1	0.98	0.09	37,37,37,37	0
58	MG	23SA	3498	1/1	0.98	0.06	38,38,38,38	0
58	MG	23SB	3397	1/1	0.98	0.06	59,59,59,59	0
58	MG	23SA	3409	1/1	0.98	0.05	42,42,42,42	0
58	MG	23SA	3428	1/1	0.98	0.07	78,78,78,78	0
59	OHX	16SA	2285	7/7	0.98	0.04	123,129,131,218	0
59	OHX	ASIB	101	7/7	0.98	0.04	114,126,131,187	0
59	OHX	23SA	3191	7/7	0.98	0.06	79,89,101,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	OHX	23SA	3193	7/7	0.98	0.08	66,70,81,129	0
59	OHX	23SA	3194	7/7	0.98	0.08	71,75,90,126	0
58	MG	23SB	3401	1/1	0.98	0.09	70,70,70,70	0
59	OHX	23SA	3196	7/7	0.98	0.10	70,74,94,114	0
59	OHX	23SA	3197	7/7	0.98	0.07	73,80,93,129	0
59	OHX	23SB	3134	7/7	0.98	0.10	82,85,92,165	0
59	OHX	23SB	3008	7/7	0.98	0.07	89,94,103,131	0
59	OHX	23SB	3012	7/7	0.98	0.08	71,76,93,139	0
59	OHX	23SB	3016	7/7	0.98	0.06	91,93,102,122	0
59	OHX	23SB	3018	7/7	0.98	0.07	53,69,86,133	0
59	OHX	23SA	3198	7/7	0.98	0.07	58,71,88,129	0
59	OHX	23SB	3021	7/7	0.98	0.08	68,77,87,136	0
60	K	16SB	2385	1/1	0.98	0.04	92,92,92,92	0
59	OHX	23SA	3199	7/7	0.98	0.06	65,73,83,129	0
60	K	23SA	3538	1/1	0.98	0.06	63,63,63,63	0
59	OHX	5SA	204	7/7	0.98	0.06	79,82,94,113	0
59	OHX	23SB	3024	7/7	0.98	0.10	69,75,81,158	0
58	MG	23SB	3402	1/1	0.98	0.05	45,45,45,45	0
59	OHX	23SA	3201	7/7	0.98	0.07	79,87,98,127	0
59	OHX	23SB	3028	7/7	0.98	0.07	85,85,101,143	0
59	OHX	23SA	3202	7/7	0.98	0.08	55,70,77,136	0
59	OHX	23SB	3031	7/7	0.98	0.07	88,95,98,151	0
59	OHX	23SA	3203	7/7	0.98	0.06	77,78,101,130	0
59	OHX	23SA	3204	7/7	0.98	0.06	66,71,91,123	0
58	MG	23SA	3074	1/1	0.98	0.04	72,72,72,72	0
59	OHX	23SA	3206	7/7	0.98	0.10	74,75,95,140	0
59	OHX	23SB	3037	7/7	0.98	0.08	97,101,106,155	0
58	MG	23SA	3383	1/1	0.98	0.05	39,39,39,39	0
58	MG	23SA	3432	1/1	0.98	0.04	67,67,67,67	0
59	OHX	23SB	3040	7/7	0.98	0.07	68,76,88,142	0
58	MG	16SA	2356	1/1	0.98	0.10	67,67,67,67	0
59	OHX	23SB	3042	7/7	0.98	0.05	101,107,110,164	0
58	MG	23SA	3508	1/1	0.98	0.05	38,38,38,38	0
59	OHX	L17A	201	7/7	0.98	0.12	63,68,78,121	0
58	MG	23SB	3409	1/1	0.98	0.04	58,58,58,58	0
58	MG	23SB	3410	1/1	0.98	0.03	75,75,75,75	0
59	OHX	23SA	3213	7/7	0.98	0.07	74,78,90,126	0
59	OHX	23SA	3216	7/7	0.98	0.08	85,94,99,152	0
59	OHX	23SA	3217	7/7	0.98	0.05	80,82,89,137	0
59	OHX	16SB	2202	7/7	0.98	0.08	86,91,97,124	0
59	OHX	16SB	2204	7/7	0.98	0.07	86,96,104,143	0
59	OHX	23SA	3218	7/7	0.98	0.09	78,86,101,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	OHX	23SB	3053	7/7	0.98	0.06	92,97,113,157	0
59	OHX	16SB	2209	7/7	0.98	0.06	90,99,108,137	0
59	OHX	23SA	3219	7/7	0.98	0.08	82,94,104,144	0
60	K	23SA	3569	1/1	0.98	0.03	46,46,46,46	0
59	OHX	23SB	3056	7/7	0.98	0.06	95,102,108,155	0
58	MG	23SA	3509	1/1	0.98	0.05	52,52,52,52	0
60	K	23SA	3573	1/1	0.98	0.06	63,63,63,63	0
59	OHX	16SB	2212	7/7	0.98	0.07	96,100,102,148	0
60	K	23SB	3459	1/1	0.98	0.07	56,56,56,56	0
58	MG	23SB	3340	1/1	0.98	0.08	45,45,45,45	0
60	K	23SA	3576	1/1	0.98	0.07	39,39,39,39	0
58	MG	23SB	3341	1/1	0.98	0.06	53,53,53,53	0
59	OHX	23SA	3313	7/7	0.98	0.10	67,73,83,167	0
59	OHX	23SA	3223	7/7	0.98	0.06	81,87,101,144	0
58	MG	16SA	2348	1/1	0.98	0.04	58,58,58,58	0
58	MG	23SA	3468	1/1	0.98	0.07	36,36,36,36	0
59	OHX	16SB	2219	7/7	0.98	0.05	103,105,116,174	0
58	MG	23SB	3345	1/1	0.98	0.05	65,65,65,65	0
58	MG	23SA	3469	1/1	0.98	0.06	40,40,40,40	0
58	MG	23SA	3436	1/1	0.98	0.10	80,80,80,80	0
59	OHX	16SB	2223	7/7	0.98	0.04	110,112,122,172	0
59	OHX	23SA	3229	7/7	0.98	0.07	81,96,99,154	0
58	MG	23SA	3514	1/1	0.98	0.13	51,51,51,51	0
58	MG	23SB	3350	1/1	0.98	0.07	37,37,37,37	0
58	MG	23SB	3351	1/1	0.98	0.04	53,53,53,53	0
58	MG	23SA	3473	1/1	0.98	0.05	67,67,67,67	0
58	MG	23SB	3353	1/1	0.98	0.05	57,57,57,57	0
59	OHX	23SA	3235	7/7	0.98	0.06	75,87,106,150	0
58	MG	16SA	2343	1/1	0.98	0.09	73,73,73,73	0
58	MG	23SB	3426	1/1	0.98	0.05	70,70,70,70	0
59	OHX	23SA	3238	7/7	0.98	0.11	64,65,76,149	0
58	MG	23SA	3517	1/1	0.98	0.07	82,82,82,82	0
58	MG	23SA	3418	1/1	0.98	0.08	36,36,36,36	0
58	MG	16SB	2328	1/1	0.98	0.08	58,58,58,58	0
58	MG	23SA	3441	1/1	0.98	0.05	43,43,43,43	0
58	MG	23SA	3521	1/1	0.98	0.04	58,58,58,58	0
58	MG	23SA	3419	1/1	0.98	0.05	64,64,64,64	0
58	MG	23SA	3090	1/1	0.98	0.13	49,49,49,49	0
58	MG	23SB	3435	1/1	0.98	0.10	94,94,94,94	0
58	MG	23SA	3481	1/1	0.98	0.10	55,55,55,55	0
58	MG	23SA	3527	1/1	0.98	0.06	42,42,42,42	0
59	OHX	23SB	3090	7/7	0.98	0.05	110,117,123,191	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	16SB	2337	1/1	0.98	0.08	100,100,100,100	0
58	MG	23SA	3062	1/1	0.98	0.10	61,61,61,61	0
59	OHX	23SA	3251	7/7	0.98	0.04	99,104,112,176	0
59	OHX	L17B	201	7/7	0.98	0.10	72,77,87,116	0
58	MG	23SA	3058	1/1	0.98	0.05	53,53,53,53	0
58	MG	23SA	3447	1/1	0.98	0.05	34,34,34,34	0
60	K	23SA	3615	1/1	0.98	0.08	69,69,69,69	0
58	MG	5SB	215	1/1	0.98	0.05	88,88,88,88	0
58	MG	23SA	3485	1/1	0.98	0.04	51,51,51,51	0
58	MG	23SA	3533	1/1	0.98	0.05	49,49,49,49	0
58	MG	23SB	3225	1/1	0.98	0.08	39,39,39,39	0
58	MG	23SA	3448	1/1	0.98	0.05	40,40,40,40	0
60	K	23SA	3621	1/1	0.98	0.08	77,77,77,77	0
58	MG	23SB	3379	1/1	0.98	0.05	41,41,41,41	0
58	MG	23SA	3449	1/1	0.98	0.05	44,44,44,44	0
58	MG	23SA	3488	1/1	0.98	0.06	49,49,49,49	0
58	MG	23SA	3407	1/1	0.98	0.05	48,48,48,48	0
59	OHX	23SA	3263	7/7	0.98	0.08	64,70,95,142	0
59	OHX	16SA	2266	7/7	0.98	0.07	89,99,109,141	0
58	MG	23SA	3490	1/1	0.98	0.07	42,42,42,42	0
59	OHX	16SA	2270	7/7	0.98	0.06	108,118,121,150	0
58	MG	23SA	3492	1/1	0.98	0.04	52,52,52,52	0
59	OHX	16SA	2272	7/7	0.98	0.07	96,111,118,140	0
58	MG	23SA	3453	1/1	0.98	0.06	34,34,34,34	0
60	K	16SA	2392	1/1	0.98	0.04	88,88,88,88	0
60	K	16SA	2393	1/1	0.98	0.07	80,80,80,80	0
60	K	16SA	2394	1/1	0.98	0.03	75,75,75,75	0
58	MG	16SB	2355	1/1	0.98	0.05	90,90,90,90	0
59	OHX	23SA	3271	7/7	0.98	0.09	70,73,91,159	0
58	MG	23SA	3494	1/1	0.98	0.05	48,48,48,48	0
58	MG	L4A	301	1/1	0.98	0.12	48,48,48,48	0
60	K	16SA	2399	1/1	0.98	0.04	65,65,65,65	0
59	OHX	16SB	2269	7/7	0.98	0.06	146,151,156,215	0
59	OHX	16SA	2277	7/7	0.98	0.07	94,95,103,165	0
58	MG	L4A	303	1/1	0.98	0.09	73,73,73,73	0
58	MG	23SA	3425	1/1	0.98	0.09	61,61,61,61	0
59	OHX	ASIA	101	7/7	0.98	0.06	100,111,125,168	0
59	OHX	L19A	201	7/7	0.99	0.05	85,89,97,137	0
58	MG	23SA	3536	1/1	0.99	0.09	36,36,36,36	0
58	MG	23SA	3459	1/1	0.99	0.04	66,66,66,66	0
59	OHX	23SA	3214	7/7	0.99	0.05	62,70,75,153	0
59	OHX	23SB	3027	7/7	0.99	0.07	78,82,92,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	OHX	23SA	3215	7/7	0.99	0.05	81,87,93,144	0
59	OHX	23SB	3029	7/7	0.99	0.05	91,95,103,141	0
58	MG	16SB	2353	1/1	0.99	0.11	76,76,76,76	0
59	OHX	16SB	2201	7/7	0.99	0.05	81,88,90,106	0
58	MG	23SA	3386	1/1	0.99	0.05	47,47,47,47	0
59	OHX	23SB	3033	7/7	0.99	0.08	79,88,93,147	0
59	OHX	16SB	2203	7/7	0.99	0.06	91,94,102,133	0
58	MG	23SA	3496	1/1	0.99	0.06	63,63,63,63	0
59	OHX	16SB	2205	7/7	0.99	0.04	105,111,117,152	0
59	OHX	16SB	2206	7/7	0.99	0.06	95,98,106,125	0
58	MG	16SB	2356	1/1	0.99	0.11	78,78,78,78	0
59	OHX	16SB	2208	7/7	0.99	0.05	79,80,93,120	0
58	MG	23SB	3348	1/1	0.99	0.12	75,75,75,75	0
58	MG	23SA	3412	1/1	0.99	0.04	40,40,40,40	0
58	MG	5SA	215	1/1	0.99	0.04	64,64,64,64	0
58	MG	16SA	2346	1/1	0.99	0.07	70,70,70,70	0
58	MG	23SB	3421	1/1	0.99	0.03	96,96,96,96	0
58	MG	23SA	3388	1/1	0.99	0.04	33,33,33,33	0
58	MG	23SA	3435	1/1	0.99	0.07	75,75,75,75	0
58	MG	L3A	302	1/1	0.99	0.04	39,39,39,39	0
58	MG	23SA	3397	1/1	0.99	0.04	46,46,46,46	0
58	MG	23SA	3502	1/1	0.99	0.07	32,32,32,32	0
58	MG	23SA	3503	1/1	0.99	0.10	70,70,70,70	0
58	MG	23SB	3359	1/1	0.99	0.12	66,66,66,66	0
58	MG	23SA	3416	1/1	0.99	0.04	63,63,63,63	0
58	MG	23SA	3398	1/1	0.99	0.04	35,35,35,35	0
58	MG	23SA	3506	1/1	0.99	0.03	39,39,39,39	0
58	MG	23SB	3432	1/1	0.99	0.04	46,46,46,46	0
58	MG	23SB	3363	1/1	0.99	0.08	47,47,47,47	0
58	MG	23SA	3470	1/1	0.99	0.05	53,53,53,53	0
58	MG	23SB	3365	1/1	0.99	0.03	45,45,45,45	0
58	MG	23SA	3471	1/1	0.99	0.02	53,53,53,53	0
58	MG	23SA	3439	1/1	0.99	0.07	38,38,38,38	0
58	MG	23SB	3438	1/1	0.99	0.05	45,45,45,45	0
60	K	23SA	3571	1/1	0.99	0.04	38,38,38,38	0
58	MG	23SB	3368	1/1	0.99	0.03	47,47,47,47	0
58	MG	23SA	3440	1/1	0.99	0.11	88,88,88,88	0
58	MG	16SA	2352	1/1	0.99	0.06	62,62,62,62	0
58	MG	23SB	3371	1/1	0.99	0.04	39,39,39,39	0
58	MG	23SA	3475	1/1	0.99	0.06	64,64,64,64	0
60	K	23SA	3577	1/1	0.99	0.03	45,45,45,45	0
58	MG	23SA	3400	1/1	0.99	0.07	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	16SA	2349	1/1	0.99	0.04	82,82,82,82	0
58	MG	23SA	3052	1/1	0.99	0.23	40,40,40,40	0
58	MG	23SB	3376	1/1	0.99	0.03	50,50,50,50	0
58	MG	23SA	3405	1/1	0.99	0.09	46,46,46,46	0
58	MG	23SA	3480	1/1	0.99	0.04	82,82,82,82	0
58	MG	23SA	3446	1/1	0.99	0.06	43,43,43,43	0
59	OHX	16SA	2260	7/7	0.99	0.06	68,70,81,89	0
59	OHX	16SA	2261	7/7	0.99	0.07	71,82,87,97	0
59	OHX	16SA	2262	7/7	0.99	0.06	62,71,88,103	0
59	OHX	16SA	2263	7/7	0.99	0.07	80,83,92,128	0
59	OHX	16SA	2264	7/7	0.99	0.05	96,101,107,133	0
58	MG	23SA	3423	1/1	0.99	0.02	50,50,50,50	0
58	MG	23SB	3382	1/1	0.99	0.05	61,61,61,61	0
59	OHX	16SA	2267	7/7	0.99	0.05	85,94,97,129	0
59	OHX	16SA	2268	7/7	0.99	0.06	96,97,109,142	0
58	MG	23SA	3520	1/1	0.99	0.13	79,79,79,79	0
59	OHX	5SB	202	7/7	0.99	0.05	96,105,116,131	0
58	MG	23SA	3406	1/1	0.99	0.04	63,63,63,63	0
58	MG	23SA	3522	1/1	0.99	0.03	73,73,73,73	0
59	OHX	PSIA	102	7/7	0.99	0.09	94,95,102,131	0
58	MG	16SA	2354	1/1	0.99	0.04	68,68,68,68	0
58	MG	23SB	3387	1/1	0.99	0.08	53,53,53,53	0
58	MG	23SA	3450	1/1	0.99	0.03	56,56,56,56	0
58	MG	16SB	2334	1/1	0.99	0.06	68,68,68,68	0
59	OHX	23SA	3178	7/7	0.99	0.10	43,55,71,95	0
59	OHX	23SA	3179	7/7	0.99	0.12	41,50,60,111	0
59	OHX	23SA	3180	7/7	0.99	0.10	70,70,90,126	0
59	OHX	23SA	3181	7/7	0.99	0.06	55,67,74,94	0
59	OHX	23SA	3182	7/7	0.99	0.06	81,85,100,104	0
59	OHX	23SA	3183	7/7	0.99	0.05	63,65,71,97	0
59	OHX	23SA	3185	7/7	0.99	0.05	69,73,78,116	0
59	OHX	23SA	3186	7/7	0.99	0.04	62,68,77,96	0
59	OHX	23SA	3187	7/7	0.99	0.06	61,66,83,110	0
59	OHX	23SA	3188	7/7	0.99	0.06	58,67,76,91	0
59	OHX	23SA	3189	7/7	0.99	0.07	60,72,78,115	0
59	OHX	23SA	3190	7/7	0.99	0.06	79,85,92,109	0
58	MG	16SB	2335	1/1	0.99	0.07	74,74,74,74	0
59	OHX	23SA	3192	7/7	0.99	0.07	68,74,81,100	0
58	MG	23SA	3525	1/1	0.99	0.10	40,40,40,40	0
58	MG	23SA	3451	1/1	0.99	0.04	33,33,33,33	0
58	MG	16SB	2338	1/1	0.99	0.05	86,86,86,86	0
58	MG	23SB	3394	1/1	0.99	0.05	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	23SA	3426	1/1	0.99	0.05	42,42,42,42	0
58	MG	23SA	3408	1/1	0.99	0.03	45,45,45,45	0
60	K	16SA	2390	1/1	0.99	0.10	67,67,67,67	0
60	K	23SA	3624	1/1	0.99	0.03	60,60,60,60	0
59	OHX	S14B	101	7/7	0.99	0.04	121,125,132,169	0
58	MG	16SB	2342	1/1	0.99	0.10	98,98,98,98	0
58	MG	23SA	3454	1/1	0.99	0.03	54,54,54,54	0
58	MG	23SA	3530	1/1	0.99	0.05	57,57,57,57	0
58	MG	16SA	2350	1/1	0.99	0.06	89,89,89,89	0
58	MG	16SB	2346	1/1	0.99	0.04	84,84,84,84	0
58	MG	23SB	3334	1/1	0.99	0.05	58,58,58,58	0
58	MG	23SA	3491	1/1	0.99	0.05	43,43,43,43	0
59	OHX	23SB	3001	7/7	0.99	0.10	59,64,68,112	0
59	OHX	23SB	3002	7/7	0.99	0.08	66,72,95,109	0
59	OHX	23SB	3004	7/7	0.99	0.04	64,70,79,95	0
59	OHX	23SB	3005	7/7	0.99	0.06	74,76,93,97	0
59	OHX	23SB	3006	7/7	0.99	0.06	70,76,84,116	0
59	OHX	23SB	3007	7/7	0.99	0.06	85,90,107,121	0
58	MG	23SB	3405	1/1	0.99	0.08	53,53,53,53	0
59	OHX	23SB	3009	7/7	0.99	0.07	75,77,79,117	0
59	OHX	23SB	3010	7/7	0.99	0.08	79,84,90,126	0
59	OHX	23SB	3011	7/7	0.99	0.07	74,84,94,103	0
58	MG	23SA	3429	1/1	0.99	0.08	60,60,60,60	0
59	OHX	23SB	3013	7/7	0.99	0.05	86,91,94,110	0
59	OHX	23SB	3014	7/7	0.99	0.04	74,88,94,117	0
59	OHX	23SB	3015	7/7	0.99	0.07	103,106,113,117	0
58	MG	23SA	3534	1/1	0.99	0.10	55,55,55,55	0
59	OHX	23SB	3017	7/7	0.99	0.06	83,87,98,124	0
58	MG	23SB	3338	1/1	0.99	0.04	48,48,48,48	0
59	OHX	23SB	3019	7/7	0.99	0.06	68,75,83,123	0
59	OHX	L4A	302	7/7	0.99	0.17	37,47,53,146	0
58	MG	23SB	3339	1/1	0.99	0.04	47,47,47,47	0
58	MG	23SA	3410	1/1	0.99	0.03	57,57,57,57	0
58	MG	23SB	3380	1/1	1.00	0.03	39,39,39,39	0
58	MG	23SA	3403	1/1	1.00	0.03	33,33,33,33	0
59	OHX	23SB	3003	7/7	1.00	0.05	75,81,93,98	0
59	OHX	23SA	3184	7/7	1.00	0.03	57,62,65,92	0
58	MG	23SB	3400	1/1	1.00	0.04	84,84,84,84	0
58	MG	23SB	3342	1/1	1.00	0.09	46,46,46,46	0
59	OHX	L4B	301	7/7	1.00	0.09	48,52,62,94	0
58	MG	23SA	3404	1/1	1.00	0.06	45,45,45,45	0
58	MG	23SA	3464	1/1	1.00	0.02	37,37,37,37	0

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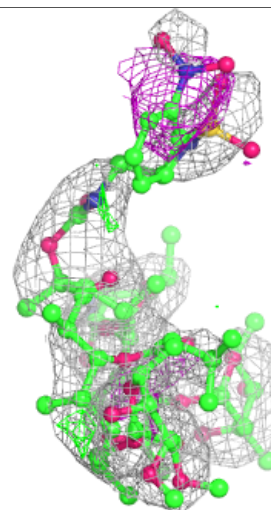
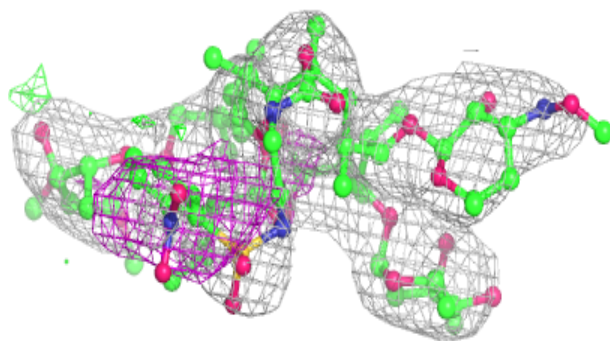
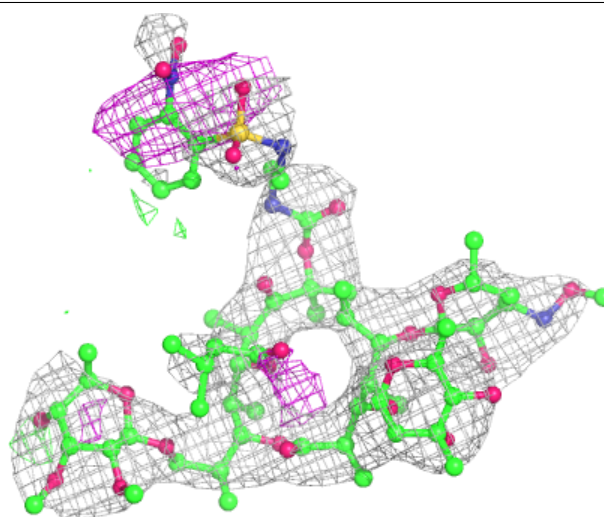
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	23SA	3455	1/1	1.00	0.11	51,51,51,51	0
58	MG	16SB	2340	1/1	1.00	0.09	64,64,64,64	0
58	MG	23SB	3354	1/1	1.00	0.03	77,77,77,77	0
58	MG	23SA	3466	1/1	1.00	0.06	57,57,57,57	0

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.

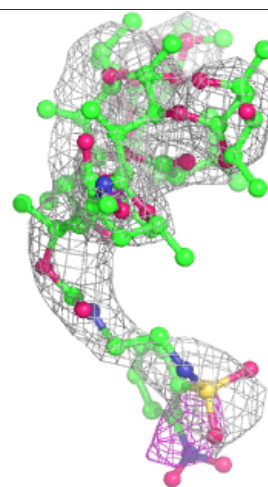
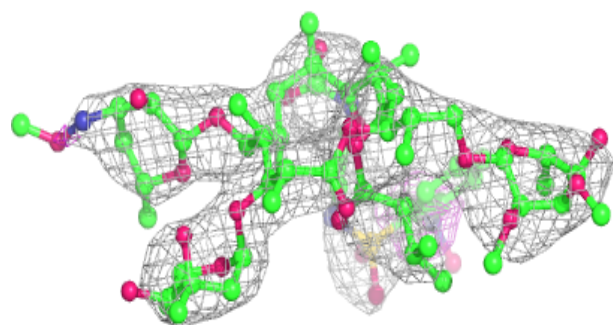
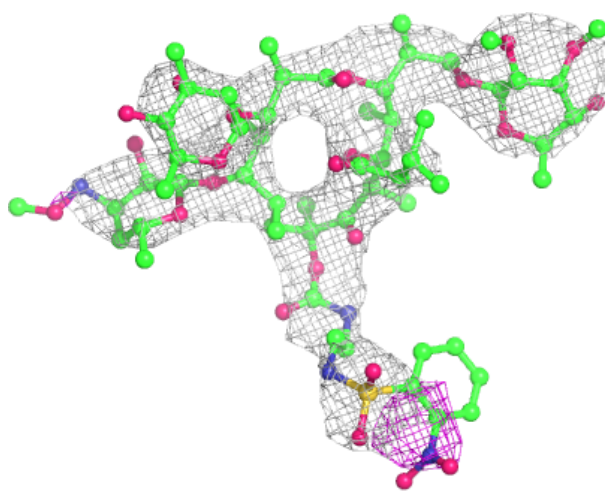
Electron density around SJE 23SA 3640:

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 SJE 23SB 3521:

$2mF_o-DF_c$ (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.