Full wwPDB X-ray Structure Validation Report (i)

Sep 16, 2026 – 03:29 pm BST

PDB ID	:	7AZO / pdb_00007azo
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

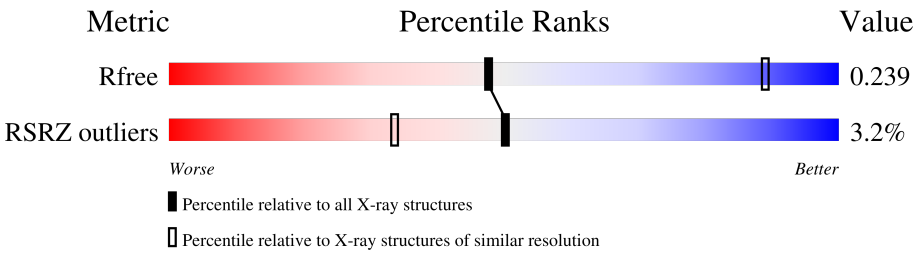
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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

2 Entry composition (i)

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
			Total	C	N	O	P			
1	16SA	1512	32509	14478	6016	10503	1512	0	0	0
1	16SB	1508	32429	14442	6008	10471	1508	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 25 is a RNA chain called RNA (30-MER).

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
27	23SA	2889	62225	27699	11629	20008	2889	0	0	0
27	23SB	2873	61886	27548	11574	19891	2873	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	L6A	171	1316	835	247	233	1	0	0	0
			Total	C	N	O	S			
33	L6B	173	1327	842	249	235	1	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	L18A	112	889	561	177	150	1	0	0	0
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
			Total	C	N	O	S			
41	L19A	137	1141	710	234	196	1	0	0	0
41	L19B	137	1141	710	234	196	1	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	L23A	93	738	480	133	124	1	0	0	0
45	L23B	94	742	482	134	125	1	0	0	0

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	L29A	69	583	363	117	101	2	0	0	0
50	L29B	71	590	367	119	103	1	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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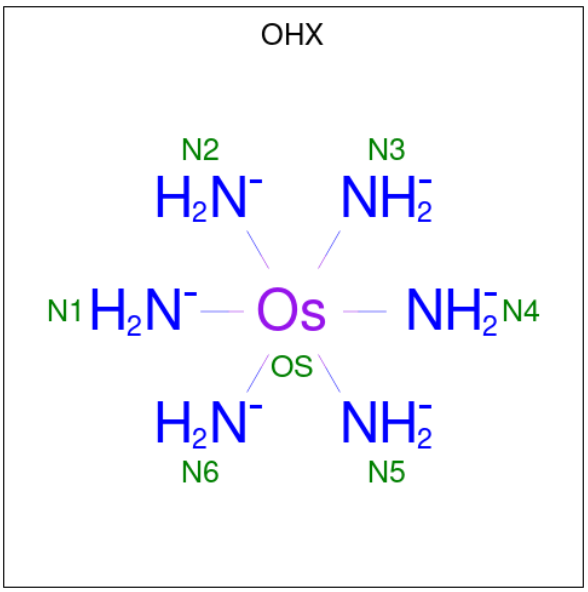
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
58	L3A	2	2	2	0	0
58	L4A	2	2	2	0	0
58	L5A	1	1	1	0	0
58	L15A	2	2	2	0	0
58	L23A	1	1	1	0	0
58	L27A	2	2	2	0	0
58	L30A	1	1	1	0	0
58	L32A	1	1	1	0	0
58	L33A	1	1	1	0	0
58	L34A	1	1	1	0	0
58	L35A	1	1	1	0	0
58	16SB	85	86	86	0	1
58	S5B	1	1	1	0	0
58	PSIB	3	3	3	0	0
58	23SB	240	241	241	0	1
58	5SB	4	4	4	0	0
58	L3B	2	2	2	0	0
58	L4B	1	1	1	0	0
58	L5B	1	1	1	0	0
58	L15B	1	1	1	0	0
58	L35B	2	2	2	0	0

- Molecule 59 is osmium (III) hexammine (CCD ID: OHX) (formula: $H_{12}N_6Os$).



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
59	23SA	1	7	6	1	0	0
			Total	N	Os		
59	23SA	1	7	6	1	0	0
			Total	N	Os		
59	23SA	1	7	6	1	0	0
			Total	N	Os		
59	23SA	1	7	6	1	0	0
			Total	N	Os		
59	23SA	1	7	6	1	0	0
			Total	N	Os		
59	23SA	1	7	6	1	0	0
			Total	N	Os		
59	23SA	1	7	6	1	0	0
			Total	N	Os		
59	23SA	1	7	6	1	0	0
			Total	N	Os		
59	23SA	1	7	6	1	0	0
			Total	N	Os		
59	23SA	1	7	6	1	0	0
			Total	N	Os		
59	23SA	1	7	6	1	0	0
			Total	N	Os		
59	23SA	1	7	6	1	0	0
			Total	N	Os		
59	5SA	1	7	6	1	0	0
			Total	N	Os		
59	5SA	1	7	6	1	0	0
			Total	N	Os		
59	5SA	1	7	6	1	0	0
			Total	N	Os		
59	5SA	1	7	6	1	0	0
			Total	N	Os		
59	5SA	1	7	6	1	0	0
			Total	N	Os		
59	5SA	1	7	6	1	0	0
			Total	N	Os		
59	5SA	1	7	6	1	0	0
			Total	N	Os		
59	5SA	1	7	6	1	0	0
			Total	N	Os		
59	5SA	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
59	5SA	1	7	6	1	0	0
			Total	N	Os		
59	5SA	1	7	6	1	0	0
			Total	N	Os		
59	L4A	1	7	6	1	0	0
			Total	N	Os		
59	L15A	1	7	6	1	0	0
			Total	N	Os		
59	L17A	1	7	6	1	0	0
			Total	N	Os		
59	L19A	1	7	6	1	0	0
			Total	N	Os		
59	L20A	1	7	6	1	0	0
			Total	N	Os		
59	L27A	1	7	6	1	0	0
			Total	N	Os		
59	L27A	1	7	6	1	0	0
			Total	N	Os		
59	L28A	1	7	6	1	0	0
			Total	N	Os		
59	L35A	1	7	6	1	0	0
			Total	N	Os		
59	16SB	1	7	6	1	0	0
			Total	N	Os		
59	16SB	1	7	6	1	0	0
			Total	N	Os		
59	16SB	1	7	6	1	0	0
			Total	N	Os		
59	16SB	1	7	6	1	0	0
			Total	N	Os		
59	16SB	1	7	6	1	0	0
			Total	N	Os		
59	16SB	1	7	6	1	0	0
			Total	N	Os		
59	16SB	1	7	6	1	0	0
			Total	N	Os		
59	16SB	1	7	6	1	0	0
			Total	N	Os		
59	16SB	1	7	6	1	0	0
			Total	N	Os		
59	16SB	1	7	6	1	0	0

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
59	16SB	1	7	6	1	0	0
			Total	N	Os		
59	16SB	1	7	6	1	0	0
			Total	N	Os		
59	16SB	1	7	6	1	0	0
			Total	N	Os		
59	16SB	1	7	6	1	0	0
			Total	N	Os		
59	16SB	1	7	6	1	0	0
			Total	N	Os		
59	S4B	1	7	6	1	0	0
			Total	N	Os		
59	S14B	1	7	6	1	0	0
			Total	N	Os		
59	ASIB	1	7	6	1	0	0
			Total	N	Os		
59	ASIB	1	7	6	1	0	0
			Total	N	Os		
59	ASIB	1	7	6	1	0	0
			Total	N	Os		
59	PSIB	1	7	6	1	0	0
			Total	N	Os		
59	PSIB	1	7	6	1	0	0
			Total	N	Os		
59	ESIB	1	7	6	1	0	0
			Total	N	Os		
59	MRNB	1	7	6	1	0	0
			Total	N	Os		
59	23SB	1	7	6	1	0	0
			Total	N	Os		
59	23SB	1	7	6	1	0	0
			Total	N	Os		
59	23SB	1	7	6	1	0	0
			Total	N	Os		
59	23SB	1	7	6	1	0	0
			Total	N	Os		
59	23SB	1	7	6	1	0	0
			Total	N	Os		
59	23SB	1	7	6	1	0	0
			Total	N	Os		
59	23SB	1	7	6	1	0	0

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

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

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

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

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

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

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

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

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

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

- Molecule 60 is POTASSIUM ION (CCD ID: K) (formula: K).

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

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

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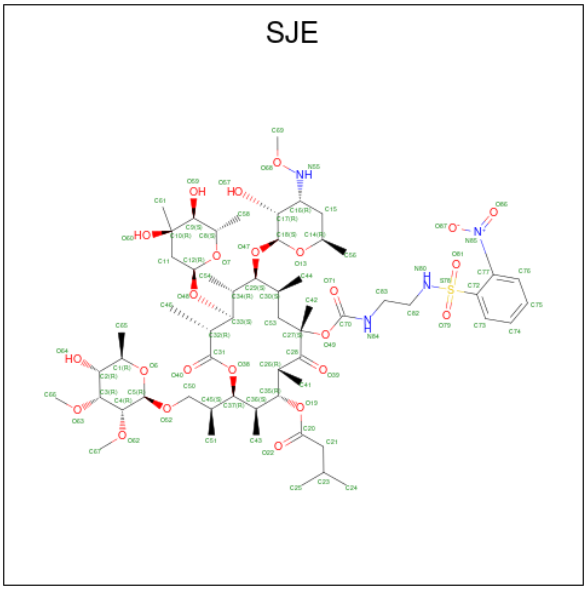
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	L5B	1	Total K 1 1	0	0
60	L15B	1	Total K 1 1	0	0
60	L16B	1	Total K 1 1	0	0

- Molecule 61 is (2R,3S,4R,5R,7S,9S,10S,11R,12S,13R)-12-(((2R,4R,5S,6S)-4,5-dihydroxy-4,6-dimethyltetrahydro-2H-pyran-2-yl)oxy)-2-((S)-1-(((2R,3R,4R,5R,6R)-5-hydroxy-3,4-dimethoxy-6-methyltetrahydro-2H-pyran-2-yl)oxy)propan-2-yl)-10-(((2S,3R,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 (CCD ID: SJE) (formula: $C_{58}H_{96}N_4O_{24}S$).



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

- Molecule 62 is water.

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	S5A	1	Total O 1 1	0	0
62	S12A	1	Total O 1 1	0	0
62	S13A	1	Total O 1 1	0	0
62	S14A	1	Total O 1 1	0	0
62	S16A	1	Total O 1 1	0	0
62	THXA	3	Total O 3 3	0	0
62	PSIA	7	Total O 7 7	0	0
62	ESIA	1	Total O 1 1	0	0
62	23SA	788	Total O 788 788	0	0
62	5SA	14	Total O 14 14	0	0
62	L2A	10	Total O 10 10	0	0
62	L3A	7	Total O 7 7	0	0
62	L4A	6	Total O 6 6	0	0
62	L15A	9	Total O 9 9	0	0
62	L16A	1	Total O 1 1	0	0
62	L17A	2	Total O 2 2	0	0
62	L18A	2	Total O 2 2	0	0
62	L19A	1	Total O 1 1	0	0
62	L23A	1	Total O 1 1	0	0
62	L27A	3	Total O 3 3	0	0
62	L30A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	L34A	1	Total O 1 1	0	0
62	L35A	1	Total O 1 1	0	0
62	16SB	157	Total O 157 157	0	0
62	S4B	2	Total O 2 2	0	0
62	S5B	1	Total O 1 1	0	0
62	S9B	1	Total O 1 1	0	0
62	S12B	2	Total O 2 2	0	0
62	S14B	2	Total O 2 2	0	0
62	23SB	519	Total O 519 519	0	0
62	5SB	5	Total O 5 5	0	0
62	L2B	12	Total O 12 12	0	0
62	L3B	6	Total O 6 6	0	0
62	L4B	1	Total O 1 1	0	0
62	L15B	7	Total O 7 7	0	0
62	L19B	1	Total O 1 1	0	0
62	L27B	2	Total O 2 2	0	0
62	L28B	1	Total O 1 1	0	0
62	L30B	1	Total O 1 1	0	0
62	L35B	6	Total O 6 6	0	0

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.15 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.214 , 0.238 0.215 , 0.239	Depositor DCC
R_{free} test set	25661 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]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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	5MC	16SA	2035	1	18,22,23	3.73	7 (38%)	26,32,35	1.07	1 (3%)
23	3AU	PSIA	47	23	24,28,29	2.80	8 (33%)	33,40,43	1.54	6 (18%)
1	2MG	16SB	1834	1	23,26,27	2.99	8 (34%)	32,38,41	2.21	12 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	PSU	PSIA	39	23	18,21,22	1.06	1 (5%)	22,30,33	1.65	3 (13%)
1	UR3	16SB	2121	1	19,22,23	2.86	7 (36%)	26,32,35	1.46	3 (11%)
27	2MA	23SA	2518	60,27	22,25,26	3.41	7 (31%)	33,37,40	2.11	10 (30%)
26	H2U	TRNA	16	26	18,21,22	2.02	4 (22%)	21,30,33	2.07	5 (23%)
1	G7M	16SB	1156	60,1	23,26,27	4.46	8 (34%)	35,39,42	3.31	13 (37%)
22	4SU	ASIA	8	22	18,21,22	1.81	4 (22%)	26,30,33	2.36	5 (19%)
26	PSU	TRNA	55	26	18,21,22	1.09	1 (5%)	22,30,33	1.77	4 (18%)
23	H2U	PSIA	16	23	18,21,22	2.01	4 (22%)	21,30,33	2.06	5 (23%)
22	PSU	ASIA	32	22	18,21,22	1.11	1 (5%)	22,30,33	1.53	4 (18%)
27	5MU	23SA	1964	60,27	19,22,23	3.78	5 (26%)	28,32,35	3.39	10 (35%)
1	M2G	16SA	1589	1	24,27,28	2.77	8 (33%)	35,40,43	1.70	9 (25%)
1	UR3	16SA	2121	1	19,22,23	2.81	8 (42%)	26,32,35	1.52	3 (11%)
23	PSU	PSIB	55	23	18,21,22	1.11	1 (5%)	22,30,33	1.67	3 (13%)
27	OMU	23SB	2567	27,58	19,22,23	2.98	8 (42%)	26,31,34	1.83	5 (19%)
23	PSU	PSIA	32	23	18,21,22	1.03	1 (5%)	22,30,33	1.59	3 (13%)
12	0TD	S12A	89	12	7,9,10	1.48	1 (14%)	6,11,13	1.87	1 (16%)
57	MIA	ASIB	37	57	28,31,32	2.27	4 (14%)	40,44,47	2.99	16 (40%)
24	MIA	ESIB	37	24	28,31,32	2.36	4 (14%)	40,44,47	3.74	15 (37%)
22	PSU	ASIA	39	22	18,21,22	1.13	1 (5%)	22,30,33	1.58	3 (13%)
23	PSU	PSIB	32	23	18,21,22	1.03	1 (5%)	22,30,33	1.69	4 (18%)
23	PSU	PSIB	39	23	18,21,22	1.11	1 (5%)	22,30,33	1.63	4 (18%)
27	PSU	23SB	2620	27	18,21,22	1.18	1 (5%)	22,30,33	1.76	3 (13%)
22	G7M	ASIA	46	22	23,26,27	4.45	8 (34%)	35,39,42	3.37	13 (37%)
23	4SU	PSIA	8	23	18,21,22	1.77	3 (16%)	26,30,33	2.51	5 (19%)
23	5MU	PSIB	54	23	19,22,23	3.90	5 (26%)	28,32,35	3.07	9 (32%)
27	OMG	23SA	2266	60,27,23	23,26,27	4.92	11 (47%)	33,38,41	4.51	18 (54%)
23	MIA	PSIA	37	23	28,31,32	2.26	4 (14%)	40,44,47	2.59	13 (32%)
1	5MC	16SB	2035	1	18,22,23	3.86	7 (38%)	26,32,35	1.10	3 (11%)
23	PSU	PSIA	55	23	18,21,22	1.21	1 (5%)	22,30,33	1.65	4 (18%)
22	PSU	ASIA	55	22	18,21,22	1.04	1 (5%)	22,30,33	1.71	4 (18%)
22	MIA	ASIA	37	22	28,31,32	2.23	4 (14%)	40,44,47	3.04	14 (35%)
27	PSU	23SA	1942	27	18,21,22	1.03	1 (5%)	22,30,33	1.79	4 (18%)
27	OMC	23SA	1945	60,27	19,22,23	1.73	4 (21%)	26,31,34	0.82	0
1	MA6	16SA	2142	1	23,26,27	1.42	5 (21%)	34,38,41	2.85	13 (38%)
27	5MC	23SA	1987	60,27	18,22,23	3.71	7 (38%)	26,32,35	0.96	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MA6	16SA	2141	1	23,26,27	1.43	5 (21%)	34,38,41	2.82	12 (35%)
27	PSU	23SA	1936	27	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)
1	5MC	16SB	1590	1	18,22,23	3.84	7 (38%)	26,32,35	1.00	1 (3%)
1	M2G	16SB	1589	1	24,27,28	2.83	8 (33%)	35,40,43	1.67	7 (20%)
1	MA6	16SB	2142	1	23,26,27	1.38	5 (21%)	34,38,41	2.81	12 (35%)
57	PSU	ASIB	32	57	18,21,22	1.02	1 (5%)	22,30,33	1.68	4 (18%)
27	5MC	23SA	1967	27	18,22,23	3.74	7 (38%)	26,32,35	1.17	1 (3%)
26	PSU	TRNA	32	26	18,21,22	1.14	1 (5%)	22,30,33	1.72	4 (18%)
27	OMG	23SB	2266	60,27,23	23,26,27	5.00	11 (47%)	33,38,41	4.61	17 (51%)
23	G7M	PSIB	46	23	23,26,27	4.53	8 (34%)	35,39,42	3.28	13 (37%)
27	2MA	23SB	2518	60,27,58	22,25,26	3.44	7 (31%)	33,37,40	2.17	11 (33%)
23	G7M	PSIA	46	23	23,26,27	4.40	8 (34%)	35,39,42	3.38	13 (37%)
1	2MG	16SA	1834	60,1	23,26,27	2.92	8 (34%)	32,38,41	2.18	12 (37%)
1	5MC	16SB	2028	1	18,22,23	3.80	7 (38%)	26,32,35	1.21	3 (11%)
1	5MC	16SA	1590	1	18,22,23	3.74	7 (38%)	26,32,35	1.07	1 (3%)
24	MIA	ESIA	37	24	28,31,32	2.35	4 (14%)	40,44,47	2.99	14 (35%)
1	4OC	16SA	2030	1	20,23,24	3.10	8 (40%)	26,32,35	0.88	1 (3%)
1	4OC	16SB	2030	58,1	20,23,24	2.85	8 (40%)	26,32,35	1.41	4 (15%)
26	4SU	TRNA	8	26	18,21,22	1.79	3 (16%)	26,30,33	2.40	5 (19%)
27	5MC	23SB	1967	27	18,22,23	3.81	7 (38%)	26,32,35	1.06	3 (11%)
23	5MU	PSIA	54	23	19,22,23	3.79	5 (26%)	28,32,35	3.16	7 (25%)
23	4SU	PSIB	8	23,58	18,21,22	1.87	5 (27%)	26,30,33	2.91	6 (23%)
26	H2U	TRNA	20	26,28	18,21,22	2.27	4 (22%)	21,30,33	1.84	5 (23%)
1	PSU	16SA	1145	58,1	18,21,22	1.14	1 (5%)	22,30,33	1.70	4 (18%)
26	5MU	TRNA	54	26	19,22,23	3.92	5 (26%)	28,32,35	3.20	9 (32%)
22	5MU	ASIA	54	22	19,22,23	3.84	5 (26%)	28,32,35	3.25	10 (35%)
27	PSU	23SA	2620	27	18,21,22	1.14	1 (5%)	22,30,33	1.82	4 (18%)
27	OMU	23SA	2567	27,58	19,22,23	2.93	8 (42%)	26,31,34	1.85	5 (19%)
27	5MC	23SB	1987	60,27	18,22,23	3.79	7 (38%)	26,32,35	0.92	1 (3%)
1	G7M	16SA	1156	60,1	23,26,27	4.40	8 (34%)	35,39,42	3.31	13 (37%)
12	0TD	S12B	89	12,1	7,9,10	1.56	1 (14%)	6,11,13	1.99	2 (33%)
1	MA6	16SB	2141	1	23,26,27	1.40	5 (21%)	34,38,41	2.64	11 (32%)
27	5MU	23SB	1940	59,27	19,22,23	3.98	5 (26%)	28,32,35	3.32	9 (32%)
27	PSU	23SB	1942	27	18,21,22	1.13	1 (5%)	22,30,33	1.64	4 (18%)
27	5MU	23SB	1964	60,27	19,22,23	3.81	5 (26%)	28,32,35	3.29	9 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	MIA	TRNA	37	27,26,37	28,31,32	2.69	8 (28%)	40,44,47	4.25	15 (37%)
1	5MC	16SB	2032	1	18,22,23	3.87	7 (38%)	26,32,35	0.94	2 (7%)
57	PSU	ASIB	39	57	18,21,22	1.11	1 (5%)	22,30,33	1.68	4 (18%)
23	MIA	PSIB	37	23	28,31,32	2.26	3 (10%)	40,44,47	2.73	14 (35%)
27	PSU	23SB	1936	27	18,21,22	1.14	1 (5%)	22,30,33	1.52	3 (13%)
57	5MU	ASIB	54	57	19,22,23	3.89	5 (26%)	28,32,35	3.16	8 (28%)
23	H2U	PSIB	16	23	18,21,22	2.05	4 (22%)	21,30,33	1.86	5 (23%)
23	3AU	PSIB	47	23	24,28,29	2.84	8 (33%)	33,40,43	1.96	8 (24%)
1	PSU	16SB	1145	58,1	18,21,22	1.11	1 (5%)	22,30,33	1.67	3 (13%)
1	5MC	16SA	2032	1	18,22,23	3.82	7 (38%)	26,32,35	0.89	2 (7%)
27	5MU	23SA	1940	27	19,22,23	4.11	5 (26%)	28,32,35	3.47	10 (35%)
1	5MC	16SA	2028	1	18,22,23	3.81	7 (38%)	26,32,35	1.09	1 (3%)
27	OMC	23SB	1945	27	19,22,23	1.80	4 (21%)	26,31,34	0.92	1 (3%)
26	PSU	TRNA	39	26	18,21,22	1.14	1 (5%)	22,30,33	1.80	5 (22%)

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	5MC	16SA	2035	1	-	0/7/25/26	0/2/2/2
23	3AU	PSIA	47	23	-	7/16/34/35	0/2/2/2
1	2MG	16SB	1834	1	-	2/9/27/28	0/3/3/3
23	PSU	PSIA	39	23	-	0/7/25/26	0/2/2/2
1	UR3	16SB	2121	1	-	0/7/25/26	0/2/2/2
27	2MA	23SA	2518	60,27	-	1/7/25/26	0/3/3/3
26	H2U	TRNA	16	26	-	3/7/38/39	0/2/2/2
1	G7M	16SB	1156	60,1	-	2/7/25/26	0/3/3/3
22	4SU	ASIA	8	22	-	1/7/25/26	0/2/2/2
26	PSU	TRNA	55	26	-	0/7/25/26	0/2/2/2
23	H2U	PSIA	16	23	-	0/7/38/39	0/2/2/2
22	PSU	ASIA	32	22	-	0/7/25/26	0/2/2/2
27	5MU	23SA	1964	60,27	-	2/7/25/26	0/2/2/2
1	M2G	16SA	1589	1	-	0/11/29/30	0/3/3/3
1	UR3	16SA	2121	1	-	0/7/25/26	0/2/2/2
23	PSU	PSIB	55	23	-	0/7/25/26	0/2/2/2
27	OMU	23SB	2567	27,58	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	PSIA	32	23	-	0/7/25/26	0/2/2/2
12	0TD	S12A	89	12	-	2/7/12/14	-
57	MIA	ASIB	37	57	-	3/15/33/34	0/3/3/3
24	MIA	ESIB	37	24	-	6/15/33/34	0/3/3/3
22	PSU	ASIA	39	22	-	0/7/25/26	0/2/2/2
23	PSU	PSIB	32	23	-	0/7/25/26	0/2/2/2
23	PSU	PSIB	39	23	-	0/7/25/26	0/2/2/2
27	PSU	23SB	2620	27	-	0/7/25/26	0/2/2/2
22	G7M	ASIA	46	22	-	2/7/25/26	0/3/3/3
23	4SU	PSIA	8	23	-	0/7/25/26	0/2/2/2
23	5MU	PSIB	54	23	-	2/7/25/26	0/2/2/2
27	OMG	23SA	2266	60,27,23	-	1/9/27/28	0/3/3/3
23	MIA	PSIA	37	23	-	5/15/33/34	0/3/3/3
1	5MC	16SB	2035	1	-	0/7/25/26	0/2/2/2
23	PSU	PSIA	55	23	-	3/7/25/26	0/2/2/2
22	PSU	ASIA	55	22	-	3/7/25/26	0/2/2/2
22	MIA	ASIA	37	22	-	6/15/33/34	0/3/3/3
27	PSU	23SA	1942	27	-	0/7/25/26	0/2/2/2
27	OMC	23SA	1945	60,27	-	1/9/27/28	0/2/2/2
1	MA6	16SA	2142	1	-	3/11/29/30	0/3/3/3
27	5MC	23SA	1987	60,27	-	0/7/25/26	0/2/2/2
1	MA6	16SA	2141	1	-	0/11/29/30	0/3/3/3
27	PSU	23SA	1936	27	-	0/7/25/26	0/2/2/2
1	5MC	16SB	1590	1	-	0/7/25/26	0/2/2/2
1	M2G	16SB	1589	1	-	0/11/29/30	0/3/3/3
1	MA6	16SB	2142	1	-	3/11/29/30	0/3/3/3
57	PSU	ASIB	32	57	-	0/7/25/26	0/2/2/2
27	5MC	23SA	1967	27	-	0/7/25/26	0/2/2/2
26	PSU	TRNA	32	26	-	0/7/25/26	0/2/2/2
27	OMG	23SB	2266	60,27,23	-	1/9/27/28	0/3/3/3
23	G7M	PSIB	46	23	-	0/7/25/26	0/3/3/3
27	2MA	23SB	2518	60,27,58	-	3/7/25/26	0/3/3/3
23	G7M	PSIA	46	23	-	2/7/25/26	0/3/3/3
1	2MG	16SA	1834	60,1	-	0/9/27/28	0/3/3/3
1	5MC	16SB	2028	1	-	0/7/25/26	0/2/2/2
1	5MC	16SA	1590	1	-	0/7/25/26	0/2/2/2
24	MIA	ESIA	37	24	-	7/15/33/34	0/3/3/3
1	4OC	16SA	2030	1	-	2/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4OC	16SB	2030	58,1	-	2/9/29/30	0/2/2/2
26	4SU	TRNA	8	26	-	2/7/25/26	0/2/2/2
27	5MC	23SB	1967	27	-	0/7/25/26	0/2/2/2
23	5MU	PSIA	54	23	-	0/7/25/26	0/2/2/2
23	4SU	PSIB	8	23,58	-	2/7/25/26	0/2/2/2
26	H2U	TRNA	20	26,28	-	5/7/38/39	0/2/2/2
1	PSU	16SA	1145	58,1	-	0/7/25/26	0/2/2/2
26	5MU	TRNA	54	26	-	2/7/25/26	0/2/2/2
22	5MU	ASIA	54	22	-	0/7/25/26	0/2/2/2
27	PSU	23SA	2620	27	-	0/7/25/26	0/2/2/2
27	OMU	23SA	2567	27,58	-	0/9/27/28	0/2/2/2
27	5MC	23SB	1987	60,27	-	0/7/25/26	0/2/2/2
1	G7M	16SA	1156	60,1	-	2/7/25/26	0/3/3/3
12	0TD	S12B	89	12,1	-	3/7/12/14	-
1	MA6	16SB	2141	1	-	0/11/29/30	0/3/3/3
27	5MU	23SB	1940	59,27	-	0/7/25/26	0/2/2/2
27	PSU	23SB	1942	27	-	0/7/25/26	0/2/2/2
27	5MU	23SB	1964	60,27	-	2/7/25/26	0/2/2/2
26	MIA	TRNA	37	27,26,37	-	6/15/33/34	0/3/3/3
1	5MC	16SB	2032	1	-	0/7/25/26	0/2/2/2
57	PSU	ASIB	39	57	-	0/7/25/26	0/2/2/2
23	MIA	PSIB	37	23	-	6/15/33/34	0/3/3/3
27	PSU	23SB	1936	27	-	0/7/25/26	0/2/2/2
57	5MU	ASIB	54	57	-	0/7/25/26	0/2/2/2
23	H2U	PSIB	16	23	-	0/7/38/39	0/2/2/2
23	3AU	PSIB	47	23	-	7/16/34/35	0/2/2/2
1	PSU	16SB	1145	58,1	-	0/7/25/26	0/2/2/2
1	5MC	16SA	2032	1	-	0/7/25/26	0/2/2/2
27	5MU	23SA	1940	27	-	3/7/25/26	0/2/2/2
1	5MC	16SA	2028	1	-	0/7/25/26	0/2/2/2
27	OMC	23SB	1945	27	-	1/9/27/28	0/2/2/2
26	PSU	TRNA	39	26	-	0/7/25/26	0/2/2/2

All (414) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	PSIB	46	G7M	C8-N7	17.80	1.65	1.33
22	ASIA	46	G7M	C8-N7	17.60	1.64	1.33
1	16SB	1156	G7M	C8-N7	17.55	1.64	1.33
23	PSIA	46	G7M	C8-N7	17.46	1.64	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16SA	1156	G7M	C8-N7	17.39	1.64	1.33
27	23SA	1940	5MU	C2-N1	13.35	1.59	1.38
27	23SB	1940	5MU	C2-N1	12.81	1.59	1.38
26	TRNA	54	5MU	C2-N1	12.72	1.58	1.38
23	PSIB	54	5MU	C2-N1	12.71	1.58	1.38
57	ASIB	54	5MU	C2-N1	12.58	1.58	1.38
27	23SB	1964	5MU	C2-N1	12.22	1.58	1.38
23	PSIA	54	5MU	C2-N1	12.17	1.58	1.38
22	ASIA	54	5MU	C2-N1	12.10	1.57	1.38
27	23SA	1964	5MU	C2-N1	11.99	1.57	1.38
27	23SB	2266	OMG	C5-N7	-11.51	1.16	1.39
27	23SA	2266	OMG	C5-N7	-11.42	1.16	1.39
27	23SB	2518	2MA	C4-N3	11.18	1.48	1.34
27	23SB	2266	OMG	C4-N3	11.08	1.60	1.34
27	23SA	2518	2MA	C4-N3	10.93	1.48	1.34
27	23SA	2266	OMG	C4-N3	10.83	1.60	1.34
1	16SB	2035	5MC	C6-C5	9.79	1.50	1.34
1	16SB	2032	5MC	C6-C5	9.64	1.50	1.34
27	23SB	1987	5MC	C6-C5	9.59	1.50	1.34
1	16SA	2028	5MC	C6-C5	9.54	1.50	1.34
27	23SA	1987	5MC	C6-C5	9.54	1.50	1.34
1	16SB	1590	5MC	C6-C5	9.43	1.50	1.34
1	16SA	1590	5MC	C6-C5	9.42	1.50	1.34
1	16SA	2032	5MC	C6-C5	9.39	1.50	1.34
27	23SB	1967	5MC	C6-C5	9.39	1.50	1.34
1	16SA	2035	5MC	C6-C5	9.38	1.50	1.34
1	16SB	2028	5MC	C6-C5	9.36	1.50	1.34
27	23SA	1967	5MC	C6-C5	9.10	1.49	1.34
23	PSIB	47	3AU	C2-N1	8.73	1.51	1.38
24	ESIB	37	MIA	C13-C14	8.60	1.57	1.32
27	23SB	2266	OMG	C4-N9	8.54	1.60	1.38
57	ASIB	37	MIA	C13-C14	8.48	1.56	1.32
23	PSIB	37	MIA	C13-C14	8.47	1.56	1.32
24	ESIA	37	MIA	C13-C14	8.45	1.56	1.32
23	PSIA	37	MIA	C13-C14	8.42	1.56	1.32
26	TRNA	37	MIA	C13-C14	8.41	1.56	1.32
22	ASIA	37	MIA	C13-C14	8.41	1.56	1.32
27	23SA	2266	OMG	C4-N9	8.26	1.59	1.38
27	23SB	2266	OMG	C8-N7	-8.24	1.09	1.32
27	23SA	2266	OMG	C8-N7	-8.12	1.09	1.32
23	PSIA	47	3AU	C2-N1	8.02	1.50	1.38
27	23SA	2266	OMG	C5-C4	7.96	1.61	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	23SB	2266	OMG	C5-C4	7.93	1.61	1.38
27	23SB	2266	OMG	C6-N1	-7.89	1.24	1.38
27	23SA	2266	OMG	C6-N1	-7.79	1.24	1.38
1	16SB	1834	2MG	C2-N3	7.57	1.46	1.31
1	16SA	1834	2MG	C2-N3	7.39	1.46	1.31
1	16SB	1590	5MC	C4-N3	7.37	1.46	1.34
1	16SA	2028	5MC	C4-N3	7.34	1.46	1.34
1	16SB	2121	UR3	C2-N1	7.31	1.49	1.38
1	16SA	2121	UR3	C2-N1	7.31	1.49	1.38
27	23SA	1967	5MC	C4-N3	7.30	1.46	1.34
1	16SB	2032	5MC	C4-N3	7.25	1.46	1.34
1	16SB	1589	M2G	C2-N2	7.20	1.49	1.35
1	16SB	2028	5MC	C4-N3	7.20	1.46	1.34
1	16SA	2032	5MC	C4-N3	7.19	1.46	1.34
27	23SB	1967	5MC	C4-N3	7.18	1.46	1.34
1	16SA	1589	M2G	C2-N2	7.12	1.48	1.35
1	16SB	1589	M2G	C4-N3	7.08	1.51	1.34
1	16SA	1590	5MC	C4-N3	7.04	1.46	1.34
26	TRNA	20	H2U	C2-N1	7.02	1.45	1.35
1	16SA	2030	4OC	C4-N3	7.01	1.45	1.32
1	16SB	2035	5MC	C4-N3	6.93	1.45	1.34
27	23SB	2567	OMU	C2-N3	6.91	1.50	1.38
27	23SB	1987	5MC	C4-N3	6.90	1.45	1.34
24	ESIA	37	MIA	C6-N6	6.88	1.45	1.34
27	23SA	2567	OMU	C2-N1	6.86	1.49	1.38
26	TRNA	37	MIA	C6-N6	6.76	1.45	1.34
24	ESIB	37	MIA	C6-N6	6.75	1.45	1.34
27	23SA	1987	5MC	C4-N3	6.67	1.45	1.34
27	23SB	1967	5MC	C2-N3	6.65	1.49	1.36
1	16SA	2035	5MC	C4-N3	6.65	1.45	1.34
1	16SA	2032	5MC	C2-N3	6.65	1.49	1.36
27	23SA	2567	OMU	C2-N3	6.58	1.49	1.38
1	16SB	2032	5MC	C2-N3	6.58	1.49	1.36
1	16SB	1590	5MC	C2-N3	6.55	1.49	1.36
23	PSIB	37	MIA	C6-N6	6.54	1.44	1.34
1	16SA	2028	5MC	C2-N3	6.50	1.49	1.36
27	23SB	1940	5MU	C4-N3	-6.48	1.26	1.38
1	16SA	1589	M2G	C4-N3	6.48	1.49	1.34
1	16SB	1834	2MG	C4-N3	6.47	1.49	1.34
27	23SA	1940	5MU	C4-N3	-6.47	1.26	1.38
1	16SB	2121	UR3	C6-C5	6.44	1.50	1.35
23	PSIA	54	5MU	C4-N3	-6.42	1.26	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16SB	2028	5MC	C2-N3	6.41	1.49	1.36
27	23SB	2567	OMU	C2-N1	6.40	1.48	1.38
1	16SB	2035	5MC	C2-N3	6.39	1.49	1.36
27	23SA	1964	5MU	C4-N3	-6.38	1.27	1.38
27	23SB	1964	5MU	C4-N3	-6.38	1.27	1.38
26	TRNA	54	5MU	C4-N3	-6.36	1.27	1.38
1	16SB	1834	2MG	C2-N2	6.35	1.47	1.33
27	23SA	1967	5MC	C2-N3	6.34	1.49	1.36
23	PSIA	37	MIA	C6-N6	6.34	1.44	1.34
57	ASIB	37	MIA	C6-N6	6.33	1.44	1.34
23	PSIA	47	3AU	C2-N3	6.32	1.49	1.38
1	16SA	2121	UR3	C6-C5	6.30	1.49	1.35
22	ASIA	54	5MU	C4-N3	-6.28	1.27	1.38
1	16SA	1834	2MG	C4-N3	6.28	1.49	1.34
23	PSIA	47	3AU	C6-C5	6.27	1.49	1.35
23	PSIB	47	3AU	C6-C5	6.26	1.49	1.35
1	16SA	1834	2MG	C2-N2	6.22	1.47	1.33
1	16SA	1590	5MC	C2-N3	6.21	1.49	1.36
1	16SA	2030	4OC	C6-C5	6.21	1.49	1.35
27	23SB	1987	5MC	C2-N3	6.19	1.48	1.36
27	23SA	1987	5MC	C2-N3	6.18	1.48	1.36
1	16SA	2035	5MC	C2-N3	6.17	1.48	1.36
23	PSIB	54	5MU	C4-N3	-6.14	1.27	1.38
1	16SB	2030	4OC	C4-N3	6.13	1.43	1.32
23	PSIB	46	G7M	C5-N7	6.11	1.46	1.39
22	ASIA	37	MIA	C6-N6	6.10	1.44	1.34
27	23SA	1940	5MU	C6-N1	6.09	1.48	1.38
57	ASIB	54	5MU	C4-N3	-6.03	1.27	1.38
23	PSIA	46	G7M	C4-N3	6.03	1.48	1.34
1	16SA	2030	4OC	C2-N3	5.96	1.48	1.36
27	23SB	2518	2MA	C2-N1	5.96	1.44	1.34
22	ASIA	46	G7M	C4-N3	5.92	1.48	1.34
23	PSIB	46	G7M	C5-C4	-5.90	1.23	1.38
27	23SA	2518	2MA	C2-N1	5.90	1.44	1.34
1	16SB	2030	4OC	C6-C5	5.88	1.48	1.35
1	16SA	1156	G7M	C5-C4	-5.84	1.23	1.38
23	PSIB	54	5MU	C2-N3	5.82	1.48	1.38
57	ASIB	54	5MU	C2-N3	5.81	1.48	1.38
23	PSIA	16	H2U	C2-N1	5.81	1.43	1.35
27	23SB	1940	5MU	C6-N1	5.81	1.48	1.38
23	PSIB	16	H2U	C2-N1	5.78	1.43	1.35
1	16SB	1156	G7M	C5-N7	5.78	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	PSIB	46	G7M	C4-N3	5.78	1.48	1.34
22	ASIA	46	G7M	C5-N7	5.77	1.45	1.39
57	ASIB	54	5MU	C6-N1	5.76	1.47	1.38
1	16SB	1156	G7M	C5-C4	-5.75	1.23	1.38
23	PSIB	47	3AU	C2-N3	5.75	1.48	1.38
26	TRNA	16	H2U	C2-N1	5.74	1.43	1.35
1	16SB	1156	G7M	C4-N3	5.73	1.47	1.34
1	16SB	1589	M2G	C2-N3	5.72	1.46	1.32
27	23SA	1940	5MU	C2-N3	5.68	1.48	1.38
22	ASIA	54	5MU	C6-N1	5.65	1.47	1.38
27	23SB	2567	OMU	C6-C5	5.65	1.48	1.35
27	23SB	1964	5MU	C2-N3	5.63	1.48	1.38
22	ASIA	54	5MU	C2-N3	5.63	1.48	1.38
26	TRNA	54	5MU	C6-N1	5.62	1.47	1.38
1	16SA	1156	G7M	C4-N3	5.60	1.47	1.34
27	23SB	1940	5MU	C2-N3	5.60	1.47	1.38
26	TRNA	54	5MU	C2-N3	5.59	1.47	1.38
27	23SA	2567	OMU	C6-C5	5.59	1.48	1.35
22	ASIA	46	G7M	C5-C4	-5.58	1.24	1.38
23	PSIB	54	5MU	C6-N1	5.57	1.47	1.38
1	16SB	2121	UR3	C2-N3	5.55	1.49	1.39
23	PSIA	46	G7M	C5-C4	-5.51	1.24	1.38
27	23SB	2518	2MA	C6-N1	5.48	1.42	1.35
23	PSIA	54	5MU	C6-N1	5.44	1.47	1.38
27	23SA	1964	5MU	C6-N1	5.36	1.47	1.38
23	PSIA	46	G7M	C5-N7	5.36	1.45	1.39
27	23SA	2518	2MA	C2-N3	5.36	1.43	1.34
27	23SA	2518	2MA	C6-N1	5.34	1.42	1.35
27	23SA	1964	5MU	C2-N3	5.33	1.47	1.38
26	TRNA	8	4SU	C5-C4	5.30	1.49	1.42
1	16SA	1589	M2G	C2-N3	5.25	1.45	1.32
1	16SB	2030	4OC	C2-N3	5.24	1.47	1.36
23	PSIA	54	5MU	C2-N3	5.22	1.47	1.38
27	23SB	1964	5MU	C6-N1	5.20	1.46	1.38
23	PSIA	8	4SU	C5-C4	5.20	1.49	1.42
1	16SA	1156	G7M	C5-N7	5.20	1.45	1.39
22	ASIA	8	4SU	C5-C4	5.16	1.49	1.42
1	16SA	2121	UR3	C2-N3	5.13	1.48	1.39
26	TRNA	37	MIA	C2-S10	5.11	1.80	1.75
22	ASIA	54	5MU	C4-C5	5.05	1.53	1.44
27	23SB	2518	2MA	C2-N3	5.05	1.43	1.34
27	23SB	1987	5MC	C4-N4	5.03	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16SB	2032	5MC	C6-N1	5.02	1.46	1.38
1	16SB	1590	5MC	C4-N4	5.02	1.47	1.34
1	16SA	1590	5MC	C4-N4	5.01	1.47	1.34
1	16SA	2028	5MC	C4-N4	5.00	1.47	1.34
27	23SB	1967	5MC	C4-N4	4.96	1.47	1.34
1	16SB	2035	5MC	C4-N4	4.96	1.47	1.34
27	23SA	1967	5MC	C4-N4	4.95	1.47	1.34
1	16SB	2032	5MC	C4-N4	4.95	1.47	1.34
1	16SB	1834	2MG	C2-N1	4.94	1.44	1.36
27	23SA	1964	5MU	C4-C5	4.94	1.53	1.44
27	23SB	1987	5MC	C6-N1	4.91	1.46	1.38
1	16SA	2035	5MC	C6-N1	4.90	1.46	1.38
1	16SA	2035	5MC	C4-N4	4.89	1.46	1.34
27	23SA	1987	5MC	C4-N4	4.88	1.46	1.34
1	16SB	2035	5MC	C6-N1	4.87	1.46	1.38
1	16SA	2032	5MC	C6-N1	4.85	1.46	1.38
1	16SB	2028	5MC	C4-N4	4.84	1.46	1.34
27	23SB	1940	5MU	C4-C5	4.83	1.52	1.44
1	16SA	2032	5MC	C4-N4	4.83	1.46	1.34
1	16SB	1590	5MC	C6-N1	4.82	1.46	1.38
26	TRNA	54	5MU	C4-C5	4.78	1.52	1.44
27	23SA	1940	5MU	C4-C5	4.77	1.52	1.44
23	PSIA	54	5MU	C4-C5	4.71	1.52	1.44
27	23SB	1967	5MC	C6-N1	4.71	1.46	1.38
1	16SB	2028	5MC	C2-N1	4.70	1.50	1.40
1	16SA	1834	2MG	C2-N1	4.70	1.44	1.36
27	23SA	1987	5MC	C6-N1	4.69	1.46	1.38
27	23SB	1964	5MU	C4-C5	4.69	1.52	1.44
23	PSIB	8	4SU	C5-C4	4.62	1.48	1.42
57	ASIB	54	5MU	C4-C5	4.62	1.52	1.44
27	23SA	1967	5MC	C2-N1	4.61	1.50	1.40
1	16SA	2028	5MC	C6-N1	4.58	1.45	1.38
1	16SB	2028	5MC	C6-N1	4.57	1.45	1.38
1	16SB	2035	5MC	C2-N1	4.54	1.49	1.40
1	16SA	1590	5MC	C6-N1	4.52	1.45	1.38
27	23SB	1967	5MC	C2-N1	4.48	1.49	1.40
27	23SB	2266	OMG	C8-N9	-4.48	1.27	1.37
23	PSIB	54	5MU	C4-C5	4.42	1.52	1.44
1	16SA	1589	M2G	C2-N1	4.39	1.47	1.36
27	23SA	2266	OMG	C8-N9	-4.36	1.27	1.37
1	16SB	2032	5MC	C2-N1	4.35	1.49	1.40
1	16SA	2030	4OC	C4-N4	4.35	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16SA	2032	5MC	C2-N1	4.35	1.49	1.40
1	16SB	1589	M2G	C2-N1	4.32	1.47	1.36
27	23SA	1967	5MC	C6-N1	4.32	1.45	1.38
1	16SA	2035	5MC	C2-N1	4.29	1.49	1.40
27	23SB	1945	OMC	C2-N3	4.29	1.45	1.36
27	23SB	1945	OMC	C4-N4	4.27	1.44	1.33
1	16SB	1590	5MC	C2-N1	4.27	1.49	1.40
27	23SA	1945	OMC	C2-N3	4.25	1.45	1.36
26	TRNA	20	H2U	C2-N3	4.23	1.45	1.38
27	23SA	1987	5MC	C2-N1	4.19	1.49	1.40
24	ESIB	37	MIA	C2-S10	4.18	1.79	1.75
27	23SB	1987	5MC	C2-N1	4.15	1.49	1.40
23	PSIB	16	H2U	C2-N3	4.13	1.45	1.38
1	16SB	2030	4OC	C2-N1	4.12	1.48	1.40
1	16SA	1156	G7M	C8-N9	4.12	1.47	1.35
27	23SB	2567	OMU	C4-N3	4.11	1.45	1.38
26	TRNA	16	H2U	C2-N3	4.10	1.45	1.38
24	ESIA	37	MIA	C2-S10	4.08	1.79	1.75
23	PSIB	8	4SU	C2-N1	4.06	1.45	1.38
27	23SA	1945	OMC	C4-N4	4.04	1.43	1.33
1	16SA	1590	5MC	C2-N1	4.00	1.48	1.40
23	PSIA	55	PSU	C6-C5	3.99	1.40	1.35
1	16SB	2030	4OC	C5-C4	3.98	1.49	1.40
1	16SB	1156	G7M	C8-N9	3.98	1.46	1.35
22	ASIA	46	G7M	C8-N9	3.97	1.46	1.35
23	PSIB	46	G7M	C8-N9	3.94	1.46	1.35
27	23SB	2518	2MA	C5-C6	3.92	1.51	1.41
1	16SA	2028	5MC	C2-N1	3.91	1.48	1.40
23	PSIA	16	H2U	C2-N3	3.89	1.44	1.38
27	23SB	1945	OMC	C5-C4	3.89	1.51	1.42
26	TRNA	32	PSU	C6-C5	3.87	1.39	1.35
23	PSIA	46	G7M	C8-N9	3.86	1.46	1.35
1	16SA	2030	4OC	C5-C4	3.85	1.49	1.40
26	TRNA	39	PSU	C6-C5	3.85	1.39	1.35
22	ASIA	32	PSU	C6-C5	3.84	1.39	1.35
1	16SA	1145	PSU	C6-C5	3.84	1.39	1.35
1	16SB	1589	M2G	C5-N7	-3.83	1.31	1.39
27	23SB	1936	PSU	C6-C5	3.82	1.39	1.35
22	ASIA	8	4SU	C2-N1	3.80	1.44	1.38
26	TRNA	8	4SU	C2-N1	3.79	1.44	1.38
27	23SB	1942	PSU	C6-C5	3.78	1.39	1.35
1	16SA	2030	4OC	C2-N1	3.78	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	PSIA	37	MIA	C2-S10	3.77	1.78	1.75
27	23SB	2620	PSU	C6-C5	3.75	1.39	1.35
23	PSIB	46	G7M	C4-N9	-3.74	1.28	1.38
22	ASIA	39	PSU	C6-C5	3.72	1.39	1.35
23	PSIA	8	4SU	C2-N1	3.71	1.44	1.38
23	PSIB	39	PSU	C6-C5	3.71	1.39	1.35
27	23SA	2567	OMU	C4-N3	3.69	1.45	1.38
1	16SB	1156	G7M	C4-N9	-3.69	1.28	1.38
23	PSIA	47	3AU	C4-N3	3.65	1.46	1.40
23	PSIB	55	PSU	C6-C5	3.65	1.39	1.35
1	16SA	1156	G7M	C4-N9	-3.63	1.28	1.38
26	TRNA	55	PSU	C6-C5	3.62	1.39	1.35
1	16SA	1589	M2G	C5-N7	-3.62	1.32	1.39
27	23SA	2518	2MA	C5-N7	-3.61	1.32	1.39
1	16SB	1145	PSU	C6-C5	3.60	1.39	1.35
22	ASIA	37	MIA	C2-S10	3.60	1.78	1.75
23	PSIB	16	H2U	C4-N3	3.57	1.43	1.37
57	ASIB	39	PSU	C6-C5	3.54	1.39	1.35
27	23SA	1945	OMC	C5-C4	3.53	1.51	1.42
57	ASIB	37	MIA	C2-S10	3.52	1.78	1.75
23	PSIB	47	3AU	C4-N3	3.50	1.45	1.40
26	TRNA	37	MIA	C4-N9	3.50	1.45	1.37
27	23SA	2620	PSU	C6-C5	3.49	1.39	1.35
22	ASIA	55	PSU	C6-C5	3.48	1.39	1.35
26	TRNA	16	H2U	C4-N3	3.47	1.43	1.37
26	TRNA	20	H2U	C4-N3	3.45	1.43	1.37
22	ASIA	46	G7M	C4-N9	-3.41	1.29	1.38
1	16SB	2141	MA6	C6-N6	3.40	1.46	1.36
27	23SA	1936	PSU	C6-C5	3.38	1.39	1.35
26	TRNA	37	MIA	C2-N3	3.35	1.39	1.34
26	TRNA	37	MIA	C5-C4	3.35	1.45	1.39
1	16SA	2142	MA6	C6-N6	3.34	1.46	1.36
23	PSIA	16	H2U	C4-N3	3.34	1.43	1.37
23	PSIA	32	PSU	C6-C5	3.30	1.39	1.35
27	23SA	1942	PSU	C6-C5	3.30	1.39	1.35
23	PSIA	39	PSU	C6-C5	3.28	1.39	1.35
1	16SB	2030	4OC	C4-N4	3.27	1.42	1.35
23	PSIB	37	MIA	C2-S10	3.24	1.78	1.75
1	16SB	2035	5MC	O2-C2	-3.24	1.17	1.23
57	ASIB	32	PSU	C6-C5	3.24	1.39	1.35
23	PSIB	8	4SU	C4-N3	3.23	1.41	1.37
1	16SA	2141	MA6	C6-N6	3.22	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16SB	2142	MA6	C6-N6	3.18	1.46	1.36
1	16SB	1834	2MG	C5-N7	-3.17	1.32	1.39
23	PSIB	32	PSU	C6-C5	3.16	1.39	1.35
23	PSIA	46	G7M	C4-N9	-3.15	1.29	1.38
1	16SA	2030	4OC	C6-N1	3.15	1.45	1.38
1	16SA	1834	2MG	O6-C6	-3.15	1.17	1.23
1	16SA	1590	5MC	O2-C2	-3.14	1.17	1.23
27	23SA	2518	2MA	C5-C6	3.12	1.49	1.41
27	23SB	1987	5MC	O2-C2	-3.08	1.18	1.23
23	PSIB	46	G7M	C2-N2	3.06	1.41	1.34
1	16SB	1156	G7M	C2-N2	3.05	1.41	1.34
1	16SB	1834	2MG	O6-C6	-3.05	1.17	1.23
1	16SA	1834	2MG	C5-N7	-3.05	1.33	1.39
27	23SB	2266	OMG	O6-C6	-3.05	1.17	1.23
22	ASIA	46	G7M	C2-N2	3.05	1.41	1.34
1	16SA	2035	5MC	O2-C2	-3.04	1.18	1.23
23	PSIA	46	G7M	C2-N2	3.03	1.41	1.34
1	16SA	1156	G7M	C2-N2	3.03	1.41	1.34
1	16SA	1589	M2G	C4-N9	-3.03	1.30	1.38
1	16SB	2028	5MC	O2-C2	-3.02	1.18	1.23
1	16SB	1590	5MC	O2-C2	-3.02	1.18	1.23
1	16SA	2030	4OC	O2-C2	-2.99	1.18	1.23
1	16SB	2030	4OC	C6-N1	2.99	1.45	1.38
1	16SA	2121	UR3	C6-N1	2.99	1.45	1.38
27	23SB	2518	2MA	C5-N7	-2.98	1.33	1.39
27	23SA	2266	OMG	O6-C6	-2.98	1.17	1.23
1	16SA	2028	5MC	O2-C2	-2.96	1.18	1.23
1	16SB	2032	5MC	O2-C2	-2.96	1.18	1.23
1	16SB	1589	M2G	C5-C6	2.94	1.55	1.44
1	16SB	2121	UR3	C6-N1	2.93	1.45	1.38
26	TRNA	37	MIA	C4-N3	2.90	1.38	1.34
1	16SA	1589	M2G	C5-C6	2.89	1.55	1.44
27	23SB	2567	OMU	O4-C4	-2.89	1.18	1.24
23	PSIA	47	3AU	C6-N1	2.88	1.45	1.38
27	23SA	2567	OMU	O4-C4	-2.85	1.19	1.24
1	16SA	2141	MA6	C8-N9	-2.85	1.32	1.37
23	PSIB	47	3AU	C6-N1	2.79	1.44	1.38
1	16SA	2032	5MC	O2-C2	-2.76	1.18	1.23
27	23SB	1967	5MC	O2-C2	-2.76	1.18	1.23
27	23SB	2266	OMG	C2-N3	2.73	1.39	1.33
23	PSIA	16	H2U	C6-N1	-2.72	1.42	1.47
27	23SA	2266	OMG	C2-N2	2.72	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16SA	2142	MA6	C5-N7	-2.72	1.33	1.39
26	TRNA	37	MIA	C5-N7	-2.72	1.33	1.39
27	23SB	2266	OMG	C2-N2	2.68	1.40	1.34
1	16SA	2142	MA6	C8-N9	-2.67	1.32	1.37
1	16SA	2141	MA6	C5-N7	-2.67	1.34	1.39
22	ASIA	8	4SU	C6-N1	2.66	1.44	1.38
23	PSIA	8	4SU	C6-N1	2.66	1.44	1.38
26	TRNA	8	4SU	C6-N1	2.65	1.44	1.38
1	16SB	2141	MA6	C8-N9	-2.65	1.32	1.37
27	23SA	1967	5MC	O2-C2	-2.64	1.18	1.23
1	16SB	2141	MA6	C5-N7	-2.64	1.34	1.39
27	23SB	2567	OMU	C6-N1	2.63	1.44	1.38
27	23SB	2518	2MA	C8-N7	2.62	1.36	1.31
1	16SA	1834	2MG	C5-C6	2.61	1.54	1.44
1	16SB	1834	2MG	C5-C6	2.60	1.54	1.44
1	16SA	1589	M2G	C6-N1	2.59	1.43	1.38
27	23SA	1987	5MC	O2-C2	-2.59	1.18	1.23
26	TRNA	16	H2U	C6-N1	-2.58	1.42	1.47
1	16SB	2142	MA6	C5-N7	-2.55	1.34	1.39
23	PSIB	16	H2U	C6-N1	-2.55	1.42	1.47
27	23SA	2567	OMU	C6-N1	2.52	1.44	1.38
1	16SA	2141	MA6	C5-C4	-2.51	1.34	1.39
1	16SA	2142	MA6	C8-N7	2.50	1.36	1.31
23	PSIB	8	4SU	C2-N3	2.50	1.42	1.38
1	16SB	1834	2MG	C6-N1	2.49	1.43	1.38
27	23SB	2567	OMU	O2-C2	-2.49	1.18	1.23
27	23SB	2266	OMG	C2-N1	-2.48	1.31	1.37
1	16SB	2142	MA6	C5-C4	-2.48	1.34	1.39
1	16SB	2142	MA6	C8-N7	2.48	1.36	1.31
1	16SB	2142	MA6	C8-N9	-2.47	1.33	1.37
27	23SA	2518	2MA	C8-N7	2.47	1.36	1.31
1	16SA	2142	MA6	C5-C4	-2.45	1.34	1.39
1	16SB	2030	4OC	O2-C2	-2.45	1.19	1.23
27	23SA	2567	OMU	C5-C4	2.45	1.49	1.43
27	23SA	2266	OMG	C2-N3	2.44	1.39	1.33
26	TRNA	20	H2U	C6-N1	-2.44	1.42	1.47
1	16SB	1589	M2G	C6-N1	2.43	1.43	1.38
1	16SB	2141	MA6	C5-C4	-2.41	1.34	1.39
57	ASIB	37	MIA	C5-N7	-2.41	1.34	1.39
23	PSIB	47	3AU	O4-C4	-2.38	1.18	1.23
23	PSIB	8	4SU	C6-N1	2.38	1.43	1.38
1	16SA	2141	MA6	C8-N7	2.36	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	PSIB	47	3AU	C5-C4	2.36	1.49	1.43
23	PSIA	47	3AU	C5-C4	2.31	1.49	1.43
27	23SB	2567	OMU	C5-C4	2.30	1.48	1.43
23	PSIA	37	MIA	C5-N7	-2.30	1.34	1.39
23	PSIA	47	3AU	O4-C4	-2.29	1.18	1.23
27	23SA	2567	OMU	O2-C2	-2.28	1.18	1.23
1	16SA	2121	UR3	C5-C4	2.28	1.49	1.43
1	16SA	2121	UR3	O4-C4	-2.25	1.18	1.23
1	16SA	1834	2MG	C6-N1	2.25	1.43	1.38
1	16SA	1156	G7M	C6-N1	-2.25	1.34	1.38
23	PSIB	47	3AU	O2-C2	-2.22	1.18	1.22
22	ASIA	37	MIA	C5-N7	-2.19	1.34	1.39
1	16SB	2121	UR3	O4-C4	-2.19	1.18	1.23
1	16SB	2121	UR3	C5-C4	2.18	1.49	1.43
1	16SB	2121	UR3	C4-N3	2.18	1.45	1.40
1	16SB	2141	MA6	C8-N7	2.17	1.35	1.31
24	ESIB	37	MIA	C5-N7	-2.15	1.35	1.39
27	23SA	2266	OMG	C2-N1	-2.15	1.32	1.37
1	16SB	1589	M2G	C4-N9	-2.14	1.32	1.38
1	16SB	1156	G7M	C6-N1	-2.12	1.34	1.38
27	23SA	1945	OMC	C6-N1	2.12	1.43	1.38
24	ESIA	37	MIA	C5-N7	-2.11	1.35	1.39
23	PSIA	46	G7M	C6-N1	-2.10	1.34	1.38
23	PSIA	47	3AU	O2-C2	-2.07	1.18	1.22
27	23SB	1945	OMC	C6-N1	2.06	1.43	1.38
22	ASIA	46	G7M	C6-N1	-2.05	1.35	1.38
1	16SA	2121	UR3	C4-N3	2.05	1.45	1.40
12	S12B	89	0TD	OD1-CG	2.04	1.28	1.22
1	16SA	2121	UR3	O2-C2	-2.03	1.18	1.22
23	PSIB	46	G7M	C5-C6	2.02	1.48	1.43
12	S12A	89	0TD	CB-CG	2.00	1.55	1.52
22	ASIA	8	4SU	C2-N3	2.00	1.41	1.38

All (573) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	ESIB	37	MIA	C11-S10-C2	15.35	113.73	102.27
26	TRNA	37	MIA	C5-C4-N3	-12.80	112.79	127.19
1	16SB	1156	G7M	CN7-N7-C5	12.37	142.13	126.77
22	ASIA	46	G7M	CN7-N7-C5	12.24	141.98	126.77
23	PSIA	46	G7M	CN7-N7-C5	11.97	141.64	126.77
1	16SA	1156	G7M	CN7-N7-C5	11.93	141.59	126.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	PSIB	46	G7M	CN7-N7-C5	11.85	141.49	126.77
27	23SA	2266	OMG	C6-C5-N7	11.62	151.84	130.25
26	TRNA	37	MIA	N3-C4-N9	11.60	143.09	126.99
27	23SB	2266	OMG	C6-C5-N7	11.57	151.76	130.25
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
24	ESIA	37	MIA	C11-S10-C2	10.71	110.27	102.27
57	ASIB	54	5MU	C5-C4-N3	10.54	124.31	115.31
22	ASIA	54	5MU	C5-C4-N3	10.45	124.23	115.31
26	TRNA	54	5MU	C5-C4-N3	10.42	124.20	115.31
1	16SA	2142	MA6	N1-C6-N6	-10.26	105.87	117.08
1	16SB	2142	MA6	N1-C6-N6	-10.09	106.06	117.08
27	23SB	2266	OMG	C8-N7-C5	10.08	122.48	104.24
23	PSIB	54	5MU	C5-C4-N3	10.08	123.91	115.31
27	23SA	2266	OMG	C8-N7-C5	9.99	122.31	104.24
27	23SB	1940	5MU	C5-C4-N3	9.86	123.73	115.31
22	ASIA	37	MIA	C12-C13-C14	-9.71	108.24	127.14
27	23SB	1964	5MU	C5-C4-N3	9.61	123.52	115.31
1	16SA	2141	MA6	N1-C6-N6	-9.60	106.59	117.08
27	23SB	2266	OMG	N9-C4-N3	9.35	144.71	125.94
23	PSIB	37	MIA	C12-C13-C14	-9.32	109.01	127.14
27	23SA	2266	OMG	N9-C4-N3	8.87	143.75	125.94
26	TRNA	37	MIA	C12-C13-C14	-8.86	109.89	127.14
57	ASIB	37	MIA	C11-S10-C2	8.77	108.81	102.27
23	PSIB	8	4SU	C4-N3-C2	-8.66	118.93	127.34
26	TRNA	37	MIA	C11-S10-C2	8.65	108.73	102.27
57	ASIB	37	MIA	C12-C13-C14	-8.58	110.45	127.14
22	ASIA	37	MIA	C11-S10-C2	8.55	108.65	102.27
23	PSIA	8	4SU	C4-N3-C2	-8.50	119.08	127.34
1	16SB	2141	MA6	N1-C6-N6	-8.18	108.14	117.08
27	23SA	2266	OMG	C6-C5-C4	-7.92	106.59	118.77
26	TRNA	8	4SU	C4-N3-C2	-7.90	119.67	127.34
27	23SB	2266	OMG	C6-C5-C4	-7.83	106.72	118.77
22	ASIA	8	4SU	C4-N3-C2	-7.69	119.87	127.34
24	ESIA	37	MIA	C12-C13-C14	-7.62	112.31	127.14
27	23SB	2266	OMG	C1'-N9-C4	7.34	148.31	126.50
57	ASIB	37	MIA	C5-C4-N3	-7.28	119.00	127.19
26	TRNA	37	MIA	C1'-N9-C8	-7.08	111.14	127.14
23	PSIA	37	MIA	C5-C4-N3	-7.02	119.29	127.19
27	23SA	1940	5MU	C4-N3-C2	-6.98	118.31	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	TRNA	37	MIA	C4-C5-C6	6.96	122.21	116.81
23	PSIB	8	4SU	C5-C4-S4	-6.95	115.51	124.47
26	TRNA	8	4SU	C5-C4-N3	6.83	121.03	114.69
27	23SA	1964	5MU	C4-N3-C2	-6.82	118.52	127.35
27	23SB	2266	OMG	C5-C6-N1	6.79	130.42	113.19
22	ASIA	46	G7M	C8-N7-C5	-6.78	99.31	107.78
27	23SB	1964	5MU	C6-C5-C4	6.74	123.67	118.03
23	PSIA	37	MIA	C12-C13-C14	-6.74	114.02	127.14
27	23SA	1964	5MU	C5-C6-N1	-6.72	116.43	123.34
27	23SA	2266	OMG	C1'-N9-C4	6.68	146.35	126.50
27	23SB	2518	2MA	C5-C4-N3	-6.67	119.68	127.19
24	ESIB	37	MIA	C5-C4-N3	-6.63	119.73	127.19
23	PSIA	46	G7M	C6-C5-N7	-6.57	124.30	132.25
27	23SB	1964	5MU	C4-N3-C2	-6.56	118.86	127.35
23	PSIA	16	H2U	C4-N3-C2	-6.53	120.38	125.79
23	PSIA	46	G7M	C8-N7-C5	-6.52	99.63	107.78
22	ASIA	37	MIA	C5-C4-N3	-6.51	119.86	127.19
27	23SA	2266	OMG	C5-C6-N1	6.50	129.70	113.19
1	16SB	1156	G7M	C8-N7-C5	-6.47	99.70	107.78
1	16SA	1156	G7M	C8-N7-C5	-6.46	99.70	107.78
23	PSIA	54	5MU	C5-C6-N1	-6.44	116.71	123.34
22	ASIA	54	5MU	C4-N3-C2	-6.44	119.02	127.35
23	PSIB	46	G7M	C8-N7-C5	-6.41	99.76	107.78
1	16SB	1834	2MG	C2-N3-C4	6.41	119.99	112.04
23	PSIA	8	4SU	C5-C4-N3	6.35	120.58	114.69
26	TRNA	37	MIA	C4-N9-C1'	6.34	141.69	126.59
26	TRNA	16	H2U	C4-N3-C2	-6.34	120.53	125.79
24	ESIA	37	MIA	C5-C4-N3	-6.29	120.12	127.19
27	23SB	1940	5MU	C4-N3-C2	-6.27	119.24	127.35
1	16SA	1834	2MG	C2-N3-C4	6.19	119.72	112.04
26	TRNA	54	5MU	C4-N3-C2	-6.18	119.35	127.35
27	23SA	2518	2MA	C5-C4-N3	-6.14	120.28	127.19
27	23SB	1940	5MU	C6-C5-C4	6.11	123.14	118.03
27	23SB	1964	5MU	C5-C6-N1	-6.10	117.06	123.34
22	ASIA	46	G7M	C6-C5-N7	-6.06	124.92	132.25
57	ASIB	54	5MU	C4-N3-C2	-6.05	119.52	127.35
27	23SA	1940	5MU	C5-C6-N1	-6.04	117.13	123.34
22	ASIA	8	4SU	C5-C4-N3	6.01	120.27	114.69
27	23SA	1964	5MU	C6-C5-C4	5.99	123.04	118.03
27	23SA	1940	5MU	C6-C5-C4	5.97	123.02	118.03
27	23SA	2567	OMU	C4-N3-C2	-5.96	118.72	126.58
22	ASIA	54	5MU	C5-C6-N1	-5.95	117.21	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	16SA	1156	G7M	C6-C5-N7	-5.93	125.07	132.25
23	PSIB	37	MIA	C5-C4-N3	-5.91	120.54	127.19
23	PSIA	54	5MU	C4-N3-C2	-5.89	119.73	127.35
27	23SB	2266	OMG	C5-C4-N3	-5.87	118.94	128.46
27	23SB	2266	OMG	C4-C5-N7	-5.81	101.52	110.72
27	23SA	2266	OMG	C4-C5-N7	-5.79	101.56	110.72
23	PSIB	54	5MU	C4-N3-C2	-5.69	119.98	127.35
1	16SB	2141	MA6	N1-C2-N3	-5.69	119.71	128.60
23	PSIB	47	3AU	C1'-N1-C2	5.68	126.57	116.99
1	16SB	2142	MA6	N1-C2-N3	-5.67	119.74	128.60
26	TRNA	54	5MU	C6-C5-C4	5.66	122.77	118.03
23	PSIB	46	G7M	N9-C8-N7	-5.64	98.25	112.21
27	23SB	2567	OMU	C4-N3-C2	-5.64	119.14	126.58
26	TRNA	54	5MU	C5-C6-N1	-5.63	117.55	123.34
23	PSIB	54	5MU	O4-C4-C5	-5.63	118.38	124.90
22	ASIA	54	5MU	C6-C5-C4	5.56	122.68	118.03
1	16SA	2142	MA6	N1-C2-N3	-5.55	119.91	128.60
57	ASIB	37	MIA	N3-C4-N9	5.55	134.69	126.99
1	16SA	2141	MA6	N1-C2-N3	-5.47	120.04	128.60
1	16SB	1156	G7M	N9-C8-N7	-5.47	98.67	112.21
23	PSIB	8	4SU	C5-C4-N3	5.45	119.75	114.69
1	16SA	1156	G7M	N9-C8-N7	-5.43	98.78	112.21
23	PSIB	47	3AU	O2-C2-N3	-5.40	114.48	121.99
27	23SB	1940	5MU	C5-C6-N1	-5.39	117.79	123.34
1	16SB	1589	M2G	C5-C4-N3	-5.39	119.72	128.46
26	TRNA	37	MIA	C15-C14-C13	-5.39	107.07	122.65
23	PSIB	16	H2U	C4-N3-C2	-5.36	121.34	125.79
27	23SA	2266	OMG	C5-C4-N3	-5.35	119.79	128.46
1	16SB	1834	2MG	C5-C4-N3	-5.34	119.79	128.46
57	ASIB	54	5MU	O4-C4-C5	-5.30	118.76	124.90
27	23SA	1940	5MU	O4-C4-C5	-5.28	118.78	124.90
23	PSIA	46	G7M	N9-C8-N7	-5.27	99.17	112.21
22	ASIA	46	G7M	N9-C8-N7	-5.26	99.19	112.21
57	ASIB	54	5MU	C5-C6-N1	-5.19	118.00	123.34
23	PSIA	54	5MU	C6-C5-C4	5.17	122.35	118.03
57	ASIB	54	5MU	C6-C5-C4	5.12	122.31	118.03
27	23SB	2266	OMG	C5-C4-N9	-5.12	96.35	105.63
26	TRNA	20	H2U	C4-N3-C2	-5.10	121.56	125.79
23	PSIA	37	MIA	N3-C4-N9	5.08	134.04	126.99
27	23SA	2266	OMG	C5-C4-N9	-5.06	96.46	105.63
23	PSIA	37	MIA	C11-S10-C2	5.05	106.04	102.27
1	16SA	1834	2MG	C5-C4-N3	-5.04	120.29	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	16SB	1156	G7M	C6-C5-N7	-5.04	126.15	132.25
1	16SB	2141	MA6	C5-C4-N3	-5.01	120.22	126.75
24	ESIB	37	MIA	C16-C14-C13	-4.99	108.23	122.65
1	16SA	2142	MA6	C5-C6-N6	4.94	133.90	125.30
27	23SB	1964	5MU	O4-C4-C5	-4.93	119.19	124.90
1	16SA	2141	MA6	C5-C4-N3	-4.92	120.33	126.75
22	ASIA	37	MIA	N3-C4-N9	4.88	133.76	126.99
1	16SA	2121	UR3	C4-N3-C2	-4.88	119.97	124.56
22	ASIA	37	MIA	C16-C14-C13	-4.86	108.60	122.65
26	TRNA	54	5MU	O4-C4-C5	-4.85	119.28	124.90
1	16SA	2141	MA6	N9-C8-N7	-4.85	107.29	113.91
24	ESIA	37	MIA	C16-C14-C13	-4.84	108.64	122.65
1	16SB	2142	MA6	C5-C4-N3	-4.80	120.49	126.75
1	16SA	2142	MA6	N9-C8-N7	-4.79	107.36	113.91
23	PSIB	46	G7M	C6-C5-N7	-4.78	126.47	132.25
27	23SA	1964	5MU	O4-C4-C5	-4.72	119.43	124.90
57	ASIB	37	MIA	C15-C14-C13	-4.69	109.08	122.65
27	23SB	1940	5MU	O4-C4-C5	-4.69	119.47	124.90
23	PSIB	37	MIA	C16-C14-C13	-4.68	109.11	122.65
23	PSIA	54	5MU	O4-C4-C5	-4.68	119.48	124.90
27	23SB	2620	PSU	C4-N3-C2	-4.66	119.63	126.34
23	PSIB	54	5MU	C6-C5-C4	4.66	121.92	118.03
26	TRNA	55	PSU	C4-N3-C2	-4.65	119.64	126.34
27	23SA	1936	PSU	N1-C2-N3	4.64	120.39	115.13
26	TRNA	39	PSU	N1-C2-N3	4.63	120.38	115.13
1	16SB	2142	MA6	C5-C6-N6	4.62	133.35	125.30
27	23SB	1940	5MU	C6-N1-C2	-4.61	116.62	121.30
1	16SA	2141	MA6	C5-C6-N6	4.61	133.33	125.30
22	ASIA	37	MIA	C15-C14-C13	-4.61	109.33	122.65
23	PSIB	8	4SU	S4-C4-N3	4.60	124.74	120.21
27	23SA	2620	PSU	N1-C2-N3	4.60	120.34	115.13
24	ESIB	37	MIA	N3-C4-N9	4.58	133.35	126.99
23	PSIB	46	G7M	C2-N3-C4	4.57	120.44	112.30
27	23SB	2266	OMG	N9-C8-N7	4.57	122.00	113.39
27	23SA	2620	PSU	C4-N3-C2	-4.56	119.77	126.34
1	16SB	1145	PSU	C4-N3-C2	-4.56	119.78	126.34
23	PSIA	46	G7M	C5-C4-N3	-4.54	119.44	128.15
26	TRNA	39	PSU	C4-N3-C2	-4.54	119.80	126.34
27	23SB	1940	5MU	C5M-C5-C6	-4.54	116.78	122.85
23	PSIA	37	MIA	C15-C14-C13	-4.54	109.53	122.65
22	ASIA	54	5MU	C5M-C5-C6	-4.54	116.79	122.85
23	PSIB	54	5MU	C6-N1-C2	-4.54	116.70	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	16SA	1589	M2G	N1-C2-N2	4.53	121.89	118.04
23	PSIB	55	PSU	C4-N3-C2	-4.53	119.82	126.34
22	ASIA	8	4SU	C5-C4-S4	-4.52	118.65	124.47
1	16SB	2142	MA6	N9-C8-N7	-4.51	107.74	113.91
27	23SA	1936	PSU	C4-N3-C2	-4.51	119.84	126.34
27	23SA	1942	PSU	C4-N3-C2	-4.51	119.84	126.34
1	16SA	1145	PSU	N1-C2-N3	4.50	120.23	115.13
26	TRNA	55	PSU	N1-C2-N3	4.48	120.21	115.13
1	16SA	2142	MA6	C5-C4-N3	-4.46	120.93	126.75
27	23SA	1942	PSU	N1-C2-N3	4.46	120.19	115.13
27	23SA	1964	5MU	C5M-C5-C6	-4.45	116.90	122.85
22	ASIA	54	5MU	O4-C4-C5	-4.45	119.75	124.90
27	23SB	2266	OMG	C1'-N9-C8	-4.44	114.05	126.70
26	TRNA	54	5MU	C5M-C5-C6	-4.44	116.92	122.85
22	ASIA	46	G7M	C4-C5-N7	4.44	114.92	107.67
23	PSIB	37	MIA	C15-C14-C13	-4.44	109.82	122.65
23	PSIA	39	PSU	C4-N3-C2	-4.43	119.95	126.34
23	PSIA	46	G7M	C4-C5-N7	4.42	114.90	107.67
27	23SB	2266	OMG	C8-N9-C4	-4.41	97.65	106.05
27	23SA	2266	OMG	N9-C8-N7	4.41	121.70	113.39
23	PSIA	8	4SU	C5-C4-S4	-4.41	118.78	124.47
23	PSIA	46	G7M	C2-N3-C4	4.40	120.15	112.30
1	16SB	1834	2MG	C2-N1-C6	-4.39	119.42	124.48
22	ASIA	55	PSU	N1-C2-N3	4.38	120.09	115.13
26	TRNA	32	PSU	C4-N3-C2	-4.38	120.03	126.34
1	16SB	2141	MA6	N9-C8-N7	-4.37	107.94	113.91
22	ASIA	46	G7M	C2-N3-C4	4.37	120.08	112.30
27	23SB	1942	PSU	C4-N3-C2	-4.37	120.05	126.34
23	PSIA	55	PSU	N1-C2-N3	4.36	120.07	115.13
24	ESIA	37	MIA	N3-C4-N9	4.35	133.03	126.99
27	23SB	2518	2MA	N9-C8-N7	-4.33	107.99	113.91
22	ASIA	39	PSU	C4-N3-C2	-4.33	120.10	126.34
1	16SB	1156	G7M	CN7-N7-C8	-4.32	118.17	124.84
57	ASIB	32	PSU	C4-N3-C2	-4.32	120.11	126.34
26	TRNA	32	PSU	N1-C2-N3	4.32	120.02	115.13
27	23SA	2567	OMU	N3-C2-N1	4.31	120.61	114.89
1	16SA	1589	M2G	C5-C4-N3	-4.31	121.47	128.46
23	PSIB	37	MIA	C6-C5-N7	4.31	137.05	132.39
23	PSIB	32	PSU	N1-C2-N3	4.30	120.00	115.13
57	ASIB	39	PSU	C4-N3-C2	-4.29	120.15	126.34
1	16SA	1156	G7M	C4-C5-N7	4.29	114.67	107.67
23	PSIB	32	PSU	C4-N3-C2	-4.28	120.17	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	PSIA	32	PSU	C4-N3-C2	-4.28	120.18	126.34
1	16SB	2030	4OC	CM4-N4-C4	-4.27	114.10	122.45
27	23SA	2266	OMG	C8-N9-C4	-4.25	97.95	106.05
57	ASIB	32	PSU	N1-C2-N3	4.25	119.94	115.13
23	PSIA	54	5MU	C5M-C5-C6	-4.24	117.18	122.85
23	PSIB	39	PSU	C4-N3-C2	-4.24	120.23	126.34
1	16SB	1156	G7M	C2-N3-C4	4.22	119.81	112.30
22	ASIA	55	PSU	C4-N3-C2	-4.21	120.28	126.34
1	16SB	1145	PSU	N1-C2-N3	4.19	119.88	115.13
22	ASIA	46	G7M	C5-C4-N3	-4.17	120.15	128.15
1	16SA	1834	2MG	C2-N1-C6	-4.17	119.69	124.48
23	PSIB	37	MIA	C5-N7-C8	4.16	109.43	103.51
1	16SA	1156	G7M	C2-N3-C4	4.16	119.71	112.30
23	PSIB	54	5MU	C5M-C5-C6	-4.16	117.30	122.85
23	PSIB	8	4SU	N3-C2-N1	4.16	120.41	114.89
24	ESIA	37	MIA	C5-N7-C8	4.15	109.41	103.51
26	TRNA	8	4SU	C5-C4-S4	-4.15	119.12	124.47
27	23SB	1964	5MU	C5M-C5-C6	-4.15	117.31	122.85
57	ASIB	54	5MU	C5M-C5-C6	-4.14	117.31	122.85
27	23SA	2518	2MA	N9-C8-N7	-4.14	108.25	113.91
23	PSIB	39	PSU	N1-C2-N3	4.13	119.81	115.13
27	23SB	1936	PSU	C4-N3-C2	-4.13	120.39	126.34
27	23SB	1942	PSU	N1-C2-N3	4.12	119.80	115.13
27	23SA	2518	2MA	N3-C4-N9	4.12	132.70	126.99
27	23SB	2620	PSU	N1-C2-N3	4.11	119.78	115.13
23	PSIB	55	PSU	N1-C2-N3	4.11	119.78	115.13
24	ESIB	37	MIA	C15-C14-C13	-4.10	110.80	122.65
23	PSIA	39	PSU	N1-C2-N3	4.09	119.77	115.13
1	16SA	1145	PSU	C4-N3-C2	-4.09	120.44	126.34
1	16SB	1156	G7M	C4-C5-N7	4.09	114.35	107.67
27	23SA	1940	5MU	C5M-C5-C6	-4.08	117.40	122.85
22	ASIA	37	MIA	C5-N7-C8	4.08	109.31	103.51
1	16SA	1590	5MC	C5-C6-N1	-4.08	119.14	123.34
23	PSIA	37	MIA	C5-N7-C8	4.06	109.28	103.51
26	TRNA	37	MIA	C5-N7-C8	4.06	109.28	103.51
24	ESIB	37	MIA	C5-N7-C8	4.06	109.28	103.51
27	23SA	1940	5MU	C6-N1-C2	-4.05	117.19	121.30
23	PSIA	8	4SU	N3-C2-N1	4.05	120.27	114.89
23	PSIB	46	G7M	C5-C6-N1	4.05	120.25	111.79
57	ASIB	37	MIA	C16-C14-C13	-4.03	110.99	122.65
1	16SA	1156	G7M	C5-C4-N3	-4.02	120.43	128.15
57	ASIB	39	PSU	N1-C2-N3	4.02	119.69	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	PSIB	46	G7M	C4-C5-N7	4.02	114.23	107.67
27	23SA	2266	OMG	O6-C6-C5	-4.01	115.97	126.60
24	ESIA	37	MIA	C15-C14-C13	-4.00	111.09	122.65
23	PSIA	32	PSU	N1-C2-N3	3.99	119.65	115.13
1	16SA	1156	G7M	CN7-N7-C8	-3.98	118.70	124.84
22	ASIA	46	G7M	CN7-N7-C8	-3.97	118.71	124.84
24	ESIB	37	MIA	C12-N6-C6	-3.96	116.67	122.55
23	PSIA	46	G7M	CN7-N7-C8	-3.96	118.73	124.84
23	PSIA	16	H2U	C5-C4-N3	3.95	121.09	116.65
27	23SB	2266	OMG	O6-C6-C5	-3.95	116.12	126.60
1	16SA	2028	5MC	C5-C6-N1	-3.95	119.27	123.34
23	PSIB	46	G7M	CN7-N7-C8	-3.95	118.75	124.84
26	TRNA	37	MIA	C16-C14-C13	-3.92	111.31	122.65
12	S12B	89	0TD	OD2-CG-CB	3.91	121.59	113.15
23	PSIB	54	5MU	C5-C6-N1	-3.90	119.32	123.34
22	ASIA	32	PSU	N1-C2-N3	3.89	119.54	115.13
1	16SB	1156	G7M	C5-C6-N1	3.89	119.91	111.79
1	16SB	2141	MA6	C5-C6-N6	3.89	132.07	125.30
23	PSIB	46	G7M	C5-C4-N3	-3.89	120.69	128.15
26	TRNA	37	MIA	C2-N3-C4	3.89	122.58	112.35
57	ASIB	37	MIA	C5-N7-C8	3.88	109.02	103.51
27	23SA	2266	OMG	C1'-N9-C8	-3.87	115.68	126.70
27	23SB	2567	OMU	N3-C2-N1	3.87	120.03	114.89
1	16SB	2121	UR3	C4-N3-C2	-3.86	120.93	124.56
23	PSIB	47	3AU	C6-N1-C2	-3.85	118.34	121.79
23	PSIA	55	PSU	C4-N3-C2	-3.85	120.79	126.34
23	PSIA	47	3AU	C1'-N1-C2	3.84	123.48	116.99
22	ASIA	32	PSU	C4-N3-C2	-3.84	120.80	126.34
22	ASIA	46	G7M	C5-C6-N1	3.84	119.81	111.79
27	23SB	2518	2MA	N3-C4-N9	3.83	132.31	126.99
23	PSIB	37	MIA	C12-N6-C6	-3.82	116.88	122.55
23	PSIB	37	MIA	C4-C5-N7	-3.82	105.97	110.62
23	PSIA	46	G7M	C5-C6-N1	3.79	119.71	111.79
1	16SA	1156	G7M	C5-C6-N1	3.79	119.70	111.79
27	23SB	1964	5MU	C6-N1-C2	-3.79	117.46	121.30
23	PSIB	37	MIA	C11-S10-C2	3.78	105.09	102.27
26	TRNA	16	H2U	C5-C4-N3	3.78	120.89	116.65
1	16SB	1589	M2G	C2-N3-C4	3.78	119.49	112.51
1	16SB	1156	G7M	C5-C4-N3	-3.77	120.91	128.15
22	ASIA	39	PSU	N1-C2-N3	3.76	119.39	115.13
27	23SA	1967	5MC	C5-C6-N1	-3.73	119.50	123.34
23	PSIB	46	G7M	C5-C4-N9	3.72	114.05	105.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	16SA	1156	G7M	C5-C4-N9	3.72	114.04	105.89
1	16SB	1156	G7M	C5-C4-N9	3.72	114.04	105.89
27	23SB	2518	2MA	C4-N9-C1'	-3.72	117.74	126.59
1	16SA	1156	G7M	O6-C6-C5	-3.71	119.69	128.06
1	16SB	2141	MA6	C2-N1-C6	3.68	120.45	111.75
23	PSIB	16	H2U	C5-C4-N3	3.67	120.78	116.65
23	PSIA	37	MIA	C16-C14-C13	-3.67	112.05	122.65
1	16SA	1589	M2G	C2-N3-C4	3.65	119.25	112.51
26	TRNA	37	MIA	C6-C5-N7	-3.64	128.46	132.39
27	23SA	1987	5MC	C5-C6-N1	-3.63	119.61	123.34
1	16SB	2028	5MC	C5-C6-N1	-3.62	119.61	123.34
23	PSIB	8	4SU	O2-C2-N1	-3.60	118.00	122.79
1	16SA	2142	MA6	C2-N1-C6	3.60	120.26	111.75
22	ASIA	46	G7M	O6-C6-C5	-3.60	119.95	128.06
27	23SB	1936	PSU	N1-C2-N3	3.59	119.20	115.13
22	ASIA	8	4SU	N3-C2-N1	3.59	119.65	114.89
1	16SA	2141	MA6	C2-N1-C6	3.57	120.17	111.75
1	16SA	2035	5MC	C5-C6-N1	-3.56	119.67	123.34
27	23SA	2266	OMG	N2-C2-N1	3.56	124.29	116.71
23	PSIA	46	G7M	O6-C6-C5	-3.55	120.06	128.06
1	16SB	2142	MA6	C2-N3-C4	3.54	120.11	111.75
23	PSIB	37	MIA	N3-C4-N9	3.53	131.89	126.99
1	16SB	2141	MA6	C4-C5-C6	3.52	119.82	115.88
1	16SB	2142	MA6	C2-N1-C6	3.51	120.05	111.75
23	PSIB	46	G7M	O6-C6-C5	-3.50	120.16	128.06
22	ASIA	46	G7M	C5-C4-N9	3.50	113.56	105.89
1	16SB	2141	MA6	C2-N3-C4	3.50	120.02	111.75
27	23SA	2567	OMU	C5-C4-N3	3.49	120.07	114.84
27	23SB	2567	OMU	C5-C4-N3	3.49	120.07	114.84
26	TRNA	54	5MU	C6-N1-C2	-3.49	117.76	121.30
23	PSIB	47	3AU	C4-N3-C2	-3.47	120.28	124.63
1	16SA	2141	MA6	C4-C5-C6	3.47	119.77	115.88
27	23SB	2266	OMG	O6-C6-N1	-3.47	113.46	120.12
23	PSIA	37	MIA	C12-N6-C6	-3.46	117.42	122.55
57	ASIB	54	5MU	C6-N1-C2	-3.45	117.81	121.30
26	TRNA	20	H2U	C5-C6-N1	3.45	122.97	111.61
1	16SB	2141	MA6	N3-C4-N9	3.43	132.73	127.08
27	23SB	1940	5MU	N3-C2-N1	3.42	119.43	114.89
27	23SB	1964	5MU	N3-C2-N1	3.42	119.42	114.89
26	TRNA	20	H2U	C5-C4-N3	3.41	120.48	116.65
1	16SB	1590	5MC	C5-C6-N1	-3.39	119.85	123.34
1	16SA	2142	MA6	C2-N3-C4	3.39	119.75	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	23SB	2518	2MA	C5-N7-C8	3.38	108.31	103.51
26	TRNA	16	H2U	N3-C2-N1	3.38	120.23	116.65
23	PSIA	46	G7M	C5-C4-N9	3.37	113.27	105.89
1	16SA	2142	MA6	C5-N7-C8	3.35	108.27	103.51
27	23SA	1940	5MU	N3-C2-N1	3.34	119.33	114.89
23	PSIA	16	H2U	N3-C2-N1	3.34	120.19	116.65
1	16SA	2141	MA6	C2-N3-C4	3.33	119.62	111.75
23	PSIB	16	H2U	C5-C6-N1	3.33	122.58	111.61
12	S12A	89	0TD	OD2-CG-CB	3.31	120.30	113.15
1	16SA	2141	MA6	C5-N7-C8	3.31	108.21	103.51
27	23SA	2518	2MA	C4-N9-C1'	-3.30	118.72	126.59
1	16SB	1156	G7M	O6-C6-C5	-3.30	120.62	128.06
24	ESIA	37	MIA	C4-C5-N7	-3.26	106.65	110.62
1	16SA	1589	M2G	N9-C8-N7	-3.24	107.29	113.39
26	TRNA	8	4SU	N3-C2-N1	3.23	119.18	114.89
26	TRNA	37	MIA	C5-C4-N9	-3.23	102.03	105.78
1	16SB	1589	M2G	N9-C4-N3	3.21	132.39	125.94
23	PSIA	47	3AU	C4-N3-C2	-3.20	120.62	124.63
1	16SA	2141	MA6	N3-C4-N9	3.19	132.34	127.08
22	ASIA	54	5MU	C6-N1-C2	-3.19	118.07	121.30
27	23SA	1942	PSU	O2-C2-N1	-3.18	119.29	122.79
23	PSIA	37	MIA	C4-C5-N7	-3.18	106.75	110.62
27	23SA	1936	PSU	O2-C2-N1	-3.15	119.32	122.79
24	ESIB	37	MIA	C4-C5-N7	-3.15	106.78	110.62
27	23SB	2518	2MA	C1'-N9-C8	3.15	134.24	127.14
23	PSIA	55	PSU	C6-N1-C2	-3.14	119.47	122.68
22	ASIA	37	MIA	C4-C5-N7	-3.13	106.80	110.62
1	16SB	1834	2MG	N9-C4-N3	3.13	132.22	125.94
1	16SA	2141	MA6	C4-N9-C8	3.11	109.10	105.73
23	PSIA	47	3AU	C6-N1-C2	-3.11	119.00	121.79
27	23SB	2567	OMU	O4-C4-C5	-3.10	119.70	125.16
1	16SB	2121	UR3	C1'-N1-C2	3.08	122.19	116.99
24	ESIB	37	MIA	C2-N3-C4	3.08	120.46	112.35
23	PSIA	37	MIA	C2-N3-C4	3.07	120.42	112.35
27	23SB	2266	OMG	N2-C2-N1	3.06	123.23	116.71
1	16SA	1156	G7M	C2-N1-C6	-3.05	119.54	125.10
1	16SA	1834	2MG	C1'-N9-C4	-3.05	117.45	126.50
57	ASIB	37	MIA	C4-C5-N7	-3.03	106.93	110.62
23	PSIA	46	G7M	C2-N1-C6	-3.03	119.58	125.10
1	16SB	2030	4OC	C2'-C1'-N1	-3.02	108.36	114.22
1	16SB	2121	UR3	C6-N1-C2	-3.02	119.08	121.79
27	23SA	2266	OMG	O6-C6-N1	-3.02	114.33	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	16SB	2142	MA6	C5-N7-C8	3.02	107.79	103.51
22	ASIA	37	MIA	C2-N3-C4	3.01	120.27	112.35
26	TRNA	20	H2U	N3-C2-N1	3.00	119.82	116.65
26	TRNA	16	H2U	C5-C6-N1	3.00	121.48	111.61
1	16SB	2141	MA6	C5-N7-C8	3.00	107.77	103.51
57	ASIB	37	MIA	C2-N3-C4	2.99	120.22	112.35
23	PSIB	46	G7M	C2-N1-C6	-2.99	119.65	125.10
22	ASIA	37	MIA	C12-N6-C6	-2.98	118.12	122.55
1	16SA	1834	2MG	N9-C8-N7	-2.96	107.82	113.39
27	23SB	1967	5MC	C5-C6-N1	-2.96	120.30	123.34
22	ASIA	37	MIA	C6-C5-N7	2.95	135.59	132.39
1	16SA	1145	PSU	C6-N1-C2	-2.95	119.67	122.68
23	PSIB	37	MIA	C2-N3-C4	2.95	120.11	112.35
22	ASIA	37	MIA	N9-C8-N7	-2.94	109.89	113.91
22	ASIA	54	5MU	N3-C2-N1	2.94	118.79	114.89
23	PSIA	16	H2U	C5-C6-N1	2.93	121.26	111.61
24	ESIA	37	MIA	N9-C8-N7	-2.91	109.93	113.91
23	PSIB	47	3AU	C5-C4-N3	2.90	119.32	115.50
23	PSIA	47	3AU	C5-C4-N3	2.90	119.32	115.50
23	PSIB	37	MIA	N9-C8-N7	-2.89	109.96	113.91
1	16SB	1156	G7M	C2-N1-C6	-2.88	119.84	125.10
24	ESIA	37	MIA	C2-N3-C4	2.88	119.94	112.35
27	23SA	2518	2MA	N6-C6-N1	2.87	121.09	117.03
22	ASIA	46	G7M	C2-N1-C6	-2.87	119.87	125.10
27	23SA	2518	2MA	N3-C2-N1	-2.85	120.48	125.72
1	16SB	1834	2MG	N9-C8-N7	-2.83	108.07	113.39
23	PSIA	47	3AU	O2-C2-N3	-2.82	118.08	121.99
1	16SB	2142	MA6	C4-C5-C6	2.81	119.03	115.88
1	16SA	1834	2MG	N9-C4-N3	2.80	131.56	125.94
27	23SB	2567	OMU	O2-C2-N1	-2.80	119.07	122.79
57	ASIB	39	PSU	O2-C2-N1	-2.79	119.71	122.79
27	23SA	1964	5MU	N3-C2-N1	2.79	118.59	114.89
24	ESIB	37	MIA	C6-C5-N7	2.78	135.40	132.39
27	23SB	1987	5MC	C5-C6-N1	-2.78	120.48	123.34
22	ASIA	55	PSU	O2-C2-N1	-2.78	119.73	122.79
26	TRNA	32	PSU	O2-C2-N1	-2.78	119.73	122.79
23	PSIA	55	PSU	O2-C2-N1	-2.77	119.74	122.79
1	16SB	2142	MA6	N3-C4-N9	2.77	131.65	127.08
22	ASIA	54	5MU	O2-C2-N1	-2.76	119.11	122.79
1	16SB	1834	2MG	C1'-N9-C4	-2.75	118.33	126.50
27	23SB	2518	2MA	N3-C2-N1	-2.74	120.68	125.72
1	16SA	2142	MA6	C4-C5-C6	2.74	118.95	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	23SA	2266	OMG	C2-N1-C6	2.74	130.09	125.10
26	TRNA	39	PSU	O2-C2-N1	-2.73	119.79	122.79
27	23SB	1964	5MU	O2-C2-N1	-2.73	119.16	122.79
1	16SA	2142	MA6	C4-N9-C8	2.70	108.66	105.73
1	16SB	2141	MA6	C4-N9-C8	2.70	108.66	105.73
26	TRNA	55	PSU	O2-C2-N1	-2.69	119.83	122.79
24	ESIA	37	MIA	C6-C5-N7	2.68	135.29	132.39
26	TRNA	37	MIA	C16-C14-C15	-2.67	108.70	114.60
57	ASIB	37	MIA	C1'-N9-C8	-2.66	121.12	127.14
26	TRNA	16	H2U	O2-C2-N1	-2.66	119.76	123.11
23	PSIA	37	MIA	C6-C5-N7	2.66	135.27	132.39
24	ESIB	37	MIA	N9-C8-N7	-2.65	110.29	113.91
23	PSIB	16	H2U	N3-C2-N1	2.65	119.45	116.65
1	16SA	1834	2MG	C1'-N9-C8	2.64	134.22	126.70
23	PSIB	47	3AU	C1'-N1-C6	-2.64	115.08	120.84
23	PSIB	54	5MU	C1'-N1-C2	2.64	122.34	117.57
26	TRNA	54	5MU	N3-C2-N1	2.62	118.37	114.89
27	23SA	2518	2MA	C1'-N9-C8	2.61	133.04	127.14
23	PSIB	46	G7M	C8-N9-C4	2.59	113.71	107.16
1	16SB	2035	5MC	C5-C6-N1	-2.59	120.68	123.34
24	ESIB	37	MIA	C16-C14-C15	-2.58	108.90	114.60
57	ASIB	32	PSU	O2-C2-N1	-2.58	119.95	122.79
27	23SA	2518	2MA	C5-N7-C8	2.58	107.17	103.51
23	PSIA	37	MIA	N9-C8-N7	-2.56	110.41	113.91
27	23SA	2567	OMU	O4-C4-C5	-2.56	120.65	125.16
24	ESIB	37	MIA	N3-C2-N1	-2.56	122.25	126.95
27	23SA	2518	2MA	C6-C5-C4	2.56	120.62	117.18
27	23SA	1964	5MU	O2-C2-N1	-2.55	119.40	122.79
1	16SB	2142	MA6	C4-N9-C8	2.54	108.49	105.73
22	ASIA	55	PSU	C6-N1-C2	-2.53	120.09	122.68
1	16SB	1589	M2G	N9-C8-N7	-2.53	108.62	113.39
23	PSIB	37	MIA	C16-C14-C15	-2.53	109.01	114.60
1	16SB	1834	2MG	C5-C6-N1	2.53	119.61	113.19
27	23SA	1936	PSU	C6-N1-C2	-2.52	120.11	122.68
27	23SB	2266	OMG	C2-N1-C6	2.51	129.68	125.10
1	16SA	2142	MA6	C4-C5-N7	-2.51	107.57	110.62
23	PSIB	39	PSU	O2-C2-N1	-2.48	120.06	122.79
1	16SA	1834	2MG	C5-C6-N1	2.48	119.48	113.19
1	16SB	1834	2MG	C1'-N9-C8	2.47	133.74	126.70
24	ESIA	37	MIA	N3-C2-N1	-2.47	122.42	126.95
23	PSIB	32	PSU	C6-N1-C2	-2.46	120.16	122.68
27	23SA	2620	PSU	C6-C5-C4	2.46	119.92	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	PSIB	47	3AU	C10-N3-C4	2.45	121.97	117.14
27	23SB	2620	PSU	O2-C2-N1	-2.45	120.10	122.79
23	PSIB	32	PSU	O2-C2-N1	-2.45	120.10	122.79
23	PSIB	54	5MU	N3-C2-N1	2.44	118.13	114.89
27	23SA	1964	5MU	C6-N1-C2	-2.43	118.83	121.30
27	23SB	2518	2MA	C4-C5-N7	-2.41	107.68	110.62
22	ASIA	37	MIA	N3-C2-N1	-2.41	122.54	126.95
27	23SA	2620	PSU	C6-N1-C2	-2.40	120.22	122.68
1	16SB	1156	G7M	C8-N9-C4	2.40	113.24	107.16
27	23SB	2266	OMG	N1-C2-N3	-2.40	118.84	123.32
27	23SB	1940	5MU	O3'-C3'-C2'	2.40	119.57	111.82
1	16SB	1589	M2G	C5-C6-N1	2.40	119.28	113.19
57	ASIB	54	5MU	N3-C2-N1	2.39	118.06	114.89
22	ASIA	32	PSU	C6-N1-C2	-2.39	120.24	122.68
1	16SA	1589	M2G	C5-C6-N1	2.38	119.22	113.19
27	23SA	1940	5MU	C1'-N1-C2	2.37	121.87	117.57
1	16SB	1834	2MG	O6-C6-C5	-2.37	120.32	126.60
1	16SB	1834	2MG	CM2-N2-C2	-2.36	118.64	123.86
27	23SB	1936	PSU	O2-C2-N1	-2.35	120.20	122.79
27	23SA	2266	OMG	N1-C2-N3	-2.35	118.93	123.32
57	ASIB	37	MIA	N9-C8-N7	-2.34	110.71	113.91
27	23SB	1942	PSU	O2-C2-N1	-2.34	120.21	122.79
26	TRNA	20	H2U	O2-C2-N3	-2.33	117.15	121.50
1	16SA	2142	MA6	N3-C4-N9	2.33	130.93	127.08
23	PSIA	37	MIA	N3-C2-N1	-2.33	122.68	126.95
22	ASIA	8	4SU	C1'-N1-C2	2.32	121.78	117.57
1	16SB	1589	M2G	O6-C6-C5	-2.32	120.44	126.60
23	PSIA	46	G7M	C8-N9-C4	2.32	113.03	107.16
27	23SA	2518	2MA	C4-N9-C8	2.32	108.24	105.73
22	ASIA	46	G7M	C8-N9-C4	2.32	113.03	107.16
23	PSIA	16	H2U	O2-C2-N1	-2.31	120.21	123.11
27	23SB	2518	2MA	CM2-C2-N1	2.31	120.76	117.15
23	PSIB	16	H2U	O2-C2-N1	-2.31	120.21	123.11
1	16SB	2032	5MC	C5-C6-N1	-2.30	120.97	123.34
1	16SA	2121	UR3	C1'-N1-C2	2.30	120.87	116.99
1	16SA	1589	M2G	O6-C6-C5	-2.29	120.52	126.60
24	ESIA	37	MIA	C2-N1-C6	2.29	121.65	117.28
23	PSIA	8	4SU	O2-C2-N1	-2.27	119.77	122.79
12	S12B	89	0TD	OD1-CG-CB	-2.27	117.70	122.44
57	ASIB	32	PSU	C6-N1-C2	-2.26	120.37	122.68
1	16SA	2030	4OC	C6-C5-C4	2.26	119.73	116.96
26	TRNA	39	PSU	C6-C5-C4	2.26	119.78	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	PSIB	37	MIA	N3-C2-N1	-2.25	122.83	126.95
23	PSIB	55	PSU	O2-C2-N1	-2.24	120.33	122.79
27	23SB	2518	2MA	C6-C5-C4	2.23	120.19	117.18
1	16SA	1156	G7M	C8-N9-C4	2.23	112.80	107.16
1	16SB	1589	M2G	C1'-N9-C8	-2.22	120.37	126.70
23	PSIA	32	PSU	O2-C2-N1	-2.22	120.34	122.79
1	16SA	1834	2MG	N1-C2-N3	-2.22	120.52	123.95
1	16SB	1834	2MG	N1-C2-N3	-2.22	120.52	123.95
26	TRNA	32	PSU	C6-N1-C2	-2.22	120.41	122.68
23	PSIB	39	PSU	C6-N1-C2	-2.22	120.42	122.68
23	PSIA	39	PSU	O2-C2-N1	-2.21	120.36	122.79
27	23SA	1942	PSU	C6-N1-C2	-2.21	120.42	122.68
1	16SB	2035	5MC	C5-C4-N3	-2.21	119.29	121.67
1	16SB	2028	5MC	C1'-N1-C6	-2.21	117.45	121.12
1	16SB	2030	4OC	C5-C6-N1	-2.21	118.11	121.81
24	ESIA	37	MIA	N6-C6-N1	2.20	121.31	118.50
57	ASIB	37	MIA	C4-N9-C1'	2.20	131.83	126.59
57	ASIB	37	MIA	C4-C5-C6	2.19	118.51	116.81
22	ASIA	39	PSU	O2-C2-N1	-2.19	120.38	122.79
23	PSIA	54	5MU	O4-C4-N3	-2.19	115.93	120.12
1	16SA	1145	PSU	O4'-C1'-C2'	2.18	108.22	105.14
57	ASIB	37	MIA	C16-C14-C15	-2.17	109.81	114.60
26	TRNA	8	4SU	C1'-N1-C2	2.17	121.50	117.57
26	TRNA	39	PSU	C6-N1-C2	-2.17	120.47	122.68
57	ASIB	39	PSU	C6-N1-C2	-2.17	120.47	122.68
1	16SA	1589	M2G	N9-C4-N3	2.17	130.29	125.94
27	23SB	1945	OMC	O2-C2-N3	-2.17	118.81	122.33
1	16SA	1834	2MG	O6-C6-C5	-2.16	120.87	126.60
27	23SA	1964	5MU	O4-C4-N3	-2.16	115.98	120.12
1	16SA	2121	UR3	C6-N1-C2	-2.14	119.87	121.79
1	16SB	2028	5MC	CM5-C5-C6	-2.14	119.99	122.85
1	16SA	2032	5MC	C5-C6-N1	-2.14	121.14	123.34
22	ASIA	54	5MU	O4-C4-N3	-2.13	116.03	120.12
1	16SA	1834	2MG	C8-N7-C5	2.13	108.10	104.24
27	23SA	2567	OMU	O2-C2-N1	-2.13	119.96	122.79
1	16SA	1834	2MG	CM2-N2-C2	-2.12	119.19	123.86
1	16SB	1834	2MG	C8-N7-C5	2.12	108.07	104.24
1	16SB	2035	5MC	O2-C2-N3	-2.11	118.89	122.33
1	16SB	2030	4OC	O2-C2-N3	-2.10	118.92	122.33
27	23SB	2518	2MA	C4-N9-C8	2.10	108.00	105.73
27	23SB	1967	5MC	CM5-C5-C6	-2.09	120.06	122.85
1	16SB	2032	5MC	C5-C4-N3	-2.09	119.42	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	TRNA	54	5MU	C1'-N1-C2	2.09	121.35	117.57
1	16SA	2141	MA6	C4-C5-N7	-2.08	108.08	110.62
22	ASIA	37	MIA	C16-C14-C15	-2.08	110.01	114.60
26	TRNA	37	MIA	N3-C2-N1	-2.08	123.14	126.95
1	16SB	1145	PSU	O4'-C1'-C2'	2.08	108.08	105.14
22	ASIA	32	PSU	O2-C2-N1	-2.08	120.50	122.79
1	16SA	1589	M2G	C8-N7-C5	2.08	108.00	104.24
57	ASIB	37	MIA	N3-C2-N1	-2.08	123.15	126.95
1	16SA	2032	5MC	CM5-C5-C6	-2.07	120.08	122.85
1	16SA	1589	M2G	C4-C5-N7	-2.07	107.45	110.72
24	ESIB	37	MIA	C2-N1-C6	2.07	121.23	117.28
26	TRNA	55	PSU	C6-N1-C2	-2.06	120.58	122.68
1	16SB	2142	MA6	C4-C5-N7	-2.05	108.12	110.62
27	23SB	1967	5MC	C5-C4-N3	-2.05	119.47	121.67
27	23SA	1940	5MU	O4-C4-N3	-2.05	116.19	120.12
1	16SA	2142	MA6	C5-C4-N9	2.03	108.14	105.78
23	PSIA	47	3AU	O31-C13-C12	2.03	120.30	113.38
27	23SB	1942	PSU	C6-N1-C2	-2.01	120.62	122.68
23	PSIB	47	3AU	O31-C13-O30	-2.01	119.53	124.09
57	ASIB	37	MIA	C6-C5-N7	2.00	134.56	132.39
27	23SA	2266	OMG	C2'-C1'-N9	-2.00	110.34	114.22

There are no chirality outliers.

All (118) 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'
22	ASIA	37	MIA	C12-C13-C14-C15
22	ASIA	37	MIA	C12-C13-C14-C16
26	TRNA	8	4SU	C3'-C4'-C5'-O5'
26	TRNA	8	4SU	O4'-C4'-C5'-O5'
26	TRNA	16	H2U	O4'-C4'-C5'-O5'
26	TRNA	16	H2U	C3'-C4'-C5'-O5'
26	TRNA	20	H2U	O4'-C4'-C5'-O5'
26	TRNA	20	H2U	C3'-C4'-C5'-O5'
26	TRNA	37	MIA	N1-C2-S10-C11
26	TRNA	37	MIA	N3-C2-S10-C11
26	TRNA	37	MIA	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
26	TRNA	37	MIA	C12-C13-C14-C16
26	TRNA	54	5MU	C3'-C4'-C5'-O5'
26	TRNA	54	5MU	O4'-C4'-C5'-O5'
1	16SB	1156	G7M	C3'-C4'-C5'-O5'
1	16SB	1834	2MG	O4'-C4'-C5'-O5'
1	16SB	1834	2MG	C3'-C4'-C5'-O5'
1	16SB	2142	MA6	O4'-C4'-C5'-O5'
23	PSIA	37	MIA	O4'-C4'-C5'-O5'
23	PSIA	37	MIA	C3'-C4'-C5'-O5'
23	PSIA	37	MIA	C12-C13-C14-C15
23	PSIB	37	MIA	C12-C13-C14-C15
23	PSIB	37	MIA	C12-C13-C14-C16
23	PSIA	47	3AU	N3-C10-C11-C12
23	PSIA	47	3AU	C10-C11-C12-C13
23	PSIA	47	3AU	C10-C11-C12-N40
23	PSIA	47	3AU	C3'-C4'-C5'-O5'
23	PSIA	47	3AU	O4'-C4'-C5'-O5'
23	PSIB	47	3AU	C2'-C1'-N1-C2
23	PSIB	54	5MU	C3'-C4'-C5'-O5'
23	PSIB	54	5MU	O4'-C4'-C5'-O5'
24	ESIA	37	MIA	N1-C2-S10-C11
24	ESIA	37	MIA	N3-C2-S10-C11
24	ESIA	37	MIA	C12-C13-C14-C15
24	ESIA	37	MIA	C12-C13-C14-C16
24	ESIB	37	MIA	O4'-C4'-C5'-O5'
24	ESIB	37	MIA	C3'-C4'-C5'-O5'
24	ESIB	37	MIA	N1-C2-S10-C11
24	ESIB	37	MIA	N3-C2-S10-C11
24	ESIB	37	MIA	C12-C13-C14-C16
27	23SA	2266	OMG	C1'-C2'-O2'-CM2
27	23SB	2266	OMG	C1'-C2'-O2'-CM2
57	ASIB	37	MIA	C12-C13-C14-C15
26	TRNA	20	H2U	C2'-C1'-N1-C2
1	16SA	2142	MA6	C3'-C4'-C5'-O5'
22	ASIA	37	MIA	C3'-C4'-C5'-O5'
1	16SB	1156	G7M	O4'-C4'-C5'-O5'
1	16SB	2142	MA6	C3'-C4'-C5'-O5'
23	PSIB	8	4SU	C3'-C4'-C5'-O5'
23	PSIB	8	4SU	O4'-C4'-C5'-O5'
23	PSIB	47	3AU	C3'-C4'-C5'-O5'
23	PSIB	47	3AU	O4'-C4'-C5'-O5'
24	ESIA	37	MIA	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
27	23SB	1964	5MU	O4'-C4'-C5'-O5'
27	23SB	2518	2MA	O4'-C4'-C5'-O5'
23	PSIB	47	3AU	C2'-C1'-N1-C6
1	16SA	2030	4OC	O4'-C4'-C5'-O5'
22	ASIA	46	G7M	C3'-C4'-C5'-O5'
1	16SB	2030	4OC	O4'-C4'-C5'-O5'
27	23SB	1964	5MU	C3'-C4'-C5'-O5'
26	TRNA	20	H2U	C2'-C1'-N1-C6
23	PSIA	55	PSU	C3'-C4'-C5'-O5'
27	23SB	2567	OMU	C3'-C4'-C5'-O5'
1	16SA	2030	4OC	C3'-C4'-C5'-O5'
22	ASIA	55	PSU	C3'-C4'-C5'-O5'
27	23SA	1940	5MU	C3'-C4'-C5'-O5'
27	23SB	2518	2MA	C3'-C4'-C5'-O5'
22	ASIA	55	PSU	O4'-C4'-C5'-O5'
27	23SB	2567	OMU	O4'-C4'-C5'-O5'
1	16SB	2030	4OC	C3'-C4'-C5'-O5'
26	TRNA	16	H2U	C4'-C5'-O5'-P
26	TRNA	37	MIA	C4'-C5'-O5'-P
23	PSIA	55	PSU	O4'-C4'-C5'-O5'
22	ASIA	46	G7M	O4'-C4'-C5'-O5'
24	ESIA	37	MIA	O4'-C4'-C5'-O5'
27	23SA	1940	5MU	O4'-C4'-C5'-O5'
57	ASIB	37	MIA	N3-C2-S10-C11
23	PSIA	55	PSU	C4'-C5'-O5'-P
12	S12B	89	0TD	SB-CB-CG-OD1
23	PSIB	37	MIA	C3'-C4'-C5'-O5'
23	PSIB	47	3AU	C11-C12-C13-O31
23	PSIB	47	3AU	C4'-C5'-O5'-P
24	ESIB	37	MIA	C4'-C5'-O5'-P
23	PSIA	46	G7M	O4'-C4'-C5'-O5'
23	PSIB	47	3AU	C11-C12-C13-O30
22	ASIA	37	MIA	N3-C2-S10-C11
23	PSIA	37	MIA	N3-C2-S10-C11
1	16SA	2142	MA6	C4'-C5'-O5'-P
22	ASIA	8	4SU	C4'-C5'-O5'-P
1	16SB	2142	MA6	C4'-C5'-O5'-P
57	ASIB	37	MIA	N1-C2-S10-C11
27	23SA	1964	5MU	O4'-C4'-C5'-O5'
24	ESIA	37	MIA	N6-C12-C13-C14
22	ASIA	37	MIA	N1-C2-S10-C11
23	PSIA	37	MIA	N1-C2-S10-C11

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Mol	Chain	Res	Type	Atoms
23	PSIB	37	MIA	N3-C2-S10-C11
22	ASIA	55	PSU	O4'-C1'-C5-C4
23	PSIA	47	3AU	C2'-C1'-N1-C6
12	S12B	89	0TD	CA-CB-SB-CSB
23	PSIA	47	3AU	C2'-C1'-N1-C2
26	TRNA	37	MIA	C2'-C1'-N9-C8
23	PSIA	46	G7M	C3'-C4'-C5'-O5'
27	23SA	1964	5MU	C3'-C4'-C5'-O5'
23	PSIB	37	MIA	N1-C2-S10-C11
27	23SA	1945	OMC	C2'-C1'-N1-C2
26	TRNA	20	H2U	C4'-C5'-O5'-P
27	23SA	2518	2MA	C4'-C5'-O5'-P
23	PSIB	37	MIA	O4'-C4'-C5'-O5'
12	S12B	89	0TD	CG-CB-SB-CSB
12	S12A	89	0TD	SB-CB-CG-OD1
27	23SB	1945	OMC	C2'-C1'-N1-C2
27	23SA	1940	5MU	C2'-C1'-N1-C2
27	23SB	2518	2MA	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	TRNA	37	MIA	0	3

4.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

4.6 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	23SB	3045	-	0,6,6	-	-	-		
59	OHX	23SB	3155	-	0,6,6	-	-	-		
59	OHX	23SA	3194	-	0,6,6	-	-	-		
59	OHX	16SB	2244	-	0,6,6	-	-	-		
59	OHX	S4A	301	4	0,6,6	-	-	-		
59	OHX	23SA	3334	-	0,6,6	-	-	-		
59	OHX	16SB	2204	-	0,6,6	-	-	-		
59	OHX	16SA	2292	-	0,6,6	-	-	-		
59	OHX	23SA	3305	-	0,6,6	-	-	-		
59	OHX	23SB	3004	-	0,6,6	-	-	-		
59	OHX	23SA	3297	-	0,6,6	-	-	-		
59	OHX	23SB	3010	-	0,6,6	-	-	-		
59	OHX	L35B	101	56	0,6,6	-	-	-		
59	OHX	23SB	3041	-	0,6,6	-	-	-		
59	OHX	23SA	3187	-	0,6,6	-	-	-		
59	OHX	23SA	3381	-	0,6,6	-	-	-		
59	OHX	23SB	3090	-	0,6,6	-	-	-		
59	OHX	23SA	3361	-	0,6,6	-	-	-		
59	OHX	16SA	2263	-	0,6,6	-	-	-		
59	OHX	23SB	3017	-	0,6,6	-	-	-		
59	OHX	23SA	3217	-	0,6,6	-	-	-		
59	OHX	23SB	3049	-	0,6,6	-	-	-		
59	OHX	23SA	3312	-	0,6,6	-	-	-		
59	OHX	23SB	3030	-	0,6,6	-	-	-		
59	OHX	16SB	2250	-	0,6,6	-	-	-		
59	OHX	23SB	3152	-	0,6,6	-	-	-		
59	OHX	23SB	3163	-	0,6,6	-	-	-		
59	OHX	23SA	3324	-	0,6,6	-	-	-		
59	OHX	23SA	3247	-	0,6,6	-	-	-		
59	OHX	23SA	3210	-	0,6,6	-	-	-		
59	OHX	23SB	3112	-	0,6,6	-	-	-		
59	OHX	16SA	2293	-	0,6,6	-	-	-		
59	OHX	23SA	3221	-	0,6,6	-	-	-		
59	OHX	23SB	3002	-	0,6,6	-	-	-		
59	OHX	L4B	301	-	0,6,6	-	-	-		
59	OHX	16SB	2208	-	0,6,6	-	-	-		
59	OHX	23SB	3140	-	0,6,6	-	-	-		
59	OHX	23SA	3207	-	0,6,6	-	-	-		
59	OHX	23SB	3058	-	0,6,6	-	-	-		
59	OHX	23SA	3189	-	0,6,6	-	-	-		
59	OHX	16SA	2321	1	0,6,6	-	-	-		
59	OHX	23SB	3137	58	0,6,6	-	-	-		
59	OHX	23SB	3100	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	OHX	ASIB	101	-	0,6,6	-	-	-		
59	OHX	23SA	3367	-	0,6,6	-	-	-		
59	OHX	23SB	3073	-	0,6,6	-	-	-		
59	OHX	23SB	3175	-	0,6,6	-	-	-		
59	OHX	23SA	3267	-	0,6,6	-	-	-		
59	OHX	23SB	3197	-	0,6,6	-	-	-		
59	OHX	23SB	3195	-	0,6,6	-	-	-		
59	OHX	16SB	2275	-	0,6,6	-	-	-		
59	OHX	23SA	3237	27	0,6,6	-	-	-		
59	OHX	23SB	3161	-	0,6,6	-	-	-		
59	OHX	23SB	3139	58	0,6,6	-	-	-		
59	OHX	5SA	213	-	0,6,6	-	-	-		
59	OHX	23SA	3275	-	0,6,6	-	-	-		
59	OHX	23SB	3024	-	0,6,6	-	-	-		
59	OHX	23SA	3283	27	0,6,6	-	-	-		
59	OHX	16SB	2215	-	0,6,6	-	-	-		
59	OHX	ESIB	101	-	0,6,6	-	-	-		
59	OHX	16SB	2223	1	0,6,6	-	-	-		
59	OHX	23SB	3196	-	0,6,6	-	-	-		
59	OHX	23SA	3329	-	0,6,6	-	-	-		
59	OHX	23SA	3244	-	0,6,6	-	-	-		
59	OHX	23SA	3379	-	0,6,6	-	-	-		
59	OHX	23SA	3354	-	0,6,6	-	-	-		
59	OHX	23SB	3026	-	0,6,6	-	-	-		
59	OHX	23SA	3261	-	0,6,6	-	-	-		
59	OHX	16SB	2210	-	0,6,6	-	-	-		
59	OHX	23SB	3101	27	0,6,6	-	-	-		
59	OHX	16SB	2264	-	0,6,6	-	-	-		
59	OHX	23SB	3065	62	0,6,6	-	-	-		
59	OHX	23SB	3122	-	0,6,6	-	-	-		
59	OHX	23SA	3314	-	0,6,6	-	-	-		
59	OHX	23SB	3154	27	0,6,6	-	-	-		
59	OHX	16SB	2217	-	0,6,6	-	-	-		
61	SJE	23SA	3640	-	87,91,91	4.12	25 (28%)	117,134,134	2.02	28 (23%)
59	OHX	5SA	209	-	0,6,6	-	-	-		
59	OHX	5SA	212	-	0,6,6	-	-	-		
59	OHX	16SA	2297	-	0,6,6	-	-	-		
59	OHX	23SB	3141	-	0,6,6	-	-	-		
59	OHX	23SB	3194	-	0,6,6	-	-	-		
59	OHX	23SB	3157	-	0,6,6	-	-	-		
59	OHX	23SA	3292	-	0,6,6	-	-	-		
59	OHX	16SA	2301	-	0,6,6	-	-	-		
59	OHX	23SB	3059	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	OHX	23SB	3115	-	0,6,6	-	-	-		
59	OHX	16SA	2306	1	0,6,6	-	-	-		
59	OHX	23SA	3279	-	0,6,6	-	-	-		
59	OHX	16SB	2272	-	0,6,6	-	-	-		
59	OHX	16SA	2277	-	0,6,6	-	-	-		
59	OHX	23SA	3289	-	0,6,6	-	-	-		
59	OHX	23SB	3061	-	0,6,6	-	-	-		
59	OHX	16SB	2269	1	0,6,6	-	-	-		
59	OHX	23SB	3179	-	0,6,6	-	-	-		
59	OHX	16SA	2299	-	0,6,6	-	-	-		
59	OHX	23SB	3009	-	0,6,6	-	-	-		
59	OHX	23SA	3190	27	0,6,6	-	-	-		
59	OHX	23SA	3213	-	0,6,6	-	-	-		
59	OHX	23SB	3131	-	0,6,6	-	-	-		
59	OHX	23SA	3355	-	0,6,6	-	-	-		
59	OHX	23SB	3168	-	0,6,6	-	-	-		
59	OHX	23SA	3365	-	0,6,6	-	-	-		
59	OHX	16SB	2234	1	0,6,6	-	-	-		
59	OHX	16SB	2243	1	0,6,6	-	-	-		
59	OHX	16SB	2254	1	0,6,6	-	-	-		
59	OHX	23SA	3225	-	0,6,6	-	-	-		
59	OHX	23SB	3198	-	0,6,6	-	-	-		
59	OHX	23SB	3042	-	0,6,6	-	-	-		
59	OHX	16SA	2333	-	0,6,6	-	-	-		
59	OHX	16SB	2258	-	0,6,6	-	-	-		
59	OHX	S19A	101	19	0,6,6	-	-	-		
59	OHX	5SB	207	-	0,6,6	-	-	-		
59	OHX	23SA	3356	-	0,6,6	-	-	-		
59	OHX	23SA	3372	-	0,6,6	-	-	-		
59	OHX	23SA	3226	-	0,6,6	-	-	-		
59	OHX	23SA	3285	-	0,6,6	-	-	-		
59	OHX	23SA	3195	58	0,6,6	-	-	-		
59	OHX	23SA	3333	-	0,6,6	-	-	-		
59	OHX	23SB	3071	-	0,6,6	-	-	-		
59	OHX	23SA	3374	-	0,6,6	-	-	-		
59	OHX	16SB	2214	1	0,6,6	-	-	-		
59	OHX	23SA	3180	27,58	0,6,6	-	-	-		
59	OHX	23SB	3170	-	0,6,6	-	-	-		
59	OHX	23SB	3182	27	0,6,6	-	-	-		
59	OHX	23SB	3171	27	0,6,6	-	-	-		
59	OHX	23SA	3342	58	0,6,6	-	-	-		
59	OHX	23SA	3277	-	0,6,6	-	-	-		
59	OHX	23SB	3173	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	OHX	23SA	3188	-	0,6,6	-	-	-		
59	OHX	23SA	3288	-	0,6,6	-	-	-		
59	OHX	L4A	302	-	0,6,6	-	-	-		
59	OHX	16SB	2278	-	0,6,6	-	-	-		
59	OHX	23SB	3022	27	0,6,6	-	-	-		
59	OHX	23SB	3074	-	0,6,6	-	-	-		
59	OHX	23SA	3273	-	0,6,6	-	-	-		
59	OHX	23SB	3187	-	0,6,6	-	-	-		
59	OHX	23SA	3366	27	0,6,6	-	-	-		
59	OHX	16SA	2294	-	0,6,6	-	-	-		
59	OHX	23SA	3345	-	0,6,6	-	-	-		
59	OHX	S14B	101	14	0,6,6	-	-	-		
59	OHX	23SB	3020	-	0,6,6	-	-	-		
59	OHX	23SB	3162	-	0,6,6	-	-	-		
59	OHX	16SB	2226	-	0,6,6	-	-	-		
59	OHX	16SA	2336	-	0,6,6	-	-	-		
59	OHX	23SB	3142	27	0,6,6	-	-	-		
59	OHX	16SB	2220	-	0,6,6	-	-	-		
59	OHX	23SB	3067	-	0,6,6	-	-	-		
59	OHX	16SA	2331	-	0,6,6	-	-	-		
59	OHX	16SA	2300	-	0,6,6	-	-	-		
59	OHX	23SA	3323	-	0,6,6	-	-	-		
59	OHX	16SB	2236	-	0,6,6	-	-	-		
59	OHX	23SB	3018	-	0,6,6	-	-	-		
59	OHX	23SA	3351	-	0,6,6	-	-	-		
59	OHX	16SB	2270	-	0,6,6	-	-	-		
59	OHX	TRNA	101	26	0,6,6	-	-	-		
59	OHX	23SA	3246	-	0,6,6	-	-	-		
59	OHX	23SB	3121	-	0,6,6	-	-	-		
59	OHX	23SB	3080	-	0,6,6	-	-	-		
59	OHX	23SA	3339	-	0,6,6	-	-	-		
59	OHX	23SA	3368	-	0,6,6	-	-	-		
59	OHX	23SA	3281	-	0,6,6	-	-	-		
59	OHX	23SB	3025	27	0,6,6	-	-	-		
59	OHX	23SB	3092	-	0,6,6	-	-	-		
59	OHX	23SA	3262	-	0,6,6	-	-	-		
59	OHX	16SA	2286	-	0,6,6	-	-	-		
59	OHX	23SB	3128	-	0,6,6	-	-	-		
59	OHX	5SB	208	28	0,6,6	-	-	-		
59	OHX	23SB	3001	-	0,6,6	-	-	-		
59	OHX	23SB	3111	-	0,6,6	-	-	-		
59	OHX	23SB	3125	-	0,6,6	-	-	-		
59	OHX	16SB	2224	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	OHX	16SB	2274	-	0,6,6	-	-	-		
59	OHX	23SA	3349	-	0,6,6	-	-	-		
59	OHX	5SB	209	-	0,6,6	-	-	-		
59	OHX	16SA	2282	-	0,6,6	-	-	-		
59	OHX	23SB	3160	-	0,6,6	-	-	-		
59	OHX	23SB	3127	-	0,6,6	-	-	-		
59	OHX	16SB	2230	1	0,6,6	-	-	-		
59	OHX	16SA	2317	-	0,6,6	-	-	-		
59	OHX	23SB	3063	27	0,6,6	-	-	-		
59	OHX	23SB	3097	-	0,6,6	-	-	-		
59	OHX	23SB	3153	-	0,6,6	-	-	-		
59	OHX	16SB	2202	-	0,6,6	-	-	-		
59	OHX	23SA	3203	-	0,6,6	-	-	-		
59	OHX	23SA	3274	-	0,6,6	-	-	-		
59	OHX	L35A	102	-	0,6,6	-	-	-		
59	OHX	23SA	3220	-	0,6,6	-	-	-		
59	OHX	16SB	2218	-	0,6,6	-	-	-		
59	OHX	23SB	3006	-	0,6,6	-	-	-		
59	OHX	23SB	3078	-	0,6,6	-	-	-		
59	OHX	16SB	2229	-	0,6,6	-	-	-		
59	OHX	23SB	3053	-	0,6,6	-	-	-		
59	OHX	23SB	3015	27	0,6,6	-	-	-		
59	OHX	16SB	2222	-	0,6,6	-	-	-		
59	OHX	23SA	3197	27	0,6,6	-	-	-		
59	OHX	23SB	3164	-	0,6,6	-	-	-		
59	OHX	16SA	2305	1	0,6,6	-	-	-		
59	OHX	23SA	3310	-	0,6,6	-	-	-		
59	OHX	16SB	2205	-	0,6,6	-	-	-		
59	OHX	16SA	2328	-	0,6,6	-	-	-		
59	OHX	16SA	2303	-	0,6,6	-	-	-		
59	OHX	23SA	3369	-	0,6,6	-	-	-		
59	OHX	23SA	3236	-	0,6,6	-	-	-		
59	OHX	23SB	3007	27	0,6,6	-	-	-		
59	OHX	ESIA	101	-	0,6,6	-	-	-		
59	OHX	16SA	2260	-	0,6,6	-	-	-		
59	OHX	23SB	3102	-	0,6,6	-	-	-		
59	OHX	16SB	2265	-	0,6,6	-	-	-		
59	OHX	23SB	3119	58	0,6,6	-	-	-		
59	OHX	23SB	3130	-	0,6,6	-	-	-		
59	OHX	16SB	2257	-	0,6,6	-	-	-		
59	OHX	23SA	3199	-	0,6,6	-	-	-		
59	OHX	16SA	2334	1	0,6,6	-	-	-		
59	OHX	23SA	3184	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	OHX	23SB	3134	-	0,6,6	-	-	-		
59	OHX	23SB	3120	-	0,6,6	-	-	-		
59	OHX	16SA	2283	-	0,6,6	-	-	-		
59	OHX	16SA	2273	1	0,6,6	-	-	-		
59	OHX	23SA	3241	27	0,6,6	-	-	-		
59	OHX	23SB	3056	-	0,6,6	-	-	-		
59	OHX	16SA	2287	-	0,6,6	-	-	-		
59	OHX	23SA	3298	-	0,6,6	-	-	-		
59	OHX	23SB	3055	-	0,6,6	-	-	-		
59	OHX	L27A	103	-	0,6,6	-	-	-		
59	OHX	23SB	3104	-	0,6,6	-	-	-		
59	OHX	23SA	3200	27	0,6,6	-	-	-		
59	OHX	16SB	2238	1	0,6,6	-	-	-		
59	OHX	16SA	2289	-	0,6,6	-	-	-		
59	OHX	23SB	3016	-	0,6,6	-	-	-		
59	OHX	23SB	3085	-	0,6,6	-	-	-		
59	OHX	23SA	3214	-	0,6,6	-	-	-		
59	OHX	23SA	3308	-	0,6,6	-	-	-		
59	OHX	23SB	3107	-	0,6,6	-	-	-		
59	OHX	23SA	3181	-	0,6,6	-	-	-		
59	OHX	23SB	3147	-	0,6,6	-	-	-		
59	OHX	16SB	2235	-	0,6,6	-	-	-		
59	OHX	23SB	3110	27	0,6,6	-	-	-		
59	OHX	23SB	3019	27	0,6,6	-	-	-		
59	OHX	23SB	3093	-	0,6,6	-	-	-		
59	OHX	PSIB	102	-	0,6,6	-	-	-		
59	OHX	23SA	3377	-	0,6,6	-	-	-		
59	OHX	16SB	2237	1	0,6,6	-	-	-		
59	OHX	23SB	3076	-	0,6,6	-	-	-		
59	OHX	23SA	3294	58	0,6,6	-	-	-		
59	OHX	23SA	3239	-	0,6,6	-	-	-		
59	OHX	16SA	2320	-	0,6,6	-	-	-		
59	OHX	23SB	3089	-	0,6,6	-	-	-		
59	OHX	23SA	3313	-	0,6,6	-	-	-		
59	OHX	23SB	3189	27	0,6,6	-	-	-		
59	OHX	16SA	2315	-	0,6,6	-	-	-		
59	OHX	23SB	3181	-	0,6,6	-	-	-		
59	OHX	16SB	2203	1	0,6,6	-	-	-		
59	OHX	23SB	3109	-	0,6,6	-	-	-		
59	OHX	16SA	2338	-	0,6,6	-	-	-		
59	OHX	23SA	3378	-	0,6,6	-	-	-		
59	OHX	MRNB	101	58	0,6,6	-	-	-		
59	OHX	23SB	3183	27	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	OHX	23SB	3185	-	0,6,6	-	-	-		
59	OHX	23SA	3253	-	0,6,6	-	-	-		
59	OHX	23SB	3149	-	0,6,6	-	-	-		
59	OHX	23SB	3106	-	0,6,6	-	-	-		
59	OHX	23SB	3146	-	0,6,6	-	-	-		
59	OHX	16SB	2262	-	0,6,6	-	-	-		
59	OHX	16SB	2247	-	0,6,6	-	-	-		
59	OHX	23SB	3039	-	0,6,6	-	-	-		
59	OHX	23SA	3268	-	0,6,6	-	-	-		
59	OHX	23SA	3315	-	0,6,6	-	-	-		
59	OHX	16SB	2216	-	0,6,6	-	-	-		
59	OHX	23SA	3192	27	0,6,6	-	-	-		
59	OHX	16SA	2308	-	0,6,6	-	-	-		
59	OHX	23SB	3113	-	0,6,6	-	-	-		
59	OHX	23SA	3317	-	0,6,6	-	-	-		
59	OHX	23SA	3260	-	0,6,6	-	-	-		
59	OHX	23SA	3306	-	0,6,6	-	-	-		
59	OHX	23SB	3013	27	0,6,6	-	-	-		
59	OHX	5SA	214	-	0,6,6	-	-	-		
59	OHX	23SA	3258	-	0,6,6	-	-	-		
59	OHX	16SA	2274	-	0,6,6	-	-	-		
59	OHX	TRNA	102	-	0,6,6	-	-	-		
59	OHX	23SA	3215	-	0,6,6	-	-	-		
59	OHX	16SB	2239	1	0,6,6	-	-	-		
59	OHX	16SA	2318	-	0,6,6	-	-	-		
59	OHX	23SA	3309	-	0,6,6	-	-	-		
59	OHX	23SB	3046	-	0,6,6	-	-	-		
59	OHX	23SB	3036	27	0,6,6	-	-	-		
59	OHX	16SB	2211	-	0,6,6	-	-	-		
59	OHX	23SB	3118	-	0,6,6	-	-	-		
59	OHX	23SB	3035	27	0,6,6	-	-	-		
59	OHX	5SA	206	-	0,6,6	-	-	-		
59	OHX	23SA	3235	-	0,6,6	-	-	-		
59	OHX	23SB	3005	-	0,6,6	-	-	-		
59	OHX	23SA	3322	-	0,6,6	-	-	-		
59	OHX	ASIA	101	-	0,6,6	-	-	-		
59	OHX	5SB	204	-	0,6,6	-	-	-		
59	OHX	23SB	3150	-	0,6,6	-	-	-		
59	OHX	16SA	2312	-	0,6,6	-	-	-		
59	OHX	16SB	2212	-	0,6,6	-	-	-		
59	OHX	23SA	3218	-	0,6,6	-	-	-		
59	OHX	23SB	3094	27	0,6,6	-	-	-		
59	OHX	23SA	3269	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	OHX	16SA	2280	-	0,6,6	-	-	-		
59	OHX	23SA	3325	-	0,6,6	-	-	-		
59	OHX	23SA	3266	-	0,6,6	-	-	-		
59	OHX	23SA	3352	-	0,6,6	-	-	-		
59	OHX	5SA	207	28	0,6,6	-	-	-		
59	OHX	23SA	3206	-	0,6,6	-	-	-		
59	OHX	PSIA	102	23	0,6,6	-	-	-		
59	OHX	23SB	3186	-	0,6,6	-	-	-		
59	OHX	23SB	3012	-	0,6,6	-	-	-		
59	OHX	23SA	3256	-	0,6,6	-	-	-		
59	OHX	23SB	3192	-	0,6,6	-	-	-		
59	OHX	5SB	203	-	0,6,6	-	-	-		
59	OHX	16SB	2225	-	0,6,6	-	-	-		
59	OHX	23SB	3032	-	0,6,6	-	-	-		
59	OHX	23SA	3249	-	0,6,6	-	-	-		
59	OHX	16SB	2233	-	0,6,6	-	-	-		
59	OHX	23SB	3143	-	0,6,6	-	-	-		
59	OHX	23SB	3144	-	0,6,6	-	-	-		
59	OHX	23SB	3075	-	0,6,6	-	-	-		
59	OHX	ASIA	102	-	0,6,6	-	-	-		
59	OHX	23SB	3190	-	0,6,6	-	-	-		
59	OHX	23SA	3347	-	0,6,6	-	-	-		
59	OHX	23SA	3302	-	0,6,6	-	-	-		
59	OHX	23SA	3242	-	0,6,6	-	-	-		
59	OHX	16SA	2339	-	0,6,6	-	-	-		
59	OHX	23SA	3252	-	0,6,6	-	-	-		
59	OHX	16SB	2267	-	0,6,6	-	-	-		
59	OHX	16SB	2273	-	0,6,6	-	-	-		
59	OHX	5SB	210	-	0,6,6	-	-	-		
59	OHX	23SA	3183	27	0,6,6	-	-	-		
59	OHX	23SA	3284	-	0,6,6	-	-	-		
59	OHX	23SB	3011	-	0,6,6	-	-	-		
59	OHX	23SB	3165	27	0,6,6	-	-	-		
59	OHX	23SB	3158	-	0,6,6	-	-	-		
59	OHX	23SA	3341	58	0,6,6	-	-	-		
59	OHX	16SB	2240	-	0,6,6	-	-	-		
59	OHX	5SB	201	-	0,6,6	-	-	-		
59	OHX	23SB	3180	-	0,6,6	-	-	-		
59	OHX	23SA	3259	-	0,6,6	-	-	-		
59	OHX	23SB	3108	27	0,6,6	-	-	-		
59	OHX	23SB	3123	-	0,6,6	-	-	-		
59	OHX	16SB	2241	-	0,6,6	-	-	-		
59	OHX	23SA	3287	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	OHX	23SB	3167	-	0,6,6	-	-	-		
59	OHX	23SA	3332	-	0,6,6	-	-	-		
59	OHX	23SA	3290	-	0,6,6	-	-	-		
59	OHX	16SB	2227	-	0,6,6	-	-	-		
59	OHX	23SA	3318	27	0,6,6	-	-	-		
59	OHX	16SA	2341	-	0,6,6	-	-	-		
59	OHX	23SA	3238	-	0,6,6	-	-	-		
59	OHX	23SA	3193	-	0,6,6	-	-	-		
59	OHX	16SB	2221	-	0,6,6	-	-	-		
59	OHX	23SA	3357	27	0,6,6	-	-	-		
59	OHX	16SA	2262	-	0,6,6	-	-	-		
59	OHX	16SB	2246	-	0,6,6	-	-	-		
59	OHX	L19A	201	41	0,6,6	-	-	-		
59	OHX	16SA	2319	-	0,6,6	-	-	-		
59	OHX	23SA	3340	-	0,6,6	-	-	-		
59	OHX	16SB	2251	1	0,6,6	-	-	-		
59	OHX	16SA	2290	-	0,6,6	-	-	-		
59	OHX	L20B	201	-	0,6,6	-	-	-		
59	OHX	16SB	2277	-	0,6,6	-	-	-		
59	OHX	23SA	3303	-	0,6,6	-	-	-		
59	OHX	16SA	2323	-	0,6,6	-	-	-		
59	OHX	16SB	2253	-	0,6,6	-	-	-		
59	OHX	16SA	2276	-	0,6,6	-	-	-		
59	OHX	23SA	3250	-	0,6,6	-	-	-		
59	OHX	16SB	2206	1	0,6,6	-	-	-		
59	OHX	23SA	3243	-	0,6,6	-	-	-		
59	OHX	23SA	3228	-	0,6,6	-	-	-		
59	OHX	23SA	3299	-	0,6,6	-	-	-		
59	OHX	23SA	3301	27	0,6,6	-	-	-		
59	OHX	23SA	3211	27	0,6,6	-	-	-		
59	OHX	16SB	2232	-	0,6,6	-	-	-		
59	OHX	23SA	3330	-	0,6,6	-	-	-		
59	OHX	23SB	3176	27	0,6,6	-	-	-		
59	OHX	23SA	3178	-	0,6,6	-	-	-		
59	OHX	16SB	2201	1	0,6,6	-	-	-		
59	OHX	23SA	3335	-	0,6,6	-	-	-		
59	OHX	ASIA	103	-	0,6,6	-	-	-		
59	OHX	23SA	3282	-	0,6,6	-	-	-		
59	OHX	23SA	3343	58	0,6,6	-	-	-		
59	OHX	16SA	2302	1	0,6,6	-	-	-		
59	OHX	23SA	3264	-	0,6,6	-	-	-		
59	OHX	23SB	3117	27	0,6,6	-	-	-		
59	OHX	L17A	201	39	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	OHX	23SB	3172	-	0,6,6	-	-	-		
59	OHX	16SB	2228	-	0,6,6	-	-	-		
59	OHX	23SA	3248	-	0,6,6	-	-	-		
59	OHX	23SB	3069	-	0,6,6	-	-	-		
59	OHX	23SA	3363	-	0,6,6	-	-	-		
59	OHX	5SB	206	-	0,6,6	-	-	-		
59	OHX	23SA	3370	27	0,6,6	-	-	-		
59	OHX	16SB	2255	-	0,6,6	-	-	-		
59	OHX	16SA	2269	-	0,6,6	-	-	-		
59	OHX	16SB	2259	-	0,6,6	-	-	-		
59	OHX	23SB	3084	-	0,6,6	-	-	-		
59	OHX	23SB	3043	-	0,6,6	-	-	-		
59	OHX	23SB	3070	-	0,6,6	-	-	-		
59	OHX	23SA	3375	-	0,6,6	-	-	-		
59	OHX	23SA	3320	27	0,6,6	-	-	-		
59	OHX	23SA	3240	-	0,6,6	-	-	-		
59	OHX	16SA	2264	-	0,6,6	-	-	-		
59	OHX	23SA	3362	-	0,6,6	-	-	-		
59	OHX	16SA	2337	-	0,6,6	-	-	-		
59	OHX	16SB	2261	-	0,6,6	-	-	-		
59	OHX	23SA	3328	-	0,6,6	-	-	-		
59	OHX	L15A	201	37	0,6,6	-	-	-		
59	OHX	23SB	3057	-	0,6,6	-	-	-		
59	OHX	23SB	3095	-	0,6,6	-	-	-		
59	OHX	23SB	3116	27	0,6,6	-	-	-		
59	OHX	23SA	3265	-	0,6,6	-	-	-		
59	OHX	23SB	3021	-	0,6,6	-	-	-		
59	OHX	23SB	3099	-	0,6,6	-	-	-		
59	OHX	23SA	3319	-	0,6,6	-	-	-		
59	OHX	23SB	3034	-	0,6,6	-	-	-		
59	OHX	16SA	2284	1	0,6,6	-	-	-		
59	OHX	23SA	3224	-	0,6,6	-	-	-		
59	OHX	16SA	2310	1	0,6,6	-	-	-		
59	OHX	ASIB	103	-	0,6,6	-	-	-		
59	OHX	23SA	3331	-	0,6,6	-	-	-		
59	OHX	16SB	2263	-	0,6,6	-	-	-		
59	OHX	23SA	3348	27	0,6,6	-	-	-		
59	OHX	23SA	3209	27	0,6,6	-	-	-		
59	OHX	16SA	2314	-	0,6,6	-	-	-		
59	OHX	23SA	3373	-	0,6,6	-	-	-		
59	OHX	23SA	3360	-	0,6,6	-	-	-		
59	OHX	5SA	205	28	0,6,6	-	-	-		
59	OHX	23SB	3136	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	OHX	23SB	3040	-	0,6,6	-	-	-		
59	OHX	MRNA	101	58	0,6,6	-	-	-		
59	OHX	16SA	2267	-	0,6,6	-	-	-		
59	OHX	23SB	3033	-	0,6,6	-	-	-		
59	OHX	23SA	3336	-	0,6,6	-	-	-		
59	OHX	23SA	3257	-	0,6,6	-	-	-		
59	OHX	23SA	3222	-	0,6,6	-	-	-		
59	OHX	16SB	2252	-	0,6,6	-	-	-		
59	OHX	16SB	2268	-	0,6,6	-	-	-		
59	OHX	23SB	3087	27	0,6,6	-	-	-		
59	OHX	16SA	2278	-	0,6,6	-	-	-		
59	OHX	23SA	3270	-	0,6,6	-	-	-		
59	OHX	23SA	3254	-	0,6,6	-	-	-		
59	OHX	16SA	2285	-	0,6,6	-	-	-		
59	OHX	23SA	3327	-	0,6,6	-	-	-		
59	OHX	16SB	2260	-	0,6,6	-	-	-		
59	OHX	23SB	3184	-	0,6,6	-	-	-		
59	OHX	23SB	3191	27	0,6,6	-	-	-		
59	OHX	23SB	3129	-	0,6,6	-	-	-		
59	OHX	23SB	3156	-	0,6,6	-	-	-		
59	OHX	23SB	3079	27	0,6,6	-	-	-		
59	OHX	16SA	2266	1	0,6,6	-	-	-		
59	OHX	23SA	3311	-	0,6,6	-	-	-		
59	OHX	23SA	3295	-	0,6,6	-	-	-		
59	OHX	23SA	3272	-	0,6,6	-	-	-		
59	OHX	23SB	3060	-	0,6,6	-	-	-		
59	OHX	16SA	2316	-	0,6,6	-	-	-		
59	OHX	23SA	3230	-	0,6,6	-	-	-		
59	OHX	23SA	3196	-	0,6,6	-	-	-		
59	OHX	16SA	2268	-	0,6,6	-	-	-		
59	OHX	23SA	3202	-	0,6,6	-	-	-		
59	OHX	16SA	2270	-	0,6,6	-	-	-		
59	OHX	23SA	3204	-	0,6,6	-	-	-		
59	OHX	23SA	3344	-	0,6,6	-	-	-		
59	OHX	23SB	3148	-	0,6,6	-	-	-		
59	OHX	23SB	3038	-	0,6,6	-	-	-		
59	OHX	16SB	2213	-	0,6,6	-	-	-		
59	OHX	23SB	3054	-	0,6,6	-	-	-		
59	OHX	23SB	3114	-	0,6,6	-	-	-		
59	OHX	23SB	3068	-	0,6,6	-	-	-		
59	OHX	23SA	3338	-	0,6,6	-	-	-		
59	OHX	23SB	3091	-	0,6,6	-	-	-		
59	OHX	23SB	3081	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	OHX	S4B	301	4	0,6,6	-	-	-		
59	OHX	23SA	3231	-	0,6,6	-	-	-		
59	OHX	16SB	2249	-	0,6,6	-	-	-		
59	OHX	23SB	3199	-	0,6,6	-	-	-		
59	OHX	16SB	2242	1	0,6,6	-	-	-		
59	OHX	23SB	3027	27	0,6,6	-	-	-		
59	OHX	23SB	3028	27	0,6,6	-	-	-		
59	OHX	16SA	2265	1	0,6,6	-	-	-		
59	OHX	16SA	2326	-	0,6,6	-	-	-		
59	OHX	23SB	3124	-	0,6,6	-	-	-		
59	OHX	23SB	3031	-	0,6,6	-	-	-		
59	OHX	16SB	2219	-	0,6,6	-	-	-		
59	OHX	23SA	3278	-	0,6,6	-	-	-		
59	OHX	16SA	2288	-	0,6,6	-	-	-		
59	OHX	23SA	3296	-	0,6,6	-	-	-		
59	OHX	23SA	3371	-	0,6,6	-	-	-		
59	OHX	23SA	3233	-	0,6,6	-	-	-		
59	OHX	23SA	3191	27	0,6,6	-	-	-		
59	OHX	23SA	3291	27	0,6,6	-	-	-		
59	OHX	16SB	2271	-	0,6,6	-	-	-		
59	OHX	16SA	2275	-	0,6,6	-	-	-		
59	OHX	16SA	2335	-	0,6,6	-	-	-		
59	OHX	23SB	3086	-	0,6,6	-	-	-		
59	OHX	23SB	3169	-	0,6,6	-	-	-		
59	OHX	16SA	2298	-	0,6,6	-	-	-		
59	OHX	23SA	3186	-	0,6,6	-	-	-		
59	OHX	23SA	3232	-	0,6,6	-	-	-		
59	OHX	23SA	3229	-	0,6,6	-	-	-		
59	OHX	ASIB	102	-	0,6,6	-	-	-		
59	OHX	23SB	3023	-	0,6,6	-	-	-		
59	OHX	23SB	3159	-	0,6,6	-	-	-		
59	OHX	23SB	3132	-	0,6,6	-	-	-		
59	OHX	16SA	2296	-	0,6,6	-	-	-		
59	OHX	23SB	3014	-	0,6,6	-	-	-		
59	OHX	23SA	3205	-	0,6,6	-	-	-		
59	OHX	23SB	3133	-	0,6,6	-	-	-		
59	OHX	16SA	2304	-	0,6,6	-	-	-		
61	SJE	23SB	3521	-	87,91,91	4.10	23 (26%)	117,134,134	1.99	22 (18%)
59	OHX	23SA	3307	-	0,6,6	-	-	-		
59	OHX	23SA	3198	-	0,6,6	-	-	-		
59	OHX	23SA	3255	-	0,6,6	-	-	-		
59	OHX	5SB	211	-	0,6,6	-	-	-		
59	OHX	23SA	3364	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	OHX	23SA	3300	-	0,6,6	-	-	-		
59	OHX	23SB	3048	27	0,6,6	-	-	-		
59	OHX	23SA	3376	-	0,6,6	-	-	-		
59	OHX	23SA	3286	-	0,6,6	-	-	-		
59	OHX	16SB	2276	-	0,6,6	-	-	-		
59	OHX	23SB	3178	-	0,6,6	-	-	-		
59	OHX	16SA	2261	1	0,6,6	-	-	-		
59	OHX	16SA	2325	-	0,6,6	-	-	-		
59	OHX	23SA	3304	42	0,6,6	-	-	-		
59	OHX	S10A	201	10,1	0,6,6	-	-	-		
59	OHX	23SA	3182	27	0,6,6	-	-	-		
59	OHX	23SB	3166	-	0,6,6	-	-	-		
59	OHX	23SA	3219	-	0,6,6	-	-	-		
59	OHX	23SA	3271	-	0,6,6	-	-	-		
59	OHX	23SA	3293	-	0,6,6	-	-	-		
59	OHX	16SA	2313	-	0,6,6	-	-	-		
59	OHX	16SA	2291	-	0,6,6	-	-	-		
59	OHX	23SB	3008	-	0,6,6	-	-	-		
59	OHX	23SA	3359	-	0,6,6	-	-	-		
59	OHX	5SB	205	28	0,6,6	-	-	-		
59	OHX	L17B	201	39	0,6,6	-	-	-		
59	OHX	23SB	3051	-	0,6,6	-	-	-		
59	OHX	16SA	2332	-	0,6,6	-	-	-		
59	OHX	16SA	2329	-	0,6,6	-	-	-		
59	OHX	23SA	3276	-	0,6,6	-	-	-		
59	OHX	23SA	3353	-	0,6,6	-	-	-		
59	OHX	16SA	2311	-	0,6,6	-	-	-		
59	OHX	L20A	201	-	0,6,6	-	-	-		
59	OHX	5SA	204	-	0,6,6	-	-	-		
59	OHX	23SA	3358	-	0,6,6	-	-	-		
59	OHX	23SB	3105	-	0,6,6	-	-	-		
59	OHX	16SB	2207	-	0,6,6	-	-	-		
59	OHX	23SB	3066	-	0,6,6	-	-	-		
59	OHX	23SA	3223	-	0,6,6	-	-	-		
59	OHX	23SB	3126	27	0,6,6	-	-	-		
59	OHX	23SB	3083	-	0,6,6	-	-	-		
59	OHX	L27A	102	48	0,6,6	-	-	-		
59	OHX	23SA	3212	27	0,6,6	-	-	-		
59	OHX	23SB	3177	-	0,6,6	-	-	-		
59	OHX	16SB	2248	-	0,6,6	-	-	-		
59	OHX	5SA	211	-	0,6,6	-	-	-		
59	OHX	23SB	3088	-	0,6,6	-	-	-		
59	OHX	23SA	3350	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	OHX	23SA	3216	-	0,6,6	-	-	-		
59	OHX	23SB	3151	-	0,6,6	-	-	-		
59	OHX	23SB	3077	27	0,6,6	-	-	-		
59	OHX	16SB	2266	-	0,6,6	-	-	-		
59	OHX	16SA	2340	-	0,6,6	-	-	-		
59	OHX	16SB	2256	1	0,6,6	-	-	-		
59	OHX	23SA	3380	27	0,6,6	-	-	-		
59	OHX	23SB	3098	-	0,6,6	-	-	-		
59	OHX	23SB	3138	27	0,6,6	-	-	-		
59	OHX	23SA	3234	-	0,6,6	-	-	-		
59	OHX	5SA	208	-	0,6,6	-	-	-		
59	OHX	16SA	2281	-	0,6,6	-	-	-		
59	OHX	23SB	3188	-	0,6,6	-	-	-		
59	OHX	23SB	3047	-	0,6,6	-	-	-		
59	OHX	5SB	202	-	0,6,6	-	-	-		
59	OHX	16SA	2272	1	0,6,6	-	-	-		
59	OHX	23SA	3208	-	0,6,6	-	-	-		
59	OHX	16SB	2231	1	0,6,6	-	-	-		
59	OHX	23SB	3052	-	0,6,6	-	-	-		
59	OHX	16SA	2307	-	0,6,6	-	-	-		
59	OHX	23SB	3082	-	0,6,6	-	-	-		
59	OHX	16SA	2322	-	0,6,6	-	-	-		
59	OHX	23SA	3321	-	0,6,6	-	-	-		
59	OHX	23SB	3135	-	0,6,6	-	-	-		
59	OHX	16SA	2330	-	0,6,6	-	-	-		
59	OHX	23SB	3044	-	0,6,6	-	-	-		
59	OHX	L28A	101	49	0,6,6	-	-	-		
59	OHX	23SB	3003	27	0,6,6	-	-	-		
59	OHX	23SA	3201	-	0,6,6	-	-	-		
59	OHX	23SA	3227	-	0,6,6	-	-	-		
59	OHX	23SB	3072	-	0,6,6	-	-	-		
59	OHX	23SB	3096	27	0,6,6	-	-	-		
59	OHX	23SA	3185	-	0,6,6	-	-	-		
59	OHX	16SA	2327	1	0,6,6	-	-	-		
59	OHX	16SB	2245	1	0,6,6	-	-	-		
59	OHX	23SA	3263	-	0,6,6	-	-	-		
59	OHX	23SB	3193	-	0,6,6	-	-	-		
59	OHX	23SA	3346	-	0,6,6	-	-	-		
59	OHX	23SB	3103	-	0,6,6	-	-	-		
59	OHX	16SA	2279	-	0,6,6	-	-	-		
59	OHX	23SA	3179	-	0,6,6	-	-	-		
59	OHX	16SB	2209	41,1	0,6,6	-	-	-		
59	OHX	23SA	3316	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	OHX	16SA	2295	-	0,6,6	-	-	-		
59	OHX	23SB	3050	-	0,6,6	-	-	-		
59	OHX	23SA	3245	-	0,6,6	-	-	-		
59	OHX	16SA	2271	-	0,6,6	-	-	-		
59	OHX	23SA	3382	-	0,6,6	-	-	-		
59	OHX	16SA	2324	-	0,6,6	-	-	-		
59	OHX	5SA	210	-	0,6,6	-	-	-		
59	OHX	23SA	3337	-	0,6,6	-	-	-		
59	OHX	23SB	3174	-	0,6,6	-	-	-		
59	OHX	23SA	3326	27	0,6,6	-	-	-		
59	OHX	16SA	2309	1	0,6,6	-	-	-		
59	OHX	PSIB	101	-	0,6,6	-	-	-		
59	OHX	23SB	3145	-	0,6,6	-	-	-		
59	OHX	23SA	3280	-	0,6,6	-	-	-		
59	OHX	23SB	3037	27	0,6,6	-	-	-		
59	OHX	23SB	3064	-	0,6,6	-	-	-		
59	OHX	23SA	3251	-	0,6,6	-	-	-		
59	OHX	23SB	3029	-	0,6,6	-	-	-		
59	OHX	23SB	3062	27	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	23SB	3521	-	-	41/101/161/161	0/5/5/5
61	SJE	23SA	3640	-	-	40/101/161/161	0/5/5/5

All (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
61	23SA	3640	SJE	O86-N85	11.11	1.41	1.22
61	23SB	3521	SJE	S78-N80	10.10	1.77	1.61
61	23SA	3640	SJE	S78-N80	10.09	1.77	1.61
61	23SA	3640	SJE	C72-S78	7.59	1.88	1.77
61	23SA	3640	SJE	C70-N84	7.30	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	23SB	3521	SJE	C70-N84	7.24	1.50	1.34
61	23SB	3521	SJE	C72-S78	7.13	1.87	1.77
61	23SB	3521	SJE	O49-C70	6.57	1.48	1.34
61	23SA	3640	SJE	O49-C70	6.54	1.47	1.34
61	23SB	3521	SJE	C61-C10	5.74	1.62	1.52
61	23SA	3640	SJE	C61-C10	5.71	1.62	1.52
61	23SA	3640	SJE	O38-C31	5.69	1.47	1.34
61	23SB	3521	SJE	O38-C31	5.45	1.47	1.34
61	23SA	3640	SJE	C77-C72	4.62	1.43	1.40
61	23SB	3521	SJE	C77-C72	4.27	1.43	1.40
61	23SB	3521	SJE	O19-C20	3.71	1.44	1.34
61	23SA	3640	SJE	O19-C20	3.58	1.44	1.34
61	23SA	3640	SJE	C21-C20	3.55	1.57	1.50
61	23SB	3521	SJE	C21-C20	3.34	1.57	1.50
61	23SA	3640	SJE	C15-C16	-3.30	1.48	1.53
61	23SB	3521	SJE	C15-C16	-3.06	1.48	1.53
61	23SB	3521	SJE	C11-C10	-3.05	1.47	1.53
61	23SB	3521	SJE	C10-C9	-2.92	1.47	1.53
61	23SA	3640	SJE	C11-C10	-2.86	1.48	1.53
61	23SA	3640	SJE	O63-C3	2.84	1.49	1.42
61	23SB	3521	SJE	O38-C37	-2.82	1.40	1.44
61	23SA	3640	SJE	O19-C35	-2.81	1.40	1.44
61	23SA	3640	SJE	O6-C5	2.80	1.49	1.41
61	23SB	3521	SJE	O19-C35	-2.77	1.40	1.44
61	23SB	3521	SJE	O6-C5	2.72	1.48	1.41
61	23SA	3640	SJE	C83-N84	2.54	1.52	1.46
61	23SA	3640	SJE	O38-C37	-2.46	1.41	1.44
61	23SA	3640	SJE	O49-C27	-2.42	1.43	1.46
61	23SA	3640	SJE	C10-C9	-2.27	1.48	1.53
61	23SB	3521	SJE	C83-N84	2.25	1.51	1.46
61	23SB	3521	SJE	O7-C12	2.24	1.47	1.42
61	23SB	3521	SJE	O49-C27	-2.22	1.43	1.46
61	23SB	3521	SJE	C53-C30	2.19	1.57	1.54
61	23SB	3521	SJE	O63-C3	2.19	1.48	1.42
61	23SA	3640	SJE	C53-C30	2.16	1.57	1.54
61	23SA	3640	SJE	C3-C4	-2.13	1.47	1.52
61	23SA	3640	SJE	C77-N85	2.09	1.49	1.45
61	23SA	3640	SJE	O7-C12	2.06	1.47	1.42

All (50) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
61	23SB	3521	SJE	O19-C20-C21	5.43	121.44	111.46
61	23SA	3640	SJE	C72-S78-N80	5.39	114.83	107.82
61	23SB	3521	SJE	O6-C1-C2	4.81	118.16	109.52
61	23SB	3521	SJE	C72-S78-N80	4.64	113.84	107.82
61	23SA	3640	SJE	O19-C20-C21	4.51	119.74	111.46
61	23SB	3521	SJE	O71-C70-N84	-4.26	118.43	124.96
61	23SA	3640	SJE	O71-C70-N84	-4.17	118.57	124.96
61	23SA	3640	SJE	O13-C14-C15	4.09	115.40	109.14
61	23SA	3640	SJE	O6-C1-C2	3.75	116.25	109.52
61	23SA	3640	SJE	C3-C2-C1	3.72	118.19	110.12
61	23SB	3521	SJE	C10-C11-C12	-3.48	108.15	114.82
61	23SB	3521	SJE	O48-C33-C34	3.36	112.27	108.22
61	23SB	3521	SJE	C3-C2-C1	3.30	117.29	110.12
61	23SB	3521	SJE	O13-C18-C17	3.19	117.10	110.35
61	23SA	3640	SJE	C65-C1-C2	-3.07	107.41	113.07
61	23SA	3640	SJE	C56-C14-C15	-3.06	108.59	113.40
61	23SB	3521	SJE	O38-C31-C32	3.04	118.23	111.56
61	23SB	3521	SJE	O7-C8-C9	3.00	115.39	110.03
61	23SA	3640	SJE	C58-C8-C9	-2.89	107.64	112.57
61	23SA	3640	SJE	O81-S78-C72	2.84	112.33	107.66
61	23SB	3521	SJE	C58-C8-C9	-2.80	107.79	112.57
61	23SA	3640	SJE	C32-C33-C34	-2.78	104.99	113.05
61	23SA	3640	SJE	C18-C17-C16	2.78	113.73	109.19
61	23SA	3640	SJE	O6-C1-C65	2.78	112.69	106.70
61	23SA	3640	SJE	C10-C11-C12	-2.76	109.52	114.82
61	23SB	3521	SJE	C15-C16-C17	2.74	115.68	109.72
61	23SA	3640	SJE	C35-O19-C20	-2.72	113.01	117.53
61	23SA	3640	SJE	O48-C33-C34	2.66	111.43	108.22
61	23SB	3521	SJE	O22-C20-C21	-2.65	118.88	124.73
61	23SA	3640	SJE	C44-C30-C53	-2.62	106.50	112.45
61	23SB	3521	SJE	C56-C14-C15	-2.60	109.32	113.40
61	23SB	3521	SJE	O47-C29-C34	2.57	111.32	108.22
61	23SA	3640	SJE	C41-C26-C35	-2.56	107.11	112.92
61	23SA	3640	SJE	C45-C37-C36	-2.55	107.49	114.29
61	23SB	3521	SJE	C32-C33-C34	-2.48	105.86	113.05
61	23SA	3640	SJE	O38-C31-C32	2.47	116.98	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	23SB	3521	SJE	C83-N84-C70	-2.46	117.95	121.89
61	23SB	3521	SJE	C77-C72-S78	-2.44	121.40	124.39
61	23SB	3521	SJE	C30-C29-C34	-2.36	108.00	114.29
61	23SA	3640	SJE	C74-C73-C72	2.30	122.97	118.78
61	23SA	3640	SJE	C75-C76-C77	2.25	122.45	118.61
61	23SA	3640	SJE	C15-C16-C17	2.16	114.41	109.72
61	23SA	3640	SJE	C73-C72-C77	-2.11	117.85	119.91
61	23SA	3640	SJE	O49-C70-O71	-2.08	121.83	125.62
61	23SA	3640	SJE	C30-C29-C34	-2.02	108.89	114.29

There are no chirality outliers.

All (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
61	23SA	3640	SJE	O49-C27-C28-O39
61	23SA	3640	SJE	C28-C27-C53-C30
61	23SA	3640	SJE	C42-C27-C53-C30
61	23SA	3640	SJE	O49-C27-C53-C30
61	23SA	3640	SJE	C34-C29-C30-C53
61	23SA	3640	SJE	O47-C29-C30-C53
61	23SA	3640	SJE	C30-C29-C34-C33
61	23SA	3640	SJE	C30-C29-C34-C54
61	23SA	3640	SJE	O47-C29-C34-C33
61	23SA	3640	SJE	O19-C35-C36-C43
61	23SA	3640	SJE	C73-C72-S78-N80
61	23SA	3640	SJE	C82-N80-S78-C72
61	23SA	3640	SJE	C82-N80-S78-O79
61	23SB	3521	SJE	C11-C12-O48-C33
61	23SB	3521	SJE	C21-C20-O19-C35
61	23SB	3521	SJE	O22-C20-O19-C35
61	23SB	3521	SJE	C28-C26-C35-O19
61	23SB	3521	SJE	C41-C26-C35-O19
61	23SB	3521	SJE	C42-C27-C28-C26
61	23SB	3521	SJE	O49-C27-C28-O39
61	23SB	3521	SJE	C28-C27-C53-C30
61	23SB	3521	SJE	C42-C27-C53-C30
61	23SB	3521	SJE	O49-C27-C53-C30

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Mol	Chain	Res	Type	Atoms
61	23SB	3521	SJE	C34-C29-C30-C53
61	23SB	3521	SJE	O47-C29-C30-C53
61	23SB	3521	SJE	C30-C29-C34-C33
61	23SB	3521	SJE	C30-C29-C34-C54
61	23SB	3521	SJE	O47-C29-C34-C33
61	23SB	3521	SJE	C72-C77-N85-O86
61	23SB	3521	SJE	C76-C77-N85-O86
61	23SB	3521	SJE	C82-N80-S78-C72
61	23SB	3521	SJE	C82-N80-S78-O79
61	23SA	3640	SJE	O71-C70-O49-C27
61	23SB	3521	SJE	O71-C70-O49-C27
61	23SA	3640	SJE	N84-C70-O49-C27
61	23SB	3521	SJE	N84-C70-O49-C27
61	23SA	3640	SJE	C73-C72-S78-O79
61	23SB	3521	SJE	C73-C72-S78-O79
61	23SB	3521	SJE	C73-C72-S78-N80
61	23SB	3521	SJE	O47-C29-C34-C54
61	23SB	3521	SJE	O7-C12-O48-C33
61	23SA	3640	SJE	C77-C72-S78-O79
61	23SB	3521	SJE	C77-C72-S78-O79
61	23SB	3521	SJE	O19-C35-C36-C43
61	23SA	3640	SJE	C26-C35-C36-C43
61	23SA	3640	SJE	C77-C72-S78-N80
61	23SA	3640	SJE	C76-C77-N85-O86
61	23SA	3640	SJE	C73-C72-S78-O81
61	23SA	3640	SJE	O47-C29-C34-C54
61	23SB	3521	SJE	C73-C72-S78-O81
61	23SA	3640	SJE	C11-C12-O48-C33
61	23SB	3521	SJE	C77-C72-S78-N80
61	23SA	3640	SJE	C4-C5-O52-C50
61	23SB	3521	SJE	C26-C35-C36-C43
61	23SA	3640	SJE	O7-C12-O48-C33
61	23SA	3640	SJE	O6-C5-O52-C50
61	23SA	3640	SJE	C77-C72-S78-O81
61	23SB	3521	SJE	C28-C26-C35-C36
61	23SA	3640	SJE	O19-C35-C36-C37
61	23SB	3521	SJE	C77-C72-S78-O81
61	23SA	3640	SJE	O47-C29-C30-C44
61	23SB	3521	SJE	O47-C29-C30-C44
61	23SA	3640	SJE	C28-C26-C35-C36
61	23SB	3521	SJE	C4-C5-O52-C50
61	23SB	3521	SJE	C82-N80-S78-O81

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Mol	Chain	Res	Type	Atoms
61	23SA	3640	SJE	C72-C77-N85-O86
61	23SB	3521	SJE	O19-C35-C36-C37
61	23SB	3521	SJE	O6-C5-O52-C50
61	23SA	3640	SJE	C34-C29-C30-C44
61	23SB	3521	SJE	C34-C29-C30-C44
61	23SB	3521	SJE	C20-C21-C23-C24
61	23SA	3640	SJE	C46-C32-C33-C34
61	23SB	3521	SJE	C41-C26-C35-C36
61	23SA	3640	SJE	C82-N80-S78-O81
61	23SA	3640	SJE	C41-C26-C35-C36
61	23SB	3521	SJE	O13-C18-O47-C29

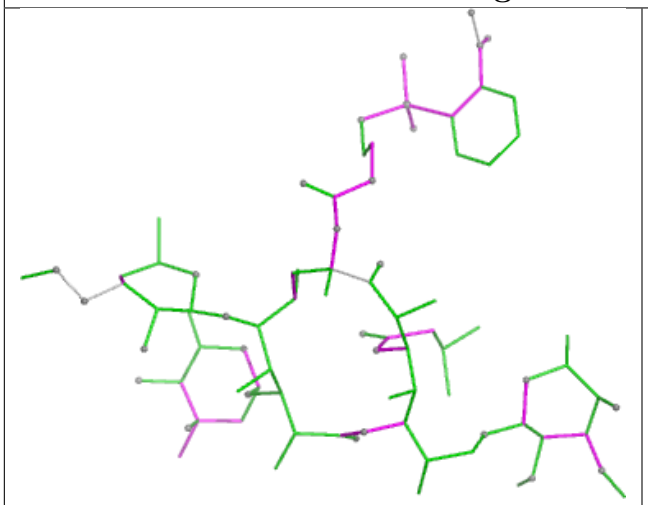
There are no ring outliers.

1 monomer is involved in 1 short contact:

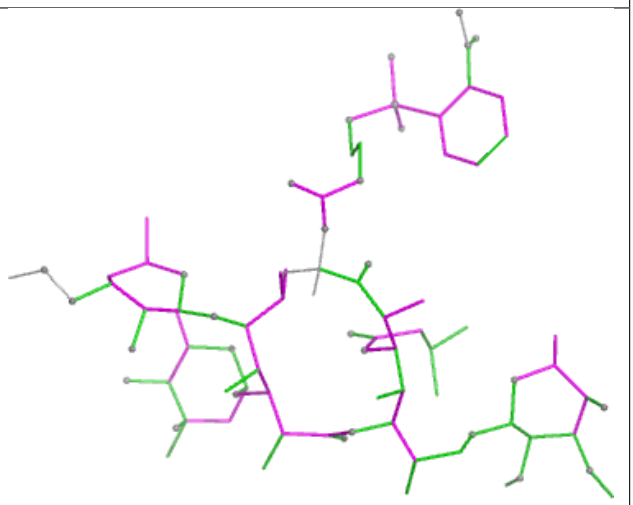
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	23SA	3304	OHX	0	1

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 then 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.

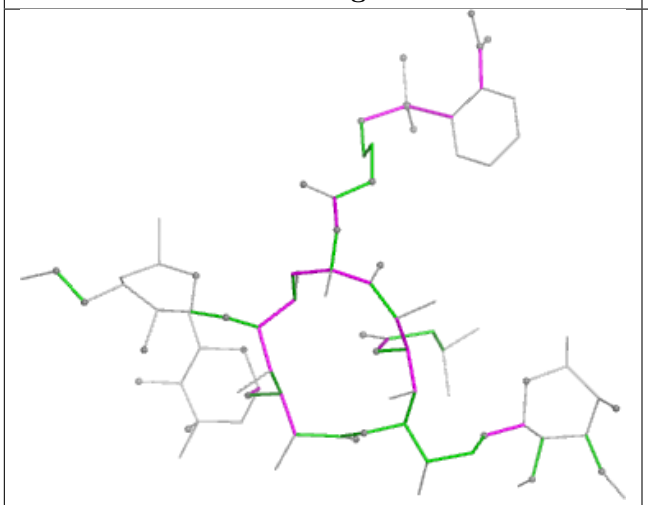
Ligand SJE 23SA 3640



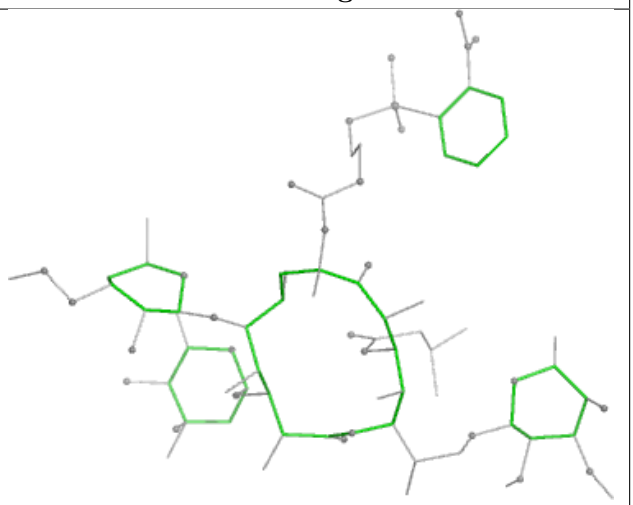
Bond lengths



Bond angles

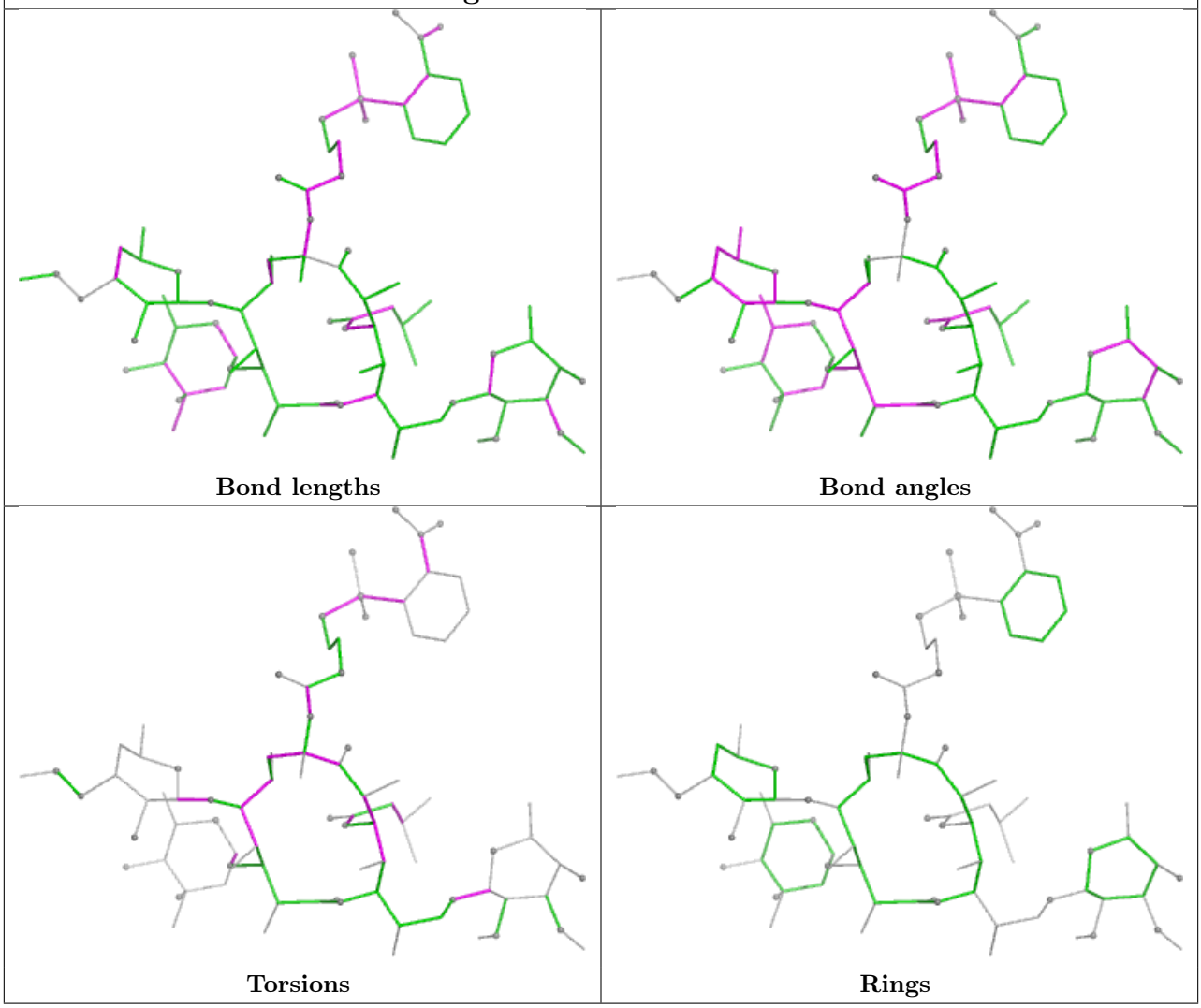


Torsions



Rings

Ligand SJE 23SB 3521



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

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%)	-0.43	4 (0%)	90	82	45, 89, 170, 260	0
1	16SB	1496/1512 (98%)	-0.61	2 (0%)	92	90	57, 100, 164, 267	0
2	S2A	237/256 (92%)	0.57	10 (4%)	40	26	91, 125, 164, 178	0
2	S2B	237/256 (92%)	0.73	12 (5%)	33	22	105, 153, 186, 205	0
3	S3A	205/239 (85%)	0.58	6 (2%)	53	35	80, 100, 141, 168	0
3	S3B	206/239 (86%)	0.50	8 (3%)	43	29	104, 128, 157, 161	0
4	S4A	208/209 (99%)	0.60	14 (6%)	24	16	75, 97, 119, 128	0
4	S4B	208/209 (99%)	0.71	14 (6%)	24	16	79, 96, 117, 138	0
5	S5A	151/162 (93%)	0.47	4 (2%)	57	38	65, 87, 108, 132	0
5	S5B	151/162 (93%)	0.39	4 (2%)	57	38	86, 105, 123, 151	0
6	S6A	101/101 (100%)	0.52	3 (2%)	52	35	70, 91, 107, 124	0
6	S6B	101/101 (100%)	0.58	6 (5%)	28	19	73, 94, 109, 132	0
7	S7A	155/156 (99%)	0.30	7 (4%)	38	25	90, 105, 129, 138	0
7	S7B	155/156 (99%)	0.21	2 (1%)	75	56	30, 115, 151, 175	0
8	S8A	138/138 (100%)	0.15	0	100	100	75, 92, 104, 114	0
8	S8B	138/138 (100%)	-0.05	1 (0%)	84	70	83, 104, 115, 125	0
9	S9A	127/128 (99%)	0.23	5 (3%)	43	29	72, 121, 140, 144	0
9	S9B	127/128 (99%)	-0.13	1 (0%)	82	68	77, 136, 152, 156	0
10	S10A	99/105 (94%)	0.28	5 (5%)	33	22	72, 124, 151, 154	0
10	S10B	99/105 (94%)	0.20	1 (1%)	79	63	104, 144, 159, 166	0
11	S11A	116/129 (89%)	0.41	2 (1%)	69	50	63, 90, 113, 142	0
11	S11B	117/129 (90%)	0.28	5 (4%)	40	25	76, 97, 122, 156	0
12	S12A	124/132 (93%)	0.55	10 (8%)	18	13	57, 66, 98, 162	0
12	S12B	124/132 (93%)	0.60	11 (8%)	15	12	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%)	0.37	8 (6%) 24 16	77, 113, 129, 138	0
13	S13B	121/126 (96%)	0.20	5 (4%) 41 27	100, 138, 150, 159	0
14	S14A	60/61 (98%)	0.21	1 (1%) 69 50	78, 90, 103, 117	0
14	S14B	59/61 (96%)	0.11	1 (1%) 69 50	106, 119, 143, 146	0
15	S15A	88/89 (98%)	0.13	0 100 100	65, 84, 108, 115	0
15	S15B	88/89 (98%)	-0.10	0 100 100	73, 96, 112, 119	0
16	S16A	83/88 (94%)	0.32	3 (3%) 46 31	86, 98, 118, 146	0
16	S16B	84/88 (95%)	0.20	1 (1%) 76 58	79, 88, 106, 144	0
17	S17A	100/105 (95%)	0.17	2 (2%) 65 46	74, 90, 101, 104	0
17	S17B	100/105 (95%)	0.09	2 (2%) 65 46	80, 97, 114, 126	0
18	S18A	71/88 (80%)	0.50	4 (5%) 30 20	72, 88, 121, 148	0
18	S18B	70/88 (79%)	0.54	3 (4%) 40 25	80, 97, 125, 148	0
19	S19A	84/93 (90%)	0.77	10 (11%) 9 7	30, 114, 133, 139	0
19	S19B	86/93 (92%)	0.43	7 (8%) 18 13	125, 151, 177, 188	0
20	S20A	99/106 (93%)	0.27	1 (1%) 79 63	58, 105, 133, 139	0
20	S20B	99/106 (93%)	-0.03	1 (1%) 79 63	60, 103, 127, 133	0
21	THXA	24/27 (88%)	-0.19	0 100 100	92, 102, 114, 129	0
21	THXB	25/27 (92%)	-0.10	0 100 100	113, 127, 143, 148	0
22	ASIA	69/76 (90%)	1.90	30 (43%) 0 0	71, 185, 223, 237	0
23	PSIA	67/76 (88%)	0.28	6 (8%) 15 11	62, 86, 106, 154	0
23	PSIB	67/76 (88%)	0.01	3 (4%) 38 25	73, 103, 134, 167	0
24	ESIA	75/76 (98%)	0.78	8 (10%) 11 9	61, 191, 216, 221	0
24	ESIB	75/76 (98%)	0.26	0 100 100	72, 196, 221, 233	0
25	MRNA	30/30 (100%)	0.98	5 (16%) 4 4	60, 150, 238, 250	0
25	MRNB	30/30 (100%)	0.25	2 (6%) 24 16	79, 168, 237, 243	0
26	TRNA	65/76 (85%)	0.38	3 (4%) 37 25	106, 176, 202, 216	0
27	23SA	2878/2911 (98%)	-0.72	13 (0%) 87 76	33, 60, 190, 262	0
27	23SB	2862/2911 (98%)	-0.50	20 (0%) 84 70	40, 76, 213, 270	0
28	5SA	122/124 (98%)	-0.77	0 100 100	57, 76, 92, 167	0
28	5SB	121/124 (97%)	-0.44	1 (0%) 82 68	80, 105, 137, 192	0
29	L2A	272/276 (98%)	-0.07	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%)	-0.11	2 (0%)	84	70	41, 62, 81, 92	0
30	L3A	204/206 (99%)	0.05	4 (1%)	65	46	41, 68, 95, 114	0
30	L3B	204/206 (99%)	0.54	12 (5%)	28	19	49, 86, 115, 128	0
31	L4A	202/210 (96%)	-0.18	2 (0%)	79	63	35, 64, 94, 117	0
31	L4B	202/210 (96%)	0.28	7 (3%)	47	31	48, 85, 113, 129	0
32	L5A	181/182 (99%)	0.17	2 (1%)	78	60	70, 87, 114, 130	0
32	L5B	181/182 (99%)	0.26	3 (1%)	69	50	100, 119, 142, 152	0
33	L6A	171/180 (95%)	0.82	14 (8%)	17	13	30, 94, 113, 136	0
33	L6B	173/180 (96%)	2.07	86 (49%)	0	0	154, 201, 242, 260	0
34	L9A	145/148 (97%)	1.00	24 (16%)	4	4	61, 116, 131, 146	0
34	L9B	146/148 (98%)	1.07	31 (21%)	2	2	75, 116, 137, 150	0
35	L13A	138/140 (98%)	0.15	4 (2%)	53	35	51, 70, 102, 112	0
35	L13B	138/140 (98%)	1.22	24 (17%)	4	4	68, 101, 130, 136	0
36	L14A	122/122 (100%)	0.24	3 (2%)	58	39	44, 62, 75, 84	0
36	L14B	122/122 (100%)	0.60	4 (3%)	49	33	62, 81, 101, 112	0
37	L15A	150/150 (100%)	-0.08	0	100	100	38, 69, 99, 141	0
37	L15B	150/150 (100%)	0.05	2 (1%)	75	56	49, 95, 127, 145	0
38	L16A	141/141 (100%)	0.26	6 (4%)	40	25	48, 66, 89, 120	0
38	L16B	141/141 (100%)	0.39	7 (4%)	34	23	58, 73, 93, 123	0
39	L17A	118/118 (100%)	-0.20	1 (0%)	82	68	49, 66, 85, 94	0
39	L17B	118/118 (100%)	-0.00	0	100	100	57, 75, 94, 111	0
40	L18A	112/112 (100%)	0.12	1 (0%)	81	65	57, 72, 99, 115	0
40	L18B	111/112 (99%)	0.02	0	100	100	73, 104, 141, 150	0
41	L19A	137/146 (93%)	0.28	2 (1%)	72	53	56, 73, 129, 158	0
41	L19B	137/146 (93%)	0.48	4 (2%)	53	35	72, 90, 167, 185	0
42	L20A	117/118 (99%)	-0.28	1 (0%)	81	65	43, 60, 88, 115	0
42	L20B	117/118 (99%)	0.80	21 (17%)	3	3	57, 94, 136, 149	0
43	L21A	101/101 (100%)	0.05	1 (0%)	79	63	44, 81, 98, 110	0
43	L21B	101/101 (100%)	1.59	31 (30%)	1	1	58, 112, 128, 142	0
44	L22A	113/113 (100%)	-0.33	1 (0%)	81	65	43, 57, 88, 128	0
44	L22B	113/113 (100%)	0.33	4 (3%)	47	31	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%)	-0.21	0 100 100	44, 57, 75, 98	0
45	L23B	94/96 (97%)	0.07	2 (2%) 63 44	58, 73, 98, 121	0
46	L24A	108/110 (98%)	0.16	2 (1%) 66 48	61, 87, 135, 151	0
46	L24B	106/110 (96%)	1.01	15 (14%) 6 5	66, 99, 145, 153	0
47	L25A	179/206 (86%)	0.53	11 (6%) 27 18	70, 104, 181, 189	0
47	L25B	176/206 (85%)	0.86	11 (6%) 26 17	107, 145, 224, 228	0
48	L27A	84/85 (98%)	-0.09	1 (1%) 76 58	45, 59, 84, 104	0
48	L27B	84/85 (98%)	0.02	4 (4%) 35 24	63, 79, 100, 128	0
49	L28A	97/98 (98%)	0.25	7 (7%) 21 15	43, 63, 110, 132	0
49	L28B	97/98 (98%)	0.28	4 (4%) 41 27	52, 75, 118, 132	0
50	L29A	69/72 (95%)	0.13	0 100 100	50, 66, 81, 105	0
50	L29B	71/72 (98%)	0.17	2 (2%) 55 36	70, 89, 109, 138	0
51	L30A	59/60 (98%)	-0.16	0 100 100	48, 66, 96, 115	0
51	L30B	59/60 (98%)	0.54	2 (3%) 48 32	69, 90, 130, 146	0
52	L31A	71/71 (100%)	0.61	3 (4%) 40 26	95, 137, 172, 175	0
52	L31B	71/71 (100%)	0.27	0 100 100	123, 160, 188, 194	0
53	L32A	56/60 (93%)	-0.14	2 (3%) 46 31	38, 70, 126, 133	0
53	L32B	56/60 (93%)	0.60	3 (5%) 31 21	47, 78, 139, 150	0
54	L33A	45/54 (83%)	1.52	12 (26%) 1 1	106, 130, 157, 160	0
54	L33B	45/54 (83%)	0.54	0 100 100	129, 157, 182, 188	0
55	L34A	48/49 (97%)	-0.43	1 (2%) 63 44	37, 42, 57, 78	0
55	L34B	49/49 (100%)	-0.21	1 (2%) 65 46	42, 51, 97, 109	0
56	L35A	64/65 (98%)	-0.36	1 (1%) 70 52	38, 54, 71, 93	0
56	L35B	64/65 (98%)	0.03	0 100 100	30, 70, 91, 116	0
57	ASIB	72/76 (94%)	0.79	10 (13%) 6 5	98, 216, 254, 258	0
All	All	21108/21740 (97%)	-0.04	675 (3%) 50 34	30, 88, 176, 270	0

All (675) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	L6B	72	ILE	7.5
4	S4A	9	CYS	6.4
34	L9A	129	THR	6.3

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Mol	Chain	Res	Type	RSRZ
22	ASIA	1	G	6.2
12	S12A	44	LYS	6.0
43	L21B	36	PRO	5.9
35	L13B	133	GLN	5.9
27	23SB	2911	G	5.8
22	ASIA	73	A	5.8
27	23SB	1110	G	5.7
2	S2B	163	PHE	5.5
27	23SB	2912	A	5.3
22	ASIA	3	C	5.2
27	23SB	572	C	5.2
33	L6B	38	SER	5.2
33	L6B	113	VAL	5.1
33	L6B	174	GLY	5.1
33	L6B	148	ILE	5.1
13	S13A	119	GLY	5.1
33	L6B	114	VAL	5.1
19	S19B	88	LYS	5.1
28	5SB	90	C	5.0
33	L6B	131	VAL	5.0
30	L3B	57	LYS	5.0
33	L6B	84	SER	5.0
4	S4B	31	CYS	4.9
34	L9B	123	LEU	4.9
4	S4A	26	CYS	4.9
30	L3B	73	GLU	4.8
34	L9A	85	GLU	4.8
27	23SB	1139	G	4.8
45	L23B	92	LEU	4.8
19	S19B	84	GLY	4.7
4	S4A	31	CYS	4.7
22	ASIA	70	G	4.7
34	L9B	80	PRO	4.6
35	L13A	96	GLU	4.6
4	S4B	24	GLU	4.6
25	MRNA	56	U	4.6
26	TRNA	73	A	4.6
4	S4B	26	CYS	4.5
35	L13B	29	LYS	4.5
43	L21B	5	VAL	4.5
33	L6B	103	LEU	4.5
12	S12B	29	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
22	ASIA	71	G	4.4
57	ASIB	1	G	4.4
13	S13A	120	LYS	4.4
4	S4B	12	CYS	4.4
43	L21B	38	LEU	4.4
48	L27B	7	LEU	4.3
36	L14B	13	ASN	4.3
35	L13B	1	MET	4.3
48	L27B	4	LYS	4.3
34	L9A	68	LEU	4.3
4	S4B	86	LYS	4.2
19	S19A	85	LYS	4.2
25	MRNA	55	U	4.2
54	L33A	9	LEU	4.2
27	23SA	1111	G	4.2
27	23SB	2913	C	4.2
22	ASIA	76	A	4.1
13	S13A	107	ALA	4.1
34	L9B	84	GLY	4.1
33	L6B	107	VAL	4.1
2	S2B	37	ASN	4.0
4	S4B	9	CYS	4.0
19	S19A	42	PRO	4.0
46	L24B	40	GLU	4.0
23	PSIA	1	G	4.0
34	L9B	140	LEU	4.0
27	23SB	1125	A	4.0
11	S11A	12	ARG	4.0
33	L6B	11	VAL	4.0
33	L6B	115	VAL	4.0
24	ESIA	14	A	4.0
43	L21B	71	LEU	3.9
34	L9B	135	GLU	3.9
46	L24B	101	LYS	3.9
33	L6B	105	LEU	3.9
2	S2B	165	VAL	3.8
19	S19A	44	MET	3.8
54	L33A	22	ALA	3.8
34	L9B	144	VAL	3.8
1	16SA	727	U	3.8
22	ASIA	72	C	3.8
42	L20B	91	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
33	L6B	35	VAL	3.7
24	ESIA	1	G	3.7
33	L6B	24	VAL	3.7
5	S5A	10	MET	3.7
32	L5A	80	PHE	3.7
2	S2A	188	ALA	3.7
22	ASIA	12	U	3.7
2	S2A	118	LEU	3.7
42	L20B	83	LEU	3.7
33	L6B	43	VAL	3.7
33	L6B	36	PRO	3.6
47	L25B	176	PRO	3.6
34	L9A	140	LEU	3.6
22	ASIA	74	C	3.6
33	L6B	102	ALA	3.6
31	L4B	131	GLY	3.6
12	S12A	126	ALA	3.6
34	L9B	146	ALA	3.6
9	S9A	127	LYS	3.6
33	L6A	172	LYS	3.6
12	S12A	58	THR	3.6
49	L28A	84	GLY	3.6
34	L9B	145	VAL	3.6
18	S18A	88	LYS	3.6
34	L9A	114	LEU	3.5
30	L3B	204	ALA	3.5
2	S2B	196	LEU	3.5
54	L33A	34	LEU	3.5
10	S10A	59	SER	3.5
43	L21B	48	GLY	3.5
33	L6B	45	VAL	3.5
34	L9B	83	ALA	3.5
34	L9A	113	ARG	3.5
25	MRNA	54	U	3.5
36	L14A	108	GLU	3.5
2	S2A	115	LEU	3.5
42	L20B	113	ALA	3.5
33	L6B	89	ILE	3.5
57	ASIB	6	G	3.5
33	L6A	34	GLU	3.4
34	L9B	122	GLU	3.4
11	S11A	25	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
13	S13B	4	ILE	3.4
33	L6B	118	PRO	3.4
22	ASIA	11	C	3.4
24	ESIA	13	C	3.4
57	ASIB	74	C	3.4
7	S7B	80	VAL	3.4
13	S13A	117	VAL	3.4
33	L6B	22	GLY	3.4
46	L24A	101	LYS	3.4
33	L6B	88	LEU	3.4
34	L9B	68	LEU	3.4
27	23SB	4	C	3.4
33	L6A	82	GLY	3.4
12	S12B	126	ALA	3.4
43	L21B	45	THR	3.4
2	S2A	148	TYR	3.4
33	L6B	71	LEU	3.4
33	L6B	151	ILE	3.4
47	L25A	107	THR	3.4
33	L6B	96	ALA	3.4
38	L16B	1	MET	3.4
1	16SB	1053	A	3.3
2	S2A	15	VAL	3.3
20	S20A	8	ARG	3.3
37	L15B	46	LYS	3.3
23	PSIB	1	G	3.3
33	L6B	150	ALA	3.3
24	ESIA	12	U	3.3
27	23SB	2910	U	3.3
33	L6B	106	THR	3.3
33	L6B	15	VAL	3.3
32	L5B	155	MET	3.3
19	S19B	82	GLY	3.3
42	L20B	111	GLU	3.3
53	L32B	53	ALA	3.3
34	L9B	143	SER	3.3
43	L21B	12	TYR	3.3
7	S7A	78	ARG	3.3
27	23SB	1137	G	3.3
33	L6B	123	PHE	3.3
50	L29B	71	ASN	3.3
34	L9A	111	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
33	L6B	99	VAL	3.2
33	L6B	169	VAL	3.2
27	23SA	1125	A	3.2
27	23SB	2914	C	3.2
57	ASIB	75	C	3.2
34	L9B	92	VAL	3.2
42	L20B	104	GLN	3.2
19	S19A	61	TYR	3.2
23	PSIB	70	G	3.2
33	L6B	129	THR	3.2
34	L9A	109	ILE	3.2
19	S19A	43	GLU	3.2
34	L9A	136	VAL	3.2
43	L21B	47	VAL	3.2
12	S12B	59	SER	3.2
27	23SA	1118	A	3.2
33	L6B	26	VAL	3.2
4	S4A	12	CYS	3.1
33	L6B	14	GLY	3.1
1	16SA	726	U	3.1
25	MRNA	53	U	3.1
3	S3B	75	VAL	3.1
35	L13B	46	VAL	3.1
33	L6B	154	PRO	3.1
27	23SB	1814	A	3.1
42	L20B	88	ILE	3.1
18	S18A	20	ALA	3.1
43	L21B	26	ASP	3.1
38	L16A	1	MET	3.1
36	L14B	91	LEU	3.1
49	L28A	85	LEU	3.1
27	23SB	5	A	3.1
2	S2A	114	ARG	3.1
22	ASIA	17	C	3.1
16	S16B	78	GLY	3.1
30	L3B	40	GLU	3.1
41	L19A	1	MET	3.1
34	L9B	139	GLN	3.0
43	L21B	35	LEU	3.0
49	L28B	64	ALA	3.0
33	L6B	133	VAL	3.0
43	L21B	85	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
38	L16A	104	PHE	3.0
35	L13B	129	PRO	3.0
46	L24B	106	LEU	3.0
54	L33A	10	LEU	3.0
20	S20B	8	ARG	3.0
33	L6B	13	LYS	3.0
33	L6B	85	LYS	3.0
43	L21B	32	THR	3.0
47	L25B	83	PRO	3.0
48	L27B	2	ALA	3.0
19	S19A	32	LYS	3.0
34	L9A	141	LYS	3.0
19	S19A	45	VAL	3.0
26	TRNA	1	G	3.0
42	L20B	90	VAL	3.0
51	L30B	58	VAL	3.0
54	L33A	48	VAL	3.0
57	ASIB	70	G	3.0
33	L6B	95	ARG	3.0
32	L5B	152	LEU	2.9
33	L6A	87	LEU	2.9
35	L13B	138	LEU	2.9
11	S11B	35	PRO	2.9
33	L6B	29	PRO	2.9
33	L6B	37	VAL	2.9
43	L21B	52	VAL	2.9
34	L9A	139	GLN	2.9
22	ASIA	68	C	2.9
16	S16A	19	ILE	2.9
12	S12A	125	ALA	2.9
23	PSIA	70	G	2.9
2	S2B	32	ILE	2.9
38	L16A	79	LEU	2.9
47	L25A	117	LEU	2.9
47	L25B	76	LEU	2.9
33	L6B	86	GLU	2.9
47	L25A	97	GLU	2.9
5	S5B	105	VAL	2.9
10	S10A	62	HIS	2.9
35	L13B	60	ILE	2.9
33	L6B	87	LEU	2.9
4	S4B	169	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
38	L16A	21	THR	2.9
54	L33A	23	THR	2.9
23	PSIA	5	G	2.9
47	L25B	116	VAL	2.9
12	S12B	82	ILE	2.9
35	L13B	137	LYS	2.9
47	L25B	41	LEU	2.9
4	S4A	102	ASP	2.9
18	S18B	24	ALA	2.9
13	S13B	87	TYR	2.9
22	ASIA	26	A	2.9
35	L13B	99	LEU	2.9
49	L28B	67	ILE	2.9
25	MRNB	57	U	2.8
33	L6B	34	GLU	2.8
33	L6B	97	ARG	2.8
17	S17A	98	LEU	2.8
34	L9B	72	LEU	2.8
43	L21B	91	TYR	2.8
33	L6B	16	SER	2.8
24	ESIA	6	G	2.8
4	S4B	34	GLU	2.8
34	L9A	135	GLU	2.8
34	L9B	78	THR	2.8
31	L4B	6	VAL	2.8
29	L2B	35	LYS	2.8
34	L9B	118	LYS	2.8
41	L19A	38	ASN	2.8
33	L6B	162	ILE	2.8
43	L21A	48	GLY	2.8
43	L21B	1	MET	2.8
46	L24B	75	ILE	2.8
6	S6B	17	SER	2.8
6	S6B	101	ALA	2.8
9	S9A	126	SER	2.8
35	L13B	132	ALA	2.8
33	L6B	19	VAL	2.8
34	L9A	116	LEU	2.8
3	S3A	80	GLY	2.8
22	ASIA	5	G	2.8
33	L6B	112	PRO	2.8
34	L9B	76	THR	2.8

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Mol	Chain	Res	Type	RSRZ
50	L29B	5	GLU	2.8
57	ASIB	76	A	2.8
22	ASIA	69	G	2.8
12	S12A	60	GLY	2.7
3	S3A	184	TYR	2.7
33	L6A	83	TYR	2.7
34	L9B	132	PRO	2.7
57	ASIB	71	G	2.7
42	L20B	94	ASN	2.7
33	L6B	136	ILE	2.7
33	L6B	120	GLY	2.7
43	L21B	30	GLY	2.7
46	L24B	58	GLY	2.7
42	L20B	99	ALA	2.7
53	L32B	2	ALA	2.7
54	L33A	31	PRO	2.7
52	L31A	59	PHE	2.7
12	S12B	60	GLY	2.7
33	L6B	145	ALA	2.7
43	L21B	79	VAL	2.7
5	S5B	13	ILE	2.7
34	L9B	134	PRO	2.7
43	L21B	50	PRO	2.7
13	S13B	8	GLU	2.7
13	S13B	5	ALA	2.7
34	L9A	123	LEU	2.7
43	L21B	14	VAL	2.7
44	L22B	111	HIS	2.7
34	L9A	80	PRO	2.6
47	L25B	80	ARG	2.6
36	L14B	59	LYS	2.6
1	16SA	986	C	2.6
22	ASIA	2	C	2.6
22	ASIA	4	C	2.6
52	L31A	52	THR	2.6
19	S19B	87	ALA	2.6
31	L4B	77	ASP	2.6
4	S4A	86	LYS	2.6
42	L20A	106	PHE	2.6
12	S12B	34	CYS	2.6
43	L21B	51	VAL	2.6
6	S6A	16	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
33	L6B	32	GLU	2.6
19	S19A	79	THR	2.6
13	S13A	114	ARG	2.6
43	L21B	99	ILE	2.6
33	L6B	55	PRO	2.6
22	ASIA	56	C	2.6
4	S4B	87	GLY	2.6
33	L6B	98	LEU	2.6
33	L6B	104	GLU	2.6
34	L9B	125	GLU	2.6
47	L25A	119	GLU	2.6
42	L20B	96	ALA	2.6
42	L20B	80	ILE	2.6
10	S10B	59	SER	2.6
24	ESIA	34	G	2.6
27	23SA	681	A	2.6
3	S3A	12	LEU	2.6
33	L6B	33	LEU	2.6
39	L17A	4	LEU	2.6
40	L18A	110	LEU	2.6
35	L13B	10	GLU	2.6
47	L25B	79	ARG	2.6
2	S2B	187	LEU	2.5
7	S7A	147	ALA	2.5
36	L14B	9	GLU	2.5
47	L25A	113	ALA	2.5
4	S4B	127	THR	2.5
7	S7A	156	TRP	2.5
7	S7A	79	ARG	2.5
9	S9A	52	ALA	2.5
12	S12A	46	ASN	2.5
19	S19B	89	ALA	2.5
43	L21B	15	GLU	2.5
43	L21B	93	GLU	2.5
46	L24B	29	GLU	2.5
27	23SA	929	G	2.5
27	23SB	2	G	2.5
13	S13A	92	HIS	2.5
4	S4A	135	LEU	2.5
6	S6A	14	LEU	2.5
13	S13A	81	LEU	2.5
3	S3B	80	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
29	L2B	212	SER	2.5
33	L6B	76	VAL	2.5
3	S3A	188	LEU	2.5
35	L13A	134	ARG	2.5
30	L3B	3	GLY	2.5
2	S2B	93	VAL	2.5
34	L9A	115	ALA	2.5
34	L9B	65	ALA	2.5
10	S10A	61	GLU	2.5
22	ASIA	25	C	2.5
23	PSIA	4	C	2.5
23	PSIA	17	C	2.5
7	S7A	85	TYR	2.5
19	S19A	84	GLY	2.5
35	L13B	57	ALA	2.4
31	L4B	78	ILE	2.4
38	L16B	104	PHE	2.4
6	S6A	84	ASN	2.4
31	L4B	72	ARG	2.4
22	ASIA	13	C	2.4
26	TRNA	34	G	2.4
42	L20B	109	LEU	2.4
38	L16B	140	ALA	2.4
47	L25A	173	ALA	2.4
2	S2A	108	ILE	2.4
33	L6B	81	GLU	2.4
33	L6B	124	GLU	2.4
31	L4B	139	PHE	2.4
33	L6B	130	ARG	2.4
41	L19B	35	LYS	2.4
7	S7A	84	ASN	2.4
34	L9B	11	ASN	2.4
22	ASIA	14	A	2.4
33	L6B	135	GLY	2.4
53	L32A	52	TYR	2.4
38	L16A	20	ALA	2.4
57	ASIB	2	C	2.4
25	MRNB	56	U	2.4
2	S2A	163	PHE	2.4
34	L9A	137	PRO	2.4
31	L4A	131	GLY	2.4
14	S14A	59	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
42	L20B	112	ARG	2.4
55	L34A	48	LYS	2.4
6	S6B	31	GLU	2.4
6	S6B	45	LEU	2.4
34	L9B	10	GLU	2.4
33	L6B	52	VAL	2.4
46	L24B	49	VAL	2.4
11	S11B	32	ILE	2.4
32	L5B	39	ILE	2.4
54	L33A	27	LYS	2.4
17	S17A	101	ARG	2.4
17	S17B	91	ARG	2.4
27	23SA	1121	A	2.4
33	L6B	18	GLU	2.4
34	L9B	85	GLU	2.4
54	L33A	24	GLU	2.4
31	L4A	6	VAL	2.4
35	L13B	36	GLY	2.3
46	L24B	108	THR	2.3
3	S3B	77	ILE	2.3
49	L28A	77	ALA	2.3
5	S5B	91	LEU	2.3
33	L6A	98	LEU	2.3
33	L6A	86	GLU	2.3
33	L6B	56	SER	2.3
11	S11B	127	LYS	2.3
2	S2B	39	ILE	2.3
18	S18B	25	THR	2.3
33	L6B	170	ARG	2.3
34	L9B	79	ILE	2.3
42	L20B	65	ILE	2.3
35	L13B	128	HIS	2.3
42	L20B	81	HIS	2.3
43	L21B	3	ALA	2.3
47	L25A	7	ALA	2.3
27	23SA	158	U	2.3
27	23SB	2600	U	2.3
41	L19B	1	MET	2.3
22	ASIA	49	C	2.3
43	L21B	40	LEU	2.3
33	L6B	119	GLU	2.3
27	23SB	161	G	2.3

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Mol	Chain	Res	Type	RSRZ
33	L6A	35	VAL	2.3
3	S3B	73	PRO	2.3
33	L6B	82	GLY	2.3
46	L24A	104	GLY	2.3
33	L6A	106	THR	2.3
19	S19B	83	HIS	2.3
35	L13A	130	HIS	2.3
12	S12B	57	LEU	2.3
27	23SB	1094	A	2.3
27	23SB	2909	U	2.3
2	S2B	15	VAL	2.3
46	L24B	63	LYS	2.3
4	S4A	35	ARG	2.3
38	L16B	68	ILE	2.3
33	L6B	165	ALA	2.3
43	L21B	31	ALA	2.3
12	S12A	64	THR	2.3
33	L6B	134	SER	2.3
35	L13B	93	THR	2.3
27	23SA	2911	G	2.3
11	S11B	36	ASP	2.3
3	S3B	64	VAL	2.3
43	L21B	46	VAL	2.3
47	L25A	116	VAL	2.3
33	L6B	21	PRO	2.3
33	L6B	39	PRO	2.3
4	S4A	90	GLY	2.3
34	L9A	84	GLY	2.3
42	L20B	82	GLY	2.3
46	L24B	41	GLY	2.3
22	ASIA	75	C	2.3
27	23SA	937	C	2.3
9	S9A	19	LEU	2.3
22	ASIA	6	G	2.2
22	ASIA	27	G	2.2
34	L9B	138	ILE	2.2
33	L6B	12	PRO	2.2
30	L3B	187	ALA	2.2
12	S12B	81	LEU	2.2
3	S3A	95	THR	2.2
35	L13B	130	HIS	2.2
12	S12A	16	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
27	23SB	1148	C	2.2
35	L13B	119	ARG	2.2
47	L25B	81	ARG	2.2
55	L34B	49	ARG	2.2
3	S3A	153	VAL	2.2
35	L13B	8	GLN	2.2
51	L30B	59	VAL	2.2
54	L33A	26	ASN	2.2
4	S4B	126	ILE	2.2
16	S16A	66	PRO	2.2
30	L3A	1	MET	2.2
35	L13B	135	PRO	2.2
44	L22A	112	GLY	2.2
22	ASIA	44	G	2.2
24	ESIA	27	G	2.2
27	23SA	1221	G	2.2
35	L13B	37	LYS	2.2
37	L15B	18	ARG	2.2
53	L32B	51	TYR	2.2
13	S13B	74	VAL	2.2
30	L3B	55	ASN	2.2
36	L14A	54	GLU	2.2
46	L24B	64	GLU	2.2
47	L25A	171	ILE	2.2
23	PSIA	67	C	2.2
3	S3B	158	GLY	2.2
4	S4B	29	PRO	2.2
5	S5A	128	PRO	2.2
8	S8B	112	LEU	2.2
33	L6B	173	PRO	2.2
34	L9B	77	LEU	2.2
36	L14A	91	LEU	2.2
46	L24B	81	LYS	2.2
41	L19B	57	PHE	2.2
44	L22B	92	ARG	2.2
47	L25A	38	TYR	2.2
52	L31A	63	TYR	2.2
4	S4A	104	VAL	2.2
34	L9A	144	VAL	2.2
22	ASIA	50	U	2.2
34	L9B	97	ILE	2.2
30	L3A	169	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
14	S14B	44	LEU	2.2
18	S18A	31	LEU	2.2
35	L13B	91	LEU	2.2
35	L13B	31	ALA	2.2
35	L13B	40	PRO	2.2
42	L20B	87	GLY	2.2
33	L6B	27	LYS	2.2
49	L28B	92	LYS	2.2
27	23SA	2913	C	2.2
34	L9B	129	THR	2.2
48	L27B	3	HIS	2.2
12	S12B	63	VAL	2.2
44	L22B	38	TYR	2.2
43	L21B	11	GLN	2.2
47	L25A	70	LEU	2.2
38	L16A	91	GLU	2.2
4	S4B	85	LYS	2.2
35	L13B	134	ARG	2.2
35	L13A	127	ASP	2.2
22	ASIA	23	A	2.2
57	ASIB	73	A	2.2
7	S7A	80	VAL	2.1
33	L6B	44	VAL	2.1
46	L24B	61	ILE	2.1
34	L9A	72	LEU	2.1
33	L6B	146	ALA	2.1
33	L6B	155	SER	2.1
33	L6A	40	GLU	2.1
30	L3B	56	PRO	2.1
38	L16B	100	GLY	2.1
27	23SB	1074	U	2.1
3	S3B	86	VAL	2.1
33	L6A	24	VAL	2.1
33	L6A	99	VAL	2.1
33	L6A	131	VAL	2.1
34	L9B	136	VAL	2.1
5	S5B	133	TYR	2.1
43	L21B	19	LYS	2.1
54	L33A	53	LYS	2.1
19	S19A	81	ARG	2.1
22	ASIA	24	G	2.1
45	L23B	91	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	S2A	119	GLU	2.1
2	S2B	167	PRO	2.1
34	L9A	143	SER	2.1
49	L28A	93	GLU	2.1
27	23SA	1123	C	2.1
33	L6B	17	VAL	2.1
46	L24B	3	VAL	2.1
1	16SA	1823	U	2.1
49	L28A	95	LEU	2.1
49	L28A	15	ALA	2.1
4	S4A	130	GLY	2.1
12	S12A	84	GLY	2.1
30	L3A	87	GLU	2.1
49	L28A	79	GLY	2.1
56	L35A	56	GLU	2.1
22	ASIA	10	G	2.1
24	ESIA	11	C	2.1
30	L3A	109	LYS	2.1
2	S2B	98	LEU	2.1
10	S10A	90	LEU	2.1
30	L3B	89	ASP	2.1
34	L9A	110	ASP	2.1
33	L6A	97	ARG	2.1
2	S2B	48	MET	2.1
13	S13A	2	ALA	2.1
32	L5A	151	ALA	2.1
25	MRNA	57	U	2.1
4	S4A	60	GLU	2.1
18	S18B	38	GLU	2.1
30	L3B	126	PRO	2.1
12	S12A	43	LYS	2.1
2	S2A	162	ILE	2.1
16	S16A	36	ILE	2.1
33	L6B	121	ILE	2.1
33	L6B	171	LEU	2.1
19	S19B	80	TYR	2.1
34	L9A	130	TYR	2.1
54	L33A	40	CYS	2.1
1	16SB	1510	G	2.1
4	S4B	2	GLY	2.1
10	S10A	47	PHE	2.1
33	L6B	117	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
5	S5A	51	VAL	2.0
11	S11B	30	VAL	2.0
33	L6B	49	VAL	2.0
42	L20B	105	VAL	2.0
47	L25B	78	LYS	2.0
53	L32A	57	VAL	2.0
47	L25B	149	SER	2.0
4	S4A	50	ARG	2.0
38	L16B	37	LEU	2.0
38	L16B	79	LEU	2.0
7	S7B	7	ALA	2.0
30	L3B	151	TYR	2.0
43	L21B	101	GLY	2.0
31	L4B	14	PRO	2.0
34	L9A	132	PRO	2.0
42	L20B	103	PRO	2.0
47	L25B	48	PHE	2.0
12	S12B	54	LYS	2.0
42	L20B	100	VAL	2.0
43	L21B	72	VAL	2.0
57	ASIB	49	C	2.0
33	L6B	152	ARG	2.0
49	L28B	95	LEU	2.0
9	S9B	58	HIS	2.0
33	L6B	163	TYR	2.0
46	L24B	60	PHE	2.0
48	L27A	69	PHE	2.0
5	S5A	9	LYS	2.0
6	S6B	18	GLN	2.0
17	S17B	100	LYS	2.0
44	L22B	113	LYS	2.0
27	23SA	703	A	2.0
4	S4A	118	ARG	2.0
9	S9A	128	ARG	2.0
12	S12B	31	ARG	2.0
18	S18A	18	ARG	2.0
30	L3B	34	VAL	2.0
42	L20B	108	GLU	2.0
6	S6B	21	LEU	2.0
3	S3B	84	ILE	2.0
41	L19B	88	ILE	2.0
23	PSIB	68	C	2.0

5.2 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
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

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

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

5.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.4 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(Å^2)	Q<0.9
58	MG	23SB	3320	1/1	-0.16	0.15	112,112,112,112	0
58	MG	16SA	2250	1/1	0.25	0.15	114,114,114,114	0
60	K	23SA	3594	1/1	0.27	0.30	127,127,127,127	0
58	MG	16SB	2304[A]	1/1	0.30	0.45	59,59,59,59	1
58	MG	16SB	2304[B]	1/1	0.30	0.45	56,56,56,56	1
58	MG	23SB	3328	1/1	0.31	0.37	102,102,102,102	0
58	MG	23SA	3152	1/1	0.40	0.27	95,95,95,95	0
60	K	S4B	302	1/1	0.44	0.21	115,115,115,115	0
58	MG	16SA	2213	1/1	0.47	0.29	103,103,103,103	0
58	MG	16SB	2313	1/1	0.48	0.19	142,142,142,142	0
58	MG	23SB	3318	1/1	0.51	0.16	88,88,88,88	0
58	MG	23SB	3262[B]	1/1	0.54	0.38	59,59,59,59	1
58	MG	23SB	3262[A]	1/1	0.54	0.38	55,55,55,55	1
58	MG	23SA	3137	1/1	0.57	0.11	89,89,89,89	0
60	K	23SA	3634	1/1	0.57	0.14	104,104,104,104	0
60	K	23SA	3539	1/1	0.57	0.10	125,125,125,125	0
58	MG	23SB	3314	1/1	0.58	0.16	89,89,89,89	0
58	MG	23SB	3212	1/1	0.58	0.23	83,83,83,83	0
58	MG	16SA	2242	1/1	0.58	0.15	93,93,93,93	0
58	MG	16SB	2343	1/1	0.58	0.12	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	K	16SA	2383	1/1	0.59	0.14	123,123,123,123	0
60	K	23SB	3519	1/1	0.59	0.15	119,119,119,119	0
60	K	16SA	2403	1/1	0.60	0.15	84,84,84,84	0
58	MG	16SA	2245	1/1	0.60	0.29	71,71,71,71	0
60	K	S20B	201	1/1	0.61	0.10	121,121,121,121	0
60	K	23SB	3492	1/1	0.61	0.09	146,146,146,146	0
58	MG	23SB	3285	1/1	0.61	0.29	77,77,77,77	0
58	MG	23SA	3110	1/1	0.62	0.27	109,109,109,109	0
58	MG	23SA	3015	1/1	0.63	0.46	91,91,91,91	0
60	K	23SA	3549	1/1	0.64	0.10	104,104,104,104	0
60	K	16SB	2364	1/1	0.64	0.10	132,132,132,132	0
60	K	16SA	2395	1/1	0.65	0.14	105,105,105,105	0
60	K	L15B	202	1/1	0.65	0.14	96,96,96,96	0
60	K	23SA	3548	1/1	0.66	0.20	100,100,100,100	0
58	MG	23SA	3127	1/1	0.66	0.18	107,107,107,107	0
58	MG	16SA	2241	1/1	0.66	0.29	81,81,81,81	0
58	MG	16SB	2322	1/1	0.66	0.16	99,99,99,99	0
60	K	16SA	2376	1/1	0.66	0.12	106,106,106,106	0
58	MG	16SB	2314	1/1	0.67	0.23	99,99,99,99	0
60	K	23SA	3563	1/1	0.67	0.12	83,83,83,83	0
58	MG	16SA	2223	1/1	0.68	0.15	102,102,102,102	0
58	MG	23SA	3154	1/1	0.68	0.19	59,59,59,59	0
58	MG	23SA	3013	1/1	0.68	0.32	69,69,69,69	0
60	K	23SA	3575	1/1	0.68	0.12	68,68,68,68	0
58	MG	16SA	2246	1/1	0.69	0.07	100,100,100,100	0
58	MG	16SB	2323	1/1	0.69	0.15	92,92,92,92	0
60	K	23SB	3515	1/1	0.69	0.08	88,88,88,88	0
58	MG	16SA	2258	1/1	0.69	0.26	95,95,95,95	0
58	MG	23SA	3103	1/1	0.69	0.17	85,85,85,85	0
60	K	16SB	2395	1/1	0.70	0.12	103,103,103,103	0
58	MG	16SA	2255	1/1	0.70	0.26	82,82,82,82	0
58	MG	23SB	3293	1/1	0.70	0.33	71,71,71,71	0
58	MG	PSIB	105	1/1	0.70	0.23	78,78,78,78	0
58	MG	16SB	2317	1/1	0.70	0.19	98,98,98,98	0
58	MG	23SA	3159	1/1	0.70	0.16	83,83,83,83	0
58	MG	23SA	3177	1/1	0.70	0.13	91,91,91,91	0
58	MG	23SB	3283	1/1	0.71	0.33	72,72,72,72	0
60	K	L3B	303	1/1	0.71	0.13	98,98,98,98	0
58	MG	23SB	3286	1/1	0.71	0.26	65,65,65,65	0
58	MG	23SA	3099	1/1	0.72	0.11	80,80,80,80	0
58	MG	23SB	3311	1/1	0.72	0.22	75,75,75,75	0
58	MG	16SA	2238	1/1	0.72	0.19	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	K	16SB	2370	1/1	0.72	0.09	135,135,135,135	0
58	MG	S5B	201	1/1	0.73	0.19	96,96,96,96	0
60	K	23SA	3545	1/1	0.73	0.15	103,103,103,103	0
58	MG	16SA	2234	1/1	0.73	0.28	83,83,83,83	0
58	MG	16SA	2249	1/1	0.73	0.24	77,77,77,77	0
60	K	23SA	3638	1/1	0.73	0.11	104,104,104,104	0
58	MG	16SA	2237	1/1	0.74	0.32	62,62,62,62	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	16SB	2324	1/1	0.74	0.17	86,86,86,86	0
58	MG	16SB	2309	1/1	0.74	0.26	77,77,77,77	0
60	K	23SA	3611	1/1	0.74	0.12	118,118,118,118	0
60	K	16SB	2396	1/1	0.74	0.15	92,92,92,92	0
60	K	16SA	2408	1/1	0.74	0.17	89,89,89,89	0
58	MG	23SA	3106	1/1	0.75	0.23	60,60,60,60	0
58	MG	16SB	2315	1/1	0.75	0.25	85,85,85,85	0
58	MG	23SA	3100	1/1	0.75	0.15	66,66,66,66	0
58	MG	23SB	3309	1/1	0.75	0.33	77,77,77,77	0
60	K	23SB	3513	1/1	0.75	0.08	127,127,127,127	0
60	K	23SA	3560	1/1	0.75	0.08	89,89,89,89	0
58	MG	23SA	3065	1/1	0.75	0.21	56,56,56,56	0
58	MG	23SB	3276	1/1	0.75	0.30	82,82,82,82	0
58	MG	PSIB	104	1/1	0.75	0.30	79,79,79,79	0
58	MG	16SA	2230	1/1	0.76	0.28	60,60,60,60	0
58	MG	23SB	3315	1/1	0.76	0.09	58,58,58,58	0
60	K	16SA	2384	1/1	0.76	0.16	106,106,106,106	0
58	MG	16SA	2252	1/1	0.76	0.21	86,86,86,86	0
58	MG	23SA	3034	1/1	0.76	0.12	60,60,60,60	0
58	MG	16SB	2284	1/1	0.76	0.19	84,84,84,84	0
58	MG	23SB	3419	1/1	0.76	0.15	99,99,99,99	0
60	K	23SA	3542	1/1	0.76	0.10	105,105,105,105	0
58	MG	L32A	101	1/1	0.77	0.12	67,67,67,67	0
58	MG	16SA	2211	1/1	0.77	0.28	70,70,70,70	0
58	MG	16SA	2224	1/1	0.77	0.17	73,73,73,73	0
60	K	16SA	2415	1/1	0.77	0.08	89,89,89,89	0
60	K	23SB	3493	1/1	0.77	0.16	98,98,98,98	0
60	K	23SB	3511	1/1	0.77	0.09	119,119,119,119	0
60	K	16SB	2388	1/1	0.77	0.08	119,119,119,119	0
60	K	16SB	2393	1/1	0.77	0.09	96,96,96,96	0
58	MG	23SB	3268	1/1	0.77	0.14	66,66,66,66	0
58	MG	16SB	2333	1/1	0.77	0.26	88,88,88,88	0
60	K	16SA	2386	1/1	0.77	0.15	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	K	23SA	3632	1/1	0.78	0.11	116,116,116,116	0
58	MG	23SB	3310	1/1	0.78	0.31	79,79,79,79	0
58	MG	16SB	2294	1/1	0.78	0.21	77,77,77,77	0
58	MG	23SB	3272	1/1	0.78	0.26	57,57,57,57	0
58	MG	16SB	2316	1/1	0.78	0.20	80,80,80,80	0
60	K	16SA	2404	1/1	0.78	0.09	114,114,114,114	0
58	MG	16SA	2218	1/1	0.78	0.39	78,78,78,78	0
58	MG	23SA	3088	1/1	0.78	0.14	72,72,72,72	0
60	K	16SA	2416	1/1	0.78	0.14	86,86,86,86	0
60	K	16SA	2418	1/1	0.78	0.17	97,97,97,97	0
60	K	S14B	102	1/1	0.78	0.08	116,116,116,116	0
60	K	S20A	201	1/1	0.78	0.08	123,123,123,123	0
58	MG	16SA	2243	1/1	0.78	0.22	89,89,89,89	0
58	MG	16SB	2287	1/1	0.78	0.19	103,103,103,103	0
58	MG	5SB	213	1/1	0.78	0.12	79,79,79,79	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
59	OHX	23SB	3192	7/7	0.78	0.10	169,174,178,271	0
59	OHX	23SB	3193	7/7	0.78	0.11	132,147,161,243	0
58	MG	23SB	3300	1/1	0.78	0.16	67,67,67,67	0
60	K	L5B	202	1/1	0.78	0.09	110,110,110,110	0
58	MG	16SB	2292	1/1	0.78	0.33	59,59,59,59	0
60	K	23SA	3586	1/1	0.79	0.09	73,73,73,73	0
58	MG	23SA	3023	1/1	0.79	0.20	77,77,77,77	0
59	OHX	23SB	3163	7/7	0.79	0.11	127,143,150,243	0
58	MG	16SB	2288	1/1	0.79	0.28	70,70,70,70	0
58	MG	16SA	2239	1/1	0.79	0.14	84,84,84,84	0
58	MG	23SB	3316	1/1	0.79	0.15	62,62,62,62	0
60	K	23SB	3501	1/1	0.79	0.12	84,84,84,84	0
58	MG	16SA	2254	1/1	0.79	0.31	67,67,67,67	0
58	MG	23SA	3427	1/1	0.79	0.12	53,53,53,53	0
58	MG	23SB	3239	1/1	0.79	0.26	50,50,50,50	0
58	MG	23SA	3142	1/1	0.79	0.28	36,36,36,36	0
58	MG	23SB	3303	1/1	0.79	0.15	66,66,66,66	0
58	MG	16SB	2281	1/1	0.79	0.23	81,81,81,81	0
58	MG	23SA	3017	1/1	0.79	0.14	73,73,73,73	0
58	MG	23SB	3297	1/1	0.80	0.25	68,68,68,68	0
58	MG	23SB	3281	1/1	0.80	0.20	77,77,77,77	0
60	K	16SA	2405	1/1	0.80	0.10	115,115,115,115	0
60	K	23SA	3547	1/1	0.80	0.11	72,72,72,72	0
58	MG	23SB	3265	1/1	0.80	0.24	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	23SA	3089	1/1	0.80	0.16	77,77,77,77	0
58	MG	23SA	3128	1/1	0.80	0.17	62,62,62,62	0
59	OHX	16SB	2261	7/7	0.80	0.10	136,151,159,251	0
58	MG	23SA	3067	1/1	0.80	0.32	71,71,71,71	0
58	MG	23SB	3284	1/1	0.81	0.32	69,69,69,69	0
58	MG	23SB	3399	1/1	0.81	0.11	88,88,88,88	0
58	MG	23SA	3095	1/1	0.81	0.12	67,67,67,67	0
58	MG	23SB	3234	1/1	0.81	0.24	55,55,55,55	0
58	MG	16SB	2295	1/1	0.81	0.27	66,66,66,66	0
58	MG	23SB	3253	1/1	0.81	0.10	78,78,78,78	0
58	MG	23SB	3257	1/1	0.81	0.26	62,62,62,62	0
59	OHX	23SA	3362	7/7	0.81	0.12	102,109,127,232	0
58	MG	23SB	3301	1/1	0.81	0.16	75,75,75,75	0
58	MG	23SB	3258	1/1	0.81	0.18	72,72,72,72	0
59	OHX	23SB	3177	7/7	0.81	0.12	117,128,145,232	0
60	K	23SB	3467	1/1	0.81	0.24	106,106,106,106	0
58	MG	23SA	3006	1/1	0.81	0.24	50,50,50,50	0
60	K	23SA	3554	1/1	0.81	0.14	87,87,87,87	0
58	MG	23SA	3130	1/1	0.81	0.14	61,61,61,61	0
58	MG	16SA	2232	1/1	0.81	0.33	66,66,66,66	0
60	K	23SB	3509	1/1	0.81	0.28	102,102,102,102	0
58	MG	23SA	3101	1/1	0.81	0.32	73,73,73,73	0
58	MG	23SA	3086	1/1	0.81	0.19	71,71,71,71	0
58	MG	16SA	2222	1/1	0.81	0.33	74,74,74,74	0
60	K	23SA	3595	1/1	0.81	0.13	71,71,71,71	0
58	MG	23SA	3059	1/1	0.81	0.20	77,77,77,77	0
58	MG	23SB	3209	1/1	0.81	0.33	63,63,63,63	0
58	MG	23SB	3322	1/1	0.81	0.17	72,72,72,72	0
58	MG	16SB	2327	1/1	0.82	0.21	93,93,93,93	0
60	K	16SB	2365	1/1	0.82	0.10	126,126,126,126	0
58	MG	23SA	3002	1/1	0.82	0.25	58,58,58,58	0
59	OHX	23SA	3353	7/7	0.82	0.11	128,135,151,244	0
60	K	PSIA	105	1/1	0.82	0.11	100,100,100,100	0
58	MG	23SB	3263	1/1	0.82	0.33	56,56,56,56	0
59	OHX	23SA	3382	7/7	0.82	0.10	86,97,101,238	0
60	K	16SB	2398	1/1	0.82	0.09	101,101,101,101	0
60	K	23SA	3544	1/1	0.82	0.08	91,91,91,91	0
58	MG	16SA	2235	1/1	0.82	0.31	80,80,80,80	0
58	MG	23SB	3267	1/1	0.82	0.16	63,63,63,63	0
58	MG	23SA	3532	1/1	0.82	0.08	100,100,100,100	0
58	MG	5SA	202	1/1	0.82	0.07	67,67,67,67	0
58	MG	16SA	2236	1/1	0.82	0.15	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	16SA	2247	1/1	0.82	0.25	66,66,66,66	0
58	MG	23SA	3060	1/1	0.82	0.22	63,63,63,63	0
58	MG	23SB	3230	1/1	0.82	0.23	66,66,66,66	0
58	MG	23SA	3148	1/1	0.82	0.05	64,64,64,64	0
58	MG	23SB	3332	1/1	0.82	0.24	67,67,67,67	0
58	MG	23SA	3063	1/1	0.82	0.18	66,66,66,66	0
60	K	23SA	3608	1/1	0.82	0.09	80,80,80,80	0
58	MG	16SB	2290	1/1	0.82	0.21	79,79,79,79	0
58	MG	23SA	3117	1/1	0.82	0.11	81,81,81,81	0
58	MG	23SA	3124	1/1	0.82	0.14	72,72,72,72	0
59	OHX	16SA	2333	7/7	0.82	0.10	128,146,168,234	0
58	MG	23SB	3201	1/1	0.83	0.23	72,72,72,72	0
58	MG	23SA	3055	1/1	0.83	0.18	51,51,51,51	0
58	MG	5SB	212	1/1	0.83	0.13	103,103,103,103	0
58	MG	23SB	3210	1/1	0.83	0.28	60,60,60,60	0
58	MG	L5B	201	1/1	0.83	0.08	122,122,122,122	0
59	OHX	16SA	2300	7/7	0.83	0.12	104,105,114,228	0
58	MG	23SB	3307	1/1	0.83	0.19	71,71,71,71	0
59	OHX	16SA	2325	7/7	0.83	0.10	137,144,157,243	0
58	MG	23SA	3108	1/1	0.83	0.23	46,46,46,46	0
59	OHX	23SA	3304	7/7	0.83	0.10	109,115,118,229	0
58	MG	16SB	2326	1/1	0.83	0.39	78,78,78,78	0
60	K	16SA	2419	1/1	0.83	0.13	95,95,95,95	0
58	MG	5SA	201	1/1	0.83	0.16	67,67,67,67	0
58	MG	16SB	2330	1/1	0.83	0.16	93,93,93,93	0
58	MG	23SB	3240	1/1	0.83	0.22	54,54,54,54	0
59	OHX	23SA	3363	7/7	0.83	0.10	109,126,158,239	0
60	K	23SB	3462	1/1	0.83	0.13	102,102,102,102	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
58	MG	23SA	3161	1/1	0.83	0.07	88,88,88,88	0
59	OHX	L28A	101	7/7	0.83	0.10	84,89,95,234	0
60	K	23SB	3494	1/1	0.83	0.12	109,109,109,109	0
60	K	23SB	3498	1/1	0.83	0.07	108,108,108,108	0
59	OHX	16SB	2257	7/7	0.83	0.10	149,153,169,230	0
58	MG	5SA	203	1/1	0.83	0.24	79,79,79,79	0
58	MG	23SA	3176	1/1	0.83	0.34	63,63,63,63	0
58	MG	L33A	101	1/1	0.83	0.26	95,95,95,95	0
59	OHX	23SB	3185	7/7	0.83	0.10	130,138,151,236	0
58	MG	23SB	3295	1/1	0.83	0.20	57,57,57,57	0
60	K	23SB	3520	1/1	0.83	0.10	107,107,107,107	0
58	MG	23SA	3036	1/1	0.83	0.18	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	3360	1/1	0.83	0.18	111,111,111,111	0
60	K	16SA	2380	1/1	0.83	0.14	91,91,91,91	0
58	MG	23SA	3118	1/1	0.84	0.14	59,59,59,59	0
58	MG	16SB	2344	1/1	0.84	0.09	107,107,107,107	0
60	K	16SB	2367	1/1	0.84	0.11	115,115,115,115	0
58	MG	23SB	3327	1/1	0.84	0.07	59,59,59,59	0
60	K	16SB	2375	1/1	0.84	0.08	106,106,106,106	0
60	K	16SB	2387	1/1	0.84	0.17	93,93,93,93	0
58	MG	16SB	2363	1/1	0.84	0.10	89,89,89,89	0
58	MG	23SA	3422	1/1	0.84	0.13	63,63,63,63	0
58	MG	23SA	3143	1/1	0.84	0.19	69,69,69,69	0
58	MG	23SB	3299	1/1	0.84	0.16	68,68,68,68	0
58	MG	23SA	3147	1/1	0.84	0.11	76,76,76,76	0
59	OHX	23SB	3140	7/7	0.84	0.10	108,117,123,240	0
58	MG	23SA	3037	1/1	0.84	0.15	88,88,88,88	0
58	MG	23SA	3051	1/1	0.84	0.29	53,53,53,53	0
59	OHX	23SB	3180	7/7	0.84	0.11	104,121,149,231	0
58	MG	23SA	3109	1/1	0.84	0.18	55,55,55,55	0
59	OHX	23SB	3186	7/7	0.84	0.11	122,128,152,228	0
60	K	23SB	3478	1/1	0.84	0.13	94,94,94,94	0
58	MG	L30A	101	1/1	0.84	0.15	54,54,54,54	0
58	MG	23SB	3218	1/1	0.84	0.21	56,56,56,56	0
58	MG	23SB	3220	1/1	0.84	0.08	72,72,72,72	0
60	K	16SA	2377	1/1	0.84	0.09	101,101,101,101	0
60	K	23SA	3584	1/1	0.84	0.06	85,85,85,85	0
58	MG	23SB	3280	1/1	0.84	0.17	59,59,59,59	0
60	K	23SB	3502	1/1	0.84	0.10	97,97,97,97	0
60	K	23SA	3588	1/1	0.84	0.27	70,70,70,70	0
59	OHX	23SA	3257	7/7	0.84	0.11	134,139,144,224	0
58	MG	23SA	3092	1/1	0.84	0.07	60,60,60,60	0
58	MG	23SA	3131	1/1	0.84	0.11	63,63,63,63	0
60	K	23SB	3517	1/1	0.84	0.24	103,103,103,103	0
59	OHX	23SA	3346	7/7	0.84	0.10	143,147,162,241	0
60	K	23SA	3625	1/1	0.84	0.08	83,83,83,83	0
58	MG	16SA	2248	1/1	0.84	0.26	83,83,83,83	0
58	MG	23SB	3319	1/1	0.84	0.11	83,83,83,83	0
59	OHX	23SA	3354	7/7	0.84	0.13	110,114,141,218	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	3116	1/1	0.85	0.20	62,62,62,62	0
59	OHX	23SB	3179	7/7	0.85	0.11	154,162,169,245	0
58	MG	16SB	2321	1/1	0.85	0.27	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	23SA	3080	1/1	0.85	0.17	57,57,57,57	0
58	MG	23SA	3081	1/1	0.85	0.20	50,50,50,50	0
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	16SB	2325	1/1	0.85	0.23	92,92,92,92	0
59	OHX	23SB	3199	7/7	0.85	0.10	100,103,106,239	0
58	MG	23SA	3445	1/1	0.85	0.12	43,43,43,43	0
60	K	23SB	3448	1/1	0.85	0.17	104,104,104,104	0
58	MG	16SB	2307	1/1	0.85	0.41	61,61,61,61	0
58	MG	23SA	3156	1/1	0.85	0.09	69,69,69,69	0
58	MG	16SB	2332	1/1	0.85	0.14	92,92,92,92	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	16SB	2312	1/1	0.85	0.12	71,71,71,71	0
60	K	16SA	2398	1/1	0.85	0.12	67,67,67,67	0
58	MG	23SA	3008	1/1	0.85	0.10	73,73,73,73	0
60	K	23SA	3617	1/1	0.85	0.10	74,74,74,74	0
59	OHX	5SA	213	7/7	0.85	0.10	118,123,145,229	0
58	MG	16SA	2229	1/1	0.85	0.23	71,71,71,71	0
58	MG	16SA	2209	1/1	0.85	0.09	86,86,86,86	0
59	OHX	16SA	2328	7/7	0.85	0.11	143,155,166,234	0
60	K	L3A	303	1/1	0.85	0.11	88,88,88,88	0
60	K	L5A	302	1/1	0.85	0.12	83,83,83,83	0
59	OHX	16SB	2272	7/7	0.85	0.10	140,141,165,247	0
58	MG	16SB	2291	1/1	0.85	0.21	73,73,73,73	0
60	K	16SB	2366	1/1	0.85	0.09	88,88,88,88	0
59	OHX	23SB	3161	7/7	0.85	0.09	142,150,169,244	0
59	OHX	TRNA	102	7/7	0.85	0.09	125,127,144,247	0
58	MG	16SA	2257	1/1	0.86	0.23	54,54,54,54	0
58	MG	L4B	302	1/1	0.86	0.29	94,94,94,94	0
60	K	16SA	2391	1/1	0.86	0.12	86,86,86,86	0
58	MG	16SA	2220	1/1	0.86	0.20	47,47,47,47	0
58	MG	16SA	2201	1/1	0.86	0.24	73,73,73,73	0
58	MG	23SA	3045	1/1	0.86	0.26	44,44,44,44	0
58	MG	23SA	3499	1/1	0.86	0.14	56,56,56,56	0
59	OHX	16SB	2264	7/7	0.86	0.09	140,157,163,237	0
60	K	16SB	2381	1/1	0.86	0.09	100,100,100,100	0
58	MG	16SB	2289	1/1	0.86	0.12	89,89,89,89	0
59	OHX	16SB	2277	7/7	0.86	0.09	99,106,111,245	0
60	K	16SB	2390	1/1	0.86	0.12	96,96,96,96	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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	3516	1/1	0.86	0.10	84,84,84,84	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
59	OHX	ASIA	102	7/7	0.86	0.11	113,120,131,219	0
58	MG	23SA	3071	1/1	0.86	0.19	77,77,77,77	0
58	MG	23SB	3279	1/1	0.86	0.23	82,82,82,82	0
58	MG	23SA	3049	1/1	0.86	0.23	57,57,57,57	0
59	OHX	23SB	3174	7/7	0.86	0.10	128,128,151,234	0
60	K	23SA	3550	1/1	0.86	0.18	81,81,81,81	0
60	K	23SA	3553	1/1	0.86	0.13	92,92,92,92	0
58	MG	23SA	3005	1/1	0.86	0.18	54,54,54,54	0
59	OHX	23SA	3312	7/7	0.86	0.23	74,87,95,219	0
58	MG	23SB	3223	1/1	0.86	0.17	79,79,79,79	0
59	OHX	23SB	3181	7/7	0.86	0.09	118,141,152,230	0
59	OHX	23SA	3347	7/7	0.86	0.10	126,132,144,218	0
58	MG	23SB	3224	1/1	0.86	0.17	68,68,68,68	0
58	MG	23SA	3083	1/1	0.86	0.18	41,41,41,41	0
58	MG	16SB	2301	1/1	0.86	0.28	68,68,68,68	0
60	K	23SB	3512	1/1	0.86	0.10	79,79,79,79	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
58	MG	L5A	301	1/1	0.86	0.25	67,67,67,67	0
58	MG	L23A	101	1/1	0.86	0.10	60,60,60,60	0
58	MG	23SA	3020	1/1	0.86	0.23	32,32,32,32	0
60	K	16SA	2379	1/1	0.86	0.07	111,111,111,111	0
58	MG	23SA	3170	1/1	0.86	0.09	69,69,69,69	0
58	MG	16SA	2226	1/1	0.86	0.11	78,78,78,78	0
58	MG	23SB	3304	1/1	0.87	0.21	68,68,68,68	0
60	K	16SB	2379	1/1	0.87	0.11	121,121,121,121	0
58	MG	16SB	2282	1/1	0.87	0.35	83,83,83,83	0
60	K	16SB	2382	1/1	0.87	0.09	94,94,94,94	0
58	MG	16SB	2296	1/1	0.87	0.19	71,71,71,71	0
59	OHX	23SA	3361	7/7	0.87	0.10	86,117,130,220	0
58	MG	23SA	3096	1/1	0.87	0.09	70,70,70,70	0
60	K	16SB	2392	1/1	0.87	0.08	117,117,117,117	0
58	MG	16SB	2361	1/1	0.87	0.08	122,122,122,122	0
58	MG	16SB	2318	1/1	0.87	0.31	65,65,65,65	0
58	MG	16SB	2302	1/1	0.87	0.35	66,66,66,66	0
58	MG	16SA	2219	1/1	0.87	0.14	74,74,74,74	0
59	OHX	23SB	3189	7/7	0.87	0.10	147,159,176,238	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	OHX	16SA	2326	7/7	0.87	0.10	127,136,164,238	0
58	MG	23SB	3255	1/1	0.87	0.29	50,50,50,50	0
58	MG	23SA	3057	1/1	0.87	0.15	44,44,44,44	0
60	K	23SB	3441	1/1	0.87	0.12	88,88,88,88	0
58	MG	16SA	2221	1/1	0.87	0.28	62,62,62,62	0
59	OHX	16SB	2246	7/7	0.87	0.10	104,108,114,227	0
60	K	23SA	3581	1/1	0.87	0.10	72,72,72,72	0
58	MG	23SB	3207	1/1	0.87	0.17	47,47,47,47	0
58	MG	23SB	3324	1/1	0.87	0.13	58,58,58,58	0
59	OHX	23SA	3258	7/7	0.87	0.09	90,100,113,211	0
59	OHX	23SA	3272	7/7	0.87	0.10	84,96,103,208	0
59	OHX	23SA	3288	7/7	0.87	0.18	82,88,106,207	0
60	K	23SA	3597	1/1	0.87	0.13	87,87,87,87	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	16SA	2389	1/1	0.87	0.13	82,82,82,82	0
59	OHX	23SB	3122	7/7	0.87	0.11	93,97,102,223	0
58	MG	23SA	3102	1/1	0.87	0.26	45,45,45,45	0
59	OHX	23SB	3127	7/7	0.87	0.09	109,115,122,246	0
58	MG	16SB	2311	1/1	0.87	0.33	84,84,84,84	0
58	MG	23SA	3537	1/1	0.87	0.14	72,72,72,72	0
59	OHX	23SB	3144	7/7	0.87	0.08	103,111,118,233	0
59	OHX	23SA	3336	7/7	0.87	0.10	112,116,141,218	0
59	OHX	23SB	3151	7/7	0.87	0.09	135,140,158,248	0
58	MG	23SA	3026	1/1	0.87	0.18	52,52,52,52	0
58	MG	23SA	3136	1/1	0.87	0.10	77,77,77,77	0
59	OHX	23SA	3349	7/7	0.87	0.09	115,126,155,229	0
60	K	16SA	2385	1/1	0.88	0.16	107,107,107,107	0
58	MG	16SA	2204	1/1	0.88	0.23	52,52,52,52	0
60	K	16SA	2387	1/1	0.88	0.10	93,93,93,93	0
59	OHX	MRNB	101	7/7	0.88	0.09	144,148,154,235	0
58	MG	23SB	3204	1/1	0.88	0.29	54,54,54,54	0
59	OHX	23SB	3114	7/7	0.88	0.08	96,100,108,207	0
58	MG	23SB	3372	1/1	0.88	0.10	50,50,50,50	0
59	OHX	23SA	3307	7/7	0.88	0.09	108,113,123,223	0
58	MG	23SB	3261	1/1	0.88	0.18	52,52,52,52	0
58	MG	23SB	3205	1/1	0.88	0.23	54,54,54,54	0
59	OHX	23SB	3132	7/7	0.88	0.09	105,111,127,226	0
58	MG	23SB	3420	1/1	0.88	0.11	62,62,62,62	0
59	OHX	23SA	3339	7/7	0.88	0.09	99,120,146,218	0
59	OHX	23SB	3143	7/7	0.88	0.09	101,107,113,221	0
59	OHX	23SA	3345	7/7	0.88	0.10	107,120,136,224	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	K	16SA	2420	1/1	0.88	0.10	99,99,99,99	0
58	MG	23SA	3171	1/1	0.88	0.11	49,49,49,49	0
59	OHX	23SB	3149	7/7	0.88	0.09	111,128,143,208	0
58	MG	23SA	3140	1/1	0.88	0.12	61,61,61,61	0
58	MG	5SB	214	1/1	0.88	0.31	56,56,56,56	0
58	MG	23SA	3097	1/1	0.88	0.25	50,50,50,50	0
58	MG	L3A	301	1/1	0.88	0.19	57,57,57,57	0
60	K	23SA	3546	1/1	0.88	0.22	94,94,94,94	0
59	OHX	16SA	2290	7/7	0.88	0.18	82,92,113,204	0
59	OHX	16SA	2292	7/7	0.88	0.11	88,100,116,196	0
58	MG	23SA	3094	1/1	0.88	0.19	55,55,55,55	0
58	MG	23SA	3144	1/1	0.88	0.20	52,52,52,52	0
58	MG	23SB	3222	1/1	0.88	0.18	64,64,64,64	0
59	OHX	23SA	3373	7/7	0.88	0.10	92,109,134,230	0
60	K	23SB	3471	1/1	0.88	0.14	106,106,106,106	0
60	K	23SB	3475	1/1	0.88	0.09	90,90,90,90	0
60	K	23SB	3476	1/1	0.88	0.22	77,77,77,77	0
58	MG	16SA	2259	1/1	0.88	0.22	47,47,47,47	0
60	K	23SB	3479	1/1	0.88	0.09	76,76,76,76	0
60	K	23SA	3562	1/1	0.88	0.05	80,80,80,80	0
58	MG	23SA	3489	1/1	0.88	0.11	36,36,36,36	0
59	OHX	16SA	2332	7/7	0.88	0.10	133,137,152,236	0
58	MG	23SA	3495	1/1	0.88	0.09	67,67,67,67	0
59	OHX	5SA	209	7/7	0.88	0.10	81,100,111,199	0
60	K	23SB	3499	1/1	0.88	0.09	85,85,85,85	0
59	OHX	16SA	2335	7/7	0.88	0.09	127,136,156,226	0
58	MG	16SB	2298	1/1	0.88	0.31	72,72,72,72	0
58	MG	23SA	3166	1/1	0.88	0.17	38,38,38,38	0
59	OHX	16SB	2249	7/7	0.88	0.09	102,104,116,221	0
58	MG	PSIB	103	1/1	0.88	0.23	52,52,52,52	0
60	K	23SA	3599	1/1	0.88	0.07	66,66,66,66	0
58	MG	23SB	3244	1/1	0.88	0.21	43,43,43,43	0
60	K	16SA	2378	1/1	0.88	0.09	93,93,93,93	0
60	K	23SA	3613	1/1	0.88	0.11	91,91,91,91	0
58	MG	23SA	3168	1/1	0.88	0.17	89,89,89,89	0
58	MG	23SA	3169	1/1	0.88	0.20	82,82,82,82	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
58	MG	L15B	201	1/1	0.89	0.15	58,58,58,58	0
59	OHX	23SB	3035	7/7	0.89	0.14	65,93,108,150	0
60	K	23SA	3635	1/1	0.89	0.04	69,69,69,69	0
59	OHX	23SA	3341	7/7	0.89	0.10	113,122,146,225	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	16SA	2205	1/1	0.89	0.26	51,51,51,51	0
58	MG	23SB	3282	1/1	0.89	0.22	64,64,64,64	0
58	MG	23SB	3254	1/1	0.89	0.25	46,46,46,46	0
58	MG	23SA	3068	1/1	0.89	0.09	64,64,64,64	0
59	OHX	23SA	3350	7/7	0.89	0.08	121,138,153,230	0
60	K	16SA	2396	1/1	0.89	0.07	103,103,103,103	0
59	OHX	16SA	2316	7/7	0.89	0.08	114,126,153,236	0
60	K	16SA	2402	1/1	0.89	0.17	89,89,89,89	0
59	OHX	16SA	2318	7/7	0.89	0.08	113,116,137,211	0
58	MG	23SA	3484	1/1	0.89	0.12	84,84,84,84	0
59	OHX	23SA	3358	7/7	0.89	0.08	129,130,145,238	0
60	K	16SB	2384	1/1	0.89	0.08	98,98,98,98	0
58	MG	23SA	3069	1/1	0.89	0.18	70,70,70,70	0
58	MG	23SB	3323	1/1	0.89	0.27	45,45,45,45	0
58	MG	23SB	3259	1/1	0.89	0.33	35,35,35,35	0
59	OHX	23SA	3365	7/7	0.89	0.08	184,185,193,269	0
58	MG	16SB	2308	1/1	0.89	0.30	59,59,59,59	0
59	OHX	23SB	3159	7/7	0.89	0.09	124,131,146,207	0
60	K	S13A	201	1/1	0.89	0.06	108,108,108,108	0
59	OHX	23SA	3370	7/7	0.89	0.11	94,101,133,213	0
60	K	PSIA	104	1/1	0.89	0.11	80,80,80,80	0
60	K	S6B	201	1/1	0.89	0.09	85,85,85,85	0
59	OHX	23SA	3371	7/7	0.89	0.09	130,141,155,222	0
58	MG	23SA	3158	1/1	0.89	0.32	77,77,77,77	0
60	K	23SA	3540	1/1	0.89	0.06	79,79,79,79	0
59	OHX	23SB	3170	7/7	0.89	0.08	132,138,158,216	0
58	MG	23SA	3139	1/1	0.89	0.17	58,58,58,58	0
60	K	23SB	3446	1/1	0.89	0.13	85,85,85,85	0
60	K	23SB	3447	1/1	0.89	0.08	97,97,97,97	0
58	MG	23SA	3121	1/1	0.89	0.18	54,54,54,54	0
59	OHX	23SB	3176	7/7	0.89	0.09	143,147,163,222	0
58	MG	23SB	3366	1/1	0.89	0.15	39,39,39,39	0
59	OHX	23SB	3178	7/7	0.89	0.10	103,113,139,232	0
58	MG	23SB	3200	1/1	0.89	0.25	39,39,39,39	0
58	MG	23SB	3388	1/1	0.89	0.12	38,38,38,38	0
59	OHX	23SA	3274	7/7	0.89	0.08	95,102,117,215	0
59	OHX	5SA	214	7/7	0.89	0.08	138,149,161,234	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
59	OHX	23SB	3188	7/7	0.89	0.08	134,155,164,228	0
58	MG	23SA	3162	1/1	0.89	0.26	62,62,62,62	0
59	OHX	23SB	3190	7/7	0.89	0.09	112,126,151,218	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	23SB	3237	1/1	0.89	0.20	73,73,73,73	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
59	OHX	23SB	3195	7/7	0.89	0.09	182,185,190,255	0
60	K	23SB	3508	1/1	0.89	0.14	76,76,76,76	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	23SA	3402	1/1	0.89	0.12	49,49,49,49	0
58	MG	23SB	3308	1/1	0.89	0.14	73,73,73,73	0
59	OHX	5SB	210	7/7	0.89	0.09	125,130,151,226	0
58	MG	23SB	3273	1/1	0.89	0.36	51,51,51,51	0
58	MG	23SA	3421	1/1	0.89	0.10	63,63,63,63	0
59	OHX	23SA	3311	7/7	0.89	0.09	99,101,117,228	0
58	MG	23SA	3163	1/1	0.89	0.19	45,45,45,45	0
58	MG	23SB	3245	1/1	0.89	0.22	45,45,45,45	0
60	K	16SA	2382	1/1	0.89	0.10	88,88,88,88	0
61	SJE	23SA	3640	87/87	0.89	0.14	44,53,86,93	0
58	MG	23SB	3260	1/1	0.90	0.34	63,63,63,63	0
58	MG	23SA	3016	1/1	0.90	0.12	59,59,59,59	0
59	OHX	23SA	3302	7/7	0.90	0.13	83,91,106,208	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	16SB	2256	7/7	0.90	0.08	125,127,138,219	0
59	OHX	5SB	208	7/7	0.90	0.10	98,111,123,206	0
58	MG	23SB	3431	1/1	0.90	0.08	113,113,113,113	0
60	K	23SA	3636	1/1	0.90	0.07	85,85,85,85	0
58	MG	23SA	3150	1/1	0.90	0.20	60,60,60,60	0
59	OHX	16SB	2262	7/7	0.90	0.08	158,164,176,252	0
58	MG	23SB	3219	1/1	0.90	0.17	61,61,61,61	0
59	OHX	23SA	3310	7/7	0.90	0.07	99,106,111,224	0
58	MG	23SA	3524	1/1	0.90	0.07	113,113,113,113	0
60	K	16SA	2381	1/1	0.90	0.09	109,109,109,109	0
58	MG	23SA	3064	1/1	0.90	0.17	55,55,55,55	0
59	OHX	23SA	3317	7/7	0.90	0.08	107,109,120,235	0
60	K	16SB	2374	1/1	0.90	0.07	94,94,94,94	0
59	OHX	ASIB	103	7/7	0.90	0.08	124,130,147,238	0
59	OHX	23SA	3318	7/7	0.90	0.09	138,157,165,234	0
58	MG	23SA	3172	1/1	0.90	0.30	58,58,58,58	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
60	K	16SB	2386	1/1	0.90	0.08	94,94,94,94	0
59	OHX	23SB	3099	7/7	0.90	0.08	87,101,111,219	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	23SA	3175	1/1	0.90	0.09	52,52,52,52	0
59	OHX	16SA	2281	7/7	0.90	0.09	106,115,123,199	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
59	OHX	23SA	3342	7/7	0.90	0.27	87,93,102,203	0
59	OHX	23SA	3343	7/7	0.90	0.10	93,117,131,217	0
58	MG	16SA	2227	1/1	0.90	0.18	56,56,56,56	0
58	MG	23SB	3312	1/1	0.90	0.17	41,41,41,41	0
60	K	16SA	2411	1/1	0.90	0.25	82,82,82,82	0
59	OHX	23SB	3131	7/7	0.90	0.08	114,116,124,216	0
58	MG	23SB	3232	1/1	0.90	0.23	60,60,60,60	0
60	K	16SA	2417	1/1	0.90	0.09	81,81,81,81	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
60	K	23SB	3445	1/1	0.90	0.09	66,66,66,66	0
59	OHX	23SB	3141	7/7	0.90	0.08	98,103,118,228	0
59	OHX	16SA	2314	7/7	0.90	0.08	119,126,128,235	0
58	MG	23SA	3019	1/1	0.90	0.10	35,35,35,35	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
58	MG	23SB	3278	1/1	0.90	0.16	45,45,45,45	0
59	OHX	23SA	3355	7/7	0.90	0.08	117,125,148,217	0
60	K	23SB	3468	1/1	0.90	0.06	97,97,97,97	0
58	MG	23SB	3236	1/1	0.90	0.28	58,58,58,58	0
60	K	23SB	3473	1/1	0.90	0.11	108,108,108,108	0
59	OHX	23SA	3360	7/7	0.90	0.10	90,94,110,208	0
59	OHX	16SA	2323	7/7	0.90	0.08	162,167,181,233	0
58	MG	16SB	2293	1/1	0.90	0.22	48,48,48,48	0
58	MG	16SA	2214	1/1	0.90	0.16	76,76,76,76	0
58	MG	23SA	3044	1/1	0.90	0.12	65,65,65,65	0
59	OHX	23SB	3168	7/7	0.90	0.10	123,133,154,222	0
60	K	23SB	3490	1/1	0.90	0.07	84,84,84,84	0
59	OHX	23SA	3368	7/7	0.90	0.10	115,130,133,209	0
59	OHX	23SB	3171	7/7	0.90	0.09	129,131,134,212	0
58	MG	23SA	3141	1/1	0.90	0.24	60,60,60,60	0
58	MG	23SA	3123	1/1	0.90	0.12	57,57,57,57	0
58	MG	23SB	3202	1/1	0.90	0.28	51,51,51,51	0
60	K	23SB	3500	1/1	0.90	0.06	80,80,80,80	0
60	K	23SA	3556	1/1	0.90	0.07	60,60,60,60	0
58	MG	23SA	3007	1/1	0.90	0.24	61,61,61,61	0
60	K	23SB	3507	1/1	0.90	0.10	72,72,72,72	0
58	MG	23SB	3292	1/1	0.90	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	OHX	23SA	3252	7/7	0.90	0.16	83,84,115,187	0
58	MG	23SB	3346	1/1	0.90	0.11	56,56,56,56	0
58	MG	23SA	3165	1/1	0.90	0.29	62,62,62,62	0
59	OHX	23SB	3183	7/7	0.90	0.08	148,155,160,237	0
59	OHX	5SA	208	7/7	0.90	0.08	98,106,114,218	0
60	K	23SB	3516	1/1	0.90	0.14	77,77,77,77	0
58	MG	23SA	3073	1/1	0.90	0.11	42,42,42,42	0
60	K	23SB	3518	1/1	0.90	0.11	86,86,86,86	0
58	MG	23SB	3296	1/1	0.90	0.42	72,72,72,72	0
59	OHX	23SA	3284	7/7	0.90	0.17	84,87,97,215	0
58	MG	23SA	3078	1/1	0.90	0.23	50,50,50,50	0
59	OHX	23SB	3191	7/7	0.90	0.09	112,116,127,213	0
59	OHX	16SB	2217	7/7	0.90	0.10	95,102,111,201	0
58	MG	16SB	2306	1/1	0.90	0.19	56,56,56,56	0
59	OHX	23SA	3377	7/7	0.91	0.08	145,154,161,239	0
59	OHX	23SB	3150	7/7	0.91	0.08	134,143,159,230	0
58	MG	L34A	101	1/1	0.91	0.22	50,50,50,50	0
60	K	16SA	2406	1/1	0.91	0.07	87,87,87,87	0
59	OHX	23SB	3153	7/7	0.91	0.08	123,135,155,235	0
60	K	16SB	2380	1/1	0.91	0.07	91,91,91,91	0
60	K	16SA	2409	1/1	0.91	0.11	81,81,81,81	0
59	OHX	23SB	3155	7/7	0.91	0.08	136,149,154,230	0
60	K	16SA	2412	1/1	0.91	0.14	92,92,92,92	0
58	MG	23SA	3061	1/1	0.91	0.10	83,83,83,83	0
58	MG	23SA	3157	1/1	0.91	0.20	39,39,39,39	0
58	MG	16SA	2240	1/1	0.91	0.32	70,70,70,70	0
58	MG	23SA	3483	1/1	0.91	0.07	92,92,92,92	0
58	MG	L3B	301	1/1	0.91	0.17	40,40,40,40	0
58	MG	16SB	2286	1/1	0.91	0.17	77,77,77,77	0
60	K	S6A	201	1/1	0.91	0.11	82,82,82,82	0
58	MG	23SA	3082	1/1	0.91	0.16	50,50,50,50	0
58	MG	23SA	3018	1/1	0.91	0.23	30,30,30,30	0
59	OHX	16SB	2222	7/7	0.91	0.10	108,112,124,190	0
59	OHX	16SB	2227	7/7	0.91	0.07	115,116,122,221	0
58	MG	23SA	3084	1/1	0.91	0.05	64,64,64,64	0
59	OHX	16SA	2286	7/7	0.91	0.24	75,88,94,169	0
60	K	23SA	3541	1/1	0.91	0.09	102,102,102,102	0
58	MG	16SB	2320	1/1	0.91	0.21	62,62,62,62	0
59	OHX	23SA	3324	7/7	0.91	0.09	85,91,107,225	0
58	MG	16SA	2231	1/1	0.91	0.20	57,57,57,57	0
58	MG	23SA	3164	1/1	0.91	0.27	61,61,61,61	0
58	MG	16SA	2203	1/1	0.91	0.33	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	16SA	2225	1/1	0.91	0.22	50,50,50,50	0
59	OHX	16SB	2263	7/7	0.91	0.08	157,159,167,234	0
58	MG	23SA	3091	1/1	0.91	0.15	66,66,66,66	0
60	K	23SA	3552	1/1	0.91	0.14	83,83,83,83	0
58	MG	23SA	3111	1/1	0.91	0.17	56,56,56,56	0
58	MG	23SB	3275	1/1	0.91	0.23	65,65,65,65	0
60	K	23SA	3555	1/1	0.91	0.17	71,71,71,71	0
58	MG	23SA	3112	1/1	0.91	0.06	60,60,60,60	0
60	K	23SB	3474	1/1	0.91	0.09	63,63,63,63	0
59	OHX	23SA	3348	7/7	0.91	0.09	138,148,158,224	0
59	OHX	16SA	2319	7/7	0.91	0.07	131,143,148,232	0
59	OHX	PSIB	102	7/7	0.91	0.08	143,157,164,248	0
58	MG	23SB	3227	1/1	0.91	0.09	76,76,76,76	0
58	MG	23SA	3115	1/1	0.91	0.21	91,91,91,91	0
58	MG	16SB	2299	1/1	0.91	0.20	50,50,50,50	0
60	K	23SB	3485	1/1	0.91	0.10	72,72,72,72	0
60	K	23SB	3487	1/1	0.91	0.06	65,65,65,65	0
59	OHX	23SB	3087	7/7	0.91	0.17	86,94,99,175	0
60	K	23SA	3587	1/1	0.91	0.07	91,91,91,91	0
59	OHX	23SB	3089	7/7	0.91	0.07	106,112,116,216	0
59	OHX	5SB	207	7/7	0.91	0.08	115,121,127,222	0
58	MG	16SA	2244	1/1	0.91	0.28	62,62,62,62	0
58	MG	23SA	3033	1/1	0.91	0.18	74,74,74,74	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	L15A	202	1/1	0.91	0.15	59,59,59,59	0
59	OHX	23SA	3359	7/7	0.91	0.08	128,136,163,233	0
58	MG	PSIA	101	1/1	0.91	0.30	54,54,54,54	0
58	MG	23SB	3336	1/1	0.91	0.08	64,64,64,64	0
58	MG	23SA	3120	1/1	0.91	0.09	67,67,67,67	0
59	OHX	23SA	3221	7/7	0.91	0.10	73,86,105,162	0
60	K	23SA	3631	1/1	0.91	0.10	78,78,78,78	0
60	K	23SB	3514	1/1	0.91	0.23	95,95,95,95	0
58	MG	16SA	2215	1/1	0.91	0.40	58,58,58,58	0
59	OHX	23SA	3367	7/7	0.91	0.08	122,139,164,218	0
58	MG	23SB	3288	1/1	0.91	0.14	72,72,72,72	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
58	MG	23SB	3291	1/1	0.91	0.14	79,79,79,79	0
58	MG	23SA	3079	1/1	0.91	0.11	76,76,76,76	0
58	MG	23SB	3389	1/1	0.91	0.09	54,54,54,54	0
58	MG	23SB	3248	1/1	0.91	0.35	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	23SB	3252	1/1	0.91	0.08	68,68,68,68	0
60	K	5SA	219	1/1	0.92	0.05	72,72,72,72	0
59	OHX	23SB	3130	7/7	0.92	0.08	106,117,124,209	0
58	MG	23SB	3203	1/1	0.92	0.29	40,40,40,40	0
58	MG	23SA	3424	1/1	0.92	0.11	36,36,36,36	0
58	MG	16SB	2319	1/1	0.92	0.33	57,57,57,57	0
58	MG	23SA	3167	1/1	0.92	0.20	77,77,77,77	0
58	MG	23SA	3040	1/1	0.92	0.21	55,55,55,55	0
59	OHX	23SB	3139	7/7	0.92	0.08	90,97,109,222	0
59	OHX	23SA	3378	7/7	0.92	0.23	81,87,102,184	0
58	MG	23SB	3429	1/1	0.92	0.16	93,93,93,93	0
59	OHX	23SB	3142	7/7	0.92	0.08	136,146,149,236	0
58	MG	23SA	3461	1/1	0.92	0.11	44,44,44,44	0
58	MG	23SA	3482	1/1	0.92	0.11	66,66,66,66	0
59	OHX	5SA	206	7/7	0.92	0.15	91,97,113,184	0
58	MG	23SB	3214	1/1	0.92	0.19	48,48,48,48	0
58	MG	L27A	101	1/1	0.92	0.17	35,35,35,35	0
58	MG	16SA	2216	1/1	0.92	0.28	46,46,46,46	0
60	K	16SA	2414	1/1	0.92	0.07	100,100,100,100	0
58	MG	L3B	302	1/1	0.92	0.11	50,50,50,50	0
60	K	16SB	2391	1/1	0.92	0.07	87,87,87,87	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
60	K	16SB	2394	1/1	0.92	0.09	92,92,92,92	0
58	MG	23SB	3264	1/1	0.92	0.08	55,55,55,55	0
58	MG	23SA	3031	1/1	0.92	0.13	58,58,58,58	0
59	OHX	23SB	3162	7/7	0.92	0.07	129,137,145,231	0
58	MG	23SA	3487	1/1	0.92	0.11	40,40,40,40	0
59	OHX	23SB	3164	7/7	0.92	0.08	124,135,157,228	0
58	MG	23SA	3046	1/1	0.92	0.19	52,52,52,52	0
59	OHX	16SB	2228	7/7	0.92	0.08	99,100,112,192	0
59	OHX	16SB	2244	7/7	0.92	0.07	99,108,114,225	0
58	MG	23SB	3269	1/1	0.92	0.25	50,50,50,50	0
58	MG	23SA	3047	1/1	0.92	0.11	52,52,52,52	0
59	OHX	23SA	3333	7/7	0.92	0.08	101,104,130,208	0
58	MG	23SB	3226	1/1	0.92	0.16	60,60,60,60	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
58	MG	23SA	3497	1/1	0.92	0.07	81,81,81,81	0
58	MG	16SB	2339	1/1	0.92	0.06	124,124,124,124	0
58	MG	23SB	3277	1/1	0.92	0.12	41,41,41,41	0
59	OHX	23SB	3182	7/7	0.92	0.08	190,192,204,241	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	OHX	16SA	2312	7/7	0.92	0.23	92,98,105,188	0
59	OHX	23SB	3184	7/7	0.92	0.08	116,132,141,221	0
59	OHX	16SB	2267	7/7	0.92	0.08	109,115,145,208	0
58	MG	23SA	3032	1/1	0.92	0.16	49,49,49,49	0
58	MG	16SB	2283	1/1	0.92	0.18	48,48,48,48	0
58	MG	23SA	3500	1/1	0.92	0.12	49,49,49,49	0
60	K	23SA	3559	1/1	0.92	0.19	82,82,82,82	0
58	MG	16SB	2310	1/1	0.92	0.39	75,75,75,75	0
58	MG	16SB	2285	1/1	0.92	0.14	65,65,65,65	0
58	MG	16SA	2212	1/1	0.92	0.18	55,55,55,55	0
60	K	23SA	3568	1/1	0.92	0.05	58,58,58,58	0
59	OHX	16SA	2324	7/7	0.92	0.08	131,145,160,226	0
58	MG	23SB	3329	1/1	0.92	0.24	64,64,64,64	0
58	MG	23SA	3014	1/1	0.92	0.28	70,70,70,70	0
58	MG	23SA	3384	1/1	0.92	0.11	43,43,43,43	0
58	MG	23SB	3246	1/1	0.92	0.34	57,57,57,57	0
59	OHX	23SB	3093	7/7	0.92	0.08	93,100,110,208	0
58	MG	16SA	2208	1/1	0.92	0.17	77,77,77,77	0
59	OHX	5SB	206	7/7	0.92	0.08	120,123,129,223	0
58	MG	23SB	3361	1/1	0.92	0.11	51,51,51,51	0
59	OHX	23SB	3104	7/7	0.92	0.08	111,116,130,225	0
60	K	23SB	3505	1/1	0.92	0.12	75,75,75,75	0
59	OHX	16SA	2340	7/7	0.92	0.08	102,105,115,209	0
59	OHX	5SB	211	7/7	0.92	0.08	134,145,159,239	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
59	OHX	L20B	201	7/7	0.92	0.16	88,95,110,186	0
58	MG	23SB	3364	1/1	0.92	0.08	65,65,65,65	0
58	MG	23SA	3134	1/1	0.92	0.11	74,74,74,74	0
60	K	23SA	3614	1/1	0.92	0.09	65,65,65,65	0
59	OHX	23SA	3364	7/7	0.92	0.08	96,103,122,203	0
58	MG	16SA	2233	1/1	0.92	0.10	71,71,71,71	0
60	K	23SA	3626	1/1	0.92	0.06	69,69,69,69	0
59	OHX	23SB	3120	7/7	0.92	0.07	94,104,115,226	0
59	OHX	23SB	3121	7/7	0.92	0.08	95,102,110,221	0
59	OHX	23SA	3239	7/7	0.92	0.08	95,99,109,191	0
60	K	L4B	303	1/1	0.92	0.07	98,98,98,98	0
58	MG	23SB	3378	1/1	0.92	0.09	70,70,70,70	0
58	MG	23SB	3384	1/1	0.92	0.09	70,70,70,70	0
59	OHX	23SB	3129	7/7	0.92	0.07	103,109,115,227	0
58	MG	23SA	3087	1/1	0.93	0.19	61,61,61,61	0
59	OHX	23SB	3158	7/7	0.93	0.08	105,107,121,203	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	K	23SA	3578	1/1	0.93	0.05	54,54,54,54	0
58	MG	16SB	2336	1/1	0.93	0.07	105,105,105,105	0
58	MG	23SA	3107	1/1	0.93	0.17	37,37,37,37	0
58	MG	23SB	3330	1/1	0.93	0.26	54,54,54,54	0
59	OHX	16SA	2327	7/7	0.93	0.07	134,143,149,217	0
58	MG	23SA	3072	1/1	0.93	0.12	68,68,68,68	0
59	OHX	16SA	2331	7/7	0.93	0.07	155,162,169,236	0
59	OHX	23SB	3167	7/7	0.93	0.08	121,136,143,203	0
60	K	23SA	3593	1/1	0.93	0.05	69,69,69,69	0
58	MG	23SB	3333	1/1	0.93	0.10	42,42,42,42	0
58	MG	16SA	2253	1/1	0.93	0.27	50,50,50,50	0
58	MG	16SB	2348	1/1	0.93	0.07	56,56,56,56	0
58	MG	16SB	2305	1/1	0.93	0.27	67,67,67,67	0
59	OHX	23SB	3173	7/7	0.93	0.07	97,115,128,200	0
59	OHX	S4A	301	7/7	0.93	0.09	118,122,140,210	0
58	MG	23SB	3241	1/1	0.93	0.13	50,50,50,50	0
58	MG	23SB	3243	1/1	0.93	0.23	30,30,30,30	0
58	MG	23SA	3437	1/1	0.93	0.23	67,67,67,67	0
59	OHX	23SA	3224	7/7	0.93	0.17	86,94,104,168	0
59	OHX	5SA	212	7/7	0.93	0.07	89,95,109,210	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
58	MG	23SB	3287	1/1	0.93	0.16	61,61,61,61	0
58	MG	23SA	3075	1/1	0.93	0.30	61,61,61,61	0
60	K	23SA	3627	1/1	0.93	0.06	67,67,67,67	0
58	MG	23SB	3381	1/1	0.93	0.10	49,49,49,49	0
58	MG	23SB	3289	1/1	0.93	0.18	72,72,72,72	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
59	OHX	23SA	3270	7/7	0.93	0.08	109,117,127,194	0
60	K	23SA	3639	1/1	0.93	0.07	80,80,80,80	0
58	MG	23SB	3386	1/1	0.93	0.07	91,91,91,91	0
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
58	MG	23SA	3452	1/1	0.93	0.11	40,40,40,40	0
58	MG	23SA	3135	1/1	0.93	0.10	55,55,55,55	0
59	OHX	23SA	3285	7/7	0.93	0.07	90,99,105,205	0
58	MG	23SB	3391	1/1	0.93	0.07	71,71,71,71	0
59	OHX	16SB	2252	7/7	0.93	0.08	109,120,138,208	0
58	MG	23SB	3396	1/1	0.93	0.07	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	OHX	23SA	3293	7/7	0.93	0.20	70,76,97,195	0
59	OHX	5SB	205	7/7	0.93	0.07	120,123,130,211	0
58	MG	23SB	3250	1/1	0.93	0.25	41,41,41,41	0
59	OHX	16SB	2259	7/7	0.93	0.07	145,150,156,224	0
58	MG	23SB	3294	1/1	0.93	0.07	55,55,55,55	0
59	OHX	5SB	209	7/7	0.93	0.08	121,127,134,216	0
59	OHX	23SA	3301	7/7	0.93	0.07	121,123,127,230	0
58	MG	L35A	101	1/1	0.93	0.16	51,51,51,51	0
58	MG	23SB	3428	1/1	0.93	0.08	84,84,84,84	0
60	K	16SA	2375	1/1	0.93	0.07	101,101,101,101	0
59	OHX	23SA	3306	7/7	0.93	0.07	100,113,126,199	0
59	OHX	16SB	2268	7/7	0.93	0.07	123,133,154,220	0
59	OHX	16SB	2271	7/7	0.93	0.07	156,167,170,247	0
58	MG	23SA	3467	1/1	0.93	0.08	41,41,41,41	0
58	MG	23SA	3472	1/1	0.93	0.14	39,39,39,39	0
59	OHX	23SA	3309	7/7	0.93	0.14	85,88,102,183	0
59	OHX	16SB	2276	7/7	0.93	0.07	131,137,146,224	0
58	MG	23SB	3437	1/1	0.93	0.29	86,86,86,86	0
58	MG	23SA	3077	1/1	0.93	0.18	48,48,48,48	0
58	MG	23SA	3003	1/1	0.93	0.15	60,60,60,60	0
59	OHX	23SA	3314	7/7	0.93	0.07	95,99,111,204	0
58	MG	23SA	3138	1/1	0.93	0.08	46,46,46,46	0
60	K	23SB	3440	1/1	0.93	0.07	94,94,94,94	0
60	K	16SA	2388	1/1	0.93	0.25	79,79,79,79	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
58	MG	23SA	3114	1/1	0.93	0.08	55,55,55,55	0
59	OHX	23SB	3067	7/7	0.93	0.09	79,95,108,174	0
59	OHX	23SA	3319	7/7	0.93	0.19	82,85,93,207	0
59	OHX	23SA	3320	7/7	0.93	0.07	94,95,109,191	0
59	OHX	23SA	3323	7/7	0.93	0.12	84,89,105,197	0
58	MG	16SA	2228	1/1	0.93	0.29	64,64,64,64	0
59	OHX	23SA	3331	7/7	0.93	0.07	91,98,108,201	0
58	MG	16SA	2217	1/1	0.93	0.14	40,40,40,40	0
60	K	23SB	3470	1/1	0.93	0.14	78,78,78,78	0
59	OHX	23SA	3334	7/7	0.93	0.07	99,115,137,214	0
60	K	23SB	3472	1/1	0.93	0.16	77,77,77,77	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
58	MG	16SA	2363	1/1	0.93	0.07	72,72,72,72	0
59	OHX	23SA	3337	7/7	0.93	0.07	109,123,134,204	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	OHX	23SA	3338	7/7	0.93	0.07	138,150,158,232	0
58	MG	23SA	3054	1/1	0.93	0.24	51,51,51,51	0
59	OHX	23SA	3340	7/7	0.93	0.08	133,146,163,217	0
58	MG	L35B	103	1/1	0.93	0.19	82,82,82,82	0
60	K	23SB	3486	1/1	0.93	0.09	73,73,73,73	0
58	MG	23SB	3213	1/1	0.93	0.16	40,40,40,40	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	23SB	3124	7/7	0.93	0.08	83,94,106,213	0
58	MG	16SA	2367	1/1	0.93	0.16	83,83,83,83	0
59	OHX	23SA	3344	7/7	0.93	0.07	95,121,141,216	0
58	MG	23SA	3146	1/1	0.93	0.23	48,48,48,48	0
58	MG	23SB	3313	1/1	0.93	0.05	48,48,48,48	0
58	MG	23SB	3266	1/1	0.93	0.17	38,38,38,38	0
59	OHX	16SA	2296	7/7	0.93	0.08	87,99,108,193	0
58	MG	16SA	2374	1/1	0.93	0.14	73,73,73,73	0
58	MG	23SA	3122	1/1	0.93	0.10	57,57,57,57	0
60	K	23SB	3504	1/1	0.93	0.09	87,87,87,87	0
60	K	23SA	3543	1/1	0.93	0.10	86,86,86,86	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	23SB	3317	1/1	0.93	0.11	78,78,78,78	0
59	OHX	16SA	2309	7/7	0.93	0.08	132,139,149,214	0
58	MG	23SA	3085	1/1	0.93	0.15	52,52,52,52	0
58	MG	23SB	3270	1/1	0.93	0.22	43,43,43,43	0
58	MG	16SA	2256	1/1	0.93	0.14	72,72,72,72	0
59	OHX	23SB	3145	7/7	0.93	0.08	106,124,142,220	0
58	MG	23SA	3393	1/1	0.93	0.09	54,54,54,54	0
58	MG	23SA	3125	1/1	0.93	0.15	62,62,62,62	0
58	MG	23SA	3411	1/1	0.93	0.10	43,43,43,43	0
58	MG	23SB	3325	1/1	0.93	0.16	47,47,47,47	0
60	K	23SA	3557	1/1	0.93	0.07	84,84,84,84	0
59	OHX	23SB	3152	7/7	0.93	0.08	103,105,129,194	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
59	OHX	23SB	3156	7/7	0.93	0.06	125,130,147,212	0
60	K	23SA	3564	1/1	0.93	0.08	72,72,72,72	0
61	SJE	23SB	3521	87/87	0.93	0.14	48,59,87,95	0
59	OHX	16SA	2274	7/7	0.94	0.14	93,97,105,164	0
59	OHX	16SB	2233	7/7	0.94	0.07	93,102,105,189	0
59	OHX	16SA	2279	7/7	0.94	0.08	118,121,129,197	0
59	OHX	16SB	2236	7/7	0.94	0.07	104,107,118,194	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	OHX	23SB	3175	7/7	0.94	0.07	138,142,159,216	0
59	OHX	16SB	2238	7/7	0.94	0.06	124,131,141,228	0
60	K	23SA	3601	1/1	0.94	0.08	55,55,55,55	0
59	OHX	16SB	2239	7/7	0.94	0.07	116,122,133,205	0
58	MG	23SA	3155	1/1	0.94	0.17	55,55,55,55	0
60	K	23SA	3606	1/1	0.94	0.05	57,57,57,57	0
59	OHX	23SA	3299	7/7	0.94	0.11	69,80,102,183	0
60	K	23SA	3609	1/1	0.94	0.06	71,71,71,71	0
60	K	23SA	3610	1/1	0.94	0.08	62,62,62,62	0
59	OHX	23SA	3300	7/7	0.94	0.06	99,105,112,220	0
60	K	23SA	3612	1/1	0.94	0.04	73,73,73,73	0
59	OHX	16SB	2247	7/7	0.94	0.08	100,103,110,200	0
58	MG	16SB	2297	1/1	0.94	0.29	64,64,64,64	0
59	OHX	16SA	2288	7/7	0.94	0.07	90,100,106,201	0
58	MG	23SB	3251	1/1	0.94	0.28	54,54,54,54	0
60	K	23SA	3619	1/1	0.94	0.04	81,81,81,81	0
58	MG	23SB	3206	1/1	0.94	0.24	34,34,34,34	0
60	K	23SA	3622	1/1	0.94	0.07	61,61,61,61	0
59	OHX	16SA	2293	7/7	0.94	0.09	92,98,111,198	0
59	OHX	23SB	3187	7/7	0.94	0.06	134,143,152,229	0
58	MG	23SA	3173	1/1	0.94	0.06	59,59,59,59	0
58	MG	23SA	3093	1/1	0.94	0.06	77,77,77,77	0
59	OHX	16SA	2297	7/7	0.94	0.07	114,122,131,209	0
59	OHX	16SA	2298	7/7	0.94	0.19	80,87,106,181	0
58	MG	16SB	2300	1/1	0.94	0.31	48,48,48,48	0
58	MG	23SB	3256	1/1	0.94	0.16	47,47,47,47	0
59	OHX	16SB	2266	7/7	0.94	0.07	135,142,152,217	0
59	OHX	23SA	3315	7/7	0.94	0.07	98,100,118,232	0
59	OHX	16SA	2301	7/7	0.94	0.07	107,112,121,213	0
59	OHX	16SB	2270	7/7	0.94	0.08	116,127,150,209	0
58	MG	16SA	2251	1/1	0.94	0.28	60,60,60,60	0
59	OHX	16SA	2305	7/7	0.94	0.07	133,141,150,228	0
59	OHX	5SB	204	7/7	0.94	0.07	98,106,120,191	0
58	MG	23SB	3356	1/1	0.94	0.07	39,39,39,39	0
59	OHX	16SB	2274	7/7	0.94	0.07	131,136,142,211	0
58	MG	23SA	3056	1/1	0.94	0.14	48,48,48,48	0
58	MG	23SA	3001	1/1	0.94	0.30	34,34,34,34	0
59	OHX	23SA	3325	7/7	0.94	0.06	89,95,103,220	0
59	OHX	16SB	2278	7/7	0.94	0.07	112,116,120,223	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	23SA	3327	7/7	0.94	0.07	88,96,114,211	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	23SB	3216	1/1	0.94	0.12	42,42,42,42	0
58	MG	16SB	2331	1/1	0.94	0.28	55,55,55,55	0
59	OHX	16SA	2313	7/7	0.94	0.07	110,116,122,207	0
58	MG	23SB	3370	1/1	0.94	0.08	49,49,49,49	0
58	MG	23SA	3160	1/1	0.94	0.13	55,55,55,55	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	3377	1/1	0.94	0.07	47,47,47,47	0
59	OHX	16SA	2317	7/7	0.94	0.09	112,120,138,202	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
58	MG	16SA	2359	1/1	0.94	0.11	62,62,62,62	0
58	MG	23SA	3010	1/1	0.94	0.17	39,39,39,39	0
58	MG	23SB	3383	1/1	0.94	0.07	77,77,77,77	0
58	MG	23SB	3302	1/1	0.94	0.17	49,49,49,49	0
58	MG	23SB	3385	1/1	0.94	0.07	82,82,82,82	0
59	OHX	23SB	3103	7/7	0.94	0.18	67,90,98,176	0
58	MG	23SA	3420	1/1	0.94	0.09	57,57,57,57	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	16SB	2341	1/1	0.94	0.07	130,130,130,130	0
58	MG	23SB	3305	1/1	0.94	0.10	65,65,65,65	0
58	MG	23SB	3390	1/1	0.94	0.10	44,44,44,44	0
60	K	16SA	2407	1/1	0.94	0.05	75,75,75,75	0
58	MG	23SB	3306	1/1	0.94	0.17	65,65,65,65	0
59	OHX	16SA	2330	7/7	0.94	0.07	153,156,163,230	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
59	OHX	23SA	3351	7/7	0.94	0.07	116,125,140,218	0
58	MG	23SB	3393	1/1	0.94	0.08	70,70,70,70	0
60	K	23SB	3464	1/1	0.94	0.07	53,53,53,53	0
60	K	23SB	3465	1/1	0.94	0.12	75,75,75,75	0
60	K	16SA	2413	1/1	0.94	0.07	84,84,84,84	0
58	MG	23SA	3505	1/1	0.94	0.11	40,40,40,40	0
58	MG	23SA	3513	1/1	0.94	0.08	84,84,84,84	0
58	MG	23SB	3417	1/1	0.94	0.06	84,84,84,84	0
58	MG	23SB	3228	1/1	0.94	0.26	43,43,43,43	0
59	OHX	16SA	2341	7/7	0.94	0.07	135,136,149,239	0
58	MG	23SA	3011	1/1	0.94	0.19	42,42,42,42	0
59	OHX	S10A	201	7/7	0.94	0.08	106,108,115,206	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	23SB	3231	1/1	0.94	0.12	51,51,51,51	0
58	MG	23SB	3271	1/1	0.94	0.20	46,46,46,46	0
59	OHX	23SA	3195	7/7	0.94	0.11	71,86,93,123	0
59	OHX	23SA	3212	7/7	0.94	0.11	51,57,86,140	0
58	MG	23SB	3430	1/1	0.94	0.09	70,70,70,70	0
58	MG	16SB	2354	1/1	0.94	0.06	102,102,102,102	0
59	OHX	23SA	3366	7/7	0.94	0.07	99,105,125,207	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	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
58	MG	23SA	3076	1/1	0.94	0.18	57,57,57,57	0
59	OHX	23SA	3372	7/7	0.94	0.08	103,116,140,217	0
58	MG	23SB	3439	1/1	0.94	0.08	87,87,87,87	0
60	K	23SB	3496	1/1	0.94	0.08	85,85,85,85	0
59	OHX	23SB	3146	7/7	0.94	0.07	98,108,114,209	0
59	OHX	23SA	3259	7/7	0.94	0.07	90,96,110,189	0
59	OHX	23SA	3376	7/7	0.94	0.08	121,128,151,229	0
59	OHX	23SA	3260	7/7	0.94	0.19	71,90,98,175	0
58	MG	23SA	3133	1/1	0.94	0.11	48,48,48,48	0
58	MG	23SA	3035	1/1	0.94	0.13	52,52,52,52	0
58	MG	23SA	3149	1/1	0.94	0.25	66,66,66,66	0
59	OHX	23SB	3154	7/7	0.94	0.09	165,172,176,225	0
59	OHX	23SA	3267	7/7	0.94	0.18	91,99,103,186	0
60	K	23SA	3558	1/1	0.94	0.10	55,55,55,55	0
59	OHX	23SA	3269	7/7	0.94	0.22	86,89,103,177	0
58	MG	23SA	3443	1/1	0.94	0.16	32,32,32,32	0
58	MG	23SA	3050	1/1	0.94	0.16	58,58,58,58	0
58	MG	5SA	216	1/1	0.94	0.07	67,67,67,67	0
59	OHX	23SB	3160	7/7	0.94	0.07	120,142,146,214	0
59	OHX	23SA	3275	7/7	0.94	0.07	100,110,119,213	0
59	OHX	23SA	3277	7/7	0.94	0.19	76,84,101,204	0
59	OHX	23SA	3278	7/7	0.94	0.07	85,98,101,210	0
60	K	23SA	3580	1/1	0.94	0.11	39,39,39,39	0
58	MG	23SA	3151	1/1	0.94	0.12	59,59,59,59	0
58	MG	16SA	2368	1/1	0.94	0.06	91,91,91,91	0
59	OHX	23SB	3166	7/7	0.94	0.08	91,100,114,205	0
58	MG	16SA	2360	1/1	0.94	0.10	72,72,72,72	0
59	OHX	16SA	2271	7/7	0.94	0.10	80,94,97,147	0
60	K	23SA	3589	1/1	0.94	0.10	85,85,85,85	0
59	OHX	23SA	3292	7/7	0.94	0.11	68,81,98,170	0
58	MG	16SA	2369	1/1	0.95	0.05	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	23SA	3174	1/1	0.95	0.11	53,53,53,53	0
58	MG	23SB	3298	1/1	0.95	0.27	55,55,55,55	0
59	OHX	16SA	2308	7/7	0.95	0.06	110,118,129,200	0
60	K	23SA	3602	1/1	0.95	0.06	67,67,67,67	0
58	MG	23SA	3477	1/1	0.95	0.11	90,90,90,90	0
58	MG	23SA	3478	1/1	0.95	0.08	50,50,50,50	0
60	K	23SA	3605	1/1	0.95	0.05	74,74,74,74	0
59	OHX	16SA	2311	7/7	0.95	0.07	102,108,117,196	0
59	OHX	16SB	2251	7/7	0.95	0.07	125,131,136,216	0
58	MG	23SA	3479	1/1	0.95	0.11	76,76,76,76	0
58	MG	23SA	3098	1/1	0.95	0.06	54,54,54,54	0
59	OHX	16SB	2254	7/7	0.95	0.07	100,105,128,186	0
58	MG	23SA	3027	1/1	0.95	0.14	45,45,45,45	0
58	MG	16SA	2371	1/1	0.95	0.05	100,100,100,100	0
58	MG	16SB	2280	1/1	0.95	0.12	59,59,59,59	0
59	OHX	16SB	2260	7/7	0.95	0.07	145,153,160,239	0
59	OHX	23SA	3316	7/7	0.95	0.06	90,97,113,204	0
58	MG	23SA	3486	1/1	0.95	0.08	42,42,42,42	0
58	MG	23SA	3048	1/1	0.95	0.14	33,33,33,33	0
58	MG	23SA	3391	1/1	0.95	0.10	37,37,37,37	0
59	OHX	16SB	2265	7/7	0.95	0.07	110,127,139,201	0
59	OHX	16SA	2320	7/7	0.95	0.08	99,106,126,191	0
58	MG	23SB	3398	1/1	0.95	0.11	46,46,46,46	0
58	MG	16SA	2202	1/1	0.95	0.20	57,57,57,57	0
60	K	23SA	3628	1/1	0.95	0.15	83,83,83,83	0
60	K	23SA	3629	1/1	0.95	0.06	65,65,65,65	0
58	MG	23SB	3406	1/1	0.95	0.16	68,68,68,68	0
59	OHX	23SA	3326	7/7	0.95	0.07	138,143,162,229	0
58	MG	23SB	3407	1/1	0.95	0.10	51,51,51,51	0
58	MG	23SB	3408	1/1	0.95	0.13	51,51,51,51	0
58	MG	23SB	3215	1/1	0.95	0.19	37,37,37,37	0
58	MG	23SB	3418	1/1	0.95	0.07	51,51,51,51	0
58	MG	16SA	2353	1/1	0.95	0.05	138,138,138,138	0
59	OHX	16SA	2329	7/7	0.95	0.06	144,149,154,226	0
58	MG	23SB	3217	1/1	0.95	0.10	48,48,48,48	0
60	K	L4A	304	1/1	0.95	0.07	77,77,77,77	0
59	OHX	5SB	203	7/7	0.95	0.07	102,107,119,182	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
58	MG	23SB	3424	1/1	0.95	0.09	71,71,71,71	0
58	MG	PSIA	103	1/1	0.95	0.08	83,83,83,83	0
60	K	16SB	2369	1/1	0.95	0.15	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	23SA	3414	1/1	0.95	0.06	50,50,50,50	0
59	OHX	23SB	3032	7/7	0.95	0.11	86,101,105,158	0
58	MG	23SA	3504	1/1	0.95	0.06	67,67,67,67	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	L35B	101	7/7	0.95	0.09	120,126,131,191	0
59	OHX	23SB	3050	7/7	0.95	0.17	74,79,98,166	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	3053	1/1	0.95	0.19	33,33,33,33	0
58	MG	23SA	3511	1/1	0.95	0.05	36,36,36,36	0
59	OHX	23SB	3061	7/7	0.95	0.07	100,105,115,190	0
60	K	16SB	2389	1/1	0.95	0.04	82,82,82,82	0
59	OHX	23SB	3062	7/7	0.95	0.06	100,103,111,185	0
58	MG	23SA	3512	1/1	0.95	0.13	45,45,45,45	0
59	OHX	23SB	3066	7/7	0.95	0.08	94,102,114,188	0
58	MG	23SA	3145	1/1	0.95	0.06	70,70,70,70	0
59	OHX	23SB	3073	7/7	0.95	0.07	89,100,113,186	0
58	MG	23SA	3515	1/1	0.95	0.06	101,101,101,101	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
59	OHX	MRNA	101	7/7	0.95	0.07	109,113,121,212	0
58	MG	23SB	3321	1/1	0.95	0.14	39,39,39,39	0
58	MG	23SA	3009	1/1	0.95	0.22	40,40,40,40	0
59	OHX	23SB	3088	7/7	0.95	0.08	110,117,123,193	0
60	K	16SA	2401	1/1	0.95	0.08	63,63,63,63	0
58	MG	23SA	3519	1/1	0.95	0.08	94,94,94,94	0
59	OHX	23SB	3092	7/7	0.95	0.16	78,84,94,180	0
58	MG	16SA	2357	1/1	0.95	0.07	63,63,63,63	0
60	K	23SB	3443	1/1	0.95	0.14	110,110,110,110	0
60	K	23SB	3444	1/1	0.95	0.07	84,84,84,84	0
58	MG	23SA	3528	1/1	0.95	0.08	42,42,42,42	0
59	OHX	23SA	3226	7/7	0.95	0.18	71,76,95,148	0
59	OHX	23SB	3102	7/7	0.95	0.06	108,115,119,215	0
59	OHX	23SA	3227	7/7	0.95	0.17	77,84,88,170	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	23SB	3106	7/7	0.95	0.08	100,119,134,193	0
60	K	23SB	3452	1/1	0.95	0.08	84,84,84,84	0
59	OHX	23SA	3236	7/7	0.95	0.18	76,86,90,178	0
60	K	23SB	3456	1/1	0.95	0.04	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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	23SB	3326	1/1	0.95	0.08	58,58,58,58	0
60	K	23SB	3463	1/1	0.95	0.06	83,83,83,83	0
59	OHX	23SA	3241	7/7	0.95	0.15	65,85,97,158	0
59	OHX	23SA	3247	7/7	0.95	0.18	85,87,97,160	0
60	K	23SB	3466	1/1	0.95	0.07	68,68,68,68	0
58	MG	23SB	3233	1/1	0.95	0.21	41,41,41,41	0
59	OHX	23SA	3254	7/7	0.95	0.14	74,86,94,175	0
60	K	23SB	3469	1/1	0.95	0.07	64,64,64,64	0
59	OHX	23SB	3116	7/7	0.95	0.07	126,131,140,206	0
58	MG	23SA	3531	1/1	0.95	0.11	69,69,69,69	0
58	MG	L35B	102	1/1	0.95	0.11	91,91,91,91	0
58	MG	16SA	2207	1/1	0.95	0.17	42,42,42,42	0
58	MG	23SA	3434	1/1	0.95	0.12	102,102,102,102	0
58	MG	23SA	3012	1/1	0.95	0.06	91,91,91,91	0
59	OHX	16SA	2276	7/7	0.95	0.12	93,96,108,169	0
59	OHX	23SB	3123	7/7	0.95	0.06	105,108,120,206	0
58	MG	16SB	2351	1/1	0.95	0.07	68,68,68,68	0
59	OHX	16SA	2280	7/7	0.95	0.07	100,102,112,186	0
59	OHX	23SA	3375	7/7	0.95	0.06	102,110,125,192	0
58	MG	23SB	3335	1/1	0.95	0.07	51,51,51,51	0
59	OHX	16SA	2283	7/7	0.95	0.06	101,107,114,179	0
59	OHX	23SA	3268	7/7	0.95	0.18	80,89,92,148	0
59	OHX	23SA	3379	7/7	0.95	0.06	102,114,136,186	0
59	OHX	16SA	2284	7/7	0.95	0.07	132,148,162,222	0
58	MG	23SA	3132	1/1	0.95	0.05	57,57,57,57	0
58	MG	16SB	2360	1/1	0.95	0.05	95,95,95,95	0
59	OHX	23SA	3273	7/7	0.95	0.16	85,96,99,180	0
59	OHX	16SA	2289	7/7	0.95	0.11	89,94,104,178	0
60	K	23SB	3495	1/1	0.95	0.05	73,73,73,73	0
58	MG	23SB	3349	1/1	0.95	0.08	71,71,71,71	0
58	MG	16SB	2303	1/1	0.95	0.17	61,61,61,61	0
58	MG	23SB	3357	1/1	0.95	0.10	65,65,65,65	0
59	OHX	23SA	3280	7/7	0.95	0.06	90,100,112,211	0
59	OHX	16SA	2294	7/7	0.95	0.07	89,94,99,207	0
59	OHX	L20A	201	7/7	0.95	0.10	80,91,102,185	0
59	OHX	L27A	102	7/7	0.95	0.18	86,89,102,190	0
58	MG	23SA	3042	1/1	0.95	0.14	47,47,47,47	0
58	MG	23SA	3043	1/1	0.95	0.18	57,57,57,57	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	K	23SB	3510	1/1	0.95	0.04	75,75,75,75	0
60	K	23SA	3565	1/1	0.95	0.07	46,46,46,46	0
59	OHX	16SB	2216	7/7	0.95	0.12	98,101,113,179	0
60	K	23SA	3570	1/1	0.95	0.07	51,51,51,51	0
58	MG	23SA	3024	1/1	0.95	0.14	45,45,45,45	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
59	OHX	23SA	3291	7/7	0.95	0.07	126,133,145,190	0
59	OHX	16SB	2224	7/7	0.95	0.06	97,105,114,200	0
58	MG	23SB	3249	1/1	0.95	0.14	56,56,56,56	0
58	MG	23SB	3369	1/1	0.95	0.07	46,46,46,46	0
59	OHX	16SB	2229	7/7	0.95	0.06	111,112,116,211	0
58	MG	23SA	3463	1/1	0.95	0.07	60,60,60,60	0
58	MG	23SA	3465	1/1	0.95	0.09	53,53,53,53	0
59	OHX	16SB	2235	7/7	0.95	0.06	105,111,120,212	0
59	OHX	16SA	2303	7/7	0.95	0.06	117,118,127,222	0
58	MG	23SB	3373	1/1	0.95	0.08	48,48,48,48	0
58	MG	23SA	3510	1/1	0.96	0.12	75,75,75,75	0
60	K	23SA	3600	1/1	0.96	0.07	68,68,68,68	0
58	MG	16SA	2344	1/1	0.96	0.06	82,82,82,82	0
58	MG	23SB	3347	1/1	0.96	0.07	65,65,65,65	0
59	OHX	16SB	2255	7/7	0.96	0.06	133,135,154,207	0
59	OHX	ESIA	101	7/7	0.96	0.07	144,159,173,194	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
58	MG	23SA	3129	1/1	0.96	0.06	54,54,54,54	0
59	OHX	23SB	3169	7/7	0.96	0.06	104,124,127,192	0
59	OHX	23SA	3332	7/7	0.96	0.06	98,103,115,190	0
58	MG	23SB	3355	1/1	0.96	0.07	65,65,65,65	0
59	OHX	16SA	2275	7/7	0.96	0.09	80,83,104,161	0
59	OHX	23SA	3335	7/7	0.96	0.13	83,87,102,172	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	16SA	2361	1/1	0.96	0.05	75,75,75,75	0
59	OHX	16SA	2278	7/7	0.96	0.06	100,115,119,183	0
58	MG	23SA	3104	1/1	0.96	0.07	63,63,63,63	0
59	OHX	23SA	3225	7/7	0.96	0.06	96,99,104,174	0
58	MG	23SB	3358	1/1	0.96	0.06	47,47,47,47	0
58	MG	23SB	3238	1/1	0.96	0.17	46,46,46,46	0
59	OHX	23SA	3230	7/7	0.96	0.09	67,77,97,168	0
58	MG	23SA	3105	1/1	0.96	0.19	59,59,59,59	0
58	MG	23SB	3362	1/1	0.96	0.06	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	16SB	2347	1/1	0.96	0.09	92,92,92,92	0
59	OHX	23SA	3237	7/7	0.96	0.11	79,89,105,162	0
58	MG	23SA	3431	1/1	0.96	0.05	79,79,79,79	0
60	K	23SA	3633	1/1	0.96	0.15	77,77,77,77	0
59	OHX	23SA	3240	7/7	0.96	0.11	69,78,93,170	0
58	MG	23SB	3367	1/1	0.96	0.09	49,49,49,49	0
59	OHX	23SA	3243	7/7	0.96	0.10	79,89,95,159	0
60	K	23SA	3637	1/1	0.96	0.13	60,60,60,60	0
59	OHX	23SA	3245	7/7	0.96	0.13	86,96,104,177	0
59	OHX	23SB	3030	7/7	0.96	0.14	80,86,109,145	0
58	MG	23SB	3242	1/1	0.96	0.19	39,39,39,39	0
59	OHX	23SB	3034	7/7	0.96	0.12	90,91,105,156	0
59	OHX	23SA	3250	7/7	0.96	0.13	58,64,77,149	0
59	OHX	16SA	2291	7/7	0.96	0.12	91,96,102,165	0
58	MG	23SA	3523	1/1	0.96	0.09	70,70,70,70	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
58	MG	16SB	2352	1/1	0.96	0.07	73,73,73,73	0
60	K	16SB	2368	1/1	0.96	0.04	103,103,103,103	0
58	MG	16SA	2362	1/1	0.96	0.12	93,93,93,93	0
58	MG	23SB	3375	1/1	0.96	0.07	66,66,66,66	0
58	MG	16SB	2357	1/1	0.96	0.06	96,96,96,96	0
59	OHX	23SB	3055	7/7	0.96	0.14	65,81,87,153	0
58	MG	16SB	2358	1/1	0.96	0.06	105,105,105,105	0
58	MG	23SA	3526	1/1	0.96	0.12	76,76,76,76	0
60	K	16SB	2378	1/1	0.96	0.07	94,94,94,94	0
59	OHX	23SB	3060	7/7	0.96	0.10	95,99,105,180	0
58	MG	16SA	2345	1/1	0.96	0.06	89,89,89,89	0
58	MG	23SA	3529	1/1	0.96	0.09	42,42,42,42	0
59	OHX	23SA	3264	7/7	0.96	0.05	98,101,114,196	0
60	K	16SB	2383	1/1	0.96	0.05	92,92,92,92	0
59	OHX	23SB	3064	7/7	0.96	0.18	77,82,98,167	0
59	OHX	23SA	3265	7/7	0.96	0.07	83,93,109,192	0
58	MG	23SA	3442	1/1	0.96	0.06	48,48,48,48	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
59	OHX	16SA	2302	7/7	0.96	0.07	105,107,113,183	0
58	MG	23SA	3038	1/1	0.96	0.15	45,45,45,45	0
58	MG	23SA	3535	1/1	0.96	0.14	59,59,59,59	0
58	MG	23SA	3004	1/1	0.96	0.24	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	16SA	2364	1/1	0.96	0.07	86,86,86,86	0
60	K	16SB	2397	1/1	0.96	0.04	97,97,97,97	0
58	MG	16SA	2365	1/1	0.96	0.09	53,53,53,53	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
58	MG	23SB	3392	1/1	0.96	0.09	52,52,52,52	0
58	MG	23SA	3462	1/1	0.96	0.07	51,51,51,51	0
59	OHX	23SA	3276	7/7	0.96	0.06	87,98,104,204	0
59	OHX	23SB	3091	7/7	0.96	0.12	81,89,94,189	0
58	MG	23SA	3066	1/1	0.96	0.18	59,59,59,59	0
58	MG	23SA	3113	1/1	0.96	0.21	52,52,52,52	0
59	OHX	23SB	3094	7/7	0.96	0.06	107,111,129,187	0
59	OHX	23SA	3279	7/7	0.96	0.06	92,97,106,198	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
58	MG	23SA	3021	1/1	0.96	0.18	40,40,40,40	0
59	OHX	23SB	3100	7/7	0.96	0.11	90,93,100,175	0
59	OHX	23SB	3101	7/7	0.96	0.07	104,111,115,185	0
59	OHX	23SA	3282	7/7	0.96	0.06	101,104,113,206	0
60	K	23SB	3453	1/1	0.96	0.05	59,59,59,59	0
58	MG	23SA	3022	1/1	0.96	0.22	40,40,40,40	0
59	OHX	5SA	207	7/7	0.96	0.06	97,103,109,176	0
60	K	23SB	3457	1/1	0.96	0.05	63,63,63,63	0
58	MG	23SA	3474	1/1	0.96	0.07	59,59,59,59	0
60	K	23SB	3460	1/1	0.96	0.06	61,61,61,61	0
58	MG	23SA	3476	1/1	0.96	0.08	51,51,51,51	0
59	OHX	5SA	210	7/7	0.96	0.17	81,88,100,168	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
59	OHX	5SA	211	7/7	0.96	0.06	101,107,113,190	0
59	OHX	23SA	3287	7/7	0.96	0.07	97,100,105,189	0
58	MG	23SB	3413	1/1	0.96	0.07	42,42,42,42	0
58	MG	23SB	3414	1/1	0.96	0.06	83,83,83,83	0
58	MG	L27A	104	1/1	0.96	0.09	65,65,65,65	0
59	OHX	23SB	3115	7/7	0.96	0.05	98,104,112,200	0
58	MG	16SA	2366	1/1	0.96	0.06	107,107,107,107	0
59	OHX	23SA	3294	7/7	0.96	0.10	85,97,105,191	0
58	MG	23SA	3070	1/1	0.96	0.24	58,58,58,58	0
59	OHX	23SA	3296	7/7	0.96	0.06	94,97,113,192	0
58	MG	16SA	2347	1/1	0.96	0.07	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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
58	MG	23SB	3422	1/1	0.96	0.07	72,72,72,72	0
59	OHX	23SB	3125	7/7	0.96	0.07	90,93,105,217	0
60	K	23SB	3482	1/1	0.96	0.04	66,66,66,66	0
58	MG	23SA	3119	1/1	0.96	0.05	61,61,61,61	0
60	K	23SA	3551	1/1	0.96	0.04	80,80,80,80	0
58	MG	23SA	3025	1/1	0.96	0.29	64,64,64,64	0
58	MG	16SA	2210	1/1	0.96	0.14	46,46,46,46	0
58	MG	16SA	2355	1/1	0.96	0.08	51,51,51,51	0
59	OHX	16SB	2221	7/7	0.96	0.05	108,115,121,190	0
59	OHX	23SA	3305	7/7	0.96	0.05	97,104,122,196	0
58	MG	23SA	3029	1/1	0.96	0.16	37,37,37,37	0
59	OHX	16SB	2225	7/7	0.96	0.10	94,95,103,163	0
59	OHX	23SB	3137	7/7	0.96	0.06	99,103,110,209	0
58	MG	23SB	3433	1/1	0.96	0.06	106,106,106,106	0
58	MG	16SA	2206	1/1	0.96	0.34	40,40,40,40	0
58	MG	23SB	3274	1/1	0.96	0.30	57,57,57,57	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
60	K	23SA	3566	1/1	0.96	0.04	51,51,51,51	0
60	K	23SB	3503	1/1	0.96	0.12	72,72,72,72	0
58	MG	23SA	3392	1/1	0.96	0.08	52,52,52,52	0
58	MG	16SA	2358	1/1	0.96	0.10	48,48,48,48	0
60	K	23SA	3574	1/1	0.96	0.04	52,52,52,52	0
58	MG	23SA	3401	1/1	0.96	0.07	63,63,63,63	0
59	OHX	16SA	2334	7/7	0.96	0.06	161,169,178,239	0
60	K	23SA	3579	1/1	0.96	0.04	60,60,60,60	0
58	MG	23SA	3153	1/1	0.96	0.12	51,51,51,51	0
58	MG	16SB	2329	1/1	0.96	0.11	63,63,63,63	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
59	OHX	16SB	2240	7/7	0.96	0.06	120,126,130,218	0
58	MG	23SB	3331	1/1	0.96	0.19	58,58,58,58	0
59	OHX	16SB	2243	7/7	0.96	0.06	115,117,121,193	0
59	OHX	16SA	2338	7/7	0.96	0.07	96,105,108,199	0
59	OHX	16SB	2245	7/7	0.96	0.06	100,107,114,181	0
60	K	23SA	3590	1/1	0.96	0.10	67,67,67,67	0
58	MG	23SA	3501	1/1	0.96	0.08	66,66,66,66	0
58	MG	23SA	3126	1/1	0.96	0.08	62,62,62,62	0
59	OHX	16SB	2248	7/7	0.96	0.05	123,130,136,226	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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
58	MG	16SA	2342	1/1	0.96	0.07	85,85,85,85	0
59	OHX	23SA	3246	7/7	0.97	0.08	88,94,111,180	0
58	MG	23SA	3028	1/1	0.97	0.23	41,41,41,41	0
59	OHX	23SA	3248	7/7	0.97	0.11	84,89,103,166	0
59	OHX	16SB	2237	7/7	0.97	0.06	109,114,118,214	0
59	OHX	23SA	3249	7/7	0.97	0.13	81,94,100,157	0
58	MG	23SA	3433	1/1	0.97	0.05	77,77,77,77	0
58	MG	16SA	2372	1/1	0.97	0.05	92,92,92,92	0
59	OHX	16SB	2241	7/7	0.97	0.06	97,104,110,191	0
59	OHX	23SA	3253	7/7	0.97	0.05	106,111,120,187	0
60	K	5SA	218	1/1	0.97	0.04	79,79,79,79	0
58	MG	16SB	2359	1/1	0.97	0.06	103,103,103,103	0
60	K	L2A	301	1/1	0.97	0.05	47,47,47,47	0
58	MG	23SB	3229	1/1	0.97	0.29	44,44,44,44	0
58	MG	23SA	3395	1/1	0.97	0.07	34,34,34,34	0
58	MG	23SA	3438	1/1	0.97	0.05	88,88,88,88	0
58	MG	16SB	2362	1/1	0.97	0.08	113,113,113,113	0
58	MG	23SA	3441	1/1	0.97	0.05	43,43,43,43	0
58	MG	23SA	3396	1/1	0.97	0.06	34,34,34,34	0
58	MG	23SB	3235	1/1	0.97	0.20	59,59,59,59	0
60	K	16SA	2397	1/1	0.97	0.07	62,62,62,62	0
58	MG	23SA	3493	1/1	0.97	0.05	44,44,44,44	0
60	K	16SA	2400	1/1	0.97	0.04	89,89,89,89	0
60	K	16SB	2371	1/1	0.97	0.05	99,99,99,99	0
60	K	16SB	2372	1/1	0.97	0.03	105,105,105,105	0
60	K	16SB	2373	1/1	0.97	0.13	93,93,93,93	0
58	MG	23SA	3399	1/1	0.97	0.05	37,37,37,37	0
58	MG	23SB	3374	1/1	0.97	0.10	48,48,48,48	0
58	MG	23SA	3444	1/1	0.97	0.10	29,29,29,29	0
58	MG	5SA	217	1/1	0.97	0.13	85,85,85,85	0
58	MG	23SA	3030	1/1	0.97	0.27	51,51,51,51	0
58	MG	16SA	2370	1/1	0.97	0.05	102,102,102,102	0
59	OHX	16SB	2258	7/7	0.97	0.05	144,147,157,204	0
58	MG	23SA	3456	1/1	0.97	0.06	50,50,50,50	0
59	OHX	16SA	2265	7/7	0.97	0.07	104,105,123,150	0
60	K	16SA	2410	1/1	0.97	0.03	77,77,77,77	0
59	OHX	16SA	2269	7/7	0.97	0.08	81,87,100,141	0
58	MG	L15A	203	1/1	0.97	0.11	65,65,65,65	0
59	OHX	16SA	2273	7/7	0.97	0.09	96,101,112,163	0
58	MG	23SA	3458	1/1	0.97	0.07	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	23SA	3460	1/1	0.97	0.09	38,38,38,38	0
58	MG	23SA	3507	1/1	0.97	0.06	55,55,55,55	0
59	OHX	23SB	3128	7/7	0.97	0.05	108,110,117,202	0
58	MG	23SB	3247	1/1	0.97	0.06	45,45,45,45	0
58	MG	23SB	3208	1/1	0.97	0.28	52,52,52,52	0
59	OHX	23SA	3281	7/7	0.97	0.11	76,91,95,177	0
58	MG	S4A	302	1/1	0.97	0.06	98,98,98,98	0
59	OHX	23SB	3133	7/7	0.97	0.05	96,99,110,198	0
59	OHX	23SA	3283	7/7	0.97	0.05	106,113,119,187	0
58	MG	23SA	3413	1/1	0.97	0.07	55,55,55,55	0
59	OHX	16SA	2282	7/7	0.97	0.12	84,85,91,155	0
58	MG	23SA	3039	1/1	0.97	0.15	30,30,30,30	0
58	MG	23SB	3395	1/1	0.97	0.11	43,43,43,43	0
58	MG	23SA	3415	1/1	0.97	0.05	67,67,67,67	0
59	OHX	23SA	3289	7/7	0.97	0.14	72,79,86,180	0
59	OHX	23SA	3290	7/7	0.97	0.12	83,93,105,198	0
59	OHX	S19A	101	7/7	0.97	0.06	115,125,129,181	0
59	OHX	16SA	2287	7/7	0.97	0.08	96,103,109,167	0
59	OHX	PSIB	101	7/7	0.97	0.08	104,107,121,137	0
59	OHX	ASIA	103	7/7	0.97	0.07	142,155,169,215	0
59	OHX	23SB	3147	7/7	0.97	0.05	109,122,129,186	0
59	OHX	ESIB	101	7/7	0.97	0.06	150,166,173,207	0
58	MG	23SB	3290	1/1	0.97	0.31	47,47,47,47	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
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
58	MG	23SA	3417	1/1	0.97	0.10	58,58,58,58	0
59	OHX	TRNA	101	7/7	0.97	0.06	135,137,154,191	0
60	K	23SB	3455	1/1	0.97	0.11	61,61,61,61	0
59	OHX	23SA	3297	7/7	0.97	0.09	97,99,109,183	0
58	MG	23SB	3403	1/1	0.97	0.06	52,52,52,52	0
59	OHX	5SA	205	7/7	0.97	0.09	75,95,106,138	0
60	K	23SA	3561	1/1	0.97	0.06	75,75,75,75	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
58	MG	23SB	3404	1/1	0.97	0.08	37,37,37,37	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
60	K	23SA	3567	1/1	0.97	0.05	46,46,46,46	0
59	OHX	23SB	3045	7/7	0.97	0.08	84,95,110,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	OHX	23SB	3046	7/7	0.97	0.09	64,76,84,147	0
60	K	23SA	3572	1/1	0.97	0.05	51,51,51,51	0
59	OHX	23SB	3047	7/7	0.97	0.11	74,90,94,149	0
59	OHX	23SA	3200	7/7	0.97	0.11	62,89,92,138	0
58	MG	16SA	2351	1/1	0.97	0.08	103,103,103,103	0
59	OHX	23SA	3207	7/7	0.97	0.11	73,78,88,136	0
59	OHX	23SA	3303	7/7	0.97	0.10	91,92,104,183	0
58	MG	23SA	3518	1/1	0.97	0.14	61,61,61,61	0
59	OHX	23SA	3209	7/7	0.97	0.08	76,90,103,134	0
60	K	23SB	3477	1/1	0.97	0.03	60,60,60,60	0
59	OHX	23SA	3210	7/7	0.97	0.11	57,67,87,122	0
59	OHX	23SB	3057	7/7	0.97	0.10	96,99,115,167	0
59	OHX	23SA	3211	7/7	0.97	0.11	61,66,83,132	0
58	MG	23SA	3058	1/1	0.97	0.04	53,53,53,53	0
59	OHX	23SA	3220	7/7	0.97	0.07	85,86,101,146	0
60	K	23SB	3484	1/1	0.97	0.07	80,80,80,80	0
58	MG	23SB	3411	1/1	0.97	0.06	41,41,41,41	0
59	OHX	23SA	3222	7/7	0.97	0.06	99,103,115,175	0
58	MG	23SB	3412	1/1	0.97	0.05	56,56,56,56	0
58	MG	23SA	3387	1/1	0.97	0.05	55,55,55,55	0
59	OHX	23SB	3065	7/7	0.97	0.10	86,93,109,147	0
58	MG	16SB	2349	1/1	0.97	0.17	90,90,90,90	0
60	K	23SB	3491	1/1	0.97	0.08	68,68,68,68	0
59	OHX	16SB	2210	7/7	0.97	0.10	96,101,107,163	0
60	K	23SA	3596	1/1	0.97	0.03	59,59,59,59	0
59	OHX	16SB	2211	7/7	0.97	0.07	101,114,117,162	0
60	K	23SA	3598	1/1	0.97	0.11	58,58,58,58	0
58	MG	23SB	3415	1/1	0.97	0.07	46,46,46,46	0
60	K	23SB	3497	1/1	0.97	0.06	48,48,48,48	0
59	OHX	23SA	3228	7/7	0.97	0.09	70,82,89,143	0
58	MG	23SB	3416	1/1	0.97	0.07	98,98,98,98	0
59	OHX	23SB	3072	7/7	0.97	0.08	81,88,103,161	0
58	MG	23SB	3337	1/1	0.97	0.06	48,48,48,48	0
59	OHX	23SA	3232	7/7	0.97	0.07	78,84,95,161	0
58	MG	23SB	3344	1/1	0.97	0.06	50,50,50,50	0
59	OHX	23SA	3234	7/7	0.97	0.08	91,94,101,156	0
60	K	23SA	3607	1/1	0.97	0.04	59,59,59,59	0
60	K	23SB	3506	1/1	0.97	0.06	75,75,75,75	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
58	MG	16SB	2350	1/1	0.97	0.08	99,99,99,99	0
59	OHX	23SB	3080	7/7	0.97	0.06	95,105,112,179	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	23SB	3221	1/1	0.97	0.14	47,47,47,47	0
59	OHX	5SB	201	7/7	0.97	0.07	103,112,120,159	0
58	MG	23SA	3389	1/1	0.97	0.06	41,41,41,41	0
60	K	23SA	3616	1/1	0.97	0.05	42,42,42,42	0
59	OHX	23SB	3083	7/7	0.97	0.05	110,114,121,181	0
58	MG	23SB	3423	1/1	0.97	0.05	73,73,73,73	0
59	OHX	16SB	2226	7/7	0.97	0.05	117,119,123,191	0
59	OHX	23SB	3086	7/7	0.97	0.10	85,86,104,167	0
58	MG	23SA	3041	1/1	0.97	0.07	32,32,32,32	0
59	OHX	23SA	3242	7/7	0.97	0.17	54,62,72,135	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
58	MG	23SB	3425	1/1	0.97	0.18	84,84,84,84	0
59	OHX	16SB	2230	7/7	0.97	0.04	126,136,146,203	0
59	OHX	23SA	3330	7/7	0.97	0.06	112,118,131,203	0
59	OHX	23SA	3244	7/7	0.97	0.10	76,82,89,144	0
58	MG	23SB	3427	1/1	0.97	0.13	49,49,49,49	0
60	K	23SA	3630	1/1	0.97	0.07	80,80,80,80	0
58	MG	23SB	3343	1/1	0.98	0.08	65,65,65,65	0
58	MG	23SA	3490	1/1	0.98	0.07	42,42,42,42	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	23SB	3345	1/1	0.98	0.05	65,65,65,65	0
58	MG	L4A	301	1/1	0.98	0.12	48,48,48,48	0
58	MG	L4A	303	1/1	0.98	0.08	73,73,73,73	0
58	MG	23SA	3492	1/1	0.98	0.04	52,52,52,52	0
60	K	16SA	2399	1/1	0.98	0.04	65,65,65,65	0
58	MG	23SB	3426	1/1	0.98	0.05	70,70,70,70	0
59	OHX	23SA	3251	7/7	0.98	0.04	99,104,112,176	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	23SB	3352	1/1	0.98	0.06	47,47,47,47	0
58	MG	23SB	3353	1/1	0.98	0.05	57,57,57,57	0
58	MG	23SA	3448	1/1	0.98	0.05	40,40,40,40	0
58	MG	23SA	3494	1/1	0.98	0.05	48,48,48,48	0
58	MG	23SA	3449	1/1	0.98	0.04	44,44,44,44	0
58	MG	23SB	3435	1/1	0.98	0.10	94,94,94,94	0
58	MG	23SA	3419	1/1	0.98	0.05	64,64,64,64	0
58	MG	23SA	3498	1/1	0.98	0.06	38,38,38,38	0
59	OHX	16SB	2269	7/7	0.98	0.06	146,151,156,215	0
58	MG	23SA	3453	1/1	0.98	0.05	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	OHX	23SA	3263	7/7	0.98	0.08	64,70,95,142	0
58	MG	16SA	2348	1/1	0.98	0.03	58,58,58,58	0
58	MG	23SA	3457	1/1	0.98	0.09	37,37,37,37	0
58	MG	23SB	3365	1/1	0.98	0.03	45,45,45,45	0
60	K	16SB	2385	1/1	0.98	0.04	92,92,92,92	0
58	MG	5SB	215	1/1	0.98	0.05	88,88,88,88	0
58	MG	23SA	3394	1/1	0.98	0.08	71,71,71,71	0
58	MG	23SA	3074	1/1	0.98	0.04	72,72,72,72	0
58	MG	23SA	3062	1/1	0.98	0.09	61,61,61,61	0
59	OHX	23SA	3271	7/7	0.98	0.09	70,73,91,159	0
59	OHX	ASIB	101	7/7	0.98	0.04	114,126,131,187	0
59	OHX	23SB	3134	7/7	0.98	0.10	82,85,92,165	0
58	MG	23SA	3508	1/1	0.98	0.05	38,38,38,38	0
60	K	23SA	3538	1/1	0.98	0.06	63,63,63,63	0
58	MG	23SA	3509	1/1	0.98	0.05	52,52,52,52	0
58	MG	23SB	3211	1/1	0.98	0.05	52,52,52,52	0
58	MG	23SA	3425	1/1	0.98	0.09	61,61,61,61	0
58	MG	23SA	3383	1/1	0.98	0.05	39,39,39,39	0
59	OHX	16SA	2266	7/7	0.98	0.07	89,99,109,141	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
58	MG	23SA	3428	1/1	0.98	0.07	78,78,78,78	0
59	OHX	23SB	3021	7/7	0.98	0.08	68,77,87,136	0
59	OHX	16SA	2270	7/7	0.98	0.06	108,118,121,150	0
58	MG	23SA	3430	1/1	0.98	0.05	74,74,74,74	0
59	OHX	23SB	3024	7/7	0.98	0.10	69,75,81,158	0
59	OHX	16SA	2272	7/7	0.98	0.07	96,111,118,140	0
58	MG	23SB	3379	1/1	0.98	0.05	41,41,41,41	0
59	OHX	23SB	3028	7/7	0.98	0.07	85,85,101,143	0
59	OHX	ASIA	101	7/7	0.98	0.06	100,111,125,168	0
59	OHX	23SB	3031	7/7	0.98	0.07	88,95,98,151	0
58	MG	16SB	2328	1/1	0.98	0.08	58,58,58,58	0
58	MG	23SA	3514	1/1	0.98	0.13	51,51,51,51	0
59	OHX	5SA	204	7/7	0.98	0.06	79,82,94,113	0
58	MG	23SA	3468	1/1	0.98	0.07	36,36,36,36	0
59	OHX	23SB	3037	7/7	0.98	0.08	97,101,106,155	0
59	OHX	16SA	2277	7/7	0.98	0.07	94,95,103,165	0
58	MG	23SA	3469	1/1	0.98	0.06	40,40,40,40	0
59	OHX	23SB	3040	7/7	0.98	0.07	68,76,88,142	0
58	MG	23SA	3090	1/1	0.98	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
60	K	23SB	3459	1/1	0.98	0.07	56,56,56,56	0
59	OHX	23SB	3042	7/7	0.98	0.05	101,107,110,164	0
59	OHX	23SA	3191	7/7	0.98	0.06	79,89,101,127	0
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
60	K	23SA	3573	1/1	0.98	0.06	63,63,63,63	0
58	MG	23SA	3473	1/1	0.98	0.05	67,67,67,67	0
59	OHX	23SA	3196	7/7	0.98	0.10	70,74,94,114	0
60	K	23SA	3576	1/1	0.98	0.07	39,39,39,39	0
59	OHX	23SA	3197	7/7	0.98	0.07	73,80,93,129	0
59	OHX	23SA	3198	7/7	0.98	0.07	58,71,88,129	0
59	OHX	L17A	201	7/7	0.98	0.12	63,68,78,121	0
59	OHX	23SA	3199	7/7	0.98	0.06	65,73,83,129	0
58	MG	23SA	3521	1/1	0.98	0.04	58,58,58,58	0
59	OHX	23SB	3053	7/7	0.98	0.06	92,97,113,157	0
59	OHX	23SA	3201	7/7	0.98	0.07	79,87,98,127	0
60	K	23SA	3585	1/1	0.98	0.08	54,54,54,54	0
59	OHX	23SA	3202	7/7	0.98	0.08	55,70,77,136	0
59	OHX	23SB	3056	7/7	0.98	0.06	95,102,108,155	0
59	OHX	23SA	3203	7/7	0.98	0.06	77,78,101,130	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	3204	7/7	0.98	0.06	66,71,91,123	0
59	OHX	16SB	2209	7/7	0.98	0.06	90,99,108,137	0
60	K	23SB	3483	1/1	0.98	0.05	69,69,69,69	0
58	MG	23SA	3432	1/1	0.98	0.03	67,67,67,67	0
59	OHX	23SA	3206	7/7	0.98	0.10	74,75,95,140	0
59	OHX	16SB	2212	7/7	0.98	0.07	96,100,102,148	0
58	MG	23SA	3385	1/1	0.98	0.05	41,41,41,41	0
58	MG	23SB	3225	1/1	0.98	0.08	39,39,39,39	0
59	OHX	16SA	2285	7/7	0.98	0.04	123,129,131,218	0
58	MG	23SA	3407	1/1	0.98	0.05	48,48,48,48	0
58	MG	23SA	3527	1/1	0.98	0.06	42,42,42,42	0
58	MG	16SB	2345	1/1	0.98	0.08	64,64,64,64	0
59	OHX	16SB	2219	7/7	0.98	0.05	103,105,116,174	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	3313	7/7	0.98	0.10	67,73,83,167	0
59	OHX	16SB	2223	7/7	0.98	0.04	110,112,122,172	0
59	OHX	23SA	3217	7/7	0.98	0.05	80,82,89,137	0
59	OHX	23SA	3218	7/7	0.98	0.09	78,86,101,146	0
59	OHX	23SA	3219	7/7	0.98	0.08	82,94,104,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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	3052	1/1	0.98	0.22	40,40,40,40	0
59	OHX	23SA	3223	7/7	0.98	0.06	81,87,101,144	0
58	MG	23SB	3401	1/1	0.98	0.09	70,70,70,70	0
60	K	23SA	3615	1/1	0.98	0.08	69,69,69,69	0
58	MG	23SB	3402	1/1	0.98	0.05	45,45,45,45	0
58	MG	23SA	3481	1/1	0.98	0.10	55,55,55,55	0
58	MG	16SA	2373	1/1	0.98	0.12	98,98,98,98	0
58	MG	23SA	3533	1/1	0.98	0.05	49,49,49,49	0
59	OHX	L17B	201	7/7	0.98	0.10	72,77,87,116	0
60	K	23SA	3621	1/1	0.98	0.08	77,77,77,77	0
59	OHX	23SA	3229	7/7	0.98	0.07	81,96,99,154	0
58	MG	23SA	3390	1/1	0.98	0.05	38,38,38,38	0
59	OHX	23SB	3090	7/7	0.98	0.05	110,117,123,191	0
58	MG	16SA	2343	1/1	0.98	0.09	73,73,73,73	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
58	MG	16SB	2355	1/1	0.98	0.05	90,90,90,90	0
59	OHX	23SA	3235	7/7	0.98	0.06	75,87,106,150	0
58	MG	23SA	3485	1/1	0.98	0.04	51,51,51,51	0
58	MG	16SA	2356	1/1	0.98	0.10	67,67,67,67	0
59	OHX	23SA	3238	7/7	0.98	0.11	64,65,76,149	0
58	MG	23SA	3418	1/1	0.98	0.08	36,36,36,36	0
58	MG	23SA	3488	1/1	0.98	0.06	49,49,49,49	0
58	MG	23SA	3447	1/1	0.98	0.05	34,34,34,34	0
60	K	L16B	201	1/1	0.98	0.04	92,92,92,92	0
58	MG	23SB	3340	1/1	0.98	0.08	45,45,45,45	0
58	MG	23SB	3341	1/1	0.98	0.06	53,53,53,53	0
59	OHX	23SB	3029	7/7	0.99	0.05	91,95,103,141	0
58	MG	16SA	2352	1/1	0.99	0.05	62,62,62,62	0
59	OHX	16SB	2203	7/7	0.99	0.06	91,94,102,133	0
58	MG	23SA	3475	1/1	0.99	0.05	64,64,64,64	0
59	OHX	23SB	3033	7/7	0.99	0.08	79,88,93,147	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	23SA	3405	1/1	0.99	0.09	46,46,46,46	0
59	OHX	16SB	2208	7/7	0.99	0.05	79,80,93,120	0
58	MG	23SA	3406	1/1	0.99	0.04	63,63,63,63	0
58	MG	23SB	3359	1/1	0.99	0.11	66,66,66,66	0
58	MG	23SA	3446	1/1	0.99	0.05	43,43,43,43	0
58	MG	23SA	3386	1/1	0.99	0.04	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	23SA	3480	1/1	0.99	0.04	82,82,82,82	0
58	MG	23SB	3363	1/1	0.99	0.08	47,47,47,47	0
58	MG	23SA	3408	1/1	0.99	0.03	45,45,45,45	0
58	MG	23SB	3432	1/1	0.99	0.04	46,46,46,46	0
58	MG	23SA	3426	1/1	0.99	0.04	42,42,42,42	0
58	MG	23SA	3517	1/1	0.99	0.08	82,82,82,82	0
58	MG	23SA	3450	1/1	0.99	0.03	56,56,56,56	0
58	MG	23SB	3368	1/1	0.99	0.03	47,47,47,47	0
58	MG	23SA	3451	1/1	0.99	0.04	33,33,33,33	0
58	MG	23SB	3438	1/1	0.99	0.05	45,45,45,45	0
58	MG	23SA	3520	1/1	0.99	0.13	79,79,79,79	0
58	MG	23SB	3371	1/1	0.99	0.04	39,39,39,39	0
58	MG	16SA	2349	1/1	0.99	0.03	82,82,82,82	0
58	MG	23SA	3522	1/1	0.99	0.03	73,73,73,73	0
58	MG	23SA	3410	1/1	0.99	0.03	57,57,57,57	0
58	MG	23SA	3454	1/1	0.99	0.03	54,54,54,54	0
58	MG	23SB	3376	1/1	0.99	0.03	50,50,50,50	0
58	MG	23SA	3525	1/1	0.99	0.10	40,40,40,40	0
58	MG	23SA	3429	1/1	0.99	0.07	60,60,60,60	0
58	MG	23SA	3388	1/1	0.99	0.04	33,33,33,33	0
58	MG	23SA	3412	1/1	0.99	0.04	40,40,40,40	0
58	MG	23SB	3382	1/1	0.99	0.04	61,61,61,61	0
60	K	23SA	3569	1/1	0.99	0.03	46,46,46,46	0
59	OHX	16SA	2260	7/7	0.99	0.06	68,70,81,89	0
60	K	23SA	3571	1/1	0.99	0.04	38,38,38,38	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	16SB	2334	1/1	0.99	0.06	68,68,68,68	0
60	K	23SA	3577	1/1	0.99	0.03	45,45,45,45	0
58	MG	16SB	2335	1/1	0.99	0.07	74,74,74,74	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	3491	1/1	0.99	0.05	43,43,43,43	0
58	MG	16SB	2337	1/1	0.99	0.08	100,100,100,100	0
58	MG	23SB	3387	1/1	0.99	0.08	53,53,53,53	0
58	MG	16SB	2338	1/1	0.99	0.05	86,86,86,86	0
58	MG	23SA	3530	1/1	0.99	0.05	57,57,57,57	0
59	OHX	PSIA	102	7/7	0.99	0.09	94,95,102,131	0
58	MG	23SA	3459	1/1	0.99	0.04	66,66,66,66	0
58	MG	16SB	2342	1/1	0.99	0.09	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	16SA	2354	1/1	0.99	0.03	68,68,68,68	0
58	MG	23SA	3397	1/1	0.99	0.04	46,46,46,46	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	5SB	202	7/7	0.99	0.05	96,105,116,131	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	23SB	3394	1/1	0.99	0.05	73,73,73,73	0
59	OHX	23SA	3192	7/7	0.99	0.07	68,74,81,100	0
58	MG	23SA	3534	1/1	0.99	0.10	55,55,55,55	0
58	MG	16SB	2346	1/1	0.99	0.04	84,84,84,84	0
58	MG	23SA	3398	1/1	0.99	0.04	35,35,35,35	0
58	MG	23SA	3536	1/1	0.99	0.09	36,36,36,36	0
58	MG	23SA	3496	1/1	0.99	0.06	63,63,63,63	0
58	MG	23SB	3334	1/1	0.99	0.05	58,58,58,58	0
58	MG	23SA	3436	1/1	0.99	0.10	80,80,80,80	0
58	MG	23SA	3416	1/1	0.99	0.04	63,63,63,63	0
58	MG	16SA	2350	1/1	0.99	0.06	89,89,89,89	0
58	MG	23SB	3405	1/1	0.99	0.07	53,53,53,53	0
58	MG	23SB	3338	1/1	0.99	0.04	48,48,48,48	0
58	MG	23SB	3339	1/1	0.99	0.04	47,47,47,47	0
59	OHX	S14B	101	7/7	0.99	0.04	121,125,132,169	0
58	MG	16SB	2353	1/1	0.99	0.11	76,76,76,76	0
58	MG	5SA	215	1/1	0.99	0.04	64,64,64,64	0
58	MG	23SA	3439	1/1	0.99	0.07	38,38,38,38	0
60	K	16SA	2390	1/1	0.99	0.10	67,67,67,67	0
58	MG	16SB	2356	1/1	0.99	0.11	78,78,78,78	0
60	K	23SA	3624	1/1	0.99	0.03	60,60,60,60	0
58	MG	23SA	3440	1/1	0.99	0.11	88,88,88,88	0
58	MG	23SA	3502	1/1	0.99	0.07	32,32,32,32	0
58	MG	L3A	302	1/1	0.99	0.04	39,39,39,39	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

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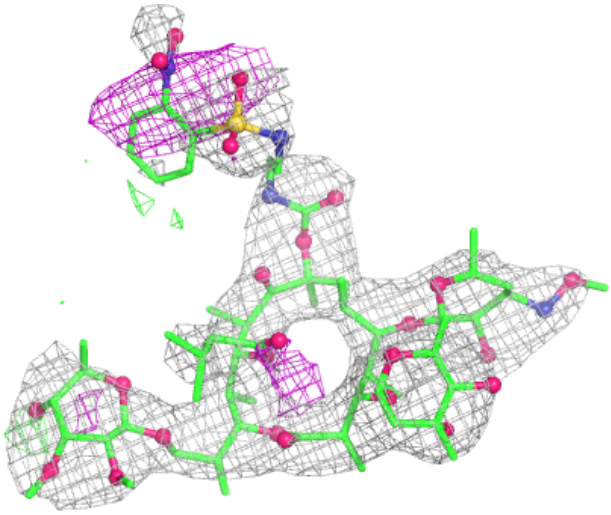
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	OHX	23SB	3005	7/7	0.99	0.06	74,76,93,97	0
59	OHX	23SB	3006	7/7	0.99	0.06	70,76,84,116	0
59	OHX	23SB	3007	7/7	0.99	0.06	85,90,107,121	0
58	MG	23SB	3348	1/1	0.99	0.12	75,75,75,75	0
59	OHX	23SB	3009	7/7	0.99	0.07	75,77,79,117	0
59	OHX	23SB	3010	7/7	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	3503	1/1	0.99	0.10	70,70,70,70	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
59	OHX	L4A	302	7/7	0.99	0.17	37,47,53,146	0
59	OHX	23SB	3017	7/7	0.99	0.06	83,87,98,124	0
59	OHX	23SA	3214	7/7	0.99	0.05	62,70,75,153	0
59	OHX	23SB	3019	7/7	0.99	0.06	68,75,83,123	0
59	OHX	23SA	3215	7/7	0.99	0.05	81,87,93,144	0
59	OHX	L19A	201	7/7	0.99	0.05	85,89,97,137	0
58	MG	23SA	3470	1/1	0.99	0.05	53,53,53,53	0
58	MG	23SA	3400	1/1	0.99	0.07	69,69,69,69	0
58	MG	23SA	3506	1/1	0.99	0.03	39,39,39,39	0
58	MG	16SA	2346	1/1	0.99	0.07	70,70,70,70	0
58	MG	23SB	3421	1/1	0.99	0.02	96,96,96,96	0
59	OHX	23SB	3027	7/7	0.99	0.07	78,82,92,125	0
59	OHX	16SB	2201	7/7	0.99	0.05	81,88,90,106	0
58	MG	23SA	3404	1/1	1.00	0.06	45,45,45,45	0
58	MG	23SA	3466	1/1	1.00	0.06	57,57,57,57	0
58	MG	23SA	3455	1/1	1.00	0.11	51,51,51,51	0
58	MG	23SA	3435	1/1	1.00	0.07	75,75,75,75	0
58	MG	23SB	3342	1/1	1.00	0.09	46,46,46,46	0
58	MG	16SB	2340	1/1	1.00	0.09	64,64,64,64	0
58	MG	23SB	3400	1/1	1.00	0.04	84,84,84,84	0
58	MG	23SB	3354	1/1	1.00	0.03	77,77,77,77	0
58	MG	23SA	3423	1/1	1.00	0.02	50,50,50,50	0
58	MG	23SA	3403	1/1	1.00	0.03	33,33,33,33	0
58	MG	23SA	3471	1/1	1.00	0.02	53,53,53,53	0
59	OHX	L4B	301	7/7	1.00	0.09	48,52,62,94	0
58	MG	23SB	3380	1/1	1.00	0.03	39,39,39,39	0
58	MG	23SA	3464	1/1	1.00	0.02	37,37,37,37	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

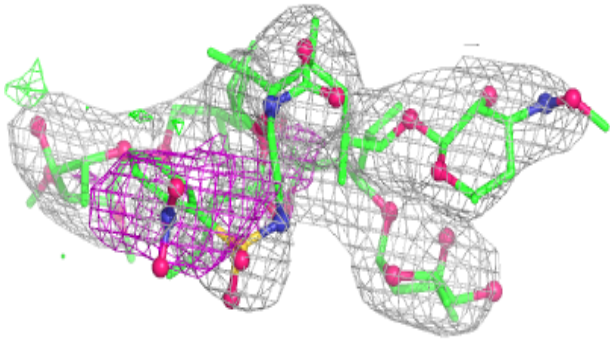
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

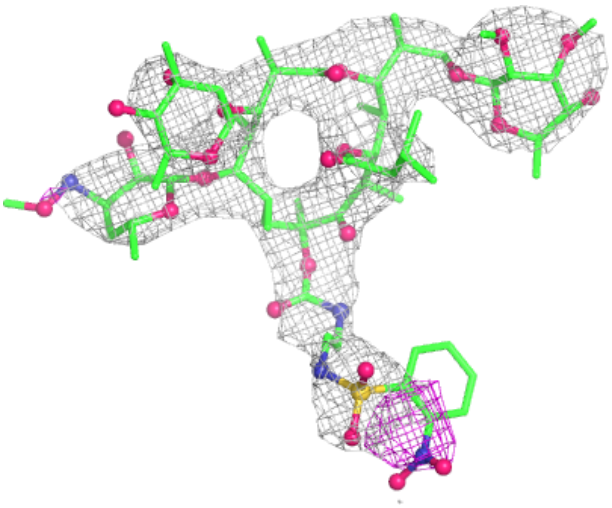
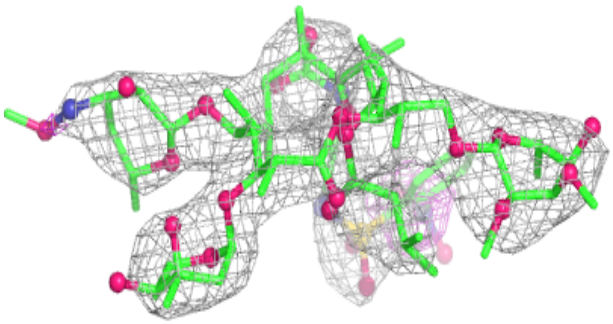
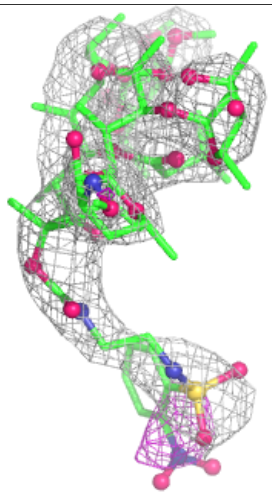
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

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)	
	

5.5 Other polymers (i)

There are no such residues in this entry.