



wwPDB X-ray Structure Validation Summary Report ⓘ

May 20, 2025 – 03:10 am BST

PDB ID : 8PNN / pdb_00008pnn
Title : 80S yeast ribosome in complex with Bromolisoclimide
Authors : Terrosu, S.; Yusupov, M.
Deposited on : 2023-06-30
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

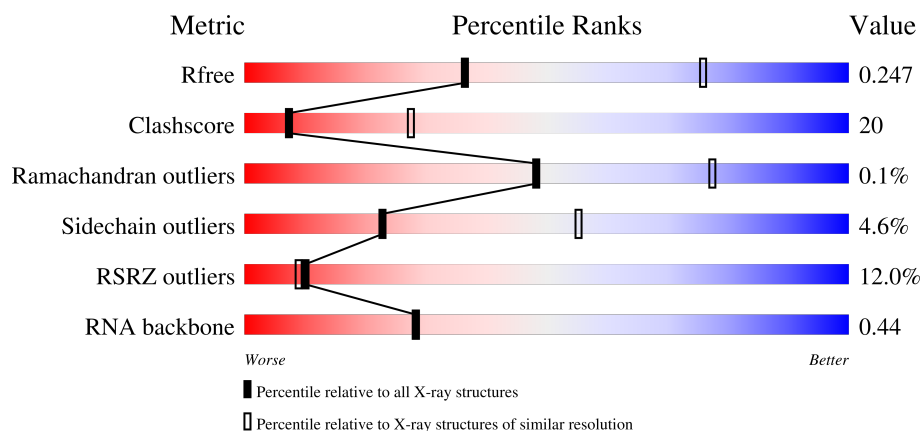
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)
RNA backbone	3690	1039 (3.10-2.70)

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

Mol	Chain	Length	Quality of chain
1	3	121	<div> <div>6%</div> <div> <div></div> <div>53%</div> <div>38%</div> <div>9%</div> </div> </div>
1	AS	121	<div> <div>2%</div> <div> <div></div> <div>50%</div> <div>45%</div> <div>6%</div> </div> </div>
2	AB	149	<div> <div>7%</div> <div> <div></div> <div>49%</div> <div>43%</div> <div>7%</div> <div>..</div> </div> </div>
2	DC	149	<div> <div>4%</div> <div> <div></div> <div>49%</div> <div>48%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	CJ	256	
3	p	256	
4	AI	120	
4	DJ	120	
5	Q	142	
5	c5	142	
6	H	236	
6	s6	236	
7	4	158	
7	AT	158	
8	AC	59	
8	DD	59	
9	CK	191	
9	q	191	
10	AJ	100	
10	DK	100	
11	R	143	
11	c6	143	
12	I	190	
12	s7	190	
13	CD	254	
13	j	254	
14	AD	105	
14	DE	105	
15	CL	221	

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Mol	Chain	Length	Quality of chain
15	r	221	
16	AK	88	
16	DL	88	
17	S	136	
17	c7	136	
18	J	200	
18	s8	200	
19	CE	387	
19	k	387	
20	AE	113	
20	DF	113	
21	CM	174	
21	s	174	
22	AL	78	
22	DM	78	
23	T	146	
23	c8	146	
24	K	197	
24	s9	197	
25	CF	362	
25	l	362	
26	AF	130	
26	DG	130	
27	CN	199	
27	t	199	

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Mol	Chain	Length	Quality of chain
28	AM	51	
28	DN	51	
29	U	144	
29	c9	144	
30	L	105	
30	c0	105	
31	CG	297	
31	m	297	
32	AG	107	
32	DH	107	
33	CO	138	
33	u	138	
34	AN	128	
34	DO	128	
35	V	121	
35	d0	121	
36	M	156	
36	c1	156	
37	CH	176	
37	n	176	
38	AH	121	
38	DI	121	
39	CP	204	
39	v	204	
40	AO	25	

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Mol	Chain	Length	Quality of chain
40	DP	25	
41	W	87	
41	d1	87	
42	O	151	
42	c3	151	
43	CI	244	
43	o	244	
44	CQ	199	
44	w	199	
45	AP	106	
45	DQ	106	
46	X	130	
46	d2	130	
47	P	138	
47	c4	138	
48	CR	184	
48	x	184	
49	AQ	92	
49	DR	92	
50	Y	145	
50	d3	145	
51	CS	186	
51	y	186	
52	p0	311	
53	Z	135	

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Mol	Chain	Length	Quality of chain
53	d4	135	
54	CT	189	
54	z	189	
55	i	273	
55	sM	273	
56	a	108	
56	d5	108	
57	0	172	
57	CU	172	
58	A	1800	
58	sR	1800	
59	b	119	
59	d6	119	
60	2	160	
60	CV	160	
61	B	252	
61	s0	252	
62	c	82	
62	d7	82	
63	5	121	
63	CW	121	
64	C	255	
64	s1	255	
65	d	67	
65	d8	67	

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Mol	Chain	Length	Quality of chain
66	6	137	
66	CX	137	
67	D	254	
67	s2	254	
68	d9	56	
68	e	56	
69	7	155	
69	CY	155	
70	E	240	
70	s3	240	
71	e0	63	
71	f	63	
72	8	142	
72	CZ	142	
73	F	261	
73	s4	261	
74	g	152	
75	1	3396	
75	AR	3396	
76	9	127	
76	DA	127	
77	G	225	
77	s5	225	
78	Rb	319	
78	h	319	

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Mol	Chain	Length	Quality of chain
79	AA	136	
79	DB	136	

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
80	OHX	1	3424	-	-	X	-
80	OHX	1	3603	-	-	X	-
80	OHX	1	3631	-	-	X	-
80	OHX	1	4028	-	-	X	-
80	OHX	1	4083	-	-	X	-
80	OHX	A	1944	-	-	X	-
80	OHX	A	1964	-	-	X	-
80	OHX	A	2003	-	-	X	-
80	OHX	A	2110	-	-	X	-
80	OHX	AK	103	-	-	X	-
80	OHX	AR	3856	-	-	X	-
80	OHX	AR	3956	-	-	X	-
80	OHX	AR	3973	-	-	X	-
80	OHX	AR	4135	-	-	X	-
80	OHX	sR	1945	-	-	X	-
80	OHX	sR	2198	-	-	X	-
81	MG	1	3500	-	-	-	X
81	MG	1	3584	-	-	-	X
81	MG	1	3900	-	-	-	X
81	MG	1	3955	-	-	-	X
81	MG	1	4041	-	-	-	X
81	MG	1	4046	-	-	-	X
81	MG	1	4109	-	-	-	X
81	MG	A	2008	-	-	-	X
81	MG	A	2021	-	-	-	X
81	MG	AR	3433	-	-	-	X
81	MG	AR	3434	-	-	-	X
81	MG	AR	3726	-	-	-	X
81	MG	AR	3905	-	-	-	X
81	MG	AR	4129	-	-	-	X
81	MG	AR	4148	-	-	-	X
81	MG	c8	202	-	-	-	X
81	MG	sR	2059	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	sR	2080	-	-	-	X
81	MG	sR	2106	-	-	-	X
81	MG	sR	2152	-	-	-	X

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 402407 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 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
1	AS	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 2 is a protein called 60S ribosomal protein L28.

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

- Molecule 3 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CJ	227	Total	C	N	O	S	0	0	0
			1762	1128	315	316	3			
3	p	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			

- Molecule 4 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 5 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Q	117	Total	C	N	O	S	0	0	0
			928	589	174	158	7			
5	c5	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	7			

- Molecule 6 is a protein called 40S ribosomal protein S6-A.

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

- Molecule 7 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	4	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			
7	AT	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 8 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	AC	54	Total	C	N	O	0	0	0
			434	271	94	69			
8	DD	58	Total	C	N	O	0	0	0
			462	289	100	73			

- Molecule 9 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	CK	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
9	q	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

- Molecule 10 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	DK	97	Total	C	N	O	S	0	0	0
			750	469	149	130	2			

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

- Molecule 11 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 12 is a protein called 40S ribosomal protein S7-A.

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

- Molecule 13 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	j	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
13	CD	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			

- Molecule 14 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AD	97	Total	C	N	O	S	0	0	0
			740	476	124	139	1			
14	DE	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			

- Molecule 15 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	CL	207	Total	C	N	O	S	0	0	0
			1685	1071	318	290	6			
15	r	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			

- Molecule 16 is a protein called 60S ribosomal protein L37-A.

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

- Molecule 17 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	S	111	Total	C	N	O	S	0	0	0
			863	536	166	159	2			
17	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

- Molecule 18 is a protein called 40S ribosomal protein S8-A.

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

- Molecule 19 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	k	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
19	CE	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

- Molecule 20 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AE	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			
20	DF	107	Total	C	N	O	S	0	0	0
			866	550	165	150	1			

- Molecule 21 is a protein called Large ribosomal subunit protein uL5B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	CM	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			
21	s	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			

- Molecule 22 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	DM	73	Total	C	N	O		0	0	0
			586	376	109	101				
22	AL	77	Total	C	N	O		0	0	0
			612	391	115	106				

- Molecule 23 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	T	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			
23	c8	135	Total	C	N	O	S	0	0	0
			1116	695	225	194	2			

- Molecule 24 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	s9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			
24	K	177	Total	C	N	O	S	0	0	0
			1436	910	277	248	1			

- Molecule 25 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	l	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
25	CF	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

- Molecule 26 is a protein called 60S ribosomal protein L32.

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

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

- Molecule 27 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	CN	193	Total	C	N	O	S	0	0	0
			1543	962	315	266				
27	t	193	Total	C	N	O	S	0	0	0
			1543	962	315	266				

- Molecule 28 is a protein called 60S ribosomal protein L39.

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

- Molecule 29 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 30 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	c0	72	Total	C	N	O	S	0	0	0
			609	395	98	114	2			
30	L	90	Total	C	N	O	S	0	0	0
			742	481	120	139	2			

- Molecule 31 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	m	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
31	CG	292	Total	C	N	O	S	0	0	0
			2348	1486	408	452	2			

- Molecule 32 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 33 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	CO	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			
33	u	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			

- Molecule 34 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 35 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	V	107	Total	C	N	O	S	0	0	0
			855	539	156	159	1			
35	d0	72	Total	C	N	O	S	0	0	0
			585	367	109	108	1			

- Molecule 36 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			
36	M	138	Total	C	N	O	S	0	0	0
			1119	718	213	185	3			

- Molecule 37 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	n	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
37	CH	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			

- Molecule 38 is a protein called 60S ribosomal protein L34-A.

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

- Molecule 39 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	CP	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			
39	v	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			

- Molecule 40 is a protein called Large ribosomal subunit protein eL41B.

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

- Molecule 41 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 42 is a protein called 40S ribosomal protein S13.

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

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

- Molecule 43 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	o	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
43	CI	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			

- Molecule 44 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	CQ	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			
44	w	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			

- Molecule 45 is a protein called 60S ribosomal protein L42-A.

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

- Molecule 46 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 47 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	c4	128	Total	C	N	O	S	0	0	0
			949	582	188	176	3			
47	P	88	Total	C	N	O	S	0	0	0
			600	361	121	117	1			

- Molecule 48 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	CR	155	Total	C	N	O	0	0	0
			1227	764	238	225			
48	x	182	Total	C	N	O	0	0	0
			1415	879	280	256			

- Molecule 49 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 50 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 51 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	CS	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			
51	y	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			

- Molecule 52 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	p0	120	Total	C	N	O	S	0	0	0
			962	618	169	172	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p0	111	GLY	ARG	conflict	UNP P05317
p0	112	LEU	ALA	conflict	UNP P05317
p0	113	THR	GLY	conflict	UNP P05317

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Chain	Residue	Modelled	Actual	Comment	Reference
p0	114	VAL	ALA	conflict	UNP P05317
p0	116	GLN	ALA	conflict	UNP P05317
p0	117	VAL	PRO	conflict	UNP P05317
p0	118	TYR	GLU	conflict	UNP P05317
p0	?	-	VAL	deletion	UNP P05317
p0	126	GLY	THR	conflict	UNP P05317
p0	127	GLN	GLY	conflict	UNP P05317
p0	128	VAL	MET	conflict	UNP P05317
p0	129	PHE	GLU	conflict	UNP P05317

- Molecule 53 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 54 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	CT	180	Total	C	N	O	0	0	0
			1461	898	317	246			
54	z	183	Total	C	N	O	0	0	0
			1482	911	320	251			

- Molecule 55 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	sM	63	Total	C	N	O	0	0	0
			475	280	99	96			
55	i	140	Total	C	N	O	0	0	0
			1010	596	202	212			

- Molecule 56 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	a	64	Total	C	N	O	0	0	0
			514	328	95	91			
56	d5	69	Total	C	N	O	0	0	0
			558	357	103	98			

- Molecule 57 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	CU	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
57	0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

- Molecule 58 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	A	1722	Total	C	N	O	P	0	0	0
			36700	16407	6500	12071	1722			
58	sR	1783	Total	C	N	O	P	0	0	0
			37990	16984	6723	12500	1783			

- Molecule 59 is a protein called Small ribosomal subunit protein eS26B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	b	93	Total	C	N	O	S	0	0	0
			743	459	156	123	5			
59	d6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

- Molecule 60 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	CV	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			
60	2	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			

- Molecule 61 is a protein called 40S ribosomal protein S0-A.

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

- Molecule 62 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 63 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
63	CW	98	Total	C	N	O	S	0	0	0
			778	505	127	146				
63	5	100	Total	C	N	O	S	0	0	0
			796	516	131	149				

- Molecule 64 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	C	116	Total	C	N	O	S	0	0	0
			943	600	171	170	2			
64	s1	216	Total	C	N	O	S	0	0	0
			1722	1091	312	315	4			

- Molecule 65 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 66 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	CX	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
66	6	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

- Molecule 67 is a protein called 40S ribosomal protein S2.

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

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

- Molecule 68 is a protein called Small ribosomal subunit protein uS14A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	e	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			
68	d9	49	Total	C	N	O	S	0	0	0
			404	249	86	65	4			

- Molecule 69 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	CY	116	Total	C	N	O	S	0	0	0
			796	501	158	136	1			
69	7	63	Total	C	N	O	S	0	0	0
			521	336	102	82	1			

- Molecule 70 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 71 is a protein called 40S ribosomal protein S30-A.

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

- Molecule 72 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	CZ	117	Total	C	N	O	S	0	0	0
			937	602	164	169	2			
72	8	117	Total	C	N	O	S	0	0	0
			937	602	164	169	2			

- Molecule 73 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 74 is a protein called Ubiquitin.

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

- Molecule 75 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	AR	3136	Total	C	N	O	P	0	0	0
			67082	29963	12096	21887	3136			
75	1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			

- Molecule 76 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
76	DA	124	Total	C	N	O	0	0	0
			976	614	190	172			
76	9	126	Total	C	N	O	0	0	0
			993	625	192	176			

- Molecule 77 is a protein called 40S ribosomal protein S5.

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

- Molecule 78 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	h	310	Total	C	N	O	S	0	0	0
			2379	1504	409	458	8			

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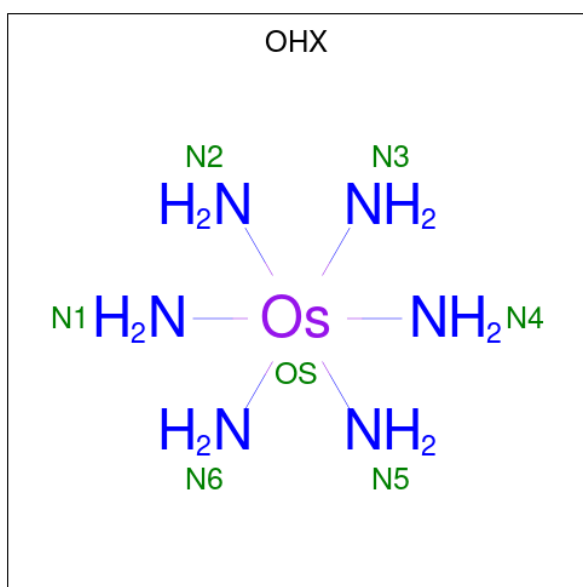
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	Rb	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 79 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 80 is osmium (III) hexammine (CCD ID: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	3	1	Total	N	Os	0	0
			7	6	1		
80	3	1	Total	N	Os	0	0
			7	6	1		
80	3	1	Total	N	Os	0	0
			7	6	1		
80	3	1	Total	N	Os	0	0
			7	6	1		
80	3	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	3	1	Total	N	Os	0	0
			7	6	1		
80	3	1	Total	N	Os	0	0
			7	6	1		
80	3	1	Total	N	Os	0	0
			7	6	1		
80	3	1	Total	N	Os	0	0
			7	6	1		
80	Q	1	Total	N	Os	0	0
			7	6	1		
80	4	1	Total	N	Os	0	0
			7	6	1		
80	4	1	Total	N	Os	0	0
			7	6	1		
80	4	1	Total	N	Os	0	0
			7	6	1		
80	4	1	Total	N	Os	0	0
			7	6	1		
80	4	1	Total	N	Os	0	0
			7	6	1		
80	4	1	Total	N	Os	0	0
			7	6	1		
80	4	1	Total	N	Os	0	0
			7	6	1		
80	4	1	Total	N	Os	0	0
			7	6	1		
80	4	1	Total	N	Os	0	0
			7	6	1		
80	4	1	Total	N	Os	0	0
			7	6	1		
80	4	1	Total	N	Os	0	0
			7	6	1		
80	4	1	Total	N	Os	0	0
			7	6	1		
80	4	1	Total	N	Os	0	0
			7	6	1		
80	AC	1	Total	N	Os	0	0
			7	6	1		
80	CK	1	Total	N	Os	0	0
			7	6	1		
80	CL	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	CL	1	Total	N	Os	0	0
			7	6	1		
80	DL	1	Total	N	Os	0	0
			7	6	1		
80	k	1	Total	N	Os	0	0
			7	6	1		
80	k	1	Total	N	Os	0	0
			7	6	1		
80	T	1	Total	N	Os	0	0
			7	6	1		
80	U	1	Total	N	Os	0	0
			7	6	1		
80	AG	1	Total	N	Os	0	0
			7	6	1		
80	CP	1	Total	N	Os	0	0
			7	6	1		
80	c3	1	Total	N	Os	0	0
			7	6	1		
80	c5	1	Total	N	Os	0	0
			7	6	1		
80	AK	1	Total	N	Os	0	0
			7	6	1		
80	AK	1	Total	N	Os	0	0
			7	6	1		
80	CS	1	Total	N	Os	0	0
			7	6	1		
80	r	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			6	5	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			6	5	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
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80	A	1	Total	N	Os	0	0
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80	A	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	A	1	Total	N	Os	0	0
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80	A	1	Total	N	Os	0	0
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80	A	1	Total	N	Os	0	0
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80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		
80	A	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	A	1	Total	N	Os	0	0
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80	A	1	Total	N	Os	0	0
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			7	6	1		
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80	A	1	Total	N	Os	0	0
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80	c8	1	Total	N	Os	0	0
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80	CV	1	Total	N	Os	0	0
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80	C	1	Total	N	Os	0	0
			7	6	1		
80	w	1	Total	N	Os	0	0
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80	CX	1	Total	N	Os	0	0
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80	x	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	1
			14	12	2		
80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
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			7	6	1		
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
80	AR	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	AR	1	Total	N	Os	0	0
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80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		
80	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	h	1	Total	N	Os	0	0
			7	6	1		
80	d4	1	Total	N	Os	0	0
			7	6	1		
80	AS	1	Total	N	Os	0	0
			7	6	1		
80	AS	1	Total	N	Os	0	0
			7	6	1		
80	AS	1	Total	N	Os	0	0
			7	6	1		
80	AS	1	Total	N	Os	0	0
			7	6	1		
80	AS	1	Total	N	Os	0	0
			7	6	1		
80	AS	1	Total	N	Os	0	0
			7	6	1		
80	AS	1	Total	N	Os	0	0
			7	6	1		
80	AS	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	sR	1	Total	N	Os	0	0
			7	6	1		
80	2	1	Total	N	Os	0	0
			7	6	1		
80	AT	1	Total	N	Os	0	0
			7	6	1		
80	AT	1	Total	N	Os	0	0
			7	6	1		
80	AT	1	Total	N	Os	0	0
			7	6	1		
80	AT	1	Total	N	Os	0	1
			14	12	2		
80	AT	1	Total	N	Os	0	0
			7	6	1		
80	AT	1	Total	N	Os	0	0
			7	6	1		
80	AT	1	Total	N	Os	0	0
			7	6	1		
80	AT	1	Total	N	Os	0	0
			7	6	1		
80	AT	1	Total	N	Os	0	0
			7	6	1		
80	AT	1	Total	N	Os	0	0
			7	6	1		
80	AT	1	Total	N	Os	0	0
			7	6	1		
80	AT	1	Total	N	Os	0	0
			7	6	1		
80	AT	1	Total	N	Os	0	0
			7	6	1		
80	Rb	1	Total	N	Os	0	0
			7	6	1		
80	DD	1	Total	N	Os	0	0
			7	6	1		
80	J	1	Total	N	Os	0	0
			7	6	1		
80	CE	1	Total	N	Os	0	0
			7	6	1		
80	CE	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	s1	1	Total	N	Os	0	0
			7	6	1		
80	CG	1	Total	N	Os	0	0
			7	6	1		
80	CG	1	Total	N	Os	0	0
			7	6	1		
80	DH	1	Total	N	Os	0	0
			7	6	1		
80	O	1	Total	N	Os	0	0
			7	6	1		
80	s4	1	Total	N	Os	0	0
			7	6	1		
80	v	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
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			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
80	1	1	Total	N	Os	0	0
			6	5	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
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80	1	1	Total	N	Os	0	0
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80	1	1	Total	N	Os	0	0
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80	1	1	Total	N	Os	0	0
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80	1	1	Total	N	Os	0	0
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80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
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80	1	1	Total	N	Os	0	0
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80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		

- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	3	12	Total	Mg	0	0
			12	12		
81	AB	7	Total	Mg	0	0
			7	7		
81	CJ	1	Total	Mg	0	0
			1	1		
81	4	20	Total	Mg	0	0
			20	20		
81	CK	2	Total	Mg	0	0
			2	2		
81	j	2	Total	Mg	0	0
			2	2		
81	CL	1	Total	Mg	0	0
			1	1		
81	DL	2	Total	Mg	0	0
			2	2		
81	s8	2	Total	Mg	0	0
			2	2		
81	k	2	Total	Mg	0	0
			2	2		
81	CM	2	Total	Mg	0	0
			2	2		
81	s9	1	Total	Mg	0	0
			1	1		
81	l	4	Total	Mg	0	0
			4	4		
81	AF	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	U	1	Total 1	Mg 1	0	0
81	m	1	Total 1	Mg 1	0	0
81	CO	1	Total 1	Mg 1	0	0
81	DO	1	Total 1	Mg 1	0	0
81	AH	1	Total 1	Mg 1	0	0
81	CP	4	Total 4	Mg 4	0	0
81	DP	1	Total 1	Mg 1	0	0
81	o	2	Total 2	Mg 2	0	0
81	CQ	3	Total 3	Mg 3	0	0
81	DQ	2	Total 2	Mg 2	0	0
81	c4	1	Total 1	Mg 1	0	0
81	CR	6	Total 6	Mg 6	0	0
81	Y	1	Total 1	Mg 1	0	0
81	AK	2	Total 2	Mg 2	0	0
81	CS	1	Total 1	Mg 1	0	0
81	c6	2	Total 2	Mg 2	0	0
81	r	3	Total 3	Mg 3	0	0
81	sM	2	Total 2	Mg 2	0	0
81	c7	1	Total 1	Mg 1	0	0
81	s	1	Total 1	Mg 1	0	0
81	CU	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	A	134	Total 134	Mg 134	0	0
81	c8	1	Total 1	Mg 1	0	0
81	t	2	Total 2	Mg 2	0	0
81	c9	1	Total 1	Mg 1	0	0
81	AO	1	Total 1	Mg 1	0	0
81	w	1	Total 1	Mg 1	0	0
81	CX	1	Total 1	Mg 1	0	0
81	D	1	Total 1	Mg 1	0	0
81	e	1	Total 1	Mg 1	0	0
81	x	8	Total 8	Mg 8	0	0
81	d2	1	Total 1	Mg 1	0	0
81	d3	3	Total 3	Mg 3	0	0
81	z	1	Total 1	Mg 1	0	0
81	AR	506	Total 506	Mg 506	0	0
81	DA	2	Total 2	Mg 2	0	0
81	d4	1	Total 1	Mg 1	0	0
81	AS	22	Total 22	Mg 22	0	0
81	sR	160	Total 160	Mg 160	0	0
81	d5	1	Total 1	Mg 1	0	0
81	AT	18	Total 18	Mg 18	0	0
81	DC	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	d6	2	Total 2	Mg 2	0	0
81	CD	3	Total 3	Mg 3	0	0
81	DD	1	Total 1	Mg 1	0	0
81	6	3	Total 3	Mg 3	0	0
81	CE	4	Total 4	Mg 4	0	0
81	s1	1	Total 1	Mg 1	0	0
81	CF	2	Total 2	Mg 2	0	0
81	s2	1	Total 1	Mg 1	0	0
81	CG	3	Total 3	Mg 3	0	0
81	DG	1	Total 1	Mg 1	0	0
81	9	1	Total 1	Mg 1	0	0
81	DH	2	Total 2	Mg 2	0	0
81	s4	2	Total 2	Mg 2	0	0
81	v	4	Total 4	Mg 4	0	0
81	CI	2	Total 2	Mg 2	0	0
81	DI	1	Total 1	Mg 1	0	0
81	1	487	Total 487	Mg 487	0	0

- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
82	DL	1	Total 1	Zn 1	0	0
82	DO	1	Total 1	Zn 1	0	0

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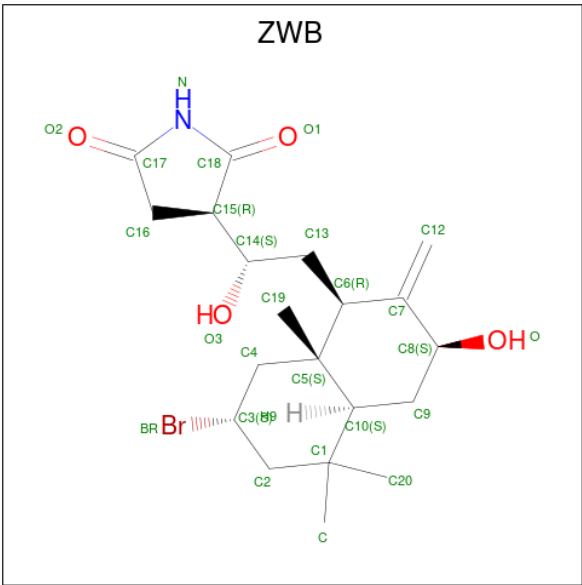
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
82	DQ	1	Total	Zn	0	0
			1	1		
82	DR	1	Total	Zn	0	0
			1	1		
82	AK	1	Total	Zn	0	0
			1	1		
82	b	1	Total	Zn	0	0
			1	1		
82	AN	1	Total	Zn	0	0
			1	1		
82	c	1	Total	Zn	0	0
			1	1		
82	AP	1	Total	Zn	0	0
			1	1		
82	e	1	Total	Zn	0	0
			1	1		
82	AQ	1	Total	Zn	0	0
			1	1		
82	g	1	Total	Zn	0	0
			1	1		
82	d6	1	Total	Zn	0	0
			1	1		
82	d7	1	Total	Zn	0	0
			1	1		
82	d9	1	Total	Zn	0	0
			1	1		

- Molecule 83 is POTASSIUM ION (CCD ID: K) (formula: K).

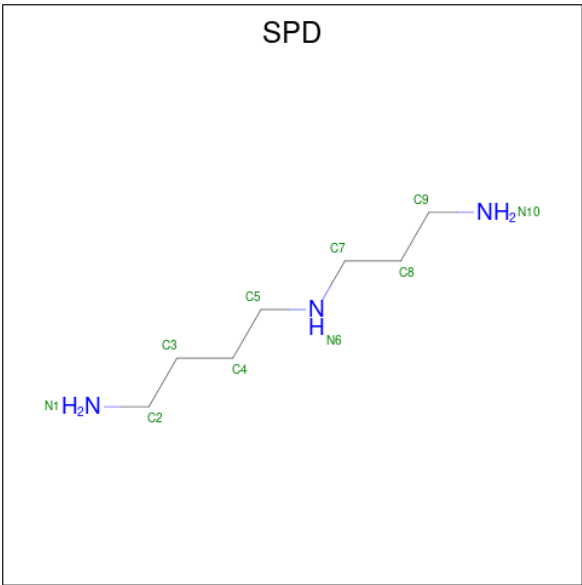
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	AR	3	Total	K	0	0
			3	3		
83	1	1	Total	K	0	0
			1	1		

- Molecule 84 is (3 {R})-3-[(1 {S})-2-[(1 {R},3 {S},4 {a} {S},7 {S},8 {a} {S})-7-bromanyl-5,5,8 {a}-trimethyl-2-methylidene-3-oxidanyl-3,4,4 {a},6,7,8-hexahydro-1 {H}-naphthalen-1-yl]-1-oxidanyl-ethyl]pyrrolidine-2,5-dione (CCD ID: ZWB) (formula: C₂₀H₃₀BrNO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
84	AR	1	Total	Br	C	N	O	0	0
			26	1	20	1	4		
84	1	1	Total	Br	C	N	O	0	0
			26	1	20	1	4		

- Molecule 85 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	AR	1	Total	C	N	0	0
			10	7	3		
85	AR	1	Total	C	N	0	0
			10	7	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	AR	1	Total	C	N	0	0
			10	7	3		
85	1	1	Total	C	N	0	0
			10	7	3		

- Molecule 86 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	3	3	Total	O	0	0
			3	3		
86	CK	3	Total	O	0	0
			3	3		
86	R	1	Total	O	0	0
			1	1		
86	s8	1	Total	O	0	0
			1	1		
86	k	1	Total	O	0	0
			1	1		
86	AE	1	Total	O	0	0
			1	1		
86	CM	1	Total	O	0	0
			1	1		
86	s9	2	Total	O	0	0
			2	2		
86	DN	2	Total	O	0	0
			2	2		
86	CP	3	Total	O	0	0
			3	3		
86	CQ	2	Total	O	0	0
			2	2		
86	CR	3	Total	O	0	0
			3	3		
86	DR	1	Total	O	0	0
			1	1		
86	AK	3	Total	O	0	0
			3	3		
86	A	46	Total	O	0	0
			46	46		
86	AR	131	Total	O	0	0
			131	131		
86	sR	61	Total	O	0	0
			61	61		

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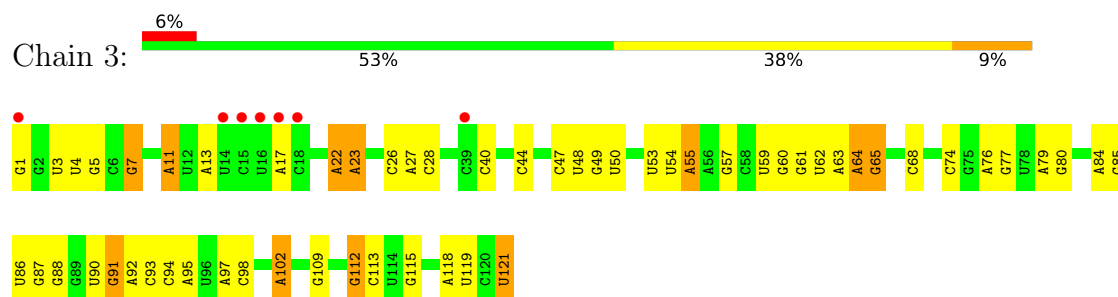
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	AT	8	Total 8	O 8	0	0
86	J	1	Total 1	O 1	0	0
86	v	1	Total 1	O 1	0	0
86	1	137	Total 137	O 137	0	0

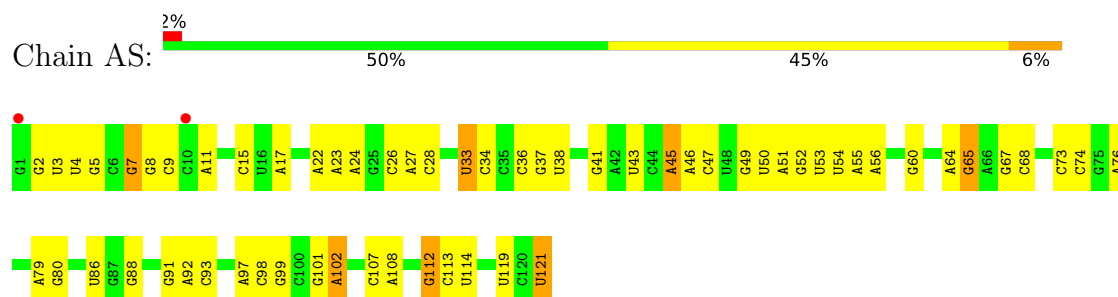
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

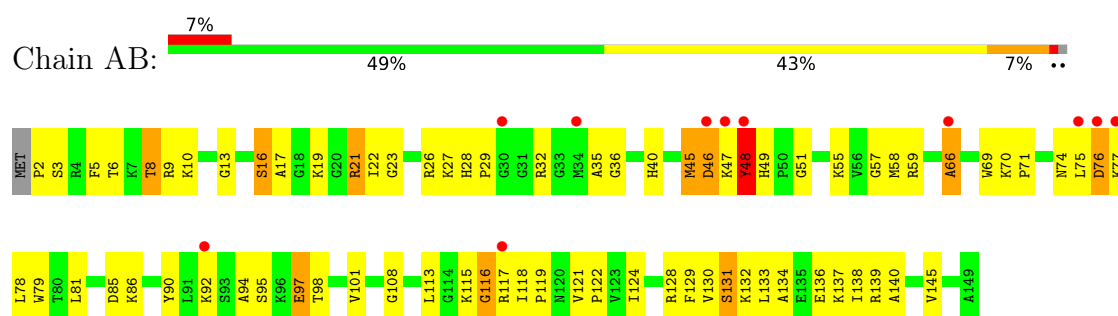
• Molecule 1: 5S ribosomal RNA



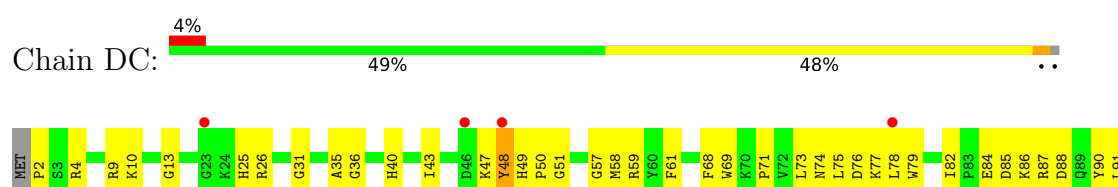
• Molecule 1: 5S ribosomal RNA



• Molecule 2: 60S ribosomal protein L28

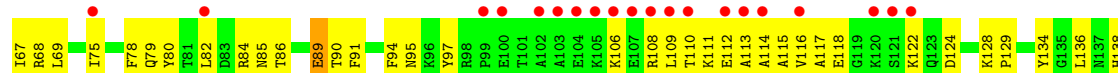
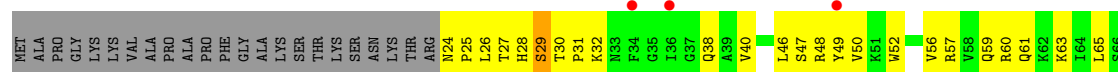


• Molecule 2: 60S ribosomal protein L28

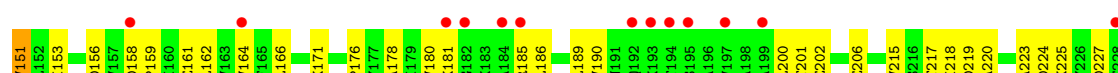




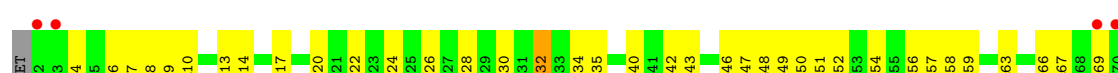
• Molecule 3: 60S ribosomal protein L8-A



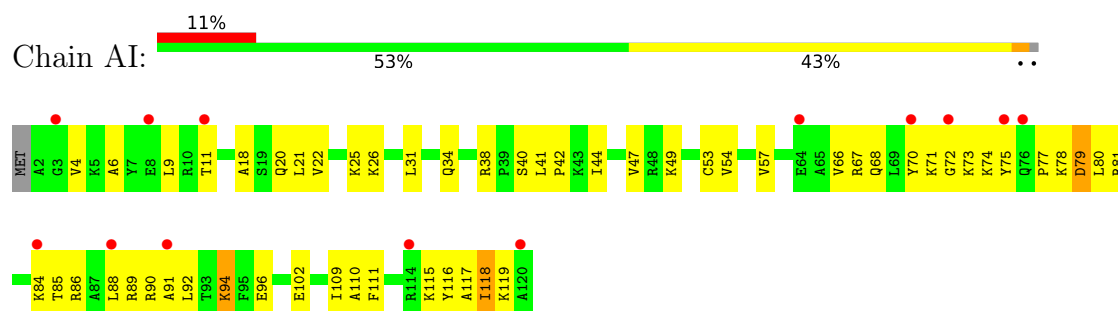
• Molecule 3: 60S ribosomal protein L8-A



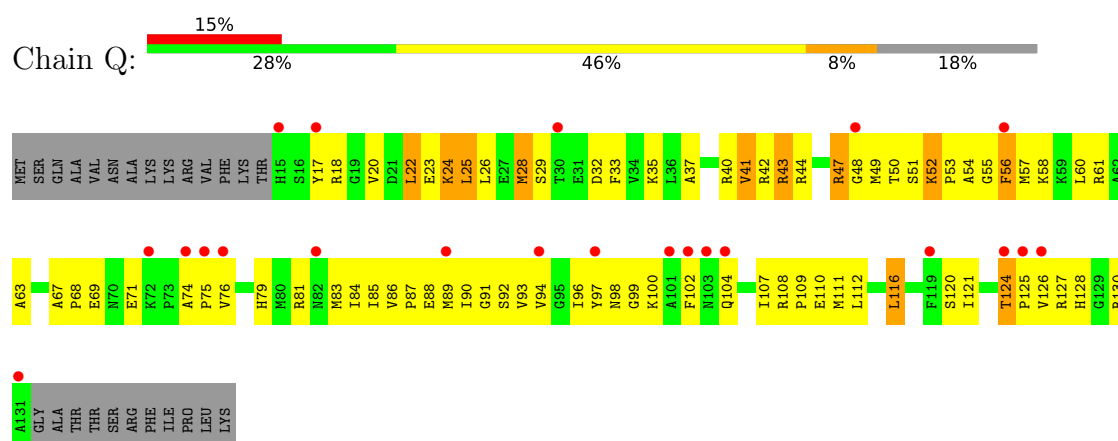
• Molecule 4: 60S ribosomal protein L35-A



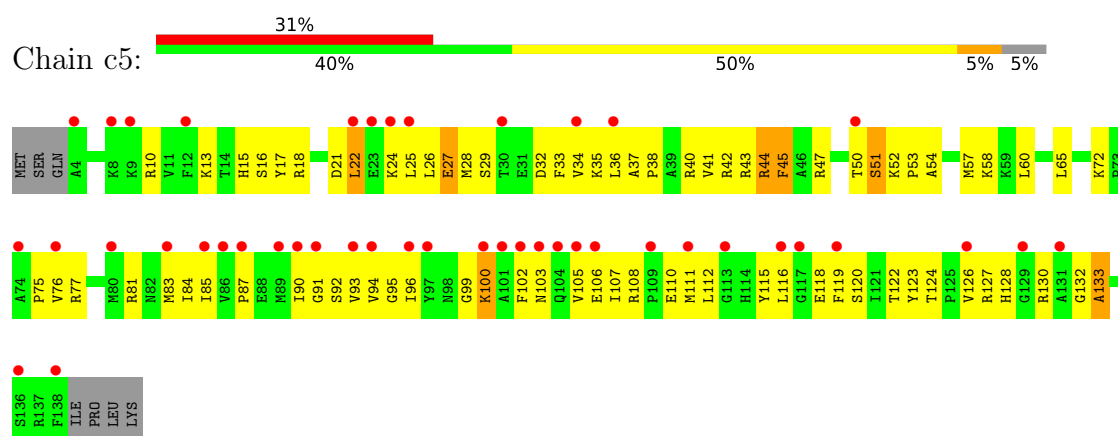
- Molecule 4: 60S ribosomal protein L35-A



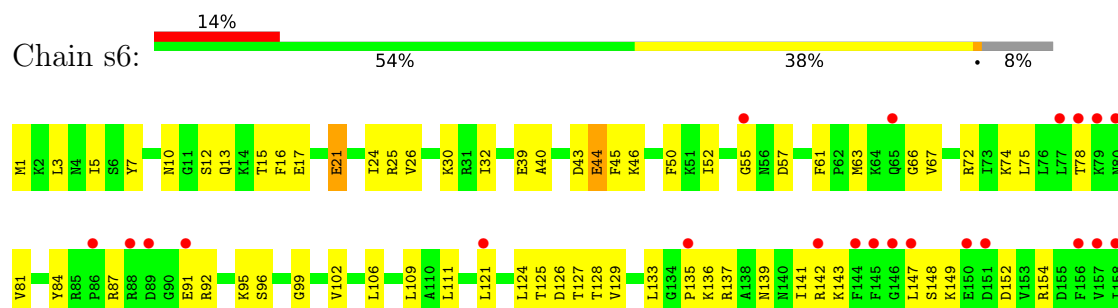
- Molecule 5: 40S ribosomal protein S15

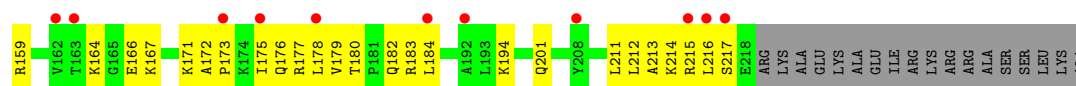


- Molecule 5: 40S ribosomal protein S15

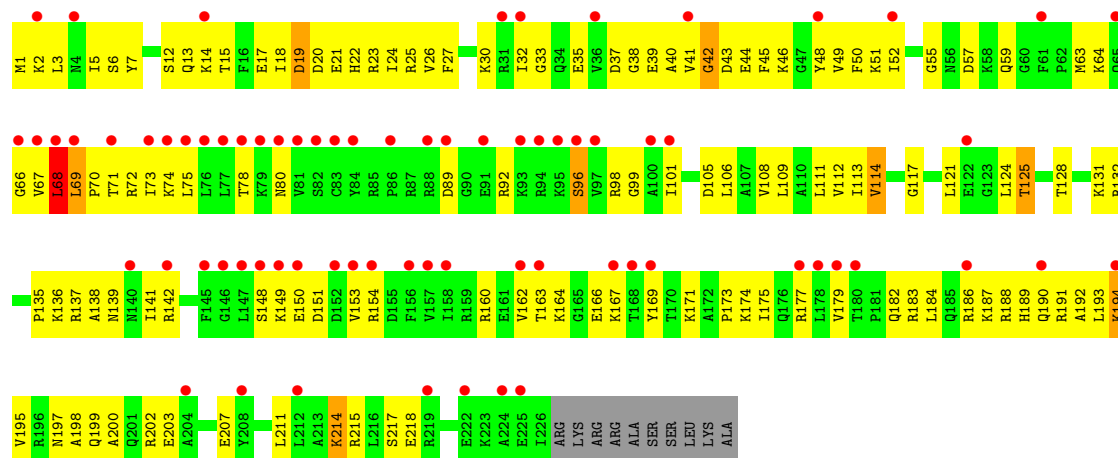
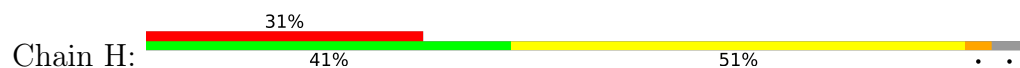


- Molecule 6: 40S ribosomal protein S6-A

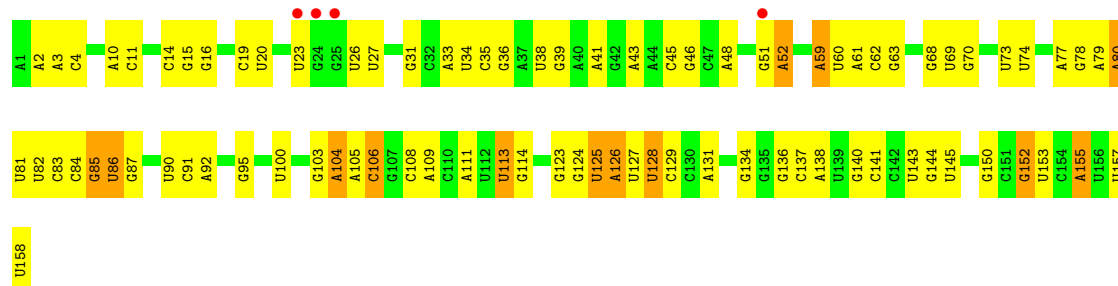




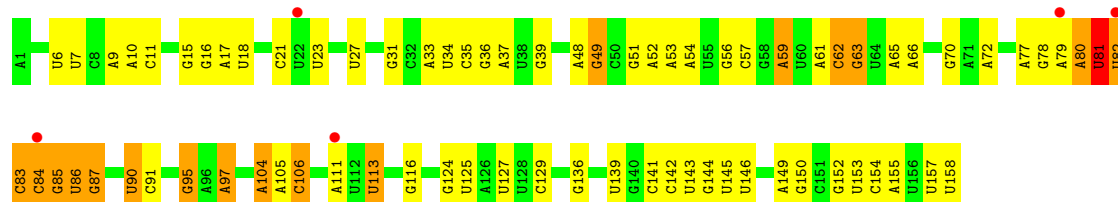
• Molecule 6: 40S ribosomal protein S6-A



• Molecule 7: 5.8S ribosomal RNA

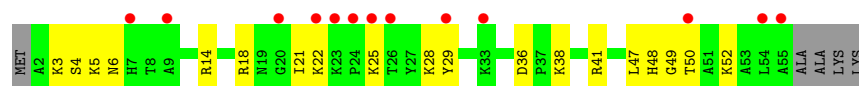


• Molecule 7: 5.8S ribosomal RNA

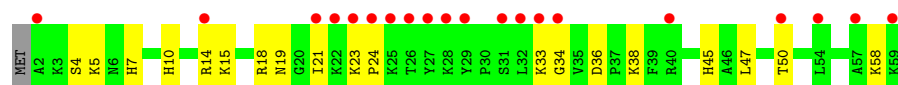


• Molecule 8: 60S ribosomal protein L29

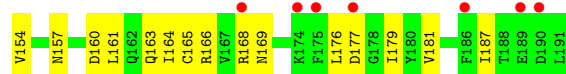
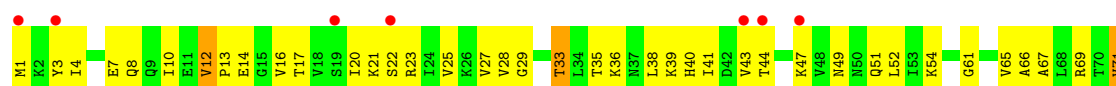




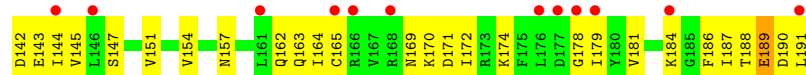
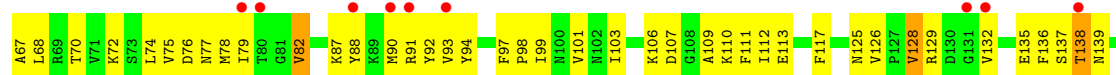
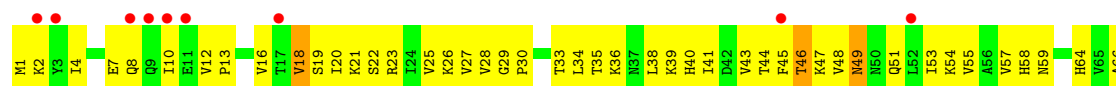
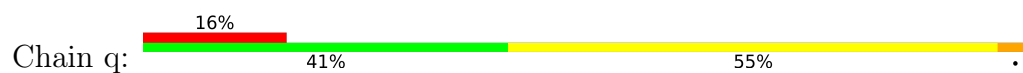
- Molecule 8: 60S ribosomal protein L29



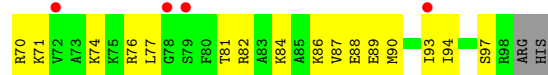
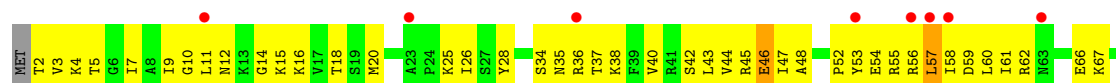
- Molecule 9: 60S ribosomal protein L9-A



- Molecule 9: 60S ribosomal protein L9-A



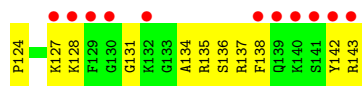
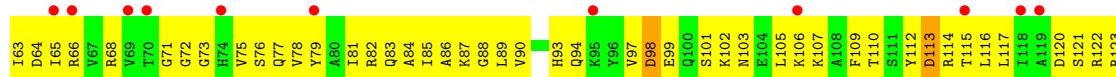
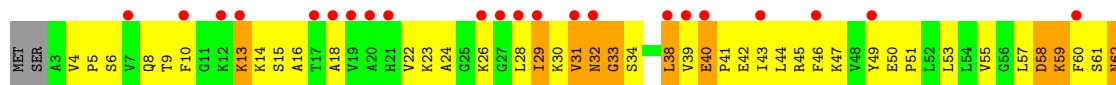
- Molecule 10: 60S ribosomal protein L36-A



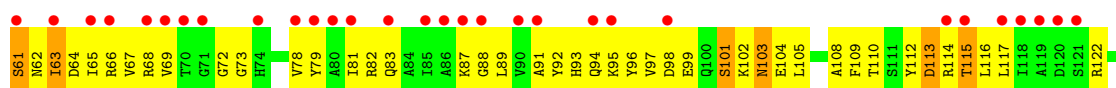
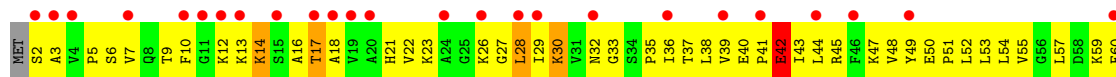
- Molecule 10: 60S ribosomal protein L36-A



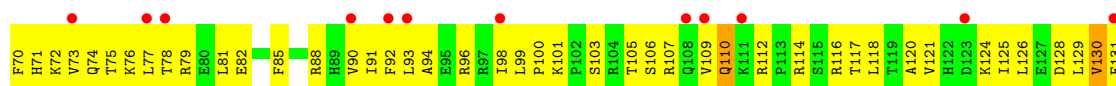
- Molecule 11: 40S ribosomal protein S16-A



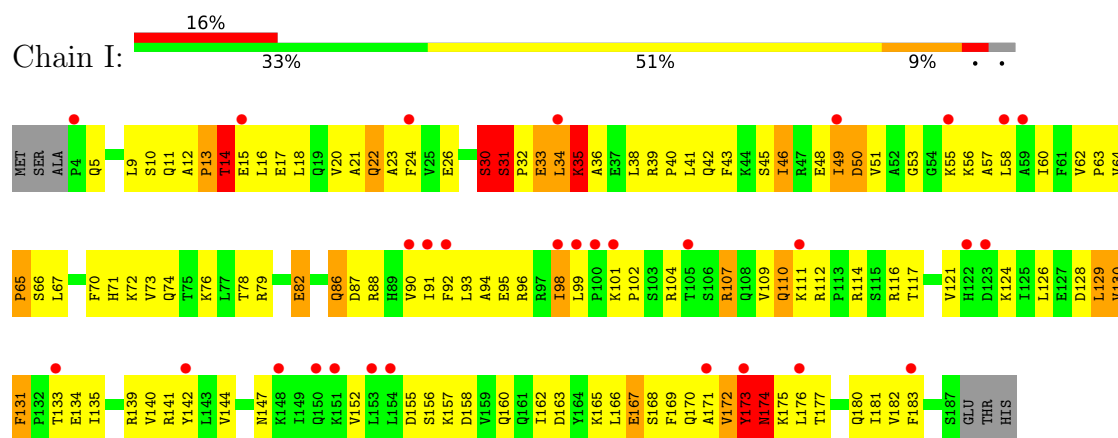
- Molecule 11: 40S ribosomal protein S16-A



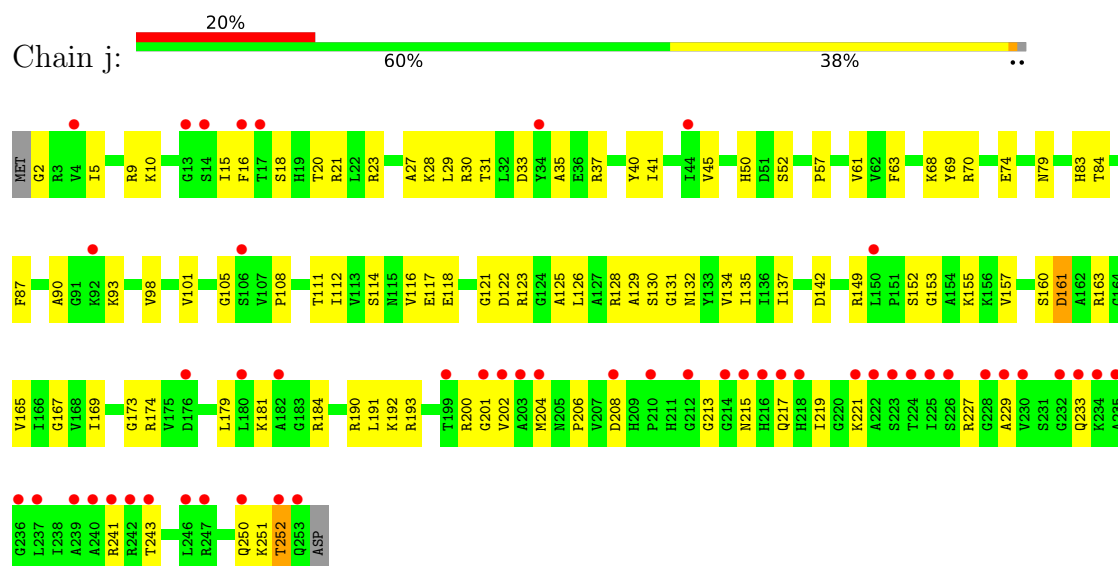
- Molecule 12: 40S ribosomal protein S7-A



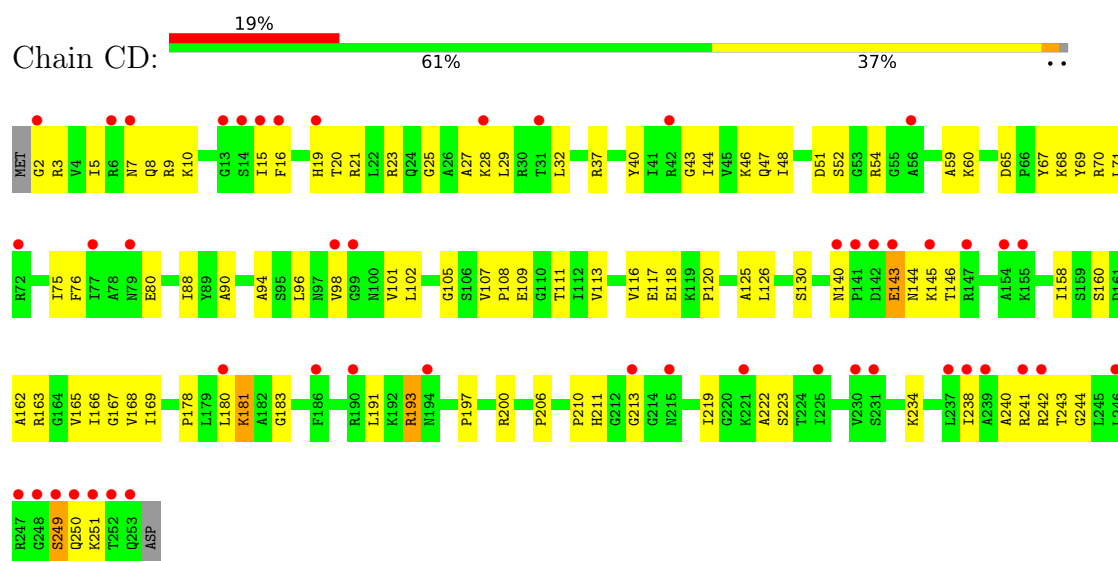
• Molecule 12: 40S ribosomal protein S7-A



• Molecule 13: 60S ribosomal protein L2-A

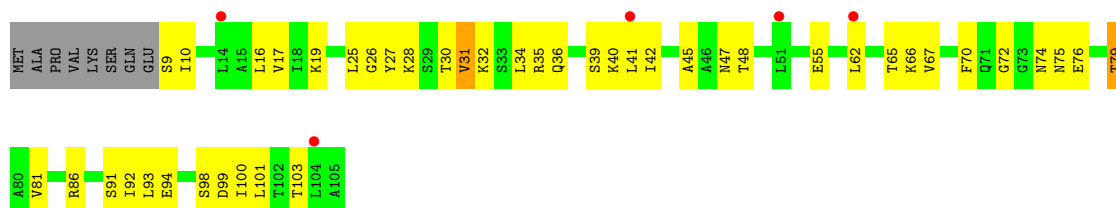


• Molecule 13: 60S ribosomal protein L2-A



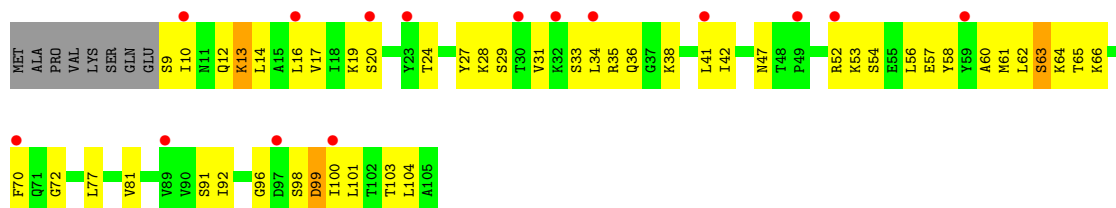
- Molecule 14: 60S ribosomal protein L30

Chain AD: 



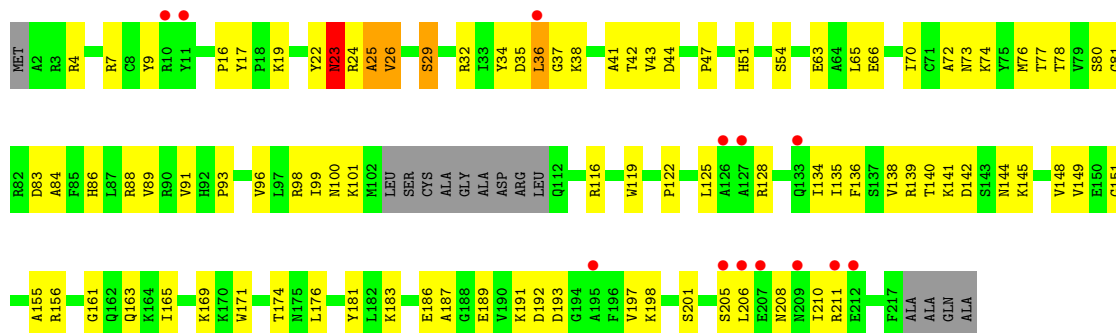
- Molecule 14: 60S ribosomal protein L30

Chain DE: 



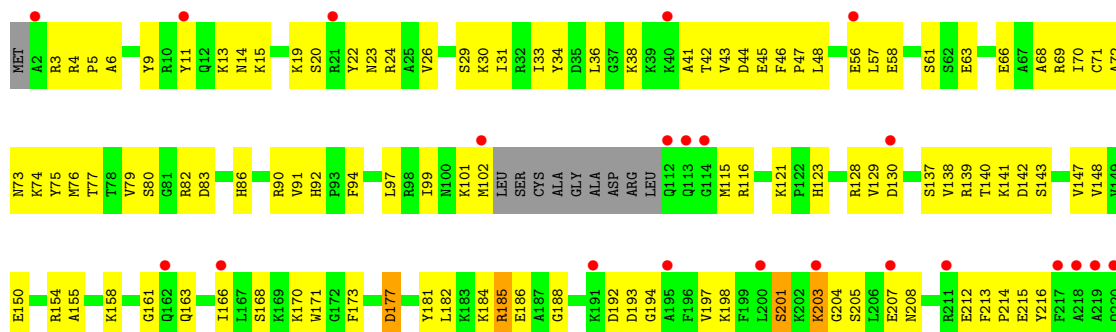
- Molecule 15: 60S ribosomal protein L10

Chain CL: 



- Molecule 15: 60S ribosomal protein L10

Chain r: 





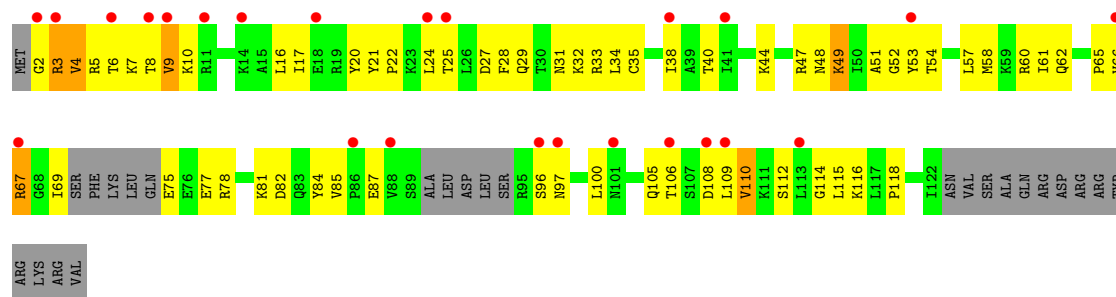
- Molecule 16: 60S ribosomal protein L37-A



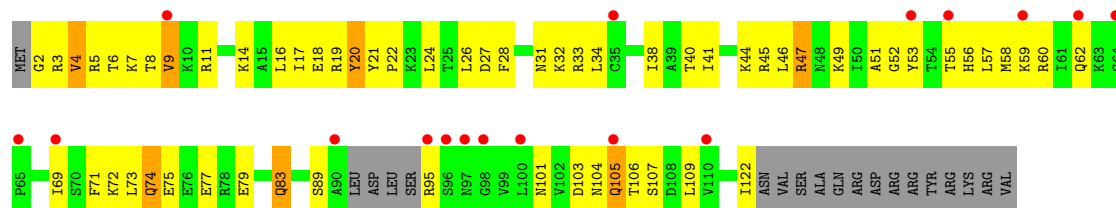
- Molecule 16: 60S ribosomal protein L37-A



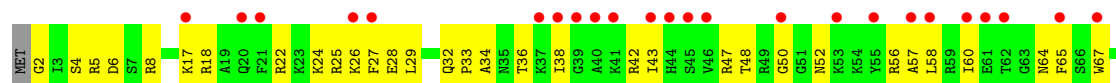
- Molecule 17: 40S ribosomal protein S17-A

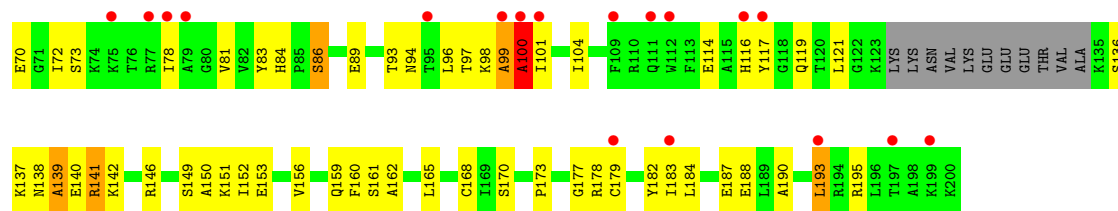


- Molecule 17: 40S ribosomal protein S17-A

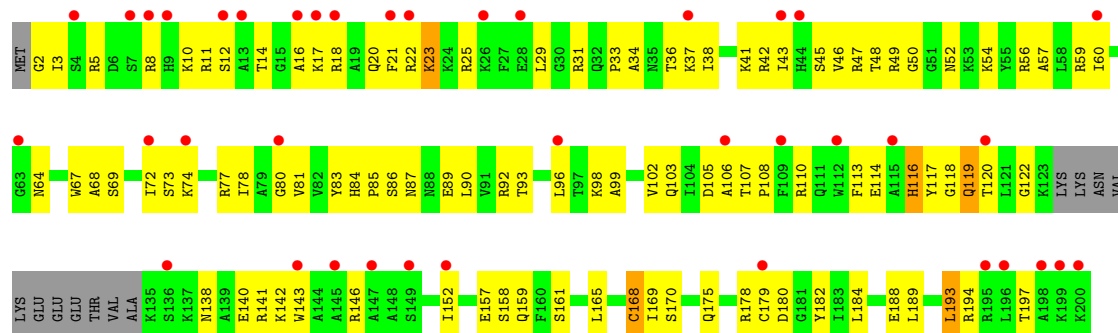
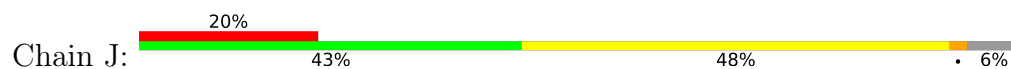


- Molecule 18: 40S ribosomal protein S8-A

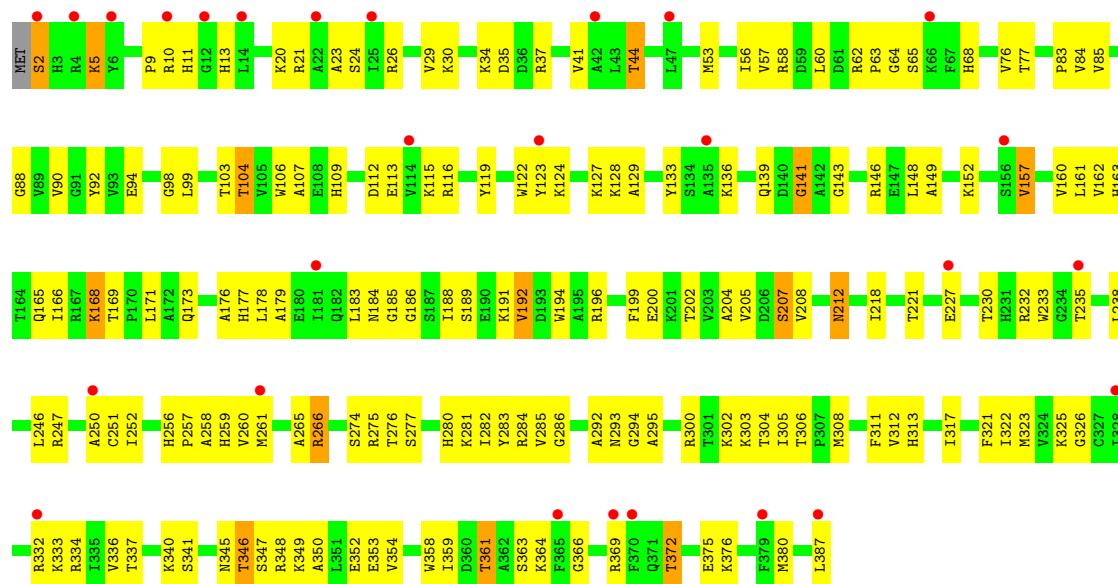




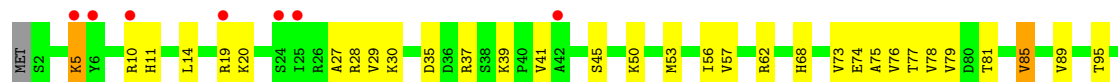
• Molecule 18: 40S ribosomal protein S8-A

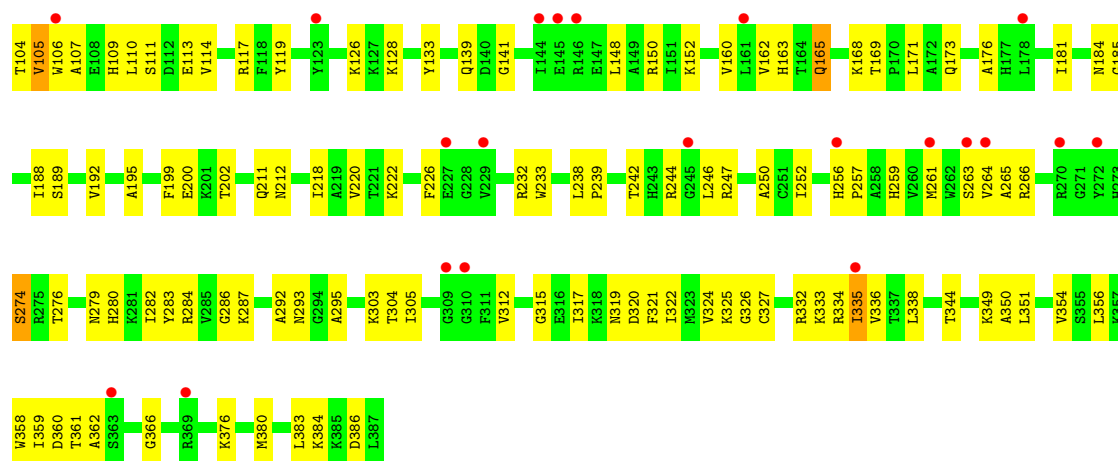


• Molecule 19: 60S ribosomal protein L3

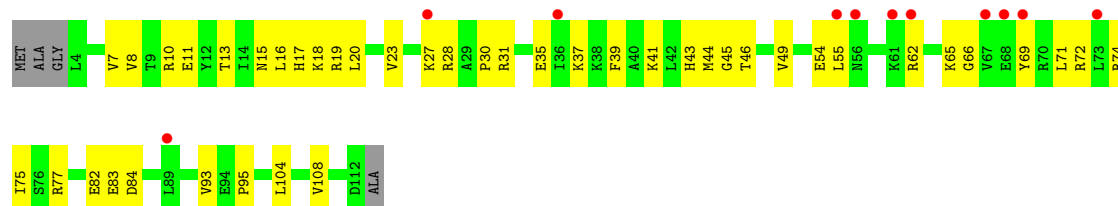


• Molecule 19: 60S ribosomal protein L3

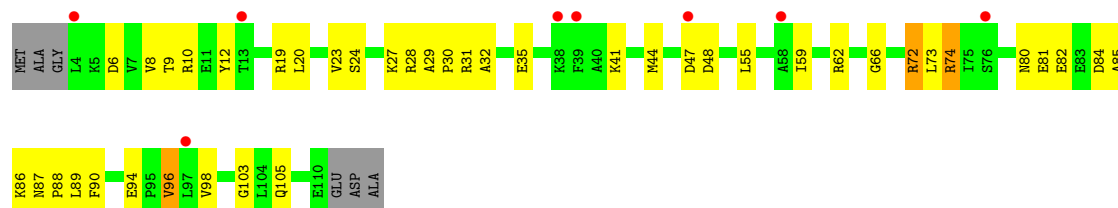




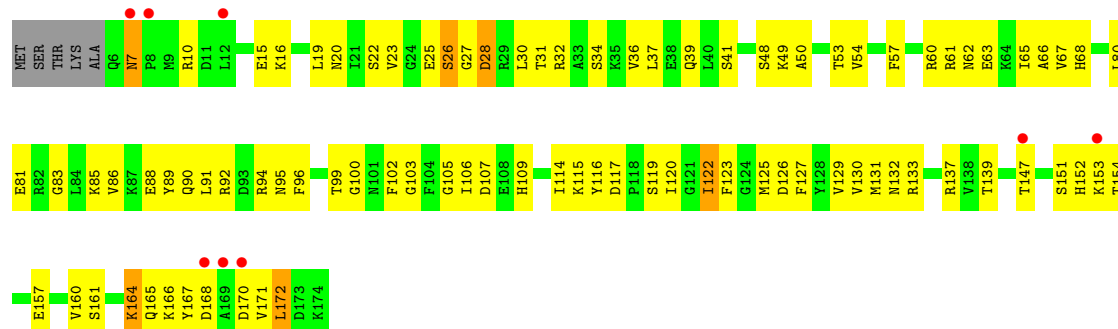
• Molecule 20: 60S ribosomal protein L31-A



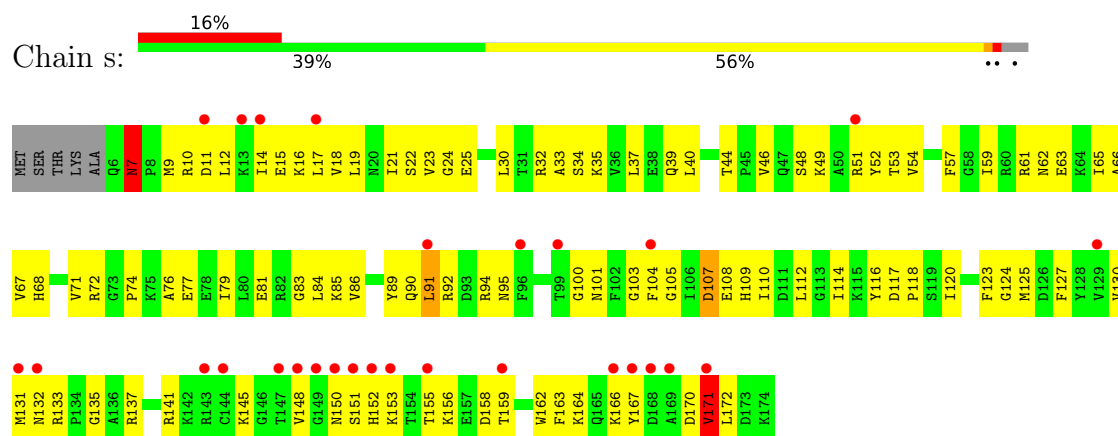
• Molecule 20: 60S ribosomal protein L31-A



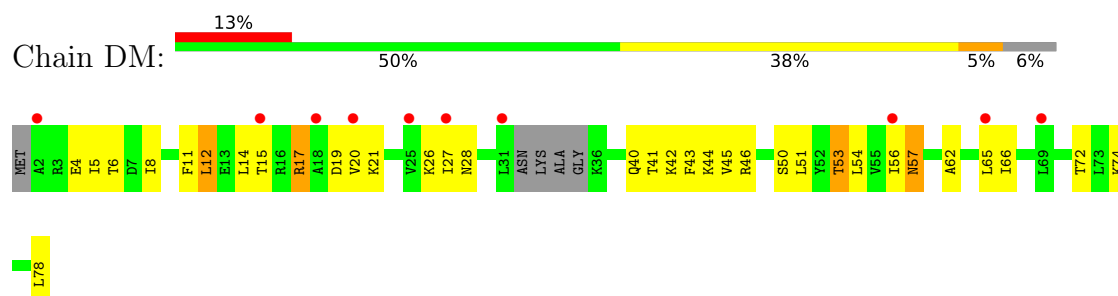
• Molecule 21: Large ribosomal subunit protein uL5B



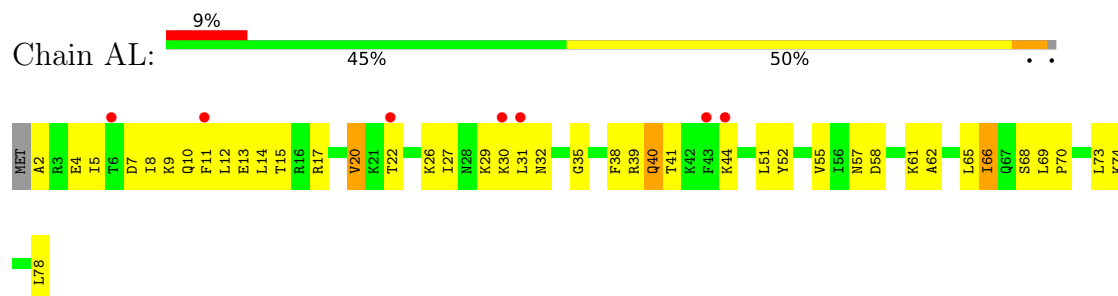
- Molecule 21: Large ribosomal subunit protein uL5B



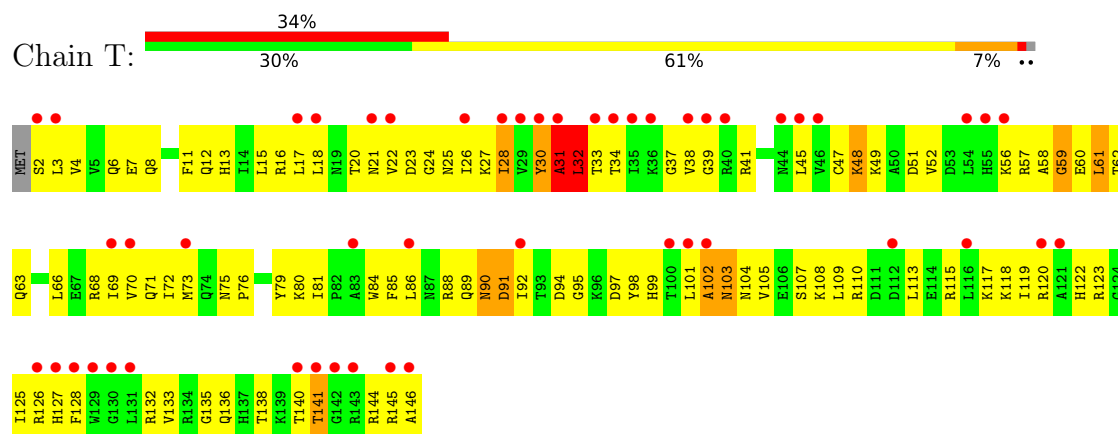
- Molecule 22: 60S ribosomal protein L38



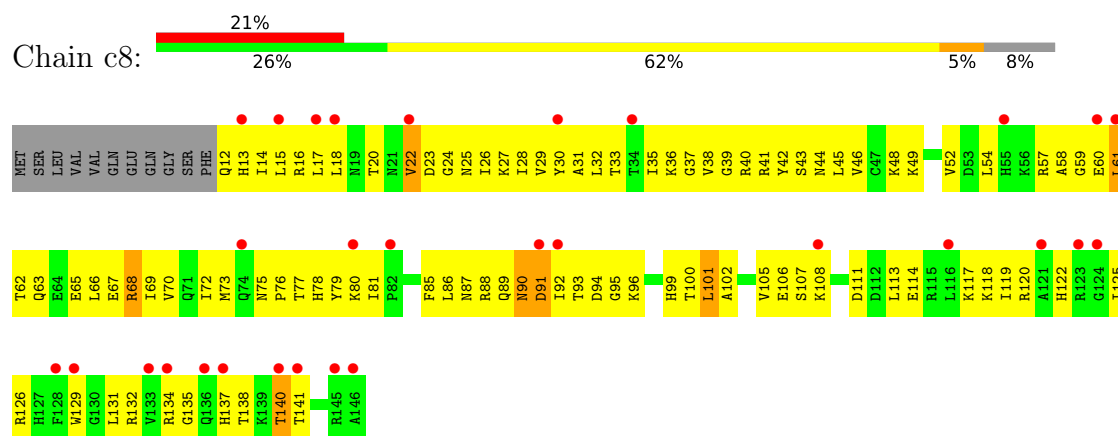
- Molecule 22: 60S ribosomal protein L38



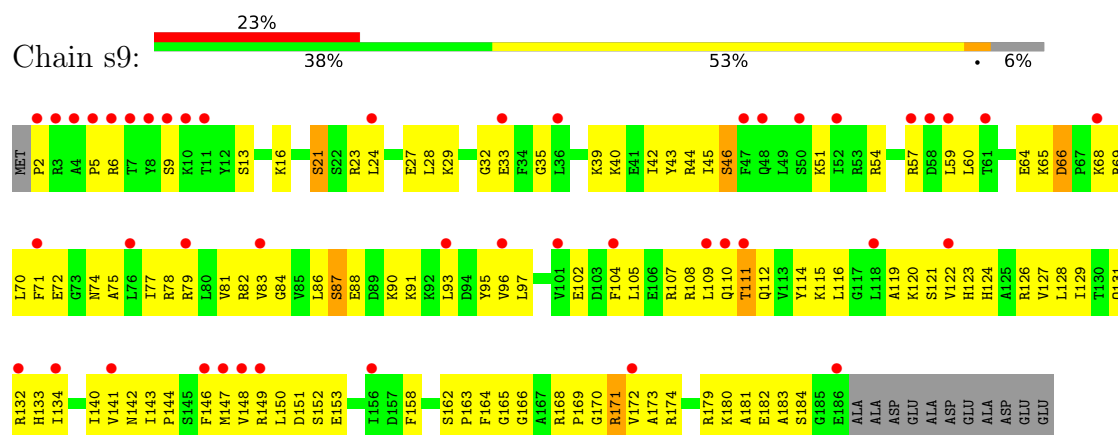
- Molecule 23: 40S ribosomal protein S18-A



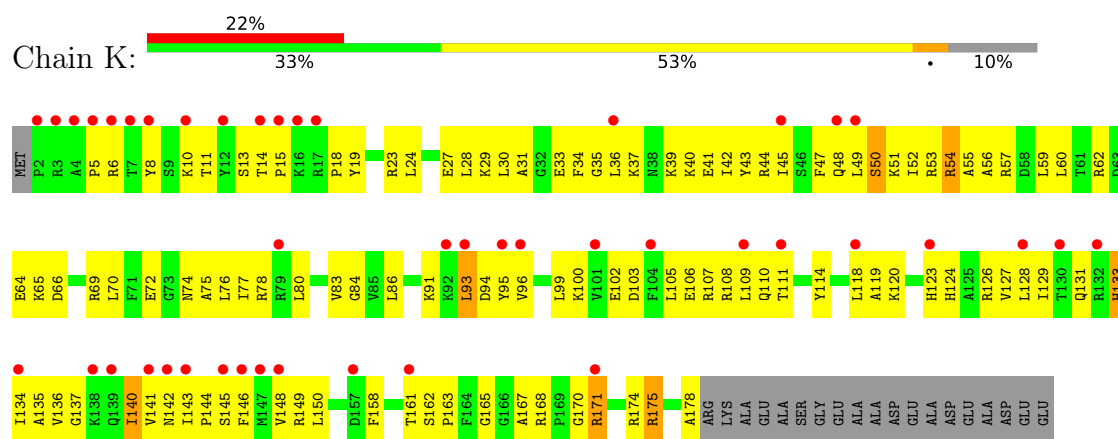
- Molecule 23: 40S ribosomal protein S18-A



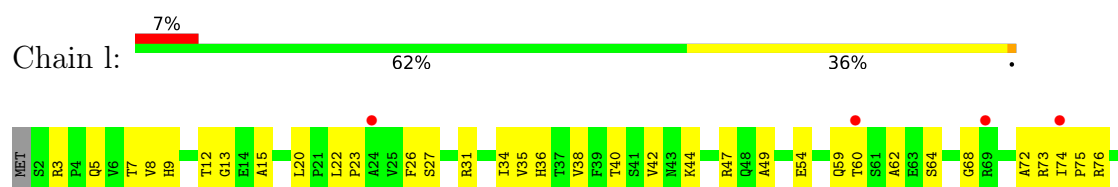
- Molecule 24: 40S ribosomal protein S9-A

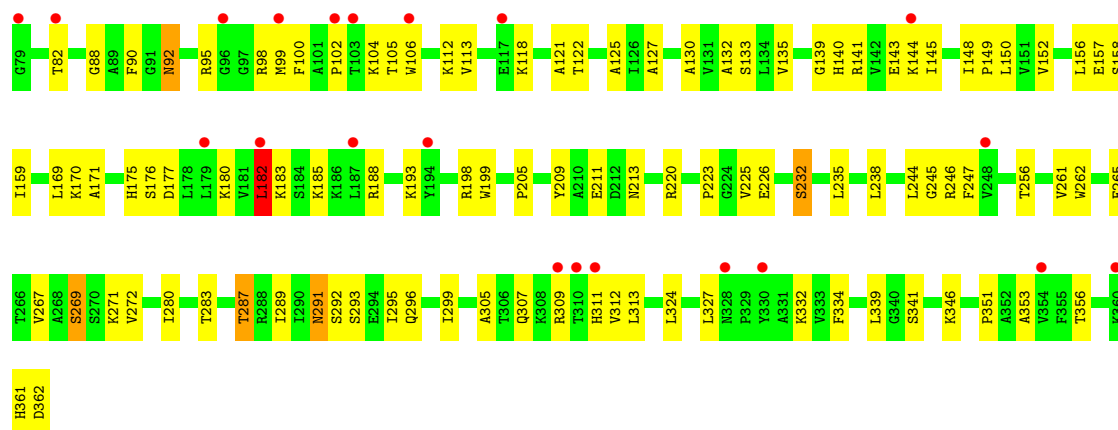


- Molecule 24: 40S ribosomal protein S9-A

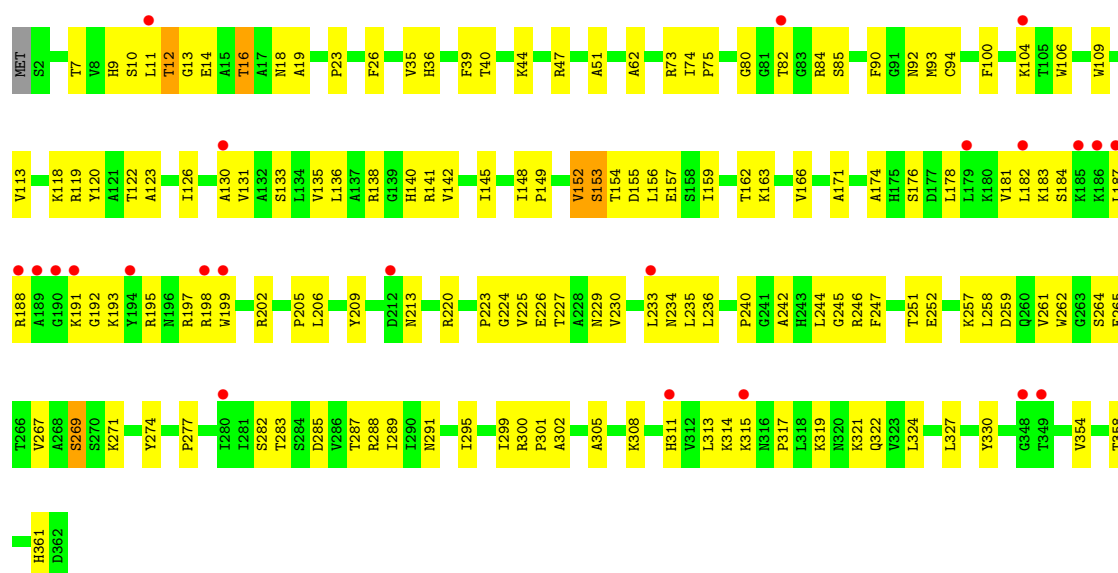


- Molecule 25: 60S ribosomal protein L4-A

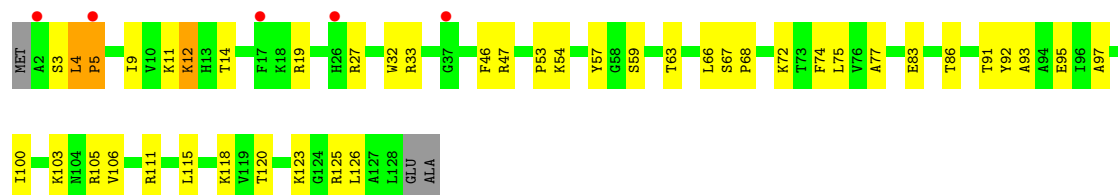




• Molecule 25: 60S ribosomal protein L4-A

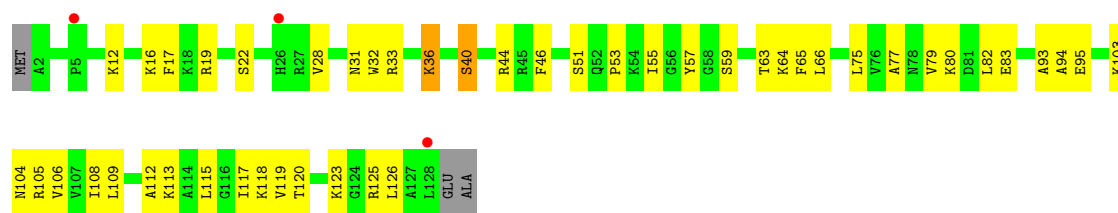


• Molecule 26: 60S ribosomal protein L32

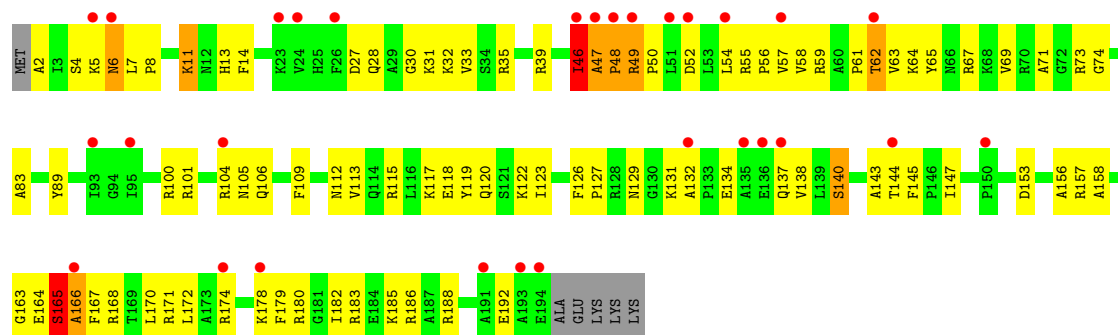


• Molecule 26: 60S ribosomal protein L32

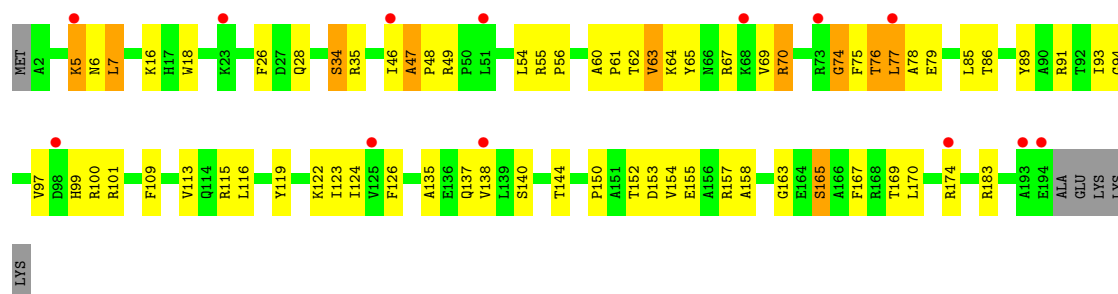




• Molecule 27: 60S ribosomal protein L13-A



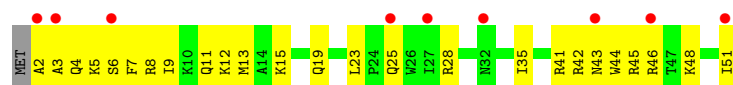
• Molecule 27: 60S ribosomal protein L13-A



• Molecule 28: 60S ribosomal protein L39



• Molecule 28: 60S ribosomal protein L39



Chain U:

36% 35% 51% 12% ...

Met

P2 G3 V4 V5 V6 V7 D8 V9 A10 A11 Q12 D13 F14 I15

Y18 L22 L28 E29 V30 P31 G32 Y33 V34 D35 I36 V37 K38 T39 S40 G42

P46 Q47 Q48 D49 A50 E51 G52 W53 F54 Y55 K56 R57 A58 S59 S60 V61 A62 R63 H64 I65 Y66 M67 R68 K69

Q70 V71 W72 V73 G74 K75 L76 N77 K78 L79 Y80 G81 G82 A83 K84

V88 R89 P90 Y91 X92 I93 I94 D95 A96 S97 G98 S99 T100 N101 I102 K103 V104 L105 Q106 A107 I108 E109 K110

T113 V114 E115 I116 S117 P118 K119

R122 I123 I124 S125 E126 N127 G128 R129 I130 D131 L132 D133

R134 I135 A136 A137 Q138 T139 L140 E141 E144

Chain c9:

14% 43% 54%

Met

M67 M68 M69 M70 M71 M72 M73 M74 M75 M76 M77 M80 M83 M84 M85 M86 M87 M88 M89 M92 M93 M94 M95 M96 M97 M98 M99 M100 M101 M102 M103 M104 M105 M108 M109 M110 M111 M112 M113 M114 M115 M116 M117 M118 M119 M122 M123 M124 M125 M128 M129 M130 M131 M132

P2 P3 P4 P5 P6 P7 P8 P9 P10 P11 P12 P13 P14 P15 P18 P21 P22 P25 P26 P27 P28 P29 P30 P31 P32 P33 P34 P35 P36 P37 P41 P42 P43 P44 P45 P46 P47 P48 P49 P50 P51 P52 P53 P54 P55 P56 P60 P61 P62 P63 P64 P65 P66

I135 A136 A137 Q138 E142 D143 E144

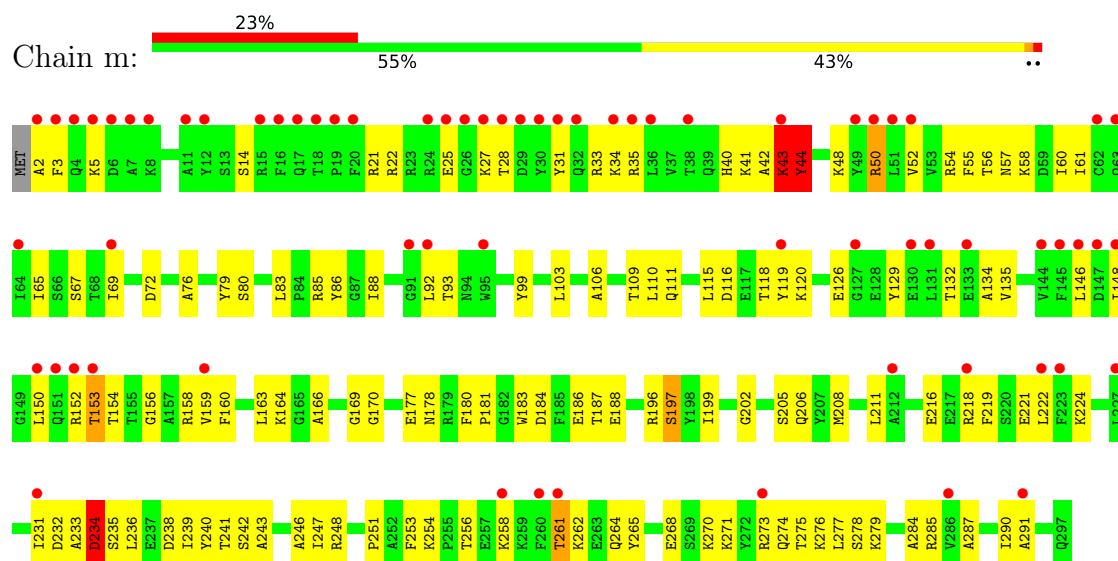
Chain c0:

Amino Acid	Frequency (bits)	Percentage
M1	0.01	19%
L2	0.01	
M3	0.01	
P4	0.01	
D7	0.01	
N8	0.01	
R9	0.01	
K10	0.01	
I11	0.01	
H12	0.01	
Q13	0.01	
Y14	0.01	
L15	0.01	
F16	0.01	
Q17	0.01	
E18	0.01	
G19	0.01	
V20	0.01	
V21	0.01	
V22	0.01	
A23	0.01	
K24	0.01	
K25	0.01	
D26	0.01	
F27	0.01	
N28	0.01	
Q29	0.01	
A30	0.01	
K31	0.01	
H32	0.01	
E33	0.01	
E34	0.01	
I35	0.01	
K38	0.01	
N39	0.01	
L40	0.01	
Y41	0.01	
V42	0.01	
I43	0.01	
K44	0.01	
A45	0.01	
L46	0.01	
Q47	0.01	
S48	0.01	
L49	0.01	
T50	0.01	
S51	0.01	
Y54	0.01	
V55	0.01	
F59	0.01	
Q62	0.01	
Y63	0.01	
Y64	0.01	
Y65	0.01	
Y66	0.01	

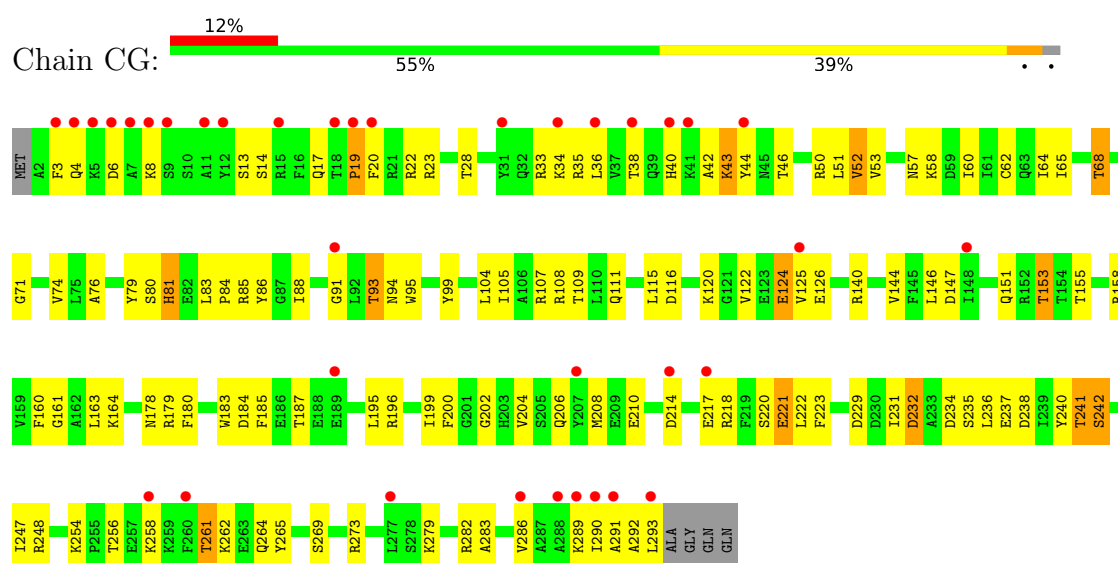
Chain L:

Position	Amino Acid	Probability
1	M	0.24
2	L	0.34
3	M	0.47
4	P	0.05
5	K	0.14
6	K	0.01
7	K	0.01
8	K	0.01
9	K	0.01
10	K	0.01
11	K	0.01
12	K	0.01
13	K	0.01
14	K	0.01
15	K	0.01
16	K	0.01
17	K	0.01
18	K	0.01
19	K	0.01
20	K	0.01
21	K	0.01
22	K	0.01
23	K	0.01
24	K	0.01
25	K	0.01
26	K	0.01
27	K	0.01
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30	K	0.01
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32	K	0.01
33	K	0.01
34	K	0.01
35	K	0.01
36	K	0.01
37	K	0.01
38	K	0.01
39	K	0.01
40	K	0.01
41	K	0.01
42	K	0.01
43	K	0.01
44	K	0.01
45	K	0.01
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60	K	0.01
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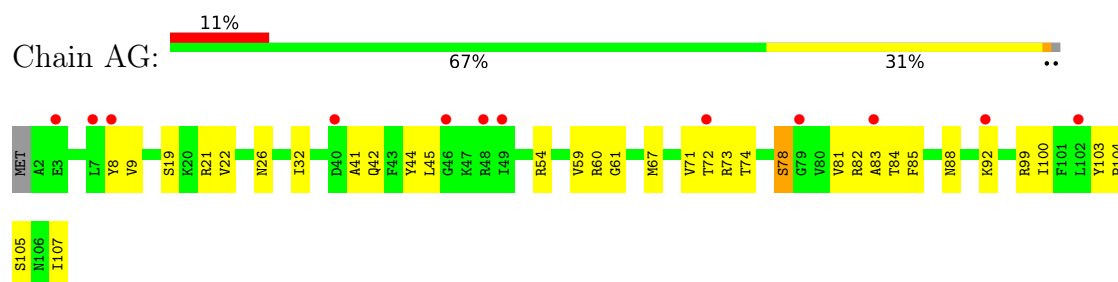
- Molecule 31: 60S ribosomal protein L5



- Molecule 31: 60S ribosomal protein L5

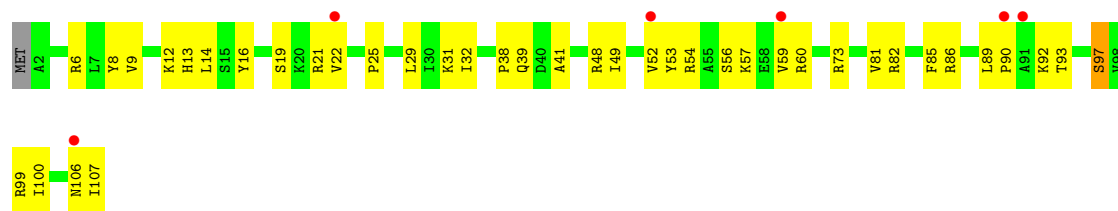


- Molecule 32: 60S ribosomal protein L33-A

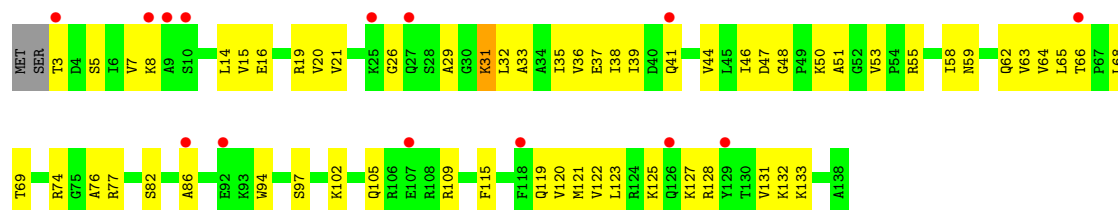


- Molecule 32: 60S ribosomal protein L33-A

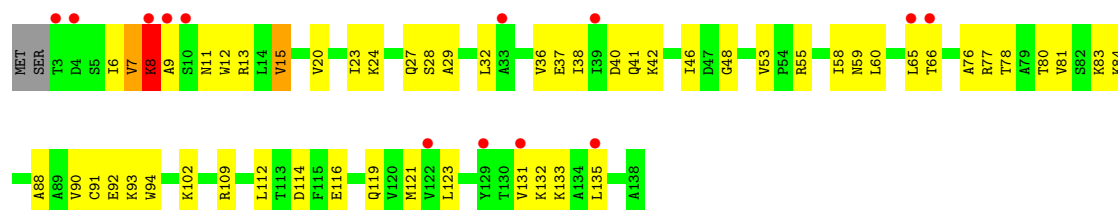




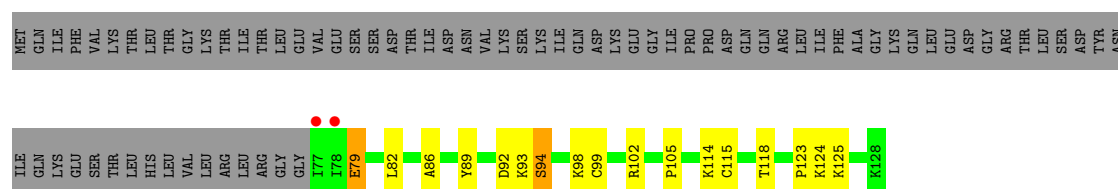
- Molecule 33: 60S ribosomal protein L14-A



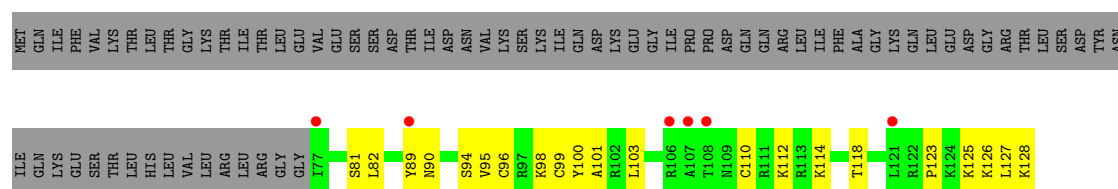
- Molecule 33: 60S ribosomal protein L14-A



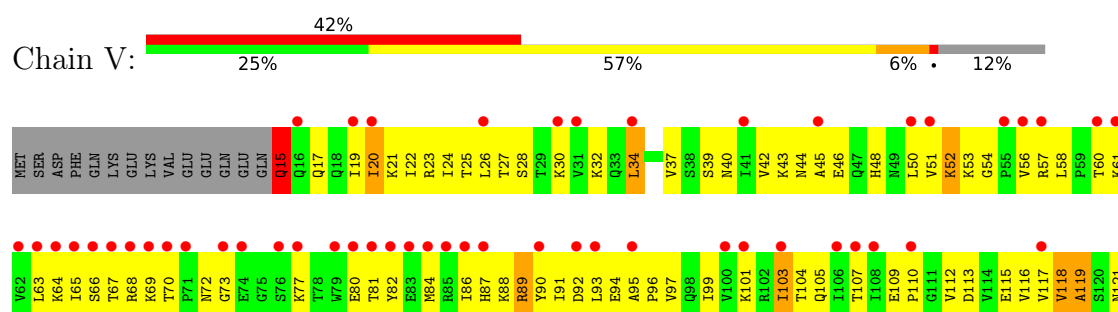
- Molecule 34: Ubiquitin-60S ribosomal protein L40



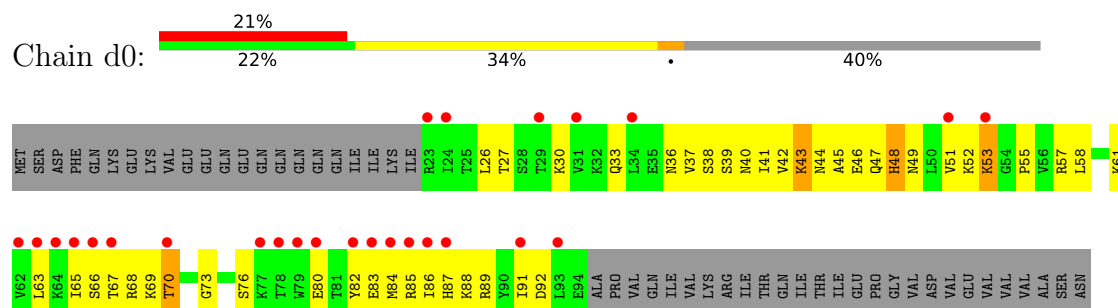
- Molecule 34: Ubiquitin-60S ribosomal protein L40



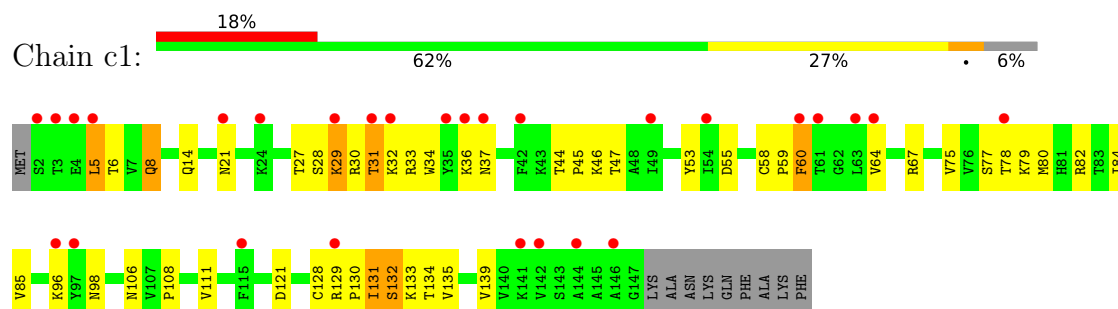
- Molecule 35: Small ribosomal subunit protein uS10



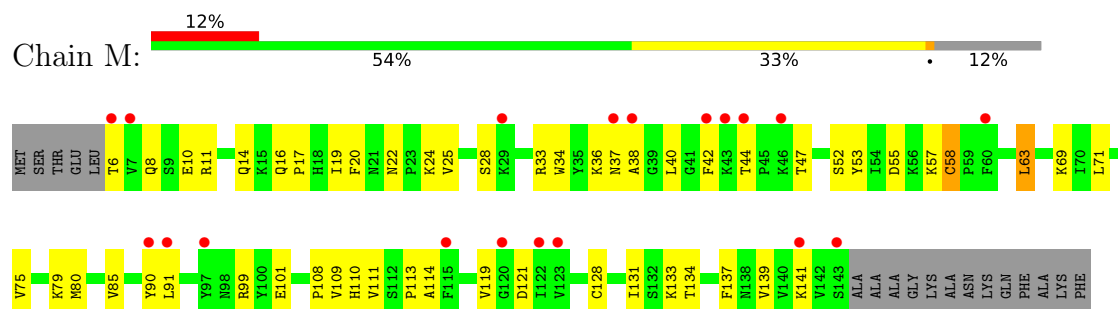
- Molecule 35: Small ribosomal subunit protein uS10



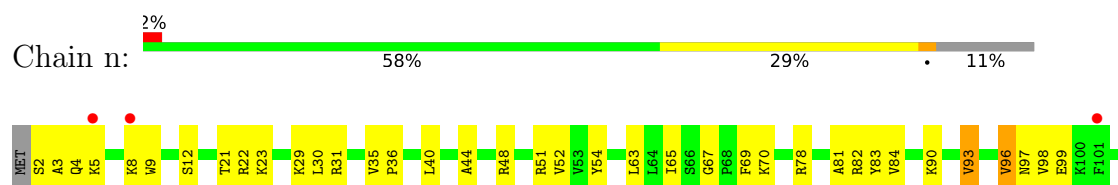
- Molecule 36: 40S ribosomal protein S11-A



- Molecule 36: 40S ribosomal protein S11-A

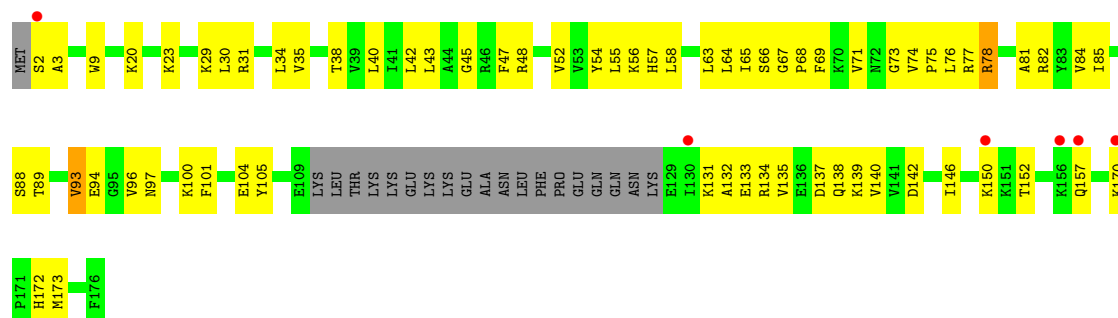


- Molecule 37: 60S ribosomal protein L6-A

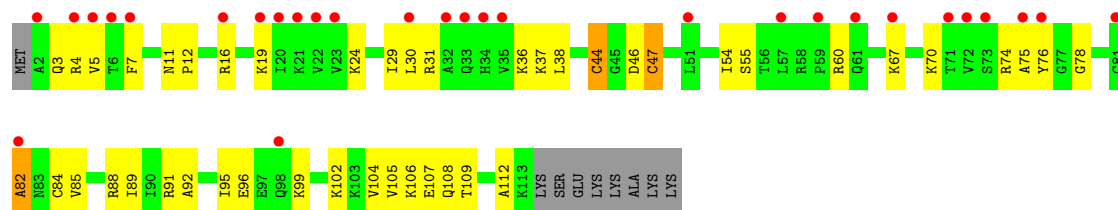




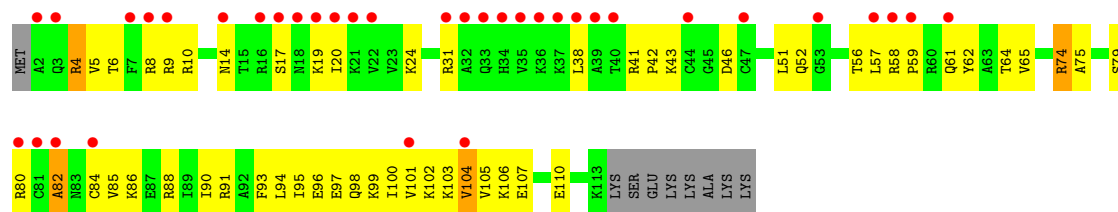
- Molecule 37: 60S ribosomal protein L6-A



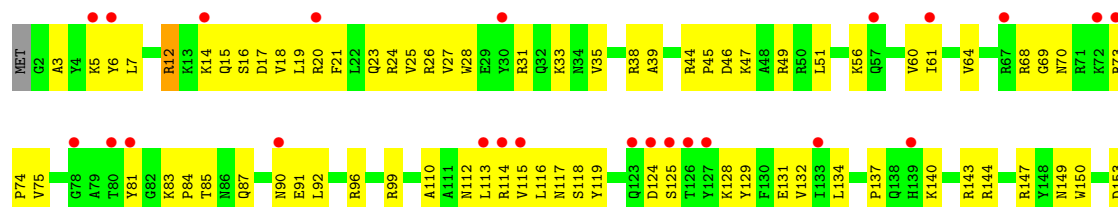
- Molecule 38: 60S ribosomal protein L34-A

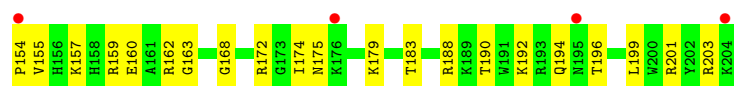


- Molecule 38: 60S ribosomal protein L34-A

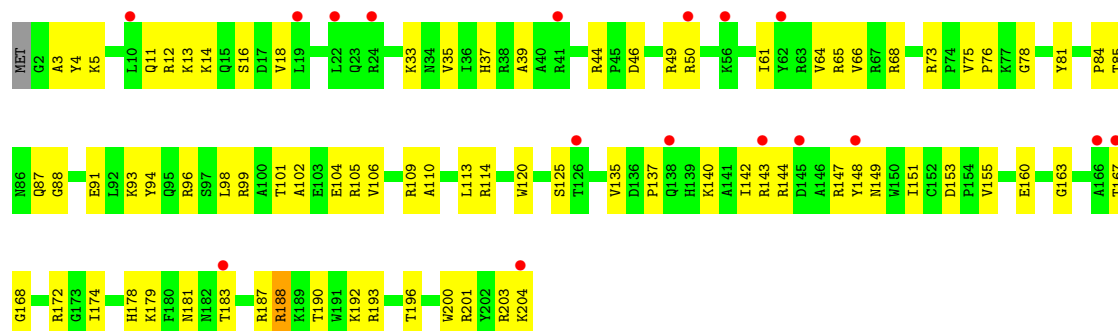


- Molecule 39: 60S ribosomal protein L15-A





- Molecule 39: 60S ribosomal protein L15-A



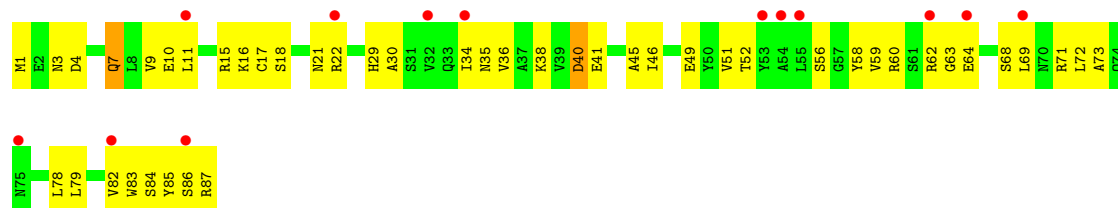
- Molecule 40: Large ribosomal subunit protein eL41B



- Molecule 40: Large ribosomal subunit protein eL41B



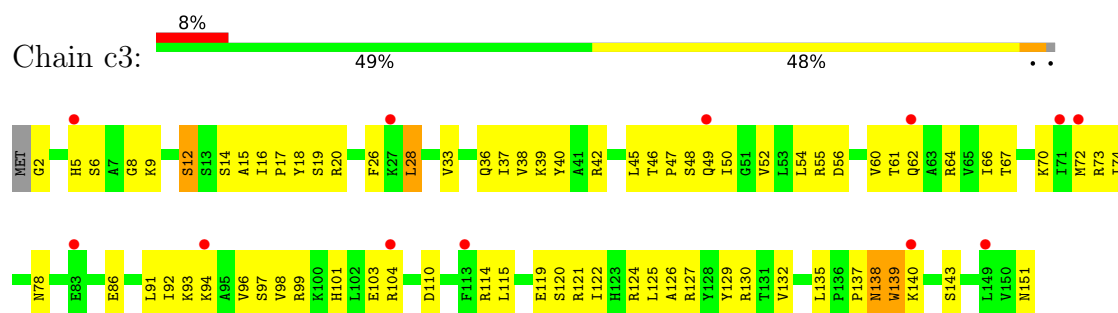
- Molecule 41: 40S ribosomal protein S21-A



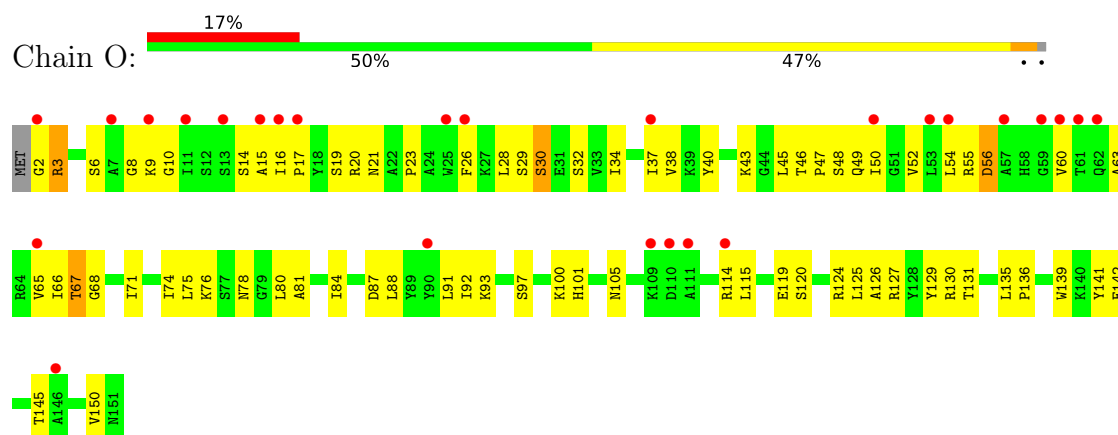
- Molecule 41: 40S ribosomal protein S21-A



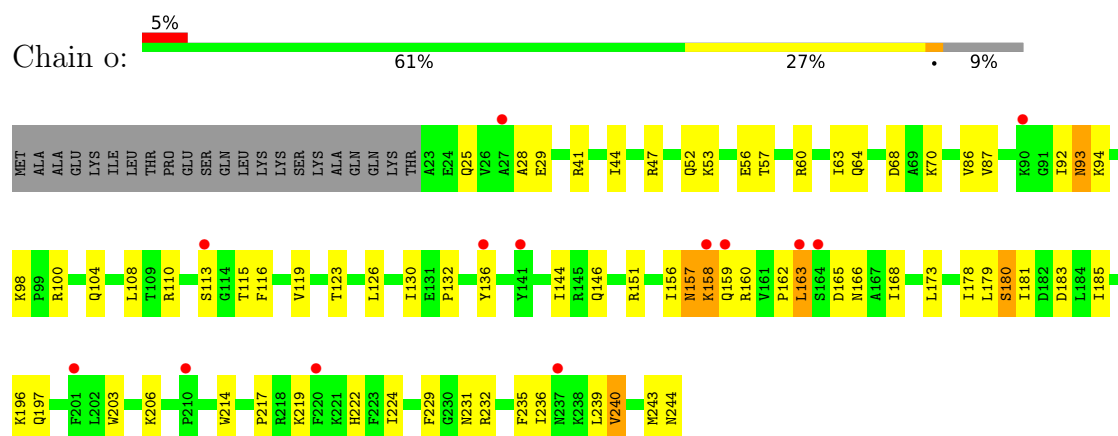
- Molecule 42: 40S ribosomal protein S13



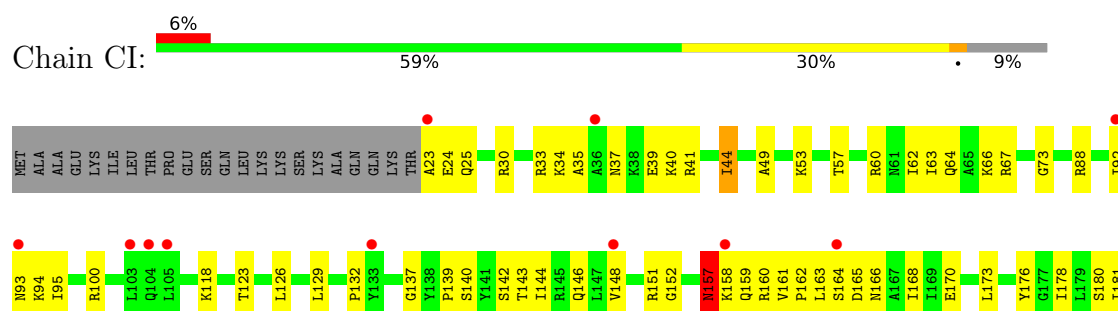
- Molecule 42: 40S ribosomal protein S13



- Molecule 43: 60S ribosomal protein L7-A

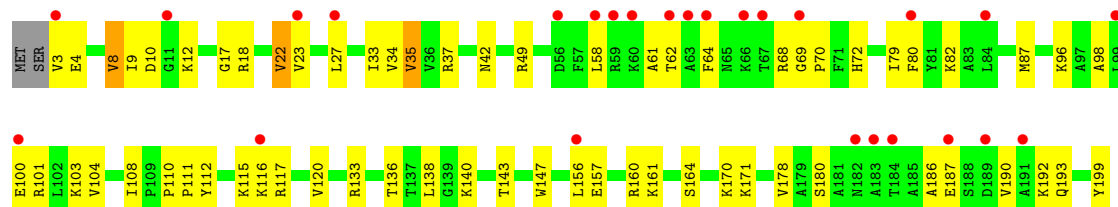


- Molecule 43: 60S ribosomal protein L7-A

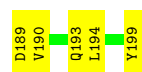
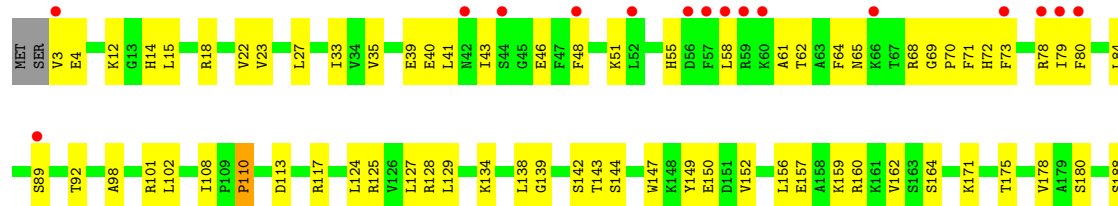




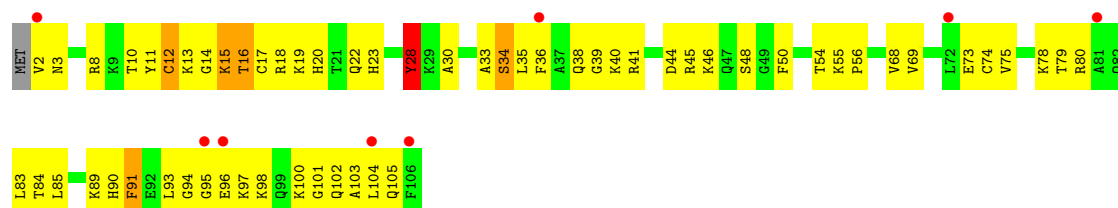
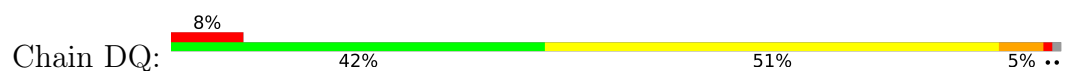
- Molecule 44: 60S ribosomal protein L16-A



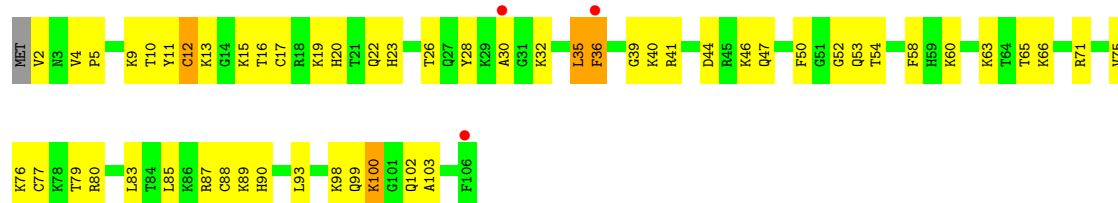
- Molecule 44: 60S ribosomal protein L16-A



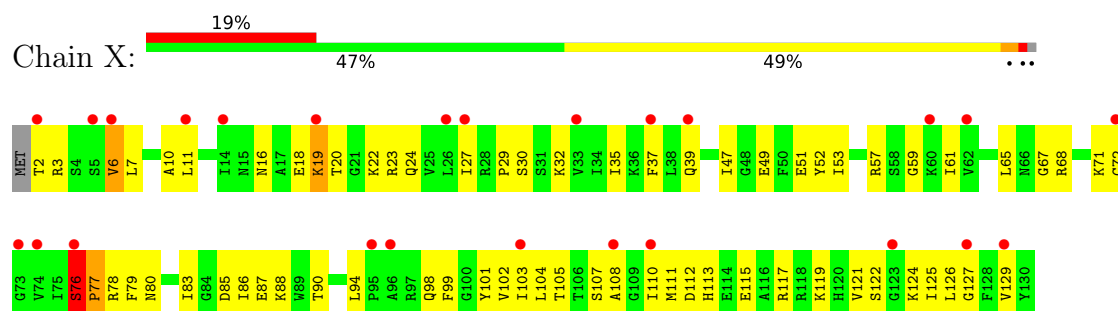
- Molecule 45: 60S ribosomal protein L42-A



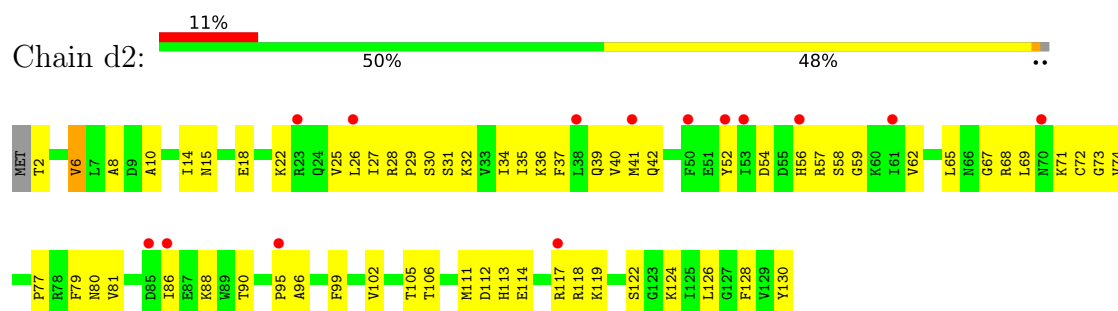
- Molecule 45: 60S ribosomal protein L42-A



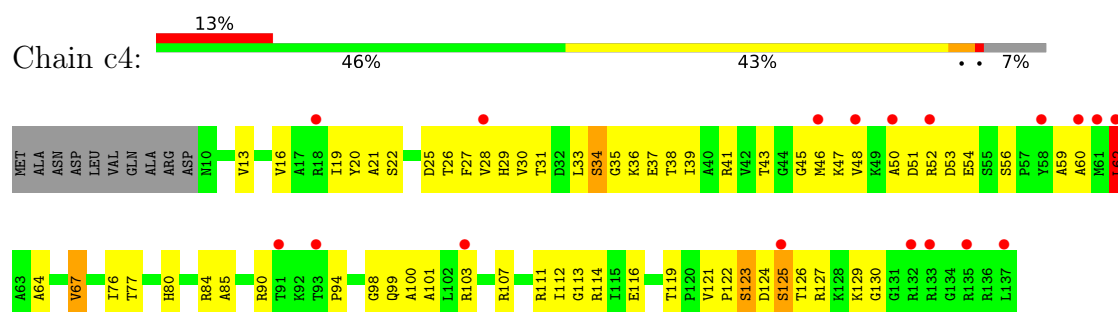
- Molecule 46: 40S ribosomal protein S22-A



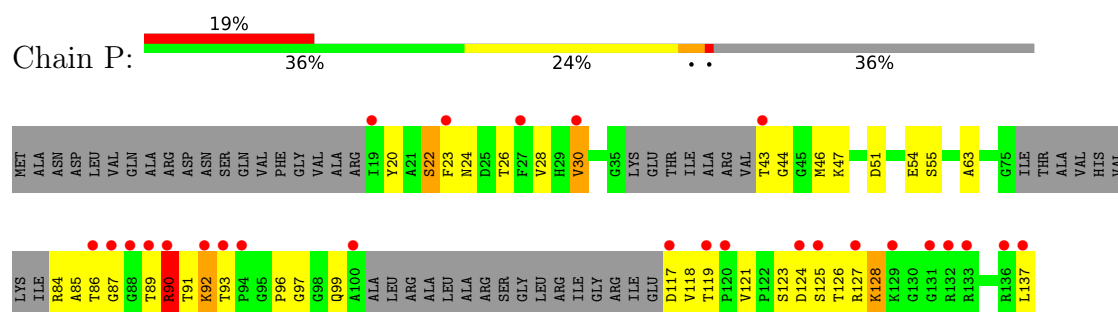
- Molecule 46: 40S ribosomal protein S22-A



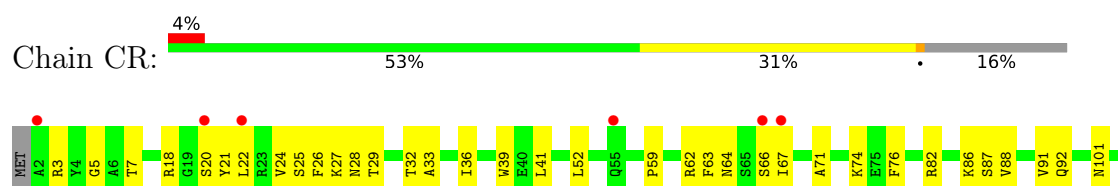
- Molecule 47: 40S ribosomal protein S14-B

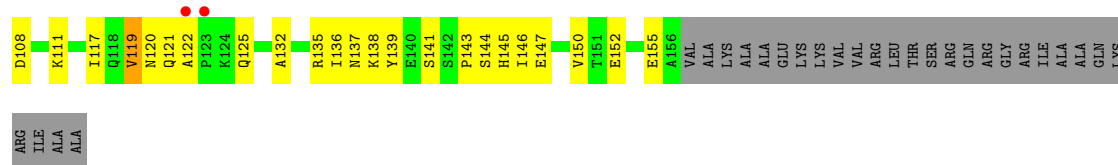


- Molecule 47: 40S ribosomal protein S14-B

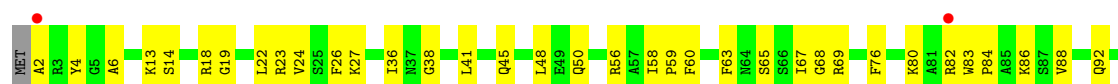


- Molecule 48: 60S ribosomal protein L17-A

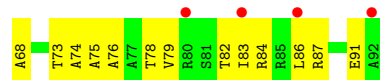
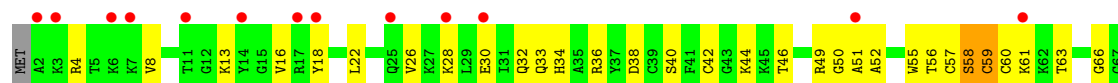




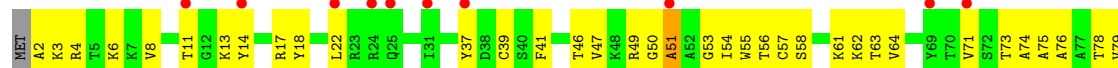
• Molecule 48: 60S ribosomal protein L17-A



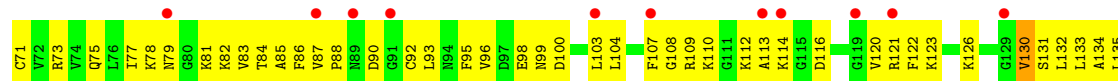
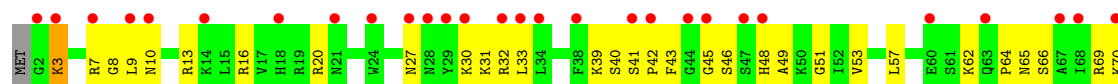
• Molecule 49: 60S ribosomal protein L43-A



• Molecule 49: 60S ribosomal protein L43-A

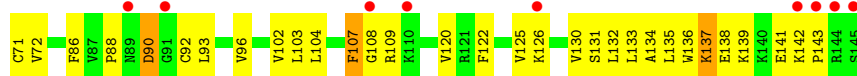


• Molecule 50: 40S ribosomal protein S23-A

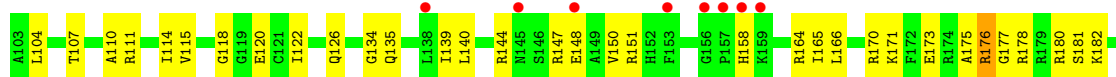
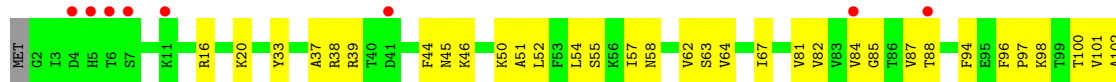




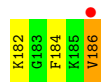
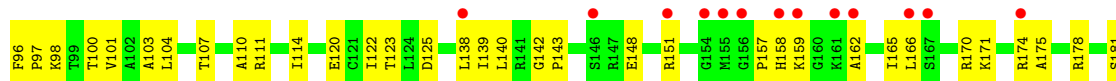
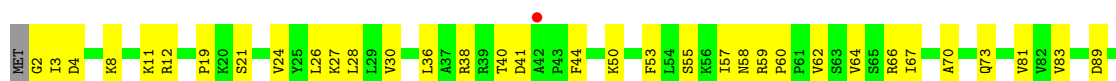
- Molecule 50: 40S ribosomal protein S23-A



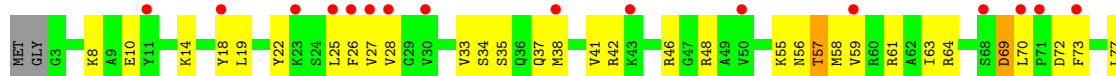
- Molecule 51: 60S ribosomal protein L18-A

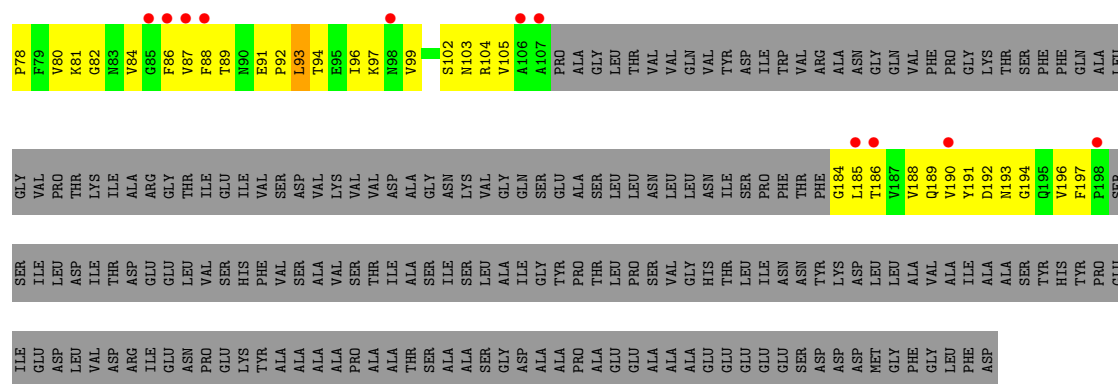


- Molecule 51: 60S ribosomal protein L18-A

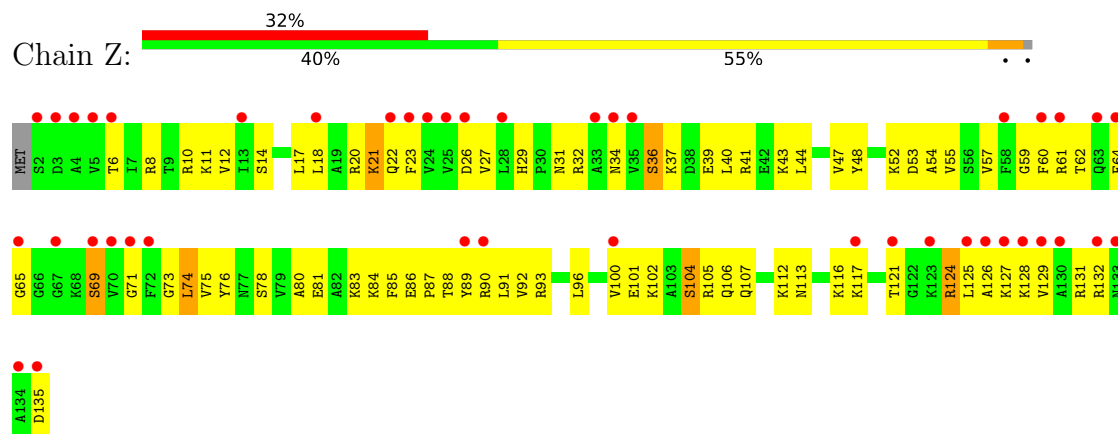


- Molecule 52: Large ribosomal subunit protein uL10

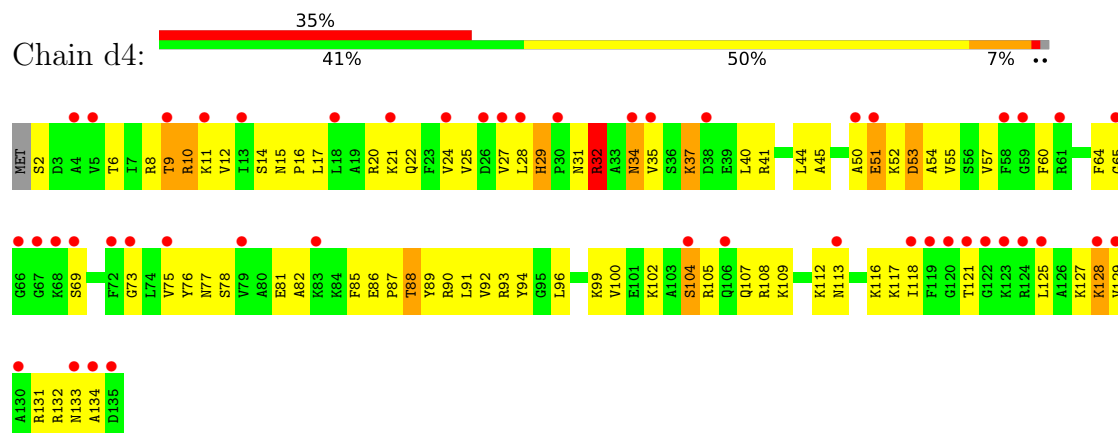




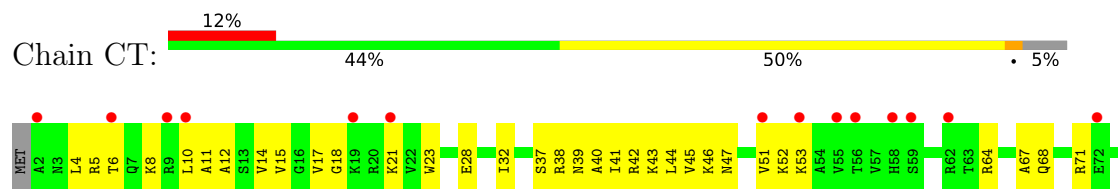
• Molecule 53: 40S ribosomal protein S24-A



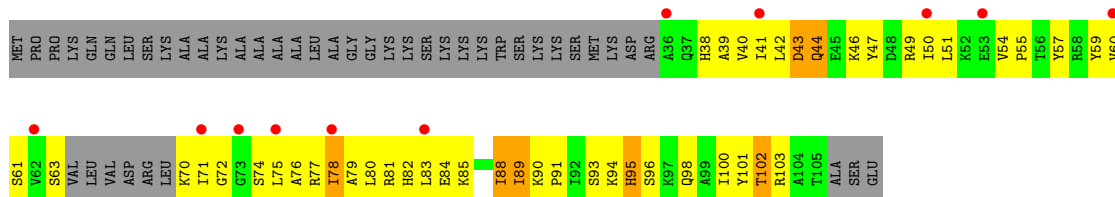
• Molecule 53: 40S ribosomal protein S24-A



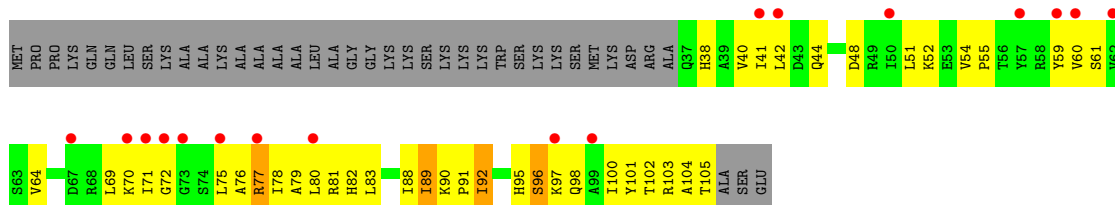
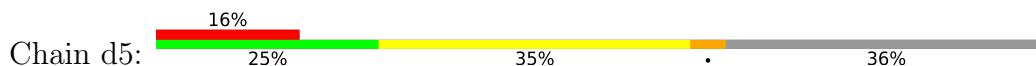
• Molecule 54: 60S ribosomal protein L19-A



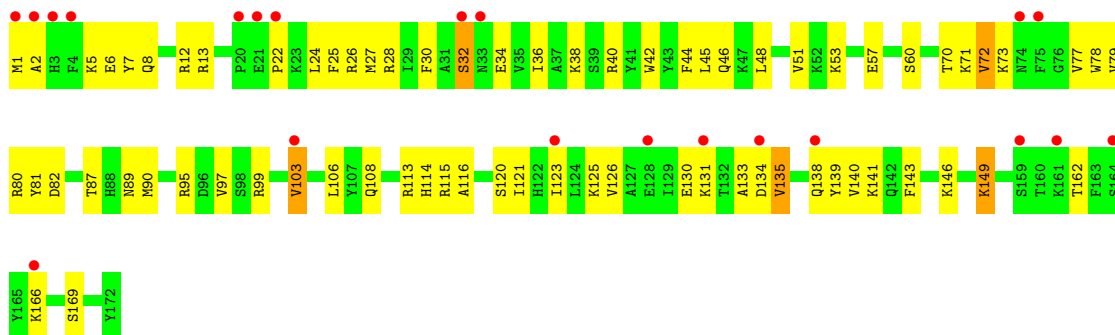
- Molecule 56: 40S ribosomal protein S25-A



- Molecule 56: 40S ribosomal protein S25-A

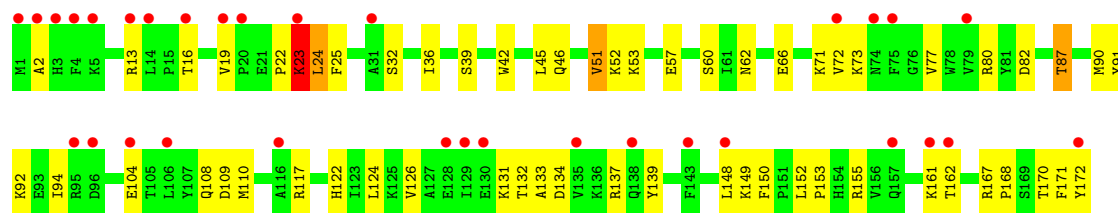


- Molecule 57: 60S ribosomal protein L20-A

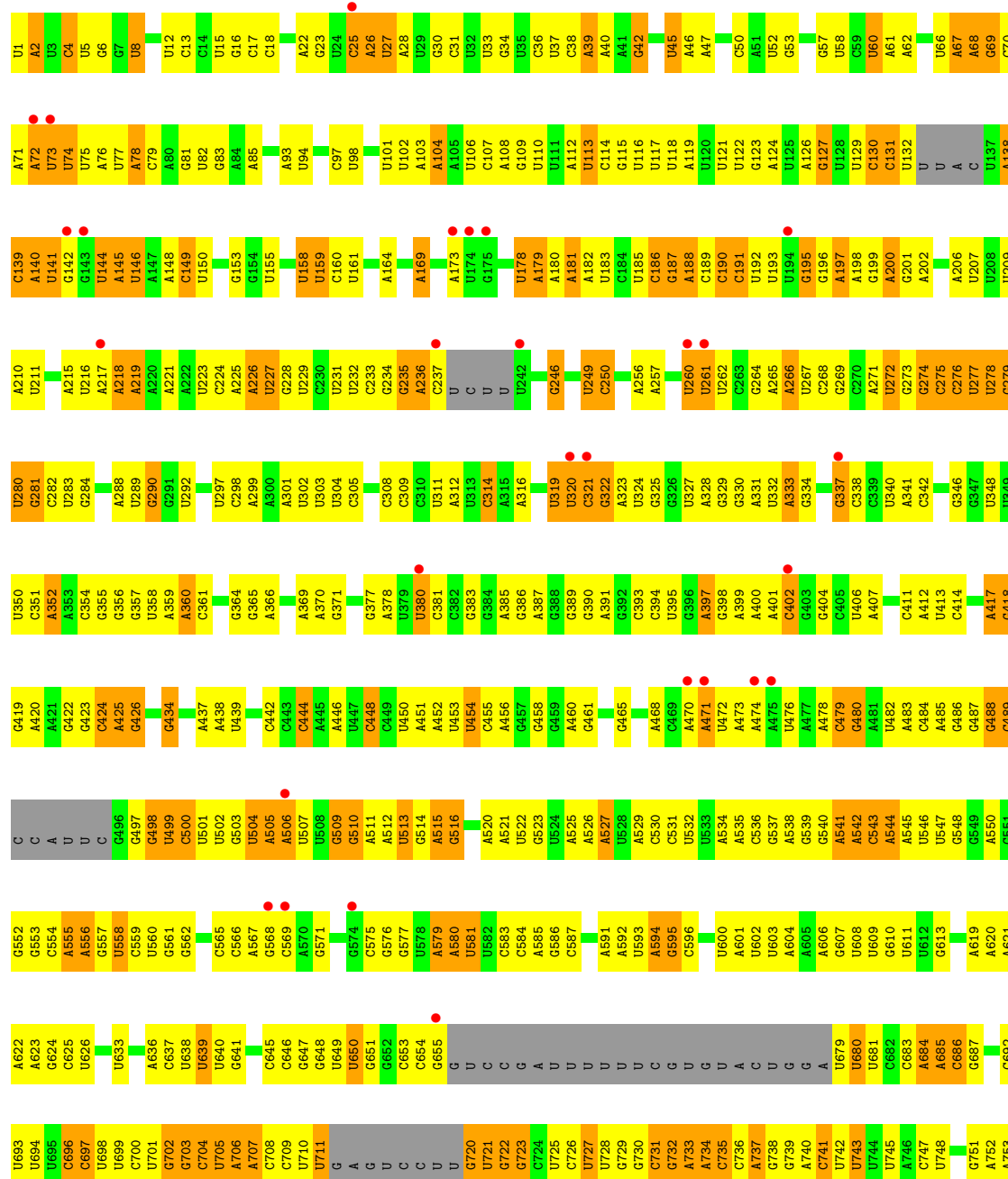


- Molecule 57: 60S ribosomal protein L20-A

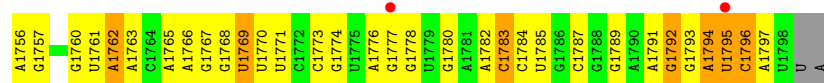




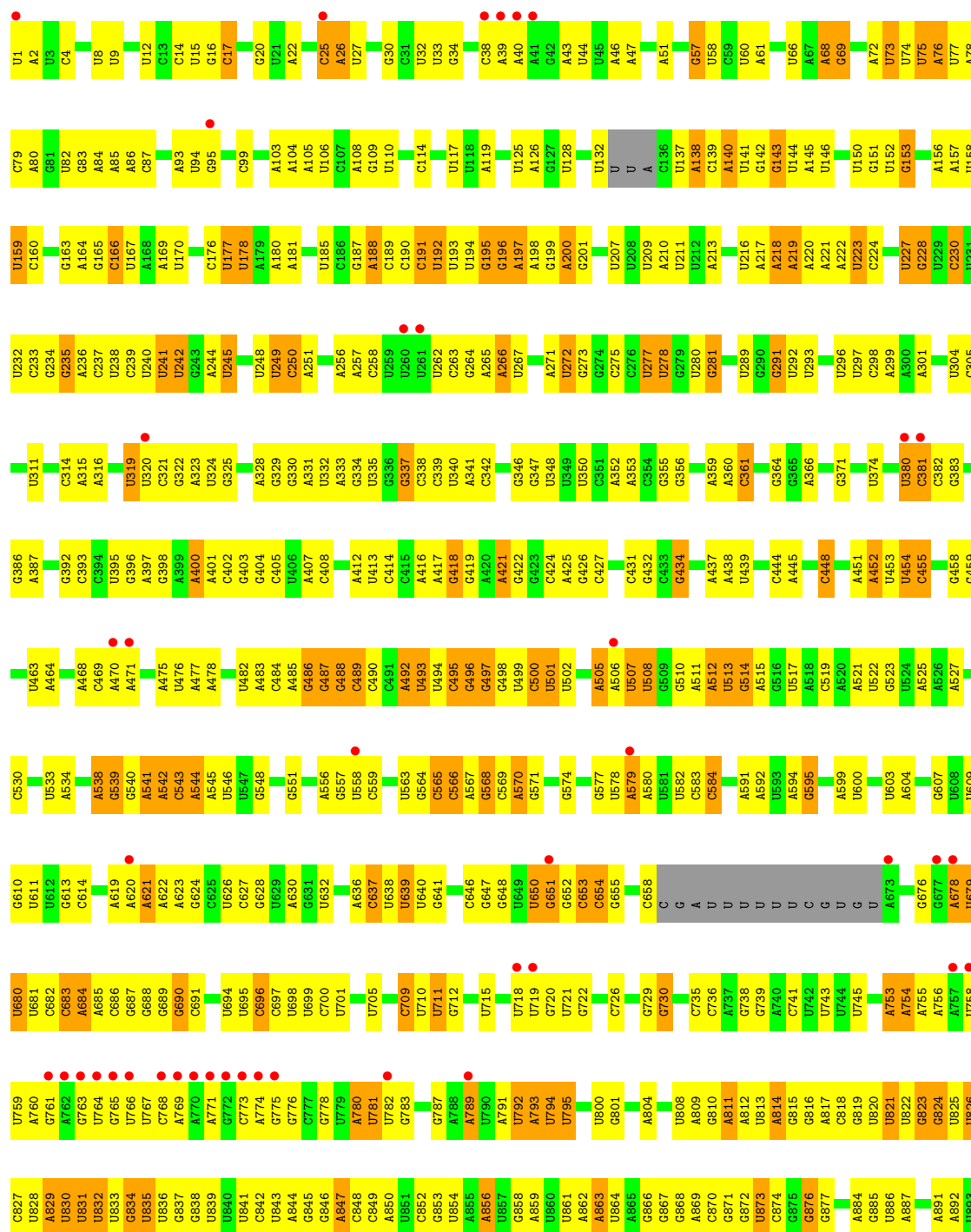
● Molecule 58: 16S ribosomal RNA

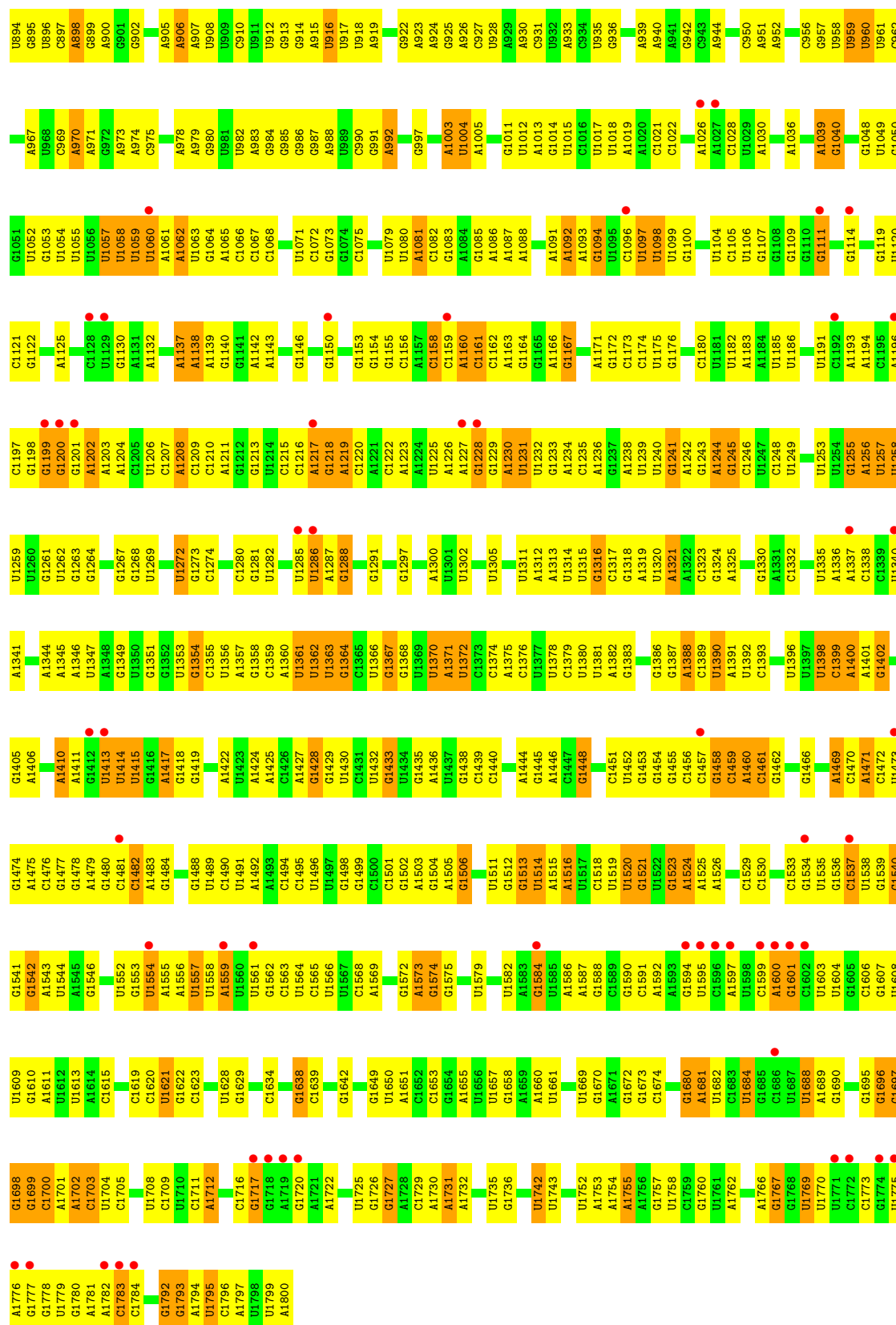


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G	A1614	A1550	C1485	A1411	C1338	U1260	G1190	G1119	A966	A891	U823	A757
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A	U1617	G1553	G1488	U1414	A1341	G1263	A1193	G1126	U968	U894	U826	
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G	G1622	U1556	U1491	A1418	A1346	U1266	U1196	G1130	A974	U830	U829	U766
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C		A1559	C1494	A1425	U1350	A1275	G1199	C1134	U978	U833	U832	U769
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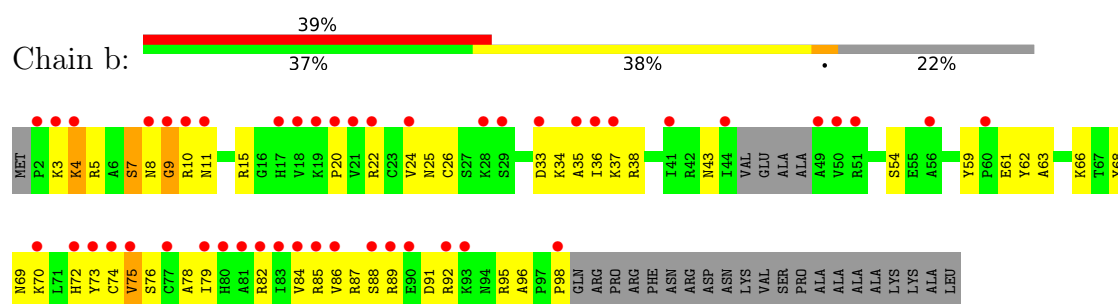


● Molecule 58: 16S ribosomal RNA

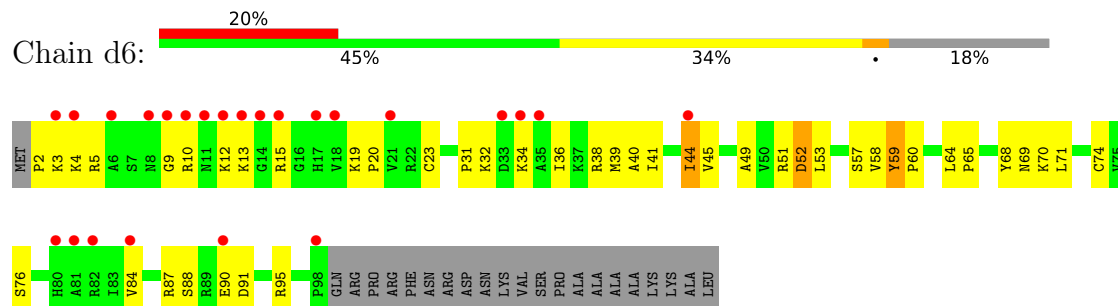




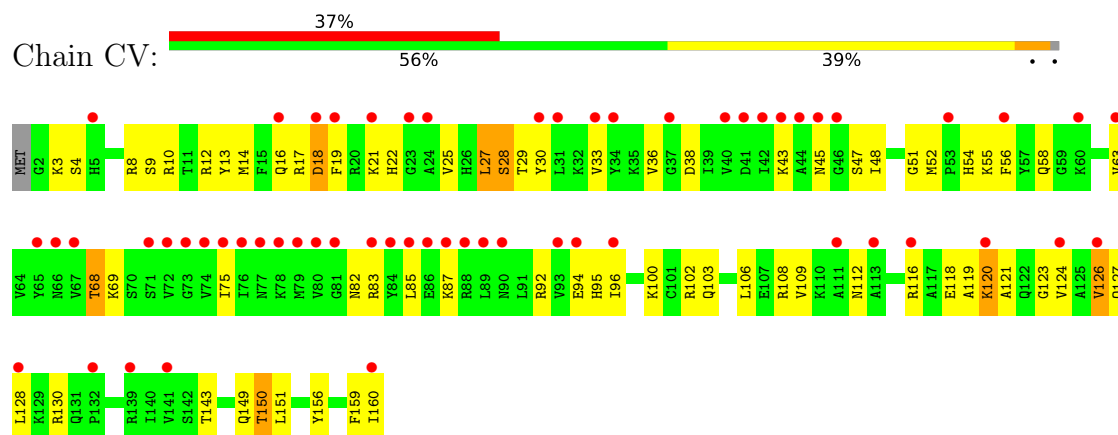
- Molecule 59: Small ribosomal subunit protein eS26B



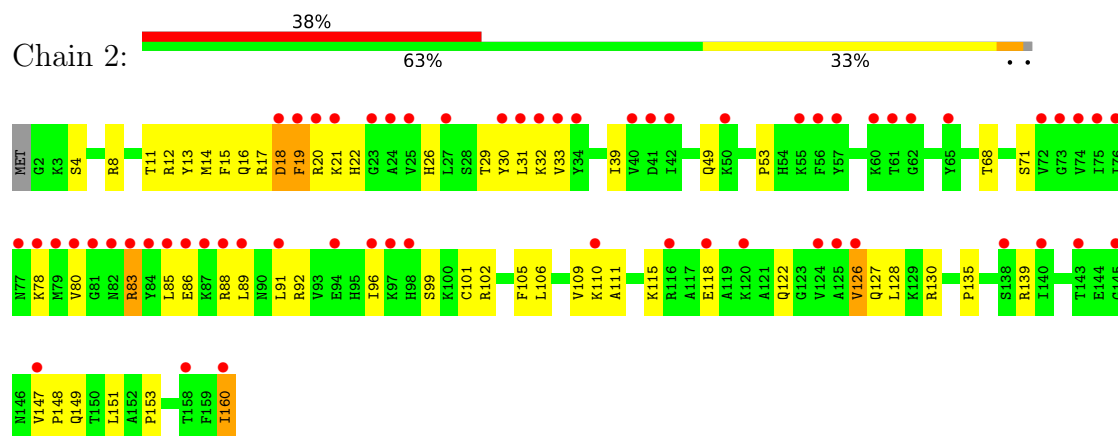
- Molecule 59: Small ribosomal subunit protein eS26B



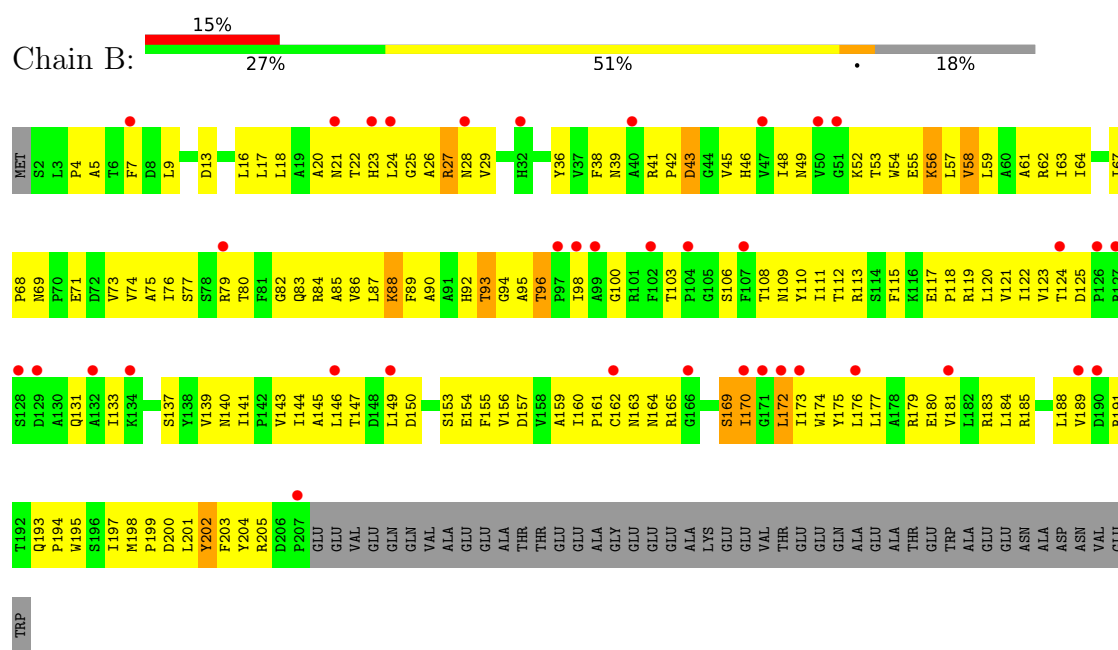
- Molecule 60: 60S ribosomal protein L21-A



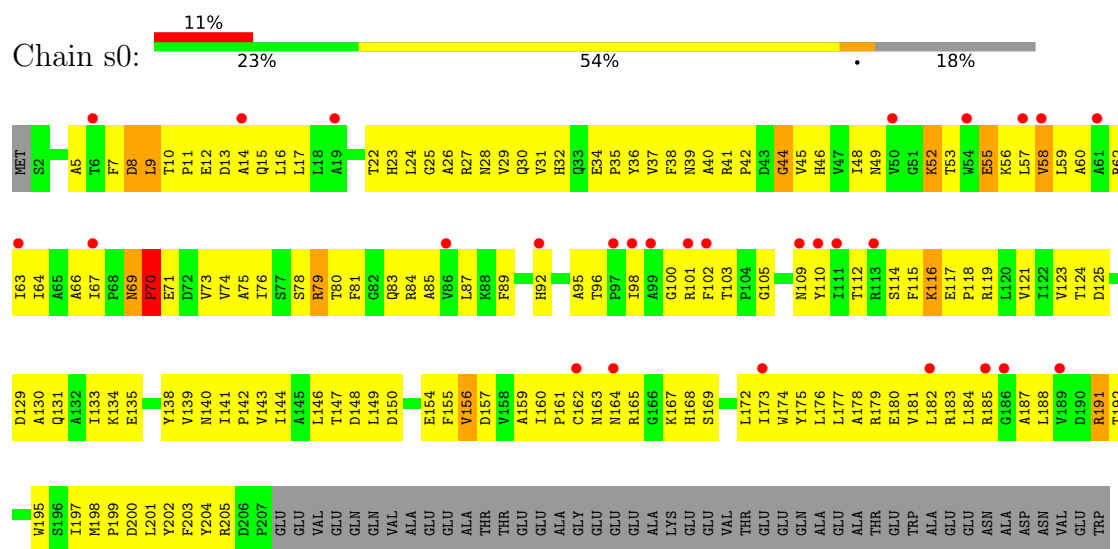
- Molecule 60: 60S ribosomal protein L21-A



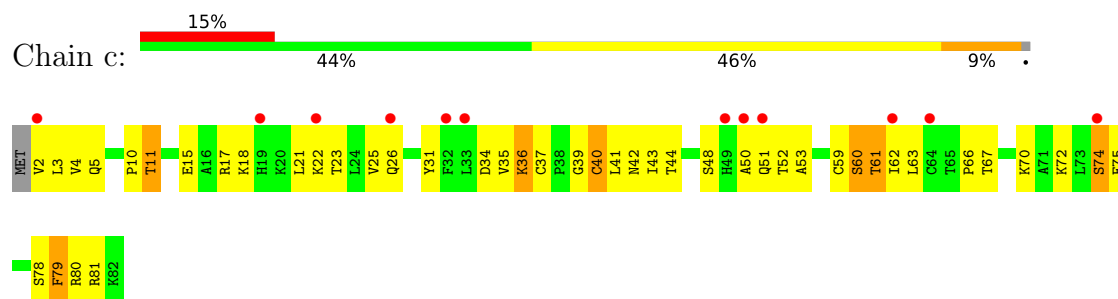
- Molecule 61: 40S ribosomal protein S0-A



• Molecule 61: 40S ribosomal protein S0-A

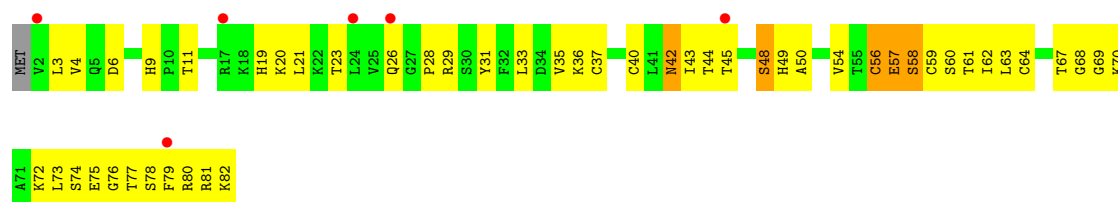


• Molecule 62: 40S ribosomal protein S27-A

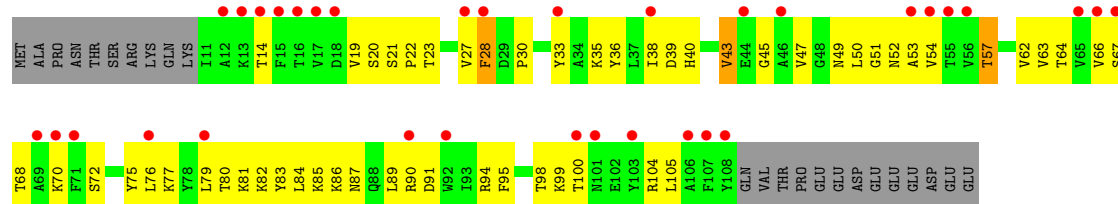


• Molecule 62: 40S ribosomal protein S27-A

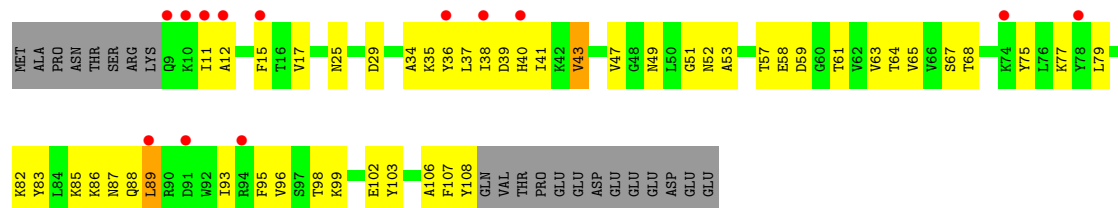




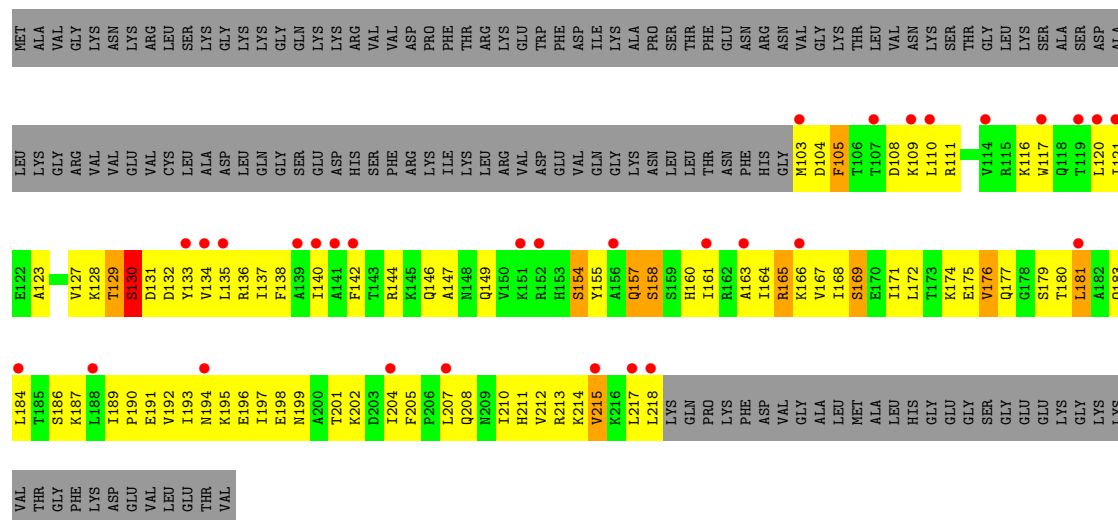
• Molecule 63: 60S ribosomal protein L22-A



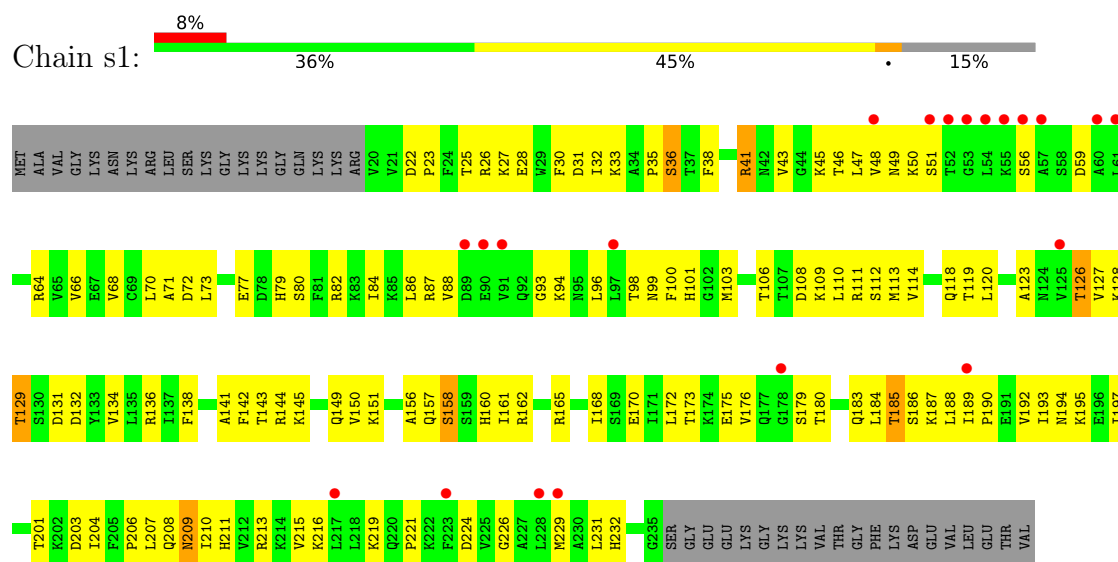
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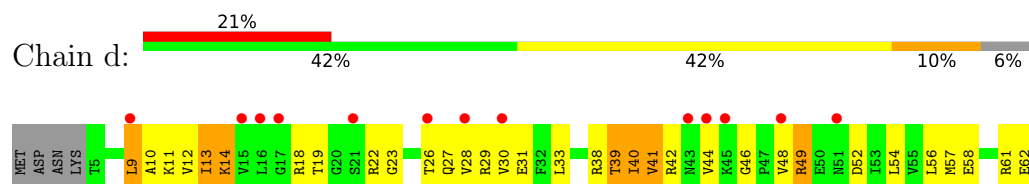
• Molecule 64: 40S ribosomal protein S1-A



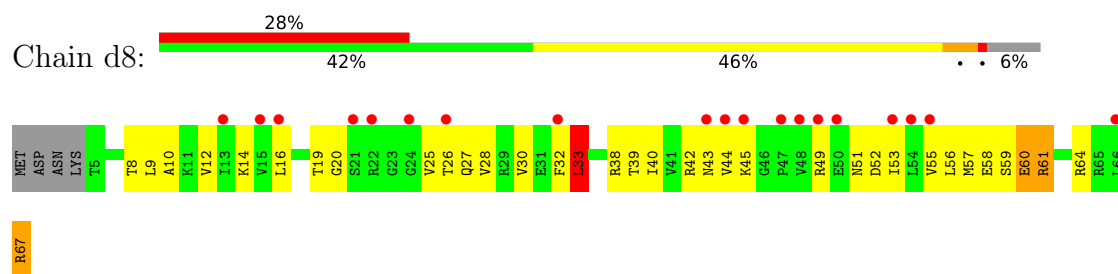
• Molecule 64: 40S ribosomal protein S1-A



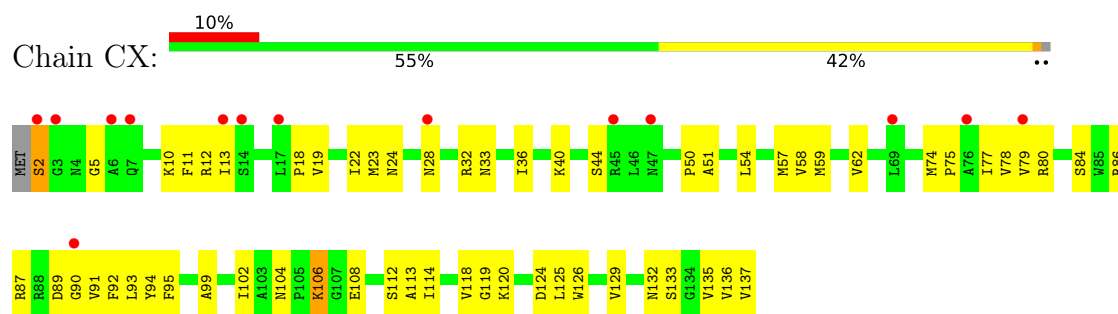
- Molecule 65: 40S ribosomal protein S28-A



- Molecule 65: 40S ribosomal protein S28-A

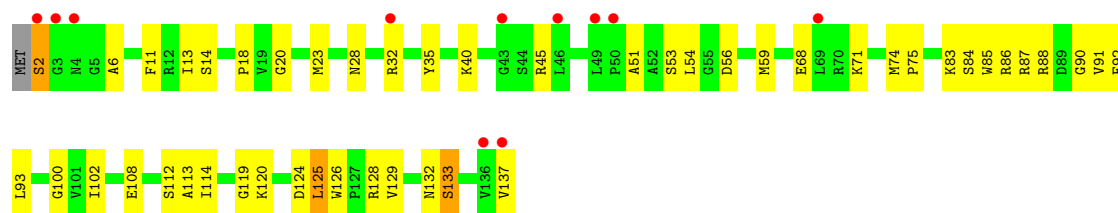


- Molecule 66: 60S ribosomal protein L23-A

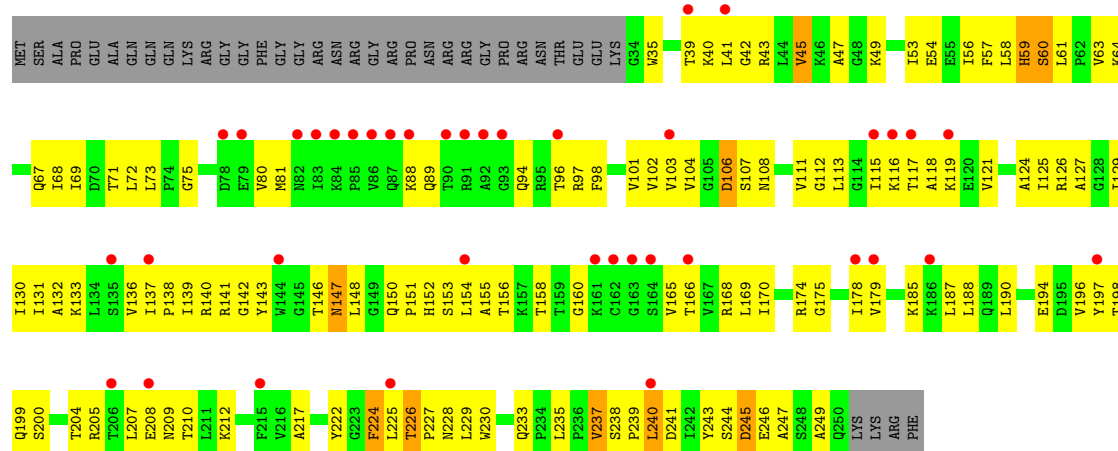


- Molecule 66: 60S ribosomal protein L23-A

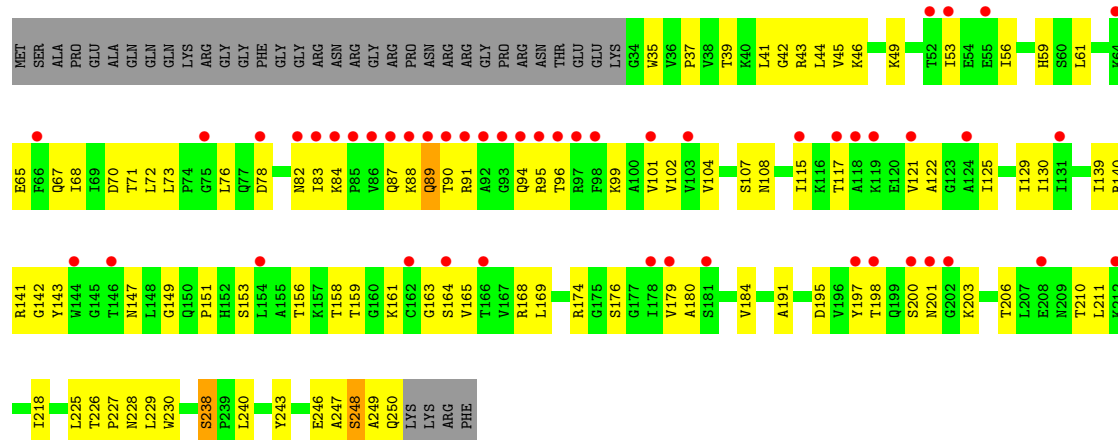




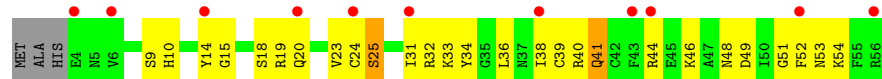
• Molecule 67: 40S ribosomal protein S2



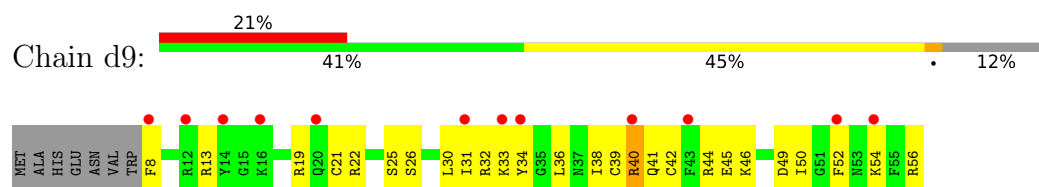
• Molecule 67: 40S ribosomal protein S2



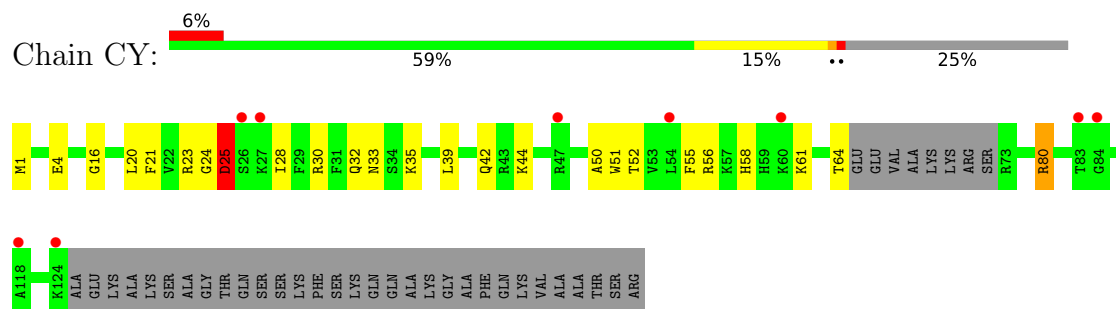
• Molecule 68: Small ribosomal subunit protein uS14A



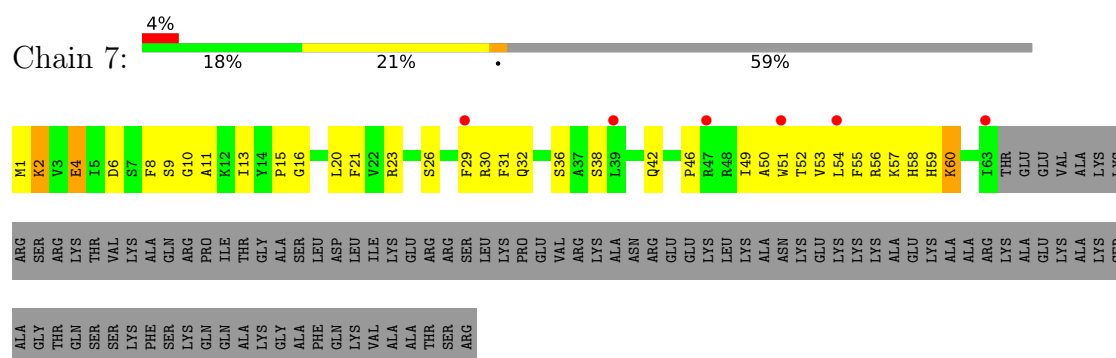
- Molecule 68: Small ribosomal subunit protein uS14A



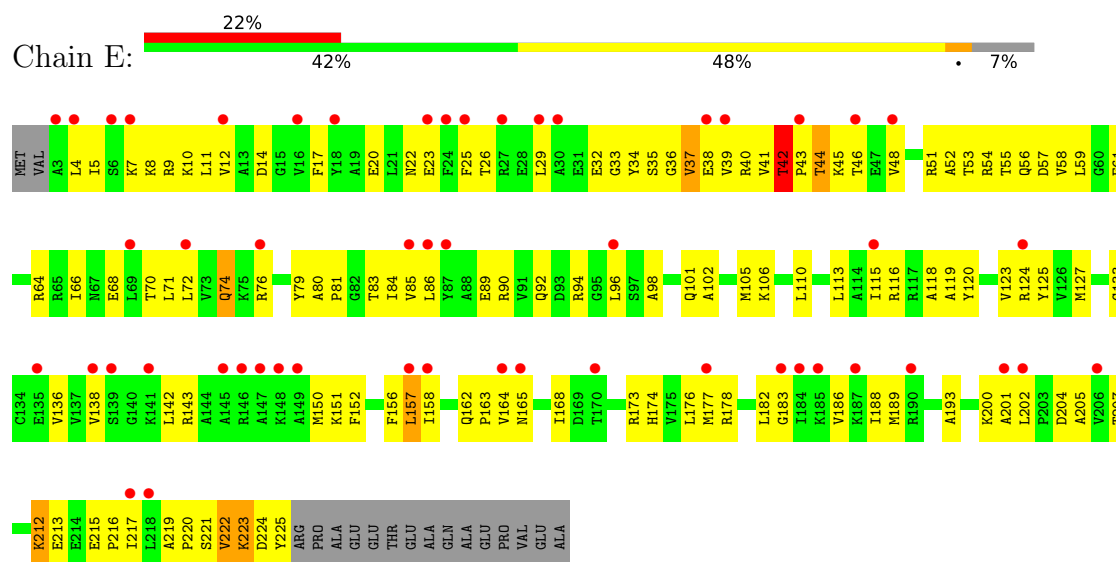
- Molecule 69: 60S ribosomal protein L24-A



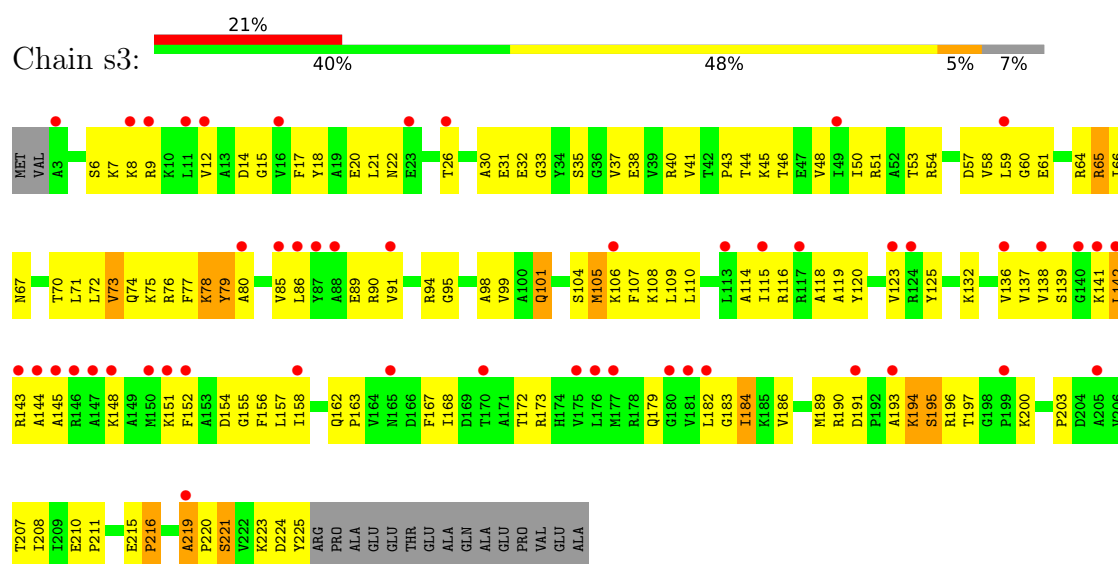
- Molecule 69: 60S ribosomal protein L24-A



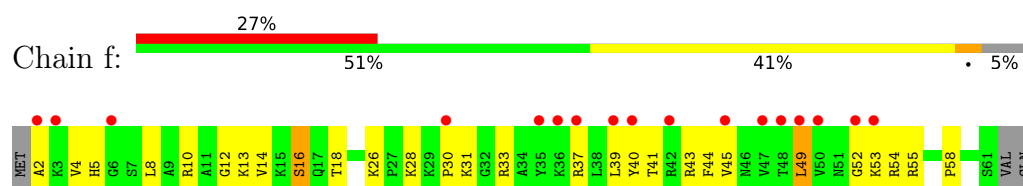
- Molecule 70: Small ribosomal subunit protein uS3



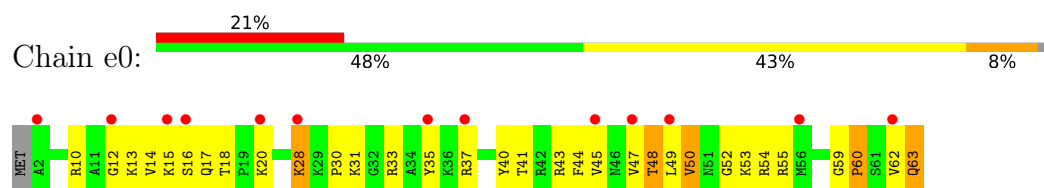
- Molecule 70: Small ribosomal subunit protein uS3



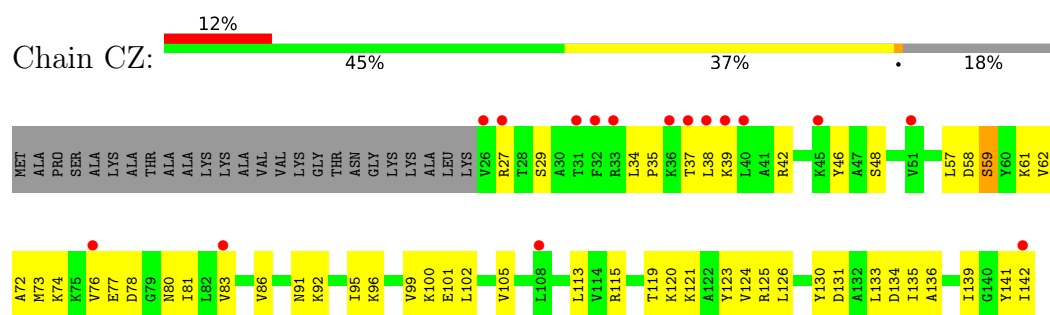
• Molecule 71: 40S ribosomal protein S30-A



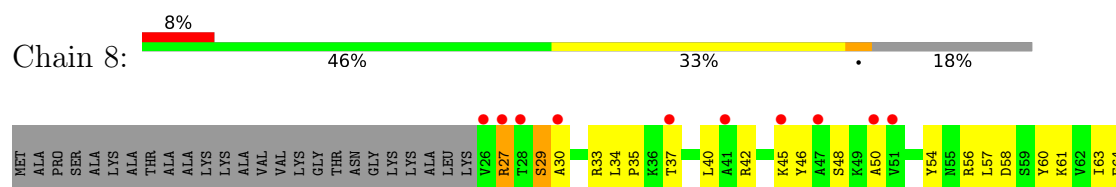
• Molecule 71: 40S ribosomal protein S30-A



• Molecule 72: 60S ribosomal protein L25

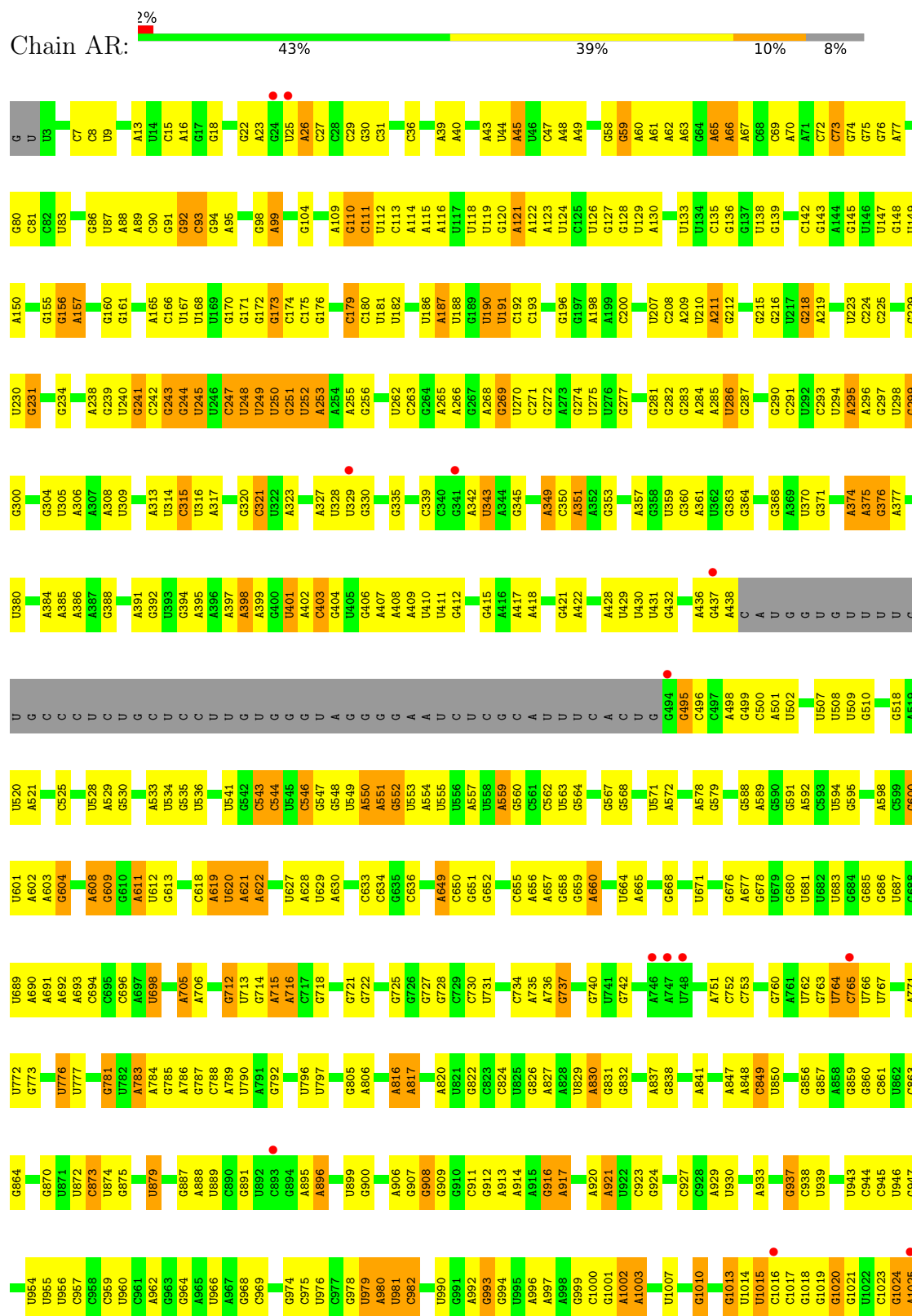


• Molecule 72: 60S ribosomal protein L25



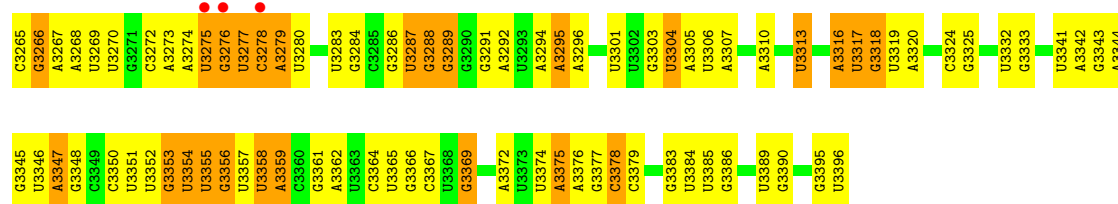


- Molecule 75: 25S ribosomal RNA

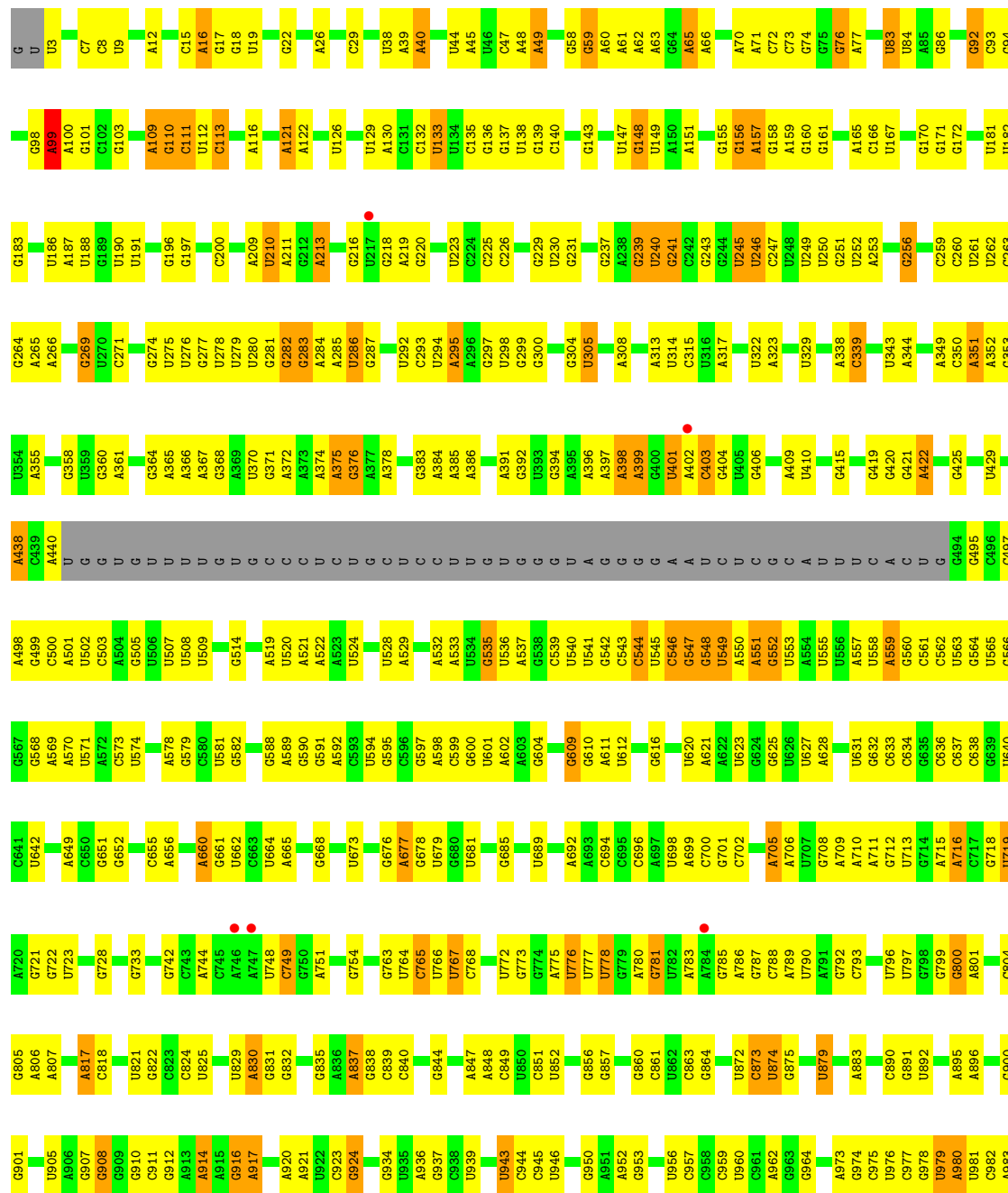
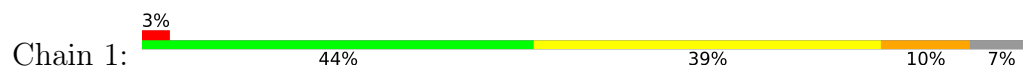


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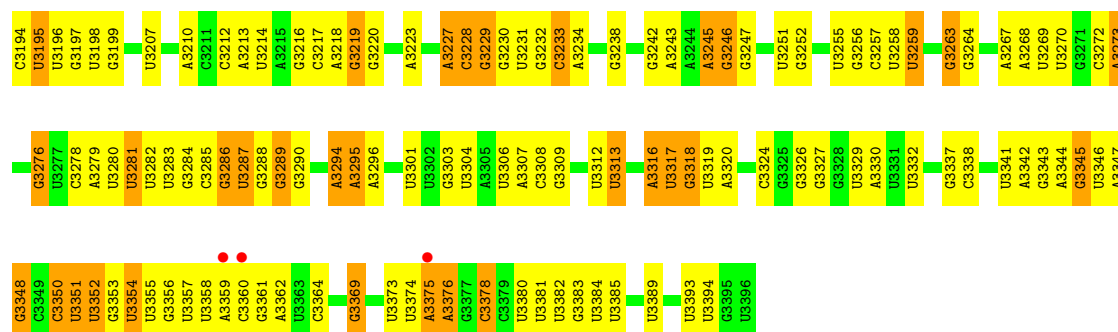


• Molecule 75: 25S ribosomal RNA

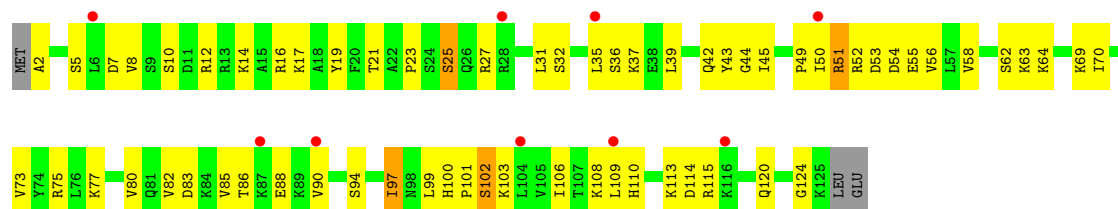


WORLDWIDE
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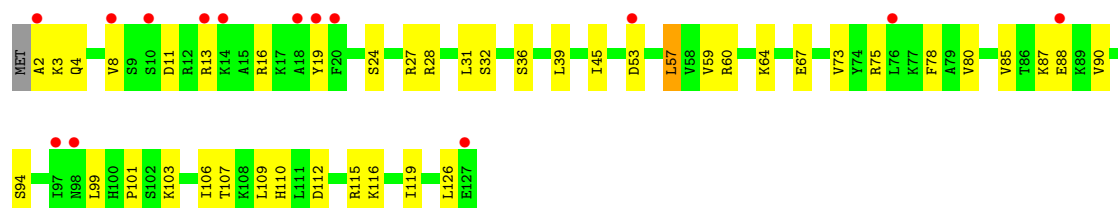
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G3045	U3046	U3047	A3048	A3049	C3053	U3056	U3057	U3058	C3059	C3060	C3061	U3064	C3065	U3066	C3067	C3072	A3073	G3074	C3075	C3076	A3077	U3078	U3079	C3080	C3081	C3082	U3083	C3084	C3085	U3086	A3087	C3088	A3089	U3090	C3091	C3092	C3093	A3094	U3095	C3096	C3097	G3102	A3103	U3106	U3107	G3108	U3111	C3112	A3113	A3114	U3117	
C2972	C2973	U2974	U2975	U2979	U2982	C2983	C2984	C2985	U2986	C2987	C3061	C2990	C2991	C2992	C2993	U2996	C2997	A3000	C3001	C3002	U2993	C3003	C3004	A3005	A3006	U3007	C3008	C3009	U3010	A3011	A3012	A3016	C3017	C3018	U3019	A3024	C3025	G3026	A3027	G3028	A3029	G3030	C3031	A3032	A3033	C3034	A3035	U3038	C3039	U3042	C3043	C3044
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G2895	A2896	A2897	G2898	C2899	A2900	U2827	U2828	U2829	U2834	U2835	C2836	U2839	C2																																							



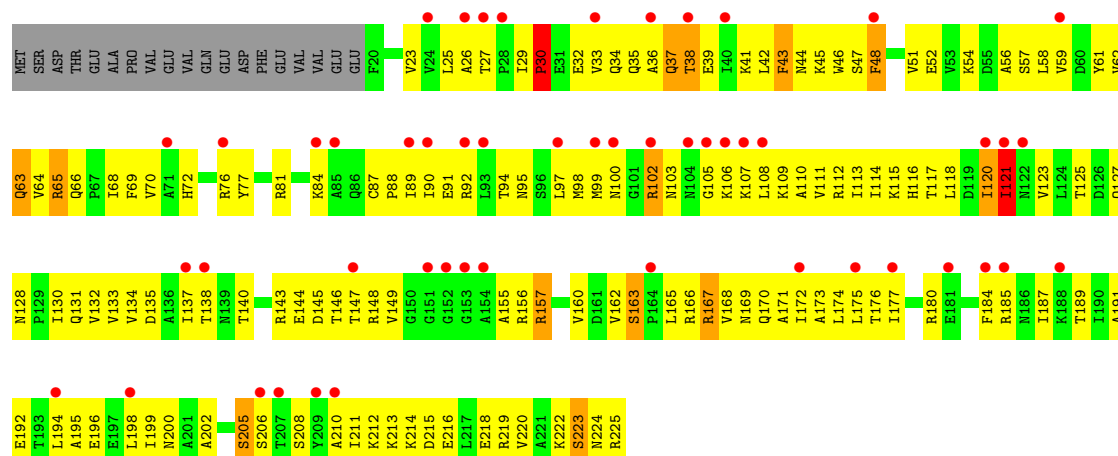
• Molecule 76: 60S ribosomal protein L26-A



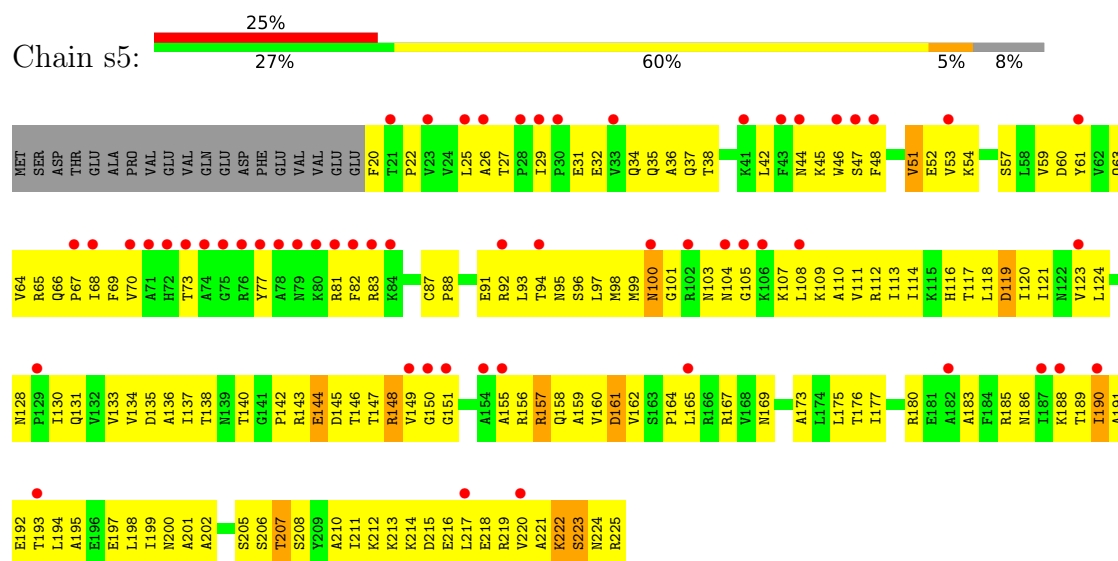
• Molecule 76: 60S ribosomal protein L26-A



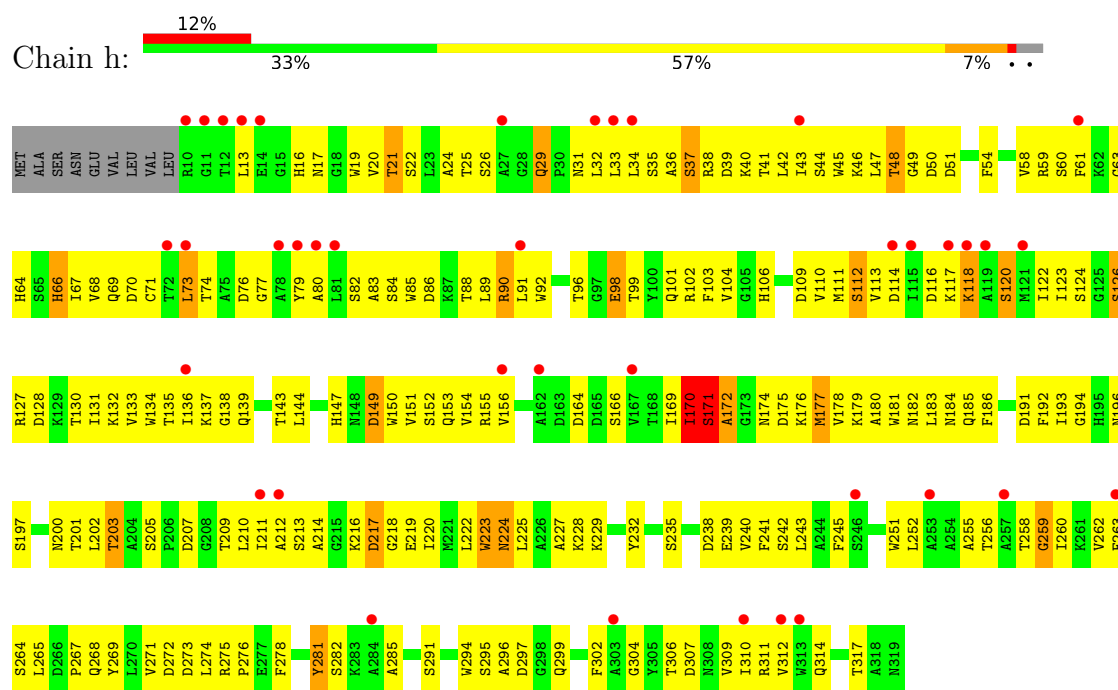
• Molecule 77: 40S ribosomal protein S5



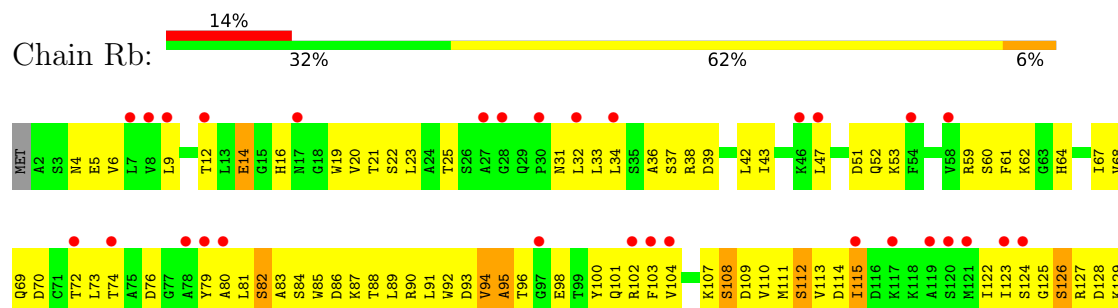
• Molecule 77: 40S ribosomal protein S5

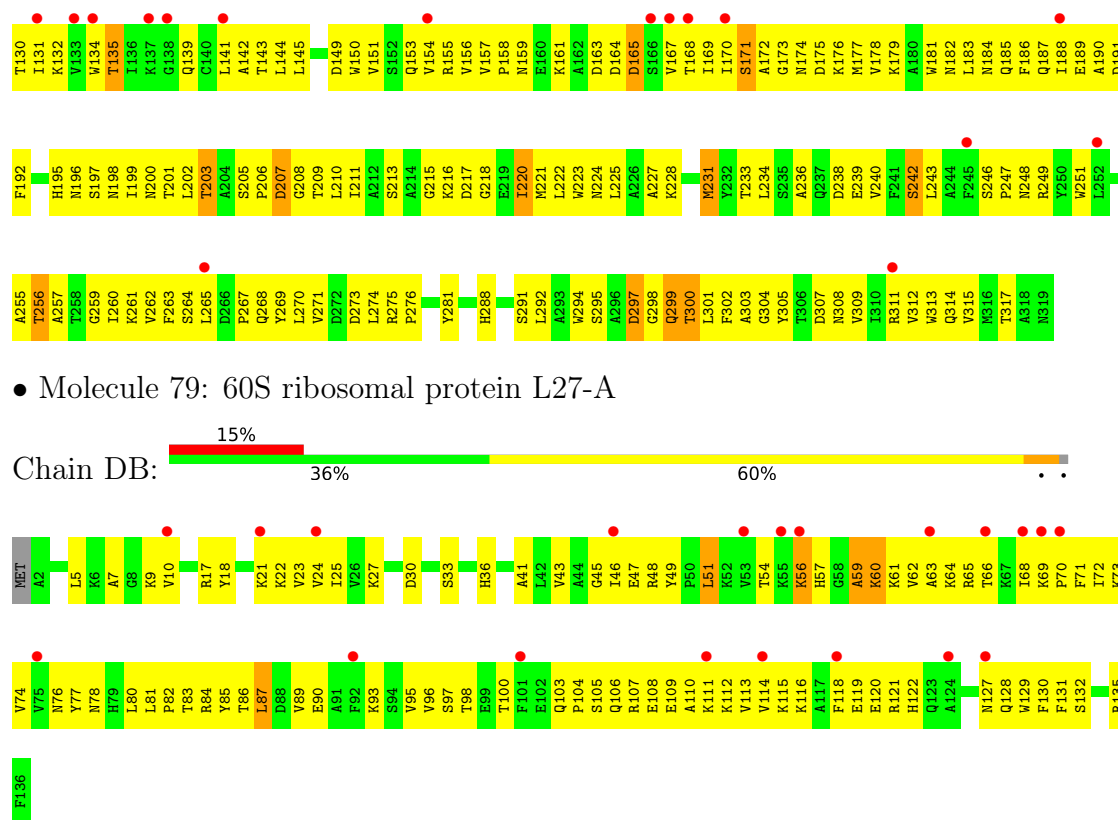


• Molecule 78: Guanine nucleotide-binding protein subunit beta-like protein

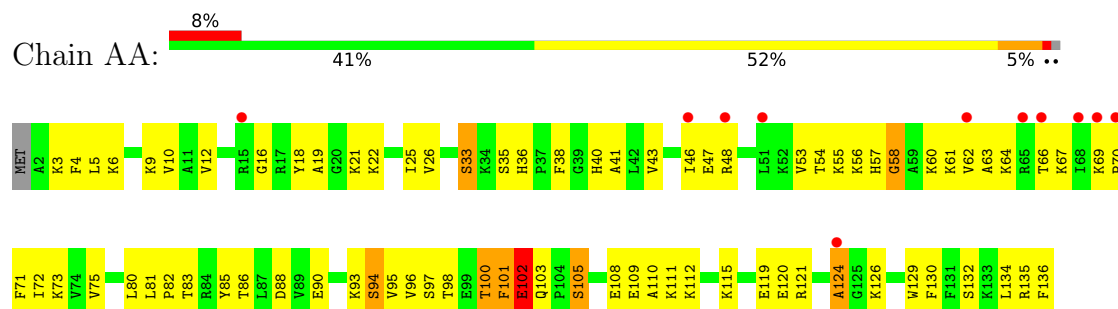


• Molecule 78: Guanine nucleotide-binding protein subunit beta-like protein





• Molecule 79: 60S ribosomal protein L27-A



• Molecule 79: 60S ribosomal protein L27-A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	302.09Å 285.96Å 433.31Å 90.00° 98.92° 90.00°	Depositor
Resolution (Å)	95.96 – 2.90 95.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (95.96-2.90) 91.1 (95.96-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.69 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.218 , 0.230 0.218 , 0.247	Depositor DCC
R_{free} test set	1573356 reflections (1.56%)	wwPDB-VP
Wilson B-factor (Å ²)	67.8	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	402407	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, ZN, MG, OHX, SPD, ZWB

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	3	0.12	0/2883	0.32	0/4491
1	AS	0.12	0/2883	0.32	0/4491
2	AB	0.24	0/1204	0.78	7/1612 (0.4%)
2	DC	0.23	0/1204	0.75	3/1612 (0.2%)
3	CJ	0.29	0/1794	0.61	0/2425
3	p	0.22	0/1836	0.55	0/2481
4	AI	0.21	0/978	0.62	2/1301 (0.2%)
4	DJ	0.20	0/978	0.65	4/1301 (0.3%)
5	Q	0.30	0/948	0.74	2/1273 (0.2%)
5	c5	0.30	0/1060	0.78	0/1426
6	H	0.29	0/1823	0.70	3/2439 (0.1%)
6	s6	0.20	0/1779	0.49	0/2379
7	4	0.12	0/3746	0.35	0/5832
7	AT	0.12	0/3746	0.34	2/5832 (0.0%)
8	AC	0.19	0/445	0.56	0/593
8	DD	0.22	0/473	0.66	0/629
9	CK	0.20	0/1539	0.50	0/2073
9	q	0.29	0/1539	0.65	0/2073
10	AJ	0.22	0/778	0.58	0/1034
10	DK	0.25	0/756	0.63	0/1005
11	R	0.27	0/1125	0.79	2/1510 (0.1%)
11	c6	0.28	0/1131	0.72	1/1518 (0.1%)
12	I	0.40	0/1506	1.05	10/2028 (0.5%)
12	s7	0.38	0/1516	0.89	3/2043 (0.1%)
13	CD	0.18	0/1948	0.50	0/2617
13	j	0.19	0/1948	0.54	0/2617
14	AD	0.21	0/748	0.51	0/1004
14	DE	0.23	0/751	0.52	0/1008
15	CL	0.20	0/1721	0.58	4/2307 (0.2%)
15	r	0.44	3/1741 (0.2%)	0.55	1/2335 (0.0%)
16	AK	0.19	0/696	0.52	0/923
16	DL	0.16	0/696	0.45	0/923

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	S	0.31	0/870	0.87	0/1165
17	c7	0.28	0/914	0.68	2/1224 (0.2%)
18	J	0.24	0/1514	0.64	0/2021
18	s8	0.23	0/1514	0.69	5/2021 (0.2%)
19	CE	0.18	0/3146	0.52	0/4228
19	k	0.19	0/3146	0.55	0/4228
20	AE	0.20	0/890	0.52	0/1196
20	DF	0.20	0/880	0.49	0/1182
21	CM	0.23	0/1374	0.56	0/1842
21	s	0.34	0/1374	0.80	5/1842 (0.3%)
22	AL	0.22	0/618	0.57	0/826
22	DM	0.23	0/591	0.56	0/789
23	T	0.39	0/1211	0.91	10/1628 (0.6%)
23	c8	0.25	0/1134	0.70	2/1524 (0.1%)
24	K	0.28	0/1461	0.71	1/1959 (0.1%)
24	s9	0.26	0/1519	0.67	1/2035 (0.0%)
25	CF	0.20	0/2800	0.53	0/3790
25	l	0.20	0/2800	0.55	1/3790 (0.0%)
26	AF	0.27	0/1041	0.56	2/1394 (0.1%)
26	DG	0.15	0/1041	0.45	0/1394
27	CN	0.25	0/1568	0.66	1/2106 (0.0%)
27	t	0.17	0/1568	0.52	0/2106
28	AM	0.18	0/443	0.54	0/588
28	DN	0.17	0/443	0.51	0/588
29	U	0.26	0/1130	0.78	3/1517 (0.2%)
29	c9	0.22	0/1130	0.56	0/1517
30	L	0.20	0/759	0.57	0/1025
30	c0	0.28	0/623	0.87	2/838 (0.2%)
31	CG	0.20	0/2398	0.54	0/3235
31	m	0.23	0/2425	0.63	5/3271 (0.2%)
32	AG	0.18	0/868	0.51	0/1168
32	DH	0.21	0/868	0.52	0/1168
33	CO	0.20	0/1068	0.51	0/1438
33	u	0.24	0/1068	0.56	1/1438 (0.1%)
34	AN	0.19	0/423	0.49	0/562
34	DO	0.21	0/423	0.55	0/562
35	V	0.35	0/865	0.84	0/1169
35	d0	0.24	0/593	0.71	0/797
36	M	0.19	0/1145	0.51	0/1543
36	c1	0.19	0/1194	0.52	0/1610
37	CH	0.20	0/1260	0.54	0/1694
37	n	0.17	0/1260	0.46	0/1694
38	AH	0.19	0/890	0.55	0/1189

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DI	0.29	0/890	0.73	0/1189
39	CP	0.16	0/1757	0.43	0/2354
39	v	0.18	0/1757	0.46	0/2354
40	AO	0.14	0/234	0.50	0/300
40	DP	0.17	0/234	0.45	0/300
41	W	0.28	0/693	0.67	0/935
41	d1	0.21	0/693	0.61	2/935 (0.2%)
42	O	0.23	0/1215	0.60	0/1638
42	c3	0.21	0/1215	0.60	2/1638 (0.1%)
43	CI	0.18	0/1821	0.52	0/2451
43	o	0.17	0/1821	0.49	0/2451
44	CQ	0.17	0/1585	0.46	0/2128
44	w	0.17	0/1585	0.48	0/2128
45	AP	0.58	0/860	0.97	0/1136
45	DQ	0.69	1/860 (0.1%)	0.99	4/1136 (0.4%)
46	X	0.31	0/1038	0.71	1/1395 (0.1%)
46	d2	0.22	0/1038	0.55	0/1395
47	P	0.29	0/605	0.88	2/813 (0.2%)
47	c4	0.23	0/960	0.66	1/1290 (0.1%)
48	CR	0.15	0/1250	0.44	0/1683
48	x	0.17	0/1438	0.47	0/1937
49	AQ	0.17	0/701	0.60	0/934
49	DR	0.17	0/701	0.62	0/934
50	Y	0.22	0/1139	0.62	0/1518
50	d3	0.26	0/1139	0.68	1/1518 (0.1%)
51	CS	0.20	0/1465	0.56	0/1965
51	y	0.19	0/1465	0.51	2/1965 (0.1%)
52	p0	0.32	0/977	0.69	0/1313
53	Z	0.30	0/1087	0.63	0/1449
53	d4	0.28	0/1087	0.76	2/1449 (0.1%)
54	CT	0.21	0/1478	0.54	0/1969
54	z	0.21	0/1499	0.55	0/1998
55	i	0.25	0/1019	0.70	1/1371 (0.1%)
55	sM	0.40	1/480 (0.2%)	0.74	1/642 (0.2%)
56	a	0.28	0/521	0.82	0/698
56	d5	0.29	0/566	0.78	1/761 (0.1%)
57	0	0.22	0/1481	0.50	0/1990
57	CU	0.17	0/1481	0.44	0/1990
58	A	0.14	0/41046	0.39	1/63949 (0.0%)
58	sR	0.14	0/42490	0.38	0/66207
59	b	0.27	0/755	0.76	0/1008
59	d6	0.45	1/782 (0.1%)	0.74	1/1047 (0.1%)
60	2	0.19	0/1300	0.53	0/1743

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	CV	0.19	0/1300	0.52	0/1743
61	B	0.32	0/1617	0.85	3/2215 (0.1%)
61	s0	0.45	0/1623	0.82	3/2222 (0.1%)
62	c	0.21	0/620	0.75	0/838
62	d7	0.27	0/620	0.81	2/838 (0.2%)
63	5	0.26	0/812	0.64	0/1099
63	CW	0.28	0/794	0.66	0/1076
64	C	0.29	0/955	0.90	4/1286 (0.3%)
64	s1	0.27	0/1748	0.62	1/2352 (0.0%)
65	d	0.26	0/499	1.14	8/670 (1.2%)
65	d8	0.37	0/499	0.91	2/670 (0.3%)
66	6	0.20	0/1018	0.50	0/1369
66	CX	0.18	0/1018	0.46	0/1369
67	D	0.25	0/1665	0.64	2/2263 (0.1%)
67	s2	0.24	0/1665	0.65	1/2263 (0.0%)
68	d9	0.30	0/412	0.73	0/544
68	e	0.21	0/452	0.71	2/600 (0.3%)
69	7	0.38	0/533	0.79	4/707 (0.6%)
69	CY	0.18	0/807	0.47	0/1087
70	E	0.31	0/1759	0.67	0/2368
70	s3	0.28	0/1759	0.74	1/2368 (0.0%)
71	e0	0.30	0/499	0.65	0/665
71	f	0.21	0/483	0.67	0/643
72	8	0.16	0/952	0.48	0/1285
72	CZ	0.18	0/952	0.54	0/1285
73	F	0.29	0/2109	0.79	6/2839 (0.2%)
73	s4	0.25	0/2109	0.65	2/2839 (0.1%)
74	g	0.30	0/577	0.89	2/770 (0.3%)
75	1	0.13	0/75394	0.37	2/117545 (0.0%)
75	AR	0.13	0/75088	0.36	1/117067 (0.0%)
76	9	0.16	0/1004	0.51	0/1341
76	DA	0.17	0/987	0.49	0/1318
77	G	0.61	3/1629 (0.2%)	0.94	7/2202 (0.3%)
77	s5	0.42	1/1629 (0.1%)	0.88	6/2202 (0.3%)
78	Rb	0.36	1/2495 (0.0%)	0.75	1/3395 (0.0%)
78	h	0.27	0/2432	0.77	8/3309 (0.2%)
79	AA	0.24	0/1118	0.61	0/1497
79	DB	0.25	0/1118	0.68	0/1497
All	All	0.20	11/423127 (0.0%)	0.49	175/621686 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	5
2	DC	0	1
3	CJ	0	2
3	p	0	2
4	AI	0	2
4	DJ	0	3
5	Q	0	3
5	c5	0	3
6	H	0	4
6	s6	0	1
9	CK	0	1
9	q	0	4
11	R	0	6
11	c6	0	2
12	I	0	19
12	s7	0	5
13	CD	0	2
13	j	0	1
14	DE	0	1
15	CL	0	3
15	r	0	2
16	AK	0	1
17	S	0	2
17	c7	0	2
18	J	0	3
18	s8	0	3
19	CE	0	2
19	k	0	2
21	CM	0	1
21	s	0	3
22	DM	0	2
23	T	0	4
23	c8	0	4
24	K	0	3
24	s9	0	3
25	CF	0	1
25	l	0	6
26	AF	0	2
26	DG	0	1
27	CN	0	6
27	t	0	4
28	DN	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
29	U	0	7
29	c9	0	1
30	L	0	1
30	c0	0	4
31	CG	0	7
31	m	0	4
32	DH	0	1
33	u	0	2
35	V	0	6
35	d0	0	4
36	c1	0	4
37	CH	0	1
38	AH	0	2
38	DI	0	2
41	d1	0	1
42	O	0	2
42	c3	0	2
43	CI	0	3
43	o	0	4
44	CQ	0	1
44	w	0	1
45	AP	0	1
46	X	0	2
46	d2	0	1
47	P	0	1
47	c4	0	2
49	AQ	0	1
49	DR	0	1
50	Y	0	2
50	d3	0	2
53	Z	0	2
53	d4	0	5
54	CT	0	4
54	z	0	3
55	i	0	5
55	sM	0	3
56	a	0	5
56	d5	0	1
57	0	0	3
57	CU	0	1
59	b	0	1
60	2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
60	CV	0	1
61	B	0	9
61	s0	0	6
62	c	0	4
62	d7	0	3
63	CW	0	1
64	C	0	6
65	d	0	1
65	d8	0	3
67	D	0	1
68	e	0	2
69	CY	0	1
70	E	0	7
70	s3	0	11
71	e0	0	4
73	F	0	5
73	s4	0	4
74	g	0	7
77	G	0	7
77	s5	0	6
78	Rb	0	4
78	h	0	7
79	AA	0	5
79	DB	0	2
All	All	0	342

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	DQ	56	PRO	N-CD	-11.46	1.31	1.47
77	G	30	PRO	CG-CD	-10.35	1.15	1.50
77	G	30	PRO	N-CA	8.28	1.57	1.47
77	G	30	PRO	CA-CB	-7.98	1.42	1.53
15	r	213	PHE	C-O	-7.96	1.20	1.23

The worst 5 of 175 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	I	173	TYR	CA-C-N	12.91	146.20	121.54
12	I	173	TYR	C-N-CA	12.91	146.20	121.54
78	h	171	SER	CA-C-N	10.69	141.95	121.54
78	h	171	SER	C-N-CA	10.69	141.95	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	B	172	LEU	CB-CG-CD1	-10.08	80.47	110.70

There are no chirality outliers.

5 of 342 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	116	GLY	Peptide
2	AB	45	MET	Peptide
2	AB	66	ALA	Peptide
2	AB	92	LYS	Peptide
2	AB	97	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	2579	0	1303	61	0
1	AS	2579	0	1304	44	0
2	AB	1173	0	1215	69	0
2	DC	1173	0	1215	87	0
3	CJ	1762	0	1839	126	0
3	p	1804	0	1877	84	0
4	AI	969	0	1078	51	0
4	DJ	969	0	1078	58	0
5	Q	928	0	958	90	0
5	c5	1039	0	1050	100	0
6	H	1799	0	1879	147	0
6	s6	1755	0	1845	82	0
7	4	3353	0	1695	78	0
7	AT	3353	0	1695	76	0
8	AC	434	0	455	22	0
8	DD	462	0	491	24	0
9	CK	1518	0	1587	72	1
9	q	1518	0	1587	110	0
10	AJ	771	0	849	40	0
10	DK	750	0	829	65	0
11	R	1105	0	1166	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	c6	1111	0	1171	117	1
12	I	1481	0	1572	150	0
12	s7	1491	0	1578	125	0
13	CD	1914	0	1981	87	0
13	j	1914	0	1981	84	0
14	AD	740	0	788	35	0
14	DE	743	0	797	51	0
15	CL	1685	0	1719	80	0
15	r	1705	0	1736	92	0
16	AK	681	0	683	26	0
16	DL	681	0	683	22	0
17	S	863	0	872	74	0
17	c7	906	0	909	73	0
18	J	1489	0	1525	103	0
18	s8	1489	0	1525	102	0
19	CE	3075	0	3142	119	0
19	k	3075	0	3142	163	0
20	AE	876	0	912	45	0
20	DF	866	0	908	30	0
21	CM	1353	0	1383	86	0
21	s	1353	0	1383	99	0
22	AL	612	0	682	30	0
22	DM	586	0	654	31	0
23	T	1192	0	1222	111	0
23	c8	1116	0	1149	105	1
24	K	1436	0	1517	134	0
24	s9	1494	0	1573	130	0
25	CF	2748	0	2859	118	0
25	l	2748	0	2858	114	0
26	AF	1020	0	1090	36	0
26	DG	1020	0	1090	40	0
27	CN	1543	0	1608	104	0
27	t	1543	0	1608	74	0
28	AM	436	0	475	24	0
28	DN	436	0	475	22	0
29	U	1112	0	1124	101	0
29	c9	1112	0	1124	91	0
30	L	742	0	715	57	0
30	c0	609	0	603	59	0
31	CG	2348	0	2301	114	0
31	m	2375	0	2325	128	0
32	AG	850	0	880	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	DH	850	0	880	38	0
33	CO	1053	0	1149	49	0
33	u	1053	0	1149	56	0
34	AN	417	0	455	17	0
34	DO	417	0	455	13	0
35	V	855	0	917	88	0
35	d0	585	0	622	41	0
36	M	1119	0	1186	54	0
36	c1	1168	0	1233	41	0
37	CH	1239	0	1326	71	0
37	n	1239	0	1326	46	0
38	AH	880	0	942	44	0
38	DI	880	0	945	58	0
39	CP	1720	0	1779	97	0
39	v	1720	0	1779	78	0
40	AO	233	0	284	13	0
40	DP	233	0	284	14	0
41	W	684	0	672	64	0
41	d1	684	0	672	40	0
42	O	1192	0	1255	65	0
42	c3	1192	0	1255	72	0
43	CI	1784	0	1862	65	0
43	o	1784	0	1862	58	0
44	CQ	1555	0	1659	55	0
44	w	1555	0	1659	65	0
45	AP	847	0	916	68	0
45	DQ	847	0	914	87	0
46	X	1021	0	1060	81	0
46	d2	1021	0	1060	64	0
47	P	600	0	559	39	0
47	c4	949	0	985	69	0
48	CR	1227	0	1236	44	0
48	x	1415	0	1432	56	0
49	AQ	694	0	734	33	0
49	DR	694	0	734	37	0
50	Y	1121	0	1196	77	0
50	d3	1121	0	1196	59	0
51	CS	1441	0	1543	61	0
51	y	1441	0	1543	65	0
52	p0	962	0	989	59	0
53	Z	1073	0	1132	101	0
53	d4	1073	0	1132	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	CT	1461	0	1558	89	0
54	z	1482	0	1578	78	0
55	i	1010	0	958	57	0
55	sM	475	0	492	35	0
56	a	514	0	545	63	0
56	d5	558	0	598	54	0
57	0	1445	0	1487	48	0
57	CU	1445	0	1487	54	0
58	A	36700	0	18465	1145	0
58	sR	37990	0	19116	989	0
59	b	743	0	788	55	0
59	d6	769	0	814	60	0
60	2	1276	0	1323	55	0
60	CV	1276	0	1323	59	0
61	B	1577	0	1567	157	0
61	s0	1583	0	1578	168	0
62	c	610	0	632	37	0
62	d7	610	0	631	60	0
63	5	796	0	812	51	0
63	CW	778	0	791	45	0
64	C	943	0	1003	93	0
64	s1	1722	0	1793	127	0
65	d	497	0	535	35	0
65	d8	497	0	535	45	0
66	6	1003	0	1048	34	0
66	CX	1003	0	1048	46	0
67	D	1635	0	1723	139	0
67	s2	1635	0	1723	81	0
68	d9	404	0	397	34	0
68	e	442	0	428	23	0
69	7	521	0	551	34	0
69	CY	796	0	701	24	0
70	E	1734	0	1817	134	0
70	s3	1734	0	1817	145	0
71	e0	491	0	542	34	0
71	f	475	0	525	36	0
72	8	937	0	994	47	0
72	CZ	937	0	994	42	0
73	F	2068	0	2154	178	0
73	s4	2068	0	2154	125	0
74	g	566	0	602	37	0
75	1	67355	0	33846	1366	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	AR	67082	0	33708	1421	0
76	9	993	0	1081	33	0
76	DA	976	0	1064	51	0
77	G	1609	0	1675	213	0
77	s5	1609	0	1675	205	0
78	Rb	2442	0	2392	249	0
78	h	2379	0	2324	206	0
79	AA	1092	0	1155	72	0
79	DB	1092	0	1155	87	0
80	1	2044	0	0	232	0
80	2	7	0	0	2	0
80	3	70	0	0	8	0
80	4	91	0	0	15	0
80	A	865	0	0	121	0
80	AC	7	0	0	1	0
80	AG	7	0	0	1	0
80	AK	14	0	0	4	0
80	AR	2089	0	0	243	0
80	AS	63	0	0	1	0
80	AT	98	0	0	8	0
80	C	7	0	0	2	0
80	CE	14	0	0	0	0
80	CG	14	0	0	2	0
80	CK	7	0	0	1	0
80	CL	14	0	0	1	0
80	CP	7	0	0	1	0
80	CS	7	0	0	0	0
80	CV	7	0	0	1	0
80	CX	7	0	0	0	0
80	DD	7	0	0	0	0
80	DH	7	0	0	1	0
80	DL	7	0	0	0	0
80	J	7	0	0	1	0
80	O	7	0	0	0	0
80	Q	7	0	0	2	0
80	Rb	7	0	0	1	0
80	T	7	0	0	2	0
80	U	7	0	0	1	0
80	c3	7	0	0	1	0
80	c5	7	0	0	1	0
80	c8	7	0	0	1	0
80	d4	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	h	7	0	0	1	0
80	k	14	0	0	3	0
80	r	7	0	0	1	0
80	s1	7	0	0	2	0
80	s4	7	0	0	0	0
80	sR	966	0	0	109	0
80	v	7	0	0	0	0
80	w	7	0	0	1	0
80	x	7	0	0	0	0
81	1	487	0	0	0	0
81	3	12	0	0	0	0
81	4	20	0	0	0	0
81	6	3	0	0	0	0
81	9	1	0	0	0	0
81	A	134	0	0	0	0
81	AB	7	0	0	0	0
81	AF	4	0	0	0	0
81	AH	1	0	0	0	0
81	AK	2	0	0	0	0
81	AO	1	0	0	0	0
81	AR	506	0	0	0	0
81	AS	22	0	0	0	0
81	AT	18	0	0	0	0
81	CD	3	0	0	0	0
81	CE	4	0	0	0	0
81	CF	2	0	0	0	0
81	CG	3	0	0	0	0
81	CI	2	0	0	0	0
81	CJ	1	0	0	0	0
81	CK	2	0	0	0	0
81	CL	1	0	0	0	0
81	CM	2	0	0	0	0
81	CO	1	0	0	0	0
81	CP	4	0	0	0	0
81	CQ	3	0	0	0	0
81	CR	6	0	0	0	0
81	CS	1	0	0	0	0
81	CU	2	0	0	0	0
81	CX	1	0	0	0	0
81	D	1	0	0	0	0
81	DA	2	0	0	0	0
81	DC	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	DD	1	0	0	0	0
81	DG	1	0	0	0	0
81	DH	2	0	0	0	0
81	DI	1	0	0	0	0
81	DL	2	0	0	0	0
81	DO	1	0	0	0	0
81	DP	1	0	0	0	0
81	DQ	2	0	0	0	0
81	U	1	0	0	0	0
81	Y	1	0	0	0	0
81	c4	1	0	0	0	0
81	c6	2	0	0	0	0
81	c7	1	0	0	0	0
81	c8	1	0	0	0	0
81	c9	1	0	0	0	0
81	d2	1	0	0	0	0
81	d3	3	0	0	0	0
81	d4	1	0	0	0	0
81	d5	1	0	0	0	0
81	d6	2	0	0	0	0
81	e	1	0	0	0	0
81	j	2	0	0	0	0
81	k	2	0	0	0	0
81	l	4	0	0	0	0
81	m	1	0	0	0	0
81	o	2	0	0	0	0
81	r	3	0	0	0	0
81	s	1	0	0	0	0
81	s1	1	0	0	0	0
81	s2	1	0	0	0	0
81	s4	2	0	0	0	0
81	s8	2	0	0	0	0
81	s9	1	0	0	0	0
81	sM	2	0	0	0	0
81	sR	160	0	0	0	0
81	t	2	0	0	0	0
81	v	4	0	0	0	0
81	w	1	0	0	0	0
81	x	8	0	0	0	0
81	z	1	0	0	0	0
82	AK	1	0	0	0	0
82	AN	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
82	AP	1	0	0	0	0
82	AQ	1	0	0	0	0
82	DL	1	0	0	0	0
82	DO	1	0	0	0	0
82	DQ	1	0	0	0	0
82	DR	1	0	0	0	0
82	b	1	0	0	0	0
82	c	1	0	0	0	0
82	d6	1	0	0	0	0
82	d7	1	0	0	0	0
82	d9	1	0	0	0	0
82	e	1	0	0	0	0
82	g	1	0	0	0	0
83	1	1	0	0	0	0
83	AR	3	0	0	0	0
84	1	26	0	0	1	0
84	AR	26	0	0	0	0
85	1	10	0	19	5	0
85	AR	30	0	57	4	0
86	1	137	0	0	8	0
86	3	3	0	0	0	0
86	A	46	0	0	0	0
86	AE	1	0	0	0	0
86	AK	3	0	0	0	0
86	AR	131	0	0	4	0
86	AT	8	0	0	0	0
86	CK	3	0	0	2	0
86	CM	1	0	0	0	0
86	CP	3	0	0	0	0
86	CQ	2	0	0	0	0
86	CR	3	0	0	1	0
86	DN	2	0	0	0	0
86	DR	1	0	0	0	0
86	J	1	0	0	1	0
86	R	1	0	0	0	0
86	k	1	0	0	0	0
86	s8	1	0	0	0	0
86	s9	2	0	0	0	0
86	sR	61	0	0	5	0
86	v	1	0	0	0	0
All	All	402407	0	291063	13733	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 13733 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:DQ:78:LYS:O	45:DQ:78:LYS:HD3	1.32	1.21
45:DQ:100:LYS:CD	45:DQ:101:GLY:H	1.60	1.15
59:b:79:ILE:HA	59:b:84:VAL:HG11	1.28	1.12
46:X:20:THR:HB	46:X:22:LYS:HD2	1.31	1.10
12:I:101:LYS:HA	12:I:112:ARG:HH12	0.93	1.07

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:CK:14:GLU:OE1	23:c8:79:TYR:OH[2_746]	2.03	0.17
11:c6:2:SER:OG	75:1:3288:G:O4'[2_656]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	146/149 (98%)	135 (92%)	11 (8%)	0	100	100
2	DC	146/149 (98%)	138 (94%)	8 (6%)	0	100	100
3	CJ	225/256 (88%)	217 (96%)	8 (4%)	0	100	100
3	p	231/256 (90%)	228 (99%)	3 (1%)	0	100	100
4	AI	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
4	DJ	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
5	Q	115/142 (81%)	106 (92%)	9 (8%)	0	100	100
5	c5	133/142 (94%)	115 (86%)	15 (11%)	3 (2%)	5	20
6	H	224/236 (95%)	215 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	s6	216/236 (92%)	211 (98%)	5 (2%)	0	100	100
8	AC	52/59 (88%)	51 (98%)	1 (2%)	0	100	100
8	DD	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
9	CK	189/191 (99%)	186 (98%)	3 (2%)	0	100	100
9	q	189/191 (99%)	181 (96%)	8 (4%)	0	100	100
10	AJ	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
10	DK	95/100 (95%)	92 (97%)	3 (3%)	0	100	100
11	R	139/143 (97%)	132 (95%)	6 (4%)	1 (1%)	19	49
11	c6	140/143 (98%)	134 (96%)	5 (4%)	1 (1%)	19	49
12	I	182/190 (96%)	162 (89%)	18 (10%)	2 (1%)	12	37
12	s7	184/190 (97%)	173 (94%)	10 (5%)	1 (0%)	25	56
13	CD	250/254 (98%)	246 (98%)	4 (2%)	0	100	100
13	j	250/254 (98%)	249 (100%)	1 (0%)	0	100	100
14	AD	95/105 (90%)	93 (98%)	2 (2%)	0	100	100
14	DE	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
15	CL	203/221 (92%)	199 (98%)	4 (2%)	0	100	100
15	r	207/221 (94%)	204 (99%)	3 (1%)	0	100	100
16	AK	85/88 (97%)	85 (100%)	0	0	100	100
16	DL	85/88 (97%)	85 (100%)	0	0	100	100
17	S	105/136 (77%)	99 (94%)	6 (6%)	0	100	100
17	c7	113/136 (83%)	109 (96%)	4 (4%)	0	100	100
18	J	184/200 (92%)	171 (93%)	13 (7%)	0	100	100
18	s8	184/200 (92%)	177 (96%)	7 (4%)	0	100	100
19	CE	384/387 (99%)	379 (99%)	5 (1%)	0	100	100
19	k	384/387 (99%)	373 (97%)	11 (3%)	0	100	100
20	AE	107/113 (95%)	104 (97%)	3 (3%)	0	100	100
20	DF	105/113 (93%)	100 (95%)	5 (5%)	0	100	100
21	CM	167/174 (96%)	161 (96%)	6 (4%)	0	100	100
21	s	167/174 (96%)	155 (93%)	12 (7%)	0	100	100
22	AL	75/78 (96%)	75 (100%)	0	0	100	100
22	DM	69/78 (88%)	67 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	T	143/146 (98%)	129 (90%)	13 (9%)	1 (1%)	19	49
23	c8	133/146 (91%)	125 (94%)	8 (6%)	0	100	100
24	K	175/197 (89%)	167 (95%)	8 (5%)	0	100	100
24	s9	183/197 (93%)	179 (98%)	4 (2%)	0	100	100
25	CF	359/362 (99%)	351 (98%)	8 (2%)	0	100	100
25	l	359/362 (99%)	343 (96%)	16 (4%)	0	100	100
26	AF	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
26	DG	125/130 (96%)	125 (100%)	0	0	100	100
27	CN	191/199 (96%)	176 (92%)	13 (7%)	2 (1%)	13	40
27	t	191/199 (96%)	182 (95%)	8 (4%)	1 (0%)	25	56
28	AM	48/51 (94%)	48 (100%)	0	0	100	100
28	DN	48/51 (94%)	48 (100%)	0	0	100	100
29	U	141/144 (98%)	132 (94%)	9 (6%)	0	100	100
29	c9	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
30	L	88/105 (84%)	82 (93%)	6 (7%)	0	100	100
30	c0	70/105 (67%)	64 (91%)	6 (9%)	0	100	100
31	CG	290/297 (98%)	285 (98%)	5 (2%)	0	100	100
31	m	294/297 (99%)	280 (95%)	13 (4%)	1 (0%)	37	66
32	AG	104/107 (97%)	102 (98%)	2 (2%)	0	100	100
32	DH	104/107 (97%)	102 (98%)	2 (2%)	0	100	100
33	CO	134/138 (97%)	134 (100%)	0	0	100	100
33	u	134/138 (97%)	131 (98%)	3 (2%)	0	100	100
34	AN	50/128 (39%)	50 (100%)	0	0	100	100
34	DO	50/128 (39%)	48 (96%)	2 (4%)	0	100	100
35	V	105/121 (87%)	98 (93%)	7 (7%)	0	100	100
35	d0	70/121 (58%)	67 (96%)	3 (4%)	0	100	100
36	M	136/156 (87%)	135 (99%)	1 (1%)	0	100	100
36	c1	144/156 (92%)	138 (96%)	6 (4%)	0	100	100
37	CH	152/176 (86%)	150 (99%)	2 (1%)	0	100	100
37	n	152/176 (86%)	152 (100%)	0	0	100	100
38	AH	110/121 (91%)	108 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	DI	110/121 (91%)	110 (100%)	0	0	100	100
39	CP	201/204 (98%)	201 (100%)	0	0	100	100
39	v	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
40	AO	23/25 (92%)	23 (100%)	0	0	100	100
40	DP	23/25 (92%)	23 (100%)	0	0	100	100
41	W	85/87 (98%)	79 (93%)	6 (7%)	0	100	100
41	d1	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
42	O	148/151 (98%)	144 (97%)	3 (2%)	1 (1%)	19	49
42	c3	148/151 (98%)	143 (97%)	5 (3%)	0	100	100
43	CI	220/244 (90%)	211 (96%)	9 (4%)	0	100	100
43	o	220/244 (90%)	211 (96%)	9 (4%)	0	100	100
44	CQ	195/199 (98%)	191 (98%)	3 (2%)	1 (0%)	25	56
44	w	195/199 (98%)	190 (97%)	5 (3%)	0	100	100
45	AP	103/106 (97%)	95 (92%)	6 (6%)	2 (2%)	6	24
45	DQ	103/106 (97%)	100 (97%)	2 (2%)	1 (1%)	13	40
46	X	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
46	d2	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
47	P	80/138 (58%)	70 (88%)	9 (11%)	1 (1%)	10	33
47	c4	126/138 (91%)	120 (95%)	5 (4%)	1 (1%)	16	45
48	CR	153/184 (83%)	152 (99%)	1 (1%)	0	100	100
48	x	180/184 (98%)	179 (99%)	1 (1%)	0	100	100
49	AQ	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
49	DR	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
50	Y	142/145 (98%)	131 (92%)	11 (8%)	0	100	100
50	d3	142/145 (98%)	133 (94%)	9 (6%)	0	100	100
51	CS	183/186 (98%)	181 (99%)	2 (1%)	0	100	100
51	y	183/186 (98%)	180 (98%)	3 (2%)	0	100	100
52	p0	116/311 (37%)	110 (95%)	5 (4%)	1 (1%)	14	43
53	Z	132/135 (98%)	128 (97%)	4 (3%)	0	100	100
53	d4	132/135 (98%)	119 (90%)	13 (10%)	0	100	100
54	CT	178/189 (94%)	175 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	z	181/189 (96%)	176 (97%)	5 (3%)	0	100	100
55	i	136/273 (50%)	124 (91%)	12 (9%)	0	100	100
55	sM	61/273 (22%)	57 (93%)	4 (7%)	0	100	100
56	a	60/108 (56%)	54 (90%)	6 (10%)	0	100	100
56	d5	67/108 (62%)	66 (98%)	1 (2%)	0	100	100
57	0	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
57	CU	170/172 (99%)	169 (99%)	1 (1%)	0	100	100
59	b	89/119 (75%)	79 (89%)	9 (10%)	1 (1%)	12	37
59	d6	95/119 (80%)	90 (95%)	4 (4%)	1 (1%)	12	37
60	2	157/160 (98%)	156 (99%)	1 (1%)	0	100	100
60	CV	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
61	B	204/252 (81%)	188 (92%)	16 (8%)	0	100	100
61	s0	204/252 (81%)	189 (93%)	15 (7%)	0	100	100
62	c	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
62	d7	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
63	5	98/121 (81%)	96 (98%)	2 (2%)	0	100	100
63	CW	96/121 (79%)	92 (96%)	4 (4%)	0	100	100
64	C	114/255 (45%)	107 (94%)	7 (6%)	0	100	100
64	s1	214/255 (84%)	211 (99%)	3 (1%)	0	100	100
65	d	61/67 (91%)	58 (95%)	3 (5%)	0	100	100
65	d8	61/67 (91%)	51 (84%)	10 (16%)	0	100	100
66	6	134/137 (98%)	134 (100%)	0	0	100	100
66	CX	134/137 (98%)	134 (100%)	0	0	100	100
67	D	215/254 (85%)	202 (94%)	12 (6%)	1 (0%)	25	56
67	s2	215/254 (85%)	210 (98%)	5 (2%)	0	100	100
68	d9	47/56 (84%)	43 (92%)	4 (8%)	0	100	100
68	e	51/56 (91%)	49 (96%)	2 (4%)	0	100	100
69	7	61/155 (39%)	61 (100%)	0	0	100	100
69	CY	112/155 (72%)	109 (97%)	3 (3%)	0	100	100
70	E	221/240 (92%)	215 (97%)	6 (3%)	0	100	100
70	s3	221/240 (92%)	210 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	e0	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
71	f	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
72	8	115/142 (81%)	114 (99%)	1 (1%)	0	100	100
72	CZ	115/142 (81%)	114 (99%)	1 (1%)	0	100	100
73	F	258/261 (99%)	246 (95%)	12 (5%)	0	100	100
73	s4	258/261 (99%)	252 (98%)	6 (2%)	0	100	100
74	g	69/152 (45%)	53 (77%)	16 (23%)	0	100	100
76	9	124/127 (98%)	124 (100%)	0	0	100	100
76	DA	122/127 (96%)	122 (100%)	0	0	100	100
77	G	204/225 (91%)	189 (93%)	13 (6%)	2 (1%)	13	40
77	s5	204/225 (91%)	193 (95%)	11 (5%)	0	100	100
78	Rb	316/319 (99%)	305 (96%)	10 (3%)	1 (0%)	37	66
78	h	308/319 (97%)	290 (94%)	18 (6%)	0	100	100
79	AA	133/136 (98%)	129 (97%)	3 (2%)	1 (1%)	16	45
79	DB	133/136 (98%)	126 (95%)	6 (4%)	1 (1%)	16	45
All	All	21536/24181 (89%)	20728 (96%)	779 (4%)	29 (0%)	48	77

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	m	234	ASP
52	p0	35	SER
11	c6	42	GLU
59	b	75	VAL
27	t	63	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	118/119 (99%)	112 (95%)	6 (5%)	20	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	DC	118/119 (99%)	116 (98%)	2 (2%)	56	83
3	CJ	182/208 (88%)	178 (98%)	4 (2%)	47	78
3	p	187/208 (90%)	183 (98%)	4 (2%)	48	78
4	AI	104/105 (99%)	100 (96%)	4 (4%)	28	63
4	DJ	104/105 (99%)	101 (97%)	3 (3%)	37	72
5	Q	97/118 (82%)	86 (89%)	11 (11%)	4	15
5	c5	103/118 (87%)	100 (97%)	3 (3%)	37	72
6	H	188/201 (94%)	179 (95%)	9 (5%)	21	54
6	s6	187/201 (93%)	184 (98%)	3 (2%)	58	84
8	AC	44/47 (94%)	43 (98%)	1 (2%)	45	77
8	DD	46/47 (98%)	46 (100%)	0	100	100
9	CK	171/171 (100%)	160 (94%)	11 (6%)	14	41
9	q	171/171 (100%)	164 (96%)	7 (4%)	26	60
10	AJ	81/82 (99%)	80 (99%)	1 (1%)	67	89
10	DK	79/82 (96%)	73 (92%)	6 (8%)	11	32
11	R	117/119 (98%)	111 (95%)	6 (5%)	20	51
11	c6	118/119 (99%)	109 (92%)	9 (8%)	11	32
12	I	165/170 (97%)	156 (94%)	9 (6%)	18	48
12	s7	165/170 (97%)	159 (96%)	6 (4%)	30	65
13	CD	193/196 (98%)	190 (98%)	3 (2%)	58	84
13	j	193/196 (98%)	188 (97%)	5 (3%)	41	74
14	AD	80/88 (91%)	78 (98%)	2 (2%)	42	75
14	DE	81/88 (92%)	78 (96%)	3 (4%)	29	64
15	CL	177/187 (95%)	172 (97%)	5 (3%)	38	73
15	r	177/187 (95%)	165 (93%)	12 (7%)	13	38
16	AK	70/71 (99%)	67 (96%)	3 (4%)	25	57
16	DL	70/71 (99%)	68 (97%)	2 (3%)	37	72
17	S	89/124 (72%)	79 (89%)	10 (11%)	5	16
17	c7	92/124 (74%)	86 (94%)	6 (6%)	14	40
18	J	150/161 (93%)	142 (95%)	8 (5%)	19	49
18	s8	150/161 (93%)	147 (98%)	3 (2%)	50	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	CE	320/323 (99%)	309 (97%)	11 (3%)	32	67
19	k	320/323 (99%)	296 (92%)	24 (8%)	11	33
20	AE	92/97 (95%)	91 (99%)	1 (1%)	70	90
20	DF	92/97 (95%)	88 (96%)	4 (4%)	25	57
21	CM	147/151 (97%)	138 (94%)	9 (6%)	15	43
21	s	147/151 (97%)	140 (95%)	7 (5%)	21	54
22	AL	68/69 (99%)	61 (90%)	7 (10%)	6	19
22	DM	66/69 (96%)	59 (89%)	7 (11%)	5	18
23	T	128/129 (99%)	118 (92%)	10 (8%)	10	31
23	c8	119/129 (92%)	111 (93%)	8 (7%)	13	39
24	K	153/166 (92%)	148 (97%)	5 (3%)	33	68
24	s9	158/166 (95%)	153 (97%)	5 (3%)	34	69
25	CF	288/289 (100%)	278 (96%)	10 (4%)	31	66
25	l	288/289 (100%)	276 (96%)	12 (4%)	25	59
26	AF	109/111 (98%)	106 (97%)	3 (3%)	38	73
26	DG	109/111 (98%)	105 (96%)	4 (4%)	29	64
27	CN	154/159 (97%)	148 (96%)	6 (4%)	27	62
27	t	154/159 (97%)	146 (95%)	8 (5%)	19	50
28	AM	45/46 (98%)	45 (100%)	0	100	100
28	DN	45/46 (98%)	41 (91%)	4 (9%)	8	26
29	U	115/116 (99%)	101 (88%)	14 (12%)	4	12
29	c9	115/116 (99%)	111 (96%)	4 (4%)	31	66
30	L	77/98 (79%)	71 (92%)	6 (8%)	10	31
30	c0	66/98 (67%)	63 (96%)	3 (4%)	23	56
31	CG	242/245 (99%)	230 (95%)	12 (5%)	20	52
31	m	244/245 (100%)	235 (96%)	9 (4%)	29	64
32	AG	90/91 (99%)	88 (98%)	2 (2%)	47	78
32	DH	90/91 (99%)	89 (99%)	1 (1%)	70	90
33	CO	107/109 (98%)	103 (96%)	4 (4%)	29	64
33	u	107/109 (98%)	105 (98%)	2 (2%)	52	81
34	AN	47/116 (40%)	46 (98%)	1 (2%)	48	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	DO	47/116 (40%)	45 (96%)	2 (4%)	25	57
35	V	100/114 (88%)	94 (94%)	6 (6%)	16	44
35	d0	68/114 (60%)	64 (94%)	4 (6%)	16	45
36	M	125/137 (91%)	120 (96%)	5 (4%)	27	61
36	c1	129/137 (94%)	123 (95%)	6 (5%)	22	55
37	CH	134/153 (88%)	130 (97%)	4 (3%)	36	71
37	n	134/153 (88%)	125 (93%)	9 (7%)	13	39
38	AH	95/103 (92%)	93 (98%)	2 (2%)	48	78
38	DI	95/103 (92%)	91 (96%)	4 (4%)	25	59
39	CP	175/176 (99%)	174 (99%)	1 (1%)	84	95
39	v	175/176 (99%)	174 (99%)	1 (1%)	84	95
40	AO	23/23 (100%)	23 (100%)	0	100	100
40	DP	23/23 (100%)	22 (96%)	1 (4%)	25	57
41	W	74/74 (100%)	71 (96%)	3 (4%)	26	60
41	d1	74/74 (100%)	69 (93%)	5 (7%)	13	38
42	O	127/128 (99%)	122 (96%)	5 (4%)	27	62
42	c3	127/128 (99%)	121 (95%)	6 (5%)	22	55
43	CI	186/205 (91%)	182 (98%)	4 (2%)	47	78
43	o	186/205 (91%)	183 (98%)	3 (2%)	58	84
44	CQ	160/162 (99%)	155 (97%)	5 (3%)	35	70
44	w	160/162 (99%)	156 (98%)	4 (2%)	42	75
45	AP	90/91 (99%)	87 (97%)	3 (3%)	33	68
45	DQ	90/91 (99%)	84 (93%)	6 (7%)	13	39
46	X	110/111 (99%)	106 (96%)	4 (4%)	30	65
46	d2	110/111 (99%)	108 (98%)	2 (2%)	54	82
47	P	53/105 (50%)	47 (89%)	6 (11%)	4	15
47	c4	97/105 (92%)	92 (95%)	5 (5%)	19	50
48	CR	125/146 (86%)	122 (98%)	3 (2%)	44	76
48	x	140/146 (96%)	133 (95%)	7 (5%)	20	52
49	AQ	71/72 (99%)	69 (97%)	2 (3%)	38	73
49	DR	71/72 (99%)	67 (94%)	4 (6%)	17	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	Y	119/120 (99%)	115 (97%)	4 (3%)	32	67
50	d3	119/120 (99%)	117 (98%)	2 (2%)	56	83
51	CS	150/151 (99%)	145 (97%)	5 (3%)	33	68
51	y	150/151 (99%)	146 (97%)	4 (3%)	40	73
52	p0	105/256 (41%)	101 (96%)	4 (4%)	28	63
53	Z	112/113 (99%)	103 (92%)	9 (8%)	10	30
53	d4	112/113 (99%)	103 (92%)	9 (8%)	10	30
54	CT	147/154 (96%)	146 (99%)	1 (1%)	81	94
54	z	149/154 (97%)	146 (98%)	3 (2%)	50	79
55	i	97/228 (42%)	87 (90%)	10 (10%)	6	19
55	sM	54/228 (24%)	51 (94%)	3 (6%)	17	47
56	a	55/89 (62%)	49 (89%)	6 (11%)	5	17
56	d5	61/89 (68%)	56 (92%)	5 (8%)	9	29
57	0	156/156 (100%)	150 (96%)	6 (4%)	28	63
57	CU	156/156 (100%)	142 (91%)	14 (9%)	8	25
59	b	81/100 (81%)	77 (95%)	4 (5%)	21	53
59	d6	83/100 (83%)	80 (96%)	3 (4%)	30	65
60	2	136/137 (99%)	131 (96%)	5 (4%)	29	64
60	CV	136/137 (99%)	124 (91%)	12 (9%)	8	26
61	B	164/210 (78%)	157 (96%)	7 (4%)	25	57
61	s0	165/210 (79%)	158 (96%)	7 (4%)	25	59
62	c	70/71 (99%)	62 (89%)	8 (11%)	4	15
62	d7	70/71 (99%)	67 (96%)	3 (4%)	25	57
63	5	87/107 (81%)	84 (97%)	3 (3%)	32	67
63	CW	85/107 (79%)	80 (94%)	5 (6%)	16	45
64	C	107/224 (48%)	98 (92%)	9 (8%)	9	28
64	s1	192/224 (86%)	184 (96%)	8 (4%)	25	59
65	d	56/60 (93%)	51 (91%)	5 (9%)	8	26
65	d8	56/60 (93%)	53 (95%)	3 (5%)	18	49
66	6	104/105 (99%)	100 (96%)	4 (4%)	28	63
66	CX	104/105 (99%)	101 (97%)	3 (3%)	37	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	D	176/205 (86%)	167 (95%)	9 (5%)	20	51
67	s2	176/205 (86%)	171 (97%)	5 (3%)	38	73
68	d9	43/49 (88%)	41 (95%)	2 (5%)	22	55
68	e	47/49 (96%)	44 (94%)	3 (6%)	14	41
69	7	55/129 (43%)	53 (96%)	2 (4%)	30	65
69	CY	58/129 (45%)	55 (95%)	3 (5%)	19	50
70	E	182/195 (93%)	173 (95%)	9 (5%)	21	53
70	s3	182/195 (93%)	173 (95%)	9 (5%)	21	53
71	e0	53/54 (98%)	50 (94%)	3 (6%)	17	47
71	f	51/54 (94%)	48 (94%)	3 (6%)	16	45
72	8	102/118 (86%)	97 (95%)	5 (5%)	21	53
72	CZ	102/118 (86%)	99 (97%)	3 (3%)	37	72
73	F	221/222 (100%)	210 (95%)	11 (5%)	20	52
73	s4	221/222 (100%)	215 (97%)	6 (3%)	40	73
74	g	62/135 (46%)	53 (86%)	9 (14%)	2	8
76	9	109/110 (99%)	108 (99%)	1 (1%)	75	92
76	DA	107/110 (97%)	100 (94%)	7 (6%)	14	40
77	G	173/191 (91%)	165 (95%)	8 (5%)	23	55
77	s5	173/191 (91%)	167 (96%)	6 (4%)	31	66
78	Rb	260/262 (99%)	237 (91%)	23 (9%)	8	26
78	h	252/262 (96%)	228 (90%)	24 (10%)	7	22
79	AA	115/116 (99%)	108 (94%)	7 (6%)	15	43
79	DB	115/116 (99%)	109 (95%)	6 (5%)	19	50
All	All	18216/20307 (90%)	17386 (95%)	830 (5%)	23	55

5 of 830 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
67	D	224	PHE
78	h	136	ILE
73	s4	246	LEU
48	x	14	SER
67	D	147	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 257 such sidechains are listed below:

Mol	Chain	Res	Type
36	M	22	ASN
76	9	98	ASN
50	Y	22	ASN
48	CR	101	ASN
73	s4	259	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	120/121 (99%)	14 (11%)	0
1	AS	120/121 (99%)	20 (16%)	1 (0%)
58	A	1716/1800 (95%)	453 (26%)	40 (2%)
58	sR	1780/1800 (98%)	464 (26%)	0
7	4	157/158 (99%)	31 (19%)	2 (1%)
7	AT	157/158 (99%)	31 (19%)	2 (1%)
75	1	3145/3396 (92%)	641 (20%)	48 (1%)
75	AR	3131/3396 (92%)	614 (19%)	48 (1%)
All	All	10326/10950 (94%)	2268 (21%)	141 (1%)

5 of 2268 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	7	G
1	3	11	A
1	3	22	A
1	3	23	A
1	3	54	U

5 of 141 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
75	1	1724	U
75	1	2112	U
75	1	2874	G
75	AR	979	U
75	AR	916	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2454 ligands modelled in this entry, 1 is modelled with single atom and 1509 are monoatomic - leaving 944 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	$\# Z > 2$
80	OHX	sR	2123	-	0,6,6	-	-	-		
80	OHX	AR	4049	-	0,6,6	-	-	-		
80	OHX	1	3873	-	0,6,6	-	-	-		
80	OHX	1	3605	-	0,6,6	-	-	-		
80	OHX	AR	4204	81	0,6,6	-	-	-		
80	OHX	AR	4017	-	0,6,6	-	-	-		
80	OHX	AR	3988	-	0,6,6	-	-	-		
80	OHX	AR	3510	-	0,6,6	-	-	-		
80	OHX	1	3488	-	0,6,6	-	-	-		
80	OHX	A	2149	-	0,6,6	-	-	-		
80	OHX	AR	3504	81	0,6,6	-	-	-		
80	OHX	A	1915	-	0,6,6	-	-	-		
80	OHX	AR	3761	-	0,6,6	-	-	-		
80	OHX	sR	2180	-	0,6,6	-	-	-		
80	OHX	A	1953	-	0,6,6	-	-	-		
80	OHX	sR	2049	-	0,6,6	-	-	-		
80	OHX	AR	3566	-	0,6,6	-	-	-		
80	OHX	1	3539	-	0,6,6	-	-	-		
80	OHX	sR	2198	-	0,6,6	-	-	-		
80	OHX	sR	2166	-	0,6,6	-	-	-		
80	OHX	1	3542	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	1	3662	-	0,6,6	-	-	-		
80	OHX	AT	207	-	0,6,6	-	-	-		
80	OHX	1	4090	81	0,6,6	-	-	-		
80	OHX	AR	3479	-	0,6,6	-	-	-		
80	OHX	U	202	-	0,6,6	-	-	-		
80	OHX	1	3792	-	0,6,6	-	-	-		
80	OHX	1	3753	-	0,6,6	-	-	-		
80	OHX	d4	201	-	0,6,6	-	-	-		
80	OHX	AR	3423	-	0,6,6	-	-	-		
80	OHX	AR	3732	-	0,6,6	-	-	-		
80	OHX	1	3423	-	0,6,6	-	-	-		
80	OHX	1	3961	-	0,6,6	-	-	-		
80	OHX	1	3964	81	0,6,6	-	-	-		
80	OHX	AR	4159	81	0,6,6	-	-	-		
80	OHX	A	2017	-	0,6,6	-	-	-		
80	OHX	AR	4046	-	0,6,6	-	-	-		
80	OHX	1	3726	-	0,6,6	-	-	-		
80	OHX	1	3784	81	0,6,6	-	-	-		
80	OHX	sR	2029	-	0,6,6	-	-	-		
80	OHX	AR	4010	-	0,6,6	-	-	-		
80	OHX	A	2082	-	0,6,6	-	-	-		
80	OHX	sR	1903	-	0,6,6	-	-	-		
80	OHX	AR	3609	-	0,6,6	-	-	-		
80	OHX	4	201	81	0,6,6	-	-	-		
80	OHX	AR	3485	-	0,6,6	-	-	-		
80	OHX	AR	3785	-	0,6,6	-	-	-		
80	OHX	1	4025	-	0,6,6	-	-	-		
80	OHX	AR	3638	-	0,6,6	-	-	-		
80	OHX	1	3850	-	0,6,6	-	-	-		
80	OHX	AR	3487	-	0,6,6	-	-	-		
80	OHX	AR	4018	-	0,6,6	-	-	-		
80	OHX	1	3545	-	0,6,6	-	-	-		
80	OHX	sR	1925	-	0,6,6	-	-	-		
80	OHX	1	3540	-	0,6,6	-	-	-		
80	OHX	A	2066	-	0,6,6	-	-	-		
80	OHX	1	3752	-	0,6,6	-	-	-		
80	OHX	AT	203	81	0,6,6	-	-	-		
80	OHX	A	2067	-	0,6,6	-	-	-		
80	OHX	AR	3642	-	0,6,6	-	-	-		
80	OHX	1	3449	-	0,6,6	-	-	-		
80	OHX	A	2103	-	0,6,6	-	-	-		
80	OHX	sR	1934	-	0,6,6	-	-	-		
80	OHX	AR	4105	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	sR	2191	-	0,6,6	-	-	-		
80	OHX	AR	3727	-	0,6,6	-	-	-		
80	OHX	AR	4104	-	0,6,6	-	-	-		
80	OHX	1	3577	-	0,6,6	-	-	-		
80	OHX	3	201	-	0,6,6	-	-	-		
80	OHX	AR	3442	-	0,6,6	-	-	-		
80	OHX	A	1905	-	0,6,6	-	-	-		
80	OHX	AR	4130	-	0,6,6	-	-	-		
80	OHX	1	3640	-	0,6,6	-	-	-		
80	OHX	1	3939	-	0,6,6	-	-	-		
80	OHX	AR	3819	-	0,6,6	-	-	-		
80	OHX	1	3751	81	0,6,6	-	-	-		
80	OHX	1	3481	-	0,6,6	-	-	-		
80	OHX	A	1944	-	0,6,6	-	-	-		
80	OHX	sR	2075	-	0,6,6	-	-	-		
80	OHX	AR	3763	-	0,6,6	-	-	-		
80	OHX	1	4058	-	0,6,6	-	-	-		
80	OHX	AR	4132	-	0,6,6	-	-	-		
80	OHX	1	3999	-	0,6,6	-	-	-		
80	OHX	AR	3861	-	0,6,6	-	-	-		
80	OHX	1	3696	81	0,6,6	-	-	-		
80	OHX	AR	3663	-	0,6,6	-	-	-		
80	OHX	sR	2039	-	0,6,6	-	-	-		
80	OHX	1	3610	-	0,6,6	-	-	-		
80	OHX	sR	1977	-	0,6,6	-	-	-		
80	OHX	AR	3725	-	0,6,6	-	-	-		
80	OHX	AR	3759	-	0,6,6	-	-	-		
80	OHX	1	3538	-	0,6,6	-	-	-		
80	OHX	CG	302	-	0,6,6	-	-	-		
80	OHX	1	3782	-	0,6,6	-	-	-		
80	OHX	1	3901	-	0,6,6	-	-	-		
80	OHX	AR	4110	-	0,6,6	-	-	-		
80	OHX	AR	3568	-	0,6,6	-	-	-		
80	OHX	AR	3944	-	0,6,6	-	-	-		
80	OHX	A	2056	-	0,6,6	-	-	-		
80	OHX	1	3517	-	0,6,6	-	-	-		
80	OHX	AR	3731	-	0,6,6	-	-	-		
80	OHX	1	4142	81	0,6,6	-	-	-		
80	OHX	A	2037	-	0,6,6	-	-	-		
80	OHX	A	1946	-	0,6,6	-	-	-		
80	OHX	sR	1991	-	0,6,6	-	-	-		
80	OHX	1	3911	-	0,6,6	-	-	-		
80	OHX	AR	3957	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	3	204	-	0,6,6	-	-	-		
80	OHX	1	3671	-	0,6,6	-	-	-		
80	OHX	1	4030	-	0,6,6	-	-	-		
80	OHX	1	4144	-	0,6,6	-	-	-		
80	OHX	AR	4045	-	0,6,6	-	-	-		
80	OHX	1	3992	-	0,6,6	-	-	-		
80	OHX	1	3639	-	0,6,6	-	-	-		
80	OHX	1	3700	-	0,6,6	-	-	-		
80	OHX	A	1904	-	0,6,6	-	-	-		
80	OHX	sR	2065	-	0,6,6	-	-	-		
80	OHX	A	1947	-	0,6,6	-	-	-		
80	OHX	A	2043	58	0,5,6	-	-	-		
80	OHX	A	2095	81	0,6,6	-	-	-		
80	OHX	1	3880	-	0,6,6	-	-	-		
80	OHX	sR	1937	-	0,6,6	-	-	-		
80	OHX	A	2053	81	0,6,6	-	-	-		
80	OHX	1	3636	-	0,6,6	-	-	-		
80	OHX	1	3451	81	0,6,6	-	-	-		
80	OHX	AR	3859	81	0,6,6	-	-	-		
80	OHX	1	3881	-	0,6,6	-	-	-		
80	OHX	1	3962	-	0,6,6	-	-	-		
80	OHX	AR	3418	-	0,6,6	-	-	-		
80	OHX	sR	1970	-	0,6,6	-	-	-		
80	OHX	1	4180	-	0,6,6	-	-	-		
80	OHX	sR	2155	-	0,6,6	-	-	-		
80	OHX	4	205	-	0,6,6	-	-	-		
80	OHX	AR	4200	-	0,6,6	-	-	-		
80	OHX	sR	2099	-	0,6,6	-	-	-		
80	OHX	AR	4172	-	0,6,6	-	-	-		
80	OHX	sR	1936	-	0,6,6	-	-	-		
80	OHX	AR	3571	-	0,6,6	-	-	-		
80	OHX	1	4060[A]	-	0,6,6	-	-	-		
80	OHX	AR	3444	-	0,6,6	-	-	-		
80	OHX	sR	2017	-	0,6,6	-	-	-		
80	OHX	1	4170	-	0,6,6	-	-	-		
80	OHX	AR	3542	-	0,6,6	-	-	-		
80	OHX	sR	1993	-	0,6,6	-	-	-		
80	OHX	AT	222	-	0,6,6	-	-	-		
80	OHX	1	3581	-	0,6,6	-	-	-		
80	OHX	AR	3483	-	0,6,6	-	-	-		
80	OHX	AR	3860	81	0,6,6	-	-	-		
80	OHX	AR	3828	81	0,6,6	-	-	-		
80	OHX	1	3813	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	c5	201	-	0,6,6	-	-	-		
80	OHX	AT	206	-	0,6,6	-	-	-		
80	OHX	AG	201	-	0,6,6	-	-	-		
80	OHX	AR	4170	-	0,6,6	-	-	-		
80	OHX	AS	219	-	0,6,6	-	-	-		
80	OHX	r	304	-	0,6,6	-	-	-		
80	OHX	1	3871	-	0,6,6	-	-	-		
80	OHX	AR	4035	-	0,6,6	-	-	-		
80	OHX	AR	4167	-	0,6,6	-	-	-		
80	OHX	AR	3417	81	0,6,6	-	-	-		
80	OHX	1	3728	81	0,6,6	-	-	-		
80	OHX	A	2151	-	0,6,6	-	-	-		
80	OHX	1	3693	-	0,6,6	-	-	-		
80	OHX	A	2063	-	0,6,6	-	-	-		
80	OHX	1	3758	-	0,6,6	-	-	-		
80	OHX	1	3941	-	0,6,6	-	-	-		
80	OHX	sR	2133	-	0,6,6	-	-	-		
80	OHX	sR	2015	-	0,6,6	-	-	-		
80	OHX	J	301	-	0,6,6	-	-	-		
80	OHX	4	207	-	0,6,6	-	-	-		
80	OHX	AR	4197	-	0,6,6	-	-	-		
80	OHX	AK	104	-	0,6,6	-	-	-		
80	OHX	1	3876	-	0,6,6	-	-	-		
80	OHX	AR	3607	-	0,6,6	-	-	-		
80	OHX	A	2006	-	0,6,6	-	-	-		
80	OHX	sR	1957	-	0,6,6	-	-	-		
80	OHX	AT	226	-	0,6,6	-	-	-		
80	OHX	1	3786	-	0,6,6	-	-	-		
80	OHX	1	3965	-	0,6,6	-	-	-		
80	OHX	1	3851	-	0,6,6	-	-	-		
80	OHX	AR	4012	-	0,6,6	-	-	-		
80	OHX	AR	3481	81	0,6,6	-	-	-		
80	OHX	A	2085	-	0,6,6	-	-	-		
80	OHX	sR	2074	81	0,6,6	-	-	-		
80	OHX	AR	3721	-	0,6,6	-	-	-		
80	OHX	A	2111	-	0,6,6	-	-	-		
80	OHX	A	1936	-	0,6,6	-	-	-		
80	OHX	A	1966	-	0,6,6	-	-	-		
80	OHX	AR	3455	-	0,6,6	-	-	-		
80	OHX	AR	4004	-	0,6,6	-	-	-		
80	OHX	1	3484	-	0,6,6	-	-	-		
80	OHX	1	3428	-	0,6,6	-	-	-		
80	OHX	1	3450	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	1	3519	-	0,6,6	-	-	-		
80	OHX	AR	3764	-	0,6,6	-	-	-		
80	OHX	1	4143	-	0,6,6	-	-	-		
80	OHX	1	3878	-	0,6,6	-	-	-		
80	OHX	A	2101	-	0,6,6	-	-	-		
80	OHX	sR	1980	-	0,6,6	-	-	-		
80	OHX	A	1945	-	0,6,6	-	-	-		
80	OHX	sR	2154	-	0,6,6	-	-	-		
80	OHX	1	4089	-	0,6,6	-	-	-		
80	OHX	A	1997	-	0,6,6	-	-	-		
80	OHX	4	208	-	0,6,6	-	-	-		
80	OHX	sR	2087	-	0,6,6	-	-	-		
80	OHX	A	2003	-	0,6,6	-	-	-		
80	OHX	1	4181	-	0,6,6	-	-	-		
80	OHX	A	2093	-	0,6,6	-	-	-		
80	OHX	AR	4165	81	0,6,6	-	-	-		
80	OHX	k	404	-	0,6,6	-	-	-		
80	OHX	AT	201	-	0,6,6	-	-	-		
80	OHX	AR	4008	-	0,6,6	-	-	-		
80	OHX	1	3512	-	0,6,6	-	-	-		
80	OHX	1	3702	-	0,6,6	-	-	-		
80	OHX	A	2139	-	0,6,6	-	-	-		
80	OHX	1	3844	-	0,6,6	-	-	-		
80	OHX	AR	4015	-	0,6,6	-	-	-		
80	OHX	A	2131	-	0,6,6	-	-	-		
80	OHX	4	202	-	0,6,6	-	-	-		
80	OHX	AR	3475	-	0,6,6	-	-	-		
80	OHX	sR	2159	-	0,6,6	-	-	-		
80	OHX	1	4029	-	0,6,6	-	-	-		
80	OHX	AR	4108	-	0,6,6	-	-	-		
80	OHX	AR	3549	-	0,6,6	-	-	-		
80	OHX	sR	2167	-	0,6,6	-	-	-		
80	OHX	3	220	81	0,6,6	-	-	-		
80	OHX	A	1923	81	0,6,6	-	-	-		
80	OHX	sR	2147	-	0,6,6	-	-	-		
80	OHX	1	3421	81	0,6,6	-	-	-		
80	OHX	sR	2170	-	0,6,6	-	-	-		
80	OHX	AR	3667[B]	-	0,6,6	-	-	-		
80	OHX	A	2142	-	0,6,6	-	-	-		
80	OHX	CV	201	-	0,6,6	-	-	-		
80	OHX	A	1927	-	0,6,6	-	-	-		
80	OHX	sR	1966	-	0,6,6	-	-	-		
80	OHX	1	3842	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	T	201	-	0,6,6	-	-	-		
80	OHX	1	3480	-	0,6,6	-	-	-		
80	OHX	AR	3611	-	0,6,6	-	-	-		
80	OHX	A	2033	-	0,6,6	-	-	-		
80	OHX	sR	1912	-	0,6,6	-	-	-		
80	OHX	A	2087	-	0,6,6	-	-	-		
80	OHX	AR	3635	-	0,6,6	-	-	-		
80	OHX	1	3453	81	0,6,6	-	-	-		
80	OHX	sR	1992	-	0,6,6	-	-	-		
80	OHX	1	4031	-	0,6,6	-	-	-		
80	OHX	CG	303	-	0,6,6	-	-	-		
80	OHX	CL	302	-	0,6,6	-	-	-		
80	OHX	AR	3413	-	0,6,6	-	-	-		
80	OHX	1	3513	-	0,6,6	-	-	-		
80	OHX	1	3996	-	0,6,6	-	-	-		
80	OHX	1	4026	-	0,6,6	-	-	-		
80	OHX	A	1914	-	0,6,6	-	-	-		
80	OHX	AR	3478	-	0,6,6	-	-	-		
80	OHX	1	3543	-	0,6,6	-	-	-		
80	OHX	AR	4006	-	0,6,6	-	-	-		
80	OHX	AR	4050	-	0,6,6	-	-	-		
80	OHX	AS	228	-	0,6,6	-	-	-		
80	OHX	1	3942	81	0,6,6	-	-	-		
80	OHX	1	4081	-	0,6,6	-	-	-		
80	OHX	1	3848	-	0,6,6	-	-	-		
80	OHX	A	2016	-	0,6,6	-	-	-		
80	OHX	Q	201	-	0,6,6	-	-	-		
80	OHX	AR	3979	-	0,6,6	-	-	-		
80	OHX	A	1984	-	0,6,6	-	-	-		
80	OHX	1	4002	80	0,6,6	-	-	-		
80	OHX	1	4146	-	0,6,6	-	-	-		
80	OHX	A	2130	80	0,6,6	-	-	-		
80	OHX	4	204	-	0,6,6	-	-	-		
80	OHX	CS	202	-	0,6,6	-	-	-		
80	OHX	AR	3446	-	0,6,6	-	-	-		
80	OHX	1	3422	81	0,6,6	-	-	-		
80	OHX	sR	2085	-	0,6,6	-	-	-		
80	OHX	AR	3987	81	0,6,6	-	-	-		
80	OHX	1	3692	-	0,6,6	-	-	-		
80	OHX	AR	3671	-	0,6,6	-	-	-		
80	OHX	1	3904	81	0,6,6	-	-	-		
80	OHX	sR	2005	-	0,6,6	-	-	-		
80	OHX	1	4061	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	1	4119	-	0,6,6	-	-	-		
80	OHX	A	1933	-	0,6,6	-	-	-		
80	OHX	AR	4073	-	0,6,6	-	-	-		
80	OHX	sR	1948	-	0,6,6	-	-	-		
80	OHX	sR	2148	-	0,6,6	-	-	-		
80	OHX	A	2055	-	0,6,6	-	-	-		
80	OHX	AR	3892	-	0,6,6	-	-	-		
80	OHX	1	3575	-	0,6,6	-	-	-		
80	OHX	1	3815	-	0,6,6	-	-	-		
80	OHX	1	3724	-	0,6,6	-	-	-		
80	OHX	sR	2112	-	0,6,6	-	-	-		
80	OHX	sR	2109	-	0,6,6	-	-	-		
80	OHX	AR	4043	-	0,6,6	-	-	-		
80	OHX	AR	3452	81	0,6,6	-	-	-		
80	OHX	AR	3515	-	0,6,6	-	-	-		
80	OHX	sR	1967	-	0,6,6	-	-	-		
80	OHX	AR	3955	-	0,6,6	-	-	-		
80	OHX	AR	3580	-	0,5,6	-	-	-		
80	OHX	AR	3893	-	0,6,6	-	-	-		
80	OHX	sR	2004	-	0,6,6	-	-	-		
80	OHX	1	4176	-	0,6,6	-	-	-		
80	OHX	AR	3851	-	0,6,6	-	-	-		
80	OHX	AR	3672	81	0,6,6	-	-	-		
80	OHX	1	4059	-	0,6,6	-	-	-		
80	OHX	AR	3980	81	0,6,6	-	-	-		
80	OHX	A	2077	-	0,6,6	-	-	-		
80	OHX	sR	2000	-	0,6,6	-	-	-		
80	OHX	sR	2037	-	0,6,6	-	-	-		
80	OHX	AR	3603	43	0,5,6	-	-	-		
80	OHX	sR	2192	-	0,6,6	-	-	-		
80	OHX	1	3725	-	0,6,6	-	-	-		
80	OHX	AR	3636	-	0,6,6	-	-	-		
80	OHX	sR	2146	-	0,6,6	-	-	-		
80	OHX	sR	2113	-	0,6,6	-	-	-		
80	OHX	AR	3547	-	0,6,6	-	-	-		
80	OHX	sR	2181	-	0,6,6	-	-	-		
80	OHX	1	3846	-	0,6,6	-	-	-		
80	OHX	1	3841	-	0,6,6	-	-	-		
80	OHX	4	232	-	0,6,6	-	-	-		
80	OHX	A	1917	-	0,6,6	-	-	-		
80	OHX	A	1926	-	0,6,6	-	-	-		
80	OHX	AR	3425	-	0,6,6	-	-	-		
80	OHX	sR	1979	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	1	3701	-	0,6,6	-	-	-		
80	OHX	AR	4078	-	0,6,6	-	-	-		
80	OHX	sR	1990	-	0,6,6	-	-	-		
80	OHX	1	3660	81	0,6,6	-	-	-		
80	OHX	A	2153	-	0,6,6	-	-	-		
80	OHX	1	3574	-	0,6,6	-	-	-		
80	OHX	1	4115	-	0,6,6	-	-	-		
80	OHX	sR	1945	-	0,6,6	-	-	-		
80	OHX	1	3601	-	0,6,6	-	-	-		
80	OHX	1	3425	-	0,6,6	-	-	-		
80	OHX	A	1995	-	0,6,6	-	-	-		
80	OHX	sR	2097	-	0,6,6	-	-	-		
80	OHX	AR	3514	-	0,6,6	-	-	-		
80	OHX	1	3790	-	0,6,6	-	-	-		
80	OHX	1	3814	-	0,6,6	-	-	-		
80	OHX	sR	1933	-	0,6,6	-	-	-		
80	OHX	AR	3830	-	0,6,6	-	-	-		
80	OHX	AR	3791	-	0,6,6	-	-	-		
80	OHX	1	3821	-	0,6,6	-	-	-		
80	OHX	AR	4166	-	0,6,6	-	-	-		
80	OHX	AR	3450	-	0,6,6	-	-	-		
80	OHX	1	3551	-	0,6,6	-	-	-		
80	OHX	A	2015	-	0,6,6	-	-	-		
80	OHX	AR	3753	-	0,6,6	-	-	-		
80	OHX	AR	4203	81	0,6,6	-	-	-		
80	OHX	AR	3516	-	0,6,6	-	-	-		
80	OHX	sR	2190	81	0,6,6	-	-	-		
80	OHX	1	4150	-	0,6,6	-	-	-		
80	OHX	1	3483	-	0,6,6	-	-	-		
80	OHX	1	3936	-	0,6,6	-	-	-		
80	OHX	1	3602	-	0,6,6	-	-	-		
80	OHX	AR	3795	-	0,6,6	-	-	-		
80	OHX	AR	3977	81	0,6,6	-	-	-		
80	OHX	AR	3923	-	0,6,6	-	-	-		
80	OHX	1	4121	81	0,6,6	-	-	-		
80	OHX	A	2094	-	0,6,6	-	-	-		
80	OHX	1	3459	-	0,6,6	-	-	-		
80	OHX	AR	4047	-	0,6,6	-	-	-		
80	OHX	AR	3911	-	0,6,6	-	-	-		
80	OHX	AR	3543	81	0,6,6	-	-	-		
80	OHX	A	2057	-	0,6,6	-	-	-		
80	OHX	A	2152	-	0,6,6	-	-	-		
80	OHX	sR	2003	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	AR	3953	-	0,6,6	-	-	-		
80	OHX	1	3489	-	0,6,6	-	-	-		
80	OHX	k	403	-	0,6,6	-	-	-		
80	OHX	sR	2063	-	0,6,6	-	-	-		
80	OHX	1	3723	-	0,6,6	-	-	-		
80	OHX	1	3755	-	0,6,6	-	-	-		
80	OHX	1	3932	81	0,6,6	-	-	-		
80	OHX	A	2102	-	0,6,6	-	-	-		
80	OHX	1	4145	-	0,6,6	-	-	-		
80	OHX	AR	4107	81	0,6,6	-	-	-		
80	OHX	AR	3942	-	0,6,6	-	-	-		
80	OHX	sR	1935	-	0,6,6	-	-	-		
80	OHX	AR	4194	-	0,6,6	-	-	-		
80	OHX	1	3819	-	0,6,6	-	-	-		
80	OHX	AR	3449	-	0,6,6	-	-	-		
80	OHX	1	3822	-	0,6,6	-	-	-		
80	OHX	sR	2062	-	0,6,6	-	-	-		
80	OHX	sR	2076	-	0,6,6	-	-	-		
80	OHX	sR	2100	-	0,6,6	-	-	-		
80	OHX	AR	3578	-	0,6,6	-	-	-		
80	OHX	AR	3855	-	0,6,6	-	-	-		
80	OHX	x	208	-	0,6,6	-	-	-		
80	OHX	sR	1924	-	0,6,6	-	-	-		
80	OHX	1	3910	-	0,6,6	-	-	-		
80	OHX	AR	3883	-	0,6,6	-	-	-		
80	OHX	AR	3692	-	0,6,6	-	-	-		
80	OHX	sR	2014	81	0,6,6	-	-	-		
80	OHX	1	3572	-	0,6,6	-	-	-		
80	OHX	AR	3411	81	0,6,6	-	-	-		
80	OHX	sR	2013	-	0,6,6	-	-	-		
80	OHX	AR	3815	-	0,6,6	-	-	-		
80	OHX	1	3991	-	0,6,6	-	-	-		
80	OHX	AR	3729	-	0,6,6	-	-	-		
80	OHX	AR	4138	-	0,6,6	-	-	-		
80	OHX	AR	3535	-	0,6,6	-	-	-		
80	OHX	1	3722	-	0,6,6	-	-	-		
80	OHX	A	2121	-	0,6,6	-	-	-		
80	OHX	AR	4019	-	0,6,6	-	-	-		
80	OHX	AR	3628	-	0,6,6	-	-	-		
80	OHX	AR	3829	-	0,6,6	-	-	-		
80	OHX	1	3694	-	0,6,6	-	-	-		
80	OHX	1	3672	-	0,6,6	-	-	-		
80	OHX	1	3791	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	1	3905	-	0,6,6	-	-	-		
80	OHX	1	4111	-	0,6,6	-	-	-		
80	OHX	AR	3728	-	0,6,6	-	-	-		
80	OHX	1	4116	-	0,6,6	-	-	-		
80	OHX	sR	1905	-	0,6,6	-	-	-		
80	OHX	A	2027	-	0,6,6	-	-	-		
80	OHX	AR	3831	-	0,6,6	-	-	-		
80	OHX	AR	3415	-	0,6,6	-	-	-		
80	OHX	sR	2040	-	0,6,6	-	-	-		
80	OHX	AR	3825	-	0,6,6	-	-	-		
80	OHX	1	3670	81	0,6,6	-	-	-		
80	OHX	4	209	-	0,6,6	-	-	-		
80	OHX	AR	3517	80	0,6,6	-	-	-		
80	OHX	AR	4139	-	0,6,6	-	-	-		
80	OHX	sR	1944	-	0,6,6	-	-	-		
80	OHX	1	3993	-	0,6,6	-	-	-		
80	OHX	sR	2156	-	0,6,6	-	-	-		
80	OHX	A	2143[A]	-	0,6,6	-	-	-		
80	OHX	1	3430	-	0,6,6	-	-	-		
80	OHX	AT	205	-	0,6,6	-	-	-		
80	OHX	1	4175	-	0,6,6	-	-	-		
80	OHX	1	3698	-	0,6,6	-	-	-		
80	OHX	A	1983	-	0,6,6	-	-	-		
80	OHX	1	3938	-	0,6,6	-	-	-		
80	OHX	1	4085	-	0,6,6	-	-	-		
80	OHX	A	1975	-	0,6,6	-	-	-		
80	OHX	A	1935	-	0,6,6	-	-	-		
80	OHX	1	3604	-	0,6,6	-	-	-		
80	OHX	A	2035	-	0,6,6	-	-	-		
80	OHX	AR	3574	-	0,6,6	-	-	-		
80	OHX	sR	1927	-	0,6,6	-	-	-		
80	OHX	1	3608	-	0,6,6	-	-	-		
80	OHX	1	3843	-	0,6,6	-	-	-		
80	OHX	AR	3511	-	0,6,6	-	-	-		
80	OHX	sR	2061	-	0,6,6	-	-	-		
80	OHX	A	2086	80	0,6,6	-	-	-		
80	OHX	sR	2188	-	0,6,6	-	-	-		
80	OHX	sR	2137	-	0,6,6	-	-	-		
80	OHX	1	3783	81	0,6,6	-	-	-		
80	OHX	1	3818	81	0,6,6	-	-	-		
80	OHX	sR	1946	-	0,6,6	-	-	-		
80	OHX	A	1967	-	0,6,6	-	-	-		
80	OHX	AR	3797	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	AR	3659	-	0,6,6	-	-	-		
80	OHX	sR	1913	-	0,6,6	-	-	-		
80	OHX	1	3518	-	0,6,6	-	-	-		
80	OHX	AR	3817	81	0,6,6	-	-	-		
80	OHX	AR	3885	-	0,6,6	-	-	-		
80	OHX	AR	3422	-	0,6,6	-	-	-		
80	OHX	1	4050	-	0,6,6	-	-	-		
80	OHX	AR	3981	-	0,6,6	-	-	-		
80	OHX	A	2026	-	0,6,6	-	-	-		
80	OHX	A	2092	-	0,6,6	-	-	-		
80	OHX	CE	402	-	0,6,6	-	-	-		
80	OHX	AR	3758	81	0,6,6	-	-	-		
80	OHX	sR	2177	-	0,6,6	-	-	-		
85	SPD	1	3478	-	9,9,9	0.31	0	8,8,8	0.87	0
80	OHX	AR	4136	-	0,6,6	-	-	-		
80	OHX	1	3785	-	0,6,6	-	-	-		
80	OHX	AR	3925	-	0,6,6	-	-	-		
80	OHX	AS	225	-	0,6,6	-	-	-		
80	OHX	A	1974	-	0,6,6	-	-	-		
80	OHX	1	4084	-	0,6,6	-	-	-		
80	OHX	1	4032	-	0,6,6	-	-	-		
80	OHX	sR	1969	-	0,6,6	-	-	-		
80	OHX	c3	201	-	0,6,6	-	-	-		
80	OHX	1	3427	-	0,6,6	-	-	-		
80	OHX	AR	3537	-	0,6,6	-	-	-		
80	OHX	AR	3545	81	0,6,6	-	-	-		
80	OHX	AR	3421	-	0,6,6	-	-	-		
80	OHX	A	1963	-	0,6,6	-	-	-		
80	OHX	AR	3477	-	0,6,6	-	-	-		
80	OHX	1	3420	-	0,6,6	-	-	-		
80	OHX	AR	3863	-	0,6,6	-	-	-		
80	OHX	sR	2089	-	0,6,6	-	-	-		
80	OHX	AR	3783	-	0,6,6	-	-	-		
80	OHX	sR	2124	-	0,6,6	-	-	-		
80	OHX	1	3612	-	0,6,6	-	-	-		
80	OHX	sR	2157	-	0,6,6	-	-	-		
80	OHX	AR	3667[A]	81	0,6,6	-	-	-		
80	OHX	1	3852	-	0,6,6	-	-	-		
80	OHX	1	4056	-	0,6,6	-	-	-		
80	OHX	AT	204[B]	-	0,6,6	-	-	-		
80	OHX	AR	4066	-	0,6,6	-	-	-		
80	OHX	AR	4128	-	0,6,6	-	-	-		
80	OHX	1	3579	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	1	4051	-	0,6,6	-	-	-		
80	OHX	1	3902	-	0,6,6	-	-	-		
80	OHX	1	3931	-	0,6,6	-	-	-		
80	OHX	1	3729	-	0,6,6	-	-	-		
80	OHX	AR	3879	-	0,6,6	-	-	-		
80	OHX	1	3571	-	0,6,6	-	-	-		
80	OHX	AR	3891	-	0,6,6	-	-	-		
80	OHX	AR	3798	81	0,6,6	-	-	-		
80	OHX	AR	3512	81	0,6,6	-	-	-		
80	OHX	sR	2041	-	0,6,6	-	-	-		
80	OHX	AT	202	-	0,6,6	-	-	-		
80	OHX	A	2047	-	0,6,6	-	-	-		
80	OHX	3	206	-	0,6,6	-	-	-		
80	OHX	sR	2122	-	0,6,6	-	-	-		
80	OHX	1	4060[B]	-	0,6,6	-	-	-		
80	OHX	sR	1902	-	0,6,6	-	-	-		
80	OHX	CE	401	-	0,6,6	-	-	-		
80	OHX	A	2113	-	0,6,6	-	-	-		
80	OHX	1	3457	-	0,6,6	-	-	-		
80	OHX	A	2119	-	0,6,6	-	-	-		
80	OHX	AR	4072	-	0,6,6	-	-	-		
80	OHX	AR	4039	-	0,6,6	-	-	-		
80	OHX	AS	230	-	0,6,6	-	-	-		
80	OHX	sR	1914	-	0,6,6	-	-	-		
80	OHX	1	3875	-	0,6,6	-	-	-		
80	OHX	1	4054	-	0,6,6	-	-	-		
80	OHX	AR	4111	-	0,6,6	-	-	-		
80	OHX	1	4173	81	0,6,6	-	-	-		
80	OHX	A	2007	-	0,6,6	-	-	-		
80	OHX	AR	3924	81	0,6,6	-	-	-		
80	OHX	AR	3984	-	0,6,6	-	-	-		
80	OHX	1	3691	-	0,6,6	-	-	-		
80	OHX	1	3669	-	0,6,6	-	-	-		
80	OHX	sR	2088	-	0,6,6	-	-	-		
80	OHX	sR	2016	-	0,6,6	-	-	-		
80	OHX	AR	4134	81	0,6,6	-	-	-		
80	OHX	sR	1955	-	0,6,6	-	-	-		
80	OHX	1	3638	-	0,6,6	-	-	-		
80	OHX	AR	3694	-	0,6,6	-	-	-		
80	OHX	AR	3956	-	0,6,6	-	-	-		
80	OHX	AR	3456	-	0,6,6	-	-	-		
80	OHX	1	3661	-	0,6,6	-	-	-		
80	OHX	3	219	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	AR	3608	-	0,6,6	-	-	-		
80	OHX	AR	3950	-	0,6,6	-	-	-		
80	OHX	1	3699	-	0,6,6	-	-	-		
80	OHX	AR	4041	-	0,6,6	-	-	-		
80	OHX	1	4120	81	0,6,6	-	-	-		
80	OHX	1	3934	81	0,6,6	-	-	-		
80	OHX	1	3731	-	0,6,6	-	-	-		
80	OHX	4	226	-	0,6,6	-	-	-		
80	OHX	A	1956	-	0,6,6	-	-	-		
80	OHX	A	2045	-	0,6,6	-	-	-		
80	OHX	1	4174	-	0,6,6	-	-	-		
80	OHX	1	3419	-	0,6,6	-	-	-		
80	OHX	1	4113	-	0,6,6	-	-	-		
80	OHX	1	4021	-	0,6,6	-	-	-		
80	OHX	1	3666	-	0,6,6	-	-	-		
80	OHX	1	3460	81	0,6,6	-	-	-		
80	OHX	AR	4109	-	0,6,6	-	-	-		
80	OHX	1	4110	-	0,6,6	-	-	-		
80	OHX	A	2096	-	0,6,6	-	-	-		
80	OHX	AR	3539	-	0,6,6	-	-	-		
80	OHX	A	2052	-	0,6,6	-	-	-		
80	OHX	DD	102	-	0,6,6	-	-	-		
80	OHX	1	3906	-	0,6,6	-	-	-		
80	OHX	1	4052	-	0,6,6	-	-	-		
80	OHX	AR	3453	80	0,5,6	-	-	-		
80	OHX	AR	3546	81	0,6,6	-	-	-		
80	OHX	AR	3975	81	0,6,6	-	-	-		
80	OHX	1	3820	-	0,6,6	-	-	-		
80	OHX	A	1973	-	0,6,6	-	-	-		
80	OHX	A	2073	-	0,6,6	-	-	-		
80	OHX	sR	2050	-	0,6,6	-	-	-		
80	OHX	AR	4140	-	0,6,6	-	-	-		
80	OHX	AR	4081	-	0,5,6	-	-	-		
80	OHX	sR	2051	-	0,6,6	-	-	-		
80	OHX	1	4140	-	0,6,6	-	-	-		
80	OHX	AR	3572	-	0,6,6	-	-	-		
80	OHX	sR	1949	-	0,6,6	-	-	-		
80	OHX	AR	3548	-	0,6,6	-	-	-		
80	OHX	A	1955	81	0,6,6	-	-	-		
80	OHX	sR	1947	-	0,6,6	-	-	-		
80	OHX	AT	227	-	0,6,6	-	-	-		
80	OHX	sR	2038	-	0,6,6	-	-	-		
80	OHX	sR	1968	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	1	3933	-	0,6,6	-	-	-		
80	OHX	1	4091	-	0,6,6	-	-	-		
80	OHX	1	3633	-	0,5,6	-	-	-		
80	OHX	AR	4101	-	0,6,6	-	-	-		
80	OHX	AC	101	-	0,6,6	-	-	-		
80	OHX	AR	3610	-	0,6,6	-	-	-		
80	OHX	sR	1926	-	0,6,6	-	-	-		
80	OHX	AR	3926	-	0,6,6	-	-	-		
80	OHX	sR	1958	81	0,6,6	-	-	-		
80	OHX	AR	4068	81	0,6,6	-	-	-		
80	OHX	AR	3821	-	0,6,6	-	-	-		
80	OHX	AR	3948	-	0,6,6	-	-	-		
80	OHX	sR	2111	-	0,6,6	-	-	-		
80	OHX	1	3788	-	0,6,6	-	-	-		
80	OHX	A	2123	-	0,5,6	-	-	-		
80	OHX	AS	221	-	0,6,6	-	-	-		
80	OHX	A	1925	-	0,6,6	-	-	-		
80	OHX	A	1913	-	0,6,6	-	-	-		
80	OHX	A	2140	-	0,6,6	-	-	-		
80	OHX	AR	3486	-	0,6,6	-	-	-		
84	ZWB	1	3578	-	26,28,28	0.58	1 (3%)	34,45,45	1.89	7 (20%)
80	OHX	Rb	401	-	0,6,6	-	-	-		
80	OHX	1	4024	-	0,6,6	-	-	-		
80	OHX	1	3606	-	0,6,6	-	-	-		
80	OHX	1	3789	-	0,6,6	-	-	-		
80	OHX	sR	1978	81	0,6,6	-	-	-		
80	OHX	AR	3630	-	0,6,6	-	-	-		
80	OHX	A	2036	-	0,6,6	-	-	-		
80	OHX	AR	3666	-	0,6,6	-	-	-		
80	OHX	1	3458	81	0,6,6	-	-	-		
80	OHX	AR	3661	81	0,6,6	-	-	-		
80	OHX	1	3845	-	0,6,6	-	-	-		
80	OHX	1	3990	81	0,6,6	-	-	-		
80	OHX	1	4112	-	0,6,6	-	-	-		
80	OHX	sR	2027	-	0,6,6	-	-	-		
80	OHX	1	3998	-	0,6,6	-	-	-		
80	OHX	sR	2168	-	0,6,6	-	-	-		
80	OHX	3	222	-	0,6,6	-	-	-		
80	OHX	A	2065	-	0,6,6	-	-	-		
80	OHX	AR	3604	-	0,6,6	-	-	-		
80	OHX	AR	3541	-	0,6,6	-	-	-		
80	OHX	1	3908	-	0,6,6	-	-	-		
80	OHX	AR	4161	81	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	AR	3952	-	0,6,6	-	-	-		
80	OHX	AR	4079	-	0,6,6	-	-	-		
80	OHX	1	3550	-	0,6,6	-	-	-		
80	OHX	AR	4014	-	0,6,6	-	-	-		
80	OHX	sR	2144	-	0,6,6	-	-	-		
80	OHX	AR	3665	-	0,6,6	-	-	-		
80	OHX	AR	4080	-	0,6,6	-	-	-		
80	OHX	1	4172	-	0,6,6	-	-	-		
80	OHX	v	305	-	0,6,6	-	-	-		
80	OHX	1	3482	-	0,6,6	-	-	-		
80	OHX	sR	2028	-	0,6,6	-	-	-		
80	OHX	sR	1923	-	0,6,6	-	-	-		
80	OHX	1	3631	-	0,6,6	-	-	-		
80	OHX	AR	3847	-	0,6,6	-	-	-		
80	OHX	AR	3857	-	0,6,6	-	-	-		
80	OHX	CX	201	-	0,6,6	-	-	-		
80	OHX	AR	4099	-	0,6,6	-	-	-		
80	OHX	sR	2073	-	0,6,6	-	-	-		
80	OHX	CK	201	-	0,6,6	-	-	-		
80	OHX	AR	3703	-	0,6,6	-	-	-		
80	OHX	AR	3827	-	0,6,6	-	-	-		
80	OHX	AR	4076	-	0,6,6	-	-	-		
80	OHX	1	3603	-	0,6,6	-	-	-		
80	OHX	1	4083	-	0,6,6	-	-	-		
80	OHX	AR	3921	-	0,6,6	-	-	-		
80	OHX	1	4179	-	0,6,6	-	-	-		
80	OHX	A	1986	-	0,6,6	-	-	-		
80	OHX	AR	3632	-	0,6,6	-	-	-		
80	OHX	h	401	-	0,6,6	-	-	-		
80	OHX	sR	2077	-	0,6,6	-	-	-		
80	OHX	sR	2135	-	0,6,6	-	-	-		
80	OHX	sR	2169	-	0,6,6	-	-	-		
80	OHX	1	3872	81	0,6,6	-	-	-		
80	OHX	1	4023	81	0,6,6	-	-	-		
80	OHX	A	1937	-	0,6,6	-	-	-		
80	OHX	1	3994	-	0,6,6	-	-	-		
80	OHX	AR	4097	-	0,6,6	-	-	-		
80	OHX	1	3971	-	0,6,6	-	-	-		
80	OHX	sR	2145	-	0,6,6	-	-	-		
80	OHX	1	3424	80	0,6,6	-	-	-		
80	OHX	A	1985	-	0,6,6	-	-	-		
80	OHX	1	3520	-	0,6,6	-	-	-		
80	OHX	1	3968	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	1	3721	-	0,6,6	-	-	-		
80	OHX	AR	3913	-	0,6,6	-	-	-		
80	OHX	AR	4196	-	0,6,6	-	-	-		
80	OHX	AS	231	-	0,6,6	-	-	-		
80	OHX	1	3548	-	0,6,6	-	-	-		
80	OHX	c8	201	-	0,6,6	-	-	-		
80	OHX	A	1996	-	0,6,6	-	-	-		
80	OHX	AR	3723	-	0,6,6	-	-	-		
80	OHX	1	3812	81	0,6,6	-	-	-		
80	OHX	AR	3765	-	0,6,6	-	-	-		
80	OHX	AR	4037	-	0,6,6	-	-	-		
80	OHX	1	4055	-	0,6,6	-	-	-		
80	OHX	AR	3480	-	0,6,6	-	-	-		
80	OHX	AR	4171	81	0,6,6	-	-	-		
80	OHX	AR	3702	-	0,6,6	-	-	-		
80	OHX	A	1924	-	0,6,6	-	-	-		
80	OHX	sR	2025	-	0,6,6	-	-	-		
80	OHX	AR	3796	-	0,6,6	-	-	-		
80	OHX	A	1954	-	0,6,6	-	-	-		
80	OHX	AR	3698	-	0,6,6	-	-	-		
80	OHX	1	3582	-	0,6,6	-	-	-		
80	OHX	1	4086	-	0,6,6	-	-	-		
80	OHX	AK	103	81	0,6,6	-	-	-		
80	OHX	AR	3973	-	0,6,6	-	-	-		
80	OHX	AR	3983	-	0,6,6	-	-	-		
80	OHX	AR	3506	-	0,6,6	-	-	-		
80	OHX	AR	3634	-	0,6,6	-	-	-		
80	OHX	AR	4048	-	0,6,6	-	-	-		
80	OHX	1	3995	-	0,6,6	-	-	-		
80	OHX	1	3569	-	0,6,6	-	-	-		
80	OHX	1	3966	-	0,6,6	-	-	-		
80	OHX	1	4022	-	0,6,6	-	-	-		
85	SPD	AR	3890	-	9,9,9	0.34	0	8,8,8	0.88	0
80	OHX	AR	3755	-	0,6,6	-	-	-		
80	OHX	1	4114	81	0,6,6	-	-	-		
80	OHX	sR	2053	-	0,6,6	-	-	-		
80	OHX	AR	4135	-	0,6,6	-	-	-		
80	OHX	AR	3640	81	0,6,6	-	-	-		
80	OHX	2	201	-	0,6,6	-	-	-		
80	OHX	1	3963	-	0,6,6	-	-	-		
80	OHX	1	4001	81	0,6,6	-	-	-		
80	OHX	AR	3751	-	0,6,6	-	-	-		
80	OHX	1	3695	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	1	4088	-	0,6,6	-	-	-		
80	OHX	1	3549	81	0,6,6	-	-	-		
80	OHX	sR	2052	-	0,6,6	-	-	-		
80	OHX	A	2133	-	0,6,6	-	-	-		
80	OHX	AR	3696	-	0,6,6	-	-	-		
80	OHX	3	203	81	0,6,6	-	-	-		
80	OHX	1	4118	-	0,6,6	-	-	-		
80	OHX	1	3479	-	0,6,6	-	-	-		
80	OHX	sR	1915	-	0,6,6	-	-	-		
80	OHX	sR	1901	-	0,6,6	-	-	-		
80	OHX	sR	2064	-	0,6,6	-	-	-		
80	OHX	1	3454	-	0,6,6	-	-	-		
80	OHX	1	3781	75	0,6,6	-	-	-		
80	OHX	1	3816	-	0,6,6	-	-	-		
80	OHX	sR	2098	-	0,6,6	-	-	-		
80	OHX	sR	1959	-	0,6,6	-	-	-		
80	OHX	1	3485	-	0,6,6	-	-	-		
80	OHX	1	4149	-	0,6,6	-	-	-		
80	OHX	AR	3895	-	0,6,6	-	-	-		
80	OHX	AR	3922	-	0,6,6	-	-	-		
80	OHX	A	1943	-	0,6,6	-	-	-		
80	OHX	A	2104	-	0,6,6	-	-	-		
80	OHX	AS	223	-	0,6,6	-	-	-		
80	OHX	1	3487	-	0,6,6	-	-	-		
80	OHX	O	201	-	0,6,6	-	-	-		
80	OHX	AR	3673	-	0,6,6	-	-	-		
80	OHX	A	2129	-	0,6,6	-	-	-		
80	OHX	AR	4074	-	0,6,6	-	-	-		
80	OHX	1	4141	81	0,6,6	-	-	-		
80	OHX	AR	3792	-	0,6,6	-	-	-		
80	OHX	AR	3639	81	0,6,6	-	-	-		
80	OHX	AR	4103	-	0,6,6	-	-	-		
80	OHX	1	3730	-	0,6,6	-	-	-		
80	OHX	1	3611	-	0,6,6	-	-	-		
80	OHX	sR	2002	-	0,6,6	-	-	-		
80	OHX	sR	2125	-	0,6,6	-	-	-		
80	OHX	AR	3448	-	0,6,6	-	-	-		
80	OHX	AR	3700	-	0,6,6	-	-	-		
80	OHX	1	3882	-	0,6,6	-	-	-		
80	OHX	AR	3881	-	0,6,6	-	-	-		
80	OHX	1	3972	81	0,6,6	-	-	-		
80	OHX	DL	102	-	0,6,6	-	-	-		
80	OHX	AR	3704	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	A	1977	-	0,6,6	-	-	-		
80	OHX	AR	4016	-	0,6,6	-	-	-		
80	OHX	1	3849	-	0,6,6	-	-	-		
80	OHX	AR	3601	-	0,6,6	-	-	-		
80	OHX	sR	2110	-	0,6,6	-	-	-		
80	OHX	AT	230	-	0,6,6	-	-	-		
80	OHX	A	1993	-	0,6,6	-	-	-		
80	OHX	A	2083	-	0,6,6	-	-	-		
80	OHX	AR	3946	-	0,6,6	-	-	-		
80	OHX	sR	2101	-	0,6,6	-	-	-		
80	OHX	A	1916	-	0,6,6	-	-	-		
80	OHX	AT	204[A]	-	0,6,6	-	-	-		
80	OHX	1	3570	-	0,6,6	-	-	-		
80	OHX	sR	2189	-	0,6,6	-	-	-		
80	OHX	1	3573	-	0,6,6	-	-	-		
80	OHX	1	3761	-	0,6,6	-	-	-		
80	OHX	1	3912	-	0,6,6	-	-	-		
80	OHX	AR	4142	81	0,6,6	-	-	-		
80	OHX	AR	4201	-	0,6,6	-	-	-		
80	OHX	A	1994	-	0,6,6	-	-	-		
80	OHX	s4	302	-	0,6,6	-	-	-		
80	OHX	1	3641	-	0,6,6	-	-	-		
80	OHX	sR	2086	-	0,6,6	-	-	-		
80	OHX	1	3490	-	0,6,6	-	-	-		
80	OHX	1	3663	-	0,6,6	-	-	-		
80	OHX	AR	3518	-	0,6,6	-	-	-		
80	OHX	1	3668	-	0,6,6	-	-	-		
80	OHX	AR	3760	-	0,6,6	-	-	-		
80	OHX	1	3732	-	0,6,6	-	-	-		
80	OHX	AS	229	-	0,6,6	-	-	-		
80	OHX	AT	208	-	0,6,6	-	-	-		
80	OHX	AR	4190	-	0,6,6	-	-	-		
80	OHX	A	2023	-	0,6,6	-	-	-		
80	OHX	sR	1989	-	0,6,6	-	-	-		
80	OHX	AR	3799	-	0,6,6	-	-	-		
80	OHX	A	2046	-	0,6,6	-	-	-		
80	OHX	1	3632	-	0,6,6	-	-	-		
80	OHX	1	4148	-	0,6,6	-	-	-		
80	OHX	3	205	-	0,6,6	-	-	-		
80	OHX	A	1965	-	0,6,6	-	-	-		
80	OHX	AR	3734	-	0,6,6	-	-	-		
80	OHX	A	2150	-	0,6,6	-	-	-		
80	OHX	DH	202	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	AR	3917	-	0,6,6	-	-	-		
80	OHX	sR	2179	-	0,6,6	-	-	-		
80	OHX	AT	228	-	0,6,6	-	-	-		
80	OHX	A	1934	-	0,6,6	-	-	-		
80	OHX	1	3546	81	0,6,6	-	-	-		
80	OHX	AR	3697	-	0,6,6	-	-	-		
80	OHX	1	3811	-	0,6,6	-	-	-		
80	OHX	A	2005	-	0,6,6	-	-	-		
80	OHX	A	2143[B]	-	0,6,6	-	-	-		
80	OHX	sR	1922	81	0,6,6	-	-	-		
80	OHX	A	2122	-	0,6,6	-	-	-		
80	OHX	AR	3473	-	0,6,6	-	-	-		
80	OHX	1	3510	-	0,6,6	-	-	-		
80	OHX	AR	3641	-	0,6,6	-	-	-		
80	OHX	AR	3576	-	0,6,6	-	-	-		
80	OHX	1	4028	-	0,6,6	-	-	-		
80	OHX	1	3759	-	0,6,6	-	-	-		
80	OHX	AR	3599	-	0,6,6	-	-	-		
80	OHX	sR	2136	-	0,6,6	-	-	-		
80	OHX	sR	1981	81	0,6,6	-	-	-		
80	OHX	AR	3419	-	0,6,6	-	-	-		
80	OHX	AR	3735	-	0,6,6	-	-	-		
80	OHX	1	4171	-	0,6,6	-	-	-		
80	OHX	A	1906	-	0,6,6	-	-	-		
80	OHX	sR	1956	-	0,6,6	-	-	-		
80	OHX	1	3609	-	0,6,6	-	-	-		
80	OHX	1	3635	-	0,6,6	-	-	-		
80	OHX	AR	3954	-	0,6,6	-	-	-		
80	OHX	1	3515	-	0,6,6	-	-	-		
80	OHX	AR	3767	-	0,6,6	-	-	-		
80	OHX	A	2110	-	0,6,6	-	-	-		
80	OHX	1	3754	-	0,6,6	-	-	-		
80	OHX	AR	3579	-	0,6,6	-	-	-		
80	OHX	sR	2178	-	0,6,6	-	-	-		
80	OHX	sR	1904	-	0,6,6	-	-	-		
80	OHX	A	2025	-	0,6,6	-	-	-		
80	OHX	AR	3701	-	0,6,6	-	-	-		
80	OHX	AR	4198	-	0,6,6	-	-	-		
80	OHX	1	3511	-	0,6,6	-	-	-		
80	OHX	A	2013	-	0,6,6	-	-	-		
80	OHX	AR	3690	-	0,6,6	-	-	-		
80	OHX	1	3909	-	0,6,6	-	-	-		
80	OHX	AR	4192	81	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	AR	3669	-	0,6,6	-	-	-		
80	OHX	sR	2121	-	0,6,6	-	-	-		
80	OHX	1	3514	-	0,6,6	-	-	-		
80	OHX	AR	3824	-	0,6,6	-	-	-		
80	OHX	A	2112	-	0,6,6	-	-	-		
80	OHX	s1	301	81	0,6,6	-	-	-		
80	OHX	1	3452	-	0,6,6	-	-	-		
80	OHX	sR	1988	81	0,6,6	-	-	-		
80	OHX	A	1907	-	0,6,6	-	-	-		
80	OHX	AR	3424	-	0,6,6	-	-	-		
80	OHX	1	3580	-	0,6,6	-	-	-		
80	OHX	4	206	-	0,6,6	-	-	-		
80	OHX	AR	4163	81	0,6,6	-	-	-		
80	OHX	AS	227	-	0,6,6	-	-	-		
84	ZWB	AR	3826	-	26,28,28	0.57	1 (3%)	34,45,45	1.91	7 (20%)
80	OHX	CP	303	-	0,6,6	-	-	-		
80	OHX	AR	3919	-	0,6,6	-	-	-		
80	OHX	A	1987	-	0,6,6	-	-	-		
80	OHX	A	1957	-	0,6,6	-	-	-		
80	OHX	AR	3915	81	0,6,6	-	-	-		
80	OHX	sR	2158	-	0,6,6	-	-	-		
80	OHX	AR	4173	-	0,6,6	-	-	-		
80	OHX	AR	3986	-	0,6,6	-	-	-		
80	OHX	3	221	-	0,6,6	-	-	-		
80	OHX	CL	301	-	0,6,6	-	-	-		
80	OHX	AR	3766	-	0,6,6	-	-	-		
80	OHX	1	4082	-	0,6,6	-	-	-		
80	OHX	1	4178	-	0,6,6	-	-	-		
80	OHX	A	1903	-	0,6,6	-	-	-		
80	OHX	A	2076	-	0,6,6	-	-	-		
80	OHX	A	1964	-	0,5,6	-	-	-		
80	OHX	AR	3484	-	0,6,6	-	-	-		
80	OHX	1	3509	-	0,6,6	-	-	-		
80	OHX	1	3879	-	0,6,6	-	-	-		
80	OHX	4	203	-	0,6,6	-	-	-		
85	SPD	AR	4164	-	9,9,9	0.33	0	8,8,8	0.89	0
80	OHX	3	202	-	0,6,6	-	-	-		
80	OHX	sR	2134	-	0,6,6	-	-	-		
80	OHX	AR	3508	-	0,6,6	-	-	-		
80	OHX	1	3634	81	0,6,6	-	-	-		
85	SPD	AR	3858	-	9,9,9	0.33	0	8,8,8	1.33	1 (12%)
80	OHX	1	3756	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	1	3642	81	0,6,6	-	-	-		
80	OHX	AR	3605	81	0,6,6	-	-	-		
80	OHX	AR	4141	-	0,6,6	-	-	-		
80	OHX	4	228	-	0,6,6	-	-	-		
80	OHX	A	1976	-	0,6,6	-	-	-		
80	OHX	AR	3540	-	0,6,6	-	-	-		
80	OHX	A	2132	-	0,6,6	-	-	-		
80	OHX	AR	3573	-	0,6,6	-	-	-		
80	OHX	1	3665	-	0,6,6	-	-	-		
80	OHX	sR	2176	-	0,6,6	-	-	-		
80	OHX	AR	3670	-	0,6,6	-	-	-		
80	OHX	AR	3793	-	0,6,6	-	-	-		
80	OHX	AR	3849	-	0,6,6	-	-	-		
80	OHX	sR	1916	-	0,6,6	-	-	-		
80	OHX	1	3762	-	0,6,6	-	-	-		
80	OHX	AR	3853	-	0,6,6	-	-	-		
80	OHX	w	201	-	0,6,6	-	-	-		
80	OHX	1	3664	-	0,6,6	-	-	-		
80	OHX	AR	3787	-	0,6,6	-	-	-		
80	OHX	AR	3757	-	0,6,6	-	-	-		
80	OHX	sR	2026	-	0,6,6	-	-	-		
80	OHX	AR	4077	-	0,6,6	-	-	-		
80	OHX	AR	3577	-	0,6,6	-	-	-		
80	OHX	AR	3894	-	0,6,6	-	-	-		
80	OHX	AR	4169	-	0,6,6	-	-	-		
80	OHX	sR	1938	-	0,6,6	-	-	-		
80	OHX	1	3903	-	0,6,6	-	-	-		
80	OHX	AR	3454	-	0,6,6	-	-	-		
80	OHX	AR	4202	-	0,6,6	-	-	-		
80	OHX	A	2072	-	0,6,6	-	-	-		
80	OHX	1	4053	81	0,6,6	-	-	-		
80	OHX	1	3970	-	0,6,6	-	-	-		
80	OHX	1	4151	-	0,6,6	-	-	-		
80	OHX	A	2062	-	0,6,6	-	-	-		
80	OHX	A	2075	-	0,6,6	-	-	-		
80	OHX	A	2141	81	0,6,6	-	-	-		
80	OHX	AR	3985	-	0,6,6	-	-	-		
80	OHX	AR	3570	81	0,6,6	-	-	-		
80	OHX	A	2120	-	0,6,6	-	-	-		
80	OHX	1	3720	-	0,6,6	-	-	-		
80	OHX	1	4000	-	0,6,6	-	-	-		
80	OHX	1	3544	-	0,6,6	-	-	-		
80	OHX	AR	3887	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	1	3874	-	0,6,6	-	-	-		
80	OHX	AR	3597	-	0,6,6	-	-	-		
80	OHX	AR	3889	-	0,6,6	-	-	-		
80	OHX	C	301	-	0,6,6	-	-	-		
80	OHX	AR	3856	-	0,6,6	-	-	-		
80	OHX	AR	3862	-	0,6,6	-	-	-		
80	OHX	AR	4042	-	0,6,6	-	-	-		
80	OHX	1	3935	-	0,6,6	-	-	-		
80	OHX	AR	3733	-	0,6,6	-	-	-		
80	OHX	AR	3823	-	0,6,6	-	-	-		
80	OHX	AR	4070	-	0,6,6	-	-	-		
80	OHX	AR	3789	-	0,6,6	-	-	-		
80	OHX	sR	1911	-	0,6,6	-	-	-		
80	OHX	1	3760	-	0,6,6	-	-	-		
80	OHX	1	3940	-	0,6,6	-	-	-		
80	OHX	1	3541	-	0,6,6	-	-	-		
80	OHX	1	3455	-	0,6,6	-	-	-		
80	OHX	1	3969	-	0,6,6	-	-	-		
80	OHX	AR	4112	-	0,6,6	-	-	-		
80	OHX	4	230	-	0,6,6	-	-	-		
80	OHX	1	3429	-	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
85	SPD	AR	4164	-	-	4/7/7/7	-
85	SPD	AR	3858	-	-	3/7/7/7	-
85	SPD	1	3478	-	-	1/7/7/7	-
84	ZWB	AR	3826	-	-	1/8/60/60	0/3/3/3
85	SPD	AR	3890	-	-	3/7/7/7	-
84	ZWB	1	3578	-	-	0/8/60/60	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	1	3578	ZWB	C5-C10	2.14	1.59	1.56
84	AR	3826	ZWB	C5-C10	2.04	1.59	1.56

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	AR	3826	ZWB	C20-C1-C2	-4.99	99.99	109.44
84	1	3578	ZWB	C20-C1-C2	-4.98	100.00	109.44
84	AR	3826	ZWB	C2-C1-C10	4.77	113.18	108.81
84	1	3578	ZWB	C2-C1-C10	4.41	112.85	108.81
84	AR	3826	ZWB	C-C1-C20	-4.33	101.52	107.89

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	AR	3858	SPD	N6-C7-C8-C9
85	AR	4164	SPD	C3-C4-C5-N6
85	AR	3890	SPD	C4-C5-N6-C7
85	AR	4164	SPD	N6-C7-C8-C9
85	AR	3858	SPD	C2-C3-C4-C5

There are no ring outliers.

539 monomers are involved in 782 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	sR	2123	OHX	2	0
80	AR	4049	OHX	1	0
80	AR	4204	OHX	1	0
80	AR	4017	OHX	1	0
80	AR	3988	OHX	1	0
80	AR	3510	OHX	2	0
80	A	2149	OHX	1	0
80	AR	3504	OHX	2	0
80	A	1915	OHX	2	0
80	AR	3761	OHX	3	0
80	sR	2180	OHX	1	0
80	A	1953	OHX	1	0
80	sR	2049	OHX	1	0
80	AR	3566	OHX	1	0
80	1	3539	OHX	2	0
80	sR	2198	OHX	5	0
80	1	3542	OHX	2	0
80	U	202	OHX	1	0
80	1	3792	OHX	1	0
80	1	3753	OHX	1	0
80	AR	3423	OHX	1	0
80	1	3423	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	1	3964	OHX	1	0
80	A	2017	OHX	1	0
80	AR	4046	OHX	2	0
80	AR	4010	OHX	1	0
80	A	2082	OHX	1	0
80	AR	3609	OHX	3	0
80	AR	3485	OHX	2	0
80	AR	3785	OHX	1	0
80	AR	3487	OHX	2	0
80	1	3545	OHX	2	0
80	1	3540	OHX	1	0
80	A	2066	OHX	2	0
80	AT	203	OHX	1	0
80	AR	3642	OHX	1	0
80	1	3449	OHX	1	0
80	A	2103	OHX	1	0
80	sR	1934	OHX	2	0
80	AR	4105	OHX	1	0
80	sR	2191	OHX	2	0
80	AR	3727	OHX	1	0
80	AR	4104	OHX	2	0
80	AR	3442	OHX	3	0
80	1	3640	OHX	1	0
80	1	3939	OHX	1	0
80	AR	3819	OHX	1	0
80	1	3751	OHX	1	0
80	A	1944	OHX	5	0
80	AR	3763	OHX	1	0
80	1	4058	OHX	1	0
80	AR	4132	OHX	1	0
80	1	3999	OHX	2	0
80	AR	3861	OHX	1	0
80	1	3696	OHX	1	0
80	1	3610	OHX	2	0
80	sR	1977	OHX	1	0
80	AR	3725	OHX	2	0
80	AR	3759	OHX	1	0
80	CG	302	OHX	1	0
80	1	3901	OHX	2	0
80	AR	3568	OHX	1	0
80	AR	3944	OHX	1	0
80	A	2037	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	sR	1991	OHX	3	0
80	AR	3957	OHX	1	0
80	3	204	OHX	1	0
80	1	3992	OHX	2	0
80	1	3639	OHX	1	0
80	1	3700	OHX	1	0
80	A	1904	OHX	1	0
80	sR	2065	OHX	1	0
80	A	2043	OHX	2	0
80	1	3880	OHX	1	0
80	1	3451	OHX	1	0
80	1	4180	OHX	1	0
80	sR	2155	OHX	1	0
80	4	205	OHX	3	0
80	AR	3571	OHX	1	0
80	sR	2017	OHX	1	0
80	1	4170	OHX	1	0
80	AR	3542	OHX	3	0
80	1	3581	OHX	1	0
80	AR	3483	OHX	3	0
80	AR	3828	OHX	1	0
80	1	3813	OHX	2	0
80	c5	201	OHX	1	0
80	AT	206	OHX	1	0
80	AG	201	OHX	1	0
80	AR	4170	OHX	1	0
80	r	304	OHX	1	0
80	AR	4035	OHX	2	0
80	AR	3417	OHX	1	0
80	1	3728	OHX	1	0
80	1	3693	OHX	1	0
80	A	2063	OHX	3	0
80	1	3941	OHX	1	0
80	sR	2133	OHX	2	0
80	J	301	OHX	1	0
80	4	207	OHX	1	0
80	A	2006	OHX	2	0
80	sR	1957	OHX	1	0
80	AT	226	OHX	1	0
80	AR	4012	OHX	1	0
80	AR	3481	OHX	3	0
80	A	2085	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	A	1936	OHX	1	0
80	A	1966	OHX	1	0
80	AR	4004	OHX	1	0
80	1	3484	OHX	1	0
80	1	3428	OHX	1	0
80	1	3450	OHX	2	0
80	AR	3764	OHX	1	0
80	1	4143	OHX	2	0
80	A	2101	OHX	1	0
80	A	1945	OHX	2	0
80	sR	2154	OHX	1	0
80	1	4089	OHX	1	0
80	A	1997	OHX	1	0
80	4	208	OHX	2	0
80	A	2003	OHX	5	0
80	A	2093	OHX	1	0
80	k	404	OHX	1	0
80	AT	201	OHX	1	0
80	A	2139	OHX	1	0
80	AR	4015	OHX	1	0
80	A	2131	OHX	1	0
80	AR	3475	OHX	1	0
80	1	4029	OHX	1	0
80	3	220	OHX	1	0
80	1	3421	OHX	1	0
80	AR	3667[B]	OHX	1	0
80	A	2142	OHX	1	0
80	CV	201	OHX	1	0
80	sR	1966	OHX	3	0
80	1	3842	OHX	2	0
80	T	201	OHX	2	0
80	1	3480	OHX	1	0
80	AR	3611	OHX	1	0
80	sR	1912	OHX	1	0
80	A	2087	OHX	1	0
80	AR	3635	OHX	1	0
80	1	3453	OHX	2	0
80	1	4031	OHX	1	0
80	CG	303	OHX	1	0
80	CL	302	OHX	1	0
80	AR	3413	OHX	1	0
80	1	3513	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	A	1914	OHX	1	0
80	AR	4006	OHX	1	0
80	1	4081	OHX	1	0
80	1	3848	OHX	1	0
80	Q	201	OHX	2	0
80	A	1984	OHX	1	0
80	1	4002	OHX	3	0
80	1	4146	OHX	1	0
80	A	2130	OHX	2	0
80	4	204	OHX	1	0
80	AR	3446	OHX	2	0
80	AR	3987	OHX	1	0
80	1	3692	OHX	2	0
80	AR	3671	OHX	2	0
80	1	3904	OHX	1	0
80	sR	2005	OHX	1	0
80	1	4061	OHX	1	0
80	A	1933	OHX	3	0
80	sR	1948	OHX	1	0
80	sR	2148	OHX	2	0
80	1	3724	OHX	1	0
80	sR	2112	OHX	1	0
80	AR	4043	OHX	2	0
80	AR	3452	OHX	1	0
80	sR	1967	OHX	1	0
80	AR	3580	OHX	1	0
80	sR	2004	OHX	1	0
80	1	4176	OHX	1	0
80	AR	3851	OHX	1	0
80	AR	3672	OHX	1	0
80	AR	3980	OHX	2	0
80	A	2077	OHX	1	0
80	sR	2037	OHX	2	0
80	AR	3603	OHX	3	0
80	1	3725	OHX	1	0
80	AR	3636	OHX	2	0
80	1	3846	OHX	1	0
80	1	3841	OHX	1	0
80	4	232	OHX	1	0
80	A	1926	OHX	1	0
80	sR	1979	OHX	1	0
80	sR	1990	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	A	2153	OHX	1	0
80	1	3574	OHX	1	0
80	sR	1945	OHX	4	0
80	1	3601	OHX	2	0
80	1	3425	OHX	1	0
80	sR	2097	OHX	1	0
80	AR	3514	OHX	2	0
80	AR	3791	OHX	3	0
80	AR	3450	OHX	1	0
80	AR	3753	OHX	1	0
80	AR	4203	OHX	1	0
80	AR	3516	OHX	1	0
80	sR	2190	OHX	1	0
80	1	4150	OHX	1	0
80	1	3483	OHX	1	0
80	1	3602	OHX	2	0
80	AR	3977	OHX	1	0
80	A	2094	OHX	1	0
80	A	2057	OHX	1	0
80	sR	2003	OHX	2	0
80	AR	3953	OHX	2	0
80	k	403	OHX	2	0
80	sR	2063	OHX	3	0
80	1	3723	OHX	2	0
80	AR	4107	OHX	1	0
80	AR	4194	OHX	1	0
80	1	3819	OHX	1	0
80	AR	3449	OHX	1	0
80	1	3822	OHX	1	0
80	sR	2062	OHX	1	0
80	sR	2100	OHX	1	0
80	AR	3578	OHX	3	0
80	AR	3883	OHX	2	0
80	sR	2014	OHX	1	0
80	sR	2013	OHX	2	0
80	AR	3815	OHX	1	0
80	1	3991	OHX	1	0
80	AR	3729	OHX	1	0
80	AR	4138	OHX	1	0
80	AR	3535	OHX	1	0
80	AR	4019	OHX	2	0
80	AR	3628	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	1	3791	OHX	1	0
80	1	4111	OHX	2	0
80	AR	3728	OHX	1	0
80	1	4116	OHX	1	0
80	sR	1905	OHX	1	0
80	AR	3831	OHX	1	0
80	AR	3415	OHX	1	0
80	AR	3825	OHX	1	0
80	4	209	OHX	2	0
80	AR	4139	OHX	1	0
80	sR	1944	OHX	2	0
80	1	3993	OHX	1	0
80	sR	2156	OHX	1	0
80	A	2143[A]	OHX	2	0
80	1	3430	OHX	1	0
80	AT	205	OHX	1	0
80	1	4175	OHX	3	0
80	1	3698	OHX	1	0
80	A	1983	OHX	2	0
80	1	4085	OHX	2	0
80	A	1935	OHX	1	0
80	A	2035	OHX	1	0
80	AR	3574	OHX	1	0
80	1	3608	OHX	2	0
80	1	3843	OHX	2	0
80	AR	3511	OHX	1	0
80	sR	2061	OHX	1	0
80	A	2086	OHX	3	0
80	sR	2188	OHX	2	0
80	1	3783	OHX	1	0
80	A	1967	OHX	1	0
80	AR	3885	OHX	1	0
80	AR	3422	OHX	1	0
80	1	4050	OHX	1	0
80	AR	3981	OHX	1	0
80	A	2026	OHX	2	0
80	A	2092	OHX	2	0
80	AR	3758	OHX	1	0
80	sR	2177	OHX	1	0
85	1	3478	SPD	5	0
80	AR	4136	OHX	1	0
80	1	3785	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	A	1974	OHX	1	0
80	1	4084	OHX	1	0
80	c3	201	OHX	1	0
80	AR	3545	OHX	1	0
80	AR	3863	OHX	1	0
80	AR	3783	OHX	1	0
80	sR	2124	OHX	1	0
80	1	3612	OHX	1	0
80	sR	2157	OHX	1	0
80	1	4056	OHX	1	0
80	AR	4066	OHX	2	0
80	1	3579	OHX	1	0
80	AR	3879	OHX	1	0
80	AR	3798	OHX	1	0
80	AR	3512	OHX	1	0
80	A	2047	OHX	1	0
80	sR	2122	OHX	1	0
80	1	3457	OHX	1	0
80	A	2119	OHX	1	0
80	AR	4072	OHX	1	0
80	AR	4039	OHX	2	0
80	1	3875	OHX	1	0
80	1	4054	OHX	1	0
80	AR	4111	OHX	1	0
80	1	4173	OHX	1	0
80	AR	3924	OHX	2	0
80	AR	3984	OHX	1	0
80	1	3691	OHX	2	0
80	1	3669	OHX	2	0
80	AR	3956	OHX	4	0
80	AR	3456	OHX	1	0
80	1	3661	OHX	2	0
80	3	219	OHX	1	0
80	AR	3950	OHX	1	0
80	AR	4041	OHX	1	0
80	1	4120	OHX	1	0
80	4	226	OHX	1	0
80	A	1956	OHX	2	0
80	A	2045	OHX	1	0
80	1	4174	OHX	2	0
80	1	4113	OHX	1	0
80	1	4021	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	1	4110	OHX	1	0
80	A	2096	OHX	1	0
80	AR	3539	OHX	2	0
80	1	3906	OHX	1	0
80	AR	3453	OHX	2	0
80	1	3820	OHX	1	0
80	A	1973	OHX	2	0
80	A	2073	OHX	2	0
80	sR	2050	OHX	1	0
80	sR	2051	OHX	2	0
80	AR	3572	OHX	1	0
80	AR	3548	OHX	2	0
80	sR	1947	OHX	2	0
80	AT	227	OHX	1	0
80	sR	2038	OHX	1	0
80	1	3933	OHX	1	0
80	1	4091	OHX	1	0
80	1	3633	OHX	2	0
80	AR	4101	OHX	1	0
80	AC	101	OHX	1	0
80	AR	3610	OHX	1	0
80	sR	1926	OHX	1	0
80	AR	3926	OHX	1	0
80	sR	1958	OHX	1	0
80	AR	4068	OHX	1	0
80	1	3788	OHX	1	0
80	A	1925	OHX	2	0
80	A	1913	OHX	2	0
84	1	3578	ZWB	1	0
80	Rb	401	OHX	1	0
80	1	4024	OHX	2	0
80	1	3606	OHX	1	0
80	1	3789	OHX	2	0
80	sR	1978	OHX	1	0
80	AR	3630	OHX	1	0
80	AR	3661	OHX	1	0
80	1	3990	OHX	2	0
80	1	4112	OHX	1	0
80	1	3998	OHX	1	0
80	3	222	OHX	2	0
80	A	2065	OHX	1	0
80	AR	3604	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	AR	3541	OHX	2	0
80	1	3908	OHX	1	0
80	AR	4161	OHX	1	0
80	AR	3952	OHX	1	0
80	sR	2144	OHX	2	0
80	1	3482	OHX	1	0
80	1	3631	OHX	5	0
80	AR	4099	OHX	1	0
80	sR	2073	OHX	1	0
80	CK	201	OHX	1	0
80	AR	3703	OHX	1	0
80	1	3603	OHX	4	0
80	1	4083	OHX	6	0
80	AR	3921	OHX	2	0
80	A	1986	OHX	3	0
80	AR	3632	OHX	1	0
80	h	401	OHX	1	0
80	sR	2135	OHX	1	0
80	1	3872	OHX	2	0
80	1	4023	OHX	2	0
80	AR	4097	OHX	1	0
80	sR	2145	OHX	2	0
80	1	3424	OHX	4	0
80	1	3721	OHX	2	0
80	AR	3913	OHX	1	0
80	AR	4196	OHX	1	0
80	c8	201	OHX	1	0
80	AR	3723	OHX	1	0
80	1	3812	OHX	1	0
80	1	4055	OHX	1	0
80	A	1924	OHX	1	0
80	sR	2025	OHX	2	0
80	1	4086	OHX	1	0
80	AK	103	OHX	4	0
80	AR	3973	OHX	4	0
80	AR	3506	OHX	1	0
80	AR	3634	OHX	1	0
80	1	3995	OHX	2	0
80	1	3966	OHX	1	0
80	1	4022	OHX	1	0
80	AR	3755	OHX	2	0
80	AR	4135	OHX	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	2	201	OHX	2	0
80	1	3963	OHX	1	0
80	AR	3751	OHX	3	0
80	1	3695	OHX	3	0
80	sR	2052	OHX	2	0
80	AR	3696	OHX	2	0
80	3	203	OHX	1	0
80	1	4118	OHX	2	0
80	1	3479	OHX	2	0
80	1	3454	OHX	1	0
80	1	3781	OHX	3	0
80	1	4149	OHX	1	0
80	AR	3895	OHX	1	0
80	A	1943	OHX	1	0
80	A	2104	OHX	1	0
80	AS	223	OHX	1	0
80	1	3487	OHX	1	0
80	A	2129	OHX	1	0
80	1	4141	OHX	2	0
80	AR	3792	OHX	1	0
80	AR	3639	OHX	1	0
80	1	3611	OHX	2	0
80	sR	2002	OHX	2	0
80	sR	2125	OHX	1	0
80	1	3882	OHX	1	0
80	AR	3881	OHX	2	0
80	AR	3704	OHX	1	0
80	A	1977	OHX	1	0
80	AR	4016	OHX	1	0
80	1	3849	OHX	1	0
80	AR	3601	OHX	1	0
80	sR	2110	OHX	1	0
80	A	2083	OHX	2	0
80	AR	3946	OHX	2	0
80	1	3570	OHX	1	0
80	sR	2189	OHX	1	0
80	AR	4142	OHX	1	0
80	AR	4201	OHX	1	0
80	A	1994	OHX	3	0
80	1	3641	OHX	1	0
80	sR	2086	OHX	1	0
80	1	3663	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	1	3668	OHX	1	0
80	AT	208	OHX	1	0
80	A	2023	OHX	1	0
80	sR	1989	OHX	2	0
80	AR	3799	OHX	1	0
80	1	3632	OHX	2	0
80	1	4148	OHX	1	0
80	A	1965	OHX	1	0
80	AR	3734	OHX	1	0
80	A	2150	OHX	3	0
80	DH	202	OHX	1	0
80	AR	3917	OHX	1	0
80	sR	2179	OHX	2	0
80	AT	228	OHX	1	0
80	A	1934	OHX	1	0
80	1	3546	OHX	1	0
80	AR	3697	OHX	1	0
80	1	3811	OHX	1	0
80	A	2005	OHX	1	0
80	A	2143[B]	OHX	1	0
80	AR	3473	OHX	1	0
80	AR	3576	OHX	1	0
80	1	4028	OHX	5	0
80	AR	3599	OHX	3	0
80	sR	2136	OHX	2	0
80	AR	3419	OHX	2	0
80	1	4171	OHX	2	0
80	A	1906	OHX	1	0
80	sR	1956	OHX	1	0
80	1	3609	OHX	1	0
80	1	3635	OHX	1	0
80	AR	3954	OHX	2	0
80	A	2110	OHX	5	0
80	AR	3579	OHX	1	0
80	sR	2178	OHX	2	0
80	sR	1904	OHX	1	0
80	A	2025	OHX	2	0
80	AR	3701	OHX	1	0
80	1	3511	OHX	1	0
80	A	2013	OHX	1	0
80	AR	3690	OHX	2	0
80	1	3909	OHX	1	0

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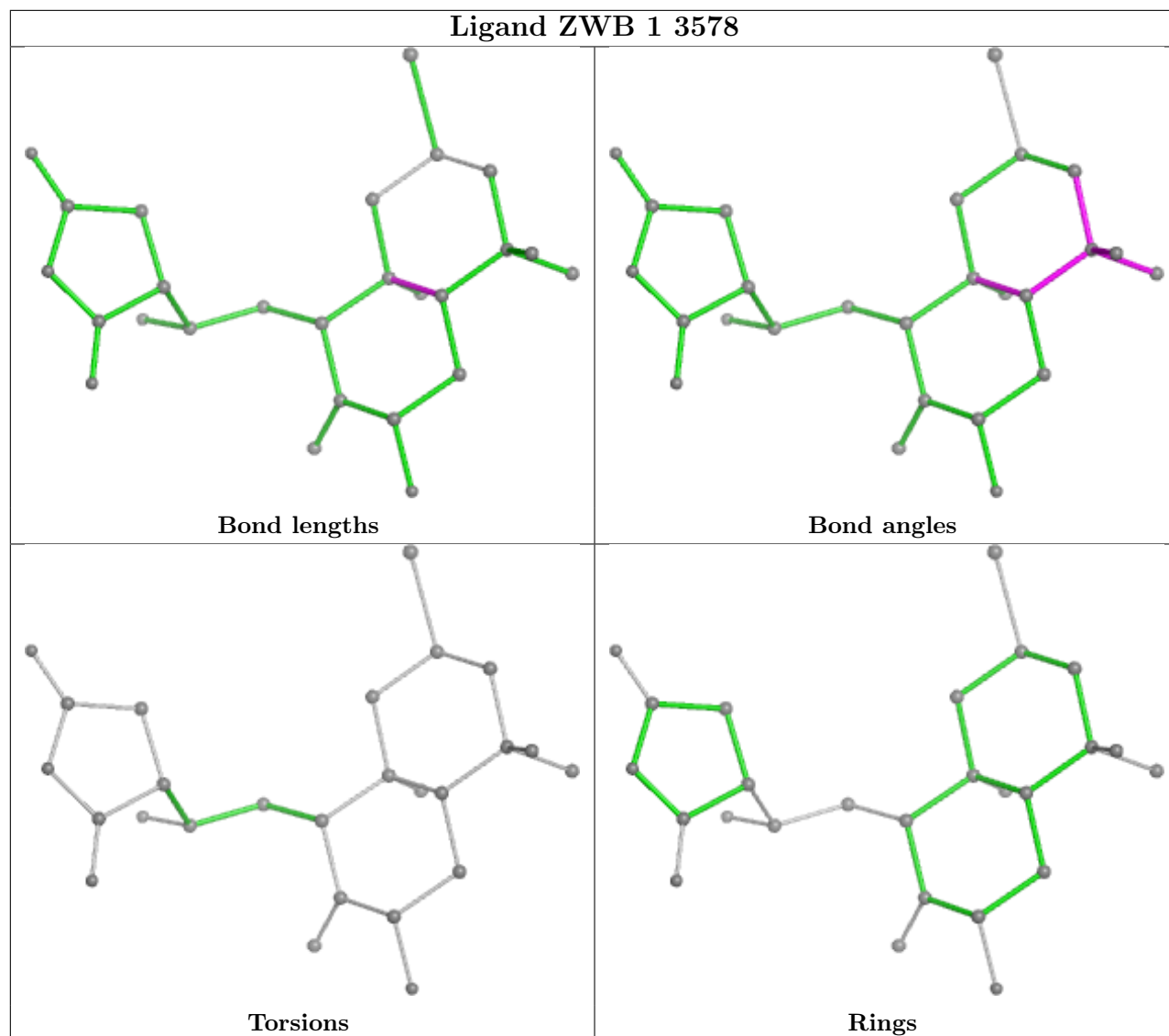
Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	AR	4192	OHX	2	0
80	sR	2121	OHX	2	0
80	s1	301	OHX	2	0
80	1	3452	OHX	2	0
80	sR	1988	OHX	1	0
80	A	1907	OHX	1	0
80	1	3580	OHX	1	0
80	AR	4163	OHX	1	0
80	CP	303	OHX	1	0
80	AR	3919	OHX	1	0
80	3	221	OHX	1	0
80	1	4082	OHX	1	0
80	1	4178	OHX	2	0
80	A	1903	OHX	2	0
80	A	1964	OHX	4	0
85	AR	4164	SPD	1	0
80	3	202	OHX	1	0
80	AR	3508	OHX	1	0
85	AR	3858	SPD	3	0
80	1	3756	OHX	1	0
80	1	3642	OHX	2	0
80	4	228	OHX	2	0
80	AR	3573	OHX	2	0
80	1	3665	OHX	1	0
80	sR	2176	OHX	1	0
80	AR	3670	OHX	1	0
80	sR	1916	OHX	2	0
80	AR	3853	OHX	1	0
80	w	201	OHX	1	0
80	AR	3787	OHX	1	0
80	sR	2026	OHX	3	0
80	AR	3577	OHX	1	0
80	AR	4169	OHX	1	0
80	A	2072	OHX	2	0
80	1	4053	OHX	2	0
80	1	3970	OHX	1	0
80	1	4151	OHX	1	0
80	A	2062	OHX	1	0
80	A	2075	OHX	1	0
80	AR	3985	OHX	1	0
80	AR	3570	OHX	1	0
80	1	4000	OHX	1	0

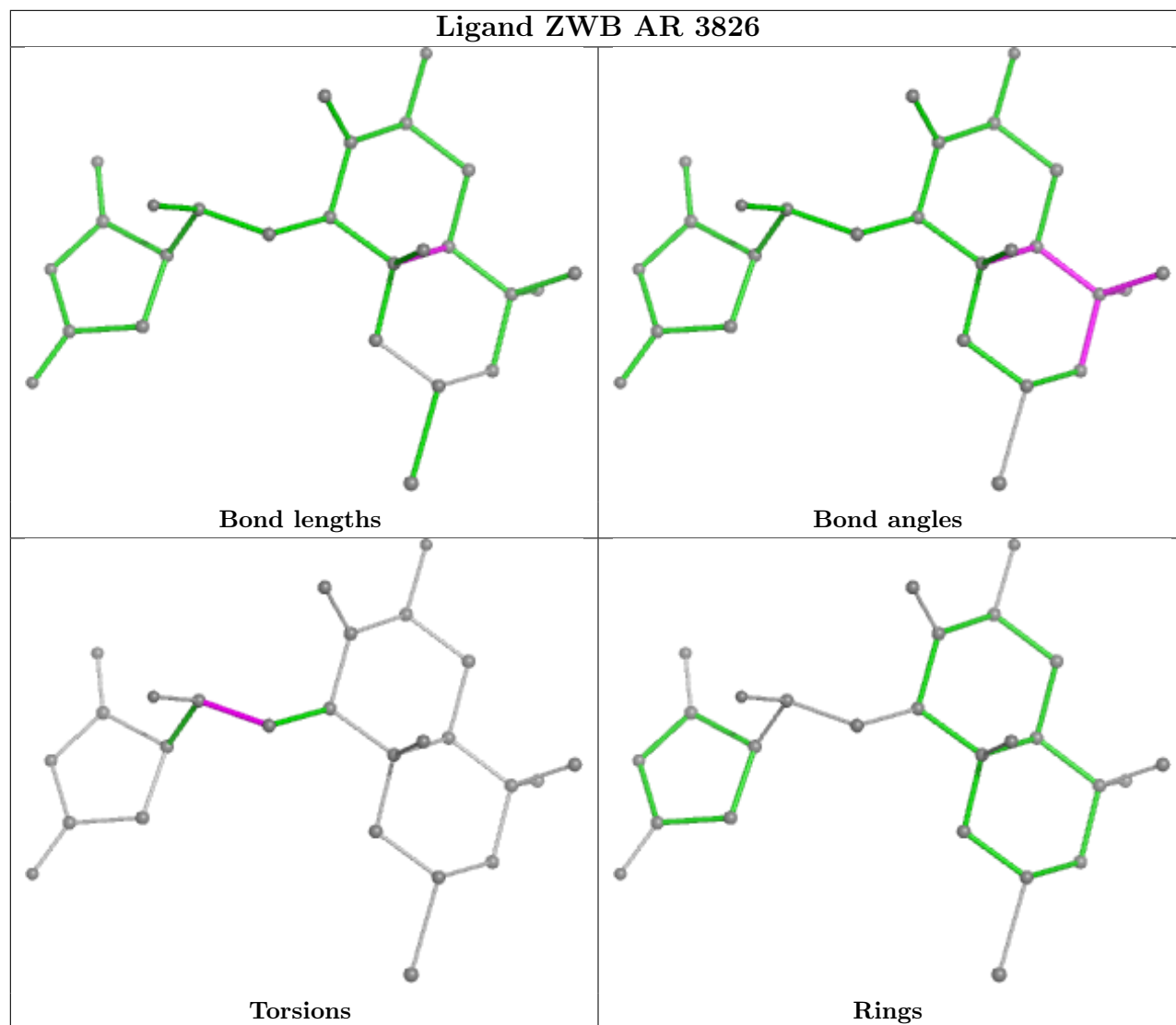
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	1	3544	OHX	1	0
80	AR	3597	OHX	2	0
80	C	301	OHX	2	0
80	AR	3856	OHX	5	0
80	AR	4042	OHX	1	0
80	1	3935	OHX	1	0
80	AR	4070	OHX	1	0
80	sR	1911	OHX	2	0
80	1	3760	OHX	1	0
80	1	3940	OHX	1	0
80	1	3541	OHX	1	0
80	1	3455	OHX	1	0
80	4	230	OHX	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	3	121/121 (100%)	0.32	7 (5%) 30 26	62, 89, 110, 152	0
1	AS	121/121 (100%)	0.03	2 (1%) 69 63	55, 75, 89, 144	0
2	AB	148/149 (99%)	0.60	11 (7%) 22 19	51, 68, 102, 119	0
2	DC	148/149 (99%)	0.66	6 (4%) 42 35	52, 72, 104, 139	0
3	CJ	227/256 (88%)	1.07	31 (13%) 8 7	79, 108, 151, 178	0
3	p	233/256 (91%)	0.88	23 (9%) 14 12	66, 95, 138, 174	0
4	AI	119/120 (99%)	0.83	13 (10%) 12 10	60, 83, 109, 123	0
4	DJ	119/120 (99%)	1.15	20 (16%) 5 4	74, 93, 122, 133	0
5	Q	117/142 (82%)	1.20	22 (18%) 4 3	84, 114, 179, 210	0
5	c5	135/142 (95%)	1.58	44 (32%) 1 1	98, 135, 180, 188	0
6	H	226/236 (95%)	1.67	73 (32%) 1 1	78, 122, 161, 191	0
6	s6	218/236 (92%)	1.04	33 (15%) 6 5	62, 100, 140, 193	0
7	4	158/158 (100%)	0.04	4 (2%) 58 52	57, 71, 131, 203	0
7	AT	158/158 (100%)	0.12	5 (3%) 50 44	60, 79, 148, 222	0
8	AC	54/59 (91%)	1.14	13 (24%) 2 2	52, 78, 116, 127	0
8	DD	58/59 (98%)	1.45	20 (34%) 1 1	55, 78, 119, 133	0
9	CK	191/191 (100%)	0.62	18 (9%) 15 13	56, 73, 114, 189	0
9	q	191/191 (100%)	1.01	30 (15%) 6 5	71, 89, 119, 176	0
10	AJ	99/100 (99%)	0.54	3 (3%) 52 47	64, 87, 129, 156	0
10	DK	97/100 (97%)	0.86	12 (12%) 9 8	81, 99, 133, 144	0
11	R	141/143 (98%)	1.53	44 (31%) 1 1	97, 127, 157, 198	0
11	c6	142/143 (99%)	1.85	60 (42%) 1 1	84, 124, 171, 206	0
12	I	184/190 (96%)	1.13	30 (16%) 5 5	89, 140, 180, 212	0
12	s7	186/190 (97%)	1.06	29 (15%) 6 5	83, 127, 189, 217	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	CD	252/254 (99%)	1.25	48 (19%) 4 3	53, 78, 107, 174	0
13	j	252/254 (99%)	1.21	51 (20%) 3 3	51, 72, 95, 137	0
14	AD	97/105 (92%)	0.64	5 (5%) 34 28	82, 102, 133, 145	0
14	DE	97/105 (92%)	0.97	15 (15%) 6 5	80, 105, 156, 170	0
15	CL	207/221 (93%)	0.69	13 (6%) 27 23	53, 73, 113, 148	0
15	r	211/221 (95%)	0.80	23 (10%) 12 10	56, 82, 127, 161	0
16	AK	87/88 (98%)	0.72	6 (6%) 24 20	53, 63, 101, 146	0
16	DL	87/88 (98%)	0.75	4 (4%) 38 32	57, 69, 111, 147	0
17	S	111/136 (81%)	1.25	24 (21%) 3 3	84, 132, 180, 201	0
17	c7	117/136 (86%)	1.10	17 (14%) 7 6	91, 123, 172, 201	0
18	J	188/200 (94%)	1.19	39 (20%) 3 3	64, 94, 139, 165	0
18	s8	188/200 (94%)	1.34	42 (22%) 3 2	67, 92, 147, 228	0
19	CE	386/387 (99%)	0.62	28 (7%) 22 19	49, 65, 93, 147	0
19	k	386/387 (99%)	0.64	27 (6%) 24 20	53, 77, 107, 149	0
20	AE	109/113 (96%)	0.90	11 (10%) 14 12	66, 87, 141, 170	0
20	DF	107/113 (94%)	0.64	8 (7%) 22 18	61, 78, 135, 193	0
21	CM	169/174 (97%)	0.55	8 (4%) 37 31	62, 86, 117, 167	0
21	s	169/174 (97%)	1.21	28 (16%) 5 5	80, 105, 135, 164	0
22	AL	77/78 (98%)	0.85	7 (9%) 16 14	83, 112, 142, 165	0
22	DM	73/78 (93%)	1.08	10 (13%) 8 7	90, 113, 136, 169	0
23	T	145/146 (99%)	1.60	49 (33%) 1 1	85, 133, 177, 203	0
23	c8	135/146 (92%)	1.34	30 (22%) 3 2	94, 120, 166, 195	0
24	K	177/197 (89%)	1.51	44 (24%) 2 2	85, 121, 158, 188	0
24	s9	185/197 (93%)	1.51	45 (24%) 2 2	69, 103, 155, 192	0
25	CF	361/362 (99%)	0.51	23 (6%) 27 22	49, 73, 103, 132	0
25	l	361/362 (99%)	0.58	25 (6%) 24 20	51, 67, 101, 128	0
26	AF	127/130 (97%)	0.50	5 (3%) 44 37	49, 61, 85, 141	0
26	DG	127/130 (97%)	0.41	3 (2%) 59 53	50, 67, 91, 146	0
27	CN	193/199 (96%)	0.95	29 (15%) 6 6	58, 87, 145, 186	0
27	t	193/199 (96%)	0.64	13 (6%) 25 21	48, 77, 130, 166	0
28	AM	50/51 (98%)	1.14	9 (18%) 4 4	56, 75, 93, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DN	50/51 (98%)	0.79	8 (16%) 6 5	64, 78, 99, 119	0
29	U	143/144 (99%)	1.72	52 (36%) 1 1	102, 130, 169, 187	0
29	c9	143/144 (99%)	1.01	20 (13%) 7 6	87, 113, 149, 199	0
30	L	90/105 (85%)	1.45	25 (27%) 2 2	90, 126, 172, 194	0
30	c0	72/105 (68%)	1.43	20 (27%) 2 2	117, 148, 175, 212	0
31	CG	292/297 (98%)	0.80	36 (12%) 9 8	60, 81, 125, 166	0
31	m	296/297 (99%)	1.30	67 (22%) 3 2	68, 101, 144, 161	0
32	AG	106/107 (99%)	0.69	12 (11%) 11 10	53, 64, 84, 107	0
32	DH	106/107 (99%)	0.57	6 (5%) 30 26	53, 63, 94, 123	0
33	CO	136/138 (98%)	0.57	14 (10%) 13 12	56, 71, 100, 139	0
33	u	136/138 (98%)	0.75	13 (9%) 15 13	64, 78, 110, 146	0
34	AN	52/128 (40%)	0.74	6 (11%) 11 9	67, 81, 113, 134	0
34	DO	52/128 (40%)	0.26	2 (3%) 44 38	53, 62, 87, 149	0
35	V	107/121 (88%)	2.22	51 (47%) 0 0	85, 135, 189, 200	0
35	d0	72/121 (59%)	2.01	26 (36%) 1 1	90, 122, 161, 190	0
36	M	138/156 (88%)	1.04	19 (13%) 8 7	73, 91, 123, 182	0
36	c1	146/156 (93%)	1.22	28 (19%) 4 3	67, 89, 145, 179	0
37	CH	156/176 (88%)	0.42	6 (3%) 44 38	57, 75, 112, 159	0
37	n	156/176 (88%)	0.27	4 (2%) 57 51	57, 71, 108, 146	0
38	AH	112/121 (92%)	1.40	29 (25%) 2 2	61, 87, 134, 166	0
38	DI	112/121 (92%)	1.53	36 (32%) 1 1	67, 92, 143, 191	0
39	CP	203/204 (99%)	1.09	28 (13%) 8 7	57, 77, 98, 116	0
39	v	203/204 (99%)	0.89	17 (8%) 18 16	50, 70, 85, 101	0
40	AO	25/25 (100%)	1.12	3 (12%) 10 9	68, 79, 98, 110	0
40	DP	25/25 (100%)	1.53	7 (28%) 2 2	61, 73, 95, 106	0
41	W	87/87 (100%)	0.94	13 (14%) 7 6	91, 123, 155, 186	0
41	d1	87/87 (100%)	1.08	10 (11%) 11 9	73, 108, 148, 172	0
42	O	150/151 (99%)	1.12	26 (17%) 5 4	79, 109, 142, 171	0
42	c3	150/151 (99%)	0.81	12 (8%) 20 17	74, 99, 131, 162	0
43	CI	222/244 (90%)	0.68	15 (6%) 25 21	52, 65, 112, 197	0
43	o	222/244 (90%)	0.58	13 (5%) 29 25	55, 68, 102, 169	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	CQ	197/199 (98%)	0.71	26 (13%) 8 7	47, 59, 96, 172	0
44	w	197/199 (98%)	0.62	16 (8%) 19 16	53, 68, 95, 139	0
45	AP	105/106 (99%)	0.47	3 (2%) 54 48	54, 75, 118, 162	0
45	DQ	105/106 (99%)	0.67	8 (7%) 21 18	56, 76, 126, 181	0
46	X	129/130 (99%)	1.09	25 (19%) 4 3	83, 105, 129, 143	0
46	d2	129/130 (99%)	0.91	14 (10%) 12 10	65, 87, 107, 130	0
47	P	88/138 (63%)	1.44	26 (29%) 1 1	80, 132, 163, 190	0
47	c4	128/138 (92%)	0.93	18 (14%) 7 6	68, 106, 146, 164	0
48	CR	155/184 (84%)	0.42	8 (5%) 34 28	52, 64, 87, 154	0
48	x	182/184 (98%)	0.44	9 (4%) 36 30	53, 67, 138, 165	0
49	AQ	91/92 (98%)	0.78	11 (12%) 10 9	61, 78, 108, 149	0
49	DR	91/92 (98%)	1.20	17 (18%) 4 3	57, 82, 111, 130	0
50	Y	144/145 (99%)	1.48	41 (28%) 1 2	73, 90, 120, 154	0
50	d3	144/145 (99%)	1.42	26 (18%) 4 4	63, 78, 113, 150	0
51	CS	185/186 (99%)	0.65	16 (8%) 18 15	57, 73, 94, 134	0
51	y	185/186 (99%)	0.69	15 (8%) 19 16	54, 68, 85, 108	0
52	p0	120/311 (38%)	1.35	27 (22%) 3 2	93, 131, 171, 202	0
53	Z	134/135 (99%)	1.47	43 (32%) 1 1	82, 121, 168, 199	0
53	d4	134/135 (99%)	1.55	47 (35%) 1 1	75, 106, 148, 184	0
54	CT	180/189 (95%)	0.79	23 (12%) 9 7	64, 86, 159, 197	0
54	z	183/189 (96%)	0.68	17 (9%) 16 14	68, 86, 150, 183	0
55	i	140/273 (51%)	1.45	37 (26%) 2 2	83, 116, 165, 182	0
55	sM	63/273 (23%)	1.15	12 (19%) 4 3	62, 131, 173, 197	0
56	a	64/108 (59%)	1.18	11 (17%) 5 4	109, 161, 200, 219	0
56	d5	69/108 (63%)	1.32	17 (24%) 2 2	116, 146, 181, 199	0
57	0	172/172 (100%)	1.05	32 (18%) 4 3	59, 76, 107, 155	0
57	CU	172/172 (100%)	0.83	21 (12%) 10 8	52, 66, 94, 124	0
58	A	1722/1800 (95%)	0.49	67 (3%) 44 37	69, 109, 207, 270	0
58	sR	1783/1800 (99%)	0.46	97 (5%) 32 28	56, 98, 220, 289	0
59	b	93/119 (78%)	2.30	47 (50%) 0 0	83, 115, 174, 207	0
59	d6	97/119 (81%)	1.31	24 (24%) 2 2	66, 90, 142, 171	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
60	2	159/160 (99%)	1.82	61 (38%)	1	1	57, 76, 125, 152	0
60	CV	159/160 (99%)	1.82	59 (37%)	1	1	54, 68, 129, 173	0
61	B	206/252 (81%)	1.25	37 (17%)	4	4	93, 130, 168, 195	0
61	s0	206/252 (81%)	1.05	28 (13%)	8	7	88, 115, 151, 181	0
62	c	81/82 (98%)	1.02	12 (14%)	7	6	96, 124, 167, 199	0
62	d7	81/82 (98%)	0.79	6 (7%)	22	19	77, 112, 170, 195	0
63	5	100/121 (82%)	0.92	13 (13%)	9	7	91, 122, 150, 165	0
63	CW	98/121 (80%)	1.89	33 (33%)	1	1	87, 115, 151, 178	0
64	C	116/255 (45%)	1.34	31 (26%)	2	2	93, 133, 175, 202	0
64	s1	216/255 (84%)	0.89	21 (9%)	15	12	77, 106, 143, 205	0
65	d	63/67 (94%)	1.51	14 (22%)	3	2	108, 156, 191, 196	0
65	d8	63/67 (94%)	1.47	19 (30%)	1	1	105, 145, 189, 210	0
66	6	136/137 (99%)	0.73	11 (8%)	19	16	54, 75, 105, 147	0
66	CX	136/137 (99%)	0.59	14 (10%)	13	12	50, 67, 97, 144	0
67	D	217/254 (85%)	1.24	39 (17%)	4	4	82, 109, 149, 184	0
67	s2	217/254 (85%)	1.27	49 (22%)	3	2	75, 100, 138, 162	0
68	d9	49/56 (87%)	1.42	12 (24%)	2	2	83, 107, 133, 148	0
68	e	53/56 (94%)	1.40	11 (20%)	3	3	83, 102, 131, 175	0
69	7	63/155 (40%)	0.75	6 (9%)	15	13	69, 83, 106, 136	0
69	CY	116/155 (74%)	0.80	9 (7%)	20	18	60, 90, 141, 192	0
70	E	223/240 (92%)	1.28	52 (23%)	2	2	87, 116, 162, 202	0
70	s3	223/240 (92%)	1.38	50 (22%)	3	2	91, 132, 174, 190	0
71	e0	62/63 (98%)	1.33	13 (20%)	3	3	73, 108, 158, 199	0
71	f	60/63 (95%)	1.49	17 (28%)	1	2	84, 124, 183, 198	0
72	8	117/142 (82%)	0.78	12 (10%)	13	12	63, 83, 111, 125	0
72	CZ	117/142 (82%)	1.01	17 (14%)	7	6	62, 88, 116, 134	0
73	F	260/261 (99%)	1.57	77 (29%)	1	1	84, 111, 143, 176	0
73	s4	260/261 (99%)	1.32	49 (18%)	4	3	76, 98, 130, 194	0
74	g	71/152 (46%)	1.57	23 (32%)	1	1	119, 156, 194, 214	0
75	1	3149/3396 (92%)	0.25	99 (3%)	51	46	47, 73, 190, 299	0
75	AR	3136/3396 (92%)	0.16	63 (2%)	64	58	48, 70, 165, 298	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
76	9	126/127 (99%)	0.75	14 (11%) 12 10	58, 76, 103, 140	0
76	DA	124/127 (97%)	0.66	9 (7%) 22 19	62, 80, 113, 139	0
77	G	206/225 (91%)	1.35	51 (24%) 2 2	103, 146, 182, 215	0
77	s5	206/225 (91%)	1.46	56 (27%) 2 2	88, 131, 177, 198	0
78	Rb	318/319 (99%)	1.06	46 (14%) 7 6	112, 154, 187, 229	0
78	h	310/319 (97%)	0.93	39 (12%) 9 8	98, 140, 182, 205	0
79	AA	135/136 (99%)	0.80	11 (8%) 19 16	83, 106, 138, 154	0
79	DB	135/136 (99%)	1.05	20 (14%) 7 6	90, 116, 151, 171	0
All	All	32216/35131 (91%)	0.79	3870 (12%) 10 9	47, 90, 165, 299	0

The worst 5 of 3870 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	CV	86	GLU	11.5
6	H	79	LYS	10.4
24	K	2	PRO	9.5
6	H	80	ASN	9.5
18	s8	61	GLU	9.5

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	A	1930	1/1	0.22	0.29	113,113,113,113	0
81	MG	1	4135	1/1	0.28	0.25	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	d5	201	1/1	0.35	0.16	109,109,109,109	0
81	MG	A	2098	1/1	0.41	0.24	113,113,113,113	0
81	MG	A	2124	1/1	0.45	0.24	104,104,104,104	0
81	MG	sR	2008	1/1	0.45	0.21	107,107,107,107	0
80	OHX	1	4143	7/7	0.49	0.17	257,269,297,380	0
81	MG	A	2040	1/1	0.50	0.23	116,116,116,116	0
81	MG	sR	1998	1/1	0.52	0.21	97,97,97,97	0
81	MG	A	1941	1/1	0.52	0.27	103,103,103,103	0
81	MG	A	1970	1/1	0.53	0.30	110,110,110,110	0
81	MG	sR	1942	1/1	0.53	0.39	112,112,112,112	0
81	MG	AR	3656	1/1	0.54	0.31	87,87,87,87	0
81	MG	1	3750	1/1	0.55	0.27	95,95,95,95	0
81	MG	1	3746	1/1	0.56	0.35	93,93,93,93	0
81	MG	A	2138	1/1	0.56	0.21	121,121,121,121	0
81	MG	1	3505	1/1	0.56	0.34	94,94,94,94	0
81	MG	1	3685	1/1	0.57	0.28	99,99,99,99	0
81	MG	1	3637	1/1	0.58	0.17	105,105,105,105	0
81	MG	AS	209	1/1	0.58	0.33	91,91,91,91	0
81	MG	AR	3715	1/1	0.58	0.15	119,119,119,119	0
81	MG	AR	4053	1/1	0.58	0.32	84,84,84,84	0
81	MG	1	3532	1/1	0.58	0.28	88,88,88,88	0
81	MG	AR	3499	1/1	0.59	0.19	86,86,86,86	0
81	MG	1	3500	1/1	0.60	0.41	94,94,94,94	0
80	OHX	1	3518	7/7	0.60	0.15	262,273,286,356	0
81	MG	1	4136	1/1	0.60	0.28	87,87,87,87	0
81	MG	AS	224	1/1	0.61	0.18	123,123,123,123	0
81	MG	AR	3645	1/1	0.61	0.24	61,61,61,61	0
81	MG	1	3521	1/1	0.62	0.30	72,72,72,72	0
81	MG	3	217	1/1	0.62	0.15	105,105,105,105	0
81	MG	1	3536	1/1	0.62	0.31	94,94,94,94	0
81	MG	1	3616	1/1	0.62	0.29	102,102,102,102	0
81	MG	6	202	1/1	0.62	0.17	98,98,98,98	0
81	MG	1	4137	1/1	0.62	0.18	85,85,85,85	0
81	MG	A	2127	1/1	0.63	0.24	97,97,97,97	0
81	MG	sR	2103	1/1	0.64	0.22	76,76,76,76	0
81	MG	CP	302	1/1	0.64	0.29	87,87,87,87	0
81	MG	A	1990	1/1	0.64	0.15	95,95,95,95	0
81	MG	AR	3637	1/1	0.64	0.19	112,112,112,112	0
81	MG	sR	1987	1/1	0.65	0.30	82,82,82,82	0
81	MG	A	1909	1/1	0.65	0.31	97,97,97,97	0
81	MG	1	3864	1/1	0.65	0.28	81,81,81,81	0
81	MG	1	3899	1/1	0.65	0.23	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	s	300	1/1	0.65	0.18	87,87,87,87	0
81	MG	sR	2080	1/1	0.65	0.42	83,83,83,83	0
81	MG	AR	3470	1/1	0.65	0.21	106,106,106,106	0
81	MG	A	2059	1/1	0.66	0.26	93,93,93,93	0
81	MG	A	2009	1/1	0.66	0.37	99,99,99,99	0
81	MG	AR	3801	1/1	0.66	0.23	94,94,94,94	0
81	MG	AR	3905	1/1	0.66	0.56	98,98,98,98	0
80	OHX	AR	3641	7/7	0.66	0.16	170,200,225,277	0
81	MG	sR	1972	1/1	0.67	0.34	94,94,94,94	0
81	MG	sR	2092	1/1	0.67	0.14	89,89,89,89	0
80	OHX	A	1904	7/7	0.67	0.17	215,216,231,306	0
81	MG	sR	2160	1/1	0.67	0.26	68,68,68,68	0
81	MG	sR	2164	1/1	0.67	0.18	93,93,93,93	0
81	MG	1	3959	1/1	0.67	0.31	84,84,84,84	0
81	MG	A	2091	1/1	0.67	0.34	89,89,89,89	0
81	MG	A	1921	1/1	0.67	0.19	85,85,85,85	0
81	MG	1	3656	1/1	0.67	0.18	89,89,89,89	0
81	MG	1	3476	1/1	0.68	0.25	91,91,91,91	0
81	MG	A	2147	1/1	0.68	0.21	94,94,94,94	0
81	MG	A	2088	1/1	0.68	0.19	93,93,93,93	0
81	MG	1	3778	1/1	0.68	0.32	79,79,79,79	0
81	MG	sR	1976	1/1	0.68	0.29	88,88,88,88	0
81	MG	sR	2130	1/1	0.68	0.32	89,89,89,89	0
81	MG	AR	4102	1/1	0.68	0.38	69,69,69,69	0
80	OHX	sR	1933	7/7	0.68	0.20	225,235,253,327	0
81	MG	A	2021	1/1	0.68	0.43	102,102,102,102	0
81	MG	sR	2059	1/1	0.68	0.42	94,94,94,94	0
81	MG	1	3748	1/1	0.69	0.34	89,89,89,89	0
80	OHX	sR	1927	7/7	0.69	0.16	222,228,250,308	0
81	MG	A	2136	1/1	0.69	0.23	78,78,78,78	0
81	MG	1	3837	1/1	0.69	0.20	80,80,80,80	0
81	MG	sR	2105	1/1	0.69	0.16	97,97,97,97	0
81	MG	1	3623	1/1	0.69	0.26	91,91,91,91	0
81	MG	AR	3708	1/1	0.69	0.23	72,72,72,72	0
81	MG	d3	202	1/1	0.69	0.37	85,85,85,85	0
81	MG	1	3507	1/1	0.69	0.39	82,82,82,82	0
81	MG	AR	4162	1/1	0.69	0.27	75,75,75,75	0
81	MG	AR	3494	1/1	0.70	0.40	79,79,79,79	0
81	MG	AR	3809	1/1	0.70	0.30	106,106,106,106	0
81	MG	sR	2058	1/1	0.70	0.25	102,102,102,102	0
81	MG	AR	3838	1/1	0.70	0.22	87,87,87,87	0
81	MG	AR	3839	1/1	0.70	0.24	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	AR	3880	1/1	0.70	0.36	78,78,78,78	0
80	OHX	sR	2170	7/7	0.71	0.17	214,222,251,318	0
81	MG	sR	1985	1/1	0.71	0.23	80,80,80,80	0
80	OHX	AR	3863	7/7	0.71	0.14	200,215,244,305	0
81	MG	AR	4129	1/1	0.71	0.56	81,81,81,81	0
80	OHX	1	3569	7/7	0.71	0.16	212,236,241,313	0
80	OHX	1	3845	7/7	0.71	0.25	202,207,214,323	0
80	OHX	AR	3895	7/7	0.71	0.13	214,216,236,300	0
81	MG	1	4105	1/1	0.71	0.35	85,85,85,85	0
81	MG	x	205	1/1	0.71	0.38	98,98,98,98	0
81	MG	sR	2082	1/1	0.71	0.40	79,79,79,79	0
81	MG	A	2020	1/1	0.71	0.32	94,94,94,94	0
81	MG	AR	3989	1/1	0.72	0.20	65,65,65,65	0
81	MG	sR	1965	1/1	0.72	0.29	74,74,74,74	0
81	MG	AO	101	1/1	0.72	0.20	85,85,85,85	0
81	MG	A	2128	1/1	0.72	0.20	129,129,129,129	0
80	OHX	A	1914	7/7	0.72	0.14	177,179,201,225	7
81	MG	1	3955	1/1	0.72	0.45	102,102,102,102	0
81	MG	AR	3414	1/1	0.72	0.32	95,95,95,95	0
81	MG	1	3678	1/1	0.72	0.36	110,110,110,110	0
80	OHX	AR	3767	7/7	0.72	0.14	189,206,233,294	0
81	MG	sR	2116	1/1	0.72	0.20	74,74,74,74	0
80	OHX	sR	1966	7/7	0.72	0.20	172,176,184,216	7
80	OHX	sR	2124	7/7	0.73	0.17	175,181,203,270	0
81	MG	A	1951	1/1	0.73	0.15	116,116,116,116	0
81	MG	sR	2033	1/1	0.73	0.37	92,92,92,92	0
81	MG	AR	3651	1/1	0.73	0.37	103,103,103,103	0
81	MG	AR	3845	1/1	0.73	0.31	86,86,86,86	0
81	MG	AR	3852	1/1	0.73	0.39	97,97,97,97	0
81	MG	AR	3866	1/1	0.73	0.37	76,76,76,76	0
81	MG	AR	3439	1/1	0.73	0.29	83,83,83,83	0
81	MG	A	2157	1/1	0.73	0.17	76,76,76,76	0
80	OHX	AR	3831	7/7	0.73	0.18	215,227,240,312	0
80	OHX	AR	3673	7/7	0.73	0.16	239,246,272,358	0
81	MG	sR	1986	1/1	0.73	0.32	88,88,88,88	0
81	MG	1	3630	1/1	0.73	0.35	88,88,88,88	0
81	MG	sR	2153	1/1	0.73	0.17	76,76,76,76	0
81	MG	AR	4098	1/1	0.73	0.36	92,92,92,92	0
81	MG	AS	215	1/1	0.74	0.36	88,88,88,88	0
81	MG	1	3439	1/1	0.74	0.30	83,83,83,83	0
80	OHX	sR	1905	7/7	0.74	0.16	242,246,272,341	0
81	MG	1	3747	1/1	0.74	0.19	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	3498	1/1	0.74	0.39	82,82,82,82	0
81	MG	sR	1939	1/1	0.74	0.31	72,72,72,72	0
81	MG	AR	3459	1/1	0.74	0.27	92,92,92,92	0
80	OHX	A	2023	7/7	0.74	0.17	218,230,246,307	0
81	MG	AR	4032	1/1	0.74	0.16	99,99,99,99	0
80	OHX	1	4058	7/7	0.74	0.15	190,199,220,296	0
81	MG	AR	4065	1/1	0.74	0.21	78,78,78,78	0
80	OHX	sR	2192	7/7	0.74	0.16	235,273,279,339	0
80	OHX	sR	2101	7/7	0.74	0.15	206,221,231,301	0
81	MG	1	4106	1/1	0.74	0.37	81,81,81,81	0
81	MG	4	233	1/1	0.74	0.32	81,81,81,81	0
81	MG	z	201	1/1	0.74	0.13	119,119,119,119	0
81	MG	U	201	1/1	0.74	0.29	79,79,79,79	0
81	MG	AR	4158	1/1	0.75	0.35	83,83,83,83	0
81	MG	sR	2007	1/1	0.75	0.32	102,102,102,102	0
81	MG	AR	3873	1/1	0.75	0.19	88,88,88,88	0
81	MG	1	3684	1/1	0.75	0.15	66,66,66,66	0
81	MG	AT	216	1/1	0.75	0.14	86,86,86,86	0
81	MG	sR	2009	1/1	0.75	0.19	74,74,74,74	0
81	MG	1	3416	1/1	0.75	0.26	97,97,97,97	0
81	MG	A	1931	1/1	0.75	0.28	73,73,73,73	0
80	OHX	AR	4081	6/7	0.75	0.16	201,217,232,296	0
81	MG	1	3776	1/1	0.75	0.29	77,77,77,77	0
81	MG	AR	3971	1/1	0.75	0.20	94,94,94,94	0
81	MG	A	2106	1/1	0.75	0.35	89,89,89,89	0
80	OHX	AS	230	7/7	0.75	0.18	176,192,209,257	0
80	OHX	A	2033	7/7	0.75	0.13	176,188,212,275	0
81	MG	A	1981	1/1	0.75	0.39	92,92,92,92	0
80	OHX	1	4181	7/7	0.75	0.21	161,174,184,296	0
81	MG	1	3977	1/1	0.75	0.26	92,92,92,92	0
81	MG	1	3985	1/1	0.75	0.16	85,85,85,85	0
81	MG	A	2089	1/1	0.75	0.17	109,109,109,109	0
81	MG	AR	4113	1/1	0.75	0.35	87,87,87,87	0
81	MG	sR	2139	1/1	0.75	0.35	72,72,72,72	0
81	MG	1	3628	1/1	0.75	0.33	85,85,85,85	0
81	MG	AR	3674	1/1	0.75	0.31	83,83,83,83	0
81	MG	sR	2152	1/1	0.76	0.43	87,87,87,87	0
80	OHX	AR	3734	7/7	0.76	0.18	113,140,173,236	0
81	MG	AR	3960	1/1	0.76	0.22	85,85,85,85	0
81	MG	A	1942	1/1	0.76	0.35	89,89,89,89	0
81	MG	sR	2196	1/1	0.76	0.18	76,76,76,76	0
81	MG	1	3715	1/1	0.76	0.30	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	AR	3735	7/7	0.76	0.12	238,247,281,344	0
80	OHX	AR	4019	7/7	0.76	0.20	210,226,253,331	0
81	MG	AR	3685	1/1	0.76	0.20	81,81,81,81	0
81	MG	c6	201	1/1	0.76	0.24	95,95,95,95	0
80	OHX	sR	2089	7/7	0.76	0.12	210,212,227,294	0
81	MG	A	2125	1/1	0.76	0.25	87,87,87,87	0
81	MG	A	1902	1/1	0.76	0.34	77,77,77,77	0
81	MG	AR	3810	1/1	0.76	0.24	78,78,78,78	0
80	OHX	A	2140	7/7	0.76	0.18	162,163,183,248	0
81	MG	1	3915	1/1	0.76	0.22	76,76,76,76	0
80	OHX	AR	3827	7/7	0.76	0.22	232,240,254,319	0
81	MG	AR	4207	1/1	0.76	0.20	62,62,62,62	0
81	MG	AR	3840	1/1	0.76	0.24	77,77,77,77	0
80	OHX	sR	2159	7/7	0.76	0.15	188,213,233,278	0
81	MG	AR	3567	1/1	0.76	0.24	86,86,86,86	0
81	MG	1	3619	1/1	0.76	0.14	74,74,74,74	0
81	MG	AR	3593	1/1	0.76	0.23	98,98,98,98	0
81	MG	AR	3621	1/1	0.76	0.30	70,70,70,70	0
80	OHX	AR	3728	7/7	0.76	0.22	155,163,186,221	7
81	MG	AR	3660	1/1	0.77	0.18	75,75,75,75	0
81	MG	AR	3495	1/1	0.77	0.35	75,75,75,75	0
81	MG	AR	4060	1/1	0.77	0.37	94,94,94,94	0
80	OHX	A	2057	7/7	0.77	0.13	208,234,250,290	0
81	MG	1	3534	1/1	0.77	0.36	85,85,85,85	0
81	MG	1	3829	1/1	0.77	0.34	69,69,69,69	0
81	MG	1	3831	1/1	0.77	0.27	94,94,94,94	0
81	MG	CK	203	1/1	0.77	0.15	142,142,142,142	0
81	MG	1	3839	1/1	0.77	0.33	82,82,82,82	0
81	MG	c7	201	1/1	0.77	0.29	97,97,97,97	0
81	MG	AR	3434	1/1	0.77	0.42	75,75,75,75	0
81	MG	1	3900	1/1	0.77	0.54	93,93,93,93	0
81	MG	c8	202	1/1	0.77	0.44	90,90,90,90	0
81	MG	A	2042	1/1	0.77	0.29	83,83,83,83	0
81	MG	CG	305	1/1	0.77	0.17	77,77,77,77	0
81	MG	1	3409	1/1	0.77	0.19	79,79,79,79	0
81	MG	1	3984	1/1	0.77	0.14	102,102,102,102	0
81	MG	CX	202	1/1	0.77	0.22	72,72,72,72	0
81	MG	1	4041	1/1	0.77	0.42	81,81,81,81	0
81	MG	sR	2106	1/1	0.77	0.44	113,113,113,113	0
81	MG	1	3440	1/1	0.77	0.30	95,95,95,95	0
80	OHX	sR	1937	7/7	0.77	0.17	191,204,230,288	0
81	MG	AR	4031	1/1	0.77	0.36	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	sR	2131	1/1	0.77	0.35	83,83,83,83	0
81	MG	3	212	1/1	0.78	0.24	74,74,74,74	0
81	MG	1	3508	1/1	0.78	0.38	60,60,60,60	0
81	MG	AR	3778	1/1	0.78	0.21	97,97,97,97	0
81	MG	A	1952	1/1	0.78	0.34	69,69,69,69	0
81	MG	AR	3598	1/1	0.78	0.26	92,92,92,92	0
81	MG	sR	2055	1/1	0.78	0.27	99,99,99,99	0
81	MG	sR	2197	1/1	0.78	0.32	56,56,56,56	0
81	MG	1	3865	1/1	0.78	0.38	76,76,76,76	0
81	MG	1	3892	1/1	0.78	0.18	85,85,85,85	0
81	MG	A	2079	1/1	0.78	0.28	96,96,96,96	0
81	MG	AR	3834	1/1	0.78	0.21	81,81,81,81	0
80	OHX	AR	3635	7/7	0.78	0.15	172,175,196,268	0
80	OHX	sR	2111	7/7	0.78	0.17	178,189,207,268	0
80	OHX	1	3702	7/7	0.78	0.14	224,242,255,311	0
81	MG	sR	1975	1/1	0.78	0.36	67,67,67,67	0
80	OHX	AR	3894	7/7	0.78	0.21	150,166,180,262	0
81	MG	sR	1984	1/1	0.78	0.20	79,79,79,79	0
81	MG	1	4003	1/1	0.78	0.18	76,76,76,76	0
81	MG	1	3468	1/1	0.78	0.23	80,80,80,80	0
81	MG	1	3474	1/1	0.78	0.16	76,76,76,76	0
80	OHX	sR	1938	7/7	0.78	0.10	261,268,281,330	0
81	MG	1	4109	1/1	0.78	0.44	73,73,73,73	0
81	MG	1	4134	1/1	0.78	0.29	80,80,80,80	0
80	OHX	A	1974	7/7	0.78	0.13	216,218,236,290	0
80	OHX	A	1997	7/7	0.78	0.14	187,196,217,293	0
81	MG	AR	3561	1/1	0.78	0.23	85,85,85,85	0
81	MG	1	3645	1/1	0.79	0.29	78,78,78,78	0
81	MG	AR	3898	1/1	0.79	0.22	83,83,83,83	0
80	OHX	AR	3511	7/7	0.79	0.19	181,183,201,235	7
81	MG	sR	2175	1/1	0.79	0.26	81,81,81,81	0
81	MG	sR	2184	1/1	0.79	0.21	103,103,103,103	0
81	MG	sR	2195	1/1	0.79	0.27	89,89,89,89	0
81	MG	AR	3433	1/1	0.79	0.48	89,89,89,89	0
81	MG	A	1928	1/1	0.79	0.35	68,68,68,68	0
80	OHX	1	4151	7/7	0.79	0.13	173,184,192,261	0
81	MG	AR	3990	1/1	0.79	0.40	66,66,66,66	0
81	MG	AR	3440	1/1	0.79	0.24	75,75,75,75	0
81	MG	AR	3443	1/1	0.79	0.27	112,112,112,112	0
81	MG	1	3823	1/1	0.79	0.29	78,78,78,78	0
81	MG	AR	3713	1/1	0.79	0.13	69,69,69,69	0
80	OHX	AR	3824	7/7	0.79	0.11	216,218,220,251	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	AR	4061	1/1	0.79	0.22	72,72,72,72	0
81	MG	CR	203	1/1	0.79	0.27	85,85,85,85	0
81	MG	AR	4071	1/1	0.79	0.31	67,67,67,67	0
81	MG	A	2144	1/1	0.79	0.36	72,72,72,72	0
81	MG	1	3866	1/1	0.79	0.24	77,77,77,77	0
81	MG	1	3870	1/1	0.79	0.35	76,76,76,76	0
81	MG	A	2145	1/1	0.79	0.38	76,76,76,76	0
80	OHX	AR	3518	7/7	0.79	0.12	183,196,218,286	0
81	MG	AR	3533	1/1	0.79	0.29	84,84,84,84	0
81	MG	1	3914	1/1	0.79	0.28	65,65,65,65	0
81	MG	1	3503	1/1	0.79	0.29	66,66,66,66	0
81	MG	1	3922	1/1	0.79	0.19	63,63,63,63	0
81	MG	1	3924	1/1	0.79	0.16	73,73,73,73	0
81	MG	AR	4153	1/1	0.79	0.23	62,62,62,62	0
81	MG	sR	2090	1/1	0.79	0.35	67,67,67,67	0
81	MG	AR	3534	1/1	0.79	0.18	52,52,52,52	0
81	MG	3	215	1/1	0.79	0.33	95,95,95,95	0
80	OHX	AR	3926	7/7	0.79	0.14	217,223,230,307	0
81	MG	AS	208	1/1	0.79	0.18	81,81,81,81	0
81	MG	1	4015	1/1	0.79	0.28	64,64,64,64	0
81	MG	A	1960	1/1	0.79	0.20	92,92,92,92	0
81	MG	1	4100	1/1	0.79	0.14	88,88,88,88	0
81	MG	1	3584	1/1	0.79	0.44	73,73,73,73	0
81	MG	sR	2129	1/1	0.79	0.13	98,98,98,98	0
81	MG	AB	206	1/1	0.79	0.30	83,83,83,83	0
80	OHX	AR	3540	7/7	0.79	0.12	205,216,234,305	0
81	MG	A	1912	1/1	0.79	0.12	101,101,101,101	0
81	MG	A	2008	1/1	0.79	0.40	63,63,63,63	0
81	MG	sR	1954	1/1	0.79	0.31	122,122,122,122	0
81	MG	1	4157	1/1	0.79	0.28	80,80,80,80	0
80	OHX	A	1944	7/7	0.80	0.12	239,242,255,328	0
81	MG	AR	4133	1/1	0.80	0.28	83,83,83,83	0
81	MG	AR	4144	1/1	0.80	0.34	63,63,63,63	0
81	MG	AR	4148	1/1	0.80	0.45	62,62,62,62	0
81	MG	AR	3726	1/1	0.80	0.45	88,88,88,88	0
81	MG	1	3659	1/1	0.80	0.32	79,79,79,79	0
81	MG	A	1972	1/1	0.80	0.48	84,84,84,84	0
80	OHX	AR	3799	7/7	0.80	0.15	193,208,227,291	0
81	MG	AR	4183	1/1	0.80	0.19	83,83,83,83	0
81	MG	AR	3803	1/1	0.80	0.53	63,63,63,63	0
81	MG	1	3736	1/1	0.80	0.23	61,61,61,61	0
81	MG	AR	3451	1/1	0.80	0.19	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	3	206	7/7	0.80	0.14	196,206,213,260	0
80	OHX	sR	1977	7/7	0.80	0.27	139,143,157,176	7
81	MG	AR	3489	1/1	0.80	0.22	70,70,70,70	0
81	MG	sR	2187	1/1	0.80	0.17	101,101,101,101	0
81	MG	sR	1918	1/1	0.80	0.35	69,69,69,69	0
80	OHX	1	3512	7/7	0.80	0.18	160,162,181,213	7
81	MG	1	3824	1/1	0.80	0.23	65,65,65,65	0
81	MG	A	2010	1/1	0.80	0.26	85,85,85,85	0
81	MG	A	2012	1/1	0.80	0.12	98,98,98,98	0
81	MG	1	3835	1/1	0.80	0.27	69,69,69,69	0
81	MG	AT	214	1/1	0.80	0.12	87,87,87,87	0
81	MG	3	213	1/1	0.80	0.15	76,76,76,76	0
81	MG	1	3847	1/1	0.80	0.17	59,59,59,59	0
80	OHX	sR	2077	7/7	0.80	0.10	228,251,270,316	0
81	MG	AR	3552	1/1	0.80	0.16	120,120,120,120	0
81	MG	AR	3558	1/1	0.80	0.33	78,78,78,78	0
81	MG	A	2148	1/1	0.80	0.24	91,91,91,91	0
80	OHX	sR	1916	7/7	0.80	0.12	224,234,257,333	0
80	OHX	1	3582	7/7	0.80	0.15	202,210,232,310	0
81	MG	t	201	1/1	0.80	0.20	94,94,94,94	0
81	MG	1	3913	1/1	0.80	0.28	69,69,69,69	0
81	MG	AR	3614	1/1	0.80	0.33	79,79,79,79	0
80	OHX	4	206	7/7	0.80	0.23	138,147,159,193	7
80	OHX	AR	3666	7/7	0.80	0.14	181,183,219,268	0
81	MG	1	3499	1/1	0.80	0.21	69,69,69,69	0
81	MG	1	3927	1/1	0.80	0.37	65,65,65,65	0
81	MG	A	2081	1/1	0.80	0.13	76,76,76,76	0
81	MG	AR	4036	1/1	0.80	0.21	105,105,105,105	0
81	MG	sR	2034	1/1	0.80	0.28	75,75,75,75	0
81	MG	sR	2035	1/1	0.80	0.16	81,81,81,81	0
80	OHX	1	3851	7/7	0.80	0.16	199,205,233,265	0
81	MG	AH	201	1/1	0.80	0.15	86,86,86,86	0
81	MG	1	3530	1/1	0.80	0.36	77,77,77,77	0
81	MG	AR	3402	1/1	0.80	0.25	80,80,80,80	0
81	MG	1	4046	1/1	0.80	0.45	67,67,67,67	0
81	MG	1	4073	1/1	0.80	0.54	80,80,80,80	0
81	MG	1	3533	1/1	0.80	0.15	74,74,74,74	0
81	MG	sR	2071	1/1	0.80	0.29	84,84,84,84	0
81	MG	AR	3412	1/1	0.80	0.33	73,73,73,73	0
81	MG	1	3556	1/1	0.80	0.24	88,88,88,88	0
81	MG	1	4128	1/1	0.80	0.32	63,63,63,63	0
81	MG	AR	3676	1/1	0.80	0.22	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	3585	1/1	0.80	0.19	62,62,62,62	0
80	OHX	1	3963	7/7	0.80	0.14	187,199,227,299	0
81	MG	A	2097	1/1	0.80	0.34	70,70,70,70	0
80	OHX	1	4001	7/7	0.80	0.14	200,223,247,306	0
82	ZN	d7	101	1/1	0.80	0.10	274,274,274,274	0
81	MG	4	217	1/1	0.81	0.19	77,77,77,77	0
81	MG	A	1908	1/1	0.81	0.28	83,83,83,83	0
81	MG	4	218	1/1	0.81	0.33	74,74,74,74	0
81	MG	A	1911	1/1	0.81	0.33	102,102,102,102	0
81	MG	4	222	1/1	0.81	0.33	76,76,76,76	0
81	MG	4	224	1/1	0.81	0.12	65,65,65,65	0
81	MG	AR	3875	1/1	0.81	0.31	64,64,64,64	0
80	OHX	1	3514	7/7	0.81	0.28	134,139,161,194	7
80	OHX	sR	1949	7/7	0.81	0.15	191,201,223,268	0
81	MG	AR	3903	1/1	0.81	0.32	87,87,87,87	0
81	MG	A	2029	1/1	0.81	0.22	103,103,103,103	0
80	OHX	1	3875	7/7	0.81	0.33	150,168,178,208	7
81	MG	sR	2142	1/1	0.81	0.16	65,65,65,65	0
81	MG	sR	2149	1/1	0.81	0.19	82,82,82,82	0
81	MG	AR	3462	1/1	0.81	0.34	59,59,59,59	0
81	MG	AR	3677	1/1	0.81	0.35	48,48,48,48	0
81	MG	CO	201	1/1	0.81	0.33	73,73,73,73	0
81	MG	AR	4022	1/1	0.81	0.25	76,76,76,76	0
81	MG	AR	4029	1/1	0.81	0.27	83,83,83,83	0
81	MG	AR	3688	1/1	0.81	0.20	96,96,96,96	0
81	MG	AR	3707	1/1	0.81	0.39	91,91,91,91	0
81	MG	A	2054	1/1	0.81	0.15	116,116,116,116	0
80	OHX	1	3882	7/7	0.81	0.17	183,192,218,268	0
81	MG	AR	4059	1/1	0.81	0.40	75,75,75,75	0
81	MG	A	2078	1/1	0.81	0.41	84,84,84,84	0
81	MG	1	4006	1/1	0.81	0.36	56,56,56,56	0
81	MG	1	3676	1/1	0.81	0.34	79,79,79,79	0
80	OHX	1	3912	7/7	0.81	0.13	195,201,237,279	0
81	MG	1	4043	1/1	0.81	0.22	84,84,84,84	0
81	MG	AR	3769	1/1	0.81	0.22	80,80,80,80	0
81	MG	1	4065	1/1	0.81	0.32	74,74,74,74	0
80	OHX	sR	2176	7/7	0.81	0.11	257,265,281,360	0
81	MG	1	4095	1/1	0.81	0.17	63,63,63,63	0
81	MG	AR	4084	1/1	0.81	0.41	78,78,78,78	0
81	MG	1	3716	1/1	0.81	0.21	71,71,71,71	0
81	MG	A	1958	1/1	0.81	0.24	95,95,95,95	0
81	MG	1	3415	1/1	0.81	0.31	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	AR	3956	7/7	0.81	0.13	179,186,190,274	0
81	MG	sR	2054	1/1	0.81	0.19	101,101,101,101	0
81	MG	x	207	1/1	0.81	0.46	96,96,96,96	0
81	MG	1	3463	1/1	0.81	0.37	81,81,81,81	0
80	OHX	AR	3760	7/7	0.81	0.12	180,200,222,280	0
81	MG	4	212	1/1	0.81	0.24	82,82,82,82	0
81	MG	1	4167	1/1	0.81	0.15	85,85,85,85	0
81	MG	AR	3583	1/1	0.81	0.28	56,56,56,56	0
81	MG	1	3805	1/1	0.82	0.23	84,84,84,84	0
80	OHX	AR	3546	7/7	0.82	0.15	168,175,206,269	0
80	OHX	AR	3604	7/7	0.82	0.12	202,209,233,275	0
80	OHX	sR	1925	7/7	0.82	0.13	201,214,232,308	0
81	MG	AR	3846	1/1	0.82	0.29	93,93,93,93	0
81	MG	s9	201	1/1	0.82	0.37	85,85,85,85	0
81	MG	1	3836	1/1	0.82	0.16	68,68,68,68	0
80	OHX	J	301	7/7	0.82	0.11	227,232,255,310	0
81	MG	sR	2068	1/1	0.82	0.23	92,92,92,92	0
81	MG	AR	3868	1/1	0.82	0.33	61,61,61,61	0
81	MG	1	3853	1/1	0.82	0.35	66,66,66,66	0
80	OHX	AR	3988	7/7	0.82	0.15	215,228,247,291	0
81	MG	AR	3522	1/1	0.82	0.26	50,50,50,50	0
80	OHX	AR	3704	7/7	0.82	0.12	183,203,221,271	0
80	OHX	1	3933	7/7	0.82	0.15	224,234,238,262	0
81	MG	sR	2095	1/1	0.82	0.17	94,94,94,94	0
81	MG	AR	3536	1/1	0.82	0.32	81,81,81,81	0
81	MG	AR	4186	1/1	0.82	0.24	68,68,68,68	0
81	MG	AR	3904	1/1	0.82	0.40	77,77,77,77	0
81	MG	DA	201	1/1	0.82	0.20	75,75,75,75	0
81	MG	A	1940	1/1	0.82	0.21	85,85,85,85	0
81	MG	1	3916	1/1	0.82	0.34	72,72,72,72	0
81	MG	AR	3914	1/1	0.82	0.37	74,74,74,74	0
81	MG	AS	214	1/1	0.82	0.29	84,84,84,84	0
81	MG	1	3926	1/1	0.82	0.14	74,74,74,74	0
81	MG	AR	3918	1/1	0.82	0.20	89,89,89,89	0
81	MG	sR	2140	1/1	0.82	0.23	80,80,80,80	0
81	MG	1	3618	1/1	0.82	0.29	60,60,60,60	0
81	MG	CP	304	1/1	0.82	0.20	66,66,66,66	0
81	MG	AR	3967	1/1	0.82	0.29	84,84,84,84	0
81	MG	AR	3968	1/1	0.82	0.31	100,100,100,100	0
80	OHX	4	202	7/7	0.82	0.13	195,206,247,301	0
81	MG	1	4004	1/1	0.82	0.44	72,72,72,72	0
81	MG	sR	1950	1/1	0.82	0.27	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	AR	3974	1/1	0.82	0.19	67,67,67,67	0
81	MG	1	3651	1/1	0.82	0.16	63,63,63,63	0
81	MG	sR	1964	1/1	0.82	0.19	84,84,84,84	0
81	MG	AR	3563	1/1	0.82	0.21	73,73,73,73	0
81	MG	A	2039	1/1	0.82	0.32	84,84,84,84	0
81	MG	AR	3771	1/1	0.82	0.28	66,66,66,66	0
81	MG	AR	3777	1/1	0.82	0.36	85,85,85,85	0
81	MG	A	1949	1/1	0.82	0.21	69,69,69,69	0
80	OHX	AR	4202	7/7	0.82	0.15	179,181,224,272	0
80	OHX	1	4032	7/7	0.82	0.15	199,216,249,292	0
81	MG	AR	3807	1/1	0.82	0.21	75,75,75,75	0
81	MG	1	3745	1/1	0.82	0.13	69,69,69,69	0
80	OHX	1	4055	7/7	0.82	0.16	149,165,178,258	0
80	OHX	A	2095	7/7	0.82	0.14	224,232,239,300	0
81	MG	AR	3629	1/1	0.82	0.18	67,67,67,67	0
81	MG	AR	3837	1/1	0.82	0.35	58,58,58,58	0
81	MG	1	3768	1/1	0.82	0.41	66,66,66,66	0
81	MG	sR	2030	1/1	0.82	0.26	83,83,83,83	0
81	MG	A	1968	1/1	0.82	0.23	72,72,72,72	0
81	MG	AR	3521	1/1	0.83	0.15	59,59,59,59	0
80	OHX	A	2073	7/7	0.83	0.16	159,176,199,269	0
81	MG	AR	3531	1/1	0.83	0.39	95,95,95,95	0
81	MG	sR	2078	1/1	0.83	0.25	97,97,97,97	0
81	MG	1	3833	1/1	0.83	0.41	74,74,74,74	0
81	MG	1	3834	1/1	0.83	0.21	77,77,77,77	0
81	MG	d2	201	1/1	0.83	0.22	70,70,70,70	0
81	MG	A	2099	1/1	0.83	0.19	82,82,82,82	0
80	OHX	sR	2154	7/7	0.83	0.15	169,180,192,259	0
80	OHX	1	3942	7/7	0.83	0.12	172,181,218,278	0
81	MG	AR	3556	1/1	0.83	0.36	62,62,62,62	0
81	MG	m	301	1/1	0.83	0.25	84,84,84,84	0
81	MG	1	3855	1/1	0.83	0.21	71,71,71,71	0
81	MG	1	3860	1/1	0.83	0.11	90,90,90,90	0
81	MG	AR	3772	1/1	0.83	0.23	63,63,63,63	0
81	MG	AS	222	1/1	0.83	0.27	72,72,72,72	0
81	MG	AR	3559	1/1	0.83	0.15	58,58,58,58	0
81	MG	sR	1907	1/1	0.83	0.43	84,84,84,84	0
81	MG	1	3885	1/1	0.83	0.47	85,85,85,85	0
81	MG	A	2030	1/1	0.83	0.17	85,85,85,85	0
81	MG	AR	3779	1/1	0.83	0.13	78,78,78,78	0
81	MG	AR	3781	1/1	0.83	0.44	72,72,72,72	0
81	MG	1	3560	1/1	0.83	0.20	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	AR	3996	1/1	0.83	0.14	69,69,69,69	0
81	MG	sR	1953	1/1	0.83	0.21	85,85,85,85	0
81	MG	A	2032	1/1	0.83	0.27	72,72,72,72	0
81	MG	AR	4024	1/1	0.83	0.37	87,87,87,87	0
80	OHX	3	220	7/7	0.83	0.13	207,211,226,304	0
80	OHX	AR	3543	7/7	0.83	0.18	139,149,171,247	0
81	MG	AR	3584	1/1	0.83	0.23	75,75,75,75	0
81	MG	1	3950	1/1	0.83	0.34	78,78,78,78	0
80	OHX	AR	3798	7/7	0.83	0.13	178,182,211,279	0
81	MG	A	1929	1/1	0.83	0.32	79,79,79,79	0
81	MG	A	1978	1/1	0.83	0.21	77,77,77,77	0
80	OHX	AR	4142	7/7	0.83	0.22	222,228,247,349	0
81	MG	1	3652	1/1	0.83	0.31	73,73,73,73	0
81	MG	1	3653	1/1	0.83	0.20	95,95,95,95	0
80	OHX	AT	227	7/7	0.83	0.15	169,171,190,250	0
81	MG	AR	3467	1/1	0.83	0.20	58,58,58,58	0
81	MG	1	4014	1/1	0.83	0.19	83,83,83,83	0
81	MG	A	1991	1/1	0.83	0.17	78,78,78,78	0
81	MG	AT	211	1/1	0.83	0.23	75,75,75,75	0
81	MG	A	2002	1/1	0.83	0.15	84,84,84,84	0
81	MG	AR	3491	1/1	0.83	0.14	58,58,58,58	0
81	MG	1	3703	1/1	0.83	0.27	54,54,54,54	0
80	OHX	sR	1955	7/7	0.83	0.16	149,157,166,190	7
81	MG	CE	405	1/1	0.83	0.42	83,83,83,83	0
81	MG	1	3719	1/1	0.83	0.40	86,86,86,86	0
81	MG	sR	2032	1/1	0.83	0.14	84,84,84,84	0
80	OHX	1	3484	7/7	0.83	0.13	145,162,170,200	7
80	OHX	1	3488	7/7	0.83	0.16	139,141,155,224	0
81	MG	AR	3874	1/1	0.83	0.33	70,70,70,70	0
81	MG	1	3418	1/1	0.83	0.21	66,66,66,66	0
81	MG	1	3431	1/1	0.83	0.20	65,65,65,65	0
81	MG	AR	3507	1/1	0.83	0.22	77,77,77,77	0
81	MG	AR	3876	1/1	0.83	0.39	95,95,95,95	0
81	MG	1	3446	1/1	0.83	0.21	75,75,75,75	0
81	MG	AR	3877	1/1	0.83	0.26	71,71,71,71	0
81	MG	1	3809	1/1	0.83	0.34	78,78,78,78	0
81	MG	1	3772	1/1	0.84	0.40	66,66,66,66	0
80	OHX	1	3813	7/7	0.84	0.11	230,237,258,309	0
80	OHX	AR	4204	7/7	0.84	0.14	163,167,190,240	0
81	MG	AR	3691	1/1	0.84	0.44	84,84,84,84	0
80	OHX	d4	201	7/7	0.84	0.12	213,222,228,282	0
81	MG	1	3464	1/1	0.84	0.26	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	4	216	1/1	0.84	0.32	73,73,73,73	0
81	MG	1	3826	1/1	0.84	0.36	51,51,51,51	0
81	MG	AR	4184	1/1	0.84	0.23	76,76,76,76	0
81	MG	1	3830	1/1	0.84	0.21	83,83,83,83	0
80	OHX	AT	208	7/7	0.84	0.13	169,188,210,283	0
81	MG	1	3494	1/1	0.84	0.28	56,56,56,56	0
80	OHX	1	3881	7/7	0.84	0.11	201,206,231,275	0
81	MG	AR	4210	1/1	0.84	0.36	77,77,77,77	0
81	MG	AR	4211	1/1	0.84	0.38	63,63,63,63	0
80	OHX	sR	1970	7/7	0.84	0.12	201,211,225,274	0
81	MG	AR	3739	1/1	0.84	0.21	59,59,59,59	0
81	MG	AR	3941	1/1	0.84	0.20	51,51,51,51	0
81	MG	sR	2104	1/1	0.84	0.21	93,93,93,93	0
81	MG	AR	3744	1/1	0.84	0.14	70,70,70,70	0
81	MG	1	3857	1/1	0.84	0.28	65,65,65,65	0
81	MG	1	3524	1/1	0.84	0.16	77,77,77,77	0
81	MG	AR	3748	1/1	0.84	0.12	69,69,69,69	0
81	MG	4	223	1/1	0.84	0.21	81,81,81,81	0
80	OHX	A	1986	7/7	0.84	0.14	107,135,150,218	0
80	OHX	1	3452	7/7	0.84	0.12	131,140,161,233	0
80	OHX	4	204	7/7	0.84	0.17	193,207,215,289	0
81	MG	1	3888	1/1	0.84	0.43	67,67,67,67	0
81	MG	sR	1929	1/1	0.84	0.50	65,65,65,65	0
81	MG	sR	1932	1/1	0.84	0.28	75,75,75,75	0
81	MG	1	3561	1/1	0.84	0.26	71,71,71,71	0
81	MG	s8	301	1/1	0.84	0.34	93,93,93,93	0
81	MG	A	2080	1/1	0.84	0.18	91,91,91,91	0
81	MG	1	3599	1/1	0.84	0.26	71,71,71,71	0
81	MG	sR	2151	1/1	0.84	0.10	93,93,93,93	0
80	OHX	AR	3987	7/7	0.84	0.14	186,199,227,276	0
80	OHX	A	2150	7/7	0.84	0.13	180,190,203,226	7
80	OHX	x	208	7/7	0.84	0.10	182,201,222,292	0
81	MG	sR	2161	1/1	0.84	0.35	67,67,67,67	0
81	MG	AR	3582	1/1	0.84	0.36	66,66,66,66	0
81	MG	AR	3426	1/1	0.84	0.12	65,65,65,65	0
81	MG	1	3958	1/1	0.84	0.13	104,104,104,104	0
81	MG	1	3644	1/1	0.84	0.28	59,59,59,59	0
81	MG	AR	4034	1/1	0.84	0.11	113,113,113,113	0
81	MG	1	3648	1/1	0.84	0.39	54,54,54,54	0
80	OHX	AR	4080	7/7	0.84	0.14	192,196,222,273	0
81	MG	sR	2194	1/1	0.84	0.19	83,83,83,83	0
80	OHX	1	3550	7/7	0.84	0.14	179,208,240,281	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	3654	1/1	0.84	0.30	77,77,77,77	0
80	OHX	1	4115	7/7	0.84	0.24	152,154,179,203	7
80	OHX	AR	3892	7/7	0.84	0.18	93,110,149,204	0
80	OHX	1	4145	7/7	0.84	0.11	205,215,222,287	0
81	MG	1	4042	1/1	0.84	0.26	95,95,95,95	0
81	MG	1	3677	1/1	0.84	0.26	72,72,72,72	0
81	MG	A	2107	1/1	0.84	0.16	111,111,111,111	0
81	MG	1	4048	1/1	0.84	0.25	57,57,57,57	0
80	OHX	A	2087	7/7	0.84	0.12	198,209,235,266	0
81	MG	sR	2006	1/1	0.84	0.37	73,73,73,73	0
81	MG	1	4074	1/1	0.84	0.26	74,74,74,74	0
81	MG	1	4077	1/1	0.84	0.20	73,73,73,73	0
81	MG	1	4080	1/1	0.84	0.41	73,73,73,73	0
81	MG	AT	221	1/1	0.84	0.39	81,81,81,81	0
81	MG	6	201	1/1	0.84	0.33	65,65,65,65	0
80	OHX	1	3612	7/7	0.84	0.10	186,196,209,291	0
81	MG	CE	404	1/1	0.84	0.37	59,59,59,59	0
81	MG	1	3733	1/1	0.84	0.23	59,59,59,59	0
81	MG	3	208	1/1	0.84	0.18	71,71,71,71	0
81	MG	1	4131	1/1	0.84	0.13	54,54,54,54	0
81	MG	1	3744	1/1	0.84	0.14	69,69,69,69	0
81	MG	A	1901	1/1	0.84	0.26	108,108,108,108	0
81	MG	AR	3476	1/1	0.84	0.19	64,64,64,64	0
80	OHX	1	3672	7/7	0.84	0.12	191,214,232,274	0
81	MG	AR	4131	1/1	0.84	0.31	60,60,60,60	0
81	MG	1	4162	1/1	0.84	0.21	70,70,70,70	0
80	OHX	AR	3610	7/7	0.84	0.14	159,169,180,243	0
82	ZN	c	101	1/1	0.84	0.13	244,244,244,244	0
80	OHX	1	3792	7/7	0.84	0.14	173,178,201,251	0
85	SPD	AR	3890	10/10	0.84	0.25	61,72,87,96	0
81	MG	AR	4208	1/1	0.85	0.23	84,84,84,84	0
80	OHX	sR	2017	7/7	0.85	0.12	169,178,200,263	0
81	MG	AR	3747	1/1	0.85	0.22	79,79,79,79	0
81	MG	3	218	1/1	0.85	0.21	89,89,89,89	0
81	MG	AR	3945	1/1	0.85	0.31	60,60,60,60	0
81	MG	A	1992	1/1	0.85	0.14	80,80,80,80	0
80	OHX	O	201	7/7	0.85	0.11	213,228,247,281	0
81	MG	A	2118	1/1	0.85	0.28	64,64,64,64	0
80	OHX	sR	2065	7/7	0.85	0.12	175,178,202,252	0
81	MG	AR	3590	1/1	0.85	0.22	82,82,82,82	0
81	MG	1	3562	1/1	0.85	0.35	84,84,84,84	0
81	MG	AR	3976	1/1	0.85	0.26	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	AR	3591	1/1	0.85	0.32	62,62,62,62	0
81	MG	1	3586	1/1	0.85	0.17	73,73,73,73	0
81	MG	1	3587	1/1	0.85	0.31	50,50,50,50	0
81	MG	sR	1920	1/1	0.85	0.16	84,84,84,84	0
81	MG	A	1910	1/1	0.85	0.12	77,77,77,77	0
81	MG	sR	1930	1/1	0.85	0.29	90,90,90,90	0
81	MG	AR	3788	1/1	0.85	0.25	75,75,75,75	0
81	MG	AR	4011	1/1	0.85	0.22	99,99,99,99	0
81	MG	AR	3800	1/1	0.85	0.28	60,60,60,60	0
80	OHX	AR	3425	7/7	0.85	0.12	171,186,220,270	0
81	MG	1	3918	1/1	0.85	0.28	66,66,66,66	0
81	MG	sR	1951	1/1	0.85	0.33	66,66,66,66	0
81	MG	sR	2193	1/1	0.85	0.16	82,82,82,82	0
80	OHX	AR	4073	7/7	0.85	0.13	163,169,201,268	0
81	MG	AR	3616	1/1	0.85	0.37	50,50,50,50	0
80	OHX	1	3490	7/7	0.85	0.15	172,190,206,246	0
81	MG	1	3954	1/1	0.85	0.17	82,82,82,82	0
81	MG	AR	3623	1/1	0.85	0.22	62,62,62,62	0
81	MG	AR	3813	1/1	0.85	0.18	70,70,70,70	0
80	OHX	AR	3454	7/7	0.85	0.15	181,184,209,223	0
81	MG	1	3960	1/1	0.85	0.11	91,91,91,91	0
80	OHX	AR	3573	7/7	0.85	0.13	190,203,218,286	0
81	MG	1	3980	1/1	0.85	0.26	73,73,73,73	0
81	MG	AT	215	1/1	0.85	0.23	76,76,76,76	0
80	OHX	c3	201	7/7	0.85	0.12	203,229,241,268	0
80	OHX	A	2036	7/7	0.85	0.14	216,231,246,295	0
80	OHX	AR	3954	7/7	0.85	0.16	135,153,172,233	0
80	OHX	AG	201	7/7	0.85	0.14	138,158,173,242	0
80	OHX	1	4085	7/7	0.85	0.13	149,156,168,251	0
80	OHX	AR	3640	7/7	0.85	0.12	174,177,203,255	0
81	MG	1	4018	1/1	0.85	0.25	71,71,71,71	0
81	MG	AR	3864	1/1	0.85	0.15	82,82,82,82	0
80	OHX	1	4118	7/7	0.85	0.14	143,162,188,246	0
81	MG	AR	4114	1/1	0.85	0.23	68,68,68,68	0
81	MG	sR	2018	1/1	0.85	0.22	65,65,65,65	0
81	MG	AR	4115	1/1	0.85	0.40	77,77,77,77	0
81	MG	AR	4124	1/1	0.85	0.23	69,69,69,69	0
81	MG	A	2064	1/1	0.85	0.09	89,89,89,89	0
80	OHX	sR	2181	7/7	0.85	0.15	193,205,243,305	0
80	OHX	1	3693	7/7	0.85	0.15	169,178,185,253	0
81	MG	1	3447	1/1	0.85	0.40	70,70,70,70	0
81	MG	1	4094	1/1	0.85	0.41	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
80	OHX	sR	2191	7/7	0.85	0.12	229,234,260,325	0
81	MG	1	4097	1/1	0.85	0.15	54,54,54,54	0
81	MG	1	3766	1/1	0.85	0.31	77,77,77,77	0
81	MG	AR	4146	1/1	0.85	0.33	56,56,56,56	0
80	OHX	1	3723	7/7	0.85	0.10	174,177,201,271	0
80	OHX	AS	231	7/7	0.85	0.11	182,211,228,262	0
81	MG	AR	4156	1/1	0.85	0.27	58,58,58,58	0
81	MG	1	3797	1/1	0.85	0.17	51,51,51,51	0
81	MG	1	3477	1/1	0.85	0.34	72,72,72,72	0
80	OHX	AR	3862	7/7	0.85	0.13	167,182,202,255	0
81	MG	AR	4160	1/1	0.85	0.17	85,85,85,85	0
81	MG	AR	3896	1/1	0.85	0.34	65,65,65,65	0
81	MG	AR	4182	1/1	0.85	0.38	82,82,82,82	0
81	MG	AR	3719	1/1	0.85	0.16	66,66,66,66	0
81	MG	1	4166	1/1	0.85	0.31	81,81,81,81	0
81	MG	1	3504	1/1	0.85	0.20	67,67,67,67	0
81	MG	1	4168	1/1	0.85	0.34	51,51,51,51	0
81	MG	AR	3720	1/1	0.85	0.26	59,59,59,59	0
80	OHX	sR	2004	7/7	0.85	0.12	178,191,214,280	0
80	OHX	1	3849	7/7	0.85	0.14	174,179,202,249	0
80	OHX	sR	2088	7/7	0.86	0.13	176,184,195,263	0
80	OHX	AR	3729	7/7	0.86	0.14	138,142,174,227	0
81	MG	CK	202	1/1	0.86	0.40	85,85,85,85	0
80	OHX	1	3910	7/7	0.86	0.12	157,174,186,248	0
81	MG	A	1979	1/1	0.86	0.20	70,70,70,70	0
80	OHX	AR	3423	7/7	0.86	0.12	177,192,201,274	0
81	MG	AR	3595	1/1	0.86	0.14	76,76,76,76	0
81	MG	A	1988	1/1	0.86	0.29	72,72,72,72	0
80	OHX	1	3510	7/7	0.86	0.13	154,162,199,234	0
80	OHX	A	2017	7/7	0.86	0.10	215,223,240,266	0
80	OHX	A	2046	7/7	0.86	0.15	185,196,209,252	0
81	MG	A	2000	1/1	0.86	0.19	88,88,88,88	0
81	MG	AT	220	1/1	0.86	0.36	79,79,79,79	0
81	MG	AR	3625	1/1	0.86	0.21	81,81,81,81	0
81	MG	x	201	1/1	0.86	0.26	58,58,58,58	0
81	MG	1	3800	1/1	0.86	0.41	76,76,76,76	0
80	OHX	sR	2125	7/7	0.86	0.13	150,154,192,259	0
81	MG	1	3806	1/1	0.86	0.21	76,76,76,76	0
81	MG	x	206	1/1	0.86	0.50	60,60,60,60	0
81	MG	AR	3910	1/1	0.86	0.12	61,61,61,61	0
81	MG	s2	301	1/1	0.86	0.37	69,69,69,69	0
80	OHX	1	4030	7/7	0.86	0.15	131,140,186,229	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	3406	1/1	0.86	0.24	76,76,76,76	0
81	MG	AR	3654	1/1	0.86	0.18	74,74,74,74	0
80	OHX	A	1957	7/7	0.86	0.15	179,186,188,239	0
80	OHX	1	3551	7/7	0.86	0.13	166,179,213,259	0
81	MG	AR	3947	1/1	0.86	0.12	82,82,82,82	0
81	MG	o	302	1/1	0.86	0.25	71,71,71,71	0
81	MG	1	3433	1/1	0.86	0.22	48,48,48,48	0
81	MG	A	2018	1/1	0.86	0.37	74,74,74,74	0
80	OHX	AR	3792	7/7	0.86	0.19	164,170,187,215	7
81	MG	CS	201	1/1	0.86	0.28	94,94,94,94	0
81	MG	A	2022	1/1	0.86	0.21	70,70,70,70	0
80	OHX	1	3581	7/7	0.86	0.13	184,188,206,246	0
81	MG	AR	3693	1/1	0.86	0.33	71,71,71,71	0
81	MG	1	3858	1/1	0.86	0.18	71,71,71,71	0
81	MG	c6	202	1/1	0.86	0.15	97,97,97,97	0
81	MG	1	3862	1/1	0.86	0.24	63,63,63,63	0
81	MG	1	3471	1/1	0.86	0.17	75,75,75,75	0
80	OHX	AR	4109	7/7	0.86	0.11	178,203,217,245	0
81	MG	1	3475	1/1	0.86	0.36	115,115,115,115	0
81	MG	AR	3999	1/1	0.86	0.28	72,72,72,72	0
81	MG	sR	1994	1/1	0.86	0.23	97,97,97,97	0
81	MG	sR	1995	1/1	0.86	0.12	67,67,67,67	0
81	MG	AR	4009	1/1	0.86	0.21	79,79,79,79	0
81	MG	1	3897	1/1	0.86	0.19	79,79,79,79	0
80	OHX	AR	3797	7/7	0.86	0.11	160,178,200,242	0
80	OHX	1	4120	7/7	0.86	0.15	191,197,213,283	0
80	OHX	1	3633	6/7	0.86	0.17	141,162,179,219	0
80	OHX	1	3665	7/7	0.86	0.15	173,175,196,260	0
80	OHX	AR	4166	7/7	0.86	0.13	171,181,206,264	0
80	OHX	AR	3924	7/7	0.86	0.11	208,220,237,300	0
81	MG	1	3917	1/1	0.86	0.23	66,66,66,66	0
81	MG	AR	3469	1/1	0.86	0.20	68,68,68,68	0
81	MG	1	3920	1/1	0.86	0.10	68,68,68,68	0
81	MG	AR	3746	1/1	0.86	0.23	70,70,70,70	0
81	MG	A	2068	1/1	0.86	0.25	87,87,87,87	0
81	MG	1	3529	1/1	0.86	0.18	77,77,77,77	0
81	MG	3	207	1/1	0.86	0.18	76,76,76,76	0
81	MG	1	3929	1/1	0.86	0.40	65,65,65,65	0
81	MG	sR	2043	1/1	0.86	0.20	81,81,81,81	0
81	MG	1	3951	1/1	0.86	0.17	66,66,66,66	0
81	MG	sR	2044	1/1	0.86	0.21	97,97,97,97	0
81	MG	AR	3750	1/1	0.86	0.10	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	3535	1/1	0.86	0.22	85,85,85,85	0
81	MG	AR	3752	1/1	0.86	0.23	74,74,74,74	0
80	OHX	1	3695	7/7	0.86	0.15	139,142,145,180	7
81	MG	1	3557	1/1	0.86	0.33	50,50,50,50	0
81	MG	A	1918	1/1	0.86	0.14	76,76,76,76	0
81	MG	sR	2067	1/1	0.86	0.21	66,66,66,66	0
80	OHX	AR	3925	7/7	0.86	0.11	185,192,232,284	0
81	MG	AR	4091	1/1	0.86	0.12	75,75,75,75	0
81	MG	AR	3776	1/1	0.86	0.43	81,81,81,81	0
81	MG	AR	4100	1/1	0.86	0.30	71,71,71,71	0
81	MG	A	1922	1/1	0.86	0.17	85,85,85,85	0
81	MG	1	3593	1/1	0.86	0.12	74,74,74,74	0
81	MG	AR	3498	1/1	0.86	0.15	77,77,77,77	0
80	OHX	AR	3697	7/7	0.86	0.10	213,216,235,298	0
81	MG	A	2090	1/1	0.86	0.37	67,67,67,67	0
80	OHX	1	3725	7/7	0.86	0.13	135,138,164,231	0
80	OHX	1	3755	7/7	0.86	0.19	140,143,159,186	7
81	MG	1	4047	1/1	0.86	0.41	89,89,89,89	0
81	MG	1	3624	1/1	0.86	0.31	83,83,83,83	0
80	OHX	1	3758	7/7	0.86	0.15	143,152,164,218	0
81	MG	1	4067	1/1	0.86	0.29	60,60,60,60	0
80	OHX	A	2063	7/7	0.86	0.12	190,197,220,285	0
81	MG	sR	2114	1/1	0.86	0.25	76,76,76,76	0
81	MG	1	3643	1/1	0.86	0.31	52,52,52,52	0
81	MG	CJ	301	1/1	0.86	0.22	81,81,81,81	0
81	MG	sR	2126	1/1	0.86	0.22	78,78,78,78	0
80	OHX	sR	2064	7/7	0.86	0.12	190,210,221,265	0
81	MG	1	3649	1/1	0.86	0.34	69,69,69,69	0
81	MG	A	2115	1/1	0.86	0.23	75,75,75,75	0
80	OHX	1	3821	7/7	0.86	0.11	174,182,217,274	0
81	MG	AR	3814	1/1	0.86	0.16	66,66,66,66	0
81	MG	AR	3816	1/1	0.86	0.80	68,68,68,68	0
81	MG	1	4127	1/1	0.86	0.22	73,73,73,73	0
80	OHX	3	222	7/7	0.86	0.15	159,162,178,196	7
81	MG	1	3658	1/1	0.86	0.11	80,80,80,80	0
80	OHX	1	3422	7/7	0.86	0.18	155,161,180,251	0
81	MG	AR	4179	1/1	0.86	0.36	58,58,58,58	0
80	OHX	AR	3957	7/7	0.86	0.11	183,195,228,289	0
80	OHX	1	3454	7/7	0.86	0.16	129,135,148,177	7
81	MG	1	3683	1/1	0.86	0.19	64,64,64,64	0
81	MG	AR	3564	1/1	0.86	0.37	86,86,86,86	0
81	MG	A	2134	1/1	0.86	0.26	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	AR	4188	1/1	0.86	0.25	66,66,66,66	0
81	MG	1	3710	1/1	0.86	0.13	74,74,74,74	0
81	MG	AR	4206	1/1	0.86	0.11	112,112,112,112	0
81	MG	sR	2182	1/1	0.86	0.18	72,72,72,72	0
81	MG	1	3717	1/1	0.86	0.12	72,72,72,72	0
85	SPD	AR	4164	10/10	0.86	0.18	49,58,67,75	0
81	MG	1	3567	1/1	0.87	0.12	87,87,87,87	0
81	MG	AR	3773	1/1	0.87	0.29	46,46,46,46	0
81	MG	CM	201	1/1	0.87	0.18	84,84,84,84	0
80	OHX	A	1976	7/7	0.87	0.15	145,170,176,208	0
81	MG	1	3863	1/1	0.87	0.34	84,84,84,84	0
81	MG	l	403	1/1	0.87	0.13	73,73,73,73	0
81	MG	AF	202	1/1	0.87	0.27	62,62,62,62	0
81	MG	1	3594	1/1	0.87	0.25	69,69,69,69	0
81	MG	AR	4003	1/1	0.87	0.23	72,72,72,72	0
81	MG	1	3883	1/1	0.87	0.26	68,68,68,68	0
81	MG	1	3613	1/1	0.87	0.42	75,75,75,75	0
81	MG	1	3614	1/1	0.87	0.25	74,74,74,74	0
81	MG	1	3890	1/1	0.87	0.22	63,63,63,63	0
81	MG	A	2069	1/1	0.87	0.17	80,80,80,80	0
81	MG	AR	3784	1/1	0.87	0.23	81,81,81,81	0
81	MG	AR	4020	1/1	0.87	0.26	60,60,60,60	0
80	OHX	AR	4050	7/7	0.87	0.10	189,201,214,253	0
80	OHX	4	209	7/7	0.87	0.14	175,184,210,270	0
81	MG	AR	3407	1/1	0.87	0.42	85,85,85,85	0
80	OHX	A	2077	7/7	0.87	0.10	248,253,272,312	0
80	OHX	sR	2148	7/7	0.87	0.10	198,217,226,295	0
80	OHX	A	1987	7/7	0.87	0.13	190,193,214,258	0
81	MG	A	1961	1/1	0.87	0.45	91,91,91,91	0
81	MG	sR	1971	1/1	0.87	0.24	67,67,67,67	0
80	OHX	AR	3703	7/7	0.87	0.14	180,186,219,267	0
81	MG	AR	4056	1/1	0.87	0.53	65,65,65,65	0
81	MG	3	209	1/1	0.87	0.32	64,64,64,64	0
81	MG	DQ	503	1/1	0.87	0.34	64,64,64,64	0
81	MG	AR	3627	1/1	0.87	0.13	88,88,88,88	0
81	MG	CR	202	1/1	0.87	0.30	66,66,66,66	0
80	OHX	AR	4110	7/7	0.87	0.10	174,201,216,255	0
81	MG	Y	201	1/1	0.87	0.25	69,69,69,69	0
81	MG	AR	4085	1/1	0.87	0.42	50,50,50,50	0
81	MG	AK	105	1/1	0.87	0.29	49,49,49,49	0
81	MG	sR	1999	1/1	0.87	0.34	59,59,59,59	0
81	MG	AR	3842	1/1	0.87	0.35	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	3973	1/1	0.87	0.14	59,59,59,59	0
81	MG	1	3680	1/1	0.87	0.18	61,61,61,61	0
81	MG	A	2109	1/1	0.87	0.27	50,50,50,50	0
80	OHX	AR	4112	7/7	0.87	0.14	163,170,210,239	0
81	MG	A	2116	1/1	0.87	0.17	68,68,68,68	0
80	OHX	CK	201	7/7	0.87	0.10	195,207,220,285	0
80	OHX	AR	4165	7/7	0.87	0.13	133,141,166,216	0
81	MG	sM	301	1/1	0.87	0.12	61,61,61,61	0
81	MG	AR	4127	1/1	0.87	0.16	71,71,71,71	0
81	MG	AR	3871	1/1	0.87	0.15	73,73,73,73	0
81	MG	AR	3492	1/1	0.87	0.42	59,59,59,59	0
81	MG	1	4033	1/1	0.87	0.19	57,57,57,57	0
81	MG	1	4038	1/1	0.87	0.11	41,41,41,41	0
81	MG	A	2126	1/1	0.87	0.28	74,74,74,74	0
80	OHX	AR	3485	7/7	0.87	0.14	136,153,182,234	0
81	MG	1	3466	1/1	0.87	0.23	55,55,55,55	0
81	MG	sR	2045	1/1	0.87	0.14	65,65,65,65	0
81	MG	AR	3496	1/1	0.87	0.21	70,70,70,70	0
80	OHX	A	1934	7/7	0.87	0.10	211,226,241,304	0
81	MG	1	4063	1/1	0.87	0.18	87,87,87,87	0
80	OHX	AR	3828	7/7	0.87	0.15	150,161,166,246	0
80	OHX	1	3663	7/7	0.87	0.16	117,135,166,229	0
81	MG	AR	3509	1/1	0.87	0.15	62,62,62,62	0
80	OHX	AR	3514	7/7	0.87	0.11	141,144,167,259	0
80	OHX	1	3972	7/7	0.87	0.12	183,191,206,271	0
81	MG	AR	3526	1/1	0.87	0.20	62,62,62,62	0
81	MG	AR	4181	1/1	0.87	0.40	73,73,73,73	0
81	MG	1	3796	1/1	0.87	0.24	79,79,79,79	0
80	OHX	1	3671	7/7	0.87	0.11	179,185,208,263	0
81	MG	1	3799	1/1	0.87	0.35	73,73,73,73	0
80	OHX	AR	3860	7/7	0.87	0.15	170,173,186,280	0
80	OHX	s4	302	7/7	0.87	0.12	180,191,211,261	0
81	MG	1	3506	1/1	0.87	0.11	61,61,61,61	0
81	MG	AR	3927	1/1	0.87	0.12	63,63,63,63	0
81	MG	AR	3929	1/1	0.87	0.18	63,63,63,63	0
80	OHX	AR	3516	7/7	0.87	0.11	175,194,219,246	0
80	OHX	1	3430	7/7	0.87	0.14	173,179,195,254	0
80	OHX	sR	1904	7/7	0.87	0.11	161,172,210,257	0
80	OHX	AR	4016	7/7	0.87	0.15	138,153,172,208	0
81	MG	AR	3964	1/1	0.87	0.24	62,62,62,62	0
81	MG	1	4139	1/1	0.87	0.35	61,61,61,61	0
81	MG	AR	3756	1/1	0.87	0.16	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	AS	207	1/1	0.87	0.17	81,81,81,81	0
81	MG	DL	104	1/1	0.87	0.31	59,59,59,59	0
81	MG	e	102	1/1	0.87	0.14	92,92,92,92	0
81	MG	AS	212	1/1	0.87	0.28	85,85,85,85	0
81	MG	AR	3972	1/1	0.87	0.19	64,64,64,64	0
80	OHX	1	3731	7/7	0.87	0.13	154,156,198,247	0
81	MG	AS	216	1/1	0.87	0.17	77,77,77,77	0
81	MG	AS	220	1/1	0.87	0.24	71,71,71,71	0
81	MG	1	3763	1/1	0.88	0.26	65,65,65,65	0
81	MG	DG	201	1/1	0.88	0.22	60,60,60,60	0
81	MG	DH	201	1/1	0.88	0.13	69,69,69,69	0
81	MG	v	304	1/1	0.88	0.27	66,66,66,66	0
81	MG	1	3774	1/1	0.88	0.11	93,93,93,93	0
81	MG	1	3402	1/1	0.88	0.28	70,70,70,70	0
81	MG	1	3404	1/1	0.88	0.45	68,68,68,68	0
81	MG	1	3779	1/1	0.88	0.32	67,67,67,67	0
81	MG	1	3795	1/1	0.88	0.21	84,84,84,84	0
81	MG	1	3405	1/1	0.88	0.30	48,48,48,48	0
80	OHX	A	1993	7/7	0.88	0.14	153,175,184,239	0
81	MG	1	3798	1/1	0.88	0.33	48,48,48,48	0
81	MG	sR	1952	1/1	0.88	0.09	83,83,83,83	0
80	OHX	1	3935	7/7	0.88	0.14	160,162,191,277	0
81	MG	1	3802	1/1	0.88	0.21	73,73,73,73	0
80	OHX	A	2111	7/7	0.88	0.10	209,217,223,286	0
81	MG	AR	4000	1/1	0.88	0.20	90,90,90,90	0
81	MG	A	2117	1/1	0.88	0.14	78,78,78,78	0
80	OHX	A	2113	7/7	0.88	0.13	180,185,203,250	0
81	MG	1	3436	1/1	0.88	0.29	67,67,67,67	0
81	MG	AR	3505	1/1	0.88	0.14	60,60,60,60	0
81	MG	AR	3754	1/1	0.88	0.10	76,76,76,76	0
81	MG	l	404	1/1	0.88	0.42	57,57,57,57	0
80	OHX	1	3543	7/7	0.88	0.17	146,148,153,194	7
80	OHX	1	3995	7/7	0.88	0.10	169,174,186,272	0
80	OHX	A	1996	7/7	0.88	0.13	165,177,183,240	0
81	MG	AR	3523	1/1	0.88	0.37	53,53,53,53	0
81	MG	AR	3525	1/1	0.88	0.42	54,54,54,54	0
81	MG	A	1980	1/1	0.88	0.23	90,90,90,90	0
81	MG	sR	1997	1/1	0.88	0.24	91,91,91,91	0
80	OHX	1	4029	7/7	0.88	0.12	140,144,175,222	0
81	MG	A	2135	1/1	0.88	0.38	101,101,101,101	0
80	OHX	sR	2113	7/7	0.88	0.10	207,224,232,283	0
81	MG	A	1989	1/1	0.88	0.15	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	AR	3786	1/1	0.88	0.35	73,73,73,73	0
81	MG	AR	4063	1/1	0.88	0.18	85,85,85,85	0
80	OHX	A	2053	7/7	0.88	0.12	193,197,222,254	0
81	MG	1	3502	1/1	0.88	0.29	68,68,68,68	0
81	MG	AR	4069	1/1	0.88	0.24	47,47,47,47	0
80	OHX	AR	4045	7/7	0.88	0.12	132,142,170,237	0
81	MG	AR	4075	1/1	0.88	0.08	95,95,95,95	0
81	MG	CP	305	1/1	0.88	0.20	80,80,80,80	0
80	OHX	sR	2147	7/7	0.88	0.11	134,151,167,228	0
81	MG	A	2155	1/1	0.88	0.26	74,74,74,74	0
81	MG	1	3887	1/1	0.88	0.32	68,68,68,68	0
80	OHX	c8	201	7/7	0.88	0.10	173,180,201,233	0
80	OHX	4	208	7/7	0.88	0.13	162,166,189,252	0
80	OHX	AR	4079	7/7	0.88	0.12	143,163,186,235	0
81	MG	AR	3581	1/1	0.88	0.22	58,58,58,58	0
81	MG	c9	201	1/1	0.88	0.12	88,88,88,88	0
81	MG	AR	3820	1/1	0.88	0.18	57,57,57,57	0
80	OHX	AR	3733	7/7	0.88	0.14	139,152,166,249	0
81	MG	AK	101	1/1	0.88	0.38	65,65,65,65	0
81	MG	D	301	1/1	0.88	0.28	78,78,78,78	0
80	OHX	AR	3422	7/7	0.88	0.14	155,163,170,249	0
80	OHX	A	2006	7/7	0.88	0.13	176,192,209,255	0
81	MG	1	3559	1/1	0.88	0.12	61,61,61,61	0
80	OHX	AR	3607	7/7	0.88	0.14	130,135,164,229	0
81	MG	AR	3596	1/1	0.88	0.16	76,76,76,76	0
81	MG	sR	2091	1/1	0.88	0.28	58,58,58,58	0
80	OHX	1	4175	7/7	0.88	0.11	192,200,214,286	0
81	MG	1	3583	1/1	0.88	0.35	64,64,64,64	0
81	MG	1	3928	1/1	0.88	0.23	62,62,62,62	0
81	MG	AR	4151	1/1	0.88	0.23	83,83,83,83	0
81	MG	1	3945	1/1	0.88	0.17	83,83,83,83	0
81	MG	AR	3602	1/1	0.88	0.18	86,86,86,86	0
80	OHX	AR	3424	7/7	0.88	0.12	136,154,167,225	0
80	OHX	sR	2198	7/7	0.88	0.16	139,151,160,170	7
81	MG	1	3592	1/1	0.88	0.13	90,90,90,90	0
80	OHX	sR	1959	7/7	0.88	0.13	171,175,197,249	0
80	OHX	AT	222	7/7	0.88	0.14	166,172,187,260	0
81	MG	AR	4174	1/1	0.88	0.27	67,67,67,67	0
81	MG	AR	3872	1/1	0.88	0.28	57,57,57,57	0
80	OHX	AR	4134	7/7	0.88	0.14	132,136,153,222	0
80	OHX	1	3753	7/7	0.88	0.15	137,142,170,240	0
81	MG	3	214	1/1	0.88	0.19	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	sR	2138	1/1	0.88	0.20	71,71,71,71	0
81	MG	1	3986	1/1	0.88	0.25	78,78,78,78	0
81	MG	AR	3631	1/1	0.88	0.19	66,66,66,66	0
80	OHX	sR	1968	7/7	0.88	0.14	160,169,183,218	0
80	OHX	CG	303	7/7	0.88	0.11	208,218,242,283	0
81	MG	AR	4191	1/1	0.88	0.19	80,80,80,80	0
81	MG	AR	3428	1/1	0.88	0.27	76,76,76,76	0
81	MG	AR	3652	1/1	0.88	0.30	72,72,72,72	0
81	MG	AR	3430	1/1	0.88	0.21	44,44,44,44	0
80	OHX	1	3762	7/7	0.88	0.11	168,177,198,260	0
81	MG	AR	3657	1/1	0.88	0.21	56,56,56,56	0
80	OHX	AR	4140	7/7	0.88	0.11	170,173,179,252	0
81	MG	sR	2165	1/1	0.88	0.28	91,91,91,91	0
81	MG	sR	2174	1/1	0.88	0.28	72,72,72,72	0
81	MG	AS	206	1/1	0.88	0.19	73,73,73,73	0
81	MG	AR	3438	1/1	0.88	0.28	76,76,76,76	0
80	OHX	A	1937	7/7	0.88	0.11	225,231,251,288	0
81	MG	1	4064	1/1	0.88	0.26	67,67,67,67	0
81	MG	sR	2186	1/1	0.88	0.39	64,64,64,64	0
80	OHX	AR	3796	7/7	0.88	0.12	142,146,160,212	0
81	MG	1	4070	1/1	0.88	0.30	68,68,68,68	0
81	MG	1	4071	1/1	0.88	0.36	58,58,58,58	0
80	OHX	CL	302	7/7	0.88	0.13	136,146,177,221	0
80	OHX	sR	2029	7/7	0.88	0.11	188,208,239,282	0
81	MG	1	4075	1/1	0.88	0.47	79,79,79,79	0
80	OHX	sR	2041	7/7	0.88	0.12	157,178,205,250	0
81	MG	AR	3460	1/1	0.88	0.21	63,63,63,63	0
81	MG	1	4092	1/1	0.88	0.25	64,64,64,64	0
81	MG	1	3681	1/1	0.88	0.34	82,82,82,82	0
81	MG	AR	3949	1/1	0.88	0.16	74,74,74,74	0
81	MG	AR	3695	1/1	0.88	0.14	68,68,68,68	0
81	MG	AR	3961	1/1	0.88	0.30	46,46,46,46	0
81	MG	1	3686	1/1	0.88	0.14	78,78,78,78	0
81	MG	1	3687	1/1	0.88	0.27	88,88,88,88	0
81	MG	1	4107	1/1	0.88	0.25	74,74,74,74	0
81	MG	AS	226	1/1	0.88	0.31	77,77,77,77	0
81	MG	1	4122	1/1	0.88	0.34	55,55,55,55	0
80	OHX	1	3852	7/7	0.88	0.12	162,170,188,224	0
81	MG	1	3713	1/1	0.88	0.15	100,100,100,100	0
81	MG	1	3714	1/1	0.88	0.18	83,83,83,83	0
81	MG	1	4132	1/1	0.88	0.45	82,82,82,82	0
81	MG	AR	3966	1/1	0.88	0.26	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	A	1938	1/1	0.88	0.26	67,67,67,67	0
80	OHX	AR	4169	7/7	0.88	0.14	123,135,144,225	0
81	MG	DC	202	1/1	0.88	0.12	65,65,65,65	0
81	MG	DD	101	1/1	0.88	0.23	58,58,58,58	0
81	MG	1	4152	1/1	0.88	0.21	79,79,79,79	0
80	OHX	AR	4173	7/7	0.88	0.18	155,167,182,240	0
81	MG	1	4159	1/1	0.88	0.14	65,65,65,65	0
81	MG	1	3737	1/1	0.88	0.27	46,46,46,46	0
81	MG	1	3740	1/1	0.88	0.11	83,83,83,83	0
80	OHX	1	3489	7/7	0.88	0.15	141,152,186,212	0
81	MG	6	203	1/1	0.88	0.35	85,85,85,85	0
81	MG	1	4169	1/1	0.88	0.39	71,71,71,71	0
80	OHX	1	3903	7/7	0.88	0.09	210,220,238,288	0
81	MG	sR	1941	1/1	0.88	0.12	66,66,66,66	0
80	OHX	sR	2076	7/7	0.88	0.13	161,166,198,249	0
80	OHX	A	1927	7/7	0.88	0.10	168,191,201,252	0
81	MG	1	3461	1/1	0.89	0.17	56,56,56,56	0
81	MG	d3	201	1/1	0.89	0.32	75,75,75,75	0
81	MG	AR	3832	1/1	0.89	0.17	80,80,80,80	0
81	MG	AR	4089	1/1	0.89	0.11	67,67,67,67	0
81	MG	1	3467	1/1	0.89	0.20	41,41,41,41	0
80	OHX	A	2075	7/7	0.89	0.13	136,149,173,223	0
81	MG	A	2050	1/1	0.89	0.13	91,91,91,91	0
80	OHX	sR	2100	7/7	0.89	0.10	164,185,201,263	0
81	MG	AR	3405	1/1	0.89	0.15	59,59,59,59	0
81	MG	sR	2042	1/1	0.89	0.18	66,66,66,66	0
81	MG	AR	3406	1/1	0.89	0.13	56,56,56,56	0
81	MG	AR	3841	1/1	0.89	0.33	68,68,68,68	0
81	MG	1	3496	1/1	0.89	0.19	60,60,60,60	0
81	MG	4	211	1/1	0.89	0.31	57,57,57,57	0
81	MG	AR	4119	1/1	0.89	0.22	70,70,70,70	0
81	MG	AR	4121	1/1	0.89	0.28	76,76,76,76	0
80	OHX	sR	1914	7/7	0.89	0.12	152,158,179,225	0
81	MG	4	213	1/1	0.89	0.31	69,69,69,69	0
80	OHX	AR	4078	7/7	0.89	0.10	136,150,160,217	0
81	MG	A	2070	1/1	0.89	0.16	83,83,83,83	0
81	MG	sR	2069	1/1	0.89	0.15	77,77,77,77	0
81	MG	AR	3429	1/1	0.89	0.31	78,78,78,78	0
80	OHX	sR	1922	7/7	0.89	0.18	117,120,138,164	7
81	MG	AR	3870	1/1	0.89	0.26	48,48,48,48	0
81	MG	sR	2081	1/1	0.89	0.21	71,71,71,71	0
81	MG	AR	3431	1/1	0.89	0.47	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	A	1964	6/7	0.89	0.16	175,178,192,284	0
80	OHX	A	2083	7/7	0.89	0.10	242,249,260,308	0
80	OHX	CS	202	7/7	0.89	0.12	161,163,173,247	0
81	MG	A	2084	1/1	0.89	0.09	95,95,95,95	0
80	OHX	1	3545	7/7	0.89	0.13	179,182,189,247	0
81	MG	A	1939	1/1	0.89	0.30	68,68,68,68	0
80	OHX	1	3940	7/7	0.89	0.10	166,192,206,267	0
81	MG	AR	3884	1/1	0.89	0.23	54,54,54,54	0
80	OHX	AR	4108	7/7	0.89	0.12	166,176,189,257	0
81	MG	AR	3897	1/1	0.89	0.23	55,55,55,55	0
80	OHX	AR	3548	7/7	0.89	0.09	145,161,180,246	0
81	MG	sR	2127	1/1	0.89	0.30	77,77,77,77	0
81	MG	1	3566	1/1	0.89	0.19	52,52,52,52	0
81	MG	AR	3461	1/1	0.89	0.29	56,56,56,56	0
81	MG	AR	4185	1/1	0.89	0.09	93,93,93,93	0
80	OHX	1	3965	7/7	0.89	0.10	202,219,236,285	0
81	MG	AR	3681	1/1	0.89	0.10	75,75,75,75	0
81	MG	AR	3466	1/1	0.89	0.07	93,93,93,93	0
80	OHX	AR	3549	7/7	0.89	0.10	172,185,212,276	0
80	OHX	1	3990	7/7	0.89	0.17	145,148,159,253	0
81	MG	sR	2143	1/1	0.89	0.17	76,76,76,76	0
80	OHX	AR	4111	7/7	0.89	0.09	202,210,243,278	0
81	MG	1	3598	1/1	0.89	0.11	71,71,71,71	0
81	MG	1	3944	1/1	0.89	0.15	62,62,62,62	0
81	MG	AR	3474	1/1	0.89	0.28	114,114,114,114	0
81	MG	1	3949	1/1	0.89	0.29	44,44,44,44	0
81	MG	AR	3938	1/1	0.89	0.25	73,73,73,73	0
81	MG	AR	3939	1/1	0.89	0.21	69,69,69,69	0
81	MG	AS	205	1/1	0.89	0.35	48,48,48,48	0
81	MG	A	1959	1/1	0.89	0.23	80,80,80,80	0
80	OHX	U	202	7/7	0.89	0.10	210,217,220,301	0
80	OHX	AR	3579	7/7	0.89	0.10	171,192,217,259	0
81	MG	sR	2172	1/1	0.89	0.14	59,59,59,59	0
80	OHX	A	2096	7/7	0.89	0.11	178,194,217,268	0
80	OHX	AR	3453	6/7	0.89	0.10	165,175,190,253	0
81	MG	AS	213	1/1	0.89	0.23	75,75,75,75	0
80	OHX	A	1984	7/7	0.89	0.22	143,146,154,164	7
81	MG	sR	2185	1/1	0.89	0.25	78,78,78,78	0
81	MG	AR	3724	1/1	0.89	0.24	63,63,63,63	0
81	MG	1	3987	1/1	0.89	0.22	71,71,71,71	0
80	OHX	AT	205	7/7	0.89	0.12	153,169,190,245	0
81	MG	AR	3737	1/1	0.89	0.24	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	sR	2000	7/7	0.89	0.17	144,159,169,189	7
81	MG	1	4008	1/1	0.89	0.15	47,47,47,47	0
81	MG	1	4010	1/1	0.89	0.24	51,51,51,51	0
81	MG	AR	3970	1/1	0.89	0.17	62,62,62,62	0
80	OHX	AR	3480	7/7	0.89	0.30	131,137,142,174	7
81	MG	sR	1906	1/1	0.89	0.23	66,66,66,66	0
80	OHX	sR	2016	7/7	0.89	0.11	139,161,187,255	0
81	MG	1	4034	1/1	0.89	0.20	43,43,43,43	0
81	MG	1	4037	1/1	0.89	0.30	69,69,69,69	0
81	MG	sR	1910	1/1	0.89	0.26	64,64,64,64	0
81	MG	1	4040	1/1	0.89	0.17	61,61,61,61	0
81	MG	AT	213	1/1	0.89	0.20	73,73,73,73	0
80	OHX	Q	201	7/7	0.89	0.09	210,216,221,251	7
80	OHX	CE	402	7/7	0.89	0.09	168,186,204,243	0
81	MG	1	4044	1/1	0.89	0.11	55,55,55,55	0
81	MG	DQ	502	1/1	0.89	0.23	70,70,70,70	0
81	MG	AT	219	1/1	0.89	0.18	69,69,69,69	0
80	OHX	sR	2028	7/7	0.89	0.11	193,200,234,275	0
80	OHX	AR	3487	7/7	0.89	0.09	200,205,227,282	0
81	MG	A	1999	1/1	0.89	0.22	93,93,93,93	0
80	OHX	AR	3642	7/7	0.89	0.10	168,176,211,258	0
81	MG	AR	4001	1/1	0.89	0.12	71,71,71,71	0
81	MG	AR	3528	1/1	0.89	0.17	76,76,76,76	0
81	MG	AR	4007	1/1	0.89	0.14	51,51,51,51	0
81	MG	1	3708	1/1	0.89	0.37	71,71,71,71	0
80	OHX	AR	4017	7/7	0.89	0.09	191,218,227,261	0
81	MG	1	3711	1/1	0.89	0.22	63,63,63,63	0
80	OHX	1	3424	7/7	0.89	0.16	146,155,175,180	7
81	MG	CE	406	1/1	0.89	0.16	86,86,86,86	0
81	MG	A	2156	1/1	0.89	0.24	93,93,93,93	0
81	MG	sR	1962	1/1	0.89	0.40	82,82,82,82	0
80	OHX	1	3761	7/7	0.89	0.10	157,190,202,238	0
81	MG	1	3718	1/1	0.89	0.22	95,95,95,95	0
80	OHX	1	3429	7/7	0.89	0.10	162,171,198,243	0
81	MG	s4	303	1/1	0.89	0.28	81,81,81,81	0
81	MG	v	303	1/1	0.89	0.37	73,73,73,73	0
81	MG	A	2011	1/1	0.89	0.10	91,91,91,91	0
81	MG	1	3401	1/1	0.89	0.15	63,63,63,63	0
81	MG	t	202	1/1	0.89	0.17	62,62,62,62	0
81	MG	1	4123	1/1	0.89	0.35	77,77,77,77	0
80	OHX	A	2123	6/7	0.89	0.10	234,247,247,263	0
80	OHX	3	204	7/7	0.89	0.11	166,172,184,236	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	r	302	1/1	0.89	0.16	66,66,66,66	0
81	MG	1	3407	1/1	0.89	0.25	48,48,48,48	0
80	OHX	AR	4049	7/7	0.89	0.12	156,174,185,253	0
81	MG	1	3410	1/1	0.89	0.12	71,71,71,71	0
81	MG	1	3412	1/1	0.89	0.19	87,87,87,87	0
81	MG	1	3413	1/1	0.89	0.29	74,74,74,74	0
80	OHX	1	3460	7/7	0.89	0.12	171,175,198,250	0
81	MG	1	3773	1/1	0.89	0.25	111,111,111,111	0
81	MG	3	216	1/1	0.89	0.08	99,99,99,99	0
80	OHX	A	2027	7/7	0.89	0.14	152,166,190,219	0
80	OHX	1	3485	7/7	0.89	0.14	46,91,115,206	0
81	MG	AB	201	1/1	0.89	0.24	56,56,56,56	0
81	MG	1	3434	1/1	0.89	0.19	59,59,59,59	0
81	MG	1	3435	1/1	0.89	0.29	63,63,63,63	0
81	MG	AR	4064	1/1	0.89	0.23	65,65,65,65	0
81	MG	AR	3811	1/1	0.89	0.36	67,67,67,67	0
81	MG	AR	3587	1/1	0.89	0.35	51,51,51,51	0
85	SPD	AR	3858	10/10	0.89	0.26	69,73,85,92	0
81	MG	AR	3588	1/1	0.89	0.19	57,57,57,57	0
81	MG	AB	204	1/1	0.89	0.35	63,63,63,63	0
81	MG	AR	4040	1/1	0.90	0.18	78,78,78,78	0
81	MG	AR	4052	1/1	0.90	0.33	59,59,59,59	0
80	OHX	AR	3985	7/7	0.90	0.11	161,171,187,252	0
80	OHX	1	4178	7/7	0.90	0.14	103,122,139,192	0
80	OHX	AR	3986	7/7	0.90	0.10	152,159,186,229	0
81	MG	1	3589	1/1	0.90	0.35	53,53,53,53	0
80	OHX	AR	3766	7/7	0.90	0.13	153,156,169,250	0
80	OHX	A	2043	6/7	0.90	0.08	266,274,275,333	0
81	MG	AR	3500	1/1	0.90	0.21	78,78,78,78	0
81	MG	AR	3501	1/1	0.90	0.16	72,72,72,72	0
81	MG	AR	3850	1/1	0.90	0.30	72,72,72,72	0
81	MG	AT	218	1/1	0.90	0.34	74,74,74,74	0
80	OHX	sR	1936	7/7	0.90	0.11	142,150,161,231	0
80	OHX	CG	302	7/7	0.90	0.10	196,201,223,255	0
80	OHX	AR	4139	7/7	0.90	0.14	137,151,161,215	0
81	MG	AT	225	1/1	0.90	0.18	52,52,52,52	0
81	MG	AR	3686	1/1	0.90	0.14	72,72,72,72	0
81	MG	d6	201	1/1	0.90	0.35	72,72,72,72	0
81	MG	1	3625	1/1	0.90	0.10	62,62,62,62	0
81	MG	CD	303	1/1	0.90	0.31	66,66,66,66	0
80	OHX	1	3909	7/7	0.90	0.08	177,204,233,266	0
80	OHX	AR	3700	7/7	0.90	0.11	148,155,174,217	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	A	1913	7/7	0.90	0.11	168,189,202,242	0
81	MG	AR	4092	1/1	0.90	0.19	64,64,64,64	0
80	OHX	AR	3893	7/7	0.90	0.11	167,178,190,237	0
81	MG	1	3925	1/1	0.90	0.17	53,53,53,53	0
80	OHX	A	2104	7/7	0.90	0.10	188,201,220,252	0
81	MG	AR	3527	1/1	0.90	0.20	98,98,98,98	0
80	OHX	1	3427	7/7	0.90	0.14	126,137,149,195	0
81	MG	sR	2001	1/1	0.90	0.14	88,88,88,88	0
80	OHX	1	3941	7/7	0.90	0.11	144,151,173,213	0
81	MG	AR	3716	1/1	0.90	0.24	62,62,62,62	0
81	MG	1	3948	1/1	0.90	0.35	53,53,53,53	0
81	MG	AR	3717	1/1	0.90	0.11	65,65,65,65	0
81	MG	AR	3886	1/1	0.90	0.14	100,100,100,100	0
81	MG	AR	4122	1/1	0.90	0.31	91,91,91,91	0
81	MG	1	3673	1/1	0.90	0.12	67,67,67,67	0
81	MG	1	3674	1/1	0.90	0.12	112,112,112,112	0
81	MG	AR	3532	1/1	0.90	0.14	48,48,48,48	0
81	MG	AR	4125	1/1	0.90	0.16	62,62,62,62	0
80	OHX	AR	4046	7/7	0.90	0.11	123,138,171,210	0
81	MG	AR	3408	1/1	0.90	0.24	67,67,67,67	0
81	MG	1	3975	1/1	0.90	0.32	69,69,69,69	0
81	MG	AR	3900	1/1	0.90	0.36	51,51,51,51	0
80	OHX	AR	3639	7/7	0.90	0.12	130,143,168,218	0
80	OHX	sR	2137	7/7	0.90	0.11	158,165,183,262	0
81	MG	AR	3738	1/1	0.90	0.17	82,82,82,82	0
81	MG	r	303	1/1	0.90	0.28	62,62,62,62	0
81	MG	AR	3912	1/1	0.90	0.21	69,69,69,69	0
81	MG	AR	3742	1/1	0.90	0.28	69,69,69,69	0
81	MG	1	3704	1/1	0.90	0.27	62,62,62,62	0
81	MG	1	4005	1/1	0.90	0.18	60,60,60,60	0
81	MG	AR	3743	1/1	0.90	0.30	79,79,79,79	0
81	MG	1	3709	1/1	0.90	0.35	60,60,60,60	0
81	MG	AR	3427	1/1	0.90	0.22	51,51,51,51	0
81	MG	sR	2066	1/1	0.90	0.25	73,73,73,73	0
81	MG	1	3712	1/1	0.90	0.17	50,50,50,50	0
81	MG	1	4017	1/1	0.90	0.12	82,82,82,82	0
80	OHX	k	403	7/7	0.90	0.11	131,142,163,209	0
81	MG	1	4019	1/1	0.90	0.30	63,63,63,63	0
81	MG	1	4020	1/1	0.90	0.26	81,81,81,81	0
81	MG	AR	3932	1/1	0.90	0.29	54,54,54,54	0
80	OHX	1	3459	7/7	0.90	0.10	142,151,174,244	0
80	OHX	A	1947	7/7	0.90	0.09	173,200,215,262	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
80	OHX	1	3729	7/7	0.90	0.11	173,176,206,241	0
81	MG	AR	3943	1/1	0.90	0.12	80,80,80,80	0
81	MG	1	3444	1/1	0.90	0.33	67,67,67,67	0
81	MG	AR	3432	1/1	0.90	0.26	46,46,46,46	0
80	OHX	1	3730	7/7	0.90	0.10	150,168,190,220	0
81	MG	4	221	1/1	0.90	0.17	68,68,68,68	0
81	MG	1	4045	1/1	0.90	0.17	101,101,101,101	0
81	MG	AR	3768	1/1	0.90	0.35	41,41,41,41	0
81	MG	AR	3437	1/1	0.90	0.16	69,69,69,69	0
81	MG	AR	4189	1/1	0.90	0.23	66,66,66,66	0
81	MG	1	4049	1/1	0.90	0.22	89,89,89,89	0
80	OHX	sR	1981	7/7	0.90	0.11	186,189,205,266	0
81	MG	AR	4199	1/1	0.90	0.08	109,109,109,109	0
81	MG	AR	4205	1/1	0.90	0.10	56,56,56,56	0
80	OHX	1	4031	7/7	0.90	0.09	234,250,262,293	0
81	MG	sR	2107	1/1	0.90	0.09	70,70,70,70	0
80	OHX	A	2122	7/7	0.90	0.13	174,186,206,230	0
80	OHX	AR	3953	7/7	0.90	0.10	145,150,180,240	0
81	MG	1	3492	1/1	0.90	0.15	69,69,69,69	0
80	OHX	A	1954	7/7	0.90	0.13	171,183,198,261	0
81	MG	A	1919	1/1	0.90	0.30	52,52,52,52	0
80	OHX	AR	3955	7/7	0.90	0.12	161,162,194,236	0
81	MG	CL	303	1/1	0.90	0.27	51,51,51,51	0
80	OHX	AR	4104	7/7	0.90	0.13	118,128,149,173	7
81	MG	1	3793	1/1	0.90	0.10	82,82,82,82	0
81	MG	AR	3464	1/1	0.90	0.18	66,66,66,66	0
80	OHX	A	2093	7/7	0.90	0.09	209,212,231,289	0
81	MG	AR	3995	1/1	0.90	0.22	69,69,69,69	0
81	MG	sR	2141	1/1	0.90	0.14	105,105,105,105	0
80	OHX	AR	3856	7/7	0.90	0.36	120,122,129,152	7
81	MG	AR	3617	1/1	0.90	0.22	49,49,49,49	0
81	MG	1	3801	1/1	0.90	0.22	70,70,70,70	0
81	MG	AR	3802	1/1	0.90	0.19	52,52,52,52	0
81	MG	1	4124	1/1	0.90	0.33	49,49,49,49	0
81	MG	AR	3468	1/1	0.90	0.14	72,72,72,72	0
81	MG	AR	3622	1/1	0.90	0.19	60,60,60,60	0
81	MG	1	3808	1/1	0.90	0.17	69,69,69,69	0
80	OHX	1	4121	7/7	0.90	0.14	146,159,178,239	0
81	MG	AR	3624	1/1	0.90	0.42	93,93,93,93	0
81	MG	A	2041	1/1	0.90	0.15	94,94,94,94	0
81	MG	sR	2163	1/1	0.90	0.06	81,81,81,81	0
81	MG	AR	4013	1/1	0.90	0.17	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
80	OHX	1	3820	7/7	0.90	0.10	235,244,261,292	0
80	OHX	sR	2053	7/7	0.90	0.09	226,229,236,264	0
81	MG	1	3552	1/1	0.90	0.28	60,60,60,60	0
81	MG	1	3554	1/1	0.90	0.21	72,72,72,72	0
81	MG	1	4160	1/1	0.90	0.16	68,68,68,68	0
81	MG	AR	3488	1/1	0.90	0.15	54,54,54,54	0
81	MG	1	4165	1/1	0.90	0.23	69,69,69,69	0
81	MG	A	2051	1/1	0.90	0.13	96,96,96,96	0
81	MG	1	3558	1/1	0.90	0.17	62,62,62,62	0
81	MG	AR	4030	1/1	0.90	0.09	85,85,85,85	0
80	OHX	1	3519	7/7	0.90	0.11	153,157,183,227	0
81	MG	AR	3646	1/1	0.90	0.34	58,58,58,58	0
81	MG	1	3854	1/1	0.90	0.23	66,66,66,66	0
81	MG	AR	3836	1/1	0.90	0.17	71,71,71,71	0
80	OHX	1	4173	7/7	0.90	0.15	130,143,169,232	0
81	MG	AR	4038	1/1	0.90	0.26	67,67,67,67	0
80	OHX	1	3670	7/7	0.91	0.14	160,165,180,237	0
81	MG	1	3838	1/1	0.91	0.12	142,142,142,142	0
80	OHX	AR	3980	7/7	0.91	0.14	147,156,173,249	0
80	OHX	1	3905	7/7	0.91	0.13	143,155,180,241	0
80	OHX	sR	1944	7/7	0.91	0.22	113,128,136,140	7
81	MG	DO	202	1/1	0.91	0.14	73,73,73,73	0
80	OHX	sR	1948	7/7	0.91	0.10	162,168,175,256	0
81	MG	1	3537	1/1	0.91	0.17	56,56,56,56	0
80	OHX	1	3911	7/7	0.91	0.12	138,160,183,214	0
81	MG	3	210	1/1	0.91	0.18	62,62,62,62	0
81	MG	A	1969	1/1	0.91	0.12	84,84,84,84	0
80	OHX	AR	4141	7/7	0.91	0.10	185,195,203,248	0
81	MG	AR	3991	1/1	0.91	0.38	57,57,57,57	0
81	MG	A	1971	1/1	0.91	0.18	72,72,72,72	0
80	OHX	sR	1903	7/7	0.91	0.10	155,166,186,239	0
81	MG	AR	3592	1/1	0.91	0.46	83,83,83,83	0
80	OHX	1	3720	7/7	0.91	0.10	169,172,198,240	0
81	MG	1	3564	1/1	0.91	0.19	50,50,50,50	0
80	OHX	AR	3829	7/7	0.91	0.13	142,152,181,252	0
81	MG	sR	2173	1/1	0.91	0.22	58,58,58,58	0
81	MG	1	3889	1/1	0.91	0.35	55,55,55,55	0
81	MG	AS	217	1/1	0.91	0.29	74,74,74,74	0
81	MG	AR	4002	1/1	0.91	0.25	62,62,62,62	0
81	MG	c4	201	1/1	0.91	0.10	66,66,66,66	0
81	MG	sR	2183	1/1	0.91	0.21	78,78,78,78	0
80	OHX	A	2045	7/7	0.91	0.11	156,178,181,226	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	3588	1/1	0.91	0.27	66,66,66,66	0
81	MG	AR	3457	1/1	0.91	0.24	61,61,61,61	0
81	MG	AR	3613	1/1	0.91	0.29	48,48,48,48	0
81	MG	A	1982	1/1	0.91	0.11	104,104,104,104	0
81	MG	sR	1909	1/1	0.91	0.21	60,60,60,60	0
80	OHX	CL	301	7/7	0.91	0.12	118,126,152,189	0
81	MG	AR	4021	1/1	0.91	0.17	69,69,69,69	0
81	MG	1	3921	1/1	0.91	0.18	56,56,56,56	0
81	MG	1	3600	1/1	0.91	0.07	45,45,45,45	0
80	OHX	sR	2099	7/7	0.91	0.14	137,142,161,207	0
81	MG	sR	1921	1/1	0.91	0.32	58,58,58,58	0
81	MG	1	3615	1/1	0.91	0.22	75,75,75,75	0
81	MG	AR	3806	1/1	0.91	0.10	58,58,58,58	0
81	MG	AT	209	1/1	0.91	0.18	65,65,65,65	0
81	MG	AT	210	1/1	0.91	0.23	60,60,60,60	0
81	MG	AR	4027	1/1	0.91	0.34	70,70,70,70	0
81	MG	AR	4028	1/1	0.91	0.14	60,60,60,60	0
81	MG	1	3946	1/1	0.91	0.15	56,56,56,56	0
81	MG	AR	3620	1/1	0.91	0.16	61,61,61,61	0
80	OHX	sR	1969	7/7	0.91	0.10	172,185,214,257	0
81	MG	AR	3463	1/1	0.91	0.30	47,47,47,47	0
80	OHX	1	3970	7/7	0.91	0.13	124,131,150,200	0
81	MG	1	3953	1/1	0.91	0.29	65,65,65,65	0
81	MG	AR	3465	1/1	0.91	0.29	103,103,103,103	0
81	MG	AB	205	1/1	0.91	0.15	65,65,65,65	0
80	OHX	sR	1915	7/7	0.91	0.14	146,150,175,209	0
81	MG	AB	207	1/1	0.91	0.18	60,60,60,60	0
81	MG	sR	1960	1/1	0.91	0.40	63,63,63,63	0
81	MG	DC	203	1/1	0.91	0.16	49,49,49,49	0
81	MG	sR	1961	1/1	0.91	0.14	66,66,66,66	0
81	MG	CD	301	1/1	0.91	0.42	75,75,75,75	0
81	MG	1	3979	1/1	0.91	0.39	44,44,44,44	0
80	OHX	AR	3825	7/7	0.91	0.13	111,135,158,197	0
81	MG	1	3655	1/1	0.91	0.18	64,64,64,64	0
81	MG	A	2137	1/1	0.91	0.19	74,74,74,74	0
81	MG	AR	3643	1/1	0.91	0.30	57,57,57,57	0
81	MG	4	210	1/1	0.91	0.46	75,75,75,75	0
80	OHX	AR	4015	7/7	0.91	0.11	151,164,187,234	0
80	OHX	sR	1988	7/7	0.91	0.14	138,142,157,191	7
81	MG	1	3675	1/1	0.91	0.16	70,70,70,70	0
80	OHX	1	4025	7/7	0.91	0.10	172,179,191,254	0
81	MG	AR	3490	1/1	0.91	0.16	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	CU	201	1/1	0.91	0.27	62,62,62,62	0
80	OHX	1	3548	7/7	0.91	0.12	152,160,181,224	0
81	MG	AR	3658	1/1	0.91	0.17	56,56,56,56	0
81	MG	A	2019	1/1	0.91	0.11	82,82,82,82	0
81	MG	AR	3662	1/1	0.91	0.16	50,50,50,50	0
81	MG	AR	3664	1/1	0.91	0.21	66,66,66,66	0
81	MG	AR	4086	1/1	0.91	0.32	73,73,73,73	0
81	MG	CI	301	1/1	0.91	0.14	72,72,72,72	0
81	MG	DI	201	1/1	0.91	0.27	57,57,57,57	0
81	MG	1	4036	1/1	0.91	0.34	43,43,43,43	0
80	OHX	1	3785	7/7	0.91	0.20	136,140,154,173	7
80	OHX	1	3789	7/7	0.91	0.12	124,147,169,207	0
80	OHX	1	3549	7/7	0.91	0.13	102,110,135,199	0
81	MG	AR	4095	1/1	0.91	0.11	72,72,72,72	0
81	MG	AR	3680	1/1	0.91	0.09	66,66,66,66	0
80	OHX	sR	1993	7/7	0.91	0.13	215,228,243,327	0
81	MG	sR	2011	1/1	0.91	0.32	76,76,76,76	0
81	MG	AR	3682	1/1	0.91	0.21	82,82,82,82	0
81	MG	sR	2021	1/1	0.91	0.18	122,122,122,122	0
81	MG	sR	2023	1/1	0.91	0.10	91,91,91,91	0
80	OHX	1	3815	7/7	0.91	0.12	135,144,167,215	0
80	OHX	1	4081	7/7	0.91	0.15	119,122,127,195	0
81	MG	AR	3687	1/1	0.91	0.12	65,65,65,65	0
81	MG	AR	3503	1/1	0.91	0.28	107,107,107,107	0
81	MG	1	3432	1/1	0.91	0.11	68,68,68,68	0
81	MG	AR	3689	1/1	0.91	0.11	86,86,86,86	0
81	MG	1	4068	1/1	0.91	0.23	57,57,57,57	0
81	MG	4	227	1/1	0.91	0.40	66,66,66,66	0
80	OHX	AR	4197	7/7	0.91	0.20	106,120,126,143	7
80	OHX	1	4113	7/7	0.91	0.14	142,155,169,228	0
81	MG	AR	3699	1/1	0.91	0.14	63,63,63,63	0
81	MG	AR	3705	1/1	0.91	0.19	55,55,55,55	0
81	MG	1	3443	1/1	0.91	0.13	66,66,66,66	0
81	MG	1	4078	1/1	0.91	0.33	51,51,51,51	0
81	MG	1	3749	1/1	0.91	0.38	75,75,75,75	0
81	MG	AR	3519	1/1	0.91	0.28	63,63,63,63	0
81	MG	1	4093	1/1	0.91	0.38	70,70,70,70	0
81	MG	AR	3520	1/1	0.91	0.27	66,66,66,66	0
80	OHX	sR	1926	7/7	0.91	0.12	159,169,176,241	0
81	MG	x	202	1/1	0.91	0.40	67,67,67,67	0
81	MG	1	4098	1/1	0.91	0.33	48,48,48,48	0
81	MG	AR	3909	1/1	0.91	0.27	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	AR	4150	1/1	0.91	0.18	66,66,66,66	0
81	MG	A	2049	1/1	0.91	0.35	62,62,62,62	0
81	MG	AR	4152	1/1	0.91	0.37	66,66,66,66	0
81	MG	1	3777	1/1	0.91	0.10	92,92,92,92	0
81	MG	j	302	1/1	0.91	0.19	57,57,57,57	0
81	MG	1	3469	1/1	0.91	0.23	77,77,77,77	0
81	MG	AR	3718	1/1	0.91	0.14	84,84,84,84	0
81	MG	1	4126	1/1	0.91	0.24	43,43,43,43	0
80	OHX	A	1917	7/7	0.91	0.10	177,189,214,249	0
80	OHX	AR	4203	7/7	0.91	0.10	209,210,222,262	0
81	MG	AR	3722	1/1	0.91	0.27	63,63,63,63	0
81	MG	A	2058	1/1	0.91	0.23	58,58,58,58	0
81	MG	AR	4177	1/1	0.91	0.24	60,60,60,60	0
81	MG	1	3493	1/1	0.91	0.35	77,77,77,77	0
81	MG	AR	4178	1/1	0.91	0.21	58,58,58,58	0
81	MG	AR	3935	1/1	0.91	0.34	76,76,76,76	0
80	OHX	1	3850	7/7	0.91	0.12	139,161,183,231	0
81	MG	A	1932	1/1	0.91	0.35	67,67,67,67	0
81	MG	AR	3401	1/1	0.91	0.24	88,88,88,88	0
80	OHX	A	1967	7/7	0.91	0.10	163,181,187,223	0
81	MG	AR	3740	1/1	0.91	0.51	48,48,48,48	0
81	MG	sR	2115	1/1	0.91	0.40	61,61,61,61	0
81	MG	CM	202	1/1	0.91	0.16	72,72,72,72	0
81	MG	1	3827	1/1	0.91	0.21	55,55,55,55	0
81	MG	sR	2118	1/1	0.91	0.24	68,68,68,68	0
80	OHX	sR	2169	7/7	0.91	0.07	205,209,212,266	0
81	MG	A	2074	1/1	0.91	0.09	111,111,111,111	0
81	MG	1	4177	1/1	0.91	0.11	103,103,103,103	0
81	MG	1	3832	1/1	0.91	0.19	68,68,68,68	0
80	OHX	AR	4018	7/7	0.91	0.13	114,126,146,224	0
81	MG	AR	3962	1/1	0.91	0.25	52,52,52,52	0
81	MG	1	3528	1/1	0.91	0.22	66,66,66,66	0
80	OHX	1	3457	7/7	0.91	0.12	147,170,174,216	0
80	OHX	A	2120	7/7	0.92	0.12	118,122,140,208	0
80	OHX	sR	1989	7/7	0.92	0.11	138,144,148,221	0
80	OHX	AT	203	7/7	0.92	0.10	141,147,166,224	0
80	OHX	AR	3830	7/7	0.92	0.10	143,150,164,242	0
80	OHX	1	3635	7/7	0.92	0.22	88,92,106,122	7
81	MG	AR	3471	1/1	0.92	0.14	74,74,74,74	0
81	MG	AR	3882	1/1	0.92	0.26	60,60,60,60	0
81	MG	AR	4147	1/1	0.92	0.23	48,48,48,48	0
81	MG	AR	3472	1/1	0.92	0.22	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
80	OHX	1	3642	7/7	0.92	0.11	135,154,167,235	0
81	MG	sR	2094	1/1	0.92	0.27	79,79,79,79	0
80	OHX	AR	3450	7/7	0.92	0.11	127,143,169,204	0
81	MG	1	3840	1/1	0.92	0.16	60,60,60,60	0
80	OHX	1	3971	7/7	0.92	0.12	169,172,179,201	0
81	MG	4	225	1/1	0.92	0.19	65,65,65,65	0
81	MG	AR	4155	1/1	0.92	0.18	60,60,60,60	0
81	MG	AR	3684	1/1	0.92	0.39	62,62,62,62	0
81	MG	AR	4157	1/1	0.92	0.08	139,139,139,139	0
81	MG	1	3522	1/1	0.92	0.18	65,65,65,65	0
81	MG	1	3859	1/1	0.92	0.20	79,79,79,79	0
81	MG	AR	3902	1/1	0.92	0.22	52,52,52,52	0
81	MG	1	3861	1/1	0.92	0.15	91,91,91,91	0
80	OHX	AR	3727	7/7	0.92	0.14	105,119,127,182	0
80	OHX	h	401	7/7	0.92	0.09	221,231,237,274	0
81	MG	sR	2117	1/1	0.92	0.14	78,78,78,78	0
80	OHX	Rb	401	7/7	0.92	0.09	219,223,240,280	0
81	MG	AR	3907	1/1	0.92	0.18	64,64,64,64	0
81	MG	1	3867	1/1	0.92	0.12	77,77,77,77	0
81	MG	AR	3493	1/1	0.92	0.31	69,69,69,69	0
81	MG	sR	2128	1/1	0.92	0.20	72,72,72,72	0
80	OHX	AR	3859	7/7	0.92	0.12	137,145,163,219	0
81	MG	A	1962	1/1	0.92	0.31	71,71,71,71	0
80	OHX	1	4002	7/7	0.92	0.14	130,136,159,170	7
80	OHX	3	203	7/7	0.92	0.11	158,163,193,220	0
81	MG	DL	101	1/1	0.92	0.31	71,71,71,71	0
80	OHX	AR	3861	7/7	0.92	0.11	135,154,157,235	0
81	MG	1	3895	1/1	0.92	0.12	64,64,64,64	0
81	MG	AR	3706	1/1	0.92	0.21	45,45,45,45	0
81	MG	1	3898	1/1	0.92	0.14	73,73,73,73	0
81	MG	AR	4187	1/1	0.92	0.17	91,91,91,91	0
81	MG	AR	3933	1/1	0.92	0.22	59,59,59,59	0
80	OHX	1	3699	7/7	0.92	0.11	122,136,171,212	0
81	MG	AR	3502	1/1	0.92	0.15	86,86,86,86	0
81	MG	1	3563	1/1	0.92	0.28	74,74,74,74	0
80	OHX	AR	4047	7/7	0.92	0.10	129,151,187,210	0
80	OHX	3	219	7/7	0.92	0.13	136,156,167,215	0
81	MG	A	2146	1/1	0.92	0.23	74,74,74,74	0
80	OHX	1	4053	7/7	0.92	0.13	103,113,141,179	0
81	MG	sR	2162	1/1	0.92	0.18	61,61,61,61	0
80	OHX	sR	2063	7/7	0.92	0.10	147,151,168,245	0
81	MG	A	2154	1/1	0.92	0.31	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	AR	3958	1/1	0.92	0.24	63,63,63,63	0
80	OHX	v	305	7/7	0.92	0.11	123,136,162,204	0
81	MG	DA	202	1/1	0.92	0.14	66,66,66,66	0
81	MG	1	3591	1/1	0.92	0.33	61,61,61,61	0
81	MG	d4	202	1/1	0.92	0.22	72,72,72,72	0
81	MG	AS	202	1/1	0.92	0.23	54,54,54,54	0
81	MG	AS	203	1/1	0.92	0.24	81,81,81,81	0
81	MG	1	3597	1/1	0.92	0.40	81,81,81,81	0
80	OHX	1	4059	7/7	0.92	0.10	154,163,171,221	0
80	OHX	1	4060[A]	7/7	0.92	0.18	117,131,137,173	7
80	OHX	1	4060[B]	7/7	0.92	0.18	116,123,133,170	7
80	OHX	1	4061	7/7	0.92	0.08	166,192,215,267	0
80	OHX	AR	3731	7/7	0.92	0.11	152,152,175,207	0
80	OHX	AR	3887	7/7	0.92	0.12	100,127,146,175	0
81	MG	AR	3969	1/1	0.92	0.19	81,81,81,81	0
81	MG	AR	3530	1/1	0.92	0.12	73,73,73,73	0
80	OHX	1	4091	7/7	0.92	0.11	153,161,180,229	0
81	MG	w	202	1/1	0.92	0.39	83,83,83,83	0
81	MG	A	2001	1/1	0.92	0.13	90,90,90,90	0
80	OHX	AR	4074	7/7	0.92	0.12	111,144,157,205	0
80	OHX	AR	3891	7/7	0.92	0.11	141,154,188,215	0
81	MG	1	3629	1/1	0.92	0.15	60,60,60,60	0
81	MG	o	301	1/1	0.92	0.14	63,63,63,63	0
81	MG	AT	212	1/1	0.92	0.28	60,60,60,60	0
81	MG	AR	3555	1/1	0.92	0.36	54,54,54,54	0
80	OHX	AR	3580	6/7	0.92	0.10	206,216,236,303	0
81	MG	AR	3557	1/1	0.92	0.26	70,70,70,70	0
81	MG	1	3989	1/1	0.92	0.28	61,61,61,61	0
81	MG	1	3646	1/1	0.92	0.14	62,62,62,62	0
81	MG	1	3647	1/1	0.92	0.25	50,50,50,50	0
81	MG	CQ	201	1/1	0.92	0.20	82,82,82,82	0
80	OHX	1	4119	7/7	0.92	0.11	133,142,161,213	0
81	MG	AR	3560	1/1	0.92	0.38	86,86,86,86	0
80	OHX	A	2132	7/7	0.92	0.14	110,121,146,208	0
81	MG	x	209	1/1	0.92	0.40	57,57,57,57	0
81	MG	AT	223	1/1	0.92	0.27	63,63,63,63	0
80	OHX	1	3759	7/7	0.92	0.10	139,155,184,228	0
81	MG	AR	3774	1/1	0.92	0.10	55,55,55,55	0
81	MG	1	3657	1/1	0.92	0.12	69,69,69,69	0
81	MG	AR	3565	1/1	0.92	0.17	71,71,71,71	0
81	MG	CR	201	1/1	0.92	0.18	79,79,79,79	0
81	MG	d6	203	1/1	0.92	0.28	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
80	OHX	A	2133	7/7	0.92	0.10	145,154,180,243	0
81	MG	CD	302	1/1	0.92	0.30	55,55,55,55	0
80	OHX	AR	3609	7/7	0.92	0.10	141,152,180,244	0
81	MG	AR	3780	1/1	0.92	0.13	71,71,71,71	0
81	MG	AR	4023	1/1	0.92	0.12	54,54,54,54	0
81	MG	A	2028	1/1	0.92	0.14	68,68,68,68	0
81	MG	AR	4025	1/1	0.92	0.22	45,45,45,45	0
81	MG	1	3682	1/1	0.92	0.34	71,71,71,71	0
80	OHX	1	4146	7/7	0.92	0.13	118,139,147,189	0
81	MG	AR	3586	1/1	0.92	0.15	70,70,70,70	0
80	OHX	1	3783	7/7	0.92	0.07	180,188,204,270	0
80	OHX	AR	3923	7/7	0.92	0.13	140,155,159,210	0
81	MG	A	2038	1/1	0.92	0.25	63,63,63,63	0
81	MG	1	3688	1/1	0.92	0.14	75,75,75,75	0
80	OHX	AR	3764	7/7	0.92	0.10	152,160,190,250	0
81	MG	AR	4033	1/1	0.92	0.09	58,58,58,58	0
81	MG	DH	203	1/1	0.92	0.09	63,63,63,63	0
81	MG	AR	3409	1/1	0.92	0.25	49,49,49,49	0
81	MG	v	301	1/1	0.92	0.18	64,64,64,64	0
81	MG	sR	1973	1/1	0.92	0.34	56,56,56,56	0
81	MG	AR	3410	1/1	0.92	0.28	68,68,68,68	0
80	OHX	sR	2112	7/7	0.92	0.10	161,169,189,235	0
81	MG	sR	1983	1/1	0.92	0.12	97,97,97,97	0
80	OHX	AR	3765	7/7	0.92	0.13	109,132,164,208	0
80	OHX	A	1966	7/7	0.92	0.09	209,220,243,268	0
81	MG	1	3403	1/1	0.92	0.23	48,48,48,48	0
80	OHX	AR	3611	7/7	0.92	0.10	187,196,211,256	0
81	MG	AR	4055	1/1	0.92	0.34	68,68,68,68	0
81	MG	AR	3812	1/1	0.92	0.21	72,72,72,72	0
81	MG	AR	4057	1/1	0.92	0.11	56,56,56,56	0
81	MG	1	4096	1/1	0.92	0.23	51,51,51,51	0
81	MG	1	3408	1/1	0.92	0.08	75,75,75,75	0
81	MG	AR	3606	1/1	0.92	0.09	97,97,97,97	0
81	MG	1	4099	1/1	0.92	0.11	60,60,60,60	0
81	MG	1	3743	1/1	0.92	0.25	63,63,63,63	0
81	MG	1	4102	1/1	0.92	0.13	59,59,59,59	0
80	OHX	4	201	7/7	0.92	0.10	125,134,161,219	0
80	OHX	A	2102	7/7	0.92	0.09	228,236,250,314	0
80	OHX	A	2103	7/7	0.92	0.12	125,137,163,193	0
81	MG	AR	3822	1/1	0.92	0.14	70,70,70,70	0
80	OHX	AR	3418	7/7	0.92	0.17	118,122,137,145	7
81	MG	CU	202	1/1	0.92	0.28	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	3426	1/1	0.92	0.10	109,109,109,109	0
81	MG	A	2061	1/1	0.92	0.13	85,85,85,85	0
80	OHX	1	3517	7/7	0.92	0.12	152,161,174,218	0
80	OHX	sR	2157	7/7	0.92	0.12	162,166,177,216	0
81	MG	1	4129	1/1	0.92	0.20	55,55,55,55	0
81	MG	1	4130	1/1	0.92	0.14	65,65,65,65	0
81	MG	sR	2020	1/1	0.92	0.20	75,75,75,75	0
80	OHX	1	3873	7/7	0.92	0.09	210,223,246,283	0
80	OHX	sR	2158	7/7	0.92	0.10	157,160,193,219	0
81	MG	1	3437	1/1	0.92	0.18	46,46,46,46	0
80	OHX	1	3880	7/7	0.92	0.10	168,178,197,228	0
80	OHX	1	3541	7/7	0.92	0.12	163,167,197,255	0
81	MG	1	4138	1/1	0.92	0.25	43,43,43,43	0
81	MG	1	3441	1/1	0.92	0.38	62,62,62,62	0
81	MG	AR	3844	1/1	0.92	0.16	68,68,68,68	0
81	MG	1	4153	1/1	0.92	0.17	53,53,53,53	0
81	MG	1	4154	1/1	0.92	0.25	40,40,40,40	0
81	MG	AB	202	1/1	0.92	0.14	69,69,69,69	0
81	MG	1	3445	1/1	0.92	0.09	79,79,79,79	0
80	OHX	A	1946	7/7	0.92	0.09	189,198,203,233	0
81	MG	AR	3848	1/1	0.92	0.14	56,56,56,56	0
81	MG	1	4164	1/1	0.92	0.24	70,70,70,70	0
80	OHX	AR	3542	7/7	0.92	0.09	125,132,169,227	0
81	MG	1	3462	1/1	0.92	0.23	60,60,60,60	0
81	MG	AR	3644	1/1	0.92	0.23	68,68,68,68	0
80	OHX	c5	201	7/7	0.92	0.07	202,217,230,262	0
80	OHX	AR	3545	7/7	0.92	0.11	112,119,146,211	0
81	MG	AR	4118	1/1	0.92	0.21	55,55,55,55	0
81	MG	1	4182	1/1	0.92	0.30	68,68,68,68	0
80	OHX	sR	2179	7/7	0.92	0.10	122,134,149,215	0
80	OHX	AR	4171	7/7	0.92	0.12	136,157,174,215	0
81	MG	sR	2060	1/1	0.92	0.18	93,93,93,93	0
80	OHX	3	205	7/7	0.92	0.11	174,178,180,221	0
80	OHX	1	3579	7/7	0.92	0.13	149,153,181,221	0
80	OHX	sR	2123	7/7	0.93	0.11	147,148,164,231	0
80	OHX	AR	3919	7/7	0.93	0.10	131,135,169,196	0
81	MG	1	3565	1/1	0.93	0.10	99,99,99,99	0
80	OHX	1	3843	7/7	0.93	0.10	128,136,161,232	0
81	MG	A	2060	1/1	0.93	0.17	69,69,69,69	0
81	MG	1	3568	1/1	0.93	0.22	68,68,68,68	0
80	OHX	AR	3922	7/7	0.93	0.08	180,186,195,225	0
81	MG	sM	302	1/1	0.93	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	sR	2136	7/7	0.93	0.10	166,172,183,239	0
81	MG	AR	3441	1/1	0.93	0.13	85,85,85,85	0
81	MG	sR	1940	1/1	0.93	0.27	77,77,77,77	0
80	OHX	AR	4107	7/7	0.93	0.11	128,131,147,207	0
80	OHX	sR	2146	7/7	0.93	0.10	107,129,155,208	0
81	MG	AR	3833	1/1	0.93	0.25	75,75,75,75	0
80	OHX	AR	3638	7/7	0.93	0.12	101,114,134,170	0
80	OHX	AR	3539	7/7	0.93	0.16	109,117,138,190	0
80	OHX	A	1973	7/7	0.93	0.10	144,152,162,242	0
80	OHX	1	3520	7/7	0.93	0.14	87,93,117,171	0
80	OHX	sR	2156	7/7	0.93	0.13	149,166,177,191	0
81	MG	1	3894	1/1	0.93	0.14	59,59,59,59	0
80	OHX	AR	3795	7/7	0.93	0.10	146,154,176,219	0
80	OHX	A	1994	7/7	0.93	0.17	123,137,148,152	7
80	OHX	A	2076	7/7	0.93	0.11	170,176,187,217	0
81	MG	AR	3648	1/1	0.93	0.32	59,59,59,59	0
80	OHX	sR	2168	7/7	0.93	0.11	127,135,148,208	0
80	OHX	AR	4138	7/7	0.93	0.09	131,133,161,222	0
81	MG	A	1920	1/1	0.93	0.18	68,68,68,68	0
80	OHX	A	1956	7/7	0.93	0.11	152,156,191,221	0
81	MG	1	3620	1/1	0.93	0.29	54,54,54,54	0
81	MG	1	3621	1/1	0.93	0.34	76,76,76,76	0
81	MG	1	3622	1/1	0.93	0.12	71,71,71,71	0
81	MG	AR	4082	1/1	0.93	0.11	62,62,62,62	0
81	MG	AR	4083	1/1	0.93	0.32	43,43,43,43	0
80	OHX	AR	3669	7/7	0.93	0.14	117,130,141,171	0
81	MG	1	3923	1/1	0.93	0.19	97,97,97,97	0
81	MG	A	2100	1/1	0.93	0.34	67,67,67,67	0
81	MG	CE	403	1/1	0.93	0.25	48,48,48,48	0
80	OHX	AR	3672	7/7	0.93	0.09	146,161,179,238	0
80	OHX	A	1926	7/7	0.93	0.11	133,156,165,203	0
81	MG	AR	3869	1/1	0.93	0.28	61,61,61,61	0
80	OHX	1	3939	7/7	0.93	0.08	182,196,224,254	0
81	MG	1	3943	1/1	0.93	0.21	64,64,64,64	0
81	MG	A	2114	1/1	0.93	0.15	64,64,64,64	0
81	MG	AR	4096	1/1	0.93	0.09	97,97,97,97	0
81	MG	9	201	1/1	0.93	0.16	67,67,67,67	0
80	OHX	sR	1980	7/7	0.93	0.12	169,174,187,224	0
81	MG	4	215	1/1	0.93	0.29	56,56,56,56	0
81	MG	1	3650	1/1	0.93	0.28	65,65,65,65	0
81	MG	s4	301	1/1	0.93	0.38	74,74,74,74	0
81	MG	AR	3678	1/1	0.93	0.40	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	1	3605	7/7	0.93	0.24	88,95,111,121	7
81	MG	v	302	1/1	0.93	0.10	75,75,75,75	0
81	MG	1	3956	1/1	0.93	0.19	66,66,66,66	0
80	OHX	AR	3981	7/7	0.93	0.14	111,118,134,189	0
80	OHX	AR	3984	7/7	0.93	0.11	114,124,142,175	0
81	MG	AR	3683	1/1	0.93	0.10	77,77,77,77	0
81	MG	4	219	1/1	0.93	0.12	58,58,58,58	0
81	MG	1	3974	1/1	0.93	0.20	69,69,69,69	0
81	MG	AR	4120	1/1	0.93	0.28	81,81,81,81	0
80	OHX	AT	201	7/7	0.93	0.10	155,164,197,212	0
80	OHX	1	3969	7/7	0.93	0.10	149,164,184,202	0
81	MG	A	1950	1/1	0.93	0.14	76,76,76,76	0
81	MG	1	3981	1/1	0.93	0.16	54,54,54,54	0
81	MG	1	3982	1/1	0.93	0.18	72,72,72,72	0
80	OHX	1	3639	7/7	0.93	0.11	141,154,162,204	0
81	MG	AR	4126	1/1	0.93	0.13	71,71,71,71	0
80	OHX	1	3640	7/7	0.93	0.09	176,184,204,244	0
81	MG	1	3679	1/1	0.93	0.32	74,74,74,74	0
81	MG	1	3988	1/1	0.93	0.25	61,61,61,61	0
80	OHX	AR	3452	7/7	0.93	0.12	119,131,142,199	0
80	OHX	AR	4170	7/7	0.93	0.12	121,152,169,213	0
81	MG	4	229	1/1	0.93	0.26	50,50,50,50	0
81	MG	1	3411	1/1	0.93	0.12	60,60,60,60	0
81	MG	4	231	1/1	0.93	0.17	86,86,86,86	0
80	OHX	A	2130	7/7	0.93	0.10	160,166,182,222	0
80	OHX	AR	3702	7/7	0.93	0.12	152,161,185,239	0
80	OHX	sR	2005	7/7	0.93	0.11	171,179,188,245	0
81	MG	sR	2057	1/1	0.93	0.18	85,85,85,85	0
81	MG	AR	4149	1/1	0.93	0.33	51,51,51,51	0
80	OHX	A	1906	7/7	0.93	0.11	131,135,145,210	0
81	MG	1	3705	1/1	0.93	0.26	60,60,60,60	0
81	MG	AR	3711	1/1	0.93	0.11	91,91,91,91	0
80	OHX	AR	4201	7/7	0.93	0.11	137,146,159,214	0
81	MG	AR	3714	1/1	0.93	0.18	58,58,58,58	0
80	OHX	sR	2027	7/7	0.93	0.10	184,190,202,212	0
80	OHX	AR	3577	7/7	0.93	0.10	123,132,150,203	0
80	OHX	AR	3578	7/7	0.93	0.11	120,143,151,223	0
80	OHX	DH	202	7/7	0.93	0.13	122,128,147,185	0
80	OHX	AR	3857	7/7	0.93	0.10	127,131,167,189	0
80	OHX	A	2007	7/7	0.93	0.08	161,182,192,238	0
81	MG	AR	3529	1/1	0.93	0.05	66,66,66,66	0
81	MG	sR	2083	1/1	0.93	0.11	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	AR	4175	1/1	0.93	0.16	69,69,69,69	0
81	MG	1	401	1/1	0.93	0.22	94,94,94,94	0
81	MG	1	3734	1/1	0.93	0.15	69,69,69,69	0
80	OHX	A	2047	7/7	0.93	0.08	192,193,212,249	0
81	MG	sR	2093	1/1	0.93	0.14	83,83,83,83	0
81	MG	1	3738	1/1	0.93	0.29	44,44,44,44	0
81	MG	1	3739	1/1	0.93	0.44	55,55,55,55	0
80	OHX	AR	3601	7/7	0.93	0.13	69,104,126,155	0
81	MG	1	3741	1/1	0.93	0.25	69,69,69,69	0
80	OHX	AR	3732	7/7	0.93	0.09	131,135,172,218	0
80	OHX	1	3732	7/7	0.93	0.14	156,162,177,226	0
80	OHX	AR	3486	7/7	0.93	0.10	153,162,171,228	0
81	MG	AR	3959	1/1	0.93	0.15	68,68,68,68	0
81	MG	AR	3741	1/1	0.93	0.29	55,55,55,55	0
80	OHX	AR	4048	7/7	0.93	0.08	160,177,199,246	0
80	OHX	A	2016	7/7	0.93	0.11	163,166,176,232	0
81	MG	x	204	1/1	0.93	0.30	68,68,68,68	0
81	MG	AR	3965	1/1	0.93	0.21	70,70,70,70	0
81	MG	1	3765	1/1	0.93	0.30	43,43,43,43	0
80	OHX	AR	3889	7/7	0.93	0.10	127,143,167,199	0
81	MG	1	3767	1/1	0.93	0.27	53,53,53,53	0
81	MG	AR	4193	1/1	0.93	0.23	73,73,73,73	0
81	MG	1	3770	1/1	0.93	0.20	61,61,61,61	0
81	MG	1	3771	1/1	0.93	0.14	67,67,67,67	0
80	OHX	1	3760	7/7	0.93	0.11	127,150,169,207	0
80	OHX	3	202	7/7	0.93	0.12	128,142,156,189	0
80	OHX	A	1924	7/7	0.93	0.12	174,176,196,234	0
81	MG	1	4101	1/1	0.93	0.37	72,72,72,72	0
81	MG	1	3775	1/1	0.93	0.19	72,72,72,72	0
81	MG	1	4103	1/1	0.93	0.44	61,61,61,61	0
81	MG	DP	101	1/1	0.93	0.12	62,62,62,62	0
81	MG	AR	3562	1/1	0.93	0.19	74,74,74,74	0
81	MG	AR	4209	1/1	0.93	0.32	51,51,51,51	0
81	MG	1	4108	1/1	0.93	0.31	43,43,43,43	0
80	OHX	AR	4077	7/7	0.93	0.08	152,175,198,246	0
81	MG	1	3780	1/1	0.93	0.17	57,57,57,57	0
80	OHX	AR	3761	7/7	0.93	0.12	125,128,143,216	0
80	OHX	1	3480	7/7	0.93	0.10	143,146,174,204	0
81	MG	1	4125	1/1	0.93	0.25	69,69,69,69	0
81	MG	CQ	202	1/1	0.93	0.25	73,73,73,73	0
81	MG	AR	3569	1/1	0.93	0.09	53,53,53,53	0
81	MG	CQ	203	1/1	0.93	0.19	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	AR	3994	1/1	0.93	0.28	61,61,61,61	0
81	MG	AR	3403	1/1	0.93	0.23	62,62,62,62	0
80	OHX	1	3790	7/7	0.93	0.10	176,182,205,237	0
80	OHX	1	3791	7/7	0.93	0.08	157,161,191,236	0
81	MG	1	3523	1/1	0.93	0.23	65,65,65,65	0
80	OHX	1	4150	7/7	0.93	0.09	136,150,180,212	0
81	MG	1	3526	1/1	0.93	0.27	48,48,48,48	0
81	MG	1	3527	1/1	0.93	0.27	64,64,64,64	0
81	MG	1	3810	1/1	0.93	0.24	58,58,58,58	0
80	OHX	A	2067	7/7	0.93	0.12	146,157,180,206	0
81	MG	AS	211	1/1	0.93	0.18	47,47,47,47	0
80	OHX	1	4171	7/7	0.93	0.12	123,134,153,188	0
81	MG	AR	3589	1/1	0.93	0.14	50,50,50,50	0
81	MG	1	3828	1/1	0.93	0.35	51,51,51,51	0
80	OHX	AR	3421	7/7	0.93	0.11	107,122,155,195	0
81	MG	sR	2171	1/1	0.93	0.17	69,69,69,69	0
81	MG	CR	204	1/1	0.93	0.33	71,71,71,71	0
81	MG	1	4163	1/1	0.93	0.18	58,58,58,58	0
81	MG	CR	205	1/1	0.93	0.08	68,68,68,68	0
80	OHX	1	3487	7/7	0.93	0.12	140,145,149,222	0
81	MG	AS	218	1/1	0.93	0.33	55,55,55,55	0
81	MG	1	3553	1/1	0.93	0.37	62,62,62,62	0
80	OHX	1	4176	7/7	0.93	0.13	99,118,130,175	0
81	MG	1	3555	1/1	0.93	0.23	58,58,58,58	0
81	MG	A	2048	1/1	0.93	0.18	83,83,83,83	0
80	OHX	1	3819	7/7	0.93	0.12	125,140,158,211	0
81	MG	AR	3804	1/1	0.93	0.29	57,57,57,57	0
81	MG	AR	3805	1/1	0.93	0.29	52,52,52,52	0
83	K	AR	3447	1/1	0.93	0.21	76,76,76,76	0
80	OHX	1	4179	7/7	0.93	0.12	108,114,124,169	0
81	MG	sR	1908	1/1	0.93	0.24	69,69,69,69	0
80	OHX	1	4180	7/7	0.93	0.09	156,162,185,239	0
80	OHX	AR	3759	7/7	0.94	0.10	156,158,169,197	0
80	OHX	A	2112	7/7	0.94	0.09	149,167,178,201	0
81	MG	AB	203	1/1	0.94	0.15	71,71,71,71	0
80	OHX	1	3604	7/7	0.94	0.13	103,113,131,145	0
80	OHX	sR	2015	7/7	0.94	0.08	202,206,209,237	0
81	MG	AR	4143	1/1	0.94	0.16	55,55,55,55	0
81	MG	AR	3930	1/1	0.94	0.31	47,47,47,47	0
80	OHX	1	3610	7/7	0.94	0.09	148,153,176,213	0
80	OHX	AT	202	7/7	0.94	0.10	117,125,151,182	0
80	OHX	AR	3517	7/7	0.94	0.10	177,194,212,283	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	3919	1/1	0.94	0.30	40,40,40,40	0
81	MG	AR	3936	1/1	0.94	0.35	62,62,62,62	0
80	OHX	AR	3636	7/7	0.94	0.12	79,101,108,183	0
80	OHX	1	3638	7/7	0.94	0.12	99,119,132,175	0
81	MG	sR	2046	1/1	0.94	0.21	60,60,60,60	0
80	OHX	AT	207	7/7	0.94	0.08	172,180,206,238	0
80	OHX	AS	227	7/7	0.94	0.12	113,120,125,158	0
81	MG	AR	4154	1/1	0.94	0.16	65,65,65,65	0
80	OHX	AS	229	7/7	0.94	0.11	127,148,155,190	0
80	OHX	A	1995	7/7	0.94	0.10	103,120,137,174	0
80	OHX	sR	2040	7/7	0.94	0.10	160,164,190,217	0
80	OHX	1	3669	7/7	0.94	0.11	133,155,168,215	0
80	OHX	A	2026	7/7	0.94	0.10	139,142,146,216	0
80	OHX	A	2055	7/7	0.94	0.12	122,143,165,180	0
80	OHX	sR	2062	7/7	0.94	0.13	68,117,130,148	0
81	MG	1	3947	1/1	0.94	0.28	48,48,48,48	0
81	MG	AR	3770	1/1	0.94	0.23	53,53,53,53	0
81	MG	AR	4176	1/1	0.94	0.15	61,61,61,61	0
81	MG	sR	2079	1/1	0.94	0.19	45,45,45,45	0
80	OHX	1	4000	7/7	0.94	0.08	179,187,199,227	0
81	MG	1	3952	1/1	0.94	0.16	59,59,59,59	0
81	MG	AR	3594	1/1	0.94	0.08	63,63,63,63	0
80	OHX	AR	3921	7/7	0.94	0.12	155,156,167,198	0
80	OHX	A	2056	7/7	0.94	0.11	154,159,170,192	0
81	MG	AR	3445	1/1	0.94	0.23	49,49,49,49	0
80	OHX	sR	1913	7/7	0.94	0.11	127,132,151,189	0
81	MG	1	3690	1/1	0.94	0.11	67,67,67,67	0
80	OHX	1	3701	7/7	0.94	0.07	187,193,207,228	0
80	OHX	sR	2075	7/7	0.94	0.10	138,147,165,200	0
80	OHX	AR	3793	7/7	0.94	0.13	79,91,117,136	0
80	OHX	A	2094	7/7	0.94	0.11	88,125,150,189	0
81	MG	A	1948	1/1	0.94	0.07	72,72,72,72	0
81	MG	AR	3619	1/1	0.94	0.27	57,57,57,57	0
80	OHX	1	4051	7/7	0.94	0.10	107,132,167,182	0
81	MG	AR	3790	1/1	0.94	0.23	62,62,62,62	0
80	OHX	sR	2087	7/7	0.94	0.12	143,156,175,225	0
81	MG	1	3983	1/1	0.94	0.17	63,63,63,63	0
81	MG	1	3465	1/1	0.94	0.30	53,53,53,53	0
80	OHX	1	3728	7/7	0.94	0.12	102,117,132,189	0
80	OHX	AR	3449	7/7	0.94	0.13	120,123,144,212	0
81	MG	AR	3997	1/1	0.94	0.16	50,50,50,50	0
81	MG	AR	3998	1/1	0.94	0.18	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
80	OHX	1	3428	7/7	0.94	0.10	164,174,189,214	0
81	MG	sR	2119	1/1	0.94	0.19	67,67,67,67	0
80	OHX	A	1907	7/7	0.94	0.11	149,160,175,208	0
80	OHX	AR	3671	7/7	0.94	0.12	90,105,113,203	0
80	OHX	1	3450	7/7	0.94	0.10	125,129,165,190	0
80	OHX	1	4062	1/7	0.94	0.13	218,218,218,218	0
81	MG	AR	4005	1/1	0.94	0.14	86,86,86,86	0
81	MG	1	4012	1/1	0.94	0.42	71,71,71,71	0
81	MG	1	4013	1/1	0.94	0.09	80,80,80,80	0
81	MG	AR	3808	1/1	0.94	0.27	58,58,58,58	0
80	OHX	AR	3547	7/7	0.94	0.12	157,159,167,227	0
81	MG	1	3742	1/1	0.94	0.10	79,79,79,79	0
81	MG	AS	204	1/1	0.94	0.22	57,57,57,57	0
80	OHX	AR	3823	7/7	0.94	0.11	84,99,126,196	0
80	OHX	1	4090	7/7	0.94	0.11	150,160,178,221	0
81	MG	1	3501	1/1	0.94	0.16	70,70,70,70	0
81	MG	AF	201	1/1	0.94	0.10	60,60,60,60	0
80	OHX	A	1985	7/7	0.94	0.12	127,134,151,181	0
81	MG	AR	3647	1/1	0.94	0.09	71,71,71,71	0
81	MG	AF	203	1/1	0.94	0.16	70,70,70,70	0
81	MG	1	4039	1/1	0.94	0.19	46,46,46,46	0
81	MG	AR	3818	1/1	0.94	0.26	43,43,43,43	0
81	MG	1	3764	1/1	0.94	0.21	58,58,58,58	0
81	MG	AF	204	1/1	0.94	0.20	79,79,79,79	0
80	OHX	AR	3694	7/7	0.94	0.15	96,108,131,157	0
81	MG	AR	3653	1/1	0.94	0.11	88,88,88,88	0
80	OHX	AR	3979	7/7	0.94	0.13	121,135,145,174	0
81	MG	1	3769	1/1	0.94	0.21	47,47,47,47	0
81	MG	AR	3655	1/1	0.94	0.12	65,65,65,65	0
81	MG	AR	3835	1/1	0.94	0.18	69,69,69,69	0
80	OHX	A	1955	7/7	0.94	0.14	112,126,144,152	0
80	OHX	1	3482	7/7	0.94	0.13	116,123,156,195	0
80	OHX	AR	3572	7/7	0.94	0.13	91,99,128,162	0
81	MG	CP	301	1/1	0.94	0.10	76,76,76,76	0
81	MG	1	4066	1/1	0.94	0.17	56,56,56,56	0
80	OHX	sR	1947	7/7	0.94	0.09	131,154,166,205	0
81	MG	1	3531	1/1	0.94	0.26	62,62,62,62	0
80	OHX	AR	3983	7/7	0.94	0.11	106,120,136,190	0
81	MG	A	1998	1/1	0.94	0.15	60,60,60,60	0
81	MG	1	4072	1/1	0.94	0.15	75,75,75,75	0
81	MG	AR	3843	1/1	0.94	0.15	47,47,47,47	0
81	MG	AR	4054	1/1	0.94	0.11	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	3794	1/1	0.94	0.21	52,52,52,52	0
81	MG	sR	1917	1/1	0.94	0.13	62,62,62,62	0
81	MG	AR	3675	1/1	0.94	0.23	39,39,39,39	0
81	MG	1	4079	1/1	0.94	0.08	47,47,47,47	0
81	MG	1	3547	1/1	0.94	0.07	87,87,87,87	0
80	OHX	A	2142	7/7	0.94	0.10	138,150,175,193	0
80	OHX	AR	3456	7/7	0.94	0.08	190,195,211,232	0
81	MG	sR	1928	1/1	0.94	0.17	67,67,67,67	0
81	MG	AR	4058	1/1	0.94	0.23	56,56,56,56	0
80	OHX	1	4148	7/7	0.94	0.10	132,137,161,196	0
80	OHX	sR	1958	7/7	0.94	0.11	122,136,154,203	0
80	OHX	A	2143[A]	7/7	0.94	0.17	119,137,140,142	7
81	MG	AR	4062	1/1	0.94	0.12	73,73,73,73	0
80	OHX	1	3816	7/7	0.94	0.12	95,116,135,160	0
80	OHX	AR	3484	7/7	0.94	0.11	164,167,180,198	0
81	MG	sR	1943	1/1	0.94	0.26	73,73,73,73	0
81	MG	AR	3867	1/1	0.94	0.28	49,49,49,49	0
80	OHX	sR	1967	7/7	0.94	0.15	94,103,133,150	0
80	OHX	A	2143[B]	7/7	0.94	0.17	131,138,141,151	7
80	OHX	1	3822	7/7	0.94	0.10	131,140,146,225	0
81	MG	AT	217	1/1	0.94	0.10	61,61,61,61	0
81	MG	AR	3524	1/1	0.94	0.30	63,63,63,63	0
80	OHX	AR	4012	7/7	0.94	0.09	113,130,148,184	0
81	MG	x	203	1/1	0.94	0.36	101,101,101,101	0
80	OHX	A	1936	7/7	0.94	0.11	153,169,179,237	0
81	MG	sR	1963	1/1	0.94	0.08	75,75,75,75	0
81	MG	AT	224	1/1	0.94	0.35	61,61,61,61	0
80	OHX	A	2153	7/7	0.94	0.09	157,162,178,201	0
81	MG	DC	201	1/1	0.94	0.14	70,70,70,70	0
81	MG	1	3590	1/1	0.94	0.10	66,66,66,66	0
81	MG	AR	4087	1/1	0.94	0.19	49,49,49,49	0
80	OHX	AR	4172	7/7	0.94	0.10	141,145,164,201	0
81	MG	AR	4090	1/1	0.94	0.18	61,61,61,61	0
80	OHX	AR	3605	7/7	0.94	0.12	88,97,123,169	0
81	MG	1	3595	1/1	0.94	0.09	64,64,64,64	0
81	MG	1	3596	1/1	0.94	0.17	73,73,73,73	0
81	MG	sR	1974	1/1	0.94	0.10	92,92,92,92	0
80	OHX	AR	3510	7/7	0.94	0.11	72,108,131,162	0
80	OHX	AR	4200	7/7	0.94	0.10	139,157,172,209	0
81	MG	1	4147	1/1	0.94	0.08	98,98,98,98	0
80	OHX	sR	2180	7/7	0.94	0.10	155,172,193,230	0
80	OHX	1	3879	7/7	0.94	0.09	112,118,142,184	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	AR	3888	1/1	0.94	0.11	93,93,93,93	0
81	MG	1	4155	1/1	0.94	0.21	61,61,61,61	0
81	MG	d3	203	1/1	0.94	0.32	63,63,63,63	0
81	MG	AR	3712	1/1	0.94	0.09	66,66,66,66	0
81	MG	AR	3538	1/1	0.94	0.18	64,64,64,64	0
81	MG	1	4161	1/1	0.94	0.20	72,72,72,72	0
80	OHX	A	1925	7/7	0.94	0.14	82,111,145,146	0
81	MG	AR	4116	1/1	0.94	0.20	63,63,63,63	0
81	MG	1	3868	1/1	0.94	0.10	39,39,39,39	0
81	MG	CF	402	1/1	0.94	0.17	77,77,77,77	0
81	MG	AR	4117	1/1	0.94	0.26	65,65,65,65	0
81	MG	1	3884	1/1	0.94	0.32	68,68,68,68	0
81	MG	AR	3553	1/1	0.94	0.30	52,52,52,52	0
81	MG	AR	3554	1/1	0.94	0.33	63,63,63,63	0
80	OHX	sR	2189	7/7	0.94	0.10	98,135,145,180	0
81	MG	1	3626	1/1	0.94	0.07	77,77,77,77	0
80	OHX	sR	2190	7/7	0.94	0.11	127,137,166,203	0
82	ZN	AP	501	1/1	0.94	0.07	114,114,114,114	0
80	OHX	1	3574	7/7	0.94	0.20	97,110,128,141	7
81	MG	1	3893	1/1	0.94	0.25	67,67,67,67	0
81	MG	AR	3404	1/1	0.94	0.10	57,57,57,57	0
80	OHX	A	1953	7/7	0.94	0.11	154,164,173,207	0
81	MG	1	3896	1/1	0.94	0.28	90,90,90,90	0
85	SPD	1	3478	10/10	0.94	0.14	44,49,53,54	0
81	MG	CF	401	1/1	0.95	0.15	64,64,64,64	0
80	OHX	AR	3576	7/7	0.95	0.11	124,127,144,210	0
80	OHX	1	3784	7/7	0.95	0.11	100,111,132,157	0
81	MG	CG	301	1/1	0.95	0.27	46,46,46,46	0
81	MG	CG	304	1/1	0.95	0.16	63,63,63,63	0
80	OHX	AR	3455	7/7	0.95	0.09	141,148,158,216	0
80	OHX	1	3786	7/7	0.95	0.12	103,123,135,174	0
80	OHX	1	3455	7/7	0.95	0.12	111,117,142,196	0
80	OHX	A	2086	7/7	0.95	0.11	129,131,136,159	0
80	OHX	1	3458	7/7	0.95	0.08	155,164,172,220	0
81	MG	sR	1996	1/1	0.95	0.18	63,63,63,63	0
81	MG	AR	4094	1/1	0.95	0.19	67,67,67,67	0
81	MG	A	2108	1/1	0.95	0.27	68,68,68,68	0
80	OHX	AR	3885	7/7	0.95	0.11	99,108,123,151	0
80	OHX	sR	1902	7/7	0.95	0.11	144,156,161,182	0
80	OHX	A	1916	7/7	0.95	0.11	109,121,160,170	0
81	MG	AR	3878	1/1	0.95	0.22	58,58,58,58	0
80	OHX	A	2003	7/7	0.95	0.09	127,142,160,202	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	A	2005	7/7	0.95	0.09	136,148,165,187	0
80	OHX	sR	1911	7/7	0.95	0.20	113,116,125,149	7
80	OHX	A	1983	7/7	0.95	0.10	158,167,170,231	0
80	OHX	AR	4076	7/7	0.95	0.11	91,96,127,164	0
80	OHX	A	2052	7/7	0.95	0.12	100,114,130,149	0
80	OHX	1	3844	7/7	0.95	0.13	111,129,153,164	0
80	OHX	AR	3508	7/7	0.95	0.12	92,116,124,175	0
81	MG	sR	2031	1/1	0.95	0.22	65,65,65,65	0
81	MG	AR	3899	1/1	0.95	0.44	59,59,59,59	0
80	OHX	4	203	7/7	0.95	0.09	124,132,160,193	0
80	OHX	sR	1924	7/7	0.95	0.11	141,146,160,213	0
80	OHX	1	3513	7/7	0.95	0.11	75,101,127,143	0
80	OHX	sR	2135	7/7	0.95	0.09	133,135,160,195	0
80	OHX	w	201	7/7	0.95	0.12	104,115,138,165	0
81	MG	1	3957	1/1	0.95	0.18	61,61,61,61	0
81	MG	AR	3906	1/1	0.95	0.22	72,72,72,72	0
81	MG	1	3417	1/1	0.95	0.33	63,63,63,63	0
80	OHX	AR	3512	7/7	0.95	0.10	98,127,134,173	0
81	MG	AR	3908	1/1	0.95	0.26	68,68,68,68	0
81	MG	sR	2047	1/1	0.95	0.14	77,77,77,77	0
81	MG	sR	2048	1/1	0.95	0.06	91,91,91,91	0
81	MG	AR	3709	1/1	0.95	0.17	48,48,48,48	0
81	MG	AR	3710	1/1	0.95	0.25	45,45,45,45	0
81	MG	AR	4145	1/1	0.95	0.26	46,46,46,46	0
81	MG	1	3706	1/1	0.95	0.13	45,45,45,45	0
81	MG	1	3707	1/1	0.95	0.30	52,52,52,52	0
80	OHX	1	3878	7/7	0.95	0.10	102,133,154,178	0
80	OHX	sR	2145	7/7	0.95	0.10	113,122,139,180	0
81	MG	1	3438	1/1	0.95	0.20	77,77,77,77	0
81	MG	AR	3916	1/1	0.95	0.32	65,65,65,65	0
80	OHX	AR	4099	7/7	0.95	0.17	75,99,113,118	0
80	OHX	AR	4103	7/7	0.95	0.10	103,109,149,159	0
81	MG	AR	3928	1/1	0.95	0.33	63,63,63,63	0
80	OHX	AR	3630	7/7	0.95	0.12	85,114,132,156	0
80	OHX	AR	3634	7/7	0.95	0.11	101,114,139,168	0
81	MG	AR	3931	1/1	0.95	0.23	43,43,43,43	0
80	OHX	A	1943	7/7	0.95	0.09	123,131,151,208	0
80	OHX	AR	3413	7/7	0.95	0.15	39,85,106,131	0
81	MG	1	4009	1/1	0.95	0.09	55,55,55,55	0
81	MG	AR	3934	1/1	0.95	0.14	84,84,84,84	0
81	MG	1	4011	1/1	0.95	0.32	61,61,61,61	0
80	OHX	sR	1946	7/7	0.95	0.10	100,106,127,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	3735	1/1	0.95	0.13	47,47,47,47	0
80	OHX	AR	3417	7/7	0.95	0.12	96,114,131,164	0
81	MG	AR	3937	1/1	0.95	0.15	70,70,70,70	0
80	OHX	AR	3952	7/7	0.95	0.10	100,111,121,201	0
80	OHX	4	230	7/7	0.95	0.09	117,120,152,169	0
81	MG	AR	3940	1/1	0.95	0.45	74,74,74,74	0
80	OHX	1	3575	7/7	0.95	0.11	106,111,128,183	0
81	MG	AR	3550	1/1	0.95	0.24	70,70,70,70	0
81	MG	1	3472	1/1	0.95	0.11	73,73,73,73	0
80	OHX	AR	3419	7/7	0.95	0.10	117,126,138,176	0
80	OHX	1	3580	7/7	0.95	0.10	116,130,136,179	0
80	OHX	AR	4135	7/7	0.95	0.12	115,123,139,193	0
80	OHX	AR	4136	7/7	0.95	0.12	94,108,125,166	0
81	MG	1	3486	1/1	0.95	0.07	78,78,78,78	0
80	OHX	1	3961	7/7	0.95	0.11	121,140,154,183	0
80	OHX	A	1965	7/7	0.95	0.12	132,146,151,177	0
80	OHX	A	2025	7/7	0.95	0.11	115,129,142,184	0
81	MG	1	3495	1/1	0.95	0.34	57,57,57,57	0
80	OHX	1	3966	7/7	0.95	0.11	95,108,138,148	0
81	MG	1	3497	1/1	0.95	0.34	55,55,55,55	0
80	OHX	1	3608	7/7	0.95	0.12	117,122,137,191	0
80	OHX	1	3609	7/7	0.95	0.10	112,134,150,179	0
80	OHX	AR	3665	7/7	0.95	0.11	97,112,130,159	0
80	OHX	1	3611	7/7	0.95	0.09	203,208,224,231	0
80	OHX	A	2066	7/7	0.95	0.10	196,204,217,231	0
81	MG	k	401	1/1	0.95	0.17	66,66,66,66	0
80	OHX	1	3991	7/7	0.95	0.11	132,137,151,170	0
80	OHX	AR	3667[A]	7/7	0.95	0.21	81,94,103,118	7
80	OHX	1	3998	7/7	0.95	0.09	162,176,186,200	0
80	OHX	AR	4161	7/7	0.95	0.12	72,99,124,129	0
81	MG	l	402	1/1	0.95	0.11	55,55,55,55	0
81	MG	1	3516	1/1	0.95	0.07	98,98,98,98	0
81	MG	AR	3978	1/1	0.95	0.21	71,71,71,71	0
80	OHX	AR	3667[B]	7/7	0.95	0.21	95,101,111,173	7
80	OHX	DL	102	7/7	0.95	0.10	106,115,136,171	0
81	MG	AR	3775	1/1	0.95	0.17	48,48,48,48	0
81	MG	AR	3993	1/1	0.95	0.14	52,52,52,52	0
81	MG	sR	2150	1/1	0.95	0.24	53,53,53,53	0
80	OHX	AR	4167	7/7	0.95	0.11	67,98,146,173	0
80	OHX	1	4028	7/7	0.95	0.09	170,184,191,217	0
80	OHX	AR	3670	7/7	0.95	0.10	95,117,134,183	0
80	OHX	AT	204[A]	7/7	0.95	0.16	105,108,134,149	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	AT	204[B]	7/7	0.95	0.16	105,111,120,152	7
80	OHX	1	3666	7/7	0.95	0.13	93,114,131,159	0
81	MG	1	3803	1/1	0.95	0.30	79,79,79,79	0
80	OHX	1	3668	7/7	0.95	0.13	90,115,123,153	0
81	MG	AS	210	1/1	0.95	0.23	68,68,68,68	0
80	OHX	sR	1992	7/7	0.95	0.12	115,129,150,192	0
81	MG	AR	3420	1/1	0.95	0.07	122,122,122,122	0
80	OHX	4	205	7/7	0.95	0.07	166,179,192,227	0
81	MG	AR	3794	1/1	0.95	0.14	96,96,96,96	0
81	MG	1	4104	1/1	0.95	0.10	59,59,59,59	0
80	OHX	1	4056	7/7	0.95	0.12	100,108,121,160	0
81	MG	AR	3600	1/1	0.95	0.25	41,41,41,41	0
81	MG	A	2031	1/1	0.95	0.13	80,80,80,80	0
80	OHX	k	404	7/7	0.95	0.10	118,130,170,181	0
81	MG	AR	3612	1/1	0.95	0.26	60,60,60,60	0
80	OHX	sR	2003	7/7	0.95	0.11	112,133,151,171	0
80	OHX	A	2035	7/7	0.95	0.09	123,133,150,188	0
81	MG	AR	3615	1/1	0.95	0.14	48,48,48,48	0
80	OHX	AT	230	7/7	0.95	0.11	117,123,146,176	0
80	OHX	1	3696	7/7	0.95	0.13	85,100,124,140	0
81	MG	AR	4026	1/1	0.95	0.06	57,57,57,57	0
81	MG	AR	3618	1/1	0.95	0.08	61,61,61,61	0
80	OHX	A	1915	7/7	0.95	0.13	130,150,162,162	0
81	MG	AR	3435	1/1	0.95	0.41	73,73,73,73	0
81	MG	A	2044	1/1	0.95	0.08	120,120,120,120	0
81	MG	sR	1919	1/1	0.95	0.11	90,90,90,90	0
81	MG	1	4133	1/1	0.95	0.15	52,52,52,52	0
80	OHX	1	3700	7/7	0.95	0.09	123,131,142,189	0
80	OHX	sR	2014	7/7	0.95	0.11	128,143,149,171	0
80	OHX	1	4086	7/7	0.95	0.11	93,106,141,160	0
80	OHX	CE	401	7/7	0.95	0.11	103,110,127,169	0
81	MG	1	3856	1/1	0.95	0.15	64,64,64,64	0
81	MG	AR	3626	1/1	0.95	0.07	115,115,115,115	0
81	MG	sR	1931	1/1	0.95	0.32	62,62,62,62	0
80	OHX	AR	4196	7/7	0.95	0.12	121,125,137,190	0
80	OHX	1	4111	7/7	0.95	0.09	98,127,155,193	0
81	MG	AR	4044	1/1	0.95	0.07	100,100,100,100	0
80	OHX	A	2037	7/7	0.95	0.15	81,119,135,141	0
80	OHX	AR	4198	7/7	0.95	0.09	100,113,141,183	0
81	MG	AR	3458	1/1	0.95	0.20	54,54,54,54	0
80	OHX	1	4116	7/7	0.95	0.10	111,120,144,193	0
80	OHX	AR	4014	7/7	0.95	0.09	156,171,186,194	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	AT	231	1/1	0.95	0.08	109,109,109,109	0
80	OHX	AR	3853	7/7	0.95	0.10	105,126,143,189	0
80	OHX	AR	3698	7/7	0.95	0.10	157,164,174,193	0
80	OHX	A	2139	7/7	0.95	0.13	100,116,133,148	0
81	MG	AR	3649	1/1	0.95	0.08	63,63,63,63	0
80	OHX	AR	3701	7/7	0.95	0.08	148,161,180,217	0
80	OHX	1	3423	7/7	0.95	0.12	90,106,135,159	0
80	OHX	sR	2051	7/7	0.95	0.11	111,123,134,177	0
80	OHX	AR	3574	7/7	0.95	0.11	88,109,132,170	0
80	OHX	1	4149	7/7	0.95	0.11	107,120,141,165	0
80	OHX	AR	4043	7/7	0.95	0.10	92,107,110,169	0
80	OHX	AS	221	7/7	0.95	0.12	114,117,134,137	0
81	MG	AR	3854	1/1	0.95	0.13	63,63,63,63	0
83	K	AR	3416	1/1	0.95	0.23	68,68,68,68	0
80	OHX	AS	223	7/7	0.95	0.12	76,104,124,162	0
83	K	AR	4195	1/1	0.95	0.10	82,82,82,82	0
83	K	1	3448	1/1	0.95	0.23	76,76,76,76	0
81	MG	AR	3865	1/1	0.95	0.13	75,75,75,75	0
80	OHX	AS	225	7/7	0.95	0.10	107,131,133,203	0
81	MG	sR	1982	1/1	0.95	0.23	68,68,68,68	0
81	MG	1	3627	1/1	0.95	0.08	71,71,71,71	0
81	MG	sR	2010	1/1	0.96	0.15	80,80,80,80	0
81	MG	AT	229	1/1	0.96	0.12	121,121,121,121	0
81	MG	AR	3992	1/1	0.96	0.28	43,43,43,43	0
81	MG	1	3976	1/1	0.96	0.45	60,60,60,60	0
80	OHX	AR	3758	7/7	0.96	0.10	82,106,127,153	0
81	MG	sR	2019	1/1	0.96	0.25	60,60,60,60	0
80	OHX	4	232	7/7	0.96	0.08	135,145,170,204	0
80	OHX	CP	303	7/7	0.96	0.09	132,143,161,209	0
81	MG	sR	2022	1/1	0.96	0.11	87,87,87,87	0
80	OHX	sR	1990	7/7	0.96	0.10	99,122,138,155	0
81	MG	AR	3497	1/1	0.96	0.10	56,56,56,56	0
80	OHX	4	207	7/7	0.96	0.08	145,159,177,218	0
80	OHX	AR	4004	7/7	0.96	0.22	65,84,108,119	0
81	MG	4	220	1/1	0.96	0.11	74,74,74,74	0
80	OHX	AR	4008	7/7	0.96	0.11	92,114,119,141	0
80	OHX	1	3483	7/7	0.96	0.14	97,112,127,155	0
80	OHX	sR	2002	7/7	0.96	0.10	97,101,116,169	0
80	OHX	AR	3763	7/7	0.96	0.08	124,128,159,189	0
80	OHX	1	3999	7/7	0.96	0.07	135,146,169,203	0
80	OHX	sR	2167	7/7	0.96	0.12	69,114,119,149	0
81	MG	1	4007	1/1	0.96	0.15	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	s1	302	1/1	0.96	0.10	90,90,90,90	0
80	OHX	AR	3603	6/7	0.96	0.10	96,98,120,185	0
80	OHX	sR	1912	7/7	0.96	0.12	59,107,123,157	0
80	OHX	1	4023	7/7	0.96	0.15	72,84,100,114	0
80	OHX	AR	3444	7/7	0.96	0.12	52,75,103,126	0
80	OHX	1	4026	7/7	0.96	0.10	109,128,151,174	0
81	MG	sR	2056	1/1	0.96	0.13	85,85,85,85	0
80	OHX	A	1975	7/7	0.96	0.09	126,149,155,179	0
81	MG	1	4016	1/1	0.96	0.09	83,83,83,83	0
80	OHX	1	3754	7/7	0.96	0.11	94,108,123,138	0
80	OHX	1	3511	7/7	0.96	0.12	80,94,109,127	0
80	OHX	4	228	7/7	0.96	0.09	93,100,130,149	0
80	OHX	AR	3789	7/7	0.96	0.10	101,108,144,162	0
81	MG	s8	302	1/1	0.96	0.31	65,65,65,65	0
80	OHX	AR	3692	7/7	0.96	0.12	102,120,131,137	0
81	MG	1	3804	1/1	0.96	0.07	70,70,70,70	0
81	MG	k	402	1/1	0.96	0.10	77,77,77,77	0
81	MG	sR	2070	1/1	0.96	0.11	100,100,100,100	0
80	OHX	sR	1923	7/7	0.96	0.10	101,113,127,171	0
81	MG	sR	2072	1/1	0.96	0.13	59,59,59,59	0
80	OHX	1	4054	7/7	0.96	0.13	72,110,116,138	0
80	OHX	A	1977	7/7	0.96	0.09	130,139,157,216	0
81	MG	AS	201	1/1	0.96	0.23	53,53,53,53	0
81	MG	1	3825	1/1	0.96	0.15	51,51,51,51	0
80	OHX	sR	2037	7/7	0.96	0.22	65,85,104,123	0
80	OHX	AR	3917	7/7	0.96	0.10	92,97,117,145	0
80	OHX	AR	3696	7/7	0.96	0.10	106,113,120,184	0
81	MG	sR	2084	1/1	0.96	0.07	90,90,90,90	0
80	OHX	A	2152	7/7	0.96	0.10	121,131,137,189	0
81	MG	1	4057	1/1	0.96	0.06	99,99,99,99	0
80	OHX	1	3788	7/7	0.96	0.08	114,118,156,186	0
81	MG	AR	4051	1/1	0.96	0.08	53,53,53,53	0
80	OHX	sR	2052	7/7	0.96	0.08	121,138,149,195	0
80	OHX	1	3546	7/7	0.96	0.11	101,127,144,161	0
80	OHX	T	201	7/7	0.96	0.12	113,126,148,149	0
81	MG	sR	2102	1/1	0.96	0.17	50,50,50,50	0
81	MG	1	4069	1/1	0.96	0.23	49,49,49,49	0
81	MG	1	3414	1/1	0.96	0.09	68,68,68,68	0
80	OHX	1	4083	7/7	0.96	0.10	105,114,119,181	0
80	OHX	1	4084	7/7	0.96	0.10	114,124,150,152	0
80	OHX	sR	1934	7/7	0.96	0.12	116,129,146,148	0
80	OHX	sR	1935	7/7	0.96	0.09	109,115,130,172	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	1	4089	7/7	0.96	0.09	124,132,153,180	0
81	MG	1	4076	1/1	0.96	0.23	79,79,79,79	0
80	OHX	r	304	7/7	0.96	0.10	92,104,129,149	0
80	OHX	AT	206	7/7	0.96	0.07	163,175,184,209	0
80	OHX	1	3818	7/7	0.96	0.10	129,146,160,198	0
80	OHX	1	3572	7/7	0.96	0.10	90,104,129,157	0
81	MG	AR	3901	1/1	0.96	0.20	47,47,47,47	0
80	OHX	AR	3632	7/7	0.96	0.14	80,116,138,143	0
81	MG	sR	2120	1/1	0.96	0.07	92,92,92,92	0
81	MG	AR	4067	1/1	0.96	0.12	97,97,97,97	0
80	OHX	AR	4192	7/7	0.96	0.14	88,97,109,121	0
80	OHX	AR	3821	7/7	0.96	0.10	90,90,105,138	0
80	OHX	1	3841	7/7	0.96	0.12	99,106,127,173	0
81	MG	A	2034	1/1	0.96	0.05	102,102,102,102	0
80	OHX	C	301	7/7	0.96	0.12	107,126,136,139	0
81	MG	sR	2132	1/1	0.96	0.11	129,129,129,129	0
81	MG	AR	3585	1/1	0.96	0.14	50,50,50,50	0
80	OHX	AT	228	7/7	0.96	0.11	91,107,141,169	0
81	MG	AR	3745	1/1	0.96	0.21	60,60,60,60	0
81	MG	1	3667	1/1	0.96	0.08	85,85,85,85	0
80	OHX	1	4141	7/7	0.96	0.11	115,123,139,169	0
81	MG	1	3886	1/1	0.96	0.21	46,46,46,46	0
80	OHX	sR	2086	7/7	0.96	0.11	122,129,151,158	0
80	OHX	1	3846	7/7	0.96	0.12	99,104,121,152	0
81	MG	AR	3749	1/1	0.96	0.19	66,66,66,66	0
80	OHX	1	3603	7/7	0.96	0.09	147,152,163,195	0
81	MG	1	3891	1/1	0.96	0.10	61,61,61,61	0
81	MG	AR	4093	1/1	0.96	0.12	75,75,75,75	0
80	OHX	AR	3950	7/7	0.96	0.08	168,177,188,199	0
80	OHX	A	2015	7/7	0.96	0.07	148,166,185,218	0
81	MG	1	3470	1/1	0.96	0.26	60,60,60,60	0
80	OHX	AR	3481	7/7	0.96	0.11	125,130,149,173	0
80	OHX	1	3871	7/7	0.96	0.11	79,108,126,141	0
81	MG	CR	206	1/1	0.96	0.08	64,64,64,64	0
80	OHX	sR	2098	7/7	0.96	0.09	116,124,148,170	0
81	MG	AR	4106	1/1	0.96	0.06	49,49,49,49	0
80	OHX	1	3874	7/7	0.96	0.13	99,105,116,147	0
80	OHX	A	1963	7/7	0.96	0.08	145,174,179,188	0
81	MG	1	3689	1/1	0.96	0.19	55,55,55,55	0
81	MG	1	3491	1/1	0.96	0.14	47,47,47,47	0
80	OHX	1	3876	7/7	0.96	0.11	109,116,128,155	0
80	OHX	sR	1957	7/7	0.96	0.08	154,157,166,196	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	A	2121	7/7	0.96	0.17	56,89,118,125	0
80	OHX	sR	2109	7/7	0.96	0.13	90,115,126,133	0
80	OHX	sR	2110	7/7	0.96	0.13	103,110,120,143	0
81	MG	A	2071	1/1	0.96	0.12	76,76,76,76	0
80	OHX	1	3636	7/7	0.96	0.12	93,109,125,136	0
81	MG	1	4156	1/1	0.96	0.32	41,41,41,41	0
80	OHX	A	2085	7/7	0.96	0.08	134,139,151,191	0
81	MG	AR	4123	1/1	0.96	0.09	71,71,71,71	0
80	OHX	1	3420	7/7	0.96	0.11	115,127,150,186	0
80	OHX	1	3906	7/7	0.96	0.10	97,110,131,151	0
81	MG	3	211	1/1	0.96	0.30	58,58,58,58	0
80	OHX	1	3908	7/7	0.96	0.10	141,149,159,183	0
81	MG	1	3930	1/1	0.96	0.08	81,81,81,81	0
80	OHX	A	1903	7/7	0.96	0.10	129,132,148,180	0
80	OHX	1	3641	7/7	0.96	0.10	97,104,114,175	0
80	OHX	A	1923	7/7	0.96	0.10	89,118,130,171	0
80	OHX	sR	2122	7/7	0.96	0.10	102,106,116,158	0
80	OHX	1	3931	7/7	0.96	0.15	60,97,110,134	0
80	OHX	AR	3663	7/7	0.96	0.10	97,103,114,150	0
80	OHX	1	3934	7/7	0.96	0.15	81,95,113,128	0
80	OHX	A	2092	7/7	0.96	0.14	105,123,128,132	0
81	MG	A	2105	1/1	0.96	0.36	68,68,68,68	0
80	OHX	1	3936	7/7	0.96	0.10	132,139,143,175	0
80	OHX	1	3938	7/7	0.96	0.10	103,115,141,172	0
80	OHX	3	201	7/7	0.96	0.11	81,111,128,140	0
80	OHX	sR	2134	7/7	0.96	0.11	114,127,138,161	0
80	OHX	AR	3753	7/7	0.96	0.14	29,67,91,113	0
84	ZWB	AR	3826	26/26	0.96	0.09	53,61,67,86	0
84	ZWB	1	3578	26/26	0.96	0.11	55,63,70,79	0
80	OHX	1	3451	7/7	0.96	0.11	62,80,119,122	0
80	OHX	sR	1978	7/7	0.96	0.13	85,101,119,155	0
80	OHX	1	3962	7/7	0.96	0.12	70,90,110,123	0
80	OHX	AS	228	7/7	0.96	0.11	106,127,137,164	0
81	MG	1	3978	1/1	0.97	0.23	60,60,60,60	0
80	OHX	AR	3479	7/7	0.97	0.08	127,134,144,164	0
80	OHX	A	2062	7/7	0.97	0.18	64,93,103,123	0
81	MG	sR	2012	1/1	0.97	0.11	48,48,48,48	0
81	MG	AR	3951	1/1	0.97	0.04	89,89,89,89	0
81	MG	AR	3762	1/1	0.97	0.06	113,113,113,113	0
80	OHX	1	3968	7/7	0.97	0.07	134,136,164,174	0
80	OHX	1	3421	7/7	0.97	0.14	62,84,89,108	0
80	OHX	AR	3851	7/7	0.97	0.10	77,102,124,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	1	3694	7/7	0.97	0.10	109,116,126,145	0
81	MG	AR	3963	1/1	0.97	0.24	47,47,47,47	0
80	OHX	sR	2097	7/7	0.97	0.16	73,88,100,123	0
81	MG	1	3997	1/1	0.97	0.05	100,100,100,100	0
80	OHX	AK	104	7/7	0.97	0.08	93,113,133,167	0
80	OHX	1	3698	7/7	0.97	0.09	82,98,108,151	0
80	OHX	1	3992	7/7	0.97	0.13	44,86,99,111	0
80	OHX	1	3993	7/7	0.97	0.08	87,101,149,162	0
81	MG	j	301	1/1	0.97	0.05	44,44,44,44	0
80	OHX	1	3994	7/7	0.97	0.11	103,120,135,142	0
80	OHX	1	3425	7/7	0.97	0.08	118,132,140,156	0
81	MG	1	3787	1/1	0.97	0.06	63,63,63,63	0
81	MG	A	2004	1/1	0.97	0.06	91,91,91,91	0
81	MG	1	3576	1/1	0.97	0.10	102,102,102,102	0
80	OHX	1	3996	7/7	0.97	0.09	95,102,128,153	0
80	OHX	AR	3855	7/7	0.97	0.08	123,132,144,163	0
80	OHX	AR	3568	7/7	0.97	0.10	87,90,111,130	0
81	MG	AR	4180	1/1	0.97	0.26	59,59,59,59	0
80	OHX	AR	3661	7/7	0.97	0.12	87,88,109,124	0
80	OHX	sR	1945	7/7	0.97	0.10	98,98,120,167	0
80	OHX	AR	3570	7/7	0.97	0.16	77,94,111,131	0
80	OHX	1	4022	7/7	0.97	0.12	66,69,120,129	0
81	MG	1	4027	1/1	0.97	0.05	82,82,82,82	0
80	OHX	1	3724	7/7	0.97	0.10	72,105,125,139	0
80	OHX	AR	3757	7/7	0.97	0.10	86,104,130,143	0
81	MG	1	4035	1/1	0.97	0.06	58,58,58,58	0
80	OHX	1	3726	7/7	0.97	0.09	69,99,135,160	0
80	OHX	AR	4163	7/7	0.97	0.09	88,119,134,153	0
80	OHX	1	3453	7/7	0.97	0.12	106,117,124,133	0
80	OHX	AR	4006	7/7	0.97	0.12	87,100,116,122	0
80	OHX	sR	2121	7/7	0.97	0.15	82,83,93,113	0
81	MG	CI	302	1/1	0.97	0.09	63,63,63,63	0
80	OHX	AR	3483	7/7	0.97	0.08	139,144,152,184	0
81	MG	AR	3436	1/1	0.97	0.06	78,78,78,78	0
80	OHX	1	3751	7/7	0.97	0.13	76,86,97,120	0
80	OHX	sR	1956	7/7	0.97	0.10	91,106,116,132	0
80	OHX	A	2082	7/7	0.97	0.13	102,111,126,134	0
80	OHX	A	2151	7/7	0.97	0.11	85,98,125,129	0
81	MG	1	3617	1/1	0.97	0.18	43,43,43,43	0
80	OHX	1	3479	7/7	0.97	0.17	73,86,98,113	0
80	OHX	A	2065	7/7	0.97	0.08	127,130,140,186	0
80	OHX	A	2129	7/7	0.97	0.11	110,118,139,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	AR	3506	7/7	0.97	0.10	76,83,100,127	0
81	MG	AR	3633	1/1	0.97	0.23	71,71,71,71	0
80	OHX	3	221	7/7	0.97	0.09	98,106,136,161	0
80	OHX	sR	2144	7/7	0.97	0.10	103,105,125,127	0
80	OHX	A	1905	7/7	0.97	0.10	117,119,125,147	0
80	OHX	AR	4194	7/7	0.97	0.10	84,96,123,142	0
80	OHX	1	4082	7/7	0.97	0.12	90,102,125,126	0
80	OHX	AR	4039	7/7	0.97	0.09	95,108,131,146	0
80	OHX	AR	4041	7/7	0.97	0.10	87,108,125,164	0
80	OHX	1	3509	7/7	0.97	0.12	59,77,89,100	0
80	OHX	AR	4042	7/7	0.97	0.09	93,106,116,129	0
80	OHX	sR	2155	7/7	0.97	0.12	93,103,118,128	0
80	OHX	AR	3446	7/7	0.97	0.09	100,112,131,144	0
80	OHX	1	3811	7/7	0.97	0.12	78,97,116,126	0
80	OHX	AR	3785	7/7	0.97	0.13	82,93,103,122	0
80	OHX	1	3814	7/7	0.97	0.12	94,96,120,134	0
80	OHX	1	4114	7/7	0.97	0.10	94,99,128,128	0
80	OHX	AR	3448	7/7	0.97	0.09	128,148,162,182	0
80	OHX	1	3515	7/7	0.97	0.08	126,138,147,181	0
80	OHX	AR	3913	7/7	0.97	0.11	68,81,103,117	0
80	OHX	sR	2166	7/7	0.97	0.12	95,104,115,118	7
81	MG	AR	3668	1/1	0.97	0.12	84,84,84,84	0
81	MG	1	3442	1/1	0.97	0.29	57,57,57,57	0
80	OHX	sR	1991	7/7	0.97	0.07	162,164,173,196	0
81	MG	1	3869	1/1	0.97	0.16	44,44,44,44	0
80	OHX	AR	3915	7/7	0.97	0.10	72,87,119,136	0
80	OHX	AR	3791	7/7	0.97	0.12	76,84,113,122	0
80	OHX	1	3542	7/7	0.97	0.12	81,88,111,123	0
80	OHX	A	2072	7/7	0.97	0.12	79,81,115,117	0
81	MG	1	3456	1/1	0.97	0.04	81,81,81,81	0
81	MG	AR	3679	1/1	0.97	0.30	47,47,47,47	0
81	MG	r	301	1/1	0.97	0.12	59,59,59,59	0
80	OHX	1	3544	7/7	0.97	0.10	97,112,128,146	0
80	OHX	AR	4068	7/7	0.97	0.14	61,71,97,121	0
80	OHX	sR	2177	7/7	0.97	0.11	94,101,103,124	0
80	OHX	1	3848	7/7	0.97	0.09	113,121,140,159	0
80	OHX	sR	2178	7/7	0.97	0.09	124,136,151,185	0
80	OHX	1	4170	7/7	0.97	0.25	80,83,96,109	0
80	OHX	AR	4070	7/7	0.97	0.12	78,81,110,131	0
80	OHX	1	4172	7/7	0.97	0.12	85,93,119,120	0
80	OHX	AR	4072	7/7	0.97	0.08	97,112,133,161	0
80	OHX	AR	3515	7/7	0.97	0.09	104,119,137,165	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	3473	1/1	0.97	0.04	64,64,64,64	0
80	OHX	CX	201	7/7	0.97	0.10	90,92,115,137	0
80	OHX	1	3872	7/7	0.97	0.14	65,75,105,126	0
80	OHX	AK	103	7/7	0.97	0.10	90,101,127,136	0
80	OHX	1	3573	7/7	0.97	0.13	48,81,107,128	0
80	OHX	AR	3411	7/7	0.97	0.13	69,77,87,117	0
81	MG	AR	4088	1/1	0.97	0.05	65,65,65,65	0
80	OHX	A	1935	7/7	0.97	0.13	113,118,135,136	0
80	OHX	sR	2025	7/7	0.97	0.20	81,89,116,116	0
80	OHX	2	201	7/7	0.97	0.16	77,91,115,125	0
80	OHX	sR	1901	7/7	0.97	0.10	89,95,104,124	0
80	OHX	AR	3415	7/7	0.97	0.09	95,106,124,131	0
80	OHX	AR	3946	7/7	0.97	0.14	57,81,99,113	0
80	OHX	1	3902	7/7	0.97	0.15	81,91,102,118	0
80	OHX	AR	3948	7/7	0.97	0.09	91,96,126,150	0
80	OHX	1	3904	7/7	0.97	0.09	105,111,126,140	0
80	OHX	sR	2039	7/7	0.97	0.10	174,179,184,190	0
80	OHX	1	3606	7/7	0.97	0.10	124,125,135,152	0
81	MG	1	4158	1/1	0.97	0.35	47,47,47,47	0
80	OHX	AR	3819	7/7	0.97	0.12	86,91,105,127	0
80	OHX	AR	4101	7/7	0.97	0.10	85,89,102,121	0
81	MG	1	3937	1/1	0.97	0.12	91,91,91,91	0
80	OHX	sR	2050	7/7	0.97	0.10	100,111,143,156	0
80	OHX	AR	3541	7/7	0.97	0.10	92,111,137,163	0
80	OHX	A	2119	7/7	0.97	0.13	96,119,128,138	0
81	MG	1	3727	1/1	0.97	0.08	85,85,85,85	0
81	MG	AR	3551	1/1	0.97	0.36	53,53,53,53	0
81	MG	AR	3736	1/1	0.97	0.04	46,46,46,46	0
80	OHX	AR	4105	7/7	0.97	0.08	119,138,143,170	0
80	OHX	sR	2061	7/7	0.97	0.13	48,71,122,122	0
80	OHX	AR	3723	7/7	0.97	0.10	97,107,122,146	0
80	OHX	AR	3725	7/7	0.97	0.10	83,100,119,133	0
81	MG	1	3525	1/1	0.97	0.16	62,62,62,62	0
80	OHX	AR	3475	7/7	0.97	0.10	59,73,121,127	0
80	OHX	AR	3477	7/7	0.97	0.10	108,122,134,157	0
80	OHX	sR	2074	7/7	0.97	0.10	63,94,116,141	0
80	OHX	s1	301	7/7	0.97	0.11	79,101,111,122	0
81	MG	4	214	1/1	0.97	0.22	50,50,50,50	0
80	OHX	AR	3977	7/7	0.97	0.10	58,82,102,127	0
80	OHX	AR	3478	7/7	0.97	0.11	88,96,106,127	0
80	OHX	AR	4130	7/7	0.97	0.10	90,104,115,129	0
80	OHX	sR	2085	7/7	0.97	0.15	53,94,119,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
80	OHX	AR	4132	7/7	0.97	0.11	91,95,117,130	0
80	OHX	1	3964	7/7	0.97	0.10	82,98,107,124	0
81	MG	1	3757	1/1	0.97	0.08	90,90,90,90	0
81	MG	sR	2108	1/1	0.98	0.07	105,105,105,105	0
80	OHX	1	3692	7/7	0.98	0.09	55,73,99,101	0
80	OHX	CV	201	7/7	0.98	0.13	61,70,85,106	0
81	MG	1	3877	1/1	0.98	0.04	59,59,59,59	0
80	OHX	AR	3817	7/7	0.98	0.11	80,82,94,115	0
80	OHX	1	4142	7/7	0.98	0.10	63,71,106,114	0
80	OHX	AR	4128	7/7	0.98	0.11	65,87,92,98	0
80	OHX	1	4144	7/7	0.98	0.09	92,123,128,150	0
80	OHX	AR	3608	7/7	0.98	0.09	99,116,127,136	0
80	OHX	AR	3566	7/7	0.98	0.10	63,65,81,100	0
80	OHX	A	1933	7/7	0.98	0.08	117,129,137,163	0
81	MG	AR	3982	1/1	0.98	0.04	79,79,79,79	0
80	OHX	AR	3751	7/7	0.98	0.15	76,80,91,105	0
81	MG	AR	4137	1/1	0.98	0.11	86,86,86,86	0
80	OHX	AT	226	7/7	0.98	0.12	61,74,87,97	0
80	OHX	A	2013	7/7	0.98	0.15	71,86,98,104	0
80	OHX	1	3932	7/7	0.98	0.10	81,94,121,122	0
81	MG	AR	3544	1/1	0.98	0.04	54,54,54,54	0
80	OHX	AR	4037	7/7	0.98	0.09	69,85,120,120	0
80	OHX	1	3721	7/7	0.98	0.14	64,73,92,124	0
80	OHX	1	3722	7/7	0.98	0.13	70,72,94,115	0
80	OHX	1	4174	7/7	0.98	0.10	94,113,124,137	0
80	OHX	AR	3755	7/7	0.98	0.10	78,83,100,114	0
80	OHX	1	3538	7/7	0.98	0.10	86,99,120,125	0
80	OHX	1	3539	7/7	0.98	0.16	75,79,103,110	0
80	OHX	1	3540	7/7	0.98	0.13	62,86,91,92	0
80	OHX	AR	3628	7/7	0.98	0.16	72,84,96,126	0
80	OHX	DD	102	7/7	0.98	0.10	55,68,98,102	0
80	OHX	AR	3690	7/7	0.98	0.13	69,79,99,125	0
80	OHX	AR	3571	7/7	0.98	0.13	57,73,96,96	0
80	OHX	sR	2013	7/7	0.98	0.15	71,79,89,94	0
81	MG	1	4087	1/1	0.98	0.04	97,97,97,97	0
80	OHX	sR	2133	7/7	0.98	0.11	72,83,103,115	0
80	OHX	1	3752	7/7	0.98	0.12	64,79,94,107	0
80	OHX	AR	3942	7/7	0.98	0.16	69,73,85,90	0
80	OHX	AR	3944	7/7	0.98	0.11	87,106,125,126	0
80	OHX	A	2101	7/7	0.98	0.10	89,95,114,146	0
80	OHX	1	3756	7/7	0.98	0.10	108,114,126,130	0
80	OHX	AR	3847	7/7	0.98	0.14	62,71,73,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	AR	3849	7/7	0.98	0.09	78,79,87,114	0
80	OHX	1	3570	7/7	0.98	0.12	68,70,95,98	0
80	OHX	1	3571	7/7	0.98	0.11	84,89,97,98	0
80	OHX	sR	2026	7/7	0.98	0.08	166,167,179,180	0
80	OHX	1	3782	7/7	0.98	0.13	86,95,106,115	0
80	OHX	AR	3535	7/7	0.98	0.10	70,75,86,107	0
81	MG	AR	3730	1/1	0.98	0.04	48,48,48,48	0
80	OHX	AR	4066	7/7	0.98	0.12	69,75,86,112	0
80	OHX	AR	3537	7/7	0.98	0.08	37,55,97,119	0
80	OHX	1	3577	7/7	0.98	0.09	106,114,127,130	0
80	OHX	A	2149	7/7	0.98	0.07	138,139,144,160	0
81	MG	1	4117	1/1	0.98	0.07	85,85,85,85	0
80	OHX	sR	2038	7/7	0.98	0.07	91,97,110,132	0
80	OHX	A	1945	7/7	0.98	0.10	121,123,137,140	0
81	MG	sR	2024	1/1	0.98	0.18	89,89,89,89	0
80	OHX	AR	4190	7/7	0.98	0.13	57,71,106,109	0
80	OHX	1	4021	7/7	0.98	0.09	66,95,105,110	0
80	OHX	1	3602	7/7	0.98	0.11	62,76,97,121	0
80	OHX	AR	3504	7/7	0.98	0.11	68,76,93,104	0
80	OHX	1	4024	7/7	0.98	0.08	93,101,118,128	0
80	OHX	1	3812	7/7	0.98	0.10	69,78,100,107	0
81	MG	sR	2036	1/1	0.98	0.08	85,85,85,85	0
80	OHX	sR	2049	7/7	0.98	0.11	58,87,100,111	0
80	OHX	AR	3473	7/7	0.98	0.14	62,73,92,118	0
80	OHX	1	3449	7/7	0.98	0.13	62,69,102,109	0
80	OHX	AR	3975	7/7	0.98	0.13	77,89,102,120	0
81	MG	1	3807	1/1	0.98	0.08	87,87,87,87	0
80	OHX	AR	3783	7/7	0.98	0.15	50,69,87,104	0
80	OHX	AR	3442	7/7	0.98	0.14	44,72,109,119	0
80	OHX	1	4050	7/7	0.98	0.11	71,83,98,100	0
80	OHX	AR	3787	7/7	0.98	0.10	107,108,135,137	0
80	OHX	1	4052	7/7	0.98	0.12	85,96,102,113	0
80	OHX	AR	3597	7/7	0.98	0.10	77,86,90,91	0
80	OHX	1	3631	7/7	0.98	0.15	56,78,96,128	0
80	OHX	1	3632	7/7	0.98	0.15	56,77,108,119	0
80	OHX	1	3842	7/7	0.98	0.11	61,93,100,112	0
80	OHX	AR	3881	7/7	0.98	0.11	62,72,95,101	0
80	OHX	1	3634	7/7	0.98	0.09	70,82,126,128	0
80	OHX	AR	4097	7/7	0.98	0.11	61,78,98,107	0
80	OHX	AR	3883	7/7	0.98	0.08	78,89,107,124	0
80	OHX	sR	2073	7/7	0.98	0.14	69,79,93,118	0
80	OHX	AR	3721	7/7	0.98	0.11	62,79,93,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	sR	2188	7/7	0.98	0.09	87,104,115,125	0
80	OHX	AR	3659	7/7	0.98	0.13	48,76,88,113	0
81	MG	AR	3782	1/1	0.98	0.08	66,66,66,66	0
80	OHX	1	3481	7/7	0.98	0.11	91,97,113,132	0
80	OHX	1	3661	7/7	0.98	0.12	66,69,85,106	0
80	OHX	1	3662	7/7	0.98	0.12	73,77,102,112	0
80	OHX	AS	219	7/7	0.98	0.12	72,95,102,124	0
80	OHX	1	4088	7/7	0.98	0.10	98,101,120,146	0
80	OHX	1	3664	7/7	0.98	0.10	82,95,112,128	0
82	ZN	b	201	1/1	0.98	0.03	96,96,96,96	0
81	MG	AR	3650	1/1	0.98	0.19	47,47,47,47	0
80	OHX	AR	3599	7/7	0.98	0.09	93,99,114,131	0
82	ZN	e	101	1/1	0.98	0.04	92,92,92,92	0
82	ZN	g	501	1/1	0.98	0.05	140,140,140,140	0
80	OHX	AC	101	7/7	0.98	0.12	53,88,102,106	0
80	OHX	4	226	7/7	0.98	0.11	62,72,92,98	0
81	MG	1	3697	1/1	0.98	0.05	76,76,76,76	0
80	OHX	1	4112	7/7	0.98	0.10	69,95,122,129	0
80	OHX	A	2110	7/7	0.98	0.10	107,112,122,141	0
81	MG	AR	3513	1/1	0.98	0.04	42,42,42,42	0
80	OHX	A	2141	7/7	0.98	0.10	79,100,125,134	0
80	OHX	AR	4010	7/7	0.98	0.14	72,79,90,116	0
80	OHX	sR	1979	7/7	0.98	0.07	147,149,160,166	0
80	OHX	1	3901	7/7	0.98	0.13	72,81,97,120	0
80	OHX	1	3691	7/7	0.98	0.15	59,74,85,120	0
81	MG	A	2024	1/1	0.99	0.04	79,79,79,79	0
80	OHX	AR	4159	7/7	0.99	0.09	68,74,99,102	0
80	OHX	AR	3815	7/7	0.99	0.20	63,74,77,106	0
80	OHX	1	3660	7/7	0.99	0.11	81,85,98,103	0
81	MG	AR	3575	1/1	0.99	0.04	62,62,62,62	0
81	MG	1	3967	1/1	0.99	0.07	39,39,39,39	0
82	ZN	DL	103	1/1	0.99	0.03	67,67,67,67	0
82	ZN	DO	201	1/1	0.99	0.03	59,59,59,59	0
82	ZN	DQ	501	1/1	0.99	0.04	120,120,120,120	0
82	ZN	DR	501	1/1	0.99	0.04	94,94,94,94	0
80	OHX	1	3419	7/7	0.99	0.13	62,81,87,99	0
82	ZN	AN	500	1/1	0.99	0.03	68,68,68,68	0
81	MG	AR	4168	1/1	0.99	0.04	42,42,42,42	0
80	OHX	AR	4035	7/7	0.99	0.11	78,79,84,102	0
80	OHX	AR	3911	7/7	0.99	0.14	66,82,90,121	0
82	ZN	AQ	501	1/1	0.99	0.03	88,88,88,88	0
81	MG	1	3907	1/1	0.99	0.09	76,76,76,76	0

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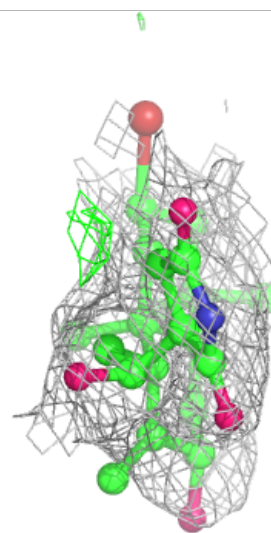
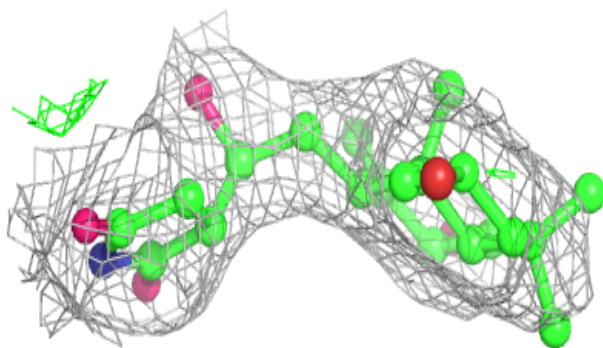
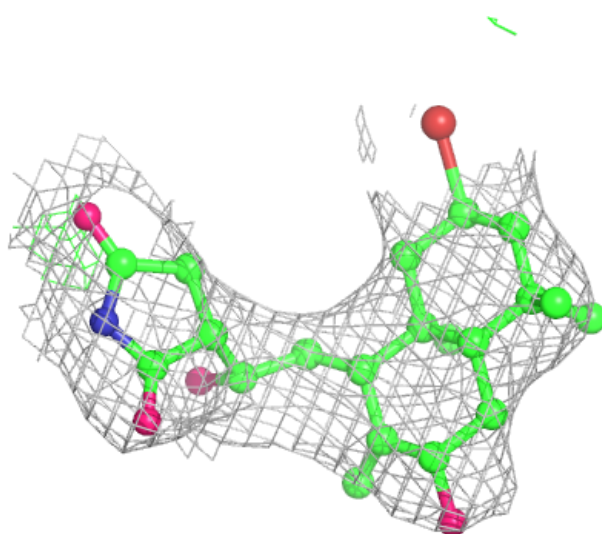
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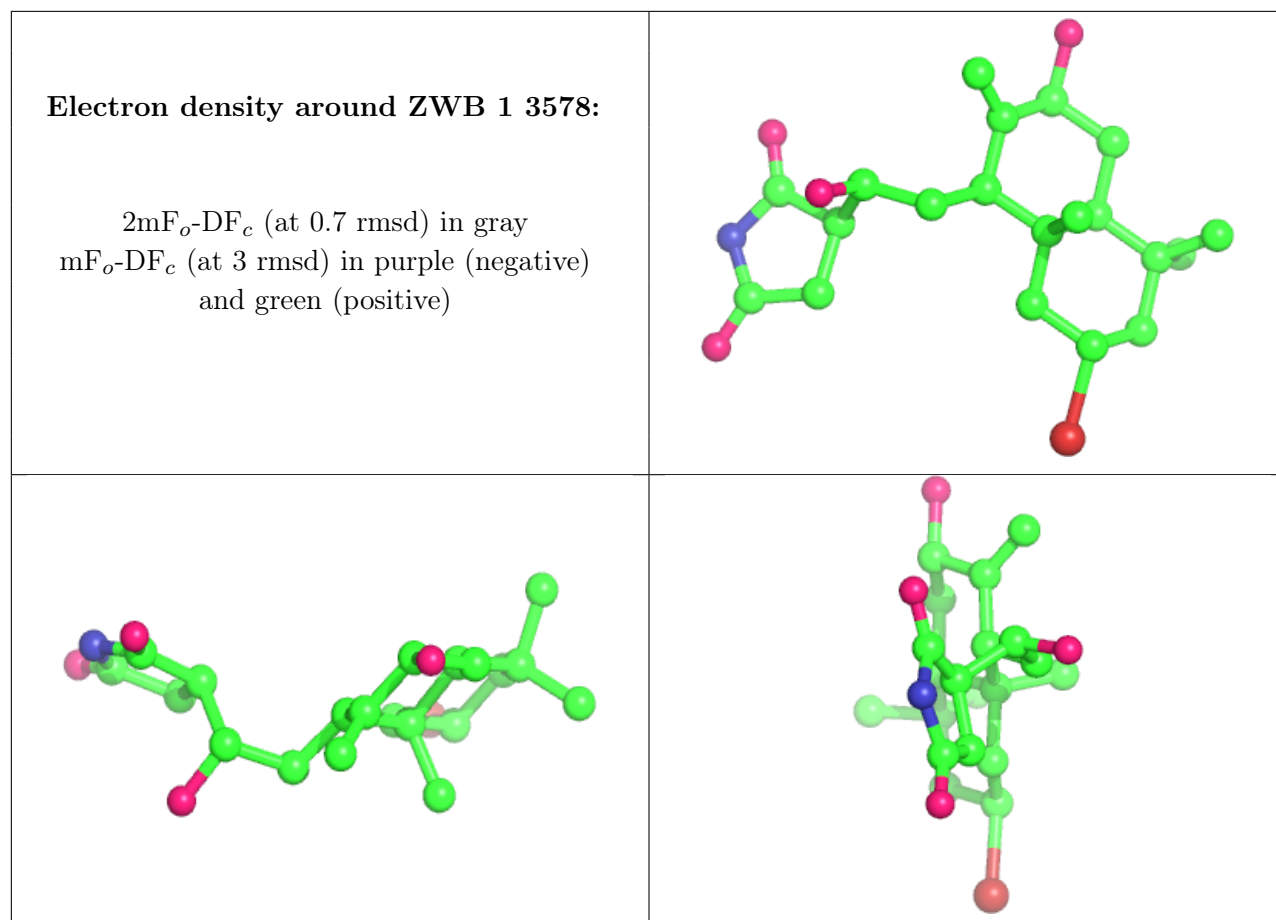
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
82	ZN	d6	202	1/1	0.99	0.02	76,76,76,76	0
80	OHX	A	2131	7/7	0.99	0.10	84,99,111,113	0
82	ZN	d9	101	1/1	0.99	0.05	105,105,105,105	0
81	MG	sR	2096	1/1	0.99	0.09	96,96,96,96	0
80	OHX	AR	3973	7/7	0.99	0.10	75,87,90,110	0
81	MG	1	3817	1/1	0.99	0.08	53,53,53,53	0
81	MG	A	2014	1/1	0.99	0.03	60,60,60,60	0
80	OHX	1	3781	7/7	0.99	0.09	100,102,116,126	0
81	MG	1	3607	1/1	0.99	0.08	61,61,61,61	0
80	OHX	1	4140	7/7	0.99	0.12	72,76,84,100	0
80	OHX	1	3601	7/7	0.99	0.12	74,83,93,99	0
80	OHX	1	4110	7/7	0.99	0.14	66,68,80,89	0
80	OHX	AR	3879	7/7	0.99	0.10	54,63,84,91	0
82	ZN	AK	102	1/1	1.00	0.02	57,57,57,57	0
81	MG	AR	3920	1/1	1.00	0.03	50,50,50,50	0
81	MG	AR	3482	1/1	1.00	0.02	50,50,50,50	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 ZWB AR 3826:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.