



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 18, 2025 – 12:46 am BST

PDB ID : 8P85 / pdb_00008p85
Title : 80S yeast ribosome in complex with Fluorolissoclimide
Authors : Terrosu, S.; Yusupov, M.
Deposited on : 2023-08-31
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) : 2.44

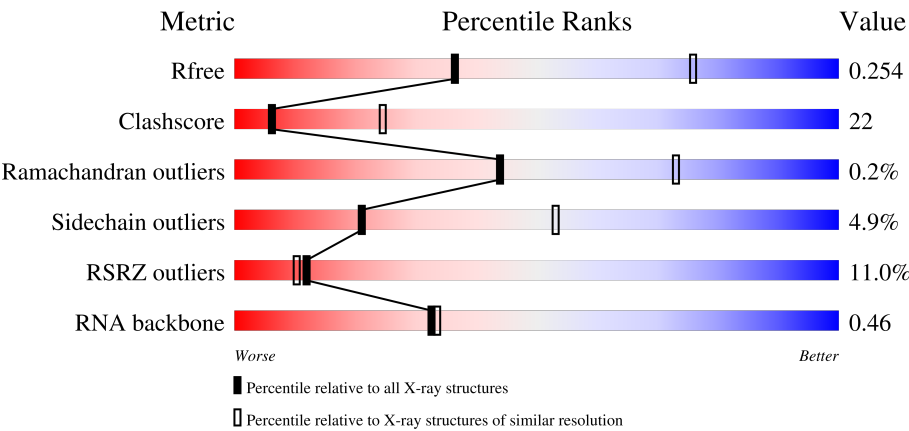
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	A	1800	<div><div>3%</div><div>30%</div><div>49%</div><div>17%</div><div></div></div>
1	sR	1800	<div><div>2%</div><div>33%</div><div>51%</div><div>16%</div><div></div></div>
2	B	252	<div><div>20%</div><div>21%</div><div>58%</div><div></div><div>18%</div></div>
2	s0	252	<div><div>14%</div><div>32%</div><div>45%</div><div></div><div>18%</div></div>

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Mol	Chain	Length	Quality of chain
3	C	255	
3	s1	255	
4	D	254	
4	s2	254	
5	E	240	
5	s3	240	
6	F	261	
6	s4	261	
7	G	225	
7	s5	225	
8	H	236	
8	s6	236	
9	I	190	
9	s7	190	
10	J	200	
10	s8	200	
11	K	197	
11	s9	197	
12	L	105	
12	c0	105	
13	M	156	
13	c1	156	
14	O	151	
14	c3	151	
15	P	138	

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Mol	Chain	Length	Quality of chain
15	c4	138	
16	Q	142	
16	c5	142	
17	R	143	
17	c6	143	
18	S	136	
18	c7	136	
19	T	146	
19	c8	146	
20	U	144	
20	c9	144	
21	V	121	
21	d0	121	
22	W	87	
22	d1	87	
23	X	130	
23	d2	130	
24	Y	145	
24	d3	145	
25	Z	135	
25	d4	135	
26	AA	136	
26	DB	136	
27	9	127	
27	DA	127	

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Mol	Chain	Length	Quality of chain
28	AB	149	
28	DC	149	
29	AC	59	
29	DD	59	
30	AD	105	
30	DE	105	
31	CD	254	
31	j	254	
32	AE	113	
32	DF	113	
33	CE	387	
33	k	387	
34	AF	130	
34	DG	130	
35	1	3396	
35	AR	3396	
36	3	121	
36	AS	121	
37	4	158	
37	AT	158	
38	CF	362	
38	l	362	
39	CG	297	
39	m	297	
40	CH	176	

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Mol	Chain	Length	Quality of chain
40	n	176	
41	CI	244	
41	o	244	
42	CJ	256	
42	p	256	
43	CK	191	
43	q	191	
44	CL	221	
44	r	221	
45	CM	174	
45	s	174	
46	CN	199	
46	t	199	
47	CO	138	
47	u	138	
48	CP	204	
48	v	204	
49	CQ	199	
49	w	199	
50	CR	184	
50	x	184	
51	CS	186	
51	y	186	
52	CT	189	
52	z	189	

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Mol	Chain	Length	Quality of chain
53	0	172	
53	CU	172	
54	2	160	
54	CV	160	
55	5	121	
55	CW	121	
56	6	137	
56	CX	137	
57	7	155	
57	CY	155	
58	8	142	
58	CZ	142	
59	AG	107	
59	DH	107	
60	AH	121	
60	DI	121	
61	AI	120	
61	DJ	120	
62	AJ	100	
62	DK	100	
63	AK	88	
63	DL	88	
64	AL	78	
64	DM	78	
65	AM	51	

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Mol	Chain	Length	Quality of chain
65	DN	51	
66	AN	128	
66	DO	128	
67	AO	25	
67	DP	25	
68	AP	106	
68	DQ	106	
69	AQ	92	
69	DR	92	
70	i	273	
70	sM	273	
71	p0	312	
72	a	108	
72	d5	108	
73	b	119	
73	d6	119	
74	c	82	
74	d7	82	
75	d	67	
75	d8	67	
76	d9	56	
76	e	56	
77	e0	63	
77	f	63	
78	e1	152	

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Mol	Chain	Length	Quality of chain
78	g	152	
79	Rb	319	
79	h	319	

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	3404	-	-	X	-
80	OHX	1	3477	-	-	X	-
80	OHX	1	4132	-	-	X	-
80	OHX	1	4156	-	-	X	-
80	OHX	1	4158	-	-	X	-
80	OHX	A	2134	-	-	X	-
80	OHX	AR	3401	-	-	X	-
80	OHX	AR	3408	-	-	X	-
80	OHX	AR	3504	-	-	X	-
80	OHX	AR	3652	-	-	X	-
80	OHX	k	403	-	-	X	-
80	OHX	sR	1957	-	-	X	-
80	OHX	sR	1975	-	-	X	-
81	MG	1	3742	-	-	-	X
81	MG	1	3897	-	-	-	X
81	MG	1	3900	-	-	-	X
81	MG	1	3920	-	-	-	X
81	MG	1	3944	-	-	-	X
81	MG	1	4039	-	-	-	X
81	MG	1	4056	-	-	-	X
81	MG	A	2008	-	-	-	X
81	MG	A	2077	-	-	-	X
81	MG	A	2097	-	-	-	X
81	MG	A	2105	-	-	-	X
81	MG	AR	3781	-	-	-	X
81	MG	AR	3783	-	-	-	X
81	MG	AR	3792	-	-	-	X
81	MG	AR	3843	-	-	-	X
81	MG	AR	3932	-	-	-	X
81	MG	AR	3945	-	-	-	X
81	MG	AR	3974	-	-	-	X
81	MG	AR	4003	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	AS	223	-	-	-	X
81	MG	CS	201	-	-	-	X
81	MG	s8	301	-	-	-	X
81	MG	sR	2064	-	-	-	X
81	MG	sR	2168	-	-	-	X
82	K	A	2161	-	-	-	X

2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 404943 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1735	Total	C	N	O	P	0	0	0
			36976	16530	6547	12164	1735			
1	sR	1783	Total	C	N	O	P	0	0	0
			37990	16984	6723	12500	1783			

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

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

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1709	1084	310	311	4			
3	s1	216	Total	C	N	O	S	0	0	0
			1722	1091	312	315	4			

- Molecule 4 is a protein called 40S ribosomal protein S2.

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

- Molecule 5 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	200	Total	C	N	O	S	0	0	0
			1583	993	294	293	3			
7	s5	199	Total	C	N	O	S	0	0	0
			1576	988	293	292	3			

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	226	Total	C	N	O	S	0	0	0
			1792	1123	346	320	3			
8	s6	218	Total	C	N	O	S	0	0	0
			1755	1102	337	313	3			

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

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

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

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

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

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	179	Total	C	N	O	S	0	0	0
			1456	922	283	250	1			
11	s9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

- Molecule 12 is a protein called Small ribosomal subunit protein eS10A, Small ribosomal subunit protein eS10A, 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	96	Total	C	N	O	S	0	0	0
			772	499	126	145	2			
12	c0	84	Total	C	N	O	S	0	0	0
			702	455	113	132	2			

- Molecule 13 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	143	Total	C	N	O	S	0	0	0
			1154	739	218	194	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

- Molecule 14 is a protein called 40S ribosomal protein S13.

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

- Molecule 15 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	c4	128	Total	C	N	O	S	0	0	0
			949	582	188	176	3			

- Molecule 16 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Q	117	Total	C	N	O	S	0	0	0
			928	589	174	158	7			
16	c5	127	Total	C	N	O	S	0	0	0
			991	629	185	170	7			

- Molecule 17 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 18 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	S	115	Total	C	N	O	S	0	0	0
			901	562	172	165	2			
18	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

- Molecule 19 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	T	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			
19	c8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			

- Molecule 20 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 21 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	V	107	Total	C	N	O	S	0	0	0
			855	539	156	159	1			
21	d0	100	Total	C	N	O	S	0	0	0
			800	509	144	146	1			

- Molecule 22 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 23 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 24 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 25 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 26 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 27 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	DA	124	Total	C	N	O	0	0	0
			976	614	190	172			
27	9	126	Total	C	N	O	0	0	0
			993	625	192	176			

- Molecule 28 is a protein called 60S ribosomal protein L28.

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

- Molecule 29 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
29	AC	58	Total	C	N	O	0	0	0
			462	289	100	73			
29	DD	58	Total	C	N	O	0	0	0
			462	289	100	73			

- Molecule 30 is a protein called 60S ribosomal protein L30.

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

- Molecule 31 is a protein called 60S ribosomal protein L2-A.

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

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

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AE	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			
32	DF	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			

- Molecule 33 is a protein called 60S ribosomal protein L3.

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

- Molecule 34 is a protein called 60S ribosomal protein L32.

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

- Molecule 35 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1	3134	Total	C	N	O	P	0	0	0
			67038	29944	12089	21871	3134			
35	AR	3147	Total	C	N	O	P	0	0	0
			67313	30067	12134	21965	3147			

- Molecule 36 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
36	AS	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 37 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	4	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			
37	AT	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 38 is a protein called 60S ribosomal protein L4-A.

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

- Molecule 39 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	m	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
39	CG	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			

- Molecule 40 is a protein called 60S ribosomal protein L6-A.

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

- Molecule 41 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 42 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	p	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
42	CJ	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			

- Molecule 43 is a protein called 60S ribosomal protein L9-A.

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

- Molecule 44 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	r	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			
44	CL	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			

- Molecule 45 is a protein called Large ribosomal subunit protein uL5B.

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

- Molecule 46 is a protein called 60S ribosomal protein L13-A.

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

- Molecule 47 is a protein called 60S ribosomal protein L14-A.

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

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

- Molecule 48 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 49 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 50 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	x	176	Total	C	N	O	S	0	0	0
			1385	861	274	250				
50	CR	155	Total	C	N	O	S	0	0	0
			1227	764	238	225				

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

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

- Molecule 52 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	z	183	Total	C	N	O	S	0	0	0
			1482	911	320	251				
52	CT	184	Total	C	N	O	S	0	0	0
			1490	917	321	252				

- Molecule 53 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
53	CU	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

- Molecule 54 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	2	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			
54	CV	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			

- Molecule 55 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	5	100	Total	C	N	O	0	0	0
			796	516	131	149			
55	CW	100	Total	C	N	O	0	0	0
			796	516	131	149			

- Molecule 56 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	6	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
56	CX	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

- Molecule 57 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	7	67	Total	C	N	O	S	0	0	0
			543	349	106	87	1			
57	CY	113	Total	C	N	O	S	0	0	0
			781	492	155	133	1			

- Molecule 58 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	8	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			
58	CZ	118	Total	C	N	O	S	0	0	0
			946	608	166	170	2			

- Molecule 59 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	AG	105	Total	C	N	O	S	0	0	0
			839	534	161	143	1			
59	DH	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			

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

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

- Molecule 61 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 62 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
62	AJ	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			
62	DK	97	Total	C	N	O	S	0	0	0
			750	469	149	130	2			

- Molecule 63 is a protein called 60S ribosomal protein L37-A.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
63	DL	86	Total	C	N	O	S	0	0	0
			676	411	147	113	5			

- Molecule 64 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	AL	77	Total	C	N	O		0	0	0
			612	391	115	106				
64	DM	77	Total	C	N	O		0	0	0
			612	391	115	106				

- Molecule 65 is a protein called 60S ribosomal protein L39.

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

- Molecule 66 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 67 is a protein called Large ribosomal subunit protein eL41B.

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

- Molecule 68 is a protein called 60S ribosomal protein L42-A.

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

- Molecule 69 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 70 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
70	i	126	Total	C	N	O		0	0	0
			939	553	188	198				
70	sM	63	Total	C	N	O		0	0	0
			475	280	99	96				

- Molecule 71 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
71	p0	123	Total	C	N	O	S	0	0	0
			977	627	172	175	3			

- Molecule 72 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	a	70	Total	C	N	O		0	0	0
			563	360	104	99				
72	d5	69	Total	C	N	O		0	0	0
			558	357	103	98				

- Molecule 73 is a protein called Small ribosomal subunit protein eS26B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
73	b	93	Total	C	N	O	S	0	0	0
			745	461	156	123	5			
73	d6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

- Molecule 74 is a protein called 40S ribosomal protein S27-A.

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

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

- Molecule 75 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 76 is a protein called Small ribosomal subunit protein uS14A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	e	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			
76	d9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			

- Molecule 77 is a protein called 40S ribosomal protein S30-A.

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

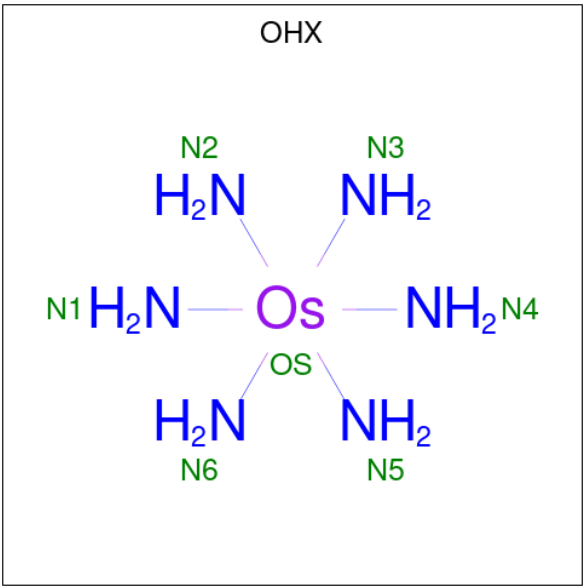
- Molecule 78 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	g	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			
78	e1	39	Total	C	N	O	S	0	0	0
			317	204	57	54	2			

- Molecule 79 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	h	312	Total	C	N	O	S	0	0	0
			2394	1515	411	460	8			
79	Rb	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- 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	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
			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
			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
			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		
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
			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	1
			14	12	2		
80	J	1	Total	N	Os	0	0
			7	6	1		
80	O	1	Total	N	Os	0	0
			7	6	1		
80	Q	1	Total	N	Os	0	0
			7	6	1		
80	S	1	Total	N	Os	0	0
			7	6	1		
80	T	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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80	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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80	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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80	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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80	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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80	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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80	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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80	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
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80	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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80	1	1	Total	N	Os	0	0
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80	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
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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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			7	6	1		
80	1	1	Total	N	Os	0	0
			7	6	1		
80	3	1	Total	N	Os	0	0
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80	3	1	Total	N	Os	0	0
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80	3	1	Total	N	Os	0	0
			7	6	1		
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80	3	1	Total	N	Os	0	0
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80	3	1	Total	N	Os	0	0
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80	3	1	Total	N	Os	0	0
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80	3	1	Total	N	Os	0	0
			7	6	1		
80	3	1	Total	N	Os	0	0
			7	6	1		
80	4	1	Total	N	Os	0	0
			7	6	1		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	r	1	Total	N	Os	0	0
			7	6	1		
80	v	1	Total	N	Os	0	0
			7	6	1		
80	x	1	Total	N	Os	0	0
			7	6	1		
80	y	1	Total	N	Os	0	0
			7	6	1		
80	z	1	Total	N	Os	0	0
			7	6	1		
80	z	1	Total	N	Os	0	0
			7	6	1		
80	2	1	Total	N	Os	0	0
			7	6	1		
80	AG	1	Total	N	Os	0	0
			7	6	1		
80	AK	1	Total	N	Os	0	0
			7	6	1		
80	AP	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
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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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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
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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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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		
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
			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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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
			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	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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			7	6	1		
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			7	6	1		
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			7	6	1		
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
			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		
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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
			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
			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
			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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			7	6	1		
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			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
			7	6	1		
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
			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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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
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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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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		

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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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80	AR	1	Total	N	Os	0	0
			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
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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
			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
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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		

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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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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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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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			7	6	1		
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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		

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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		
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		
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	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		
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
			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	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		
80	AR	1	Total	N	Os	0	0
			6	5	1		
80	AR	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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	AS	1	Total	N	Os	0	0
			7	6	1		
80	AS	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	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	CG	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	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	CL	1	Total	N	Os	0	0
			6	5	1		
80	CP	1	Total	N	Os	0	0
			7	6	1		
80	CS	1	Total	N	Os	0	0
			7	6	1		
80	CX	1	Total	N	Os	0	0
			7	6	1		
80	DH	1	Total	N	Os	0	0
			7	6	1		
80	DK	1	Total	N	Os	0	0
			7	6	1		
80	DL	1	Total	N	Os	0	0
			7	6	1		
80	DQ	1	Total	N	Os	0	0
			7	6	1		
80	e	1	Total	N	Os	0	0
			7	6	1		
80	h	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		

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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	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	Rb	1	Total	N	Os	0	0
			7	6	1		
80	s1	1	Total	N	Os	0	0
			7	6	1		
80	s4	1	Total	N	Os	0	0
			7	6	1		
80	s8	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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
80	c8	1	Total	N	Os	0	0
			7	6	1		
80	d4	1	Total	N	Os	0	0
			7	6	1		
80	d6	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	A	139	Total	Mg	0	0
			139	139		
81	D	1	Total	Mg	0	0
			1	1		
81	F	1	Total	Mg	0	0
			1	1		
81	O	1	Total	Mg	0	0
			1	1		
81	P	1	Total	Mg	0	0
			1	1		
81	DA	2	Total	Mg	0	0
			2	2		
81	AB	3	Total	Mg	0	0
			3	3		
81	AC	1	Total	Mg	0	0
			1	1		
81	DC	2	Total	Mg	0	0
			2	2		
81	CD	2	Total	Mg	0	0
			2	2		
81	CE	3	Total	Mg	0	0
			3	3		
81	AF	2	Total	Mg	0	0
			2	2		
81	1	489	Total	Mg	0	0
			489	489		
81	3	12	Total	Mg	0	0
			12	12		
81	4	21	Total	Mg	0	0
			21	21		
81	j	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	k	1	Total 1	Mg 1	0	0
81	l	4	Total 4	Mg 4	0	0
81	m	1	Total 1	Mg 1	0	0
81	o	1	Total 1	Mg 1	0	0
81	r	3	Total 3	Mg 3	0	0
81	s	1	Total 1	Mg 1	0	0
81	t	3	Total 3	Mg 3	0	0
81	v	5	Total 5	Mg 5	0	0
81	w	1	Total 1	Mg 1	0	0
81	x	8	Total 8	Mg 8	0	0
81	z	2	Total 2	Mg 2	0	0
81	6	3	Total 3	Mg 3	0	0
81	8	3	Total 3	Mg 3	0	0
81	9	1	Total 1	Mg 1	0	0
81	AH	1	Total 1	Mg 1	0	0
81	AK	3	Total 3	Mg 3	0	0
81	AN	1	Total 1	Mg 1	0	0
81	AR	534	Total 534	Mg 534	0	0
81	AS	18	Total 18	Mg 18	0	0
81	AT	15	Total 15	Mg 15	0	0
81	CF	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	CG	1	Total 1	Mg 1	0	0
81	CI	2	Total 2	Mg 2	0	0
81	CK	2	Total 2	Mg 2	0	0
81	CL	1	Total 1	Mg 1	0	0
81	CM	2	Total 2	Mg 2	0	0
81	CO	1	Total 1	Mg 1	0	0
81	CP	3	Total 3	Mg 3	0	0
81	CQ	3	Total 3	Mg 3	0	0
81	CR	6	Total 6	Mg 6	0	0
81	CS	1	Total 1	Mg 1	0	0
81	CU	2	Total 2	Mg 2	0	0
81	CX	1	Total 1	Mg 1	0	0
81	CY	1	Total 1	Mg 1	0	0
81	DH	2	Total 2	Mg 2	0	0
81	DI	1	Total 1	Mg 1	0	0
81	DL	1	Total 1	Mg 1	0	0
81	DO	1	Total 1	Mg 1	0	0
81	DP	1	Total 1	Mg 1	0	0
81	DQ	3	Total 3	Mg 3	0	0
81	DR	2	Total 2	Mg 2	0	0
81	sM	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
81	b	1	Total Mg 1 1	0	0
81	sR	143	Total Mg 143 143	0	0
81	s1	1	Total Mg 1 1	0	0
81	s2	1	Total Mg 1 1	0	0
81	s4	2	Total Mg 2 2	0	0
81	s8	3	Total Mg 3 3	0	0
81	c1	1	Total Mg 1 1	0	0
81	c4	2	Total Mg 2 2	0	0
81	c6	2	Total Mg 2 2	0	0
81	c8	2	Total Mg 2 2	0	0
81	c9	1	Total Mg 1 1	0	0
81	d2	1	Total Mg 1 1	0	0
81	d3	3	Total Mg 3 3	0	0
81	d4	2	Total Mg 2 2	0	0
81	d5	1	Total Mg 1 1	0	0
81	d6	2	Total Mg 2 2	0	0
81	d9	1	Total Mg 1 1	0	0

- Molecule 82 is POTASSIUM ION (CCD ID: K) (formula: K).

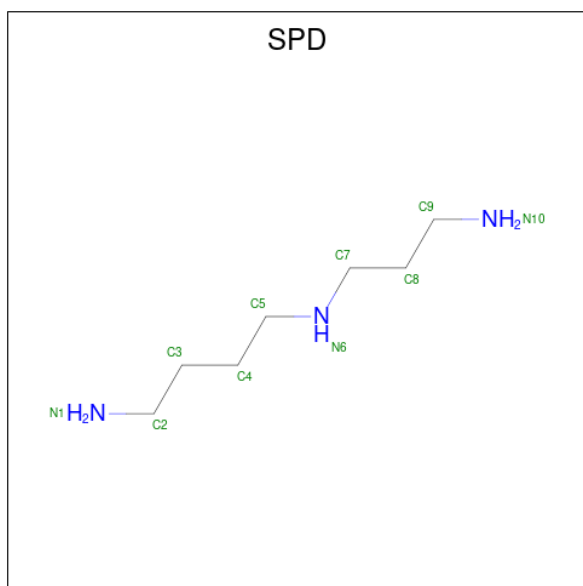
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	A	2	Total K 2 2	0	0
82	AR	1	Total K 1 1	0	0

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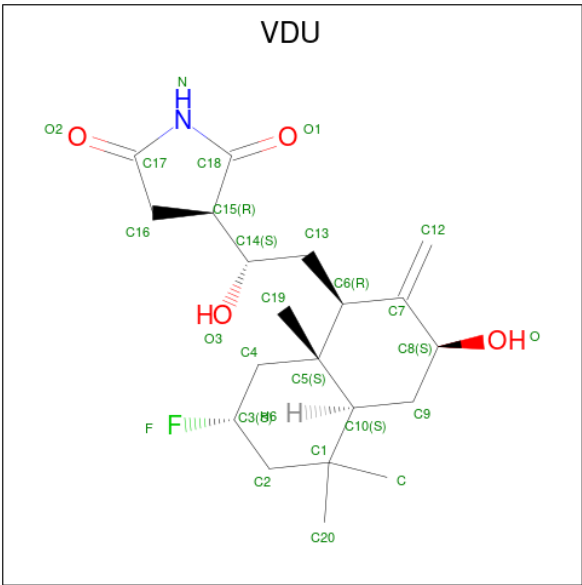
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	CK	1	Total K 1 1	0	0

- Molecule 83 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	1	1	Total C N 10 7 3	0	0
83	AR	1	Total C N 10 7 3	0	0

- Molecule 84 is fluorolissoclimide (CCD ID: VDU) (formula: $C_{20}H_{30}FNO_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

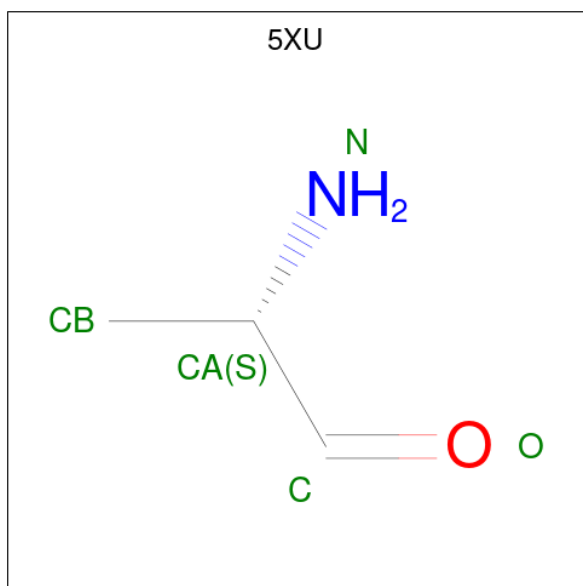
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	AK	1	Total	Zn	0	0
			1	1		
85	AN	1	Total	Zn	0	0
			1	1		
85	AP	1	Total	Zn	0	0
			1	1		
85	AQ	1	Total	Zn	0	0
			1	1		
85	DI	1	Total	Zn	0	0
			1	1		
85	DL	1	Total	Zn	0	0
			1	1		
85	DO	1	Total	Zn	0	0
			1	1		
85	DQ	1	Total	Zn	0	0
			1	1		
85	DR	1	Total	Zn	0	0
			1	1		
85	b	1	Total	Zn	0	0
			1	1		

Continued on next page...

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	c	1	Total	Zn	0	0
			1	1		
85	e	1	Total	Zn	0	0
			1	1		
85	g	1	Total	Zn	0	0
			1	1		
85	d6	1	Total	Zn	0	0
			1	1		
85	d7	1	Total	Zn	0	0
			1	1		
85	d9	1	Total	Zn	0	0
			1	1		
85	e1	1	Total	Zn	0	0
			1	1		

- Molecule 86 is (2 {S})-2-azanylpropanal (CCD ID: 5XU) (formula: C₃H₇NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
86	s3	1	Total	C	N	O	0	0
			5	3	1	1		
86	s3	1	Total	C	N	O	0	0
			4	2	1	1		
86	c0	1	Total	C	N	O	0	0
			5	3	1	1		
86	c0	1	Total	C	N	O	0	0
			5	3	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
86	c0	1	Total	C	N	O	0	0
			5	3	1	1		

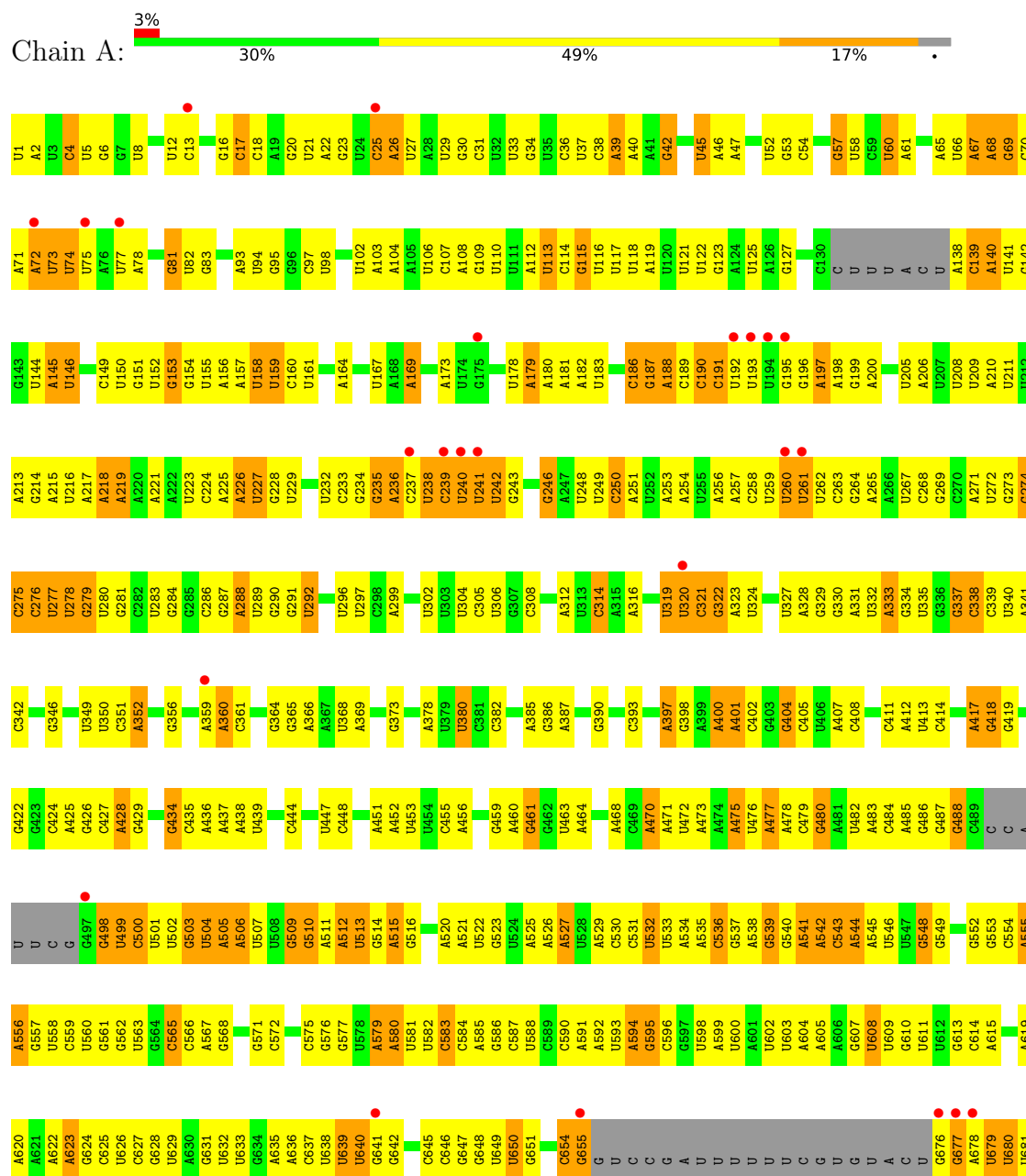
- Molecule 87 is water.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
87	A	44	Total	O			0	0
			44	44				
87	F	1	Total	O			0	0
			1	1				
87	CD	1	Total	O			0	0
			1	1				
87	AF	3	Total	O			0	0
			3	3				
87	1	60	Total	O			0	0
			60	60				
87	8	6	Total	O			0	0
			6	6				
87	AO	1	Total	O			0	0
			1	1				
87	i	1	Total	O			0	0
			1	1				
87	AR	81	Total	O			0	0
			81	81				
87	AT	2	Total	O			0	0
			2	2				
87	CP	3	Total	O			0	0
			3	3				
87	CR	1	Total	O			0	0
			1	1				
87	DG	3	Total	O			0	0
			3	3				
87	sR	24	Total	O			0	0
			24	24				

3 Residue-property plots

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

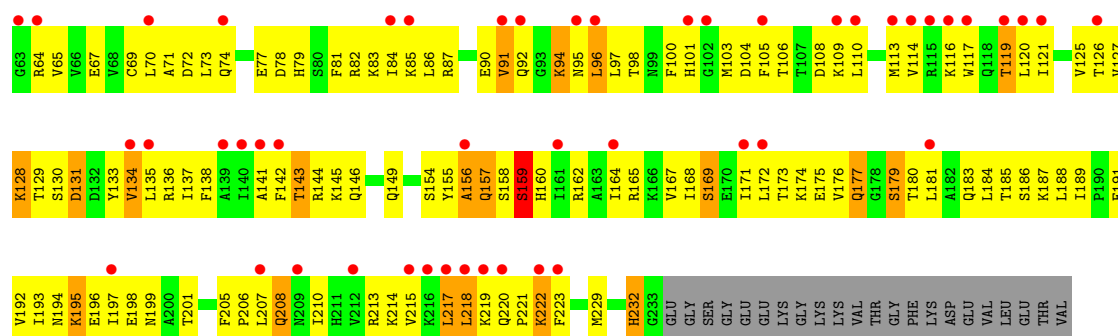
• Molecule 1: 16S ribosomal RNA



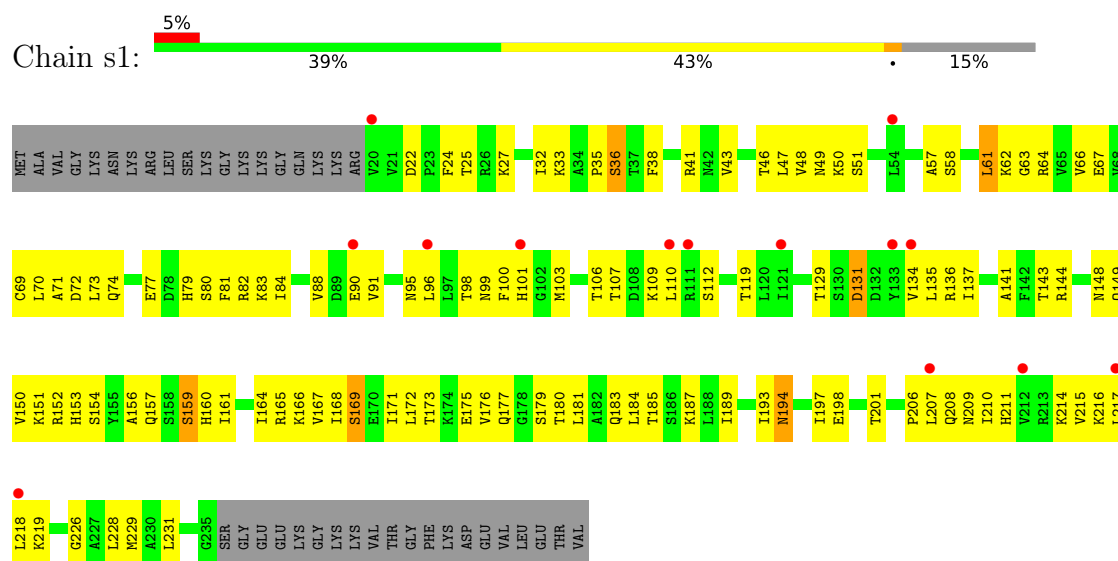




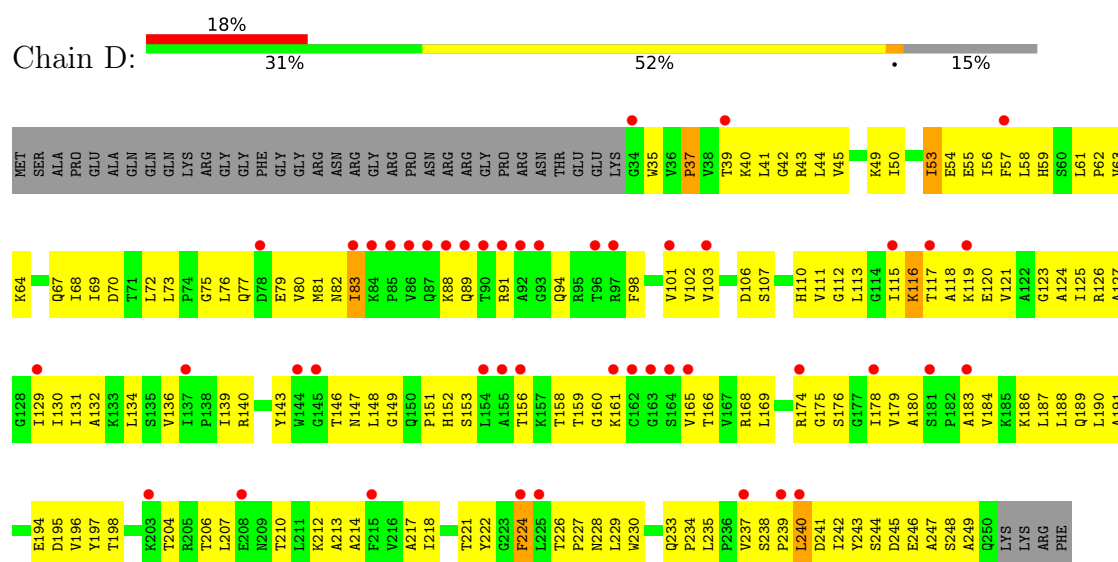




• Molecule 3: 40S ribosomal protein S1-A

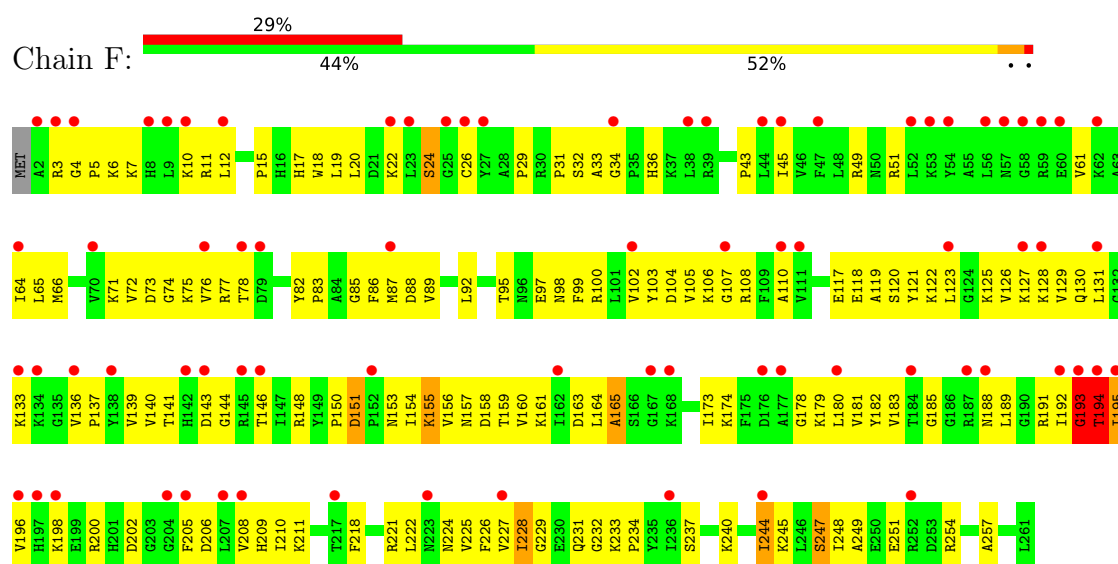


• Molecule 4: 40S ribosomal protein S2

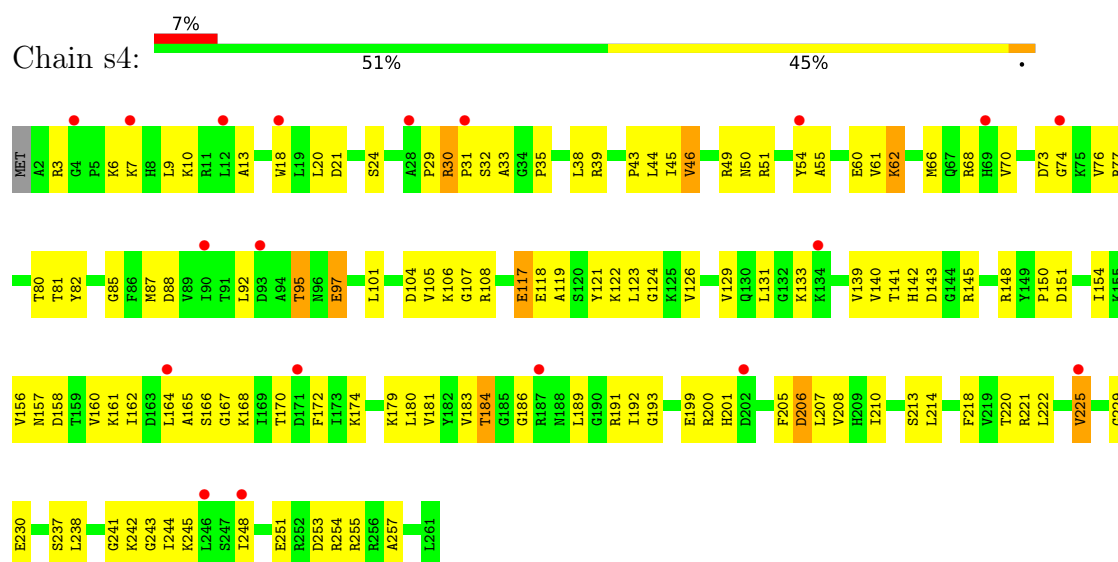


• Molecule 4: 40S ribosomal protein S2

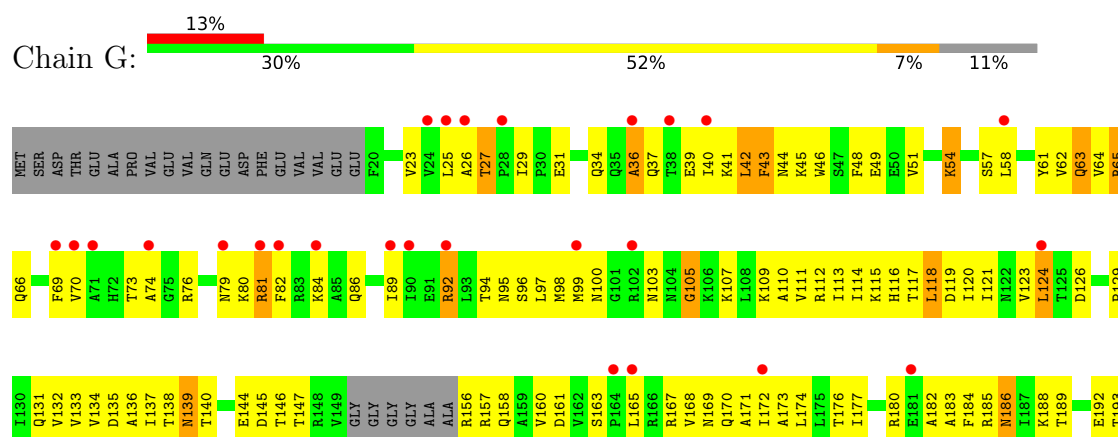


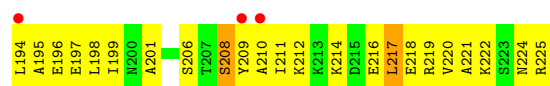


• Molecule 6: 40S ribosomal protein S4-A

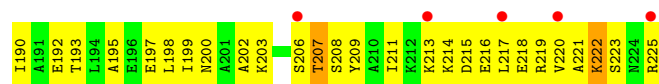
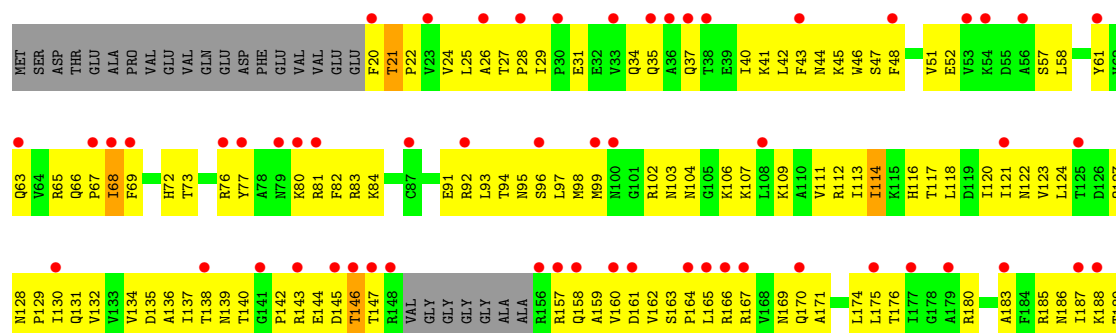


• Molecule 7: 40S ribosomal protein S5

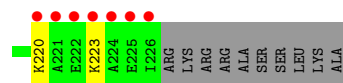
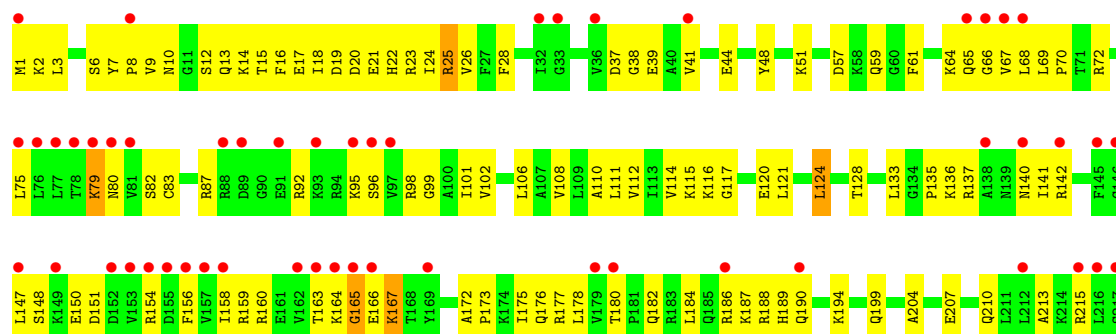




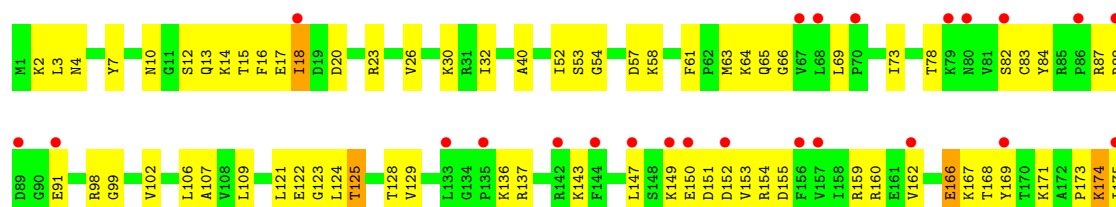
• Molecule 7: 40S ribosomal protein S5

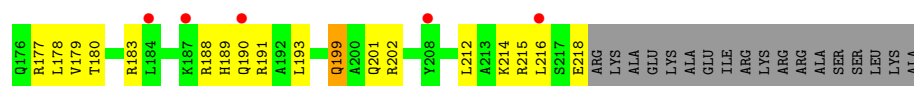


• Molecule 8: 40S ribosomal protein S6-A

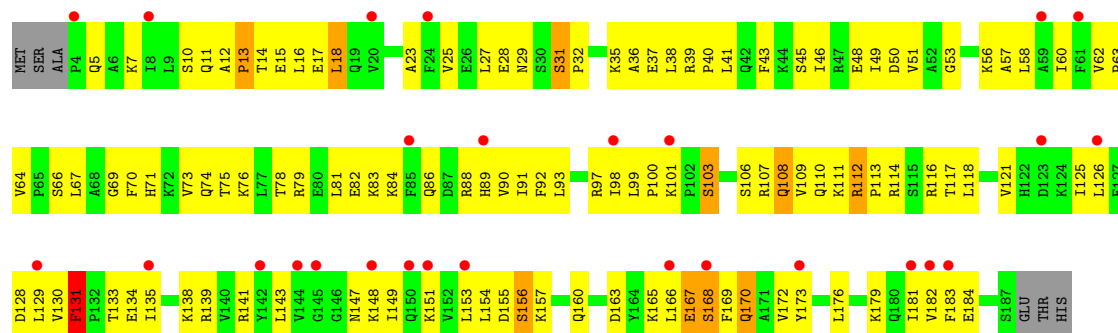


• Molecule 8: 40S ribosomal protein S6-A

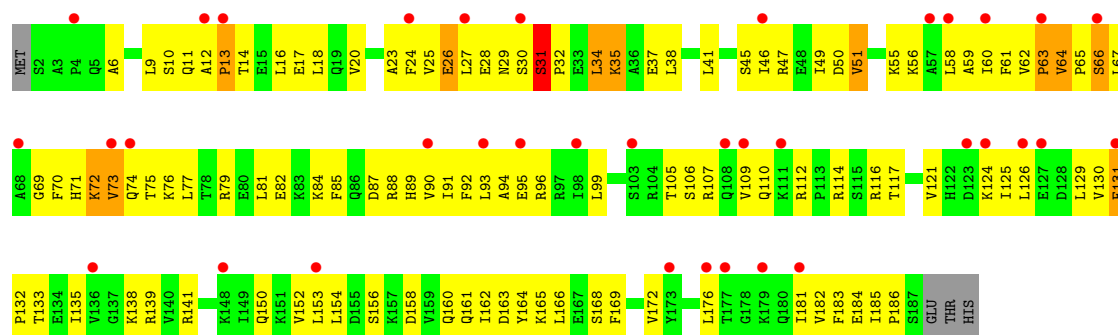




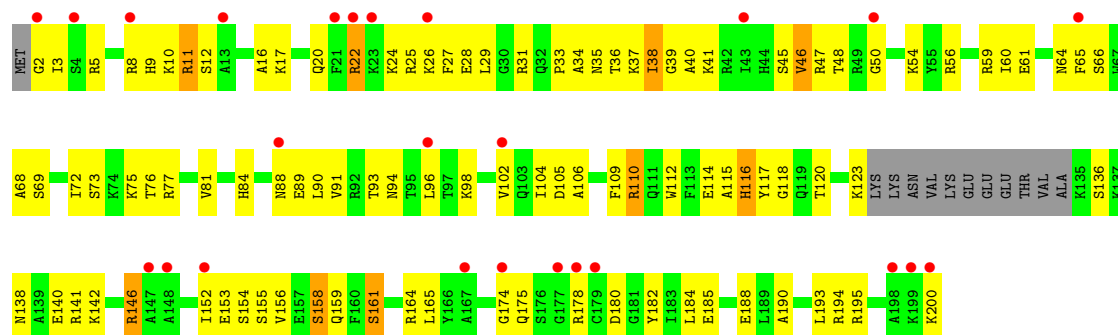
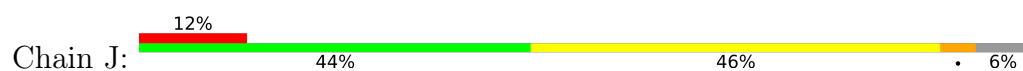
• Molecule 9: 40S ribosomal protein S7-A



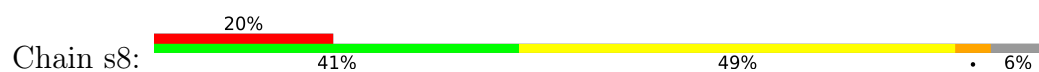
• Molecule 9: 40S ribosomal protein S7-A

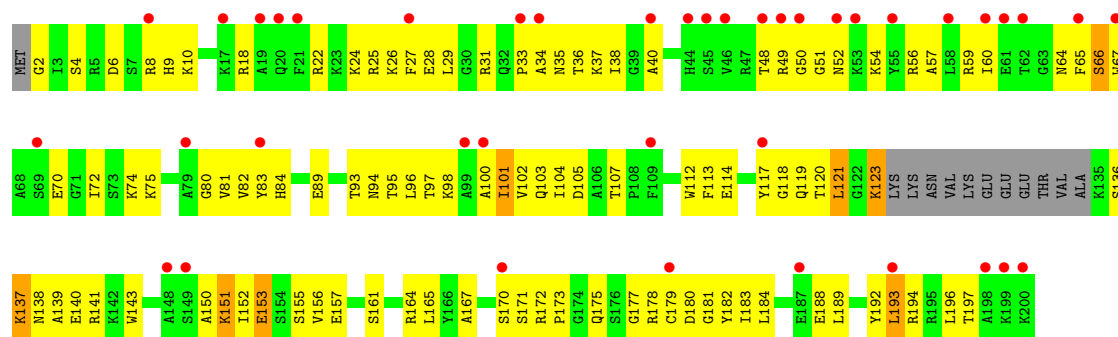


• Molecule 10: 40S ribosomal protein S8-A

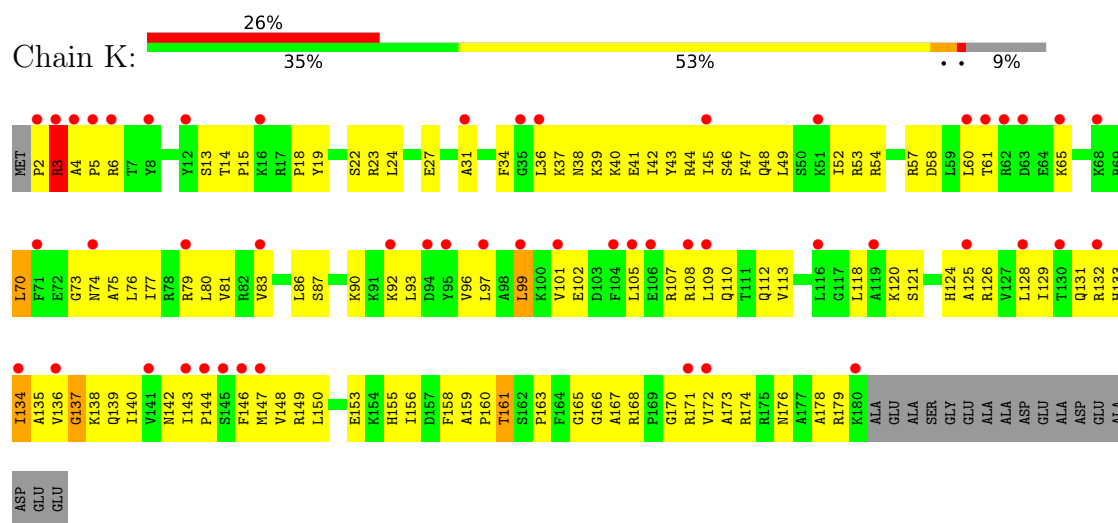


• Molecule 10: 40S ribosomal protein S8-A

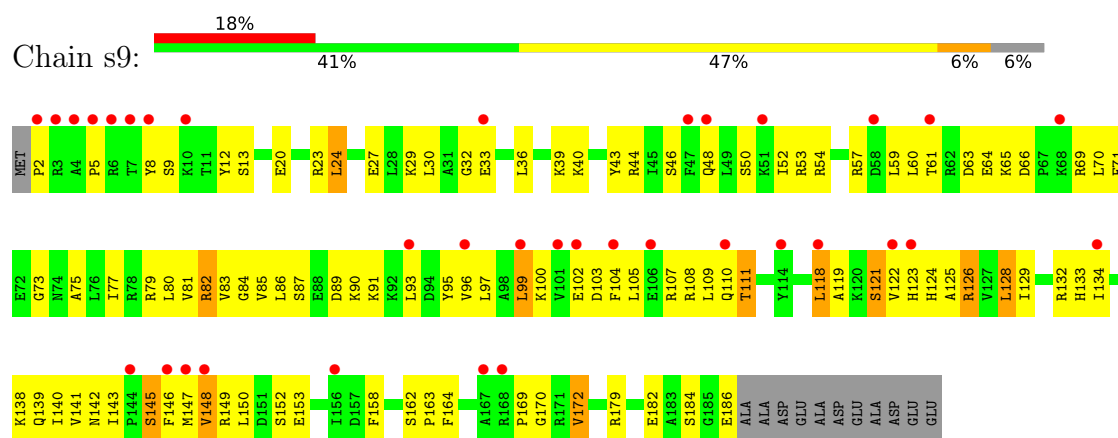




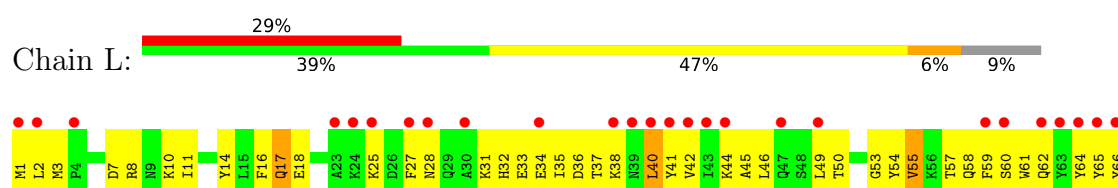
• Molecule 11: 40S ribosomal protein S9-A

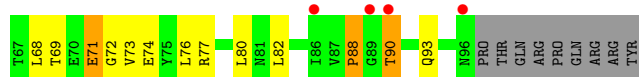


• Molecule 11: 40S ribosomal protein S9-A

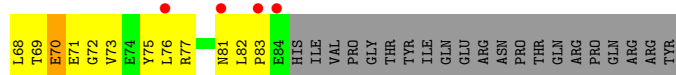
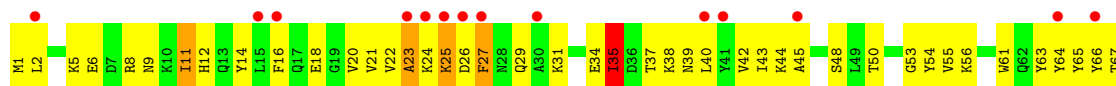


• Molecule 12: Small ribosomal subunit protein eS10A, Small ribosomal subunit protein eS10A, 40S ribosomal protein S10-A

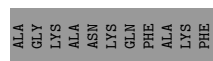
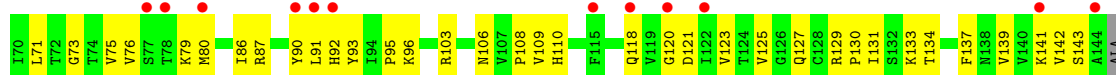
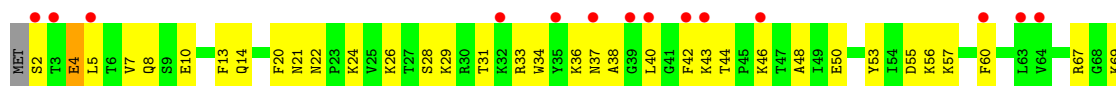




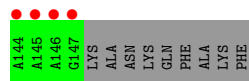
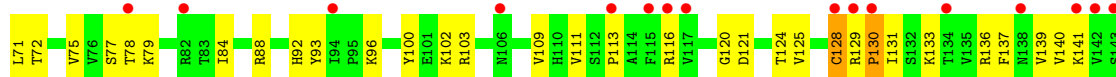
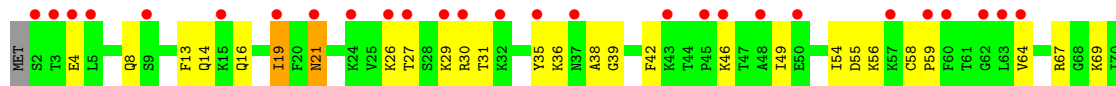
- Molecule 12: Small ribosomal subunit protein eS10A, Small ribosomal subunit protein eS10A, 40S ribosomal protein S10-A



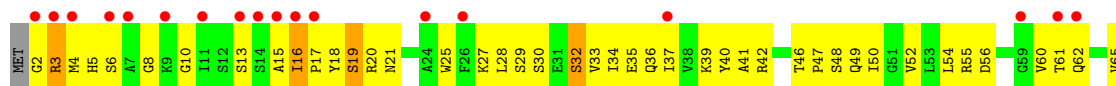
- Molecule 13: 40S ribosomal protein S11-A

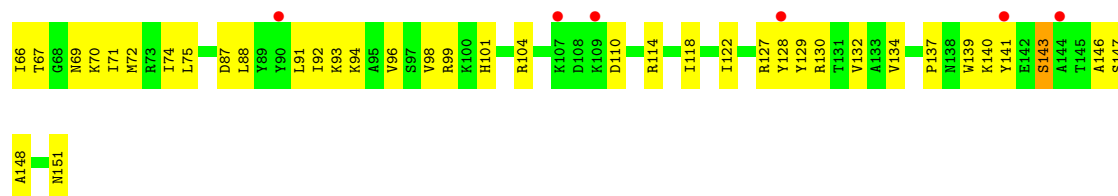


- Molecule 13: 40S ribosomal protein S11-A

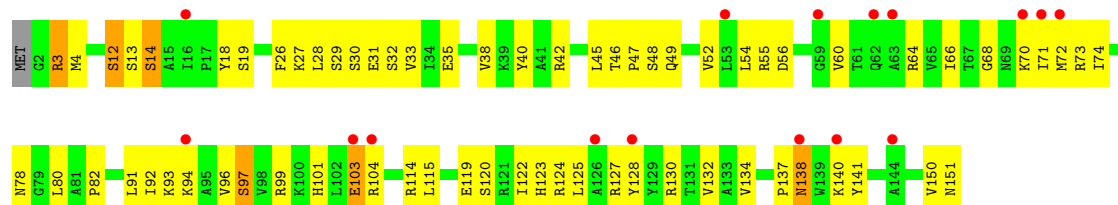


- Molecule 14: 40S ribosomal protein S13

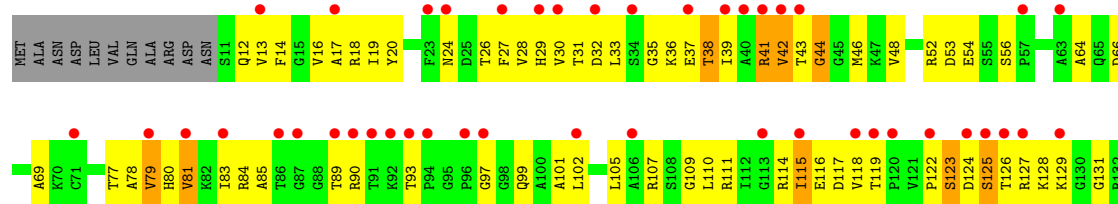




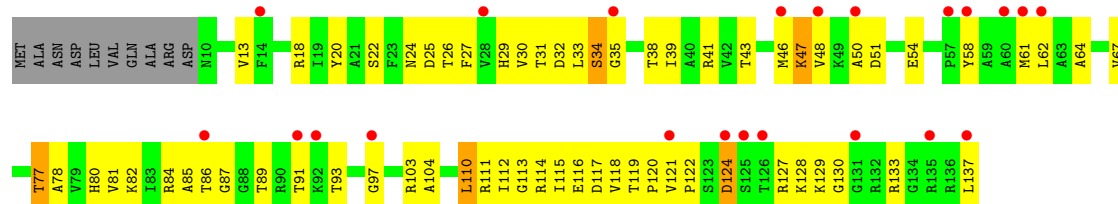
- Molecule 14: 40S ribosomal protein S13



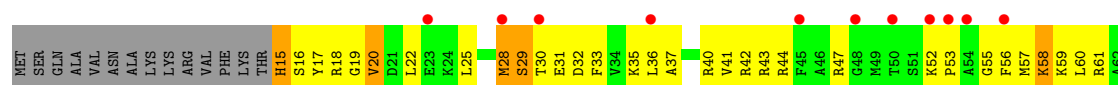
- Molecule 15: 40S ribosomal protein S14-B

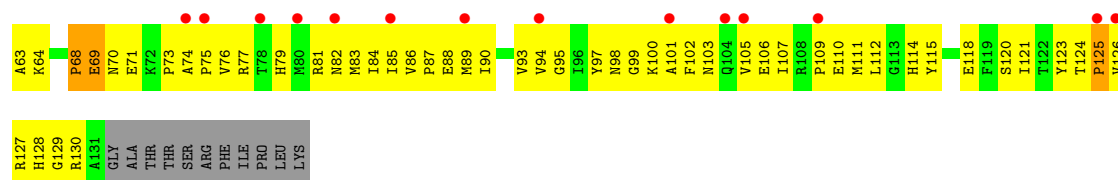


- Molecule 15: 40S ribosomal protein S14-B

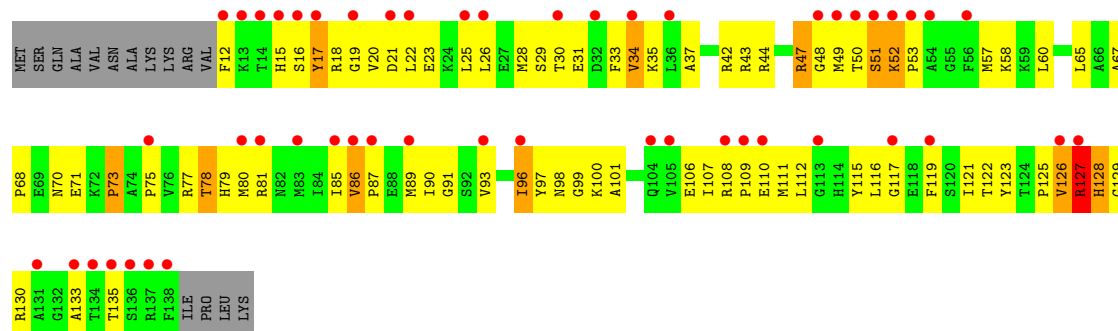


- Molecule 16: 40S ribosomal protein S15

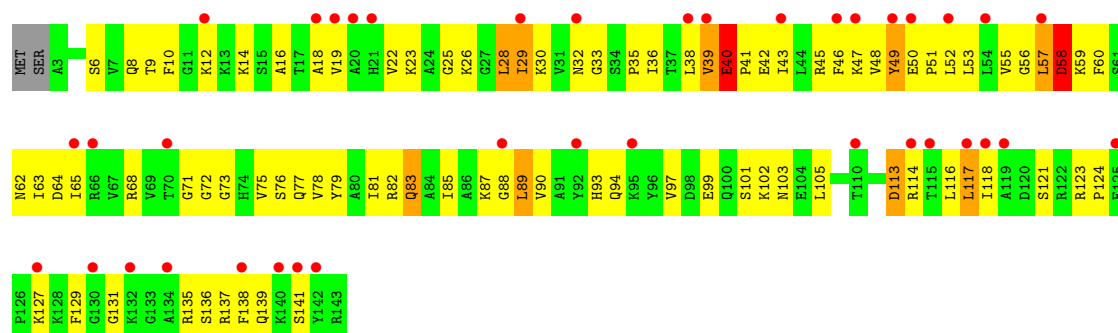




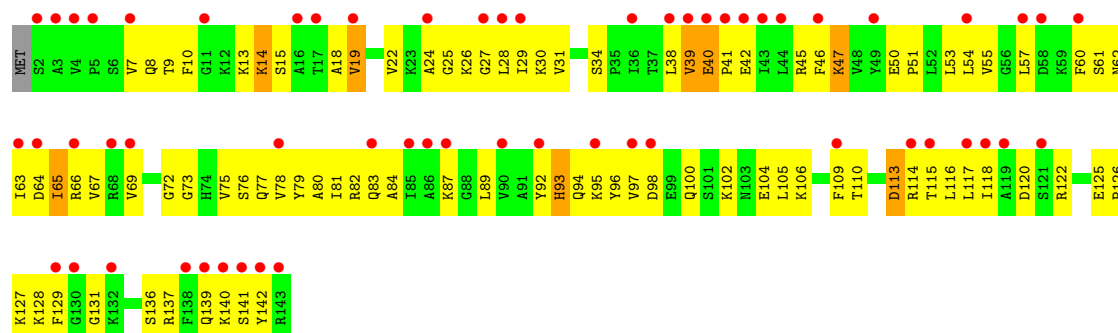
• Molecule 16: 40S ribosomal protein S15



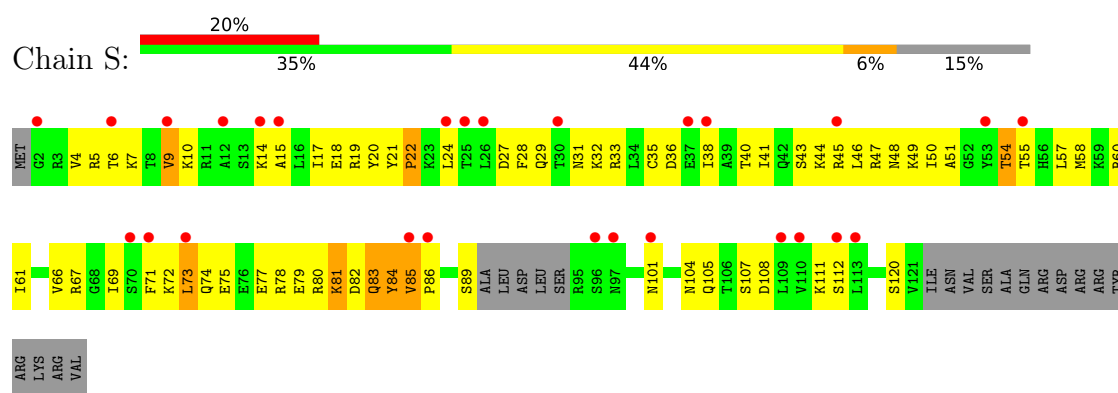
• Molecule 17: 40S ribosomal protein S16-A



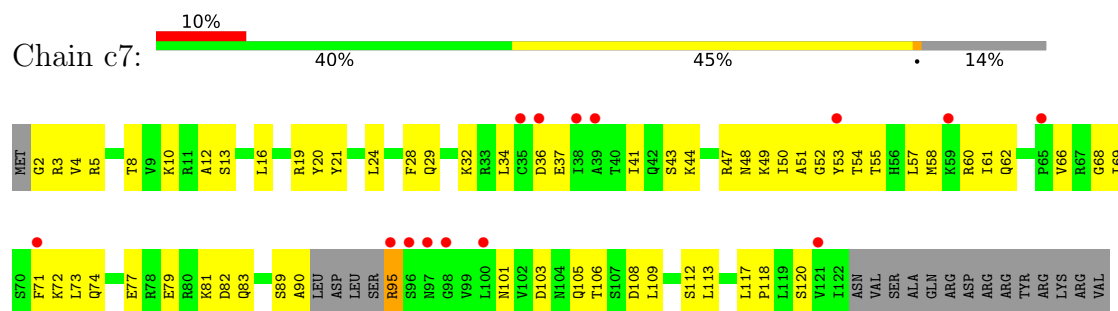
• Molecule 17: 40S ribosomal protein S16-A



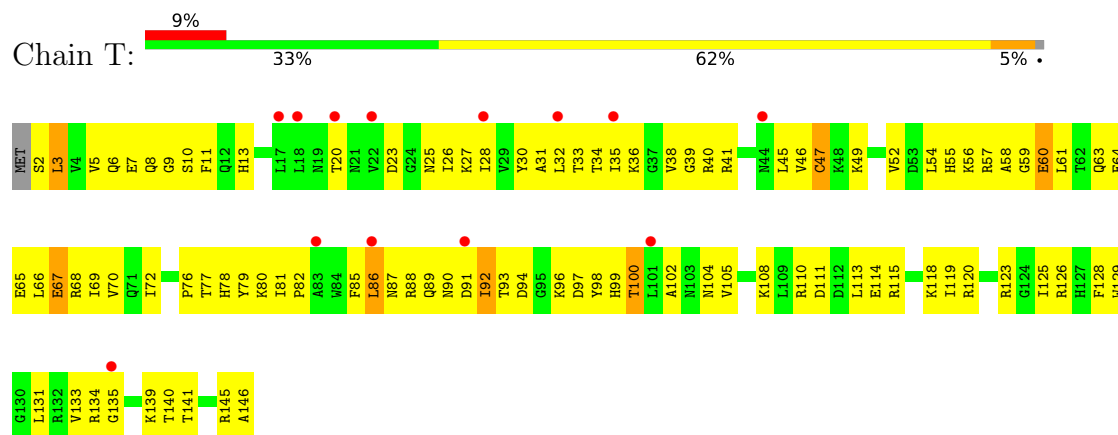
• Molecule 18: 40S ribosomal protein S17-A



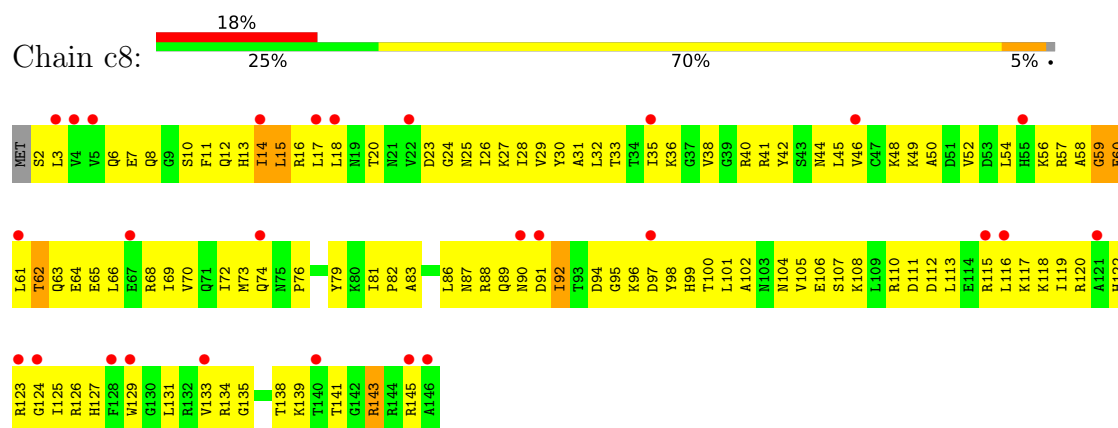
• Molecule 18: 40S ribosomal protein S17-A



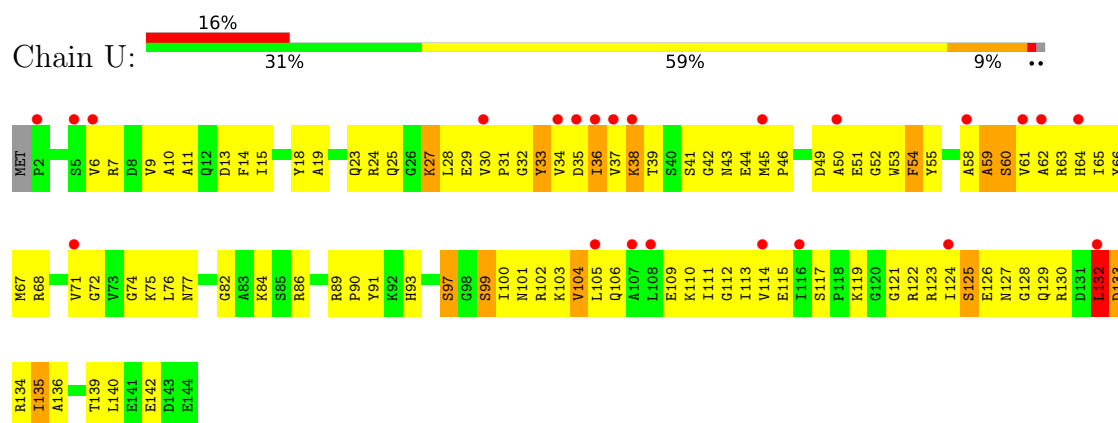
• Molecule 19: 40S ribosomal protein S18-A



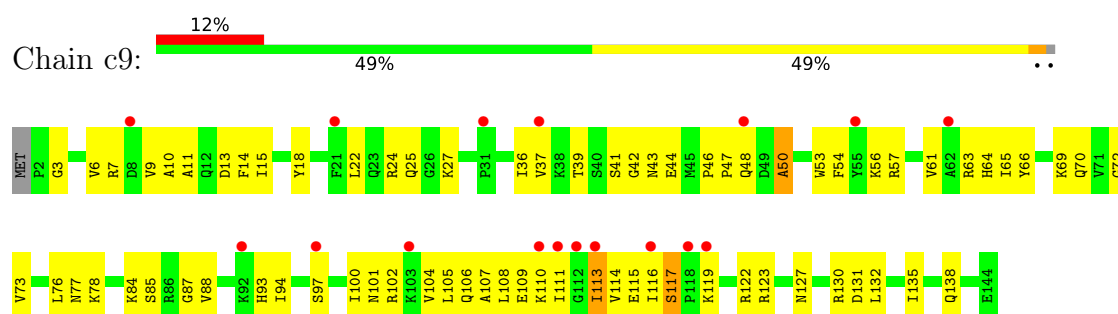
• Molecule 19: 40S ribosomal protein S18-A



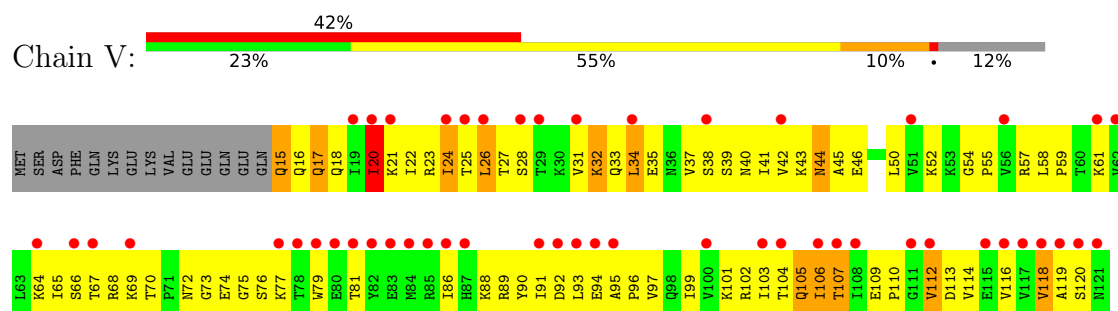
- Molecule 20: 40S ribosomal protein S19-A



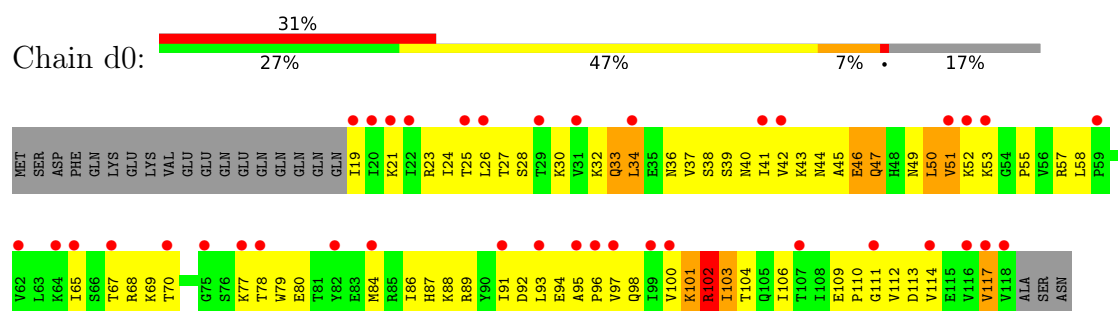
- Molecule 20: 40S ribosomal protein S19-A



- Molecule 21: Small ribosomal subunit protein uS10

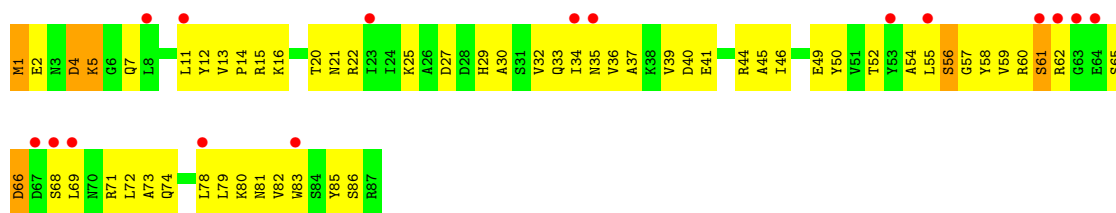


- Molecule 21: Small ribosomal subunit protein uS10

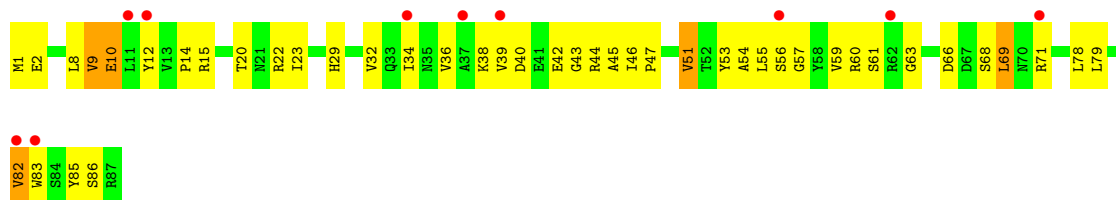


- Molecule 22: 40S ribosomal protein S21-A

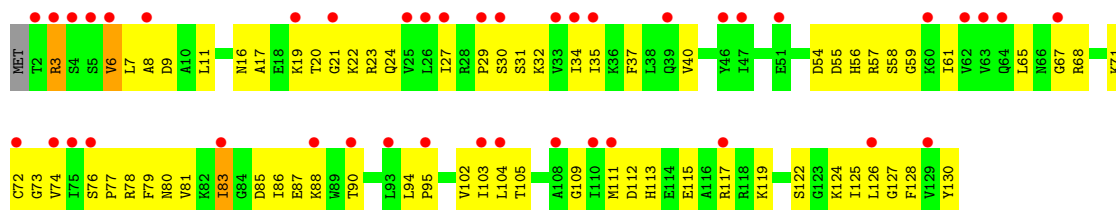




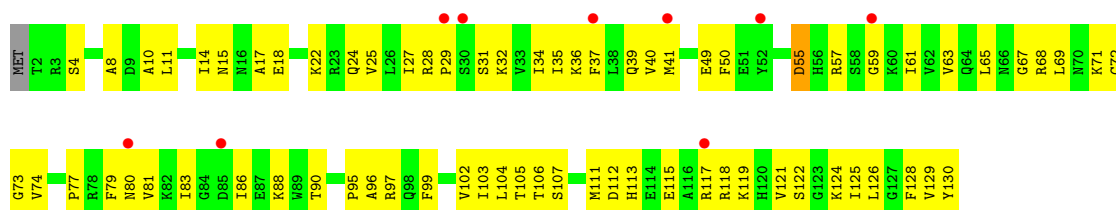
• Molecule 22: 40S ribosomal protein S21-A



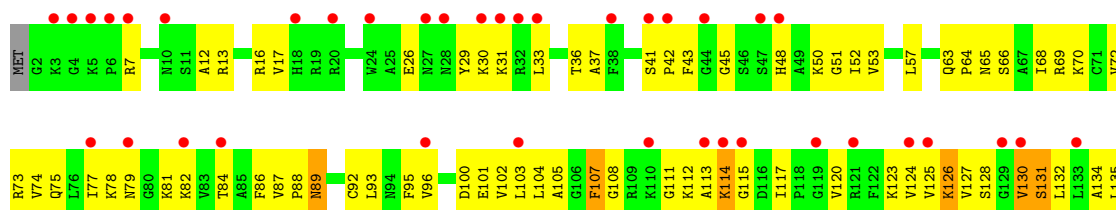
• Molecule 23: 40S ribosomal protein S22-A

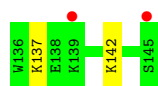


• Molecule 23: 40S ribosomal protein S22-A

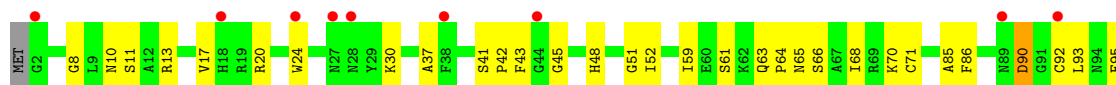


• Molecule 24: 40S ribosomal protein S23-A

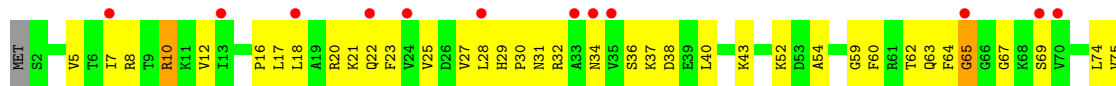




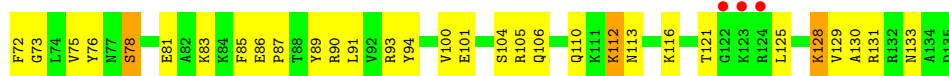
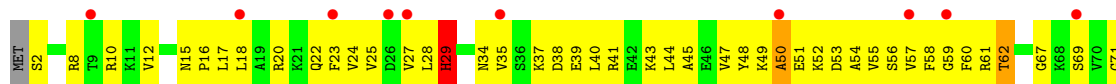
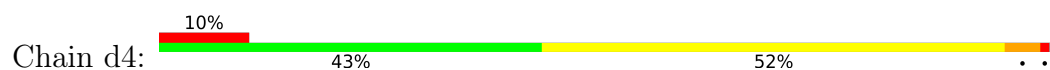
- Molecule 24: 40S ribosomal protein S23-A



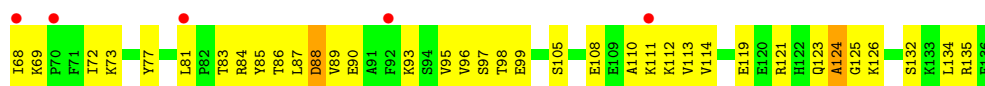
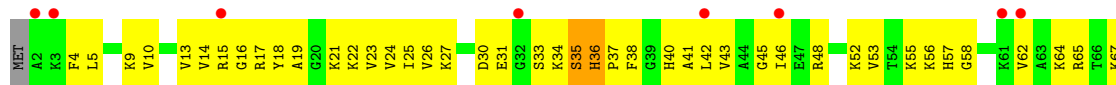
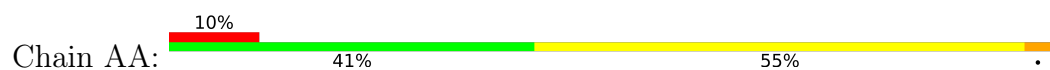
- Molecule 25: 40S ribosomal protein S24-A



- Molecule 25: 40S ribosomal protein S24-A

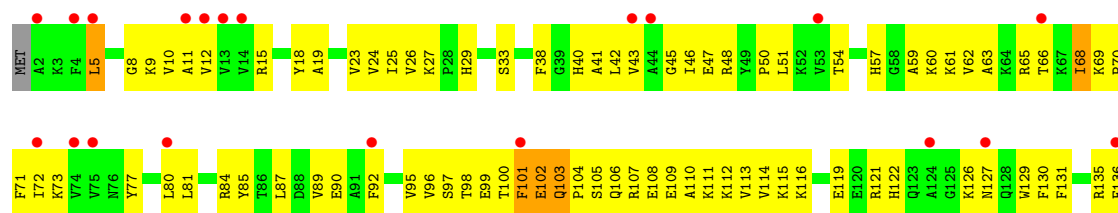


- Molecule 26: 60S ribosomal protein L27-A

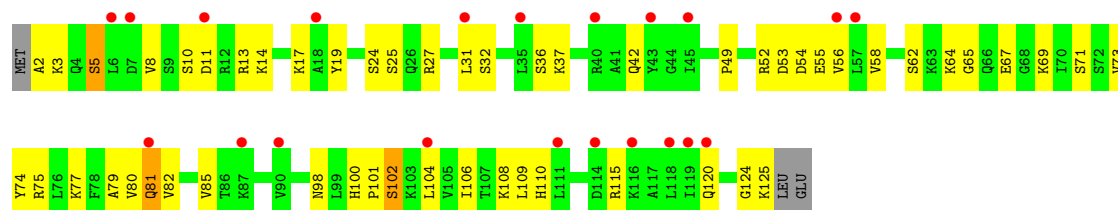


- Molecule 26: 60S ribosomal protein L27-A

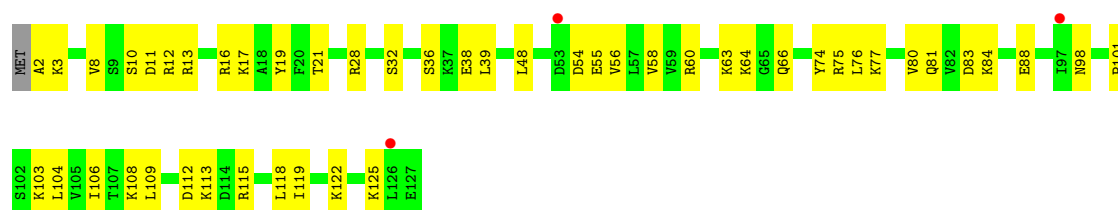




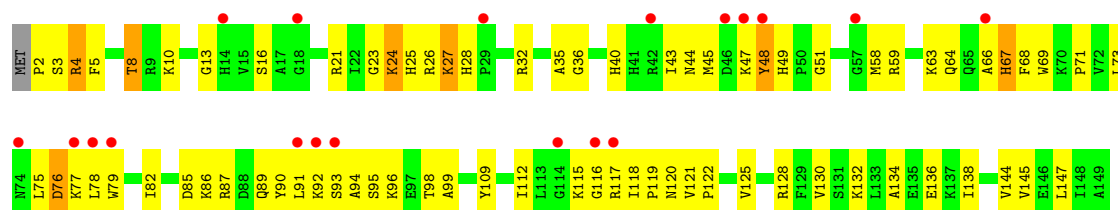
• Molecule 27: 60S ribosomal protein L26-A



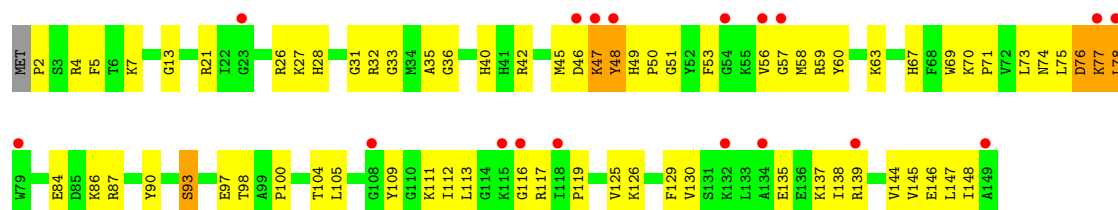
• Molecule 27: 60S ribosomal protein L26-A



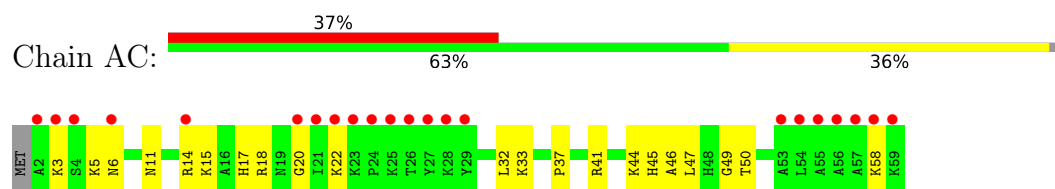
• Molecule 28: 60S ribosomal protein L28



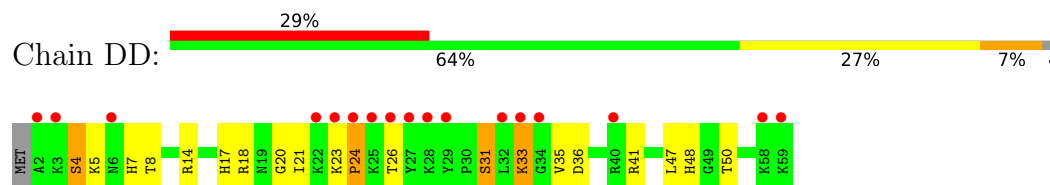
• Molecule 28: 60S ribosomal protein L28



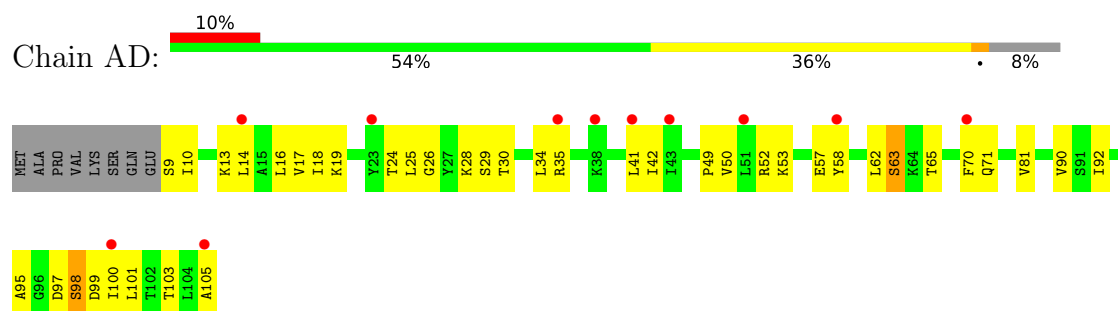
- Molecule 29: 60S ribosomal protein L29



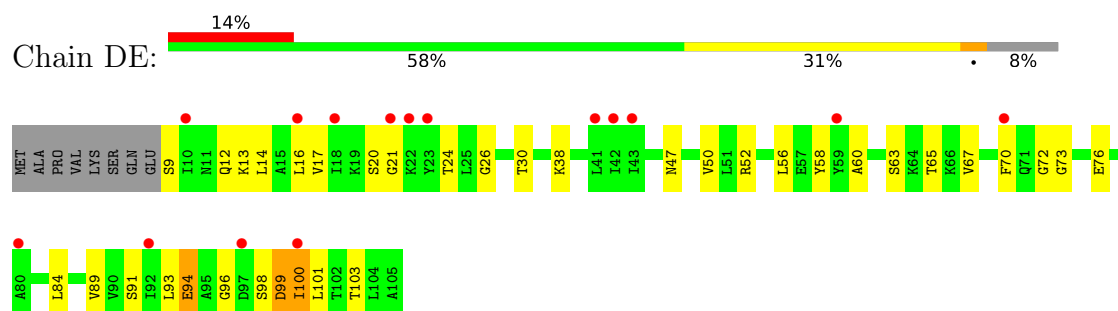
- Molecule 29: 60S ribosomal protein L29



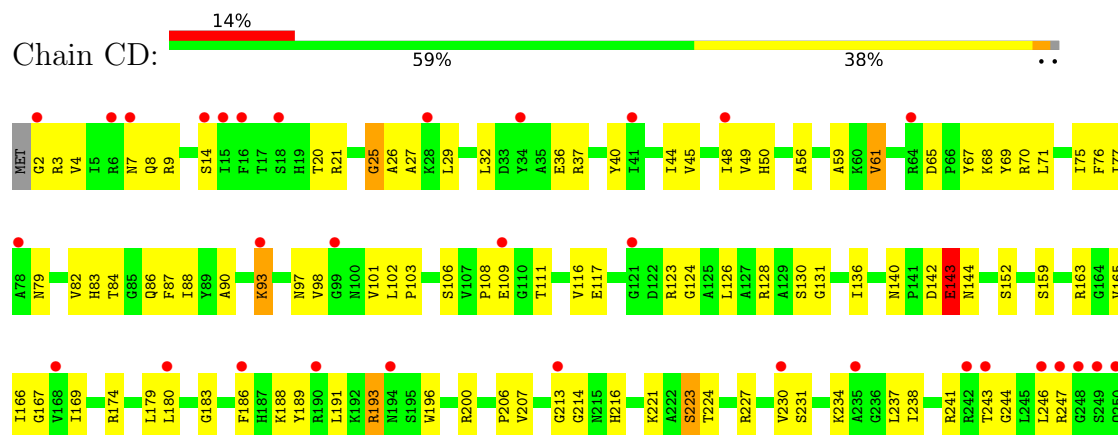
- Molecule 30: 60S ribosomal protein L30



- Molecule 30: 60S ribosomal protein L30



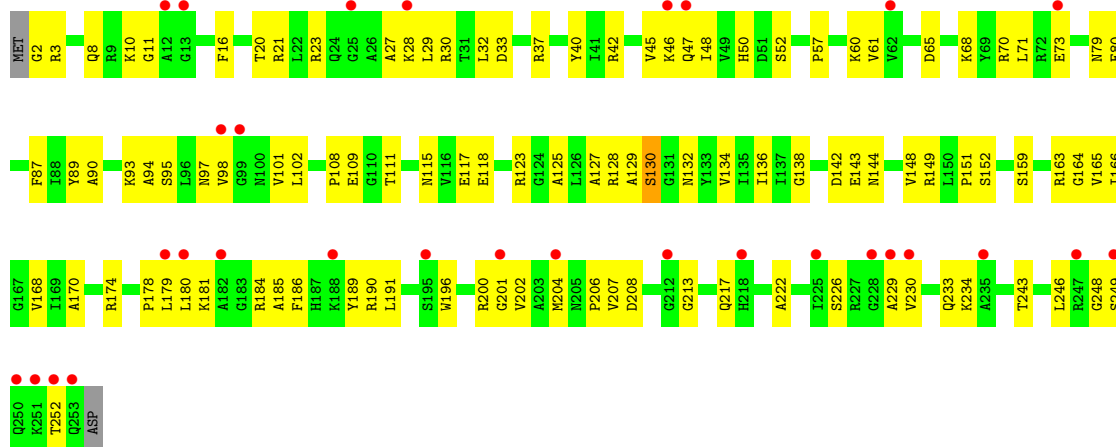
- Molecule 31: 60S ribosomal protein L2-A





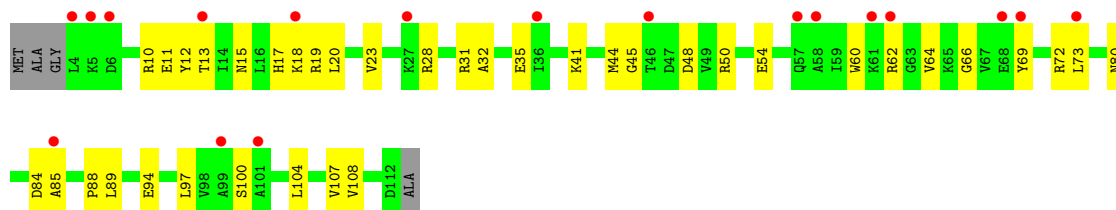
• Molecule 31: 60S ribosomal protein L2-A

Chain j: 12% 57% 41%



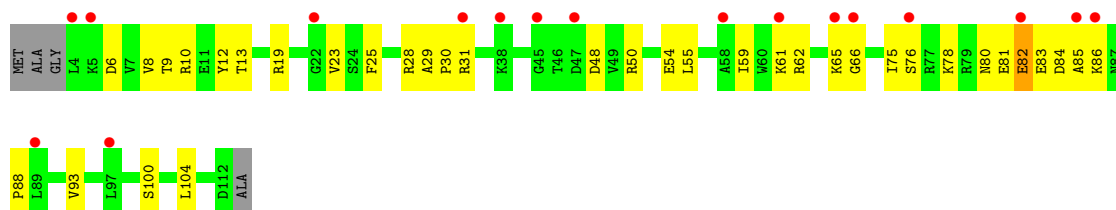
• Molecule 32: 60S ribosomal protein L31-A

Chain AE: 16% 63% 34%



• Molecule 32: 60S ribosomal protein L31-A

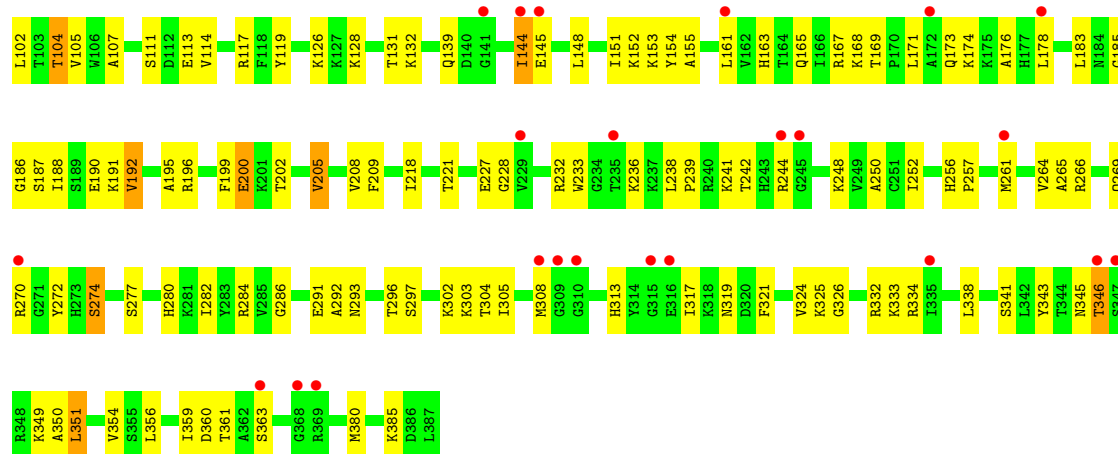
Chain DF: 15% 65% 31%



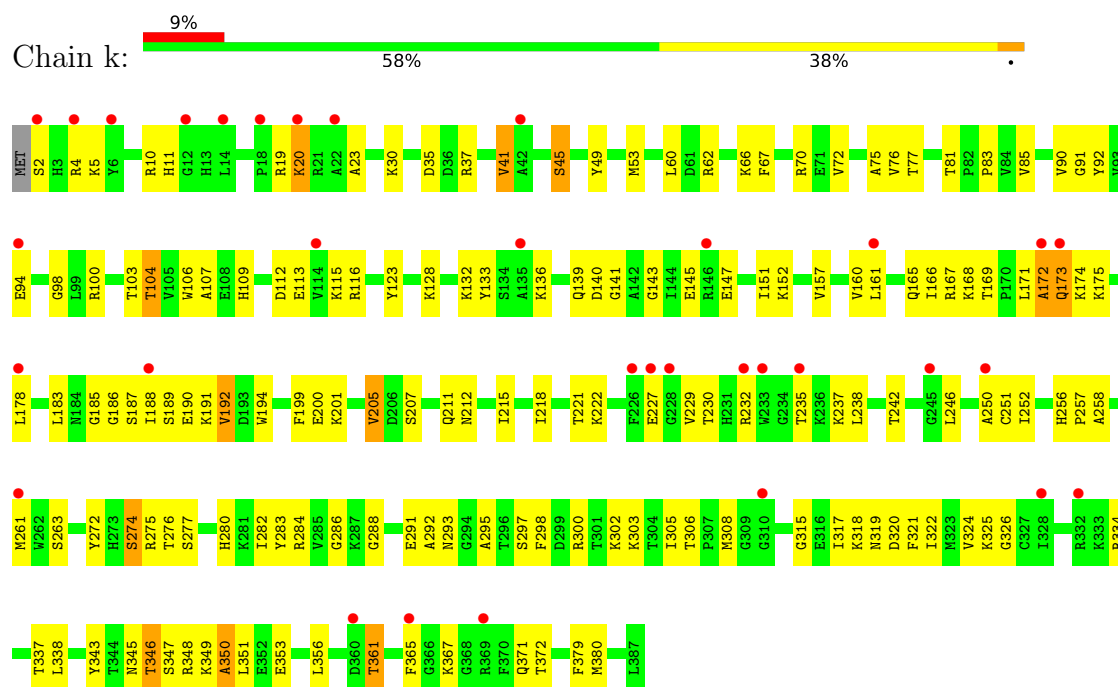
• Molecule 33: 60S ribosomal protein L3

Chain CE: 7% 61% 36%

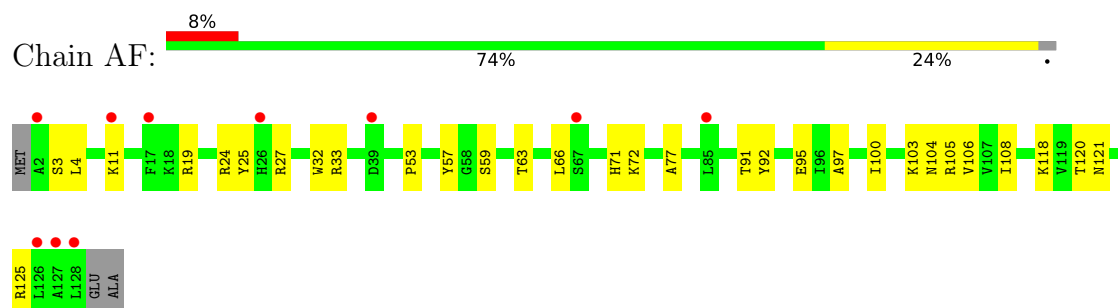




• Molecule 33: 60S ribosomal protein L3

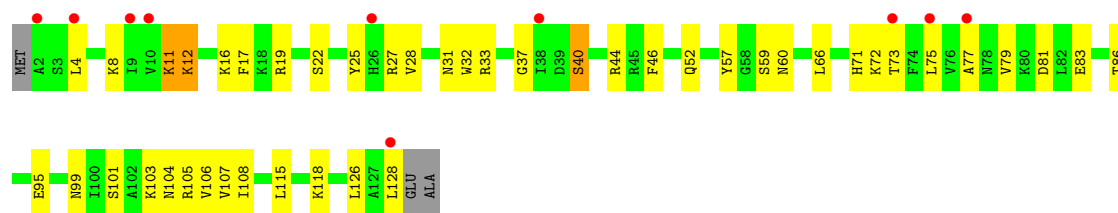


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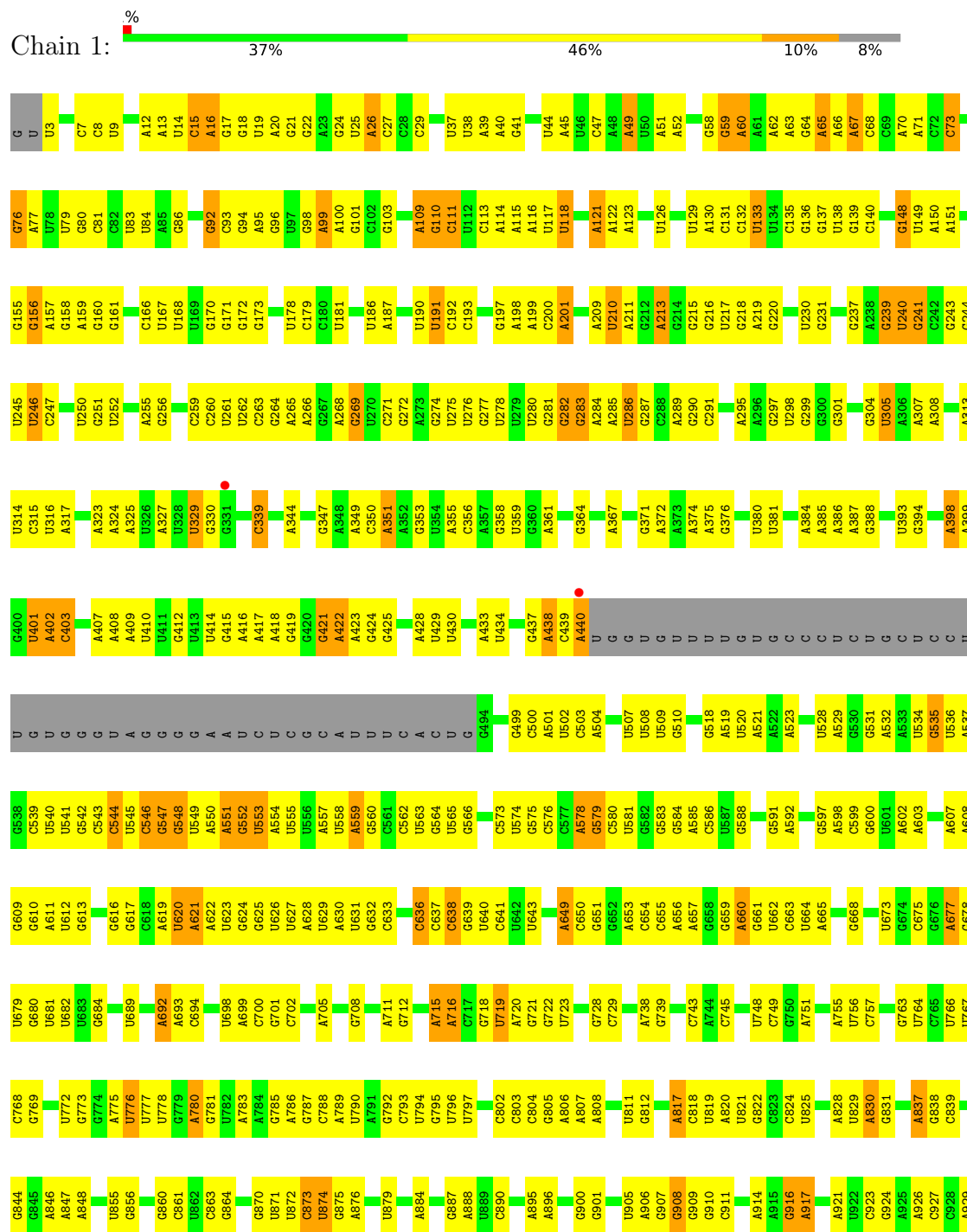


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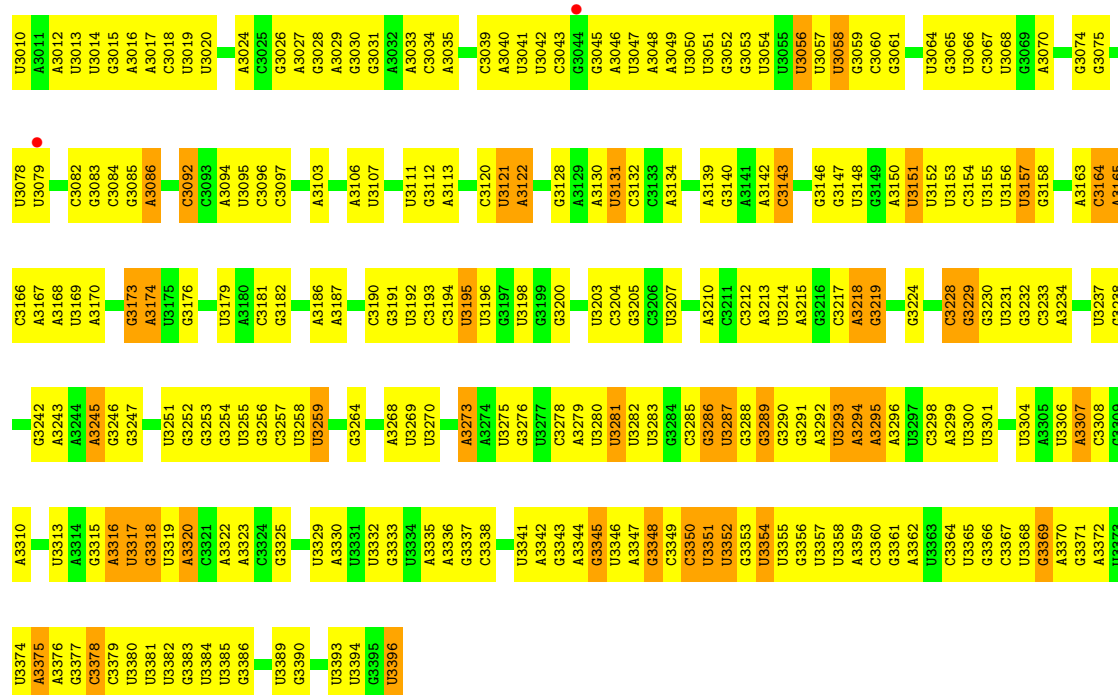


● Molecule 35: 25S ribosomal RNA

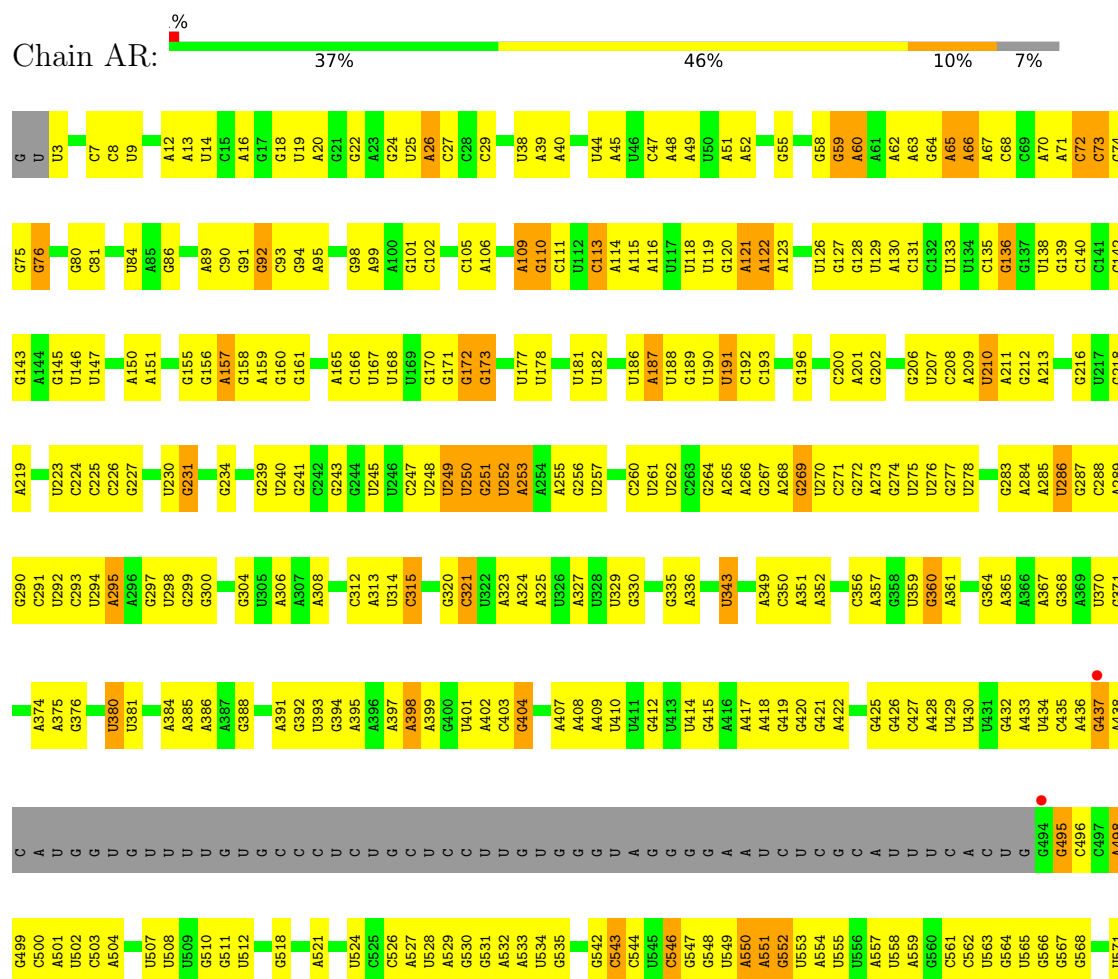


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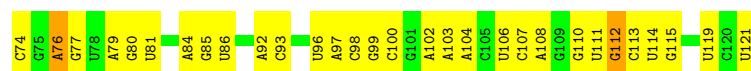


• Molecule 35: 25S ribosomal RNA

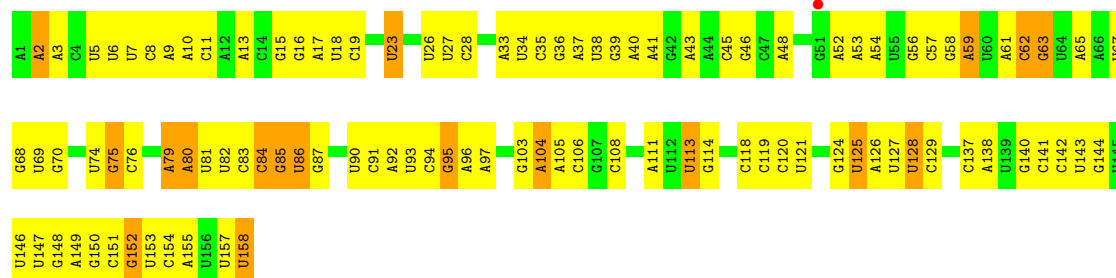


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G1640	U1493	C1423	U1336	C1248	G1173	U1090	C1016	U952	G870	U789	A705	U627
U1641	U1494	U1424	A1337	G1249	C1174	A1093	C1017	C953	U871	G791	G712	A628
A1642	U1495	U1425	G1338	U1250	G1175	U1094	G1018	G954	U872	G792	U713	U629
A1643	C1496	G1426	U1339	A1251	C1176	U1095	G1019	U955	C873	C793	U714	A630
G1644	C1497	U1427	U1340	U1252	G1177	U1096	G1020	U956	U874	U794	A715	U631
U1645	A1498	U1428	U1341	C1254	U1180	G1097	G1021	U957	C875	G795	A716	G632
U1646	C1499	U1429	G1342	C1255	U1181	A1098	U1022	C958	U879	U796	C717	C633
U1647	C1502	U1430	U1343	U1256	C1182	G1101	G1024	C959	A884	U797	G718	C634
U1648	A1503	G1431	U1344	C1257	C1183	A1102	A1025	U960	U887	G798	G635	G635
U1649	A1504	C1432	G1345	U1258	U1184	A1103	A1026	C961	G800	U799	C636	C636
U1650	C1505	A1433	U1346	U1259	C1185	G1104	A1027	A962	U888	C802	G721	G639
U1651	U1507	G1434	U1347	A1260	U1190	A1105	U1028	G963	U889			
A1654	U1508	U1435	U1348									
G1655	U1509	U1436	G1349									
A1656	G1507	G1437	G1350									
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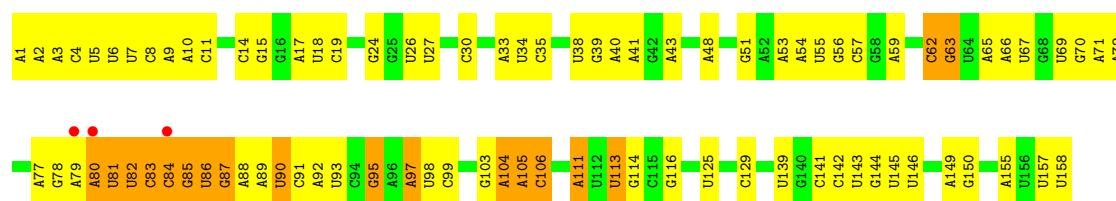




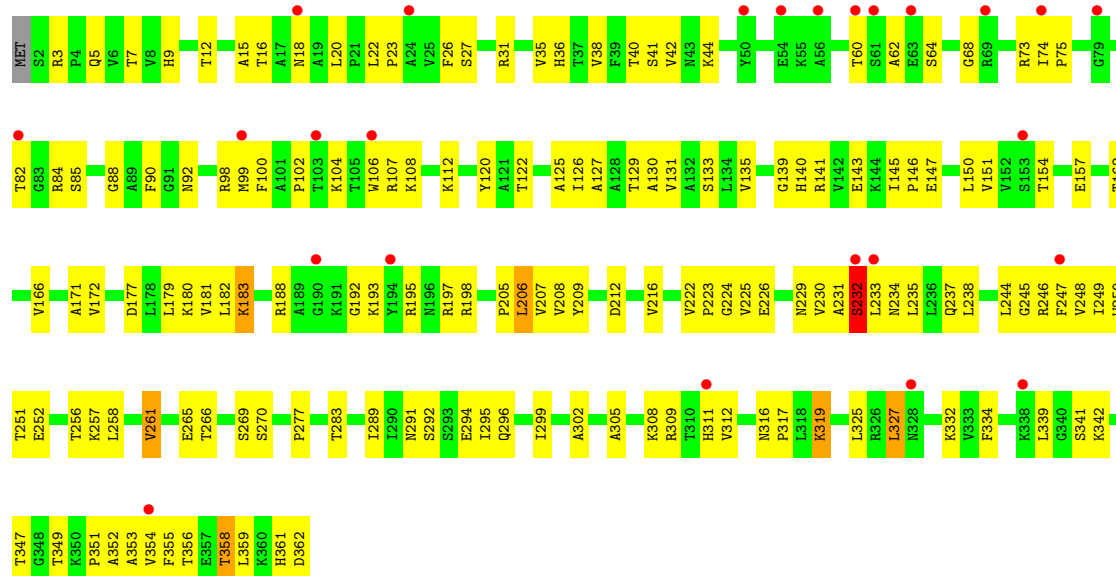
- Molecule 37: 5.8S ribosomal RNA



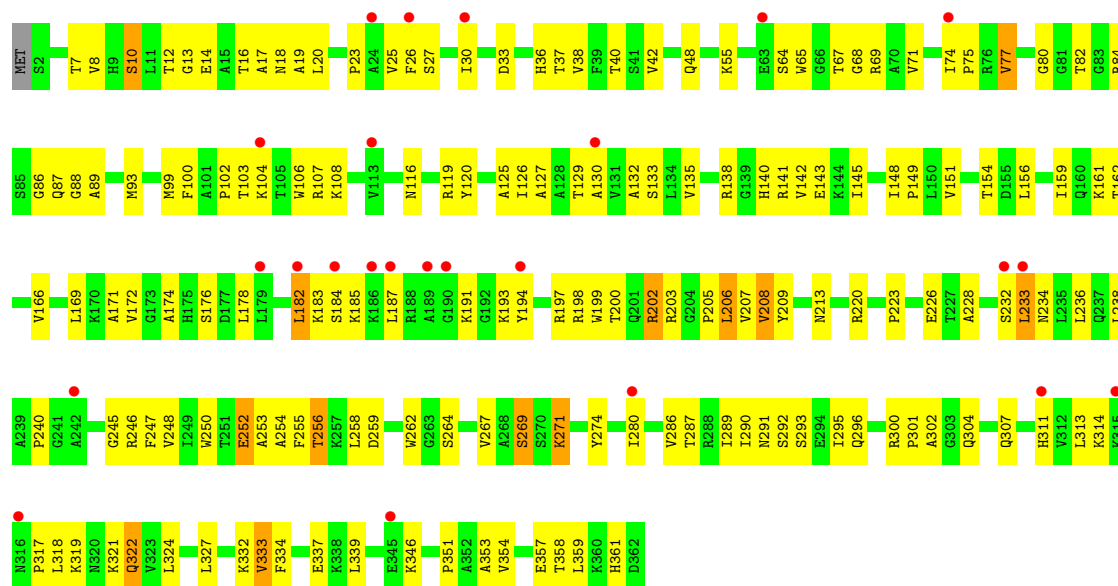
- Molecule 37: 5.8S ribosomal RNA



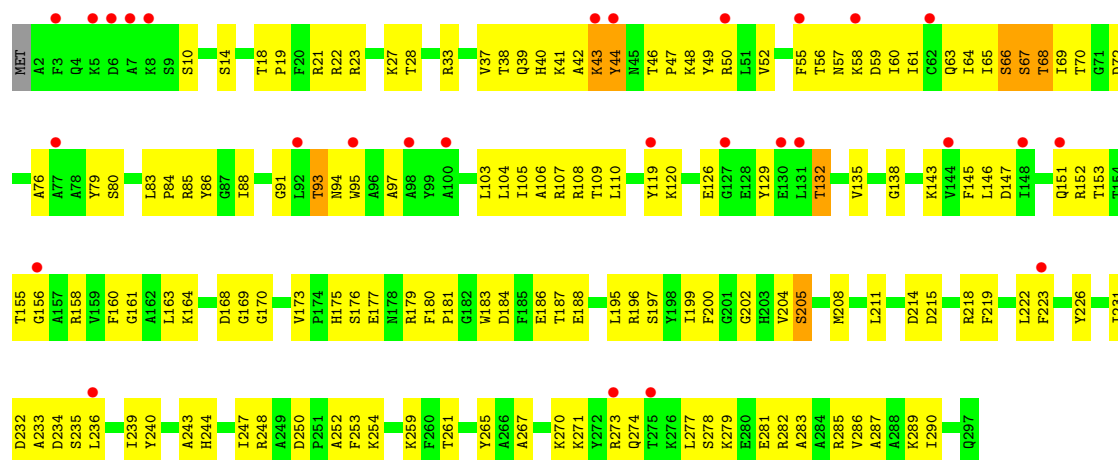
- Molecule 38: 60S ribosomal protein L4-A



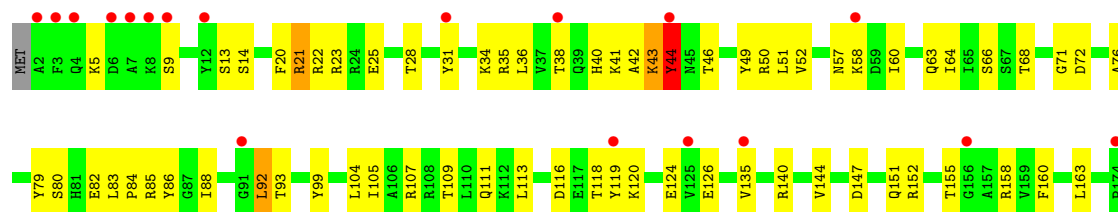
- Molecule 38: 60S ribosomal protein L4-A

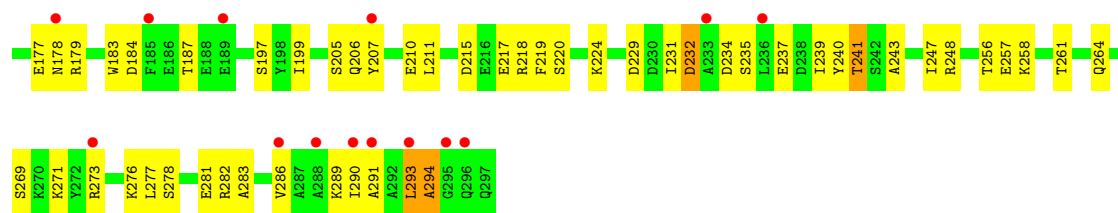


• Molecule 39: 60S ribosomal protein L5

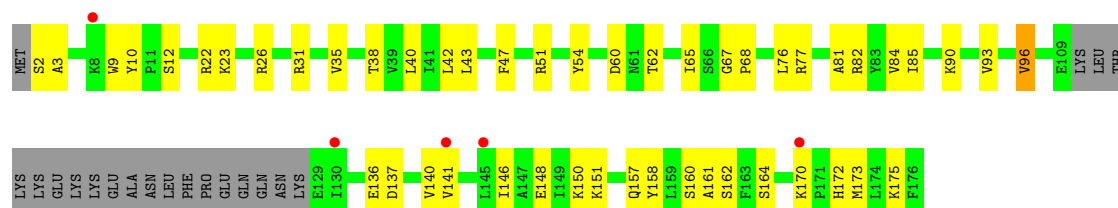


• Molecule 39: 60S ribosomal protein L5

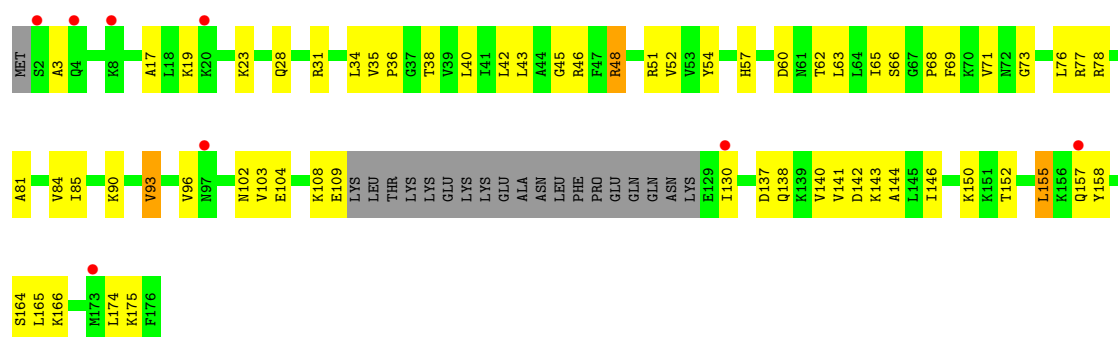




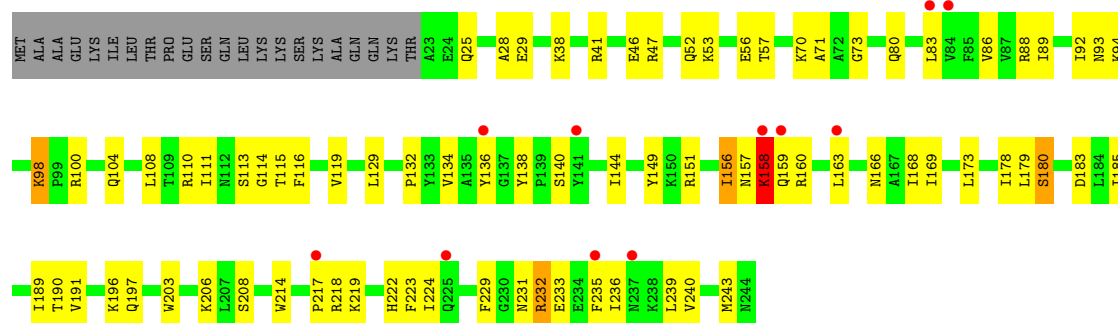
• Molecule 40: 60S ribosomal protein L6-A



• Molecule 40: 60S ribosomal protein L6-A

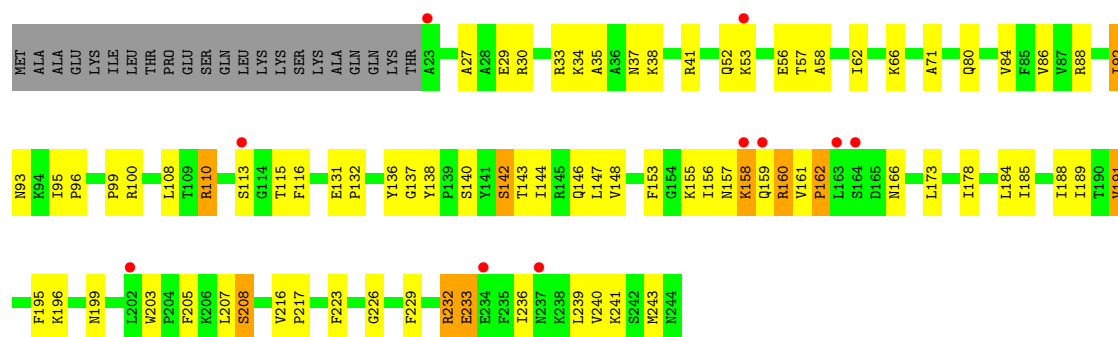


• Molecule 41: 60S ribosomal protein L7-A

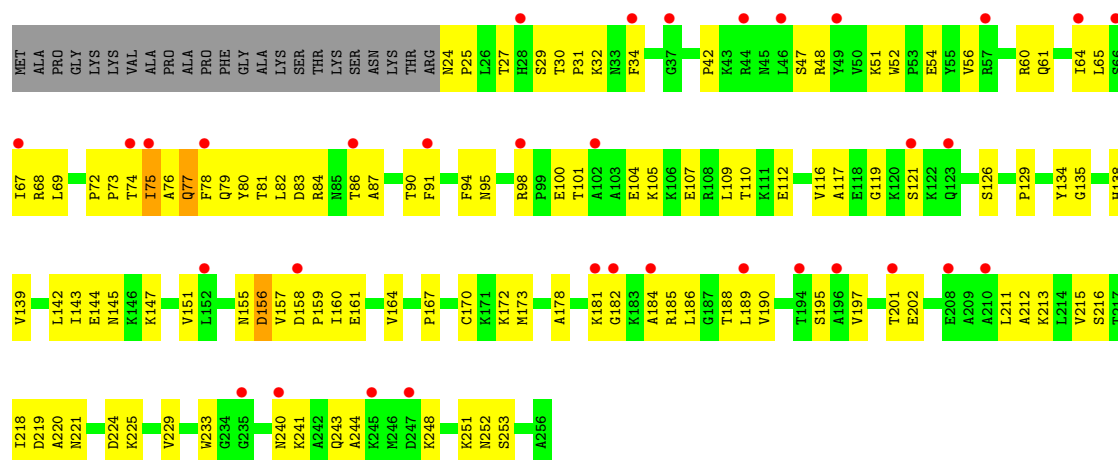


• Molecule 41: 60S ribosomal protein L7-A

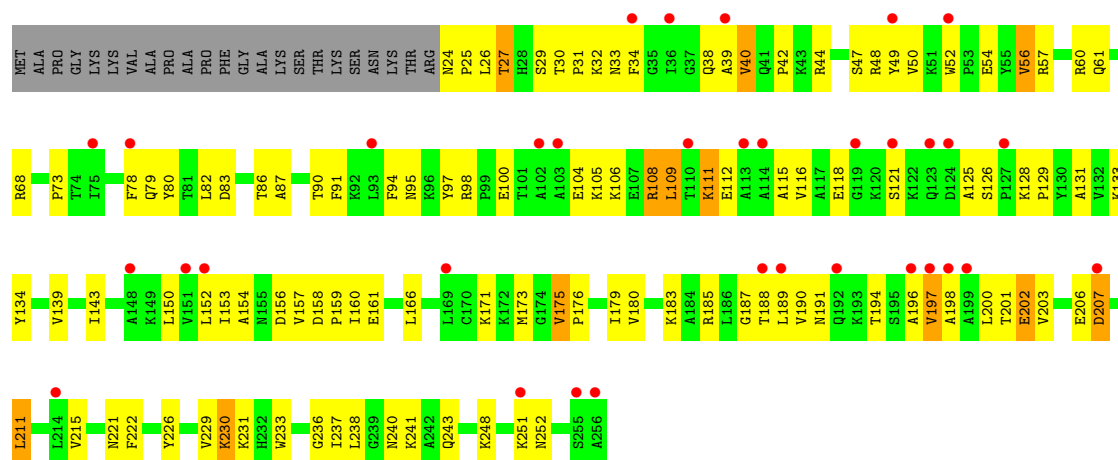




• Molecule 42: 60S ribosomal protein L8-A

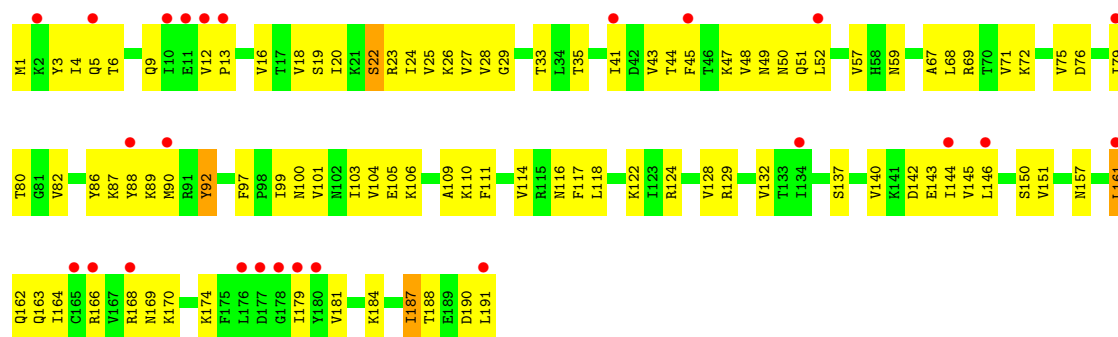


• Molecule 42: 60S ribosomal protein L8-A

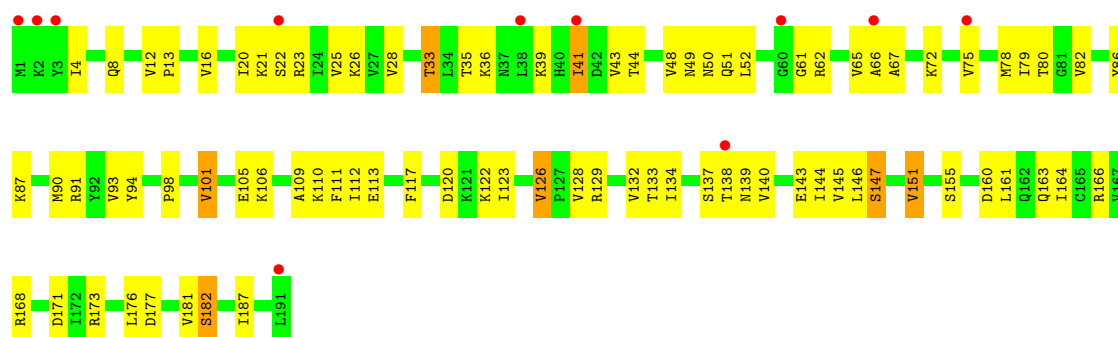


• Molecule 43: 60S ribosomal protein L9-A

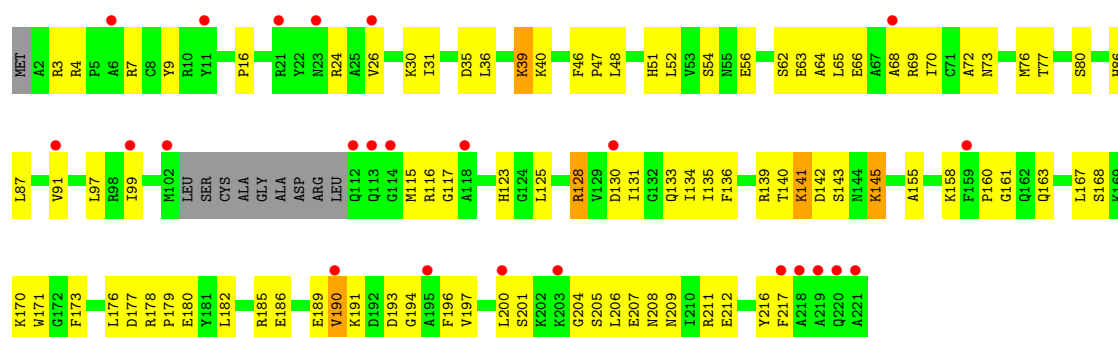




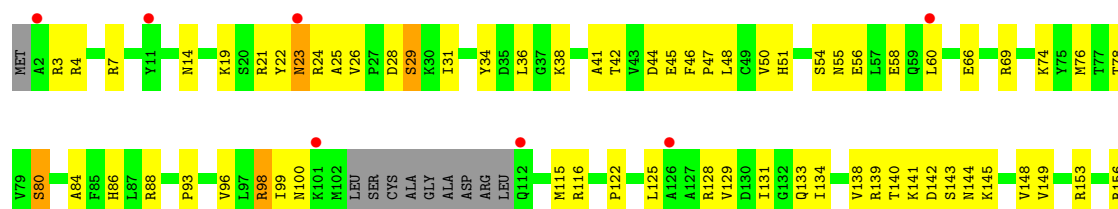
• Molecule 43: 60S ribosomal protein L9-A

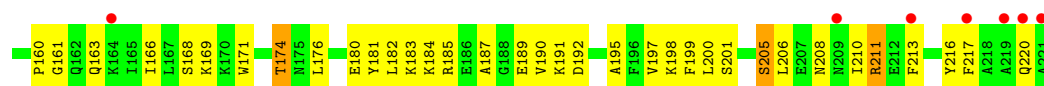


• Molecule 44: 60S ribosomal protein L10

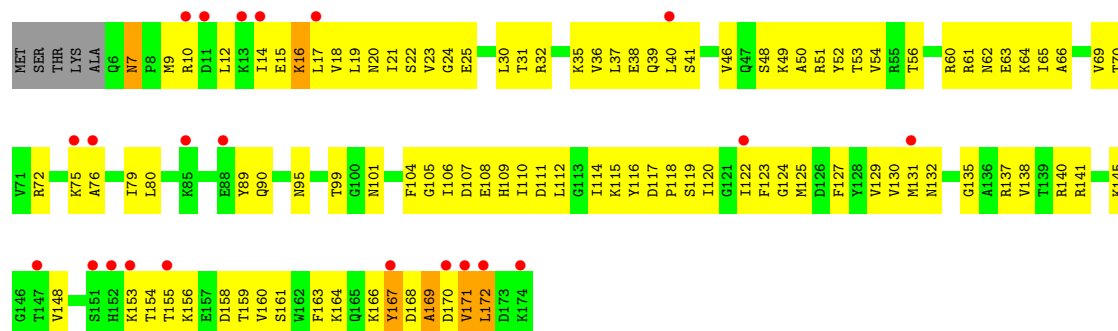


• Molecule 44: 60S ribosomal protein L10

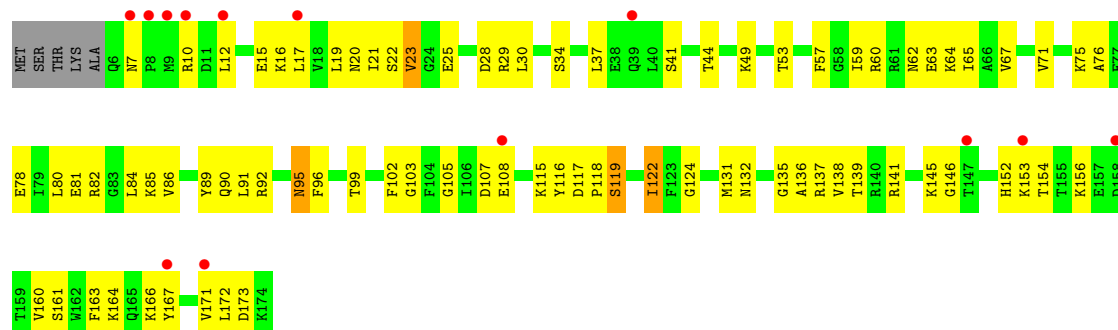




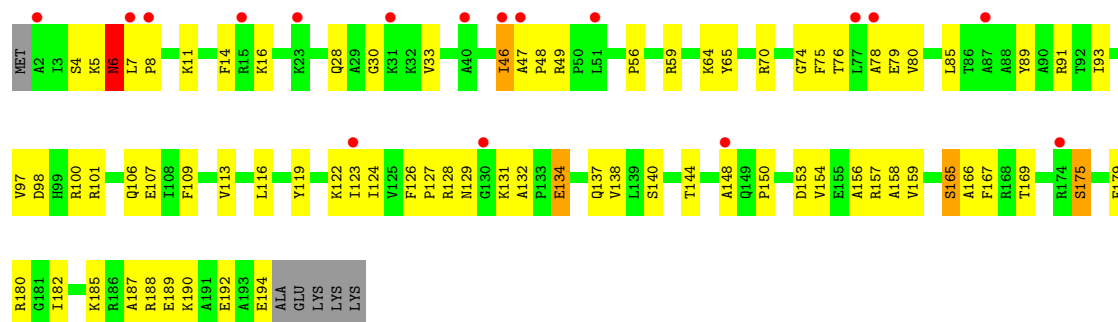
• Molecule 45: Large ribosomal subunit protein uL5B



• Molecule 45: Large ribosomal subunit protein uL5B

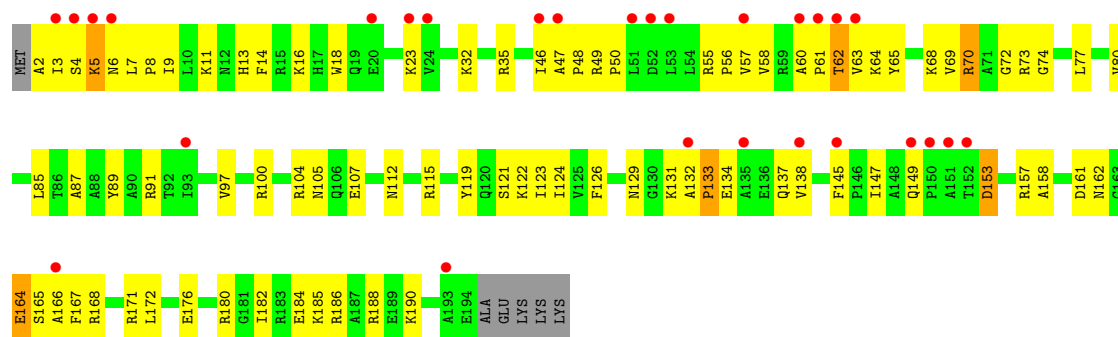


• Molecule 46: 60S ribosomal protein L13-A

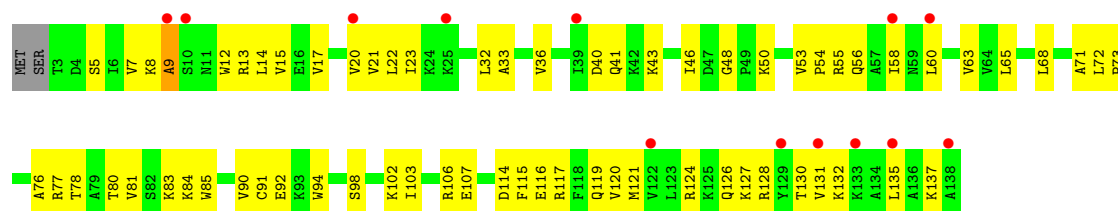


• Molecule 46: 60S ribosomal protein L13-A

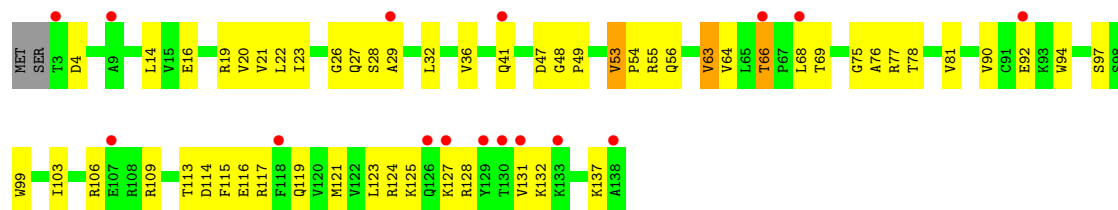




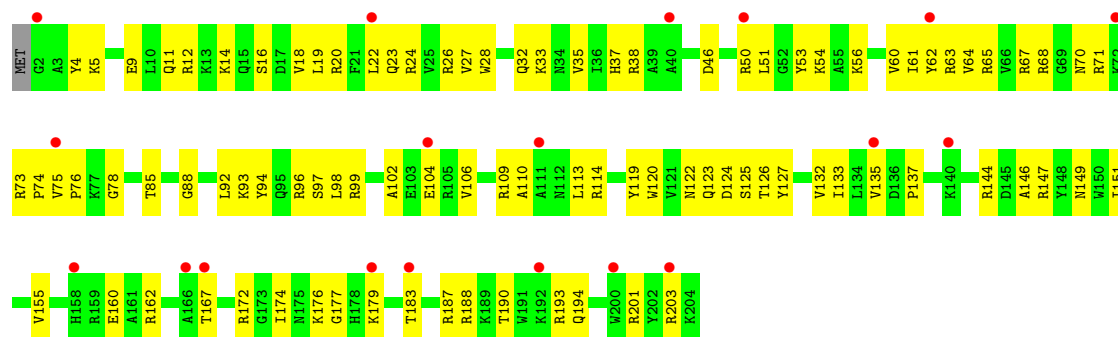
• Molecule 47: 60S ribosomal protein L14-A



• Molecule 47: 60S ribosomal protein L14-A

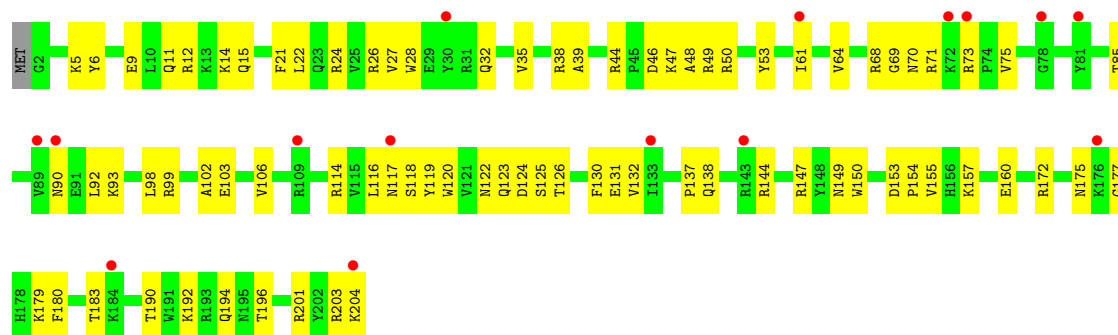


• Molecule 48: 60S ribosomal protein L15-A

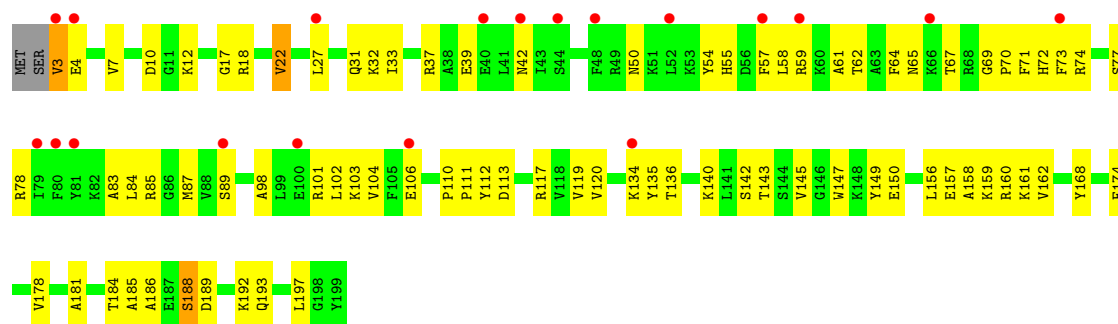


• Molecule 48: 60S ribosomal protein L15-A

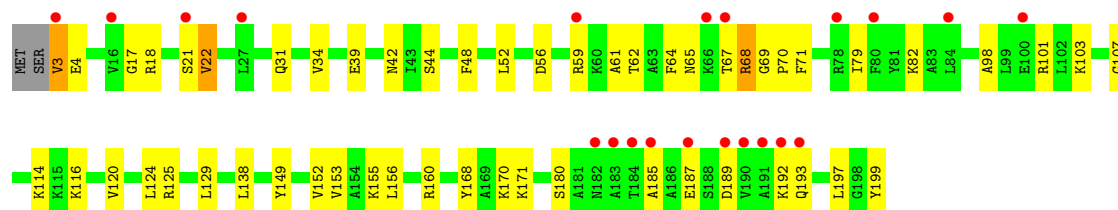
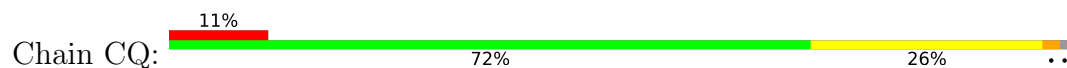




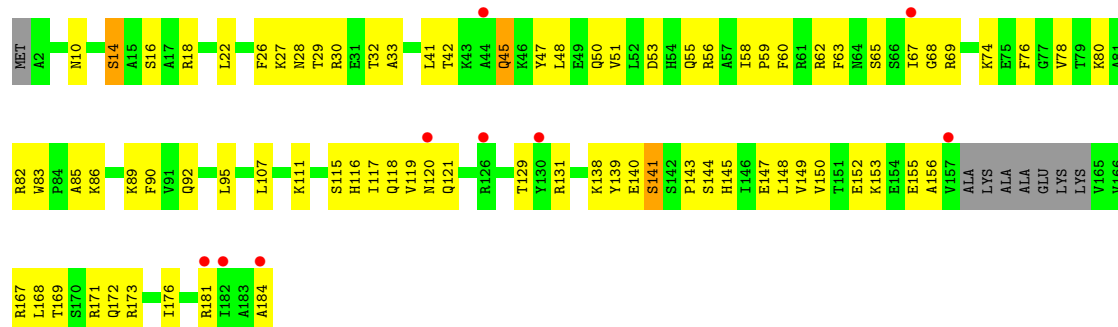
• Molecule 49: 60S ribosomal protein L16-A



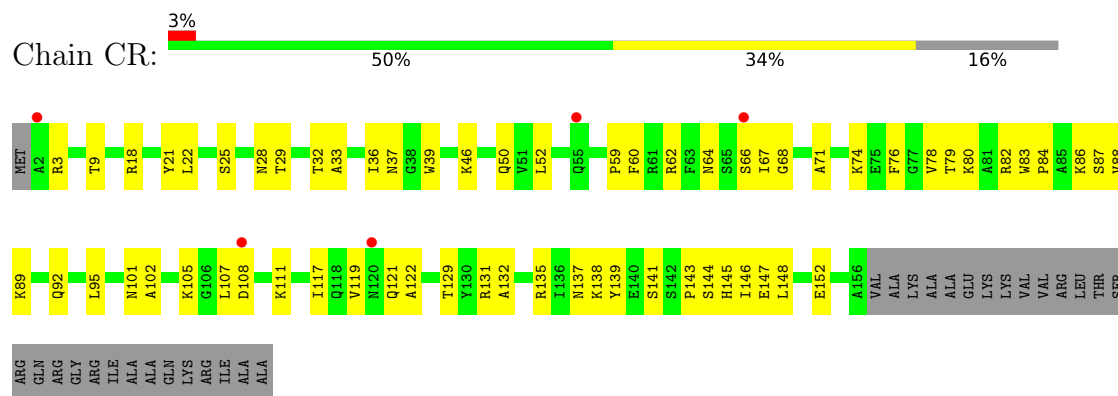
• Molecule 49: 60S ribosomal protein L16-A



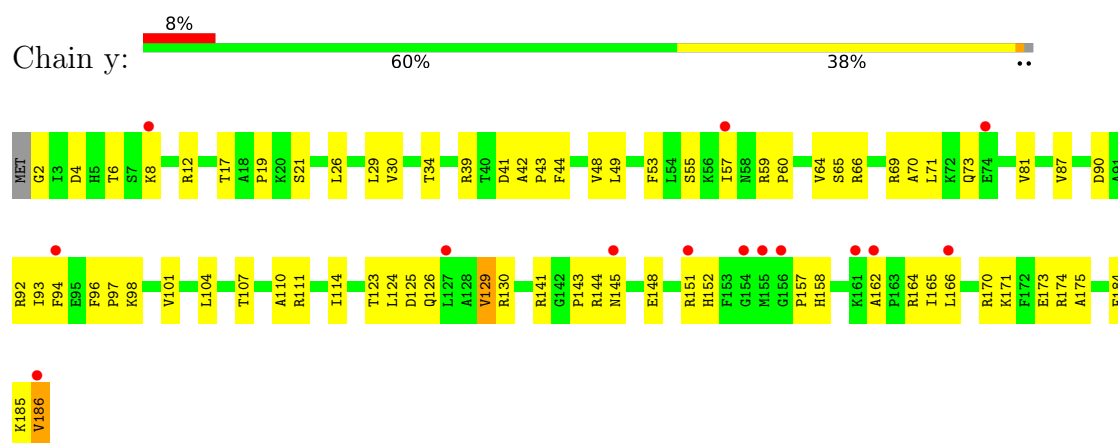
• Molecule 50: 60S ribosomal protein L17-A



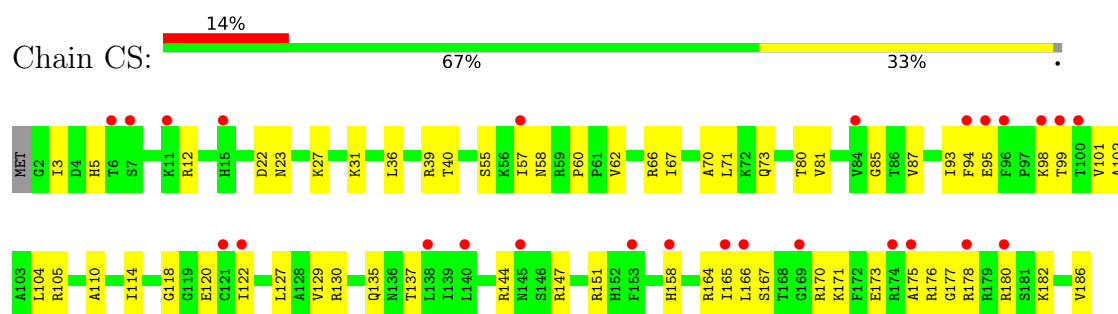
- Molecule 50: 60S ribosomal protein L17-A



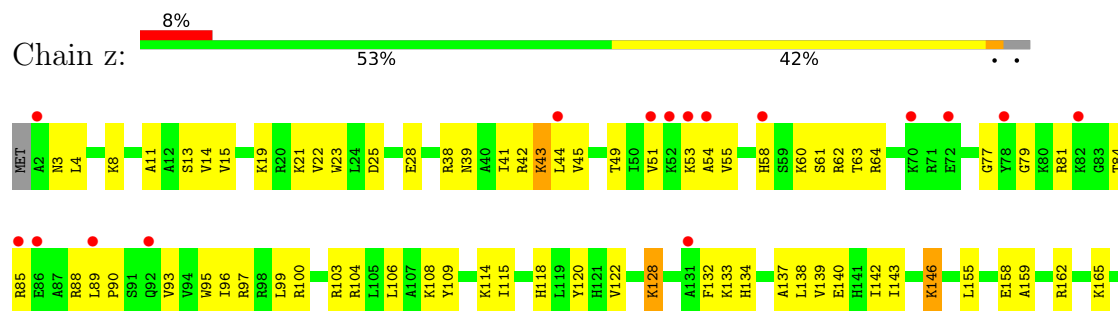
- Molecule 51: 60S ribosomal protein L18-A

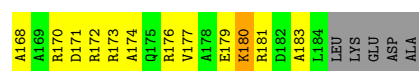


- Molecule 51: 60S ribosomal protein L18-A

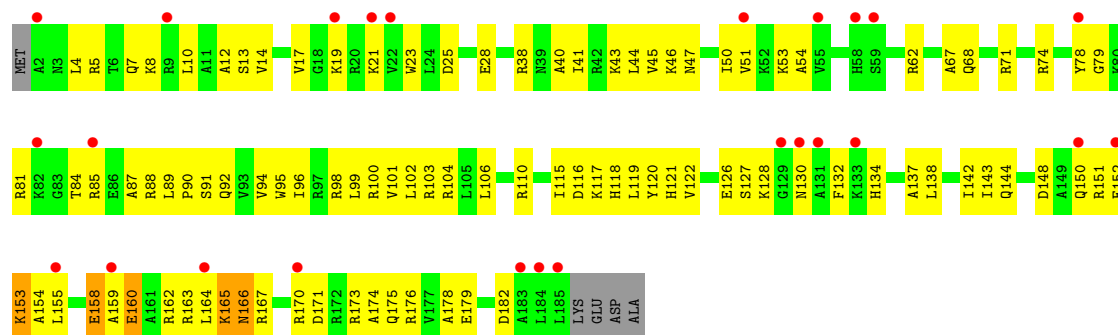


- Molecule 52: 60S ribosomal protein L19-A

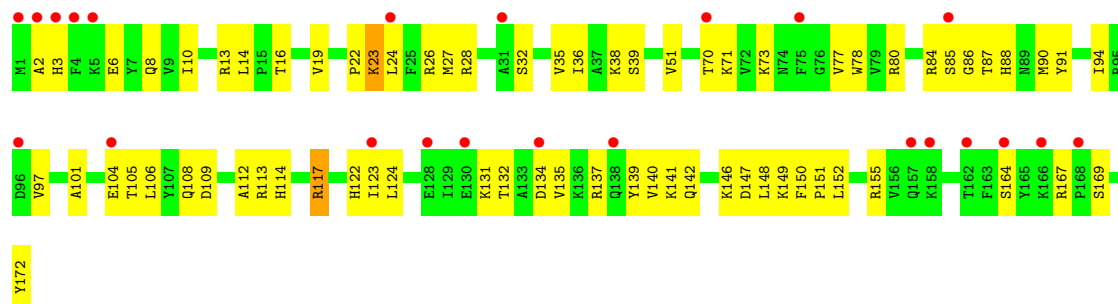




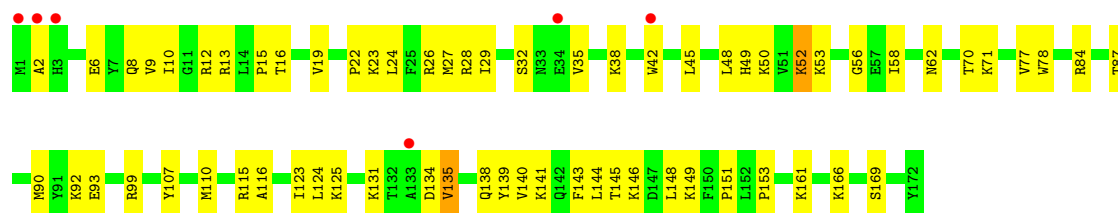
• Molecule 52: 60S ribosomal protein L19-A



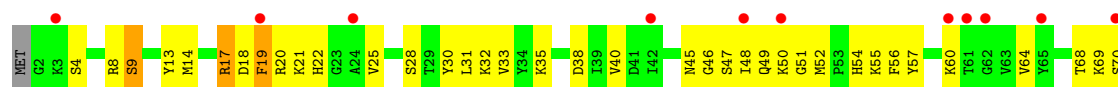
• Molecule 53: 60S ribosomal protein L20-A

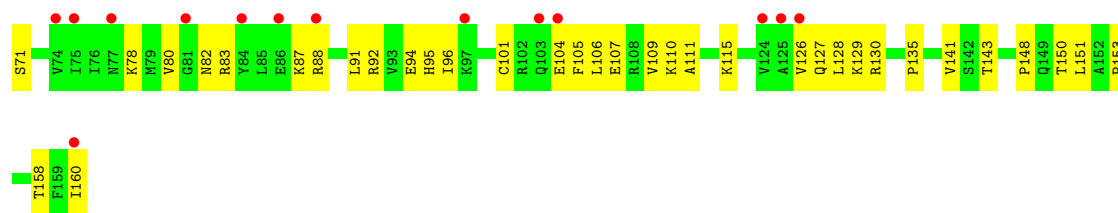


• Molecule 53: 60S ribosomal protein L20-A

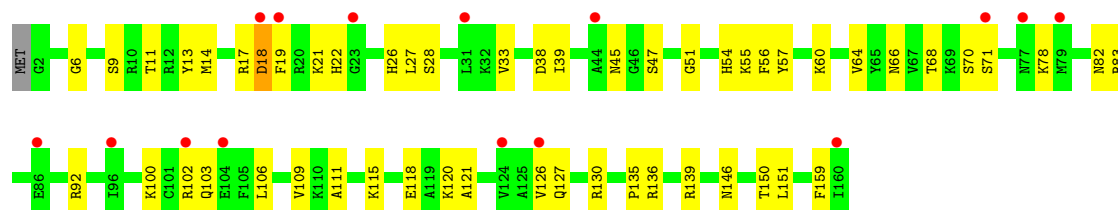


• Molecule 54: 60S ribosomal protein L21-A

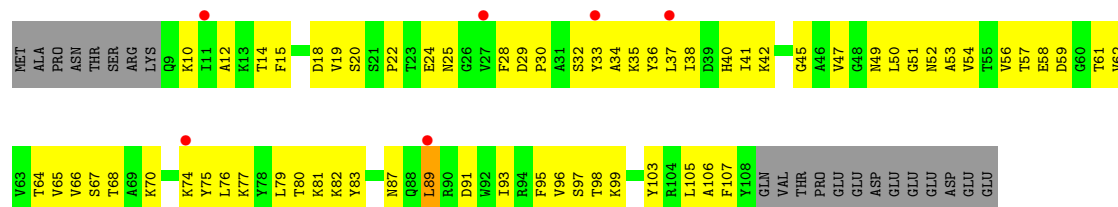




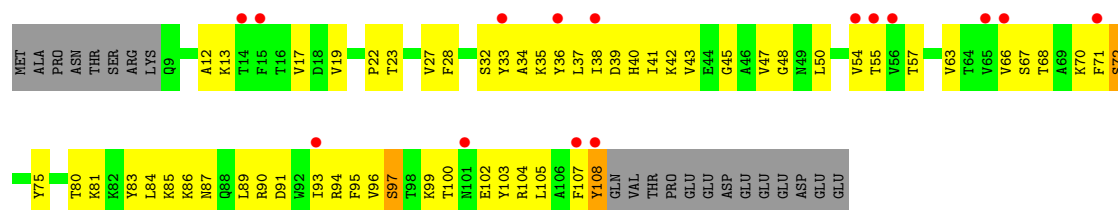
• Molecule 54: 60S ribosomal protein L21-A



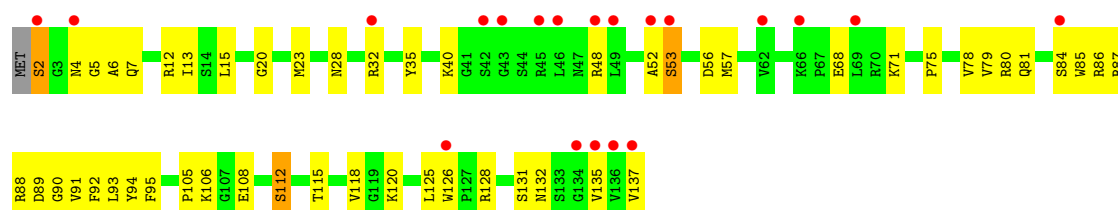
• Molecule 55: 60S ribosomal protein L22-A



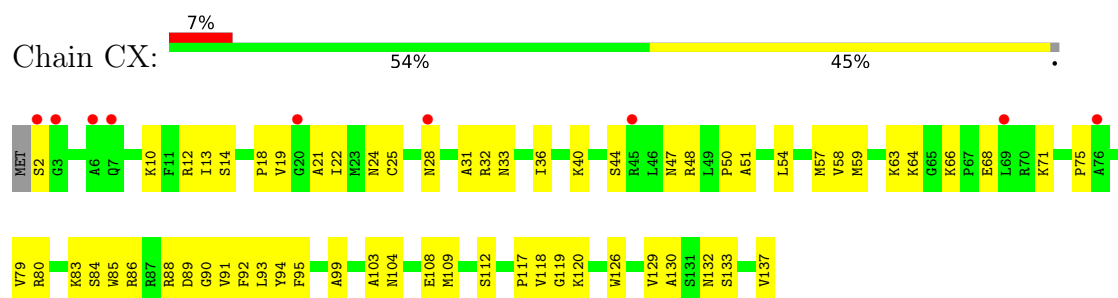
• Molecule 55: 60S ribosomal protein L22-A



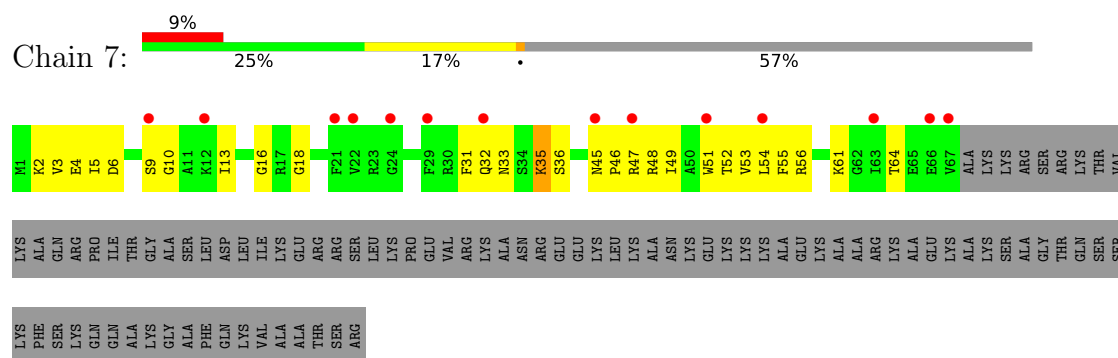
• Molecule 56: 60S ribosomal protein L23-A

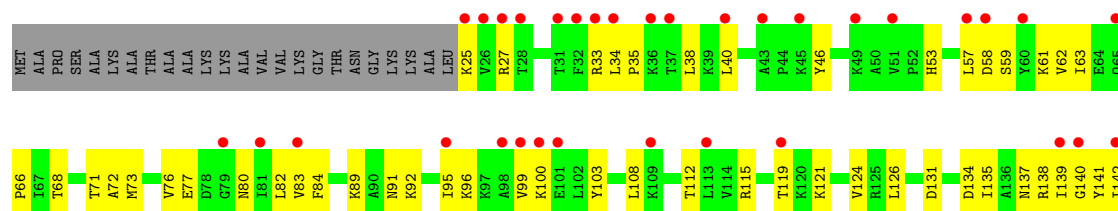


- Molecule 56: 60S ribosomal protein L23-A

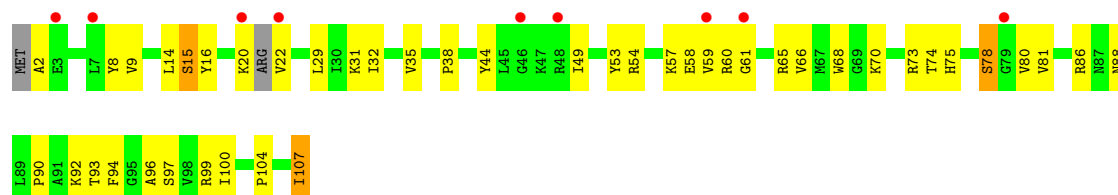


- Molecule 57: 60S ribosomal protein L24-A

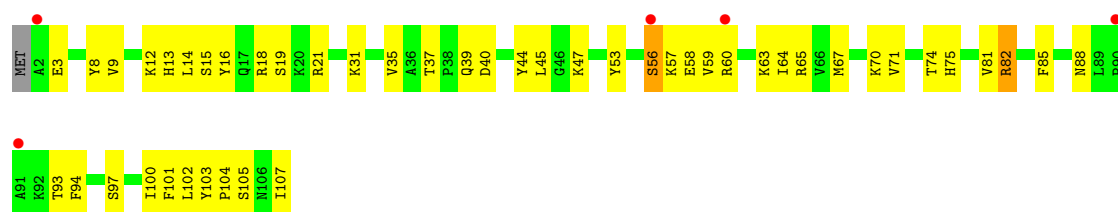




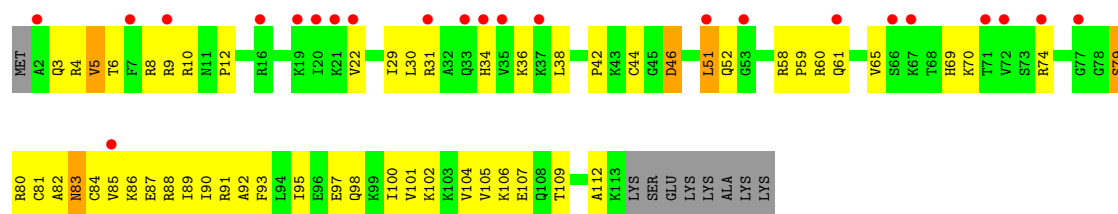
• Molecule 59: 60S ribosomal protein L33-A



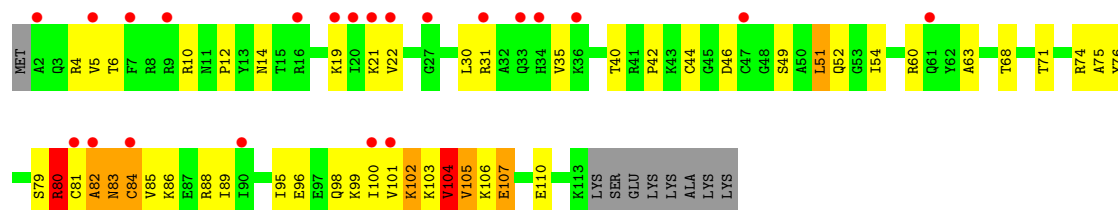
• Molecule 59: 60S ribosomal protein L33-A



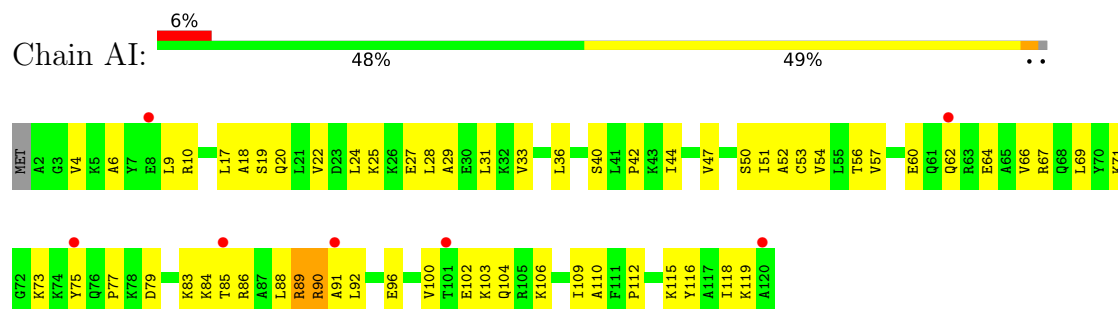
• Molecule 60: 60S ribosomal protein L34-A



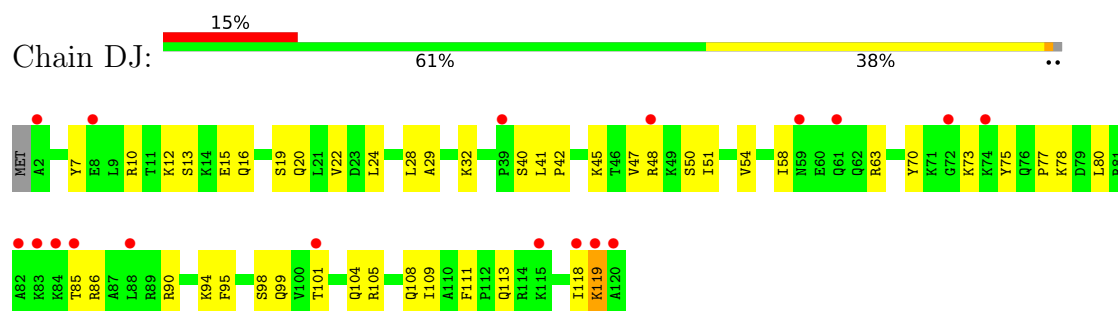
• Molecule 60: 60S ribosomal protein L34-A



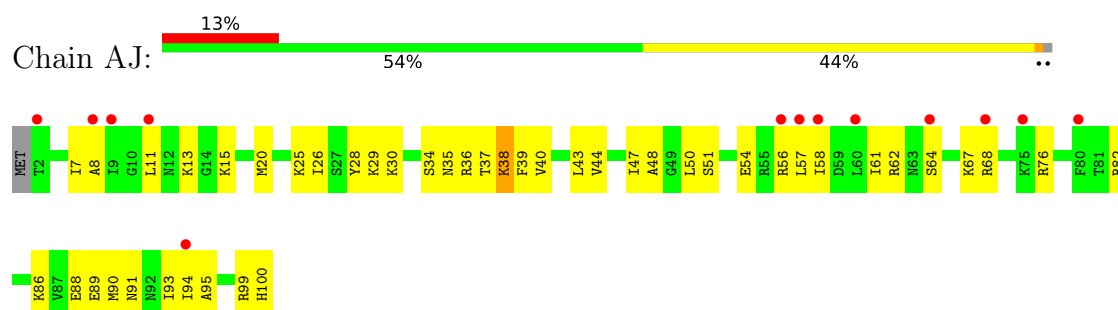
- Molecule 61: 60S ribosomal protein L35-A



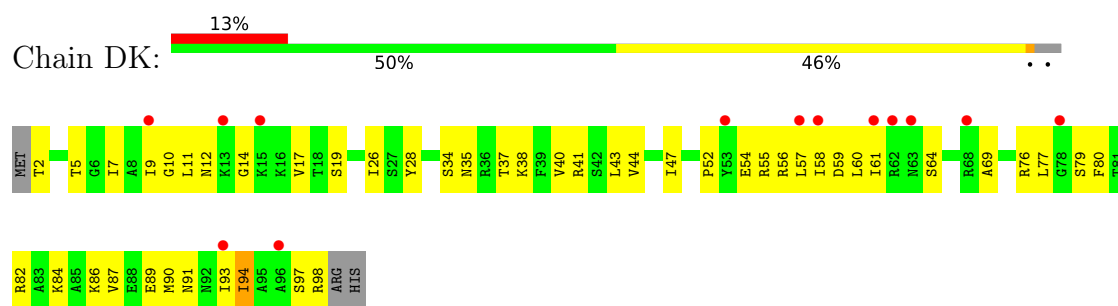
- Molecule 61: 60S ribosomal protein L35-A



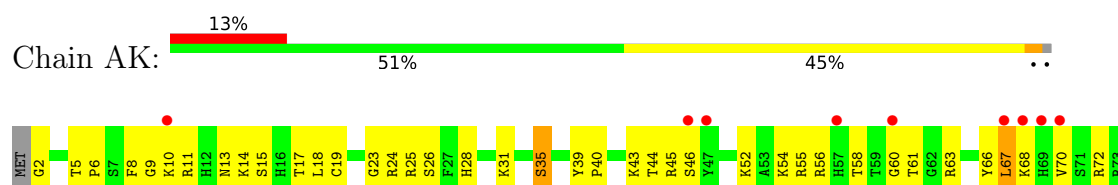
- Molecule 62: 60S ribosomal protein L36-A

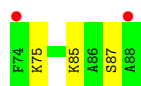


- Molecule 62: 60S ribosomal protein L36-A

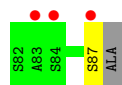


- Molecule 63: 60S ribosomal protein L37-A

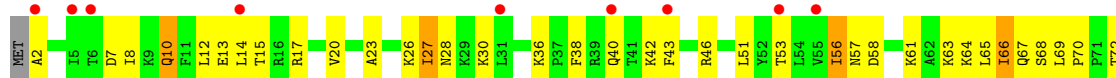




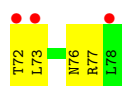
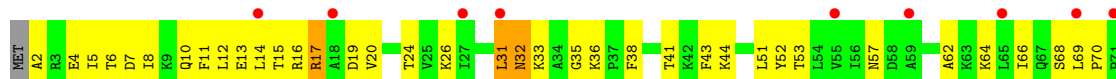
- Molecule 63: 60S ribosomal protein L37-A



- Molecule 64: 60S ribosomal protein L38



- Molecule 64: 60S ribosomal protein L38



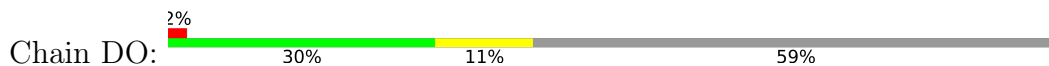
- Molecule 65: 60S ribosomal protein L39

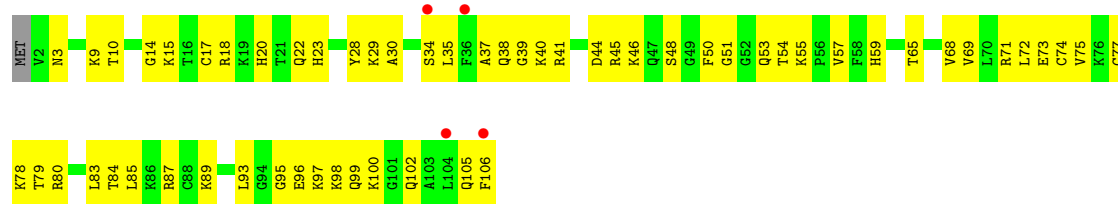


- Molecule 65: 60S ribosomal protein L39

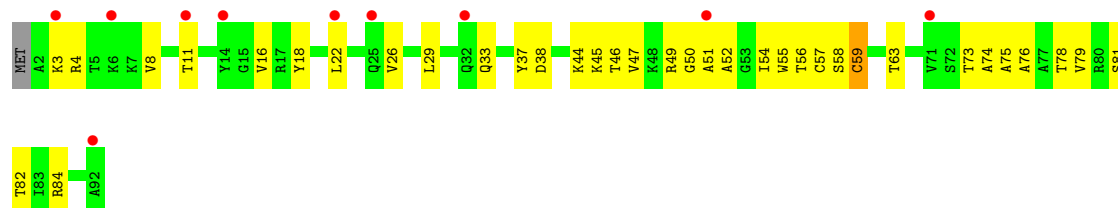


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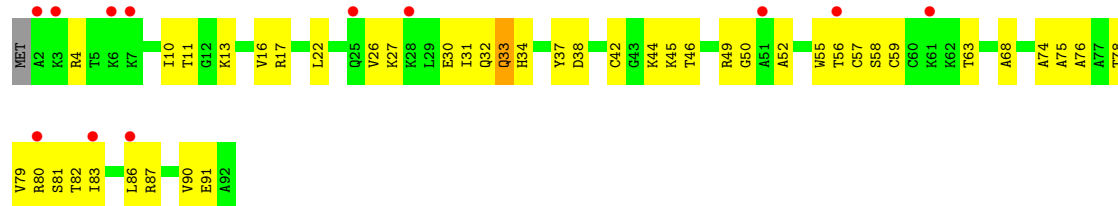




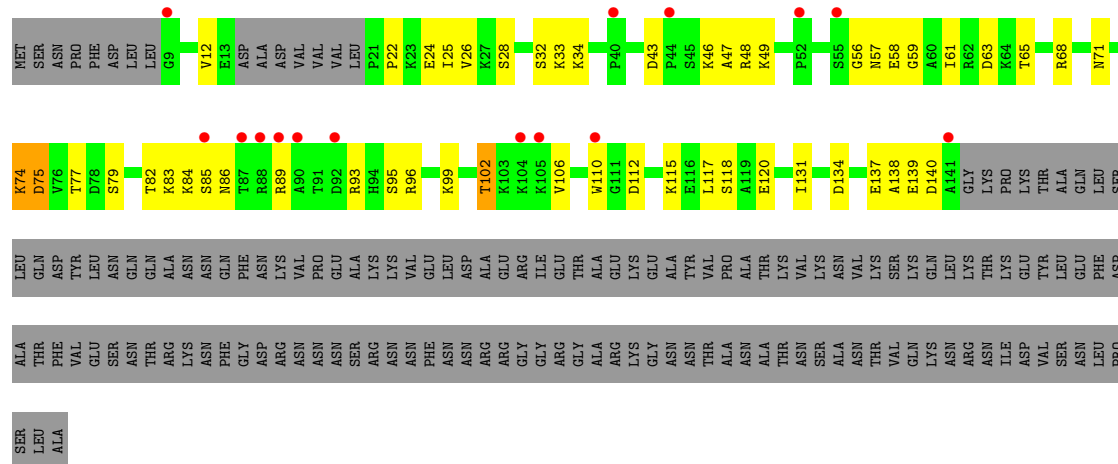
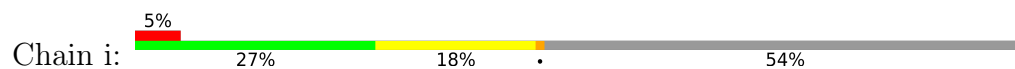
- Molecule 69: 60S ribosomal protein L43-A



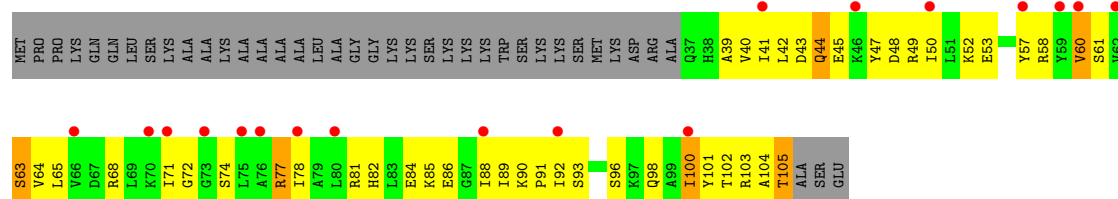
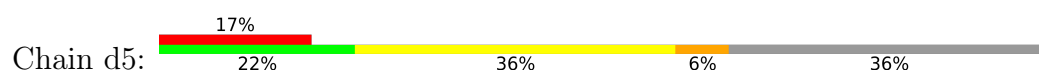
- Molecule 69: 60S ribosomal protein L43-A



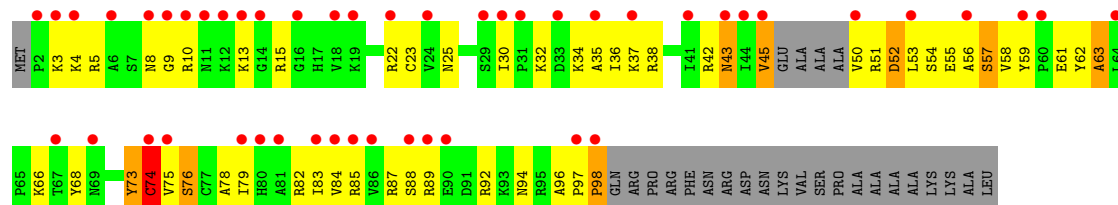
- Molecule 70: Suppressor protein STM1



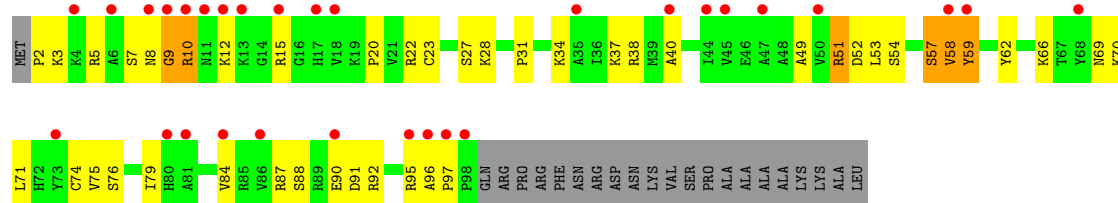
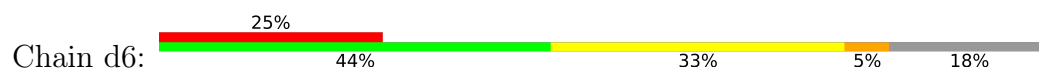
- Molecule 70: Suppressor protein STM1



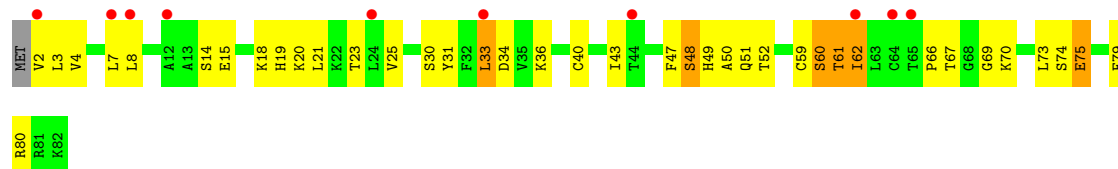
• Molecule 73: Small ribosomal subunit protein eS26B



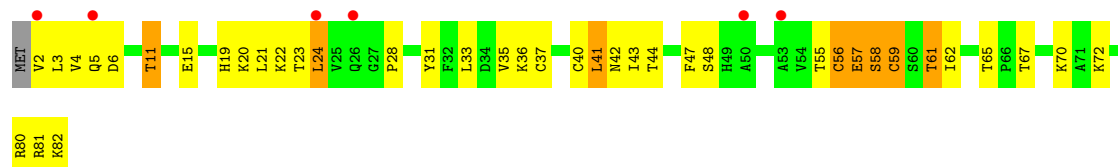
• Molecule 73: Small ribosomal subunit protein eS26B



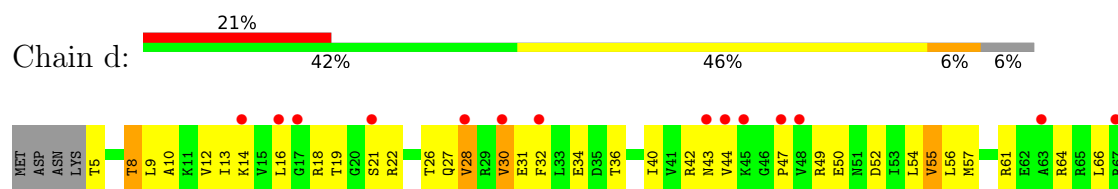
• Molecule 74: 40S ribosomal protein S27-A



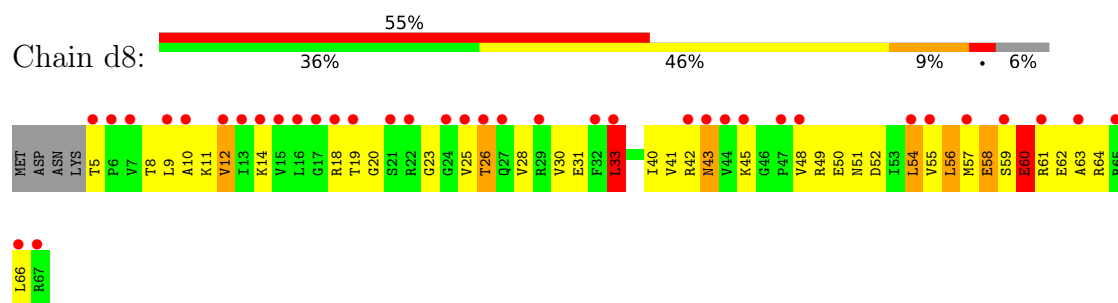
• Molecule 74: 40S ribosomal protein S27-A



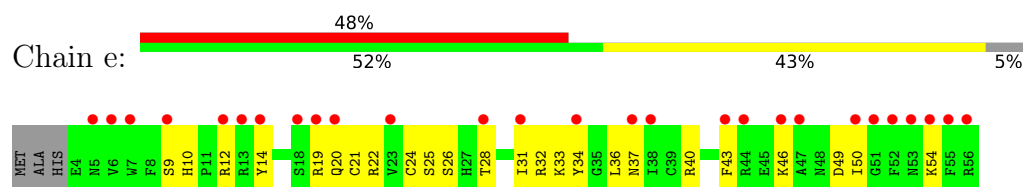
• Molecule 75: 40S ribosomal protein S28-A



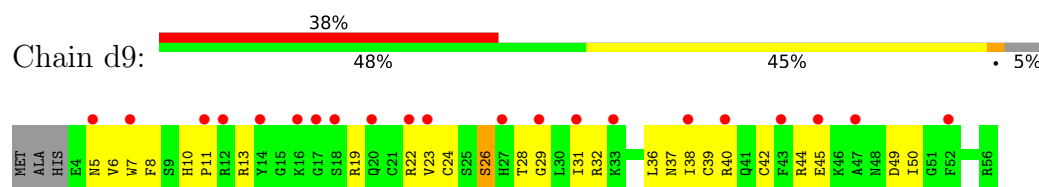
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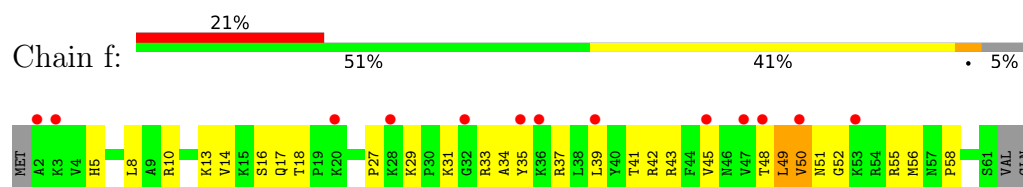
• Molecule 76: Small ribosomal subunit protein uS14A



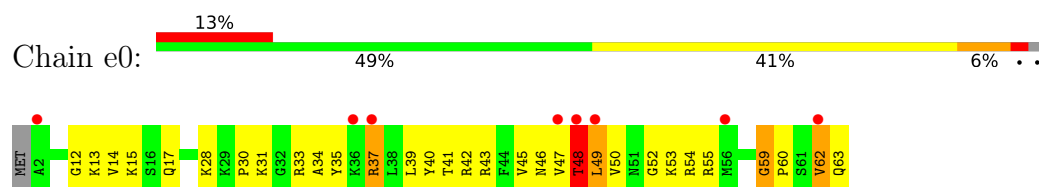
• Molecule 76: Small ribosomal subunit protein uS14A



• Molecule 77: 40S ribosomal protein S30-A



• Molecule 77: 40S ribosomal protein S30-A



• Molecule 78: Ubiquitin



A318	A319	L252	A253	A254	A255	T256	A257	T258	G259	L260	K261	V262	F263	S264	L265	D266	P267	Q268	Y269	L270	V271	L274	R275	P276	F277	F278	Y281	S282	K283	E286	S291	L292	A293	W294	S295	A296	D297	G298	Q299	T300	L301	F302	A303	G304	T306	D307	N308	V309	I310	R311	V312	W313	Q314	V315	M316	T317	MET	A2	E5	V6	L7	V8	L9	R10	L13	E14	G15	H16	N17	G18	W19	V20	T21	S22	L23	A24	T25	S26	A27	G28	Q29	P30	N31	L32	L33	L34	S35	A36	S37	R38	D39	L42	I43	S44	W45	K46	L47	T48	G49	D50	D51	Q52	K53	F54	V58	R59	S60	F61	K62	G63	H64	S65	H66	I67	W68	Q69	D70	C71	T72	L73	T74	A75	D76	G77	A78	Y79	A80	L81	S82	A83	S84	W85	D86	K87	T88	L89	R90	L91	W92	D93	W94	A95	T96	E97	E98	T99	Y100	Q101	R102	F103	V104	G105	H106	K107	S108	D109	V110	M111	S112	V113	D114	I115	D116	K117	A118	A119	S120	W121	I122	I123	S124	G125	S126	R127	D128	K129	K132	V133	W134	I136	K137	G138	Q139	C140	L141	A142	T143	G146	D149	W150	V151	S152	Q153	V154	R155	V156	V157	P158	N159	E160	K161	A162	D163	S166	V167	T168	I169	I170	S171	A172	G173	N174	D175	K176	M177	V178	K179	A180	W181	N182	L183	N184	Q185	F186	Q187	I188	E189	A190	D191	F192	N196	S197	N198	I199	N200	T201	L202	T203	A204	S205	P206	D207	G208	T209	L210	I211	A212	S213	A214	G215	K216	D217	G218	E219	I220	M221	L222	W223	N224	L225	A226	A227	K228	K229	A230	M231	T232	T233	L234	S235	A236	Q237	D238	E239	V240	F241	S242	L243	A244	F245	S246	P247	W248	R249	Y250	W251
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	303.68Å 287.58Å 435.09Å 90.00° 98.93° 90.00°	Depositor
Resolution (Å)	207.60 – 2.90 207.60 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (207.60-2.90) 88.5 (207.60-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.50 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.0	Depositor
R, R_{free}	0.220 , 0.223 0.232 , 0.254	Depositor DCC
R_{free} test set	1593386 reflections (1.55%)	wwPDB-VP
Wilson B-factor (Å ²)	61.4	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	404943	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.39% 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: VDU, K, SPD, ZN, 5XU, OHX, MG

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	A	0.17	0/41356	0.40	0/64437
1	sR	0.16	0/42490	0.38	3/66207 (0.0%)
2	B	0.48	0/1617	1.16	9/2215 (0.4%)
2	s0	0.40	0/1623	1.00	10/2222 (0.5%)
3	C	0.48	0/1735	1.47	31/2335 (1.3%)
3	s1	0.24	0/1748	0.75	0/2352
4	D	0.34	0/1665	0.86	2/2263 (0.1%)
4	s2	0.28	0/1665	0.80	2/2263 (0.1%)
5	E	0.32	0/1759	0.89	0/2368
5	s3	0.34	0/1759	1.02	7/2368 (0.3%)
6	F	0.44	1/2109 (0.0%)	1.03	14/2839 (0.5%)
6	s4	0.27	0/2109	0.81	2/2839 (0.1%)
7	G	0.42	0/1602	1.14	8/2165 (0.4%)
7	s5	0.41	0/1595	0.94	2/2155 (0.1%)
8	H	0.31	0/1815	0.86	5/2428 (0.2%)
8	s6	0.29	0/1779	0.72	0/2379
9	I	0.43	0/1506	1.14	11/2028 (0.5%)
9	s7	0.38	0/1516	1.11	14/2043 (0.7%)
10	J	0.29	0/1514	0.90	4/2021 (0.2%)
10	s8	0.30	0/1514	0.76	1/2021 (0.0%)
11	K	0.43	0/1481	1.01	5/1984 (0.3%)
11	s9	0.29	0/1519	0.87	3/2035 (0.1%)
12	L	0.44	0/789	1.05	8/1067 (0.7%)
12	c0	0.35	0/718	1.03	4/968 (0.4%)
13	M	0.28	0/1180	0.76	3/1591 (0.2%)
13	c1	0.28	0/1194	0.78	4/1610 (0.2%)
14	O	0.29	0/1215	0.72	0/1638
14	c3	0.25	0/1215	0.85	6/1638 (0.4%)
15	P	0.45	0/901	1.15	8/1217 (0.7%)
15	c4	0.26	0/960	0.98	2/1290 (0.2%)
16	Q	0.41	0/948	1.38	12/1273 (0.9%)
16	c5	0.39	1/1012 (0.1%)	1.16	9/1360 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	R	0.39	0/1125	1.22	10/1510 (0.7%)
17	c6	0.44	2/1131 (0.2%)	1.02	8/1518 (0.5%)
18	S	0.41	0/910	1.13	11/1219 (0.9%)
18	c7	0.29	0/914	0.92	2/1224 (0.2%)
19	T	0.39	0/1211	1.03	2/1628 (0.1%)
19	c8	0.32	0/1211	0.91	3/1628 (0.2%)
20	U	0.42	0/1130	1.30	11/1517 (0.7%)
20	c9	0.26	0/1130	0.74	1/1517 (0.1%)
21	V	0.44	0/865	1.24	10/1169 (0.9%)
21	d0	0.32	0/810	1.31	14/1095 (1.3%)
22	W	0.37	0/693	0.99	1/935 (0.1%)
22	d1	0.27	0/693	0.93	6/935 (0.6%)
23	X	0.35	0/1038	0.96	0/1395
23	d2	0.24	0/1038	0.78	3/1395 (0.2%)
24	Y	0.28	0/1139	0.94	6/1518 (0.4%)
24	d3	0.22	0/1139	0.77	0/1518
25	Z	0.30	0/1087	0.86	1/1449 (0.1%)
25	d4	0.32	0/1087	1.07	8/1449 (0.6%)
26	AA	0.24	0/1118	0.87	5/1497 (0.3%)
26	DB	0.51	2/1118 (0.2%)	1.02	7/1497 (0.5%)
27	9	0.22	0/1004	0.65	0/1341
27	DA	0.18	0/987	0.62	0/1318
28	AB	0.29	0/1204	0.88	5/1612 (0.3%)
28	DC	0.31	0/1204	0.97	9/1612 (0.6%)
29	AC	0.18	0/473	0.79	2/629 (0.3%)
29	DD	0.22	0/473	0.86	1/629 (0.2%)
30	AD	0.26	0/751	0.67	0/1008
30	DE	0.23	0/751	0.67	0/1008
31	CD	0.22	0/1948	0.71	2/2617 (0.1%)
31	j	0.23	0/1948	0.72	1/2617 (0.0%)
32	AE	0.21	0/890	0.65	0/1196
32	DF	0.21	0/890	0.79	5/1196 (0.4%)
33	CE	0.20	0/3146	0.65	3/4228 (0.1%)
33	k	0.24	0/3146	0.70	5/4228 (0.1%)
34	AF	0.15	0/1041	0.62	2/1394 (0.1%)
34	DG	0.17	0/1041	0.61	2/1394 (0.1%)
35	1	0.15	0/75038	0.37	1/116986 (0.0%)
35	AR	0.15	0/75347	0.37	0/117472
36	3	0.14	0/2883	0.32	0/4491
36	AS	0.13	0/2883	0.33	0/4491
37	4	0.14	0/3746	0.37	0/5832
37	AT	0.13	0/3746	0.34	0/5832
38	CF	0.25	0/2800	0.74	5/3790 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	l	0.23	0/2800	0.82	7/3790 (0.2%)
39	CG	0.28	0/2425	0.84	5/3271 (0.2%)
39	m	0.30	0/2425	0.85	2/3271 (0.1%)
40	CH	0.20	0/1260	0.65	0/1694
40	n	0.21	0/1260	0.62	0/1694
41	CI	0.22	0/1821	0.76	5/2451 (0.2%)
41	o	0.24	0/1821	0.82	3/2451 (0.1%)
42	CJ	0.35	0/1836	0.88	4/2481 (0.2%)
42	p	0.35	1/1836 (0.1%)	0.83	7/2481 (0.3%)
43	CK	0.22	0/1539	0.65	0/2073
43	q	0.28	0/1539	0.78	1/2073 (0.0%)
44	CL	0.21	0/1741	0.68	2/2335 (0.1%)
44	r	0.27	0/1741	0.71	0/2335
45	CM	0.27	0/1374	0.77	0/1842
45	s	0.36	0/1374	1.03	7/1842 (0.4%)
46	CN	0.29	0/1568	0.90	6/2106 (0.3%)
46	t	0.32	0/1568	0.84	3/2106 (0.1%)
47	CO	0.20	0/1068	0.64	0/1438
47	u	0.25	0/1068	0.62	0/1438
48	CP	0.19	0/1757	0.54	0/2354
48	v	0.22	0/1757	0.61	0/2354
49	CQ	0.18	0/1585	0.59	0/2128
49	w	0.22	0/1585	0.62	0/2128
50	CR	0.18	0/1250	0.66	0/1683
50	x	0.21	0/1407	0.66	0/1892
51	CS	0.22	0/1465	0.67	0/1965
51	y	0.22	0/1465	0.65	2/1965 (0.1%)
52	CT	0.27	0/1507	0.87	11/2009 (0.5%)
52	z	0.33	0/1499	0.78	3/1998 (0.2%)
53	0	0.24	0/1481	0.72	1/1990 (0.1%)
53	CU	0.17	0/1481	0.62	0/1990
54	2	0.24	0/1300	0.72	1/1743 (0.1%)
54	CV	0.22	0/1300	0.72	0/1743
55	5	0.36	0/812	0.87	0/1099
55	CW	0.32	0/812	0.83	0/1099
56	6	0.23	0/1018	0.64	0/1369
56	CX	0.21	0/1018	0.58	0/1369
57	7	0.27	0/555	0.68	0/738
57	CY	0.21	0/792	0.67	2/1066 (0.2%)
58	8	0.23	0/979	0.72	0/1321
58	CZ	0.23	0/961	0.66	1/1296 (0.1%)
59	AG	0.24	0/856	0.77	2/1151 (0.2%)
59	DH	0.22	0/868	0.75	0/1168

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	AH	0.32	0/890	0.82	3/1189 (0.3%)
60	DI	0.44	0/890	0.97	4/1189 (0.3%)
61	AI	0.26	0/978	0.88	5/1301 (0.4%)
61	DJ	0.25	0/978	0.64	0/1301
62	AJ	0.25	0/778	0.71	0/1034
62	DK	0.26	0/756	0.71	0/1005
63	AK	0.20	0/696	0.67	1/923 (0.1%)
63	DL	0.19	0/691	0.60	0/916
64	AL	0.29	0/618	0.78	0/826
64	DM	0.28	0/618	1.06	6/826 (0.7%)
65	AM	0.23	0/443	0.72	0/588
65	DN	0.17	0/443	0.63	1/588 (0.2%)
66	AN	0.27	0/423	0.67	0/562
66	DO	0.24	0/423	0.63	0/562
67	AO	0.17	0/234	0.74	0/300
67	DP	0.15	0/234	0.58	0/300
68	AP	0.49	0/860	0.89	2/1136 (0.2%)
68	DQ	0.45	0/860	0.88	0/1136
69	AQ	0.22	0/701	0.80	0/934
69	DR	0.22	0/701	0.77	0/934
70	i	0.30	0/948	0.79	0/1270
70	sM	0.33	0/480	0.94	2/642 (0.3%)
71	p0	0.63	4/992 (0.4%)	0.90	2/1334 (0.1%)
72	a	0.39	0/571	1.18	2/768 (0.3%)
72	d5	0.40	0/566	1.02	3/761 (0.4%)
73	b	0.43	0/757	1.41	9/1011 (0.9%)
73	d6	0.29	0/782	1.00	6/1047 (0.6%)
74	c	0.34	0/620	1.04	4/838 (0.5%)
74	d7	0.77	3/620 (0.5%)	1.43	9/838 (1.1%)
75	d	0.30	0/499	0.81	0/670
75	d8	0.43	0/499	1.15	5/670 (0.7%)
76	d9	0.33	0/452	0.89	2/600 (0.3%)
76	e	0.34	0/452	0.74	0/600
77	e0	0.37	0/499	0.94	3/665 (0.5%)
77	f	0.53	1/483 (0.2%)	1.07	2/643 (0.3%)
78	e1	0.56	0/322	1.91	12/429 (2.8%)
78	g	0.41	0/577	1.55	11/770 (1.4%)
79	Rb	0.39	0/2495	1.07	14/3395 (0.4%)
79	h	0.33	0/2447	1.03	9/3330 (0.3%)
All	All	0.23	15/425385 (0.0%)	0.61	533/624774 (0.1%)

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	s0	0	1
3	C	0	1
6	F	0	3
9	I	0	2
11	K	0	1
16	Q	0	1
16	c5	0	1
17	R	0	3
20	U	0	1
21	d0	0	1
23	X	0	1
25	d4	0	2
26	DB	0	2
38	l	0	1
60	DI	0	1
73	b	0	1
73	d6	0	1
74	d7	0	1
78	e1	0	1
All	All	0	26

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	d7	58	SER	CA-CB	-10.23	1.36	1.53
17	c6	65	ILE	CG1-CD1	8.39	1.84	1.51
71	p0	91	GLU	N-CA	-7.99	1.35	1.46
16	c5	52	LYS	C-O	-7.67	1.20	1.23
77	f	51	ASN	CG-ND2	-7.22	1.18	1.33

The worst 5 of 533 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	d7	58	SER	CA-C-N	19.73	161.37	126.45
74	d7	58	SER	C-N-CA	19.73	161.37	126.45
73	b	74	CYS	CA-C-N	18.15	154.64	121.97
73	b	74	CYS	C-N-CA	18.15	154.64	121.97
7	G	65	ARG	CA-C-N	17.23	152.72	121.70

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	36	SER	Peptide
6	F	193	GLY	Peptide
6	F	194	THR	Peptide,Mainchain
9	I	131	PHE	Peptide,Mainchain
11	K	3	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	A	36976	0	18602	1337	2
1	sR	37990	0	19115	1204	1
2	B	1577	0	1567	195	0
2	s0	1583	0	1578	129	0
3	C	1709	0	1784	210	0
3	s1	1722	0	1793	115	0
4	D	1635	0	1723	176	0
4	s2	1635	0	1723	97	0
5	E	1734	0	1817	117	0
5	s3	1734	0	1817	154	0
6	F	2068	0	2154	170	0
6	s4	2068	0	2154	119	0
7	G	1583	0	1652	169	0
7	s5	1576	0	1643	174	0
8	H	1792	0	1871	109	0
8	s6	1755	0	1846	87	0
9	I	1481	0	1572	138	0
9	s7	1491	0	1578	119	0
10	J	1489	0	1525	104	0
10	s8	1489	0	1525	102	0
11	K	1456	0	1543	129	0
11	s9	1494	0	1573	123	0
12	L	772	0	727	66	0
12	c0	702	0	675	59	0
13	M	1154	0	1220	68	0
13	c1	1168	0	1233	55	0
14	O	1192	0	1255	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	c3	1192	0	1255	64	0
15	P	891	0	883	97	0
15	c4	949	0	985	71	0
16	Q	928	0	958	87	0
16	c5	991	0	1010	96	0
17	R	1105	0	1166	107	0
17	c6	1111	0	1171	99	0
18	S	901	0	917	89	0
18	c7	906	0	909	67	0
19	T	1192	0	1222	137	0
19	c8	1192	0	1222	129	0
20	U	1112	0	1124	139	0
20	c9	1112	0	1124	82	0
21	V	855	0	917	97	0
21	d0	800	0	869	71	0
22	W	684	0	672	79	0
22	d1	684	0	672	43	0
23	X	1021	0	1060	83	0
23	d2	1021	0	1060	77	0
24	Y	1121	0	1196	68	0
24	d3	1121	0	1196	52	0
25	Z	1073	0	1132	71	0
25	d4	1073	0	1132	65	0
26	AA	1092	0	1155	65	0
26	DB	1092	0	1155	100	0
27	9	993	0	1081	34	0
27	DA	976	0	1064	49	0
28	AB	1173	0	1215	81	0
28	DC	1173	0	1215	85	0
29	AC	462	0	491	19	0
29	DD	462	0	491	19	0
30	AD	743	0	797	36	0
30	DE	743	0	797	38	0
31	CD	1914	0	1981	96	0
31	j	1914	0	1981	89	0
32	AE	876	0	912	30	0
32	DF	876	0	912	21	0
33	CE	3075	0	3142	126	0
33	k	3075	0	3142	148	0
34	AF	1020	0	1090	25	0
34	DG	1020	0	1090	33	0
35	1	67038	0	33689	1718	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	AR	67313	0	33825	1747	1
36	3	2579	0	1304	71	0
36	AS	2579	0	1304	58	0
37	4	3353	0	1695	95	1
37	AT	3353	0	1695	89	0
38	CF	2748	0	2859	121	0
38	l	2748	0	2859	119	0
39	CG	2375	0	2325	107	1
39	m	2375	0	2325	152	0
40	CH	1239	0	1326	57	0
40	n	1239	0	1326	36	0
41	CI	1784	0	1862	70	0
41	o	1784	0	1862	81	0
42	CJ	1804	0	1877	114	1
42	p	1804	0	1877	100	1
43	CK	1518	0	1587	67	1
43	q	1518	0	1587	102	0
44	CL	1705	0	1736	75	0
44	r	1705	0	1736	78	0
45	CM	1353	0	1383	76	1
45	s	1353	0	1383	112	0
46	CN	1543	0	1608	104	0
46	t	1543	0	1608	100	0
47	CO	1053	0	1149	51	0
47	u	1053	0	1149	64	0
48	CP	1720	0	1778	79	0
48	v	1720	0	1779	96	0
49	CQ	1555	0	1659	38	1
49	w	1555	0	1659	70	0
50	CR	1227	0	1236	51	0
50	x	1385	0	1413	65	0
51	CS	1441	0	1543	57	0
51	y	1441	0	1543	61	0
52	CT	1490	0	1589	91	0
52	z	1482	0	1578	75	0
53	0	1445	0	1487	68	0
53	CU	1445	0	1487	55	0
54	2	1276	0	1323	75	0
54	CV	1276	0	1323	51	0
55	5	796	0	812	58	0
55	CW	796	0	812	58	0
56	6	1003	0	1047	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CX	1003	0	1048	52	0
57	7	543	0	564	21	0
57	CY	781	0	694	26	0
58	8	964	0	1024	44	0
58	CZ	946	0	1007	40	0
59	AG	839	0	866	41	0
59	DH	850	0	880	38	0
60	AH	880	0	942	48	0
60	DI	880	0	943	83	0
61	AI	969	0	1078	49	0
61	DJ	969	0	1078	40	0
62	AJ	771	0	849	49	0
62	DK	750	0	829	48	0
63	AK	681	0	682	39	0
63	DL	676	0	678	30	0
64	AL	612	0	682	43	0
64	DM	612	0	682	37	0
65	AM	436	0	475	20	0
65	DN	436	0	475	16	0
66	AN	417	0	455	21	0
66	DO	417	0	455	15	0
67	AO	233	0	284	13	0
67	DP	233	0	284	9	0
68	AP	847	0	914	62	0
68	DQ	847	0	914	73	0
69	AQ	694	0	734	33	0
69	DR	694	0	734	34	0
70	i	939	0	920	68	0
70	sM	475	0	492	38	0
71	p0	977	0	989	59	0
72	a	563	0	603	80	0
72	d5	558	0	598	60	0
73	b	745	0	792	77	0
73	d6	769	0	814	54	0
74	c	610	0	633	35	0
74	d7	610	0	632	50	0
75	d	497	0	535	39	0
75	d8	497	0	535	53	0
76	d9	442	0	428	29	0
76	e	442	0	428	28	0
77	e0	491	0	542	40	0
77	f	475	0	525	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
78	e1	317	0	323	36	0
78	g	566	0	602	52	0
79	Rb	2442	0	2392	282	0
79	h	2394	0	2344	239	0
80	1	2137	0	0	228	0
80	2	7	0	0	0	0
80	3	77	0	0	6	0
80	4	119	0	0	14	0
80	A	902	0	0	103	0
80	AC	7	0	0	2	0
80	AE	7	0	0	0	0
80	AG	7	0	0	1	0
80	AK	7	0	0	0	0
80	AP	7	0	0	3	0
80	AR	2238	0	0	259	0
80	AS	70	0	0	3	0
80	AT	98	0	0	8	0
80	CE	14	0	0	2	0
80	CG	21	0	0	2	0
80	CK	7	0	0	1	0
80	CL	20	0	0	3	0
80	CP	7	0	0	1	0
80	CS	7	0	0	2	0
80	CX	7	0	0	0	0
80	DD	7	0	0	2	0
80	DH	7	0	0	1	0
80	DK	7	0	0	1	0
80	DL	7	0	0	1	0
80	DQ	7	0	0	3	0
80	J	7	0	0	2	0
80	O	7	0	0	2	0
80	Q	7	0	0	1	0
80	Rb	7	0	0	2	0
80	S	7	0	0	1	0
80	T	7	0	0	1	0
80	c3	7	0	0	0	0
80	c5	7	0	0	2	0
80	c8	7	0	0	0	0
80	d4	7	0	0	0	0
80	d6	7	0	0	0	0
80	e	7	0	0	1	0
80	h	7	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	k	21	0	0	5	0
80	l	7	0	0	2	0
80	n	7	0	0	1	0
80	r	7	0	0	0	0
80	s1	7	0	0	1	0
80	s4	7	0	0	0	0
80	s8	7	0	0	1	0
80	sR	1063	0	0	130	0
80	v	7	0	0	1	0
80	x	7	0	0	2	0
80	y	7	0	0	0	0
80	z	14	0	0	1	0
81	1	489	0	0	0	0
81	3	12	0	0	0	0
81	4	21	0	0	0	0
81	6	3	0	0	0	0
81	8	3	0	0	0	0
81	9	1	0	0	0	0
81	A	139	0	0	0	0
81	AB	3	0	0	0	0
81	AC	1	0	0	0	0
81	AF	2	0	0	0	0
81	AH	1	0	0	0	0
81	AK	3	0	0	0	0
81	AN	1	0	0	0	0
81	AR	534	0	0	0	0
81	AS	18	0	0	0	0
81	AT	15	0	0	0	0
81	CD	2	0	0	0	0
81	CE	3	0	0	0	0
81	CF	2	0	0	0	0
81	CG	1	0	0	0	0
81	CI	2	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	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	CX	1	0	0	0	0
81	CY	1	0	0	0	0
81	D	1	0	0	0	0
81	DA	2	0	0	0	0
81	DC	2	0	0	0	0
81	DH	2	0	0	0	0
81	DI	1	0	0	0	0
81	DL	1	0	0	0	0
81	DO	1	0	0	0	0
81	DP	1	0	0	0	0
81	DQ	3	0	0	0	0
81	DR	2	0	0	0	0
81	F	1	0	0	0	0
81	O	1	0	0	0	0
81	P	1	0	0	0	0
81	b	1	0	0	0	0
81	c1	1	0	0	0	0
81	c4	2	0	0	0	0
81	c6	2	0	0	0	0
81	c8	2	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	2	0	0	0	0
81	d5	1	0	0	0	0
81	d6	2	0	0	0	0
81	d9	1	0	0	0	0
81	j	3	0	0	0	0
81	k	1	0	0	0	0
81	l	4	0	0	0	0
81	m	1	0	0	0	0
81	o	1	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	3	0	0	0	0
81	sM	2	0	0	0	0
81	sR	143	0	0	0	0
81	t	3	0	0	0	0
81	v	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	w	1	0	0	0	0
81	x	8	0	0	0	0
81	z	2	0	0	0	0
82	A	2	0	0	0	0
82	AR	1	0	0	0	0
82	CK	1	0	0	0	0
83	1	10	0	19	3	0
83	AR	10	0	19	3	0
84	1	26	0	0	1	0
84	AR	26	0	0	2	0
85	AK	1	0	0	0	0
85	AN	1	0	0	0	0
85	AP	1	0	0	0	0
85	AQ	1	0	0	0	0
85	DI	1	0	0	0	0
85	DL	1	0	0	0	0
85	DO	1	0	0	0	0
85	DQ	1	0	0	0	0
85	DR	1	0	0	0	0
85	b	1	0	0	0	0
85	c	1	0	0	0	0
85	d6	1	0	0	0	0
85	d7	1	0	0	0	0
85	d9	1	0	0	0	0
85	e	1	0	0	0	0
85	e1	1	0	0	0	0
85	g	1	0	0	0	0
86	c0	15	0	14	1	0
86	s3	9	0	6	0	0
87	1	60	0	0	12	0
87	8	6	0	0	1	0
87	A	44	0	0	3	0
87	AF	3	0	0	0	0
87	AO	1	0	0	0	0
87	AR	81	0	0	4	0
87	AT	2	0	0	0	0
87	CD	1	0	0	0	0
87	CP	3	0	0	0	0
87	CR	1	0	0	1	0
87	DG	3	0	0	0	0
87	F	1	0	0	0	0
87	i	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	sR	24	0	0	2	0
All	All	404943	0	293267	15297	6

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 22.

The worst 5 of 15297 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)
17:c6:65:ILE:CG1	17:c6:65:ILE:CD1	1.84	1.50
68:AP:71:ARG:NH2	68:AP:80:ARG:HH21	1.01	1.50
68:AP:71:ARG:HH21	68:AP:80:ARG:NH2	1.11	1.42
68:DQ:15:LYS:O	68:DQ:15:LYS:HD2	1.25	1.33
79:Rb:199:ILE:HA	79:Rb:215:GLY:HA3	1.28	1.15

The worst 5 of 6 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)
43:CK:138:THR:OG1	45:CM:75:LYS:NZ[2_746]	1.98	0.22
35:AR:1242:G:O6	39:CG:206:GLN:NE2[2_746]	2.10	0.10
1:A:221:A:O5'	42:p:84:ARG:NH2[2_645]	2.13	0.07
42:CJ:111:LYS:NZ	1:sR:823:G:O2'[2_656]	2.17	0.03
1:A:236:A:O2'	37:4:158:U:O2'[2_645]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	204/252 (81%)	186 (91%)	18 (9%)	0	100	100
2	s0	204/252 (81%)	191 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	212/255 (83%)	197 (93%)	15 (7%)	0	100	100
3	s1	214/255 (84%)	212 (99%)	2 (1%)	0	100	100
4	D	215/254 (85%)	207 (96%)	8 (4%)	0	100	100
4	s2	215/254 (85%)	208 (97%)	7 (3%)	0	100	100
5	E	221/240 (92%)	215 (97%)	6 (3%)	0	100	100
5	s3	221/240 (92%)	213 (96%)	5 (2%)	3 (1%)	9	31
6	F	258/261 (99%)	253 (98%)	4 (2%)	1 (0%)	30	60
6	s4	258/261 (99%)	257 (100%)	1 (0%)	0	100	100
7	G	196/225 (87%)	191 (97%)	5 (3%)	0	100	100
7	s5	195/225 (87%)	188 (96%)	7 (4%)	0	100	100
8	H	224/236 (95%)	222 (99%)	2 (1%)	0	100	100
8	s6	216/236 (92%)	210 (97%)	5 (2%)	1 (0%)	25	56
9	I	182/190 (96%)	174 (96%)	7 (4%)	1 (0%)	25	56
9	s7	184/190 (97%)	174 (95%)	8 (4%)	2 (1%)	12	37
10	J	184/200 (92%)	177 (96%)	7 (4%)	0	100	100
10	s8	184/200 (92%)	181 (98%)	2 (1%)	1 (0%)	25	56
11	K	177/197 (90%)	171 (97%)	5 (3%)	1 (1%)	22	52
11	s9	183/197 (93%)	181 (99%)	2 (1%)	0	100	100
12	L	94/105 (90%)	89 (95%)	5 (5%)	0	100	100
12	c0	82/105 (78%)	74 (90%)	6 (7%)	2 (2%)	5	19
13	M	141/156 (90%)	139 (99%)	2 (1%)	0	100	100
13	c1	144/156 (92%)	140 (97%)	4 (3%)	0	100	100
14	O	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
14	c3	148/151 (98%)	141 (95%)	7 (5%)	0	100	100
15	P	125/138 (91%)	120 (96%)	5 (4%)	0	100	100
15	c4	126/138 (91%)	120 (95%)	4 (3%)	2 (2%)	8	28
16	Q	115/142 (81%)	107 (93%)	8 (7%)	0	100	100
16	c5	125/142 (88%)	117 (94%)	6 (5%)	2 (2%)	8	28
17	R	139/143 (97%)	136 (98%)	3 (2%)	0	100	100
17	c6	140/143 (98%)	137 (98%)	2 (1%)	1 (1%)	19	49
18	S	111/136 (82%)	108 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	c7	113/136 (83%)	110 (97%)	2 (2%)	1 (1%)	14	43
19	T	143/146 (98%)	138 (96%)	3 (2%)	2 (1%)	9	31
19	c8	143/146 (98%)	132 (92%)	8 (6%)	3 (2%)	5	22
20	U	141/144 (98%)	134 (95%)	7 (5%)	0	100	100
20	c9	141/144 (98%)	141 (100%)	0	0	100	100
21	V	105/121 (87%)	100 (95%)	4 (4%)	1 (1%)	13	40
21	d0	98/121 (81%)	95 (97%)	3 (3%)	0	100	100
22	W	85/87 (98%)	80 (94%)	5 (6%)	0	100	100
22	d1	85/87 (98%)	81 (95%)	3 (4%)	1 (1%)	11	35
23	X	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
23	d2	127/130 (98%)	127 (100%)	0	0	100	100
24	Y	142/145 (98%)	131 (92%)	10 (7%)	1 (1%)	19	49
24	d3	142/145 (98%)	135 (95%)	7 (5%)	0	100	100
25	Z	132/135 (98%)	130 (98%)	2 (2%)	0	100	100
25	d4	132/135 (98%)	125 (95%)	7 (5%)	0	100	100
26	AA	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
26	DB	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
27	9	124/127 (98%)	124 (100%)	0	0	100	100
27	DA	122/127 (96%)	122 (100%)	0	0	100	100
28	AB	146/149 (98%)	140 (96%)	4 (3%)	2 (1%)	9	31
28	DC	146/149 (98%)	142 (97%)	4 (3%)	0	100	100
29	AC	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
29	DD	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
30	AD	95/105 (90%)	95 (100%)	0	0	100	100
30	DE	95/105 (90%)	95 (100%)	0	0	100	100
31	CD	250/254 (98%)	248 (99%)	2 (1%)	0	100	100
31	j	250/254 (98%)	250 (100%)	0	0	100	100
32	AE	107/113 (95%)	104 (97%)	3 (3%)	0	100	100
32	DF	107/113 (95%)	102 (95%)	5 (5%)	0	100	100
33	CE	384/387 (99%)	380 (99%)	4 (1%)	0	100	100
33	k	384/387 (99%)	378 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	AF	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
34	DG	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
38	CF	359/362 (99%)	356 (99%)	3 (1%)	0	100	100
38	l	359/362 (99%)	353 (98%)	5 (1%)	1 (0%)	37	66
39	CG	294/297 (99%)	288 (98%)	4 (1%)	2 (1%)	19	49
39	m	294/297 (99%)	286 (97%)	8 (3%)	0	100	100
40	CH	152/176 (86%)	151 (99%)	1 (1%)	0	100	100
40	n	152/176 (86%)	152 (100%)	0	0	100	100
41	CI	220/244 (90%)	213 (97%)	6 (3%)	1 (0%)	25	56
41	o	220/244 (90%)	218 (99%)	2 (1%)	0	100	100
42	CJ	231/256 (90%)	224 (97%)	7 (3%)	0	100	100
42	p	231/256 (90%)	230 (100%)	1 (0%)	0	100	100
43	CK	189/191 (99%)	188 (100%)	1 (0%)	0	100	100
43	q	189/191 (99%)	184 (97%)	5 (3%)	0	100	100
44	CL	207/221 (94%)	205 (99%)	2 (1%)	0	100	100
44	r	207/221 (94%)	204 (99%)	3 (1%)	0	100	100
45	CM	167/174 (96%)	164 (98%)	3 (2%)	0	100	100
45	s	167/174 (96%)	158 (95%)	9 (5%)	0	100	100
46	CN	191/199 (96%)	180 (94%)	11 (6%)	0	100	100
46	t	191/199 (96%)	184 (96%)	7 (4%)	0	100	100
47	CO	134/138 (97%)	134 (100%)	0	0	100	100
47	u	134/138 (97%)	132 (98%)	1 (1%)	1 (1%)	19	49
48	CP	201/204 (98%)	201 (100%)	0	0	100	100
48	v	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
49	CQ	195/199 (98%)	195 (100%)	0	0	100	100
49	w	195/199 (98%)	195 (100%)	0	0	100	100
50	CR	153/184 (83%)	153 (100%)	0	0	100	100
50	x	172/184 (94%)	171 (99%)	1 (1%)	0	100	100
51	CS	183/186 (98%)	183 (100%)	0	0	100	100
51	y	183/186 (98%)	180 (98%)	3 (2%)	0	100	100
52	CT	182/189 (96%)	177 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	z	181/189 (96%)	180 (99%)	1 (1%)	0	100	100
53	0	170/172 (99%)	170 (100%)	0	0	100	100
53	CU	170/172 (99%)	169 (99%)	1 (1%)	0	100	100
54	2	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
54	CV	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
55	5	98/121 (81%)	98 (100%)	0	0	100	100
55	CW	98/121 (81%)	98 (100%)	0	0	100	100
56	6	134/137 (98%)	134 (100%)	0	0	100	100
56	CX	134/137 (98%)	134 (100%)	0	0	100	100
57	7	65/155 (42%)	65 (100%)	0	0	100	100
57	CY	109/155 (70%)	107 (98%)	2 (2%)	0	100	100
58	8	119/142 (84%)	119 (100%)	0	0	100	100
58	CZ	116/142 (82%)	116 (100%)	0	0	100	100
59	AG	101/107 (94%)	99 (98%)	2 (2%)	0	100	100
59	DH	104/107 (97%)	102 (98%)	2 (2%)	0	100	100
60	AH	110/121 (91%)	109 (99%)	1 (1%)	0	100	100
60	DI	110/121 (91%)	108 (98%)	1 (1%)	1 (1%)	14	43
61	AI	117/120 (98%)	111 (95%)	5 (4%)	1 (1%)	14	43
61	DJ	117/120 (98%)	114 (97%)	1 (1%)	2 (2%)	7	27
62	AJ	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
62	DK	95/100 (95%)	94 (99%)	1 (1%)	0	100	100
63	AK	85/88 (97%)	85 (100%)	0	0	100	100
63	DL	84/88 (96%)	84 (100%)	0	0	100	100
64	AL	75/78 (96%)	75 (100%)	0	0	100	100
64	DM	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
65	AM	48/51 (94%)	48 (100%)	0	0	100	100
65	DN	48/51 (94%)	48 (100%)	0	0	100	100
66	AN	50/128 (39%)	50 (100%)	0	0	100	100
66	DO	50/128 (39%)	48 (96%)	2 (4%)	0	100	100
67	AO	23/25 (92%)	23 (100%)	0	0	100	100
67	DP	23/25 (92%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	AP	103/106 (97%)	96 (93%)	7 (7%)	0	100	100
68	DQ	103/106 (97%)	101 (98%)	2 (2%)	0	100	100
69	AQ	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
69	DR	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
70	i	122/273 (45%)	121 (99%)	0	1 (1%)	16	45
70	sM	61/273 (22%)	54 (88%)	7 (12%)	0	100	100
71	p0	119/312 (38%)	117 (98%)	2 (2%)	0	100	100
72	a	68/108 (63%)	66 (97%)	2 (3%)	0	100	100
72	d5	67/108 (62%)	65 (97%)	2 (3%)	0	100	100
73	b	89/119 (75%)	83 (93%)	6 (7%)	0	100	100
73	d6	95/119 (80%)	90 (95%)	5 (5%)	0	100	100
74	c	79/82 (96%)	76 (96%)	1 (1%)	2 (2%)	4	18
74	d7	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
75	d	61/67 (91%)	61 (100%)	0	0	100	100
75	d8	61/67 (91%)	58 (95%)	3 (5%)	0	100	100
76	d9	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
76	e	51/56 (91%)	51 (100%)	0	0	100	100
77	e0	60/63 (95%)	59 (98%)	0	1 (2%)	7	27
77	f	58/63 (92%)	58 (100%)	0	0	100	100
78	e1	35/152 (23%)	30 (86%)	4 (11%)	1 (3%)	3	15
78	g	69/152 (45%)	64 (93%)	5 (7%)	0	100	100
79	Rb	316/319 (99%)	309 (98%)	6 (2%)	1 (0%)	37	66
79	h	310/319 (97%)	299 (96%)	9 (3%)	2 (1%)	22	52
All	All	21787/24334 (90%)	21256 (98%)	486 (2%)	45 (0%)	44	73

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	112	ARG
11	K	134	ILE
19	T	3	LEU
19	T	92	ILE
24	Y	89	ASN

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	B	164/210 (78%)	158 (96%)	6 (4%)	29	64
2	s0	165/210 (79%)	156 (94%)	9 (6%)	18	48
3	C	191/224 (85%)	174 (91%)	17 (9%)	8	26
3	s1	192/224 (86%)	182 (95%)	10 (5%)	19	50
4	D	176/205 (86%)	170 (97%)	6 (3%)	32	67
4	s2	176/205 (86%)	168 (96%)	8 (4%)	23	56
5	E	182/195 (93%)	173 (95%)	9 (5%)	21	53
5	s3	182/195 (93%)	175 (96%)	7 (4%)	28	63
6	F	221/222 (100%)	216 (98%)	5 (2%)	45	77
6	s4	221/222 (100%)	206 (93%)	15 (7%)	13	38
7	G	173/191 (91%)	163 (94%)	10 (6%)	17	46
7	s5	172/191 (90%)	167 (97%)	5 (3%)	37	72
8	H	187/201 (93%)	178 (95%)	9 (5%)	21	54
8	s6	187/201 (93%)	177 (95%)	10 (5%)	19	49
9	I	165/170 (97%)	157 (95%)	8 (5%)	21	54
9	s7	165/170 (97%)	155 (94%)	10 (6%)	15	43
10	J	150/161 (93%)	136 (91%)	14 (9%)	7	23
10	s8	150/161 (93%)	141 (94%)	9 (6%)	16	44
11	K	155/166 (93%)	147 (95%)	8 (5%)	19	50
11	s9	158/166 (95%)	146 (92%)	12 (8%)	11	32
12	L	77/98 (79%)	72 (94%)	5 (6%)	14	40
12	c0	73/98 (74%)	69 (94%)	4 (6%)	18	48
13	M	129/137 (94%)	126 (98%)	3 (2%)	45	77
13	c1	129/137 (94%)	125 (97%)	4 (3%)	35	70
14	O	127/128 (99%)	120 (94%)	7 (6%)	18	48
14	c3	127/128 (99%)	122 (96%)	5 (4%)	27	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	P	81/105 (77%)	75 (93%)	6 (7%)	11	34
15	c4	97/105 (92%)	91 (94%)	6 (6%)	15	43
16	Q	97/118 (82%)	89 (92%)	8 (8%)	9	29
16	c5	101/118 (86%)	90 (89%)	11 (11%)	5	17
17	R	117/119 (98%)	103 (88%)	14 (12%)	4	13
17	c6	118/119 (99%)	114 (97%)	4 (3%)	32	67
18	S	94/124 (76%)	88 (94%)	6 (6%)	14	41
18	c7	92/124 (74%)	90 (98%)	2 (2%)	47	78
19	T	128/129 (99%)	120 (94%)	8 (6%)	15	42
19	c8	128/129 (99%)	123 (96%)	5 (4%)	27	62
20	U	115/116 (99%)	105 (91%)	10 (9%)	8	27
20	c9	115/116 (99%)	111 (96%)	4 (4%)	31	66
21	V	100/114 (88%)	89 (89%)	11 (11%)	5	16
21	d0	94/114 (82%)	87 (93%)	7 (7%)	11	34
22	W	74/74 (100%)	66 (89%)	8 (11%)	5	17
22	d1	74/74 (100%)	70 (95%)	4 (5%)	18	49
23	X	110/111 (99%)	108 (98%)	2 (2%)	54	82
23	d2	110/111 (99%)	110 (100%)	0	100	100
24	Y	119/120 (99%)	115 (97%)	4 (3%)	32	67
24	d3	119/120 (99%)	114 (96%)	5 (4%)	25	59
25	Z	112/113 (99%)	108 (96%)	4 (4%)	30	65
25	d4	112/113 (99%)	106 (95%)	6 (5%)	18	49
26	AA	115/116 (99%)	109 (95%)	6 (5%)	19	50
26	DB	115/116 (99%)	111 (96%)	4 (4%)	31	66
27	9	109/110 (99%)	106 (97%)	3 (3%)	38	73
27	DA	107/110 (97%)	101 (94%)	6 (6%)	17	47
28	AB	118/119 (99%)	111 (94%)	7 (6%)	16	45
28	DC	118/119 (99%)	112 (95%)	6 (5%)	20	51
29	AC	46/47 (98%)	46 (100%)	0	100	100
29	DD	46/47 (98%)	42 (91%)	4 (9%)	8	27
30	AD	81/88 (92%)	76 (94%)	5 (6%)	15	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	DE	81/88 (92%)	77 (95%)	4 (5%)	21	53
31	CD	193/196 (98%)	183 (95%)	10 (5%)	19	50
31	j	193/196 (98%)	190 (98%)	3 (2%)	58	84
32	AE	92/97 (95%)	88 (96%)	4 (4%)	25	57
32	DF	92/97 (95%)	89 (97%)	3 (3%)	33	68
33	CE	320/323 (99%)	300 (94%)	20 (6%)	15	42
33	k	320/323 (99%)	303 (95%)	17 (5%)	19	49
34	AF	109/111 (98%)	109 (100%)	0	100	100
34	DG	109/111 (98%)	104 (95%)	5 (5%)	23	55
38	CF	288/289 (100%)	266 (92%)	22 (8%)	11	32
38	l	288/289 (100%)	273 (95%)	15 (5%)	19	50
39	CG	244/245 (100%)	232 (95%)	12 (5%)	21	53
39	m	244/245 (100%)	234 (96%)	10 (4%)	26	60
40	CH	134/153 (88%)	131 (98%)	3 (2%)	47	78
40	n	134/153 (88%)	129 (96%)	5 (4%)	29	64
41	CI	186/205 (91%)	178 (96%)	8 (4%)	25	57
41	o	186/205 (91%)	179 (96%)	7 (4%)	28	63
42	CJ	187/208 (90%)	176 (94%)	11 (6%)	16	45
42	p	187/208 (90%)	185 (99%)	2 (1%)	70	90
43	CK	171/171 (100%)	161 (94%)	10 (6%)	17	46
43	q	171/171 (100%)	165 (96%)	6 (4%)	31	66
44	CL	177/187 (95%)	167 (94%)	10 (6%)	17	47
44	r	177/187 (95%)	170 (96%)	7 (4%)	27	61
45	CM	147/151 (97%)	136 (92%)	11 (8%)	11	33
45	s	147/151 (97%)	142 (97%)	5 (3%)	32	67
46	CN	154/159 (97%)	148 (96%)	6 (4%)	27	62
46	t	154/159 (97%)	150 (97%)	4 (3%)	41	74
47	CO	107/109 (98%)	103 (96%)	4 (4%)	29	64
47	u	107/109 (98%)	106 (99%)	1 (1%)	75	92
48	CP	175/176 (99%)	175 (100%)	0	100	100
48	v	175/176 (99%)	173 (99%)	2 (1%)	70	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	CQ	160/162 (99%)	153 (96%)	7 (4%)	24	57
49	w	160/162 (99%)	156 (98%)	4 (2%)	42	75
50	CR	125/146 (86%)	121 (97%)	4 (3%)	34	69
50	x	140/146 (96%)	134 (96%)	6 (4%)	25	57
51	CS	150/151 (99%)	146 (97%)	4 (3%)	40	73
51	y	150/151 (99%)	142 (95%)	8 (5%)	19	49
52	CT	150/154 (97%)	147 (98%)	3 (2%)	50	79
52	z	149/154 (97%)	144 (97%)	5 (3%)	32	67
53	0	156/156 (100%)	153 (98%)	3 (2%)	52	81
53	CU	156/156 (100%)	149 (96%)	7 (4%)	23	56
54	2	136/137 (99%)	132 (97%)	4 (3%)	37	72
54	CV	136/137 (99%)	133 (98%)	3 (2%)	47	78
55	5	87/107 (81%)	83 (95%)	4 (5%)	23	55
55	CW	87/107 (81%)	83 (95%)	4 (5%)	23	55
56	6	104/105 (99%)	97 (93%)	7 (7%)	13	39
56	CX	104/105 (99%)	103 (99%)	1 (1%)	73	91
57	7	56/129 (43%)	54 (96%)	2 (4%)	30	65
57	CY	58/129 (45%)	58 (100%)	0	100	100
58	8	104/118 (88%)	99 (95%)	5 (5%)	21	54
58	CZ	103/118 (87%)	101 (98%)	2 (2%)	52	81
59	AG	89/91 (98%)	86 (97%)	3 (3%)	32	67
59	DH	90/91 (99%)	86 (96%)	4 (4%)	24	57
60	AH	95/103 (92%)	89 (94%)	6 (6%)	15	42
60	DI	95/103 (92%)	90 (95%)	5 (5%)	19	49
61	AI	104/105 (99%)	103 (99%)	1 (1%)	73	91
61	DJ	104/105 (99%)	104 (100%)	0	100	100
62	AJ	81/82 (99%)	76 (94%)	5 (6%)	15	43
62	DK	79/82 (96%)	75 (95%)	4 (5%)	20	51
63	AK	70/71 (99%)	67 (96%)	3 (4%)	25	57
63	DL	70/71 (99%)	67 (96%)	3 (4%)	25	57
64	AL	68/69 (99%)	59 (87%)	9 (13%)	3	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	DM	68/69 (99%)	65 (96%)	3 (4%)	24	57
65	AM	45/46 (98%)	44 (98%)	1 (2%)	47	78
65	DN	45/46 (98%)	44 (98%)	1 (2%)	47	78
66	AN	47/116 (40%)	44 (94%)	3 (6%)	14	41
66	DO	47/116 (40%)	47 (100%)	0	100	100
67	AO	23/23 (100%)	22 (96%)	1 (4%)	25	57
67	DP	23/23 (100%)	21 (91%)	2 (9%)	8	27
68	AP	90/91 (99%)	86 (96%)	4 (4%)	24	57
68	DQ	90/91 (99%)	89 (99%)	1 (1%)	70	90
69	AQ	71/72 (99%)	70 (99%)	1 (1%)	62	86
69	DR	71/72 (99%)	68 (96%)	3 (4%)	25	59
70	i	97/228 (42%)	90 (93%)	7 (7%)	12	35
70	sM	54/228 (24%)	51 (94%)	3 (6%)	17	47
71	p0	105/254 (41%)	97 (92%)	8 (8%)	11	32
72	a	61/89 (68%)	57 (93%)	4 (7%)	14	39
72	d5	61/89 (68%)	55 (90%)	6 (10%)	6	21
73	b	82/100 (82%)	75 (92%)	7 (8%)	8	27
73	d6	83/100 (83%)	79 (95%)	4 (5%)	21	54
74	c	70/71 (99%)	65 (93%)	5 (7%)	12	36
74	d7	70/71 (99%)	65 (93%)	5 (7%)	12	36
75	d	56/60 (93%)	49 (88%)	7 (12%)	3	12
75	d8	56/60 (93%)	47 (84%)	9 (16%)	2	6
76	d9	47/49 (96%)	44 (94%)	3 (6%)	14	41
76	e	47/49 (96%)	45 (96%)	2 (4%)	25	57
77	e0	53/54 (98%)	49 (92%)	4 (8%)	11	33
77	f	51/54 (94%)	48 (94%)	3 (6%)	16	45
78	e1	34/135 (25%)	31 (91%)	3 (9%)	8	26
78	g	62/135 (46%)	53 (86%)	9 (14%)	2	8
79	Rb	260/262 (99%)	237 (91%)	23 (9%)	8	26
79	h	254/262 (97%)	232 (91%)	22 (9%)	8	27
All	All	18444/20440 (90%)	17546 (95%)	898 (5%)	21	53

5 of 898 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	CF	322	GLN
75	d8	60	GLU
58	CZ	59	SER
74	d7	41	LEU
12	c0	27	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 272 such sidechains are listed below:

Mol	Chain	Res	Type
6	s4	57	ASN
8	s6	190	GLN
23	d2	70	ASN
45	s	68	HIS
44	r	59	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1730/1800 (96%)	436 (25%)	44 (2%)
1	sR	1780/1800 (98%)	431 (24%)	0
35	1	3128/3396 (92%)	570 (18%)	44 (1%)
35	AR	3143/3396 (92%)	573 (18%)	48 (1%)
36	3	120/121 (99%)	15 (12%)	1 (0%)
36	AS	120/121 (99%)	18 (15%)	2 (1%)
37	4	157/158 (99%)	33 (21%)	2 (1%)
37	AT	157/158 (99%)	29 (18%)	1 (0%)
All	All	10335/10950 (94%)	2105 (20%)	142 (1%)

5 of 2105 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	4	C
1	A	8	U
1	A	17	C
1	A	25	C

5 of 142 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	AR	1820	U
35	AR	2255	A
35	AR	3157	U
35	1	763	G
35	1	588	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 2541 ligands modelled in this entry, 1523 are monoatomic - leaving 1018 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	AR	3434	-	0,6,6	-	-	-		
80	OHX	1	3426	-	0,6,6	-	-	-		
80	OHX	AR	3510	-	0,6,6	-	-	-		
80	OHX	sR	2011	-	0,6,6	-	-	-		
80	OHX	sR	2001	-	0,6,6	-	-	-		
80	OHX	sR	1905	-	0,6,6	-	-	-		
80	OHX	sR	1989	-	0,6,6	-	-	-		
80	OHX	sR	2028	-	0,6,6	-	-	-		
80	OHX	1	3514	-	0,6,6	-	-	-		
80	OHX	sR	1902	-	0,6,6	-	-	-		
80	OHX	1	3485	-	0,6,6	-	-	-		
80	OHX	1	3428	-	0,6,6	-	-	-		
80	OHX	A	1948	80	0,6,6	-	-	-		
80	OHX	1	4171	-	0,4,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	A	2150	-	0,6,6	-	-	-		
80	OHX	1	3407	-	0,6,6	-	-	-		
80	OHX	1	4149	-	0,6,6	-	-	-		
80	OHX	AR	3550	-	0,6,6	-	-	-		
80	OHX	sR	2015	-	0,6,6	-	-	-		
80	OHX	1	4128	-	0,6,6	-	-	-		
80	OHX	l	403	-	0,6,6	-	-	-		
80	OHX	AR	3614	-	0,6,6	-	-	-		
80	OHX	AR	3544	-	0,6,6	-	-	-		
80	OHX	1	3413	-	0,6,6	-	-	-		
80	OHX	A	1941	-	0,6,6	-	-	-		
80	OHX	A	1957	-	0,6,6	-	-	-		
80	OHX	1	3487	-	0,6,6	-	-	-		
80	OHX	1	3520[A]	-	0,6,6	-	-	-		
80	OHX	1	3628	-	0,6,6	-	-	-		
80	OHX	AR	3421	-	0,6,6	-	-	-		
80	OHX	AR	3480	-	0,6,6	-	-	-		
80	OHX	AR	3630	-	0,6,6	-	-	-		
80	OHX	AR	3517	-	0,6,6	-	-	-		
80	OHX	sR	1926	81	0,6,6	-	-	-		
80	OHX	sR	1986	-	0,6,6	-	-	-		
80	OHX	1	3402	-	0,6,6	-	-	-		
80	OHX	1	3602	-	0,6,6	-	-	-		
80	OHX	AR	3556	-	0,6,6	-	-	-		
80	OHX	AR	3596	-	0,6,6	-	-	-		
80	OHX	A	1959	-	0,6,6	-	-	-		
80	OHX	AR	3591	-	0,6,6	-	-	-		
80	OHX	1	3463	81	0,6,6	-	-	-		
80	OHX	1	3569	-	0,6,6	-	-	-		
80	OHX	1	3575	-	0,6,6	-	-	-		
80	OHX	AR	3503	-	0,6,6	-	-	-		
80	OHX	sR	1978	-	0,6,6	-	-	-		
80	OHX	sR	1906	-	0,6,6	-	-	-		
80	OHX	1	3504	-	0,6,6	-	-	-		
80	OHX	AR	3478	-	0,6,6	-	-	-		
80	OHX	AR	3693	-	0,6,6	-	-	-		
80	OHX	AR	3469	-	0,6,6	-	-	-		
80	OHX	AR	3435	81	0,6,6	-	-	-		
80	OHX	sR	1908	-	0,6,6	-	-	-		
80	OHX	1	4139	-	0,6,6	-	-	-		
86	5XU	c0	203	86	3,4,4	0.79	0	2,4,4	1.08	0
80	OHX	A	2139	-	0,6,6	-	-	-		
80	OHX	1	3461	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	4	214	-	0,6,6	-	-	-		
80	OHX	sR	1954	-	0,6,6	-	-	-		
80	OHX	1	3565	-	0,6,6	-	-	-		
80	OHX	1	3608	-	0,6,6	-	-	-		
80	OHX	AR	3450	-	0,6,6	-	-	-		
80	OHX	AR	3699	-	0,6,6	-	-	-		
80	OHX	4	201	-	0,6,6	-	-	-		
80	OHX	sR	1990	-	0,6,6	-	-	-		
80	OHX	sR	1903	81	0,6,6	-	-	-		
80	OHX	1	3422	-	0,6,6	-	-	-		
80	OHX	AR	3518	-	0,6,6	-	-	-		
80	OHX	sR	1971	-	0,6,6	-	-	-		
80	OHX	1	3506	-	0,6,6	-	-	-		
80	OHX	A	1946	-	0,6,6	-	-	-		
80	OHX	1	4146	-	0,6,6	-	-	-		
80	OHX	3	223	-	0,6,6	-	-	-		
80	OHX	A	1933	-	0,6,6	-	-	-		
80	OHX	sR	1910	-	0,6,6	-	-	-		
80	OHX	sR	2023	-	0,6,6	-	-	-		
80	OHX	A	1924	-	0,6,6	-	-	-		
80	OHX	c5	201	-	0,6,6	-	-	-		
80	OHX	AR	3613	81	0,6,6	-	-	-		
80	OHX	AR	3482	-	0,6,6	-	-	-		
80	OHX	1	4156	-	0,5,6	-	-	-		
80	OHX	AR	3668	-	0,6,6	-	-	-		
80	OHX	1	3468	-	0,6,6	-	-	-		
80	OHX	z	201	-	0,6,6	-	-	-		
80	OHX	A	1967	-	0,6,6	-	-	-		
80	OHX	A	2123	-	0,6,6	-	-	-		
80	OHX	sR	1964	-	0,6,6	-	-	-		
80	OHX	1	3609	-	0,6,6	-	-	-		
80	OHX	AR	3560	-	0,6,6	-	-	-		
80	OHX	AR	3593	-	0,6,6	-	-	-		
80	OHX	AR	3690	-	0,6,6	-	-	-		
80	OHX	1	4166	-	0,6,6	-	-	-		
80	OHX	A	1937	-	0,6,6	-	-	-		
80	OHX	1	4162	-	0,6,6	-	-	-		
80	OHX	1	3432	-	0,6,6	-	-	-		
80	OHX	A	2146	-	0,6,6	-	-	-		
80	OHX	1	3427	81	0,6,6	-	-	-		
80	OHX	AR	3535	-	0,6,6	-	-	-		
80	OHX	AR	3601	81	0,6,6	-	-	-		
80	OHX	AR	3650	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	AR	3404	-	0,6,6	-	-	-		
80	OHX	A	2124	-	0,6,6	-	-	-		
80	OHX	AR	3540	-	0,6,6	-	-	-		
80	OHX	AR	3470	-	0,6,6	-	-	-		
80	OHX	1	4132	-	0,6,6	-	-	-		
80	OHX	1	4151	-	0,6,6	-	-	-		
80	OHX	AR	3669	-	0,6,6	-	-	-		
80	OHX	sR	1922	-	0,6,6	-	-	-		
80	OHX	1	4159	-	0,6,6	-	-	-		
80	OHX	AR	3439	-	0,6,6	-	-	-		
80	OHX	CG	303	-	0,6,6	-	-	-		
80	OHX	1	3522	-	0,6,6	-	-	-		
80	OHX	A	1977	-	0,6,6	-	-	-		
80	OHX	1	3508	81	0,6,6	-	-	-		
80	OHX	AR	3463	-	0,6,6	-	-	-		
80	OHX	AT	210	-	0,6,6	-	-	-		
80	OHX	1	4138	-	0,6,6	-	-	-		
80	OHX	A	1922	-	0,6,6	-	-	-		
80	OHX	sR	1901	-	0,6,6	-	-	-		
80	OHX	sR	1904	-	0,6,6	-	-	-		
80	OHX	sR	2025	-	0,6,6	-	-	-		
80	OHX	A	2154	-	0,6,6	-	-	-		
80	OHX	1	3520[B]	-	0,6,6	-	-	-		
80	OHX	sR	1923	-	0,6,6	-	-	-		
80	OHX	1	3440	-	0,6,6	-	-	-		
80	OHX	1	3441	-	0,6,6	-	-	-		
80	OHX	s4	301	-	0,6,6	-	-	-		
80	OHX	1	3622	-	0,6,6	-	-	-		
80	OHX	1	3626	-	0,6,6	-	-	-		
80	OHX	h	401	-	0,6,6	-	-	-		
80	OHX	sR	1976	81	0,6,6	-	-	-		
80	OHX	AR	3623	-	0,6,6	-	-	-		
80	OHX	1	3640	-	0,6,6	-	-	-		
80	OHX	sR	1994	-	0,6,6	-	-	-		
80	OHX	AR	3417	-	0,6,6	-	-	-		
80	OHX	A	1949	81	0,6,6	-	-	-		
80	OHX	AR	3527	81	0,6,6	-	-	-		
80	OHX	1	3507	-	0,6,6	-	-	-		
80	OHX	AR	3604	-	0,6,6	-	-	-		
80	OHX	AR	3642	-	0,6,6	-	-	-		
80	OHX	1	3496	-	0,6,6	-	-	-		
80	OHX	sR	2005	-	0,6,6	-	-	-		
80	OHX	1	3638	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	1	3546	-	0,6,6	-	-	-		
80	OHX	1	3590	-	0,6,6	-	-	-		
80	OHX	A	2158	-	0,6,6	-	-	-		
80	OHX	A	1975	-	0,6,6	-	-	-		
80	OHX	A	2130	-	0,6,6	-	-	-		
80	OHX	1	3470	-	0,6,6	-	-	-		
80	OHX	1	4163	81	0,6,6	-	-	-		
80	OHX	AS	209	-	0,6,6	-	-	-		
80	OHX	AT	204	-	0,6,6	-	-	-		
80	OHX	1	3451	-	0,6,6	-	-	-		
80	OHX	1	3636	81	0,6,6	-	-	-		
80	OHX	4	215	-	0,6,6	-	-	-		
80	OHX	AR	3626	-	0,6,6	-	-	-		
80	OHX	AS	203	-	0,6,6	-	-	-		
80	OHX	A	1926	81	0,6,6	-	-	-		
80	OHX	4	236	-	0,6,6	-	-	-		
80	OHX	A	1915	-	0,6,6	-	-	-		
80	OHX	sR	1936	-	0,6,6	-	-	-		
80	OHX	1	4147	-	0,6,6	-	-	-		
80	OHX	CE	401	-	0,6,6	-	-	-		
80	OHX	2	201	-	0,6,6	-	-	-		
80	OHX	AR	3570	-	0,6,6	-	-	-		
80	OHX	sR	2182	-	0,6,6	-	-	-		
80	OHX	AR	3457	-	0,6,6	-	-	-		
80	OHX	sR	1975	-	0,6,6	-	-	-		
80	OHX	3	203	81	0,6,6	-	-	-		
80	OHX	AR	3427	-	0,6,6	-	-	-		
80	OHX	1	3536	81	0,6,6	-	-	-		
80	OHX	sR	1921	-	0,6,6	-	-	-		
80	OHX	AR	3602	-	0,6,6	-	-	-		
80	OHX	sR	1929	81	0,6,6	-	-	-		
80	OHX	1	3499	-	0,6,6	-	-	-		
80	OHX	3	202	-	0,6,6	-	-	-		
80	OHX	1	3625	-	0,6,6	-	-	-		
80	OHX	sR	2000	-	0,6,6	-	-	-		
80	OHX	1	3443	-	0,6,6	-	-	-		
80	OHX	AR	3579	-	0,6,6	-	-	-		
80	OHX	A	1904	-	0,6,6	-	-	-		
80	OHX	AR	3698	-	0,6,6	-	-	-		
80	OHX	A	2159[B]	-	0,6,6	-	-	-		
80	OHX	AR	3582	-	0,6,6	-	-	-		
80	OHX	AS	210	-	0,6,6	-	-	-		
80	OHX	AR	3509	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	sR	1935	-	0,6,6	-	-	-		
80	OHX	AR	3426	-	0,6,6	-	-	-		
80	OHX	AR	3584	-	0,6,6	-	-	-		
80	OHX	AR	3600	-	0,6,6	-	-	-		
80	OHX	1	3411	-	0,6,6	-	-	-		
80	OHX	1	3484	81	0,6,6	-	-	-		
80	OHX	A	1906	-	0,6,6	-	-	-		
80	OHX	1	4148	-	0,6,6	-	-	-		
80	OHX	AR	3549	-	0,6,6	-	-	-		
80	OHX	AR	3438	-	0,6,6	-	-	-		
80	OHX	sR	1939	-	0,6,6	-	-	-		
83	SPD	AR	4200	-	9,9,9	0.33	0	8,8,8	1.12	1 (12%)
80	OHX	AR	3461	81	0,6,6	-	-	-		
80	OHX	sR	1919	-	0,6,6	-	-	-		
80	OHX	A	1905	-	0,6,6	-	-	-		
80	OHX	sR	2185	-	0,5,6	-	-	-		
80	OHX	1	3447	81	0,6,6	-	-	-		
80	OHX	A	1960	-	0,6,6	-	-	-		
80	OHX	A	2118	-	0,6,6	-	-	-		
80	OHX	1	4155	-	0,6,6	-	-	-		
80	OHX	4	212	-	0,6,6	-	-	-		
80	OHX	1	3631	-	0,6,6	-	-	-		
80	OHX	1	3532	-	0,6,6	-	-	-		
80	OHX	1	3421	-	0,6,6	-	-	-		
80	OHX	AR	3621	81	0,6,6	-	-	-		
80	OHX	A	1920	-	0,6,6	-	-	-		
80	OHX	1	3577	-	0,6,6	-	-	-		
80	OHX	A	1907	-	0,6,6	-	-	-		
80	OHX	AR	3531	81	0,6,6	-	-	-		
80	OHX	sR	2035	-	0,6,6	-	-	-		
80	OHX	AR	3681	-	0,6,6	-	-	-		
80	OHX	1	3406	-	0,6,6	-	-	-		
80	OHX	1	3548	81	0,6,6	-	-	-		
80	OHX	A	2143	81	0,6,6	-	-	-		
80	OHX	1	3551	-	0,6,6	-	-	-		
80	OHX	k	403	-	0,6,6	-	-	-		
80	OHX	1	4125	-	0,6,6	-	-	-		
80	OHX	AR	3619	-	0,6,6	-	-	-		
80	OHX	sR	1997	-	0,6,6	-	-	-		
80	OHX	AR	3498	-	0,6,6	-	-	-		
80	OHX	1	3620	-	0,6,6	-	-	-		
80	OHX	AR	3590	-	0,6,6	-	-	-		
80	OHX	1	3476	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	1	3607	-	0,6,6	-	-	-		
80	OHX	AR	3636	-	0,6,6	-	-	-		
80	OHX	AR	4232	-	0,6,6	-	-	-		
80	OHX	1	3630	-	0,6,6	-	-	-		
80	OHX	s8	302	-	0,6,6	-	-	-		
80	OHX	AR	3647	-	0,6,6	-	-	-		
80	OHX	AR	3670	-	0,6,6	-	-	-		
80	OHX	sR	1927	-	0,6,6	-	-	-		
80	OHX	1	4150	-	0,6,6	-	-	-		
80	OHX	AR	3423	-	0,6,6	-	-	-		
80	OHX	AR	3500	-	0,6,6	-	-	-		
80	OHX	AR	3545	-	0,6,6	-	-	-		
80	OHX	A	2151	-	0,6,6	-	-	-		
80	OHX	AR	4231	81	0,6,6	-	-	-		
80	OHX	sR	1988	-	0,6,6	-	-	-		
80	OHX	1	3558	-	0,6,6	-	-	-		
80	OHX	sR	1950	-	0,6,6	-	-	-		
80	OHX	1	3481	-	0,6,6	-	-	-		
80	OHX	sR	1925	81	0,6,6	-	-	-		
80	OHX	A	2145	-	0,6,6	-	-	-		
80	OHX	sR	1956	-	0,6,6	-	-	-		
80	OHX	AR	3660	-	0,6,6	-	-	-		
80	OHX	AR	3682	81	0,6,6	-	-	-		
80	OHX	A	1921	-	0,6,6	-	-	-		
80	OHX	1	3478	-	0,6,6	-	-	-		
80	OHX	AR	3537	81	0,6,6	-	-	-		
80	OHX	AR	4225	-	0,6,6	-	-	-		
80	OHX	AR	4228	-	0,6,6	-	-	-		
80	OHX	AR	3643	-	0,6,6	-	-	-		
80	OHX	sR	1973	-	0,6,6	-	-	-		
80	OHX	AR	3473	-	0,6,6	-	-	-		
80	OHX	1	4127	-	0,6,6	-	-	-		
80	OHX	AR	3441	81	0,6,6	-	-	-		
80	OHX	sR	1943	-	0,6,6	-	-	-		
80	OHX	A	1981	-	0,6,6	-	-	-		
80	OHX	1	3599	-	0,6,6	-	-	-		
80	OHX	AR	3519	-	0,6,6	-	-	-		
80	OHX	r	304	-	0,6,6	-	-	-		
80	OHX	sR	1959	-	0,6,6	-	-	-		
80	OHX	AR	3640	81	0,6,6	-	-	-		
80	OHX	AR	3665	-	0,6,6	-	-	-		
80	OHX	AT	214	-	0,6,6	-	-	-		
80	OHX	1	4109	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	AR	3680	-	0,6,6	-	-	-		
80	OHX	A	1961	-	0,6,6	-	-	-		
80	OHX	A	1964	-	0,6,6	-	-	-		
80	OHX	A	1971	-	0,6,6	-	-	-		
80	OHX	1	3490	81	0,6,6	-	-	-		
80	OHX	sR	2006	-	0,6,6	-	-	-		
80	OHX	1	3581	-	0,6,6	-	-	-		
80	OHX	1	4122	-	0,6,6	-	-	-		
80	OHX	1	3431	-	0,6,6	-	-	-		
80	OHX	sR	2187	-	0,6,6	-	-	-		
80	OHX	1	3542	-	0,6,6	-	-	-		
80	OHX	1	3619	-	0,6,6	-	-	-		
80	OHX	1	4141	-	0,6,6	-	-	-		
80	OHX	1	4123	-	0,6,6	-	-	-		
80	OHX	AR	3674	-	0,6,6	-	-	-		
80	OHX	1	4173	-	0,6,6	-	-	-		
80	OHX	1	3525	-	0,6,6	-	-	-		
80	OHX	1	4182	-	0,6,6	-	-	-		
80	OHX	1	3597	-	0,6,6	-	-	-		
80	OHX	AR	3437	-	0,6,6	-	-	-		
80	OHX	CK	202	-	0,6,6	-	-	-		
80	OHX	AR	3574	-	0,6,6	-	-	-		
80	OHX	A	2141	-	0,6,6	-	-	-		
80	OHX	1	3423	-	0,6,6	-	-	-		
80	OHX	AR	3505	-	0,6,6	-	-	-		
80	OHX	AR	3546	-	0,6,6	-	-	-		
80	OHX	AR	3638	-	0,6,6	-	-	-		
80	OHX	sR	2178	-	0,6,6	-	-	-		
80	OHX	A	2147	-	0,6,6	-	-	-		
80	OHX	1	3502	-	0,6,6	-	-	-		
80	OHX	AR	3629	81	0,6,6	-	-	-		
80	OHX	1	3501	-	0,6,6	-	-	-		
80	OHX	1	3617	-	0,6,6	-	-	-		
80	OHX	sR	1979	-	0,6,6	-	-	-		
80	OHX	s1	301	81	0,6,6	-	-	-		
80	OHX	AS	204	-	0,6,6	-	-	-		
80	OHX	AR	3624	-	0,6,6	-	-	-		
80	OHX	1	3618[A]	-	0,6,6	-	-	-		
80	OHX	A	2119	-	0,6,6	-	-	-		
80	OHX	AS	208	-	0,6,6	-	-	-		
80	OHX	sR	1914	-	0,6,6	-	-	-		
80	OHX	AR	3562	-	0,6,6	-	-	-		
80	OHX	1	3601	81	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	A	1978	-	0,6,6	-	-	-		
80	OHX	c8	202	-	0,6,6	-	-	-		
80	OHX	1	3580	-	0,6,6	-	-	-		
80	OHX	A	1976	-	0,6,6	-	-	-		
80	OHX	sR	1934	81	0,6,6	-	-	-		
80	OHX	AS	206	-	0,6,6	-	-	-		
80	OHX	1	4167	-	0,6,6	-	-	-		
80	OHX	sR	1931	-	0,6,6	-	-	-		
80	OHX	AR	3671	-	0,6,6	-	-	-		
80	OHX	1	3497	-	0,6,6	-	-	-		
80	OHX	sR	1918	-	0,6,6	-	-	-		
80	OHX	sR	2033	-	0,6,6	-	-	-		
80	OHX	1	3583	-	0,6,6	-	-	-		
80	OHX	sR	1983	-	0,6,6	-	-	-		
80	OHX	AR	3692	81	0,6,6	-	-	-		
80	OHX	CL	301	-	0,6,6	-	-	-		
80	OHX	1	3561	-	0,6,6	-	-	-		
80	OHX	AR	3589	-	0,6,6	-	-	-		
80	OHX	AR	3606	-	0,6,6	-	-	-		
80	OHX	A	1903	81	0,6,6	-	-	-		
80	OHX	1	3454	-	0,6,6	-	-	-		
80	OHX	1	4161	81	0,6,6	-	-	-		
80	OHX	A	1973	-	0,6,6	-	-	-		
80	OHX	DL	102	-	0,6,6	-	-	-		
80	OHX	AR	3578	-	0,6,6	-	-	-		
80	OHX	AR	3532	-	0,6,6	-	-	-		
80	OHX	AR	3611	-	0,6,6	-	-	-		
80	OHX	sR	1987	-	0,6,6	-	-	-		
80	OHX	1	3404	-	0,6,6	-	-	-		
80	OHX	1	3540	-	0,6,6	-	-	-		
80	OHX	1	3472	-	0,6,6	-	-	-		
80	OHX	AR	3513[A]	-	0,6,6	-	-	-		
80	OHX	AR	4224	81	0,6,6	-	-	-		
80	OHX	sR	2008	-	0,6,6	-	-	-		
80	OHX	A	1911	81	0,6,6	-	-	-		
80	OHX	sR	1947	-	0,6,6	-	-	-		
80	OHX	1	3491	-	0,6,6	-	-	-		
80	OHX	e	102	-	0,6,6	-	-	-		
80	OHX	1	3418	81	0,6,6	-	-	-		
80	OHX	sR	1912	-	0,6,6	-	-	-		
80	OHX	AR	3462	-	0,6,6	-	-	-		
80	OHX	AR	3533	-	0,6,6	-	-	-		
80	OHX	AR	3597	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	1	3494	-	0,6,6	-	-	-		
80	OHX	AR	3507	-	0,6,6	-	-	-		
80	OHX	1	3430	81	0,6,6	-	-	-		
80	OHX	1	3409	-	0,6,6	-	-	-		
80	OHX	A	1934	-	0,6,6	-	-	-		
80	OHX	1	4175	-	0,6,6	-	-	-		
80	OHX	A	2136	-	0,6,6	-	-	-		
80	OHX	AR	3666	-	0,6,6	-	-	-		
80	OHX	CE	402	-	0,6,6	-	-	-		
80	OHX	A	1927	-	0,6,6	-	-	-		
80	OHX	1	4158	-	0,6,6	-	-	-		
80	OHX	AR	3676	-	0,6,6	-	-	-		
80	OHX	A	1929	-	0,6,6	-	-	-		
80	OHX	A	2133	-	0,6,6	-	-	-		
80	OHX	1	3465	-	0,6,6	-	-	-		
80	OHX	AR	3460	-	0,6,6	-	-	-		
80	OHX	AR	3443	-	0,6,6	-	-	-		
80	OHX	A	1945	-	0,6,6	-	-	-		
80	OHX	1	3541	-	0,6,6	-	-	-		
80	OHX	AR	3637	-	0,6,6	-	-	-		
80	OHX	sR	1963	-	0,6,6	-	-	-		
86	5XU	s3	302	86	3,3,4	0.63	0	0,2,4	-	-
80	OHX	sR	1998	-	0,6,6	-	-	-		
80	OHX	1	3612	-	0,6,6	-	-	-		
80	OHX	1	3488	-	0,6,6	-	-	-		
80	OHX	A	1956	-	0,6,6	-	-	-		
80	OHX	AR	3408	-	0,6,6	-	-	-		
80	OHX	AR	3569	-	0,6,6	-	-	-		
80	OHX	AR	3678	-	0,6,6	-	-	-		
80	OHX	AT	209	-	0,6,6	-	-	-		
80	OHX	AR	3552	81	0,6,6	-	-	-		
80	OHX	sR	2021	-	0,6,6	-	-	-		
80	OHX	AR	3696	-	0,6,6	-	-	-		
80	OHX	AR	3514	-	0,6,6	-	-	-		
80	OHX	AR	4227	-	0,6,6	-	-	-		
80	OHX	AR	3502	-	0,6,6	-	-	-		
80	OHX	AR	3471	-	0,6,6	-	-	-		
80	OHX	AR	3700[B]	-	0,6,6	-	-	-		
80	OHX	AR	3583	-	0,6,6	-	-	-		
80	OHX	AR	4237	-	0,5,6	-	-	-		
80	OHX	DQ	203	81	0,6,6	-	-	-		
80	OHX	1	3444	-	0,6,6	-	-	-		
80	OHX	AR	3418	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	1	3618[B]	-	0,6,6	-	-	-		
80	OHX	sR	2016	-	0,6,6	-	-	-		
80	OHX	AR	3608	-	0,6,6	-	-	-		
80	OHX	sR	2190	-	0,6,6	-	-	-		
80	OHX	AR	3440	-	0,6,6	-	-	-		
80	OHX	AR	3477	-	0,6,6	-	-	-		
80	OHX	1	4177	-	0,6,6	-	-	-		
80	OHX	sR	1942	-	0,6,6	-	-	-		
80	OHX	sR	1980	-	0,6,6	-	-	-		
80	OHX	1	4169	-	0,6,6	-	-	-		
80	OHX	AR	3415	81	0,6,6	-	-	-		
80	OHX	AR	4235	-	0,6,6	-	-	-		
80	OHX	1	3604	-	0,6,6	-	-	-		
80	OHX	1	3467	-	0,6,6	-	-	-		
80	OHX	A	1939	-	0,6,6	-	-	-		
80	OHX	AR	3530	-	0,6,6	-	-	-		
80	OHX	AR	4206	-	0,6,6	-	-	-		
80	OHX	1	4157	-	0,6,6	-	-	-		
80	OHX	AR	3581	-	0,6,6	-	-	-		
80	OHX	AR	3559	-	0,6,6	-	-	-		
80	OHX	4	205	-	0,6,6	-	-	-		
80	OHX	AR	3467	81	0,6,6	-	-	-		
80	OHX	AR	3628	-	0,6,6	-	-	-		
80	OHX	AR	3652	-	0,6,6	-	-	-		
80	OHX	1	3489	81	0,6,6	-	-	-		
80	OHX	sR	1999	-	0,6,6	-	-	-		
80	OHX	1	3616	-	0,6,6	-	-	-		
80	OHX	AR	3431	-	0,6,6	-	-	-		
80	OHX	AR	3520	-	0,6,6	-	-	-		
80	OHX	AR	3595	-	0,6,6	-	-	-		
80	OHX	1	3480	-	0,6,6	-	-	-		
80	OHX	A	2144	-	0,6,6	-	-	-		
80	OHX	sR	1948	-	0,6,6	-	-	-		
80	OHX	sR	1981	-	0,6,6	-	-	-		
80	OHX	AR	3528	81	0,6,6	-	-	-		
80	OHX	J	301	-	0,6,6	-	-	-		
80	OHX	AR	3575	-	0,6,6	-	-	-		
80	OHX	sR	1995	-	0,6,6	-	-	-		
80	OHX	AT	203	-	0,6,6	-	-	-		
80	OHX	AR	3609	-	0,6,6	-	-	-		
80	OHX	1	3429	-	0,6,6	-	-	-		
80	OHX	A	1972	-	0,6,6	-	-	-		
80	OHX	AR	3432	81	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	AR	3475	-	0,6,6	-	-	-		
80	OHX	AR	3697	-	0,6,6	-	-	-		
80	OHX	AT	208	-	0,6,6	-	-	-		
80	OHX	AR	3695	-	0,6,6	-	-	-		
80	OHX	AR	3513[B]	-	0,6,6	-	-	-		
80	OHX	1	3513	-	0,6,6	-	-	-		
80	OHX	1	3603	-	0,6,6	-	-	-		
80	OHX	1	3473	-	0,6,6	-	-	-		
80	OHX	AR	3541	-	0,6,6	-	-	-		
80	OHX	sR	2004	-	0,6,6	-	-	-		
80	OHX	1	3567	-	0,6,6	-	-	-		
80	OHX	AR	3599	-	0,6,6	-	-	-		
80	OHX	c3	201	-	0,6,6	-	-	-		
80	OHX	1	4180	-	0,5,6	-	-	-		
80	OHX	1	3531	-	0,6,6	-	-	-		
80	OHX	AR	3515	-	0,6,6	-	-	-		
80	OHX	A	1963	-	0,6,6	-	-	-		
80	OHX	AR	3662	-	0,6,6	-	-	-		
80	OHX	1	3549	-	0,6,6	-	-	-		
80	OHX	1	3516	-	0,6,6	-	-	-		
80	OHX	CP	302	-	0,6,6	-	-	-		
80	OHX	1	3605	-	0,6,6	-	-	-		
80	OHX	3	205	-	0,6,6	-	-	-		
80	OHX	1	4174	-	0,6,6	-	-	-		
80	OHX	1	3629	-	0,6,6	-	-	-		
80	OHX	1	3437	-	0,6,6	-	-	-		
80	OHX	1	3482	-	0,6,6	-	-	-		
80	OHX	1	3595	-	0,6,6	-	-	-		
80	OHX	AR	3472	-	0,6,6	-	-	-		
80	OHX	A	1930	-	0,6,6	-	-	-		
80	OHX	AR	3651	-	0,6,6	-	-	-		
80	OHX	A	1952	-	0,6,6	-	-	-		
80	OHX	sR	1993	-	0,6,6	-	-	-		
80	OHX	4	213	-	0,6,6	-	-	-		
80	OHX	AR	3474	81	0,6,6	-	-	-		
80	OHX	AK	104	81	0,6,6	-	-	-		
80	OHX	AR	3673	-	0,6,6	-	-	-		
80	OHX	AR	3655	-	0,6,6	-	-	-		
80	OHX	1	3635	-	0,6,6	-	-	-		
80	OHX	AR	3487	-	0,6,6	-	-	-		
80	OHX	AR	3424	-	0,6,6	-	-	-		
80	OHX	A	1910	-	0,6,6	-	-	-		
80	OHX	A	1902	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	AR	3430	81	0,6,6	-	-	-		
80	OHX	AR	3494	-	0,6,6	-	-	-		
80	OHX	1	3639	-	0,6,6	-	-	-		
80	OHX	AR	3511	-	0,6,6	-	-	-		
80	OHX	sR	1911	-	0,6,6	-	-	-		
80	OHX	sR	1924	-	0,6,6	-	-	-		
80	OHX	1	3537	-	0,6,6	-	-	-		
80	OHX	AR	3588	-	0,6,6	-	-	-		
80	OHX	1	3547	-	0,6,6	-	-	-		
80	OHX	1	3632	-	0,6,6	-	-	-		
80	OHX	sR	1991	-	0,6,6	-	-	-		
80	OHX	1	4130	-	0,6,6	-	-	-		
80	OHX	AR	3538	-	0,6,6	-	-	-		
80	OHX	1	4176	-	0,6,6	-	-	-		
80	OHX	AR	3476	-	0,6,6	-	-	-		
80	OHX	AR	3607	-	0,6,6	-	-	-		
80	OHX	1	3448	-	0,6,6	-	-	-		
80	OHX	1	3408	-	0,6,6	-	-	-		
80	OHX	AR	3568	-	0,6,6	-	-	-		
80	OHX	sR	2009	-	0,6,6	-	-	-		
80	OHX	A	2149	-	0,6,6	-	-	-		
80	OHX	sR	1916[A]	-	0,6,6	-	-	-		
80	OHX	AR	3555	-	0,6,6	-	-	-		
80	OHX	AR	3610	-	0,6,6	-	-	-		
80	OHX	A	1909	-	0,6,6	-	-	-		
80	OHX	1	3419	-	0,6,6	-	-	-		
80	OHX	A	2152	-	0,6,6	-	-	-		
80	OHX	1	3510	-	0,6,6	-	-	-		
80	OHX	AR	3571	-	0,6,6	-	-	-		
80	OHX	AR	3620	81	0,6,6	-	-	-		
80	OHX	A	2131	-	0,6,6	-	-	-		
80	OHX	sR	2014	-	0,6,6	-	-	-		
80	OHX	A	2110	-	0,6,6	-	-	-		
80	OHX	sR	1968	-	0,6,6	-	-	-		
80	OHX	1	3453	-	0,6,6	-	-	-		
80	OHX	1	3452	-	0,6,6	-	-	-		
80	OHX	sR	1917	-	0,6,6	-	-	-		
80	OHX	AR	3508	-	0,6,6	-	-	-		
80	OHX	1	3459	-	0,6,6	-	-	-		
80	OHX	1	3417	-	0,6,6	-	-	-		
80	OHX	1	3533	-	0,6,6	-	-	-		
80	OHX	AR	3664	81	0,6,6	-	-	-		
80	OHX	AT	211	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	AR	3444	-	0,6,6	-	-	-		
80	OHX	A	1942	81	0,6,6	-	-	-		
80	OHX	AS	228	-	0,6,6	-	-	-		
80	OHX	1	3633	-	0,6,6	-	-	-		
80	OHX	1	3606	81	0,6,6	-	-	-		
80	OHX	1	3592	-	0,6,6	-	-	-		
80	OHX	1	3576	-	0,6,6	-	-	-		
80	OHX	3	206	-	0,6,6	-	-	-		
80	OHX	1	3457	-	0,6,6	-	-	-		
80	OHX	1	3563	-	0,6,6	-	-	-		
80	OHX	1	4154	-	0,6,6	-	-	-		
80	OHX	1	3589	-	0,6,6	-	-	-		
86	5XU	c0	201	86	3,4,4	0.80	0	2,4,4	0.64	0
80	OHX	AR	4234	-	0,6,6	-	-	-		
80	OHX	1	3538	-	0,6,6	-	-	-		
80	OHX	1	3434	-	0,6,6	-	-	-		
80	OHX	1	3545	-	0,6,6	-	-	-		
80	OHX	sR	1938	-	0,6,6	-	-	-		
80	OHX	A	1962	-	0,6,6	-	-	-		
80	OHX	1	3553	-	0,6,6	-	-	-		
80	OHX	1	3615	-	0,6,6	-	-	-		
80	OHX	1	3579	-	0,6,6	-	-	-		
80	OHX	A	2153	-	0,6,6	-	-	-		
80	OHX	sR	1982	-	0,6,6	-	-	-		
80	OHX	AR	3635	-	0,6,6	-	-	-		
80	OHX	4	210	-	0,6,6	-	-	-		
80	OHX	1	3587	-	0,6,6	-	-	-		
80	OHX	AR	3468	-	0,6,6	-	-	-		
80	OHX	AR	3536	-	0,6,6	-	-	-		
80	OHX	1	3534	-	0,6,6	-	-	-		
80	OHX	AR	3625	-	0,6,6	-	-	-		
80	OHX	AR	3686	-	0,6,6	-	-	-		
80	OHX	sR	2024	-	0,6,6	-	-	-		
80	OHX	AR	3522	-	0,6,6	-	-	-		
80	OHX	1	3495	-	0,6,6	-	-	-		
80	OHX	1	3458	-	0,6,6	-	-	-		
80	OHX	AR	3491	-	0,6,6	-	-	-		
80	OHX	AP	502	81	0,6,6	-	-	-		
80	OHX	AR	3672	-	0,6,6	-	-	-		
80	OHX	1	3416	81	0,6,6	-	-	-		
80	OHX	AR	3402	-	0,6,6	-	-	-		
80	OHX	1	3641	-	0,6,6	-	-	-		
80	OHX	sR	1966	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	A	2117	-	0,6,6	-	-	-		
80	OHX	1	3492	-	0,6,6	-	-	-		
80	OHX	AR	3612	-	0,6,6	-	-	-		
80	OHX	AR	3506	-	0,6,6	-	-	-		
80	OHX	1	3544	81	0,6,6	-	-	-		
80	OHX	3	204	-	0,6,6	-	-	-		
80	OHX	AR	3656	-	0,6,6	-	-	-		
80	OHX	A	1931	-	0,6,6	-	-	-		
80	OHX	sR	2032	-	0,6,6	-	-	-		
80	OHX	A	1966	-	0,6,6	-	-	-		
80	OHX	1	3486	-	0,6,6	-	-	-		
80	OHX	AR	3420	81	0,6,6	-	-	-		
80	OHX	AR	3558	-	0,6,6	-	-	-		
80	OHX	A	2148	-	0,6,6	-	-	-		
80	OHX	1	3425	-	0,6,6	-	-	-		
80	OHX	1	3524	-	0,6,6	-	-	-		
80	OHX	1	4129	-	0,6,6	-	-	-		
80	OHX	AR	3646	-	0,6,6	-	-	-		
80	OHX	CG	302	-	0,6,6	-	-	-		
80	OHX	sR	1933	-	0,6,6	-	-	-		
80	OHX	1	3446	81	0,6,6	-	-	-		
80	OHX	1	3521	-	0,6,6	-	-	-		
80	OHX	AR	3410	81	0,6,6	-	-	-		
80	OHX	AR	3481	-	0,6,6	-	-	-		
80	OHX	1	3585	-	0,6,6	-	-	-		
80	OHX	A	2129	-	0,6,6	-	-	-		
80	OHX	AR	3616	-	0,6,6	-	-	-		
80	OHX	1	3477	-	0,6,6	-	-	-		
80	OHX	1	3414	-	0,6,6	-	-	-		
80	OHX	1	3530	-	0,6,6	-	-	-		
80	OHX	1	3573	-	0,6,6	-	-	-		
80	OHX	AR	3521	-	0,6,6	-	-	-		
80	OHX	1	3543	-	0,6,6	-	-	-		
80	OHX	sR	1920	-	0,6,6	-	-	-		
80	OHX	AR	3454	-	0,6,6	-	-	-		
80	OHX	1	3433	-	0,6,6	-	-	-		
80	OHX	1	3572	-	0,6,6	-	-	-		
80	OHX	1	4152	-	0,6,6	-	-	-		
80	OHX	AR	3406	-	0,6,6	-	-	-		
80	OHX	sR	1916[B]	-	0,6,6	-	-	-		
80	OHX	A	1940	-	0,6,6	-	-	-		
80	OHX	1	3526	-	0,6,6	-	-	-		
80	OHX	AR	3433	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	1	3412	-	0,6,6	-	-	-		
80	OHX	AG	201	-	0,6,6	-	-	-		
80	OHX	AR	3659	-	0,6,6	-	-	-		
80	OHX	sR	1957	-	0,6,6	-	-	-		
80	OHX	sR	1930	-	0,6,6	-	-	-		
80	OHX	AR	3667	-	0,6,6	-	-	-		
80	OHX	d6	201	-	0,6,6	-	-	-		
80	OHX	AR	3466	-	0,6,6	-	-	-		
80	OHX	AR	3633	-	0,6,6	-	-	-		
80	OHX	1	4134	-	0,6,6	-	-	-		
80	OHX	AR	3446	-	0,6,6	-	-	-		
80	OHX	sR	2174	-	0,6,6	-	-	-		
80	OHX	A	1980	-	0,6,6	-	-	-		
80	OHX	1	3557	-	0,6,6	-	-	-		
80	OHX	1	3559	-	0,6,6	-	-	-		
80	OHX	1	4153	-	0,6,6	-	-	-		
80	OHX	AR	3542	-	0,6,6	-	-	-		
80	OHX	Q	201	-	0,6,6	-	-	-		
80	OHX	AR	3661	-	0,6,6	-	-	-		
80	OHX	AR	4230	-	0,6,6	-	-	-		
80	OHX	AR	3553	-	0,6,6	-	-	-		
80	OHX	1	4165	-	0,6,6	-	-	-		
80	OHX	1	3552	-	0,6,6	-	-	-		
80	OHX	1	3568	-	0,6,6	-	-	-		
80	OHX	1	4140	81	0,6,6	-	-	-		
80	OHX	A	2115	-	0,6,6	-	-	-		
80	OHX	1	4133	-	0,6,6	-	-	-		
80	OHX	sR	1951	-	0,6,6	-	-	-		
80	OHX	sR	1907	-	0,6,6	-	-	-		
80	OHX	1	3500	-	0,6,6	-	-	-		
80	OHX	1	3593	-	0,6,6	-	-	-		
80	OHX	3	221	-	0,6,6	-	-	-		
80	OHX	AR	3403	-	0,6,6	-	-	-		
80	OHX	A	1908	-	0,6,6	-	-	-		
80	OHX	1	3594	-	0,6,6	-	-	-		
80	OHX	AR	3534	-	0,6,6	-	-	-		
80	OHX	AR	3632	-	0,6,6	-	-	-		
80	OHX	1	4126	-	0,6,6	-	-	-		
80	OHX	AR	3419	-	0,6,6	-	-	-		
80	OHX	1	4135	-	0,6,6	-	-	-		
80	OHX	AR	3501	-	0,6,6	-	-	-		
80	OHX	1	3535	-	0,6,6	-	-	-		
80	OHX	k	402	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	AR	3644	81	0,6,6	-	-	-		
80	OHX	AR	3663	-	0,6,6	-	-	-		
80	OHX	AR	3566	-	0,6,6	-	-	-		
80	OHX	1	3556	-	0,6,6	-	-	-		
80	OHX	1	3582	-	0,6,6	-	-	-		
80	OHX	sR	1992	-	0,6,6	-	-	-		
80	OHX	sR	1909	-	0,6,6	-	-	-		
83	SPD	1	4106	-	9,9,9	0.32	0	8,8,8	0.81	0
80	OHX	A	2140	-	0,6,6	-	-	-		
80	OHX	AR	3452	-	0,6,6	-	-	-		
80	OHX	1	4144	-	0,6,6	-	-	-		
80	OHX	1	3600	-	0,6,6	-	-	-		
80	OHX	A	1968	-	0,6,6	-	-	-		
80	OHX	CX	201	-	0,6,6	-	-	-		
80	OHX	A	1925	-	0,6,6	-	-	-		
80	OHX	A	2125	-	0,6,6	-	-	-		
80	OHX	n	201	-	0,6,6	-	-	-		
80	OHX	AR	3447	-	0,6,6	-	-	-		
80	OHX	1	3528	-	0,6,6	-	-	-		
80	OHX	1	3450	-	0,6,6	-	-	-		
80	OHX	1	3613	-	0,6,6	-	-	-		
80	OHX	AR	3414	-	0,6,6	-	-	-		
80	OHX	AR	3525	-	0,6,6	-	-	-		
80	OHX	AR	3561	-	0,6,6	-	-	-		
80	OHX	AR	3493	-	0,6,6	-	-	-		
80	OHX	A	2128	81	0,6,6	-	-	-		
80	OHX	1	4164	81	0,6,6	-	-	-		
80	OHX	AR	3631	-	0,6,6	-	-	-		
80	OHX	A	2121	-	0,6,6	-	-	-		
80	OHX	A	2134	-	0,6,6	-	-	-		
80	OHX	4	204	-	0,6,6	-	-	-		
80	OHX	AR	3401	-	0,6,6	-	-	-		
80	OHX	sR	2012	-	0,6,6	-	-	-		
80	OHX	1	3623	-	0,6,6	-	-	-		
80	OHX	sR	1969	-	0,6,6	-	-	-		
80	OHX	AR	3548	-	0,6,6	-	-	-		
80	OHX	CS	202	-	0,6,6	-	-	-		
80	OHX	sR	1915	-	0,6,6	-	-	-		
80	OHX	sR	2183	-	0,6,6	-	-	-		
80	OHX	A	1970	-	0,6,6	-	-	-		
80	OHX	AR	3551	-	0,6,6	-	-	-		
80	OHX	4	209	-	0,6,6	-	-	-		
80	OHX	AC	102	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	AR	3587	-	0,6,6	-	-	-		
80	OHX	1	3588	-	0,6,6	-	-	-		
80	OHX	1	4136	-	0,6,6	-	-	-		
80	OHX	1	4172	-	0,6,6	-	-	-		
80	OHX	AR	3701	-	0,6,6	-	-	-		
80	OHX	sR	1967	-	0,6,6	-	-	-		
80	OHX	A	2127	-	0,6,6	-	-	-		
80	OHX	1	3512	-	0,6,6	-	-	-		
80	OHX	sR	2027	-	0,6,6	-	-	-		
80	OHX	1	3562	-	0,6,6	-	-	-		
80	OHX	AR	3455	-	0,5,6	-	-	-		
80	OHX	AR	3564	81	0,6,6	-	-	-		
80	OHX	sR	2180	-	0,6,6	-	-	-		
80	OHX	sR	1974	-	0,6,6	-	-	-		
80	OHX	AR	3512	-	0,6,6	-	-	-		
80	OHX	1	3445	81	0,6,6	-	-	-		
80	OHX	y	201	-	0,6,6	-	-	-		
80	OHX	1	3527	-	0,6,6	-	-	-		
80	OHX	AR	3495	-	0,6,6	-	-	-		
80	OHX	A	1901	-	0,6,6	-	-	-		
80	OHX	AR	4229	-	0,6,6	-	-	-		
80	OHX	sR	1958	-	0,6,6	-	-	-		
80	OHX	sR	2179	-	0,6,6	-	-	-		
80	OHX	AR	3445	-	0,6,6	-	-	-		
80	OHX	sR	1955	-	0,6,6	-	-	-		
80	OHX	AR	4238	-	0,6,6	-	-	-		
80	OHX	AR	3409	-	0,6,6	-	-	-		
80	OHX	AR	3489	-	0,6,6	-	-	-		
80	OHX	AR	3594	-	0,6,6	-	-	-		
80	OHX	1	3420	-	0,6,6	-	-	-		
80	OHX	1	3570	-	0,6,6	-	-	-		
80	OHX	sR	2189	-	0,6,6	-	-	-		
80	OHX	1	3442	-	0,6,6	-	-	-		
80	OHX	A	1979	-	0,6,6	-	-	-		
80	OHX	1	3410	-	0,6,6	-	-	-		
80	OHX	AT	215	-	0,6,6	-	-	-		
80	OHX	sR	2019	-	0,6,6	-	-	-		
80	OHX	A	1936	-	0,6,6	-	-	-		
80	OHX	AR	3465	-	0,6,6	-	-	-		
80	OHX	1	3554	-	0,6,6	-	-	-		
80	OHX	sR	2029	-	0,6,6	-	-	-		
80	OHX	AR	3585	-	0,6,6	-	-	-		
80	OHX	1	4108	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	1	3529	-	0,6,6	-	-	-		
80	OHX	1	3515	-	0,6,6	-	-	-		
80	OHX	sR	2026	-	0,6,6	-	-	-		
80	OHX	sR	2186	-	0,6,6	-	-	-		
80	OHX	AR	3425	-	0,6,6	-	-	-		
80	OHX	sR	2022	-	0,6,6	-	-	-		
80	OHX	AR	4213	81	0,6,6	-	-	-		
80	OHX	sR	1984	-	0,6,6	-	-	-		
80	OHX	1	3578	81	0,6,6	-	-	-		
80	OHX	1	4143	-	0,6,6	-	-	-		
80	OHX	DK	201	-	0,6,6	-	-	-		
80	OHX	4	203	-	0,6,6	-	-	-		
80	OHX	AR	3685	-	0,6,6	-	-	-		
80	OHX	AR	3412	-	0,6,6	-	-	-		
80	OHX	sR	1961	-	0,6,6	-	-	-		
80	OHX	AR	3645	-	0,6,6	-	-	-		
80	OHX	A	1923	-	0,6,6	-	-	-		
80	OHX	1	3539	81	0,6,6	-	-	-		
80	OHX	sR	2003	-	0,6,6	-	-	-		
80	OHX	A	1913	-	0,6,6	-	-	-		
80	OHX	sR	2013	-	0,6,6	-	-	-		
80	OHX	1	3584	-	0,6,6	-	-	-		
80	OHX	d4	201	-	0,6,6	-	-	-		
80	OHX	Rb	401	-	0,6,6	-	-	-		
80	OHX	sR	2034	-	0,6,6	-	-	-		
80	OHX	1	3456	-	0,6,6	-	-	-		
80	OHX	AR	3657	-	0,6,6	-	-	-		
80	OHX	sR	1965	-	0,6,6	-	-	-		
80	OHX	AR	3456	-	0,6,6	-	-	-		
80	OHX	AR	3617	-	0,6,6	-	-	-		
80	OHX	AR	3691	-	0,6,6	-	-	-		
80	OHX	1	4170	-	0,6,6	-	-	-		
80	OHX	1	3439	-	0,6,6	-	-	-		
80	OHX	DD	101	-	0,6,6	-	-	-		
80	OHX	1	3498	-	0,6,6	-	-	-		
80	OHX	AE	201	-	0,6,6	-	-	-		
80	OHX	AR	3436	-	0,6,6	-	-	-		
80	OHX	1	3460	-	0,6,6	-	-	-		
80	OHX	1	4124	-	0,6,6	-	-	-		
80	OHX	A	2137	-	0,6,6	-	-	-		
80	OHX	A	2159[A]	-	0,6,6	-	-	-		
80	OHX	AT	205	-	0,6,6	-	-	-		
80	OHX	AR	3653	81	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	sR	1944	-	0,6,6	-	-	-		
80	OHX	3	222	-	0,6,6	-	-	-		
80	OHX	A	1950	-	0,6,6	-	-	-		
80	OHX	sR	1962	-	0,6,6	-	-	-		
80	OHX	A	1974	-	0,6,6	-	-	-		
80	OHX	1	3469	81	0,6,6	-	-	-		
80	OHX	1	3435	-	0,6,6	-	-	-		
80	OHX	A	1928	-	0,6,6	-	-	-		
80	OHX	AR	3499	-	0,6,6	-	-	-		
80	OHX	A	2114	-	0,6,6	-	-	-		
80	OHX	sR	1953	-	0,6,6	-	-	-		
80	OHX	O	201	-	0,6,6	-	-	-		
80	OHX	k	404	-	0,6,6	-	-	-		
80	OHX	A	1943	-	0,6,6	-	-	-		
80	OHX	1	3624	-	0,6,6	-	-	-		
80	OHX	CG	304	-	0,6,6	-	-	-		
80	OHX	A	2116	-	0,6,6	-	-	-		
80	OHX	AR	3453	-	0,6,6	-	-	-		
80	OHX	AR	3658	-	0,6,6	-	-	-		
86	5XU	s3	301	86	3,4,4	0.69	0	2,4,4	2.03	1 (50%)
80	OHX	1	3550	-	0,6,6	-	-	-		
80	OHX	1	3627	-	0,6,6	-	-	-		
80	OHX	AR	3648	-	0,6,6	-	-	-		
80	OHX	1	3598	-	0,6,6	-	-	-		
80	OHX	AR	4233	81	0,6,6	-	-	-		
80	OHX	sR	2002	-	0,6,6	-	-	-		
80	OHX	AR	3464	-	0,6,6	-	-	-		
80	OHX	AR	3459	81	0,6,6	-	-	-		
80	OHX	AR	3504	-	0,6,6	-	-	-		
80	OHX	CL	302	-	0,6,6	-	-	-		
80	OHX	AR	3524	-	0,6,6	-	-	-		
80	OHX	sR	2010	-	0,6,6	-	-	-		
80	OHX	sR	1949	-	0,6,6	-	-	-		
80	OHX	AR	4236	-	0,6,6	-	-	-		
80	OHX	AR	3586	-	0,6,6	-	-	-		
80	OHX	3	201	-	0,6,6	-	-	-		
80	OHX	A	1916	-	0,6,6	-	-	-		
80	OHX	1	3462	-	0,6,6	-	-	-		
80	OHX	A	1954	-	0,6,6	-	-	-		
80	OHX	1	3519	-	0,6,6	-	-	-		
80	OHX	1	3505	-	0,6,6	-	-	-		
80	OHX	1	4181	80	0,6,6	-	-	-		
80	OHX	sR	2017	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	AR	3413	-	0,6,6	-	-	-		
80	OHX	4	207	-	0,6,6	-	-	-		
80	OHX	1	3503	-	0,6,6	-	-	-		
80	OHX	1	3479	-	0,6,6	-	-	-		
80	OHX	A	2156	80	0,5,6	-	-	-		
80	OHX	AR	3679	-	0,6,6	-	-	-		
80	OHX	AR	3684	-	0,6,6	-	-	-		
80	OHX	1	4142	-	0,6,6	-	-	-		
80	OHX	A	2135	-	0,6,6	-	-	-		
80	OHX	1	3621	-	0,6,6	-	-	-		
80	OHX	AR	3485	-	0,6,6	-	-	-		
80	OHX	AR	3654	-	0,6,6	-	-	-		
80	OHX	AR	3526	-	0,6,6	-	-	-		
80	OHX	1	4168	-	0,6,6	-	-	-		
80	OHX	sR	1937	-	0,6,6	-	-	-		
80	OHX	1	3566	-	0,6,6	-	-	-		
80	OHX	sR	1945	-	0,6,6	-	-	-		
80	OHX	A	2122	-	0,6,6	-	-	-		
80	OHX	A	1932	-	0,6,6	-	-	-		
80	OHX	sR	2018	-	0,6,6	-	-	-		
80	OHX	AT	207	-	0,6,6	-	-	-		
80	OHX	AR	3483	-	0,6,6	-	-	-		
80	OHX	A	1914	-	0,6,6	-	-	-		
80	OHX	sR	2176	-	0,6,6	-	-	-		
80	OHX	1	3466	80	0,5,6	-	-	-		
80	OHX	AR	3496	-	0,6,6	-	-	-		
80	OHX	1	3523	-	0,6,6	-	-	-		
80	OHX	1	3591	-	0,6,6	-	-	-		
80	OHX	1	3634	-	0,6,6	-	-	-		
80	OHX	AR	3422	-	0,6,6	-	-	-		
80	OHX	sR	2188	-	0,6,6	-	-	-		
80	OHX	DH	202	-	0,6,6	-	-	-		
80	OHX	1	3509	-	0,6,6	-	-	-		
80	OHX	AR	3677	-	0,6,6	-	-	-		
80	OHX	sR	1913	-	0,6,6	-	-	-		
80	OHX	1	3555	-	0,6,6	-	-	-		
80	OHX	AR	4226	-	0,6,6	-	-	-		
80	OHX	A	1953	-	0,6,6	-	-	-		
80	OHX	1	4160	-	0,6,6	-	-	-		
80	OHX	4	206	-	0,6,6	-	-	-		
80	OHX	AR	3565	81	0,6,6	-	-	-		
80	OHX	AT	213	-	0,6,6	-	-	-		
80	OHX	sR	1977	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	1	3493	81	0,6,6	-	-	-		
80	OHX	AR	3448	-	0,6,6	-	-	-		
80	OHX	AR	3529	-	0,6,6	-	-	-		
80	OHX	A	1918	-	0,6,6	-	-	-		
80	OHX	AR	3618	-	0,6,6	-	-	-		
80	OHX	AR	3492	-	0,6,6	-	-	-		
80	OHX	AR	3484	-	0,6,6	-	-	-		
80	OHX	AR	3689	-	0,6,6	-	-	-		
80	OHX	1	3610	-	0,6,6	-	-	-		
80	OHX	z	204	-	0,6,6	-	-	-		
80	OHX	AR	3516	-	0,6,6	-	-	-		
80	OHX	A	1969	-	0,6,6	-	-	-		
80	OHX	AR	3486	-	0,6,6	-	-	-		
80	OHX	AR	3563	-	0,6,6	-	-	-		
80	OHX	1	3401	-	0,6,6	-	-	-		
80	OHX	1	3415	-	0,6,6	-	-	-		
80	OHX	x	209	-	0,6,6	-	-	-		
80	OHX	sR	1952	-	0,6,6	-	-	-		
80	OHX	AR	3416	-	0,6,6	-	-	-		
80	OHX	1	3449	-	0,6,6	-	-	-		
80	OHX	T	201	-	0,6,6	-	-	-		
80	OHX	1	3637	-	0,6,6	-	-	-		
80	OHX	AR	3428	-	0,6,6	-	-	-		
80	OHX	AR	3490	-	0,6,6	-	-	-		
80	OHX	sR	1985	-	0,6,6	-	-	-		
80	OHX	sR	1940	-	0,6,6	-	-	-		
80	OHX	sR	1970	81	0,6,6	-	-	-		
80	OHX	A	1912	-	0,6,6	-	-	-		
80	OHX	A	2120	-	0,6,6	-	-	-		
80	OHX	AR	3598	-	0,6,6	-	-	-		
84	VDU	1	4195	-	28,28,28	0.39	0	35,45,45	1.03	2 (5%)
80	OHX	AR	3639	-	0,6,6	-	-	-		
80	OHX	4	238	-	0,6,6	-	-	-		
80	OHX	AR	3547	81	0,6,6	-	-	-		
80	OHX	AR	3539	-	0,6,6	-	-	-		
80	OHX	1	3614	-	0,6,6	-	-	-		
80	OHX	1	3405	-	0,6,6	-	-	-		
80	OHX	1	3483	-	0,6,6	-	-	-		
80	OHX	AS	205	81	0,6,6	-	-	-		
80	OHX	AR	3576	-	0,6,6	-	-	-		
80	OHX	1	4145	-	0,6,6	-	-	-		
80	OHX	3	219	-	0,6,6	-	-	-		
80	OHX	sR	1972	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	1	4131	81	0,6,6	-	-	-		
80	OHX	1	4137	-	0,6,6	-	-	-		
80	OHX	AR	3572	-	0,6,6	-	-	-		
80	OHX	A	2142	-	0,6,6	-	-	-		
80	OHX	v	301	-	0,6,6	-	-	-		
80	OHX	AR	3479	-	0,6,6	-	-	-		
80	OHX	AR	3429	-	0,6,6	-	-	-		
80	OHX	1	3560	-	0,6,6	-	-	-		
80	OHX	A	1951	-	0,6,6	-	-	-		
80	OHX	CL	304	-	0,5,6	-	-	-		
80	OHX	A	1947	-	0,6,6	-	-	-		
80	OHX	1	3455	-	0,6,6	-	-	-		
80	OHX	1	3517	-	0,6,6	-	-	-		
80	OHX	1	3564	81	0,6,6	-	-	-		
80	OHX	AR	3577	-	0,6,6	-	-	-		
80	OHX	AR	3675	-	0,6,6	-	-	-		
80	OHX	sR	2020	-	0,6,6	-	-	-		
80	OHX	AR	3557	81	0,6,6	-	-	-		
80	OHX	AR	3605	-	0,6,6	-	-	-		
80	OHX	4	237	-	0,6,6	-	-	-		
86	5XU	c0	202	86	3,4,4	0.84	0	2,4,4	0.93	0
80	OHX	AR	3523	-	0,6,6	-	-	-		
80	OHX	AT	212	-	0,6,6	-	-	-		
80	OHX	AR	3554	-	0,6,6	-	-	-		
80	OHX	S	201	-	0,6,6	-	-	-		
80	OHX	A	1955	-	0,6,6	-	-	-		
80	OHX	sR	1928	-	0,6,6	-	-	-		
80	OHX	A	2157	-	0,6,6	-	-	-		
80	OHX	sR	2181	-	0,6,6	-	-	-		
80	OHX	A	1935	-	0,6,6	-	-	-		
80	OHX	AR	3603	-	0,6,6	-	-	-		
80	OHX	1	3464	-	0,6,6	-	-	-		
80	OHX	AR	3627	-	0,6,6	-	-	-		
80	OHX	sR	1946	-	0,6,6	-	-	-		
80	OHX	3	220	-	0,6,6	-	-	-		
80	OHX	sR	2030	-	0,6,6	-	-	-		
80	OHX	1	3611	-	0,6,6	-	-	-		
80	OHX	A	2126	-	0,6,6	-	-	-		
80	OHX	AT	201	-	0,6,6	-	-	-		
80	OHX	sR	2007	-	0,6,6	-	-	-		
84	VDU	AR	4255	-	28,28,28	0.39	0	35,45,45	1.03	2 (5%)
80	OHX	AT	206	-	0,6,6	-	-	-		
80	OHX	1	3586	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	A	1919	-	0,6,6	-	-	-		
80	OHX	1	4179	-	0,6,6	-	-	-		
80	OHX	A	1965	-	0,6,6	-	-	-		
80	OHX	1	4178	-	0,6,6	-	-	-		
80	OHX	1	3518	-	0,6,6	-	-	-		
80	OHX	A	2132	-	0,6,6	-	-	-		
80	OHX	AR	3622	-	0,6,6	-	-	-		
80	OHX	AR	3683	-	0,6,6	-	-	-		
80	OHX	A	1917	-	0,6,6	-	-	-		
80	OHX	AR	3497	81	0,6,6	-	-	-		
80	OHX	A	1938	-	0,6,6	-	-	-		
80	OHX	1	3574	-	0,6,6	-	-	-		
80	OHX	A	1944	-	0,6,6	-	-	-		
80	OHX	AR	3543	-	0,6,6	-	-	-		
80	OHX	AR	3649	-	0,6,6	-	-	-		
80	OHX	sR	1941	-	0,6,6	-	-	-		
80	OHX	sR	1996	-	0,6,6	-	-	-		
80	OHX	AR	3688	-	0,6,6	-	-	-		
80	OHX	1	3471	-	0,6,6	-	-	-		
80	OHX	AR	3411	-	0,6,6	-	-	-		
80	OHX	1	3436	81	0,6,6	-	-	-		
80	OHX	1	3403	-	0,6,6	-	-	-		
80	OHX	AR	3687	-	0,6,6	-	-	-		
80	OHX	sR	2184	-	0,6,6	-	-	-		
80	OHX	sR	1960	-	0,6,6	-	-	-		
80	OHX	AR	3694	-	0,6,6	-	-	-		
80	OHX	4	208	81	0,6,6	-	-	-		
80	OHX	sR	2031	-	0,6,6	-	-	-		
80	OHX	A	2138	-	0,6,6	-	-	-		
80	OHX	AR	3449	-	0,6,6	-	-	-		
80	OHX	AR	3458	-	0,6,6	-	-	-		
80	OHX	AR	3407	-	0,6,6	-	-	-		
80	OHX	1	3475	-	0,6,6	-	-	-		
80	OHX	1	3596	81	0,6,6	-	-	-		
80	OHX	A	1958	-	0,6,6	-	-	-		
80	OHX	AR	3451	-	0,6,6	-	-	-		
80	OHX	AR	3567	-	0,6,6	-	-	-		
80	OHX	AR	3641	-	0,6,6	-	-	-		
80	OHX	1	3474	-	0,6,6	-	-	-		
80	OHX	AS	202	-	0,6,6	-	-	-		
80	OHX	AR	3615	-	0,6,6	-	-	-		
80	OHX	sR	1932	-	0,6,6	-	-	-		
80	OHX	1	3424	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	OHX	1	3571	-	0,6,6	-	-	-		
80	OHX	1	3511	-	0,6,6	-	-	-		
80	OHX	AS	207	-	0,6,6	-	-	-		
80	OHX	1	3438	81	0,6,6	-	-	-		
80	OHX	4	211	-	0,6,6	-	-	-		
80	OHX	AR	3580	-	0,6,6	-	-	-		
80	OHX	AR	3405	-	0,6,6	-	-	-		
80	OHX	AR	3634	-	0,6,6	-	-	-		
80	OHX	AR	3700[A]	-	0,6,6	-	-	-		
80	OHX	sR	2177	-	0,6,6	-	-	-		
80	OHX	AR	3592	81	0,6,6	-	-	-		
80	OHX	AR	3442	-	0,6,6	-	-	-		
80	OHX	AR	3573	-	0,6,6	-	-	-		
80	OHX	AR	3488	-	0,6,6	-	-	-		
80	OHX	A	2155	-	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
86	5XU	s3	302	86	-	0/0/1/2	-
86	5XU	c0	202	86	-	0/0/2/2	-
86	5XU	c0	203	86	-	0/0/2/2	-
84	VDU	AR	4255	-	-	0/8/60/60	0/3/3/3
83	SPD	AR	4200	-	-	4/7/7/7	-
83	SPD	1	4106	-	-	3/7/7/7	-
84	VDU	1	4195	-	-	0/8/60/60	0/3/3/3
86	5XU	c0	201	86	-	0/0/2/2	-
86	5XU	s3	301	86	-	0/0/2/2	-

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	1	4195	VDU	C1-C10-C5	-4.36	111.80	116.78
84	AR	4255	VDU	C1-C10-C5	-4.36	111.81	116.78
86	s3	301	5XU	CB-CA-N	-2.33	102.48	109.85
83	AR	4200	SPD	C8-C7-N6	-2.15	106.33	112.14
84	AR	4255	VDU	C9-C8-C7	2.08	113.69	110.84

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	AR	4200	SPD	N6-C7-C8-C9
83	1	4106	SPD	N6-C7-C8-C9
83	AR	4200	SPD	C8-C7-N6-C5
83	1	4106	SPD	C3-C4-C5-N6
83	1	4106	SPD	C8-C7-N6-C5

There are no ring outliers.

563 monomers are involved in 814 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	AR	3434	OHX	1	0
80	1	3426	OHX	1	0
80	AR	3510	OHX	1	0
80	sR	2011	OHX	1	0
80	sR	2001	OHX	1	0
80	sR	1905	OHX	1	0
80	sR	1989	OHX	1	0
80	sR	2028	OHX	2	0
80	sR	1902	OHX	1	0
80	1	3485	OHX	1	0
80	1	4171	OHX	1	0
80	1	3407	OHX	1	0
80	1	4149	OHX	1	0
80	AR	3550	OHX	1	0
80	sR	2015	OHX	1	0
80	1	4128	OHX	1	0
80	l	403	OHX	2	0
80	AR	3614	OHX	1	0
80	AR	3544	OHX	1	0
80	1	3487	OHX	1	0
80	1	3520[A]	OHX	1	0
80	AR	3421	OHX	1	0
80	AR	3517	OHX	1	0
80	sR	1926	OHX	1	0
80	1	3402	OHX	1	0
80	1	3602	OHX	1	0
80	AR	3556	OHX	1	0
80	A	1959	OHX	1	0
80	AR	3591	OHX	1	0
80	sR	1978	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	sR	1906	OHX	1	0
80	1	3504	OHX	1	0
80	AR	3435	OHX	1	0
80	sR	1908	OHX	1	0
80	1	4139	OHX	1	0
80	sR	1954	OHX	3	0
80	1	3565	OHX	1	0
80	AR	3450	OHX	1	0
80	AR	3699	OHX	1	0
80	4	201	OHX	2	0
80	sR	1990	OHX	2	0
80	sR	1903	OHX	3	0
80	1	3422	OHX	1	0
80	AR	3518	OHX	1	0
80	1	3506	OHX	1	0
80	A	1946	OHX	2	0
80	1	4146	OHX	3	0
80	3	223	OHX	1	0
80	A	1933	OHX	1	0
80	sR	1910	OHX	2	0
80	sR	2023	OHX	3	0
80	c5	201	OHX	2	0
80	AR	3613	OHX	1	0
80	1	4156	OHX	5	0
80	AR	3668	OHX	2	0
80	A	1967	OHX	2	0
80	A	2123	OHX	2	0
80	sR	1964	OHX	3	0
80	AR	3593	OHX	2	0
80	AR	3690	OHX	1	0
80	1	4166	OHX	3	0
80	A	1937	OHX	1	0
80	A	2146	OHX	1	0
80	AR	3650	OHX	1	0
80	AR	3404	OHX	1	0
80	A	2124	OHX	1	0
80	AR	3540	OHX	1	0
80	AR	3470	OHX	2	0
80	1	4132	OHX	4	0
80	1	4151	OHX	1	0
80	AR	3669	OHX	1	0
80	sR	1922	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	1	4159	OHX	2	0
80	AR	3439	OHX	1	0
80	CG	303	OHX	2	0
80	1	3508	OHX	1	0
80	AR	3463	OHX	3	0
80	1	4138	OHX	1	0
80	A	1922	OHX	2	0
80	sR	1923	OHX	1	0
80	1	3440	OHX	2	0
80	1	3622	OHX	1	0
80	h	401	OHX	2	0
80	sR	1976	OHX	1	0
80	AR	3623	OHX	1	0
80	1	3640	OHX	2	0
80	sR	1994	OHX	1	0
80	AR	3417	OHX	1	0
80	AR	3527	OHX	1	0
80	A	1975	OHX	1	0
80	A	2130	OHX	1	0
80	1	4163	OHX	2	0
80	1	3451	OHX	1	0
80	4	215	OHX	1	0
80	4	236	OHX	1	0
80	sR	1936	OHX	1	0
80	1	4147	OHX	2	0
80	CE	401	OHX	2	0
80	AR	3570	OHX	1	0
80	AR	3457	OHX	1	0
80	sR	1975	OHX	4	0
80	AR	3427	OHX	2	0
80	AR	3602	OHX	1	0
80	sR	1929	OHX	1	0
80	1	3499	OHX	2	0
80	1	3625	OHX	1	0
80	AR	3579	OHX	2	0
80	AR	3509	OHX	1	0
80	sR	1935	OHX	1	0
80	AR	3426	OHX	3	0
80	AR	3584	OHX	2	0
80	AR	3600	OHX	1	0
80	1	3411	OHX	1	0
80	A	1906	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	1	4148	OHX	1	0
80	AR	3549	OHX	1	0
80	AR	3438	OHX	2	0
83	AR	4200	SPD	3	0
80	sR	2185	OHX	3	0
80	1	3447	OHX	1	0
80	A	2118	OHX	1	0
80	1	4155	OHX	1	0
80	1	3631	OHX	3	0
80	A	1907	OHX	2	0
80	AR	3531	OHX	1	0
80	A	2143	OHX	1	0
80	k	403	OHX	4	0
80	1	4125	OHX	3	0
80	sR	1997	OHX	3	0
80	AR	3590	OHX	1	0
80	1	3476	OHX	1	0
80	AR	4232	OHX	1	0
80	1	3630	OHX	1	0
80	s8	302	OHX	1	0
80	sR	1927	OHX	1	0
80	1	4150	OHX	2	0
80	A	2151	OHX	3	0
80	AR	4231	OHX	1	0
80	sR	1988	OHX	2	0
80	sR	1950	OHX	1	0
80	A	2145	OHX	1	0
80	AR	3660	OHX	2	0
80	AR	3682	OHX	1	0
80	AR	3537	OHX	1	0
80	AR	4225	OHX	1	0
80	AR	3643	OHX	1	0
80	AR	3473	OHX	2	0
80	1	4127	OHX	2	0
80	AR	3441	OHX	1	0
80	sR	1959	OHX	2	0
80	AR	3640	OHX	2	0
80	1	4109	OHX	1	0
80	A	1961	OHX	2	0
80	A	1971	OHX	1	0
80	1	3490	OHX	1	0
80	sR	2006	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	1	4122	OHX	1	0
80	1	3431	OHX	1	0
80	1	3542	OHX	1	0
80	1	3619	OHX	1	0
80	1	4141	OHX	3	0
80	1	4123	OHX	1	0
80	1	4182	OHX	1	0
80	AR	3437	OHX	1	0
80	CK	202	OHX	1	0
80	A	2141	OHX	1	0
80	AR	3505	OHX	1	0
80	sR	2178	OHX	1	0
80	A	2147	OHX	1	0
80	1	3502	OHX	2	0
80	1	3501	OHX	1	0
80	1	3617	OHX	1	0
80	sR	1979	OHX	1	0
80	s1	301	OHX	1	0
80	AS	204	OHX	2	0
80	A	2119	OHX	1	0
80	AR	3562	OHX	2	0
80	A	1978	OHX	1	0
80	1	3580	OHX	1	0
80	A	1976	OHX	1	0
80	1	4167	OHX	1	0
80	sR	1931	OHX	2	0
80	sR	1918	OHX	2	0
80	AR	3692	OHX	2	0
80	CL	301	OHX	2	0
80	AR	3606	OHX	1	0
80	1	3454	OHX	3	0
80	1	4161	OHX	1	0
80	A	1973	OHX	2	0
80	DL	102	OHX	1	0
80	AR	3532	OHX	1	0
80	1	3404	OHX	5	0
80	AR	4224	OHX	2	0
80	e	102	OHX	1	0
80	1	3418	OHX	1	0
80	sR	1912	OHX	1	0
80	AR	3533	OHX	1	0
80	AR	3597	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	1	3494	OHX	1	0
80	AR	3507	OHX	1	0
80	A	2136	OHX	2	0
80	AR	3666	OHX	1	0
80	A	1927	OHX	1	0
80	1	4158	OHX	4	0
80	AR	3676	OHX	2	0
80	A	2133	OHX	2	0
80	AR	3443	OHX	1	0
80	1	3541	OHX	2	0
80	AR	3637	OHX	1	0
80	sR	1998	OHX	1	0
80	1	3612	OHX	1	0
80	1	3488	OHX	1	0
80	A	1956	OHX	1	0
80	AR	3408	OHX	5	0
80	AR	3678	OHX	1	0
80	AT	209	OHX	2	0
80	AR	3552	OHX	1	0
80	AR	3696	OHX	1	0
80	AR	4227	OHX	2	0
80	AR	3700[B]	OHX	1	0
80	AR	3583	OHX	3	0
80	AR	4237	OHX	1	0
80	DQ	203	OHX	3	0
80	1	3444	OHX	1	0
80	AR	3418	OHX	2	0
80	sR	2016	OHX	1	0
80	AR	3608	OHX	1	0
80	AR	3477	OHX	1	0
80	1	4177	OHX	2	0
80	sR	1980	OHX	2	0
80	1	4169	OHX	1	0
80	AR	3415	OHX	1	0
80	AR	4235	OHX	1	0
80	1	3604	OHX	1	0
80	1	3467	OHX	1	0
80	A	1939	OHX	1	0
80	AR	3559	OHX	1	0
80	AR	3628	OHX	1	0
80	AR	3652	OHX	4	0
80	1	3616	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	AR	3520	OHX	2	0
80	A	2144	OHX	2	0
80	AR	3528	OHX	1	0
80	J	301	OHX	2	0
80	AT	203	OHX	1	0
80	1	3429	OHX	2	0
80	A	1972	OHX	1	0
80	AR	3432	OHX	1	0
80	AR	3475	OHX	1	0
80	AT	208	OHX	1	0
80	AR	3695	OHX	1	0
80	AR	3513[B]	OHX	1	0
80	1	3513	OHX	1	0
80	1	3473	OHX	1	0
80	AR	3541	OHX	1	0
80	sR	2004	OHX	1	0
80	1	4180	OHX	3	0
80	CP	302	OHX	1	0
80	1	3605	OHX	1	0
80	1	4174	OHX	1	0
80	1	3629	OHX	1	0
80	1	3437	OHX	1	0
80	AR	3651	OHX	1	0
80	4	213	OHX	1	0
80	AR	3474	OHX	1	0
80	AR	3673	OHX	2	0
80	AR	3487	OHX	1	0
80	AR	3424	OHX	1	0
80	A	1910	OHX	2	0
80	sR	1924	OHX	1	0
80	1	3537	OHX	1	0
80	sR	1991	OHX	2	0
80	1	4130	OHX	3	0
80	AR	3538	OHX	1	0
80	AR	3476	OHX	1	0
80	AR	3607	OHX	3	0
80	1	3408	OHX	2	0
80	AR	3568	OHX	1	0
80	A	2149	OHX	3	0
80	AR	3555	OHX	1	0
80	1	3419	OHX	1	0
80	A	2152	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	1	3510	OHX	1	0
80	AR	3571	OHX	1	0
80	AR	3620	OHX	1	0
80	A	2131	OHX	1	0
80	sR	1917	OHX	1	0
80	AR	3508	OHX	1	0
80	1	3533	OHX	1	0
80	AR	3664	OHX	1	0
80	AT	211	OHX	2	0
80	A	1942	OHX	1	0
80	1	3633	OHX	1	0
80	1	3576	OHX	1	0
80	1	3563	OHX	2	0
80	1	4154	OHX	1	0
86	c0	201	5XU	1	0
80	AR	4234	OHX	3	0
80	1	3538	OHX	1	0
80	1	3434	OHX	1	0
80	sR	1938	OHX	1	0
80	1	3553	OHX	1	0
80	1	3615	OHX	1	0
80	A	2153	OHX	1	0
80	4	210	OHX	2	0
80	AR	3468	OHX	1	0
80	AR	3536	OHX	1	0
80	sR	2024	OHX	2	0
80	AR	3522	OHX	1	0
80	1	3458	OHX	1	0
80	AP	502	OHX	3	0
80	AR	3672	OHX	2	0
80	AR	3402	OHX	1	0
80	A	2117	OHX	2	0
80	1	3492	OHX	1	0
80	3	204	OHX	1	0
80	sR	2032	OHX	2	0
80	1	3486	OHX	1	0
80	AR	3420	OHX	2	0
80	1	3425	OHX	1	0
80	1	3524	OHX	1	0
80	1	4129	OHX	3	0
80	sR	1933	OHX	1	0
80	1	3446	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	AR	3410	OHX	2	0
80	A	2129	OHX	1	0
80	AR	3616	OHX	1	0
80	1	3477	OHX	4	0
80	1	3414	OHX	1	0
80	1	3530	OHX	1	0
80	AR	3521	OHX	1	0
80	sR	1920	OHX	1	0
80	AR	3454	OHX	1	0
80	1	3433	OHX	2	0
80	1	3572	OHX	1	0
80	1	4152	OHX	1	0
80	AR	3406	OHX	3	0
80	sR	1916[B]	OHX	1	0
80	AR	3433	OHX	1	0
80	1	3412	OHX	1	0
80	AG	201	OHX	1	0
80	sR	1957	OHX	4	0
80	sR	1930	OHX	3	0
80	AR	3466	OHX	2	0
80	1	4134	OHX	2	0
80	AR	3446	OHX	1	0
80	A	1980	OHX	1	0
80	1	4153	OHX	1	0
80	AR	3542	OHX	3	0
80	Q	201	OHX	1	0
80	AR	3553	OHX	2	0
80	1	4165	OHX	2	0
80	A	2115	OHX	1	0
80	sR	1951	OHX	1	0
80	sR	1907	OHX	1	0
80	1	3500	OHX	1	0
80	1	3593	OHX	1	0
80	3	221	OHX	1	0
80	AR	3403	OHX	2	0
80	A	1908	OHX	2	0
80	AR	3534	OHX	1	0
80	1	4126	OHX	1	0
80	AR	3419	OHX	1	0
80	1	4135	OHX	1	0
80	AR	3501	OHX	3	0
80	k	402	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	1	3556	OHX	1	0
80	1	3582	OHX	1	0
80	sR	1992	OHX	1	0
80	sR	1909	OHX	1	0
83	1	4106	SPD	3	0
80	AR	3452	OHX	1	0
80	1	4144	OHX	2	0
80	1	3600	OHX	2	0
80	A	2125	OHX	1	0
80	n	201	OHX	1	0
80	AR	3447	OHX	3	0
80	1	3450	OHX	1	0
80	AR	3414	OHX	2	0
80	AR	3525	OHX	1	0
80	A	2128	OHX	1	0
80	1	4164	OHX	2	0
80	A	2121	OHX	2	0
80	A	2134	OHX	4	0
80	AR	3401	OHX	4	0
80	sR	2012	OHX	1	0
80	sR	1969	OHX	2	0
80	AR	3548	OHX	1	0
80	CS	202	OHX	2	0
80	sR	1915	OHX	1	0
80	A	1970	OHX	1	0
80	AR	3551	OHX	1	0
80	AC	102	OHX	2	0
80	AR	3587	OHX	1	0
80	1	4172	OHX	1	0
80	AR	3701	OHX	1	0
80	sR	1967	OHX	1	0
80	A	2127	OHX	2	0
80	1	3512	OHX	1	0
80	1	3562	OHX	2	0
80	AR	3455	OHX	3	0
80	1	3445	OHX	1	0
80	A	1901	OHX	1	0
80	AR	4229	OHX	2	0
80	sR	1958	OHX	3	0
80	AR	3445	OHX	1	0
80	sR	1955	OHX	1	0
80	AR	3409	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	AR	3489	OHX	2	0
80	1	3420	OHX	2	0
80	A	1979	OHX	2	0
80	1	3410	OHX	2	0
80	AT	215	OHX	1	0
80	AR	3465	OHX	1	0
80	1	4108	OHX	1	0
80	AR	4213	OHX	1	0
80	sR	1984	OHX	2	0
80	1	4143	OHX	2	0
80	DK	201	OHX	1	0
80	4	203	OHX	2	0
80	AR	3412	OHX	1	0
80	AR	3645	OHX	1	0
80	A	1923	OHX	1	0
80	1	3539	OHX	1	0
80	Rb	401	OHX	2	0
80	sR	2034	OHX	1	0
80	1	3456	OHX	1	0
80	sR	1965	OHX	2	0
80	AR	3456	OHX	1	0
80	AR	3691	OHX	1	0
80	1	4170	OHX	3	0
80	DD	101	OHX	2	0
80	1	3498	OHX	1	0
80	AR	3436	OHX	1	0
80	1	4124	OHX	1	0
80	A	2137	OHX	1	0
80	A	2159[A]	OHX	2	0
80	3	222	OHX	2	0
80	A	1950	OHX	1	0
80	A	1974	OHX	2	0
80	1	3469	OHX	1	0
80	AR	3499	OHX	1	0
80	A	2114	OHX	3	0
80	O	201	OHX	2	0
80	1	3624	OHX	2	0
80	A	2116	OHX	2	0
80	AR	3453	OHX	2	0
80	AR	3658	OHX	1	0
80	1	3550	OHX	1	0
80	1	3627	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	AR	4233	OHX	3	0
80	sR	2002	OHX	1	0
80	AR	3464	OHX	1	0
80	AR	3504	OHX	4	0
80	CL	302	OHX	1	0
80	sR	2010	OHX	2	0
80	sR	1949	OHX	2	0
80	3	201	OHX	1	0
80	A	1916	OHX	1	0
80	1	3519	OHX	1	0
80	1	3505	OHX	1	0
80	1	4181	OHX	2	0
80	sR	2017	OHX	1	0
80	4	207	OHX	1	0
80	1	3503	OHX	1	0
80	1	3479	OHX	1	0
80	A	2156	OHX	1	0
80	AR	3684	OHX	1	0
80	1	4142	OHX	2	0
80	A	2135	OHX	2	0
80	1	3621	OHX	1	0
80	AR	3526	OHX	1	0
80	sR	1937	OHX	1	0
80	1	3566	OHX	1	0
80	A	2122	OHX	2	0
80	AT	207	OHX	1	0
80	sR	2176	OHX	1	0
80	1	3466	OHX	1	0
80	AR	3496	OHX	2	0
80	sR	2188	OHX	3	0
80	DH	202	OHX	1	0
80	1	3509	OHX	1	0
80	sR	1913	OHX	3	0
80	1	3555	OHX	1	0
80	AR	4226	OHX	1	0
80	1	4160	OHX	1	0
80	4	206	OHX	1	0
80	AR	3565	OHX	1	0
80	sR	1977	OHX	1	0
80	1	3493	OHX	2	0
80	A	1918	OHX	1	0
80	AR	3484	OHX	1	0

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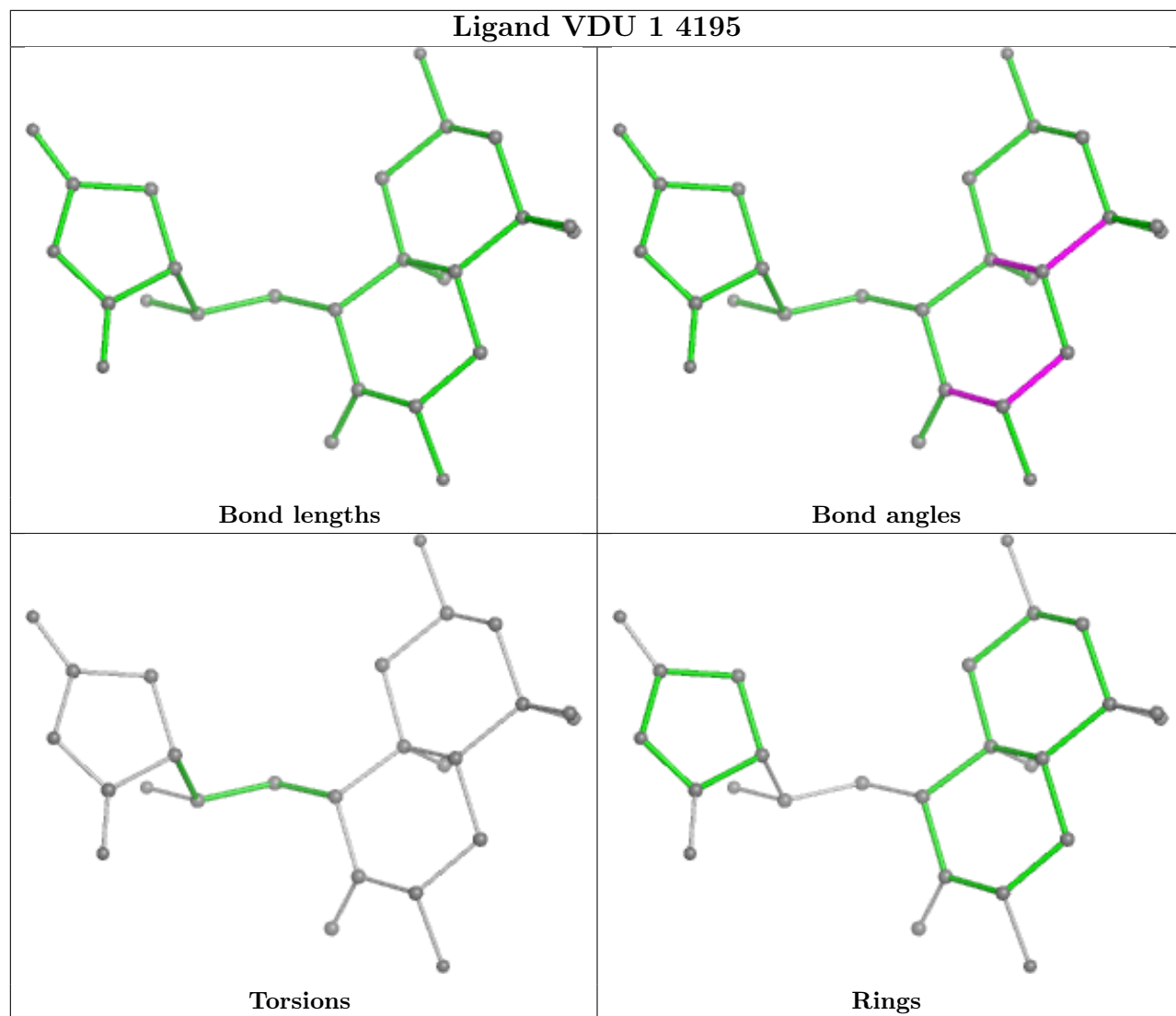
Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	z	204	OHX	1	0
80	AR	3516	OHX	2	0
80	A	1969	OHX	1	0
80	AR	3486	OHX	1	0
80	1	3401	OHX	1	0
80	1	3415	OHX	1	0
80	x	209	OHX	2	0
80	AR	3416	OHX	1	0
80	T	201	OHX	1	0
80	1	3637	OHX	1	0
80	AR	3428	OHX	2	0
80	AR	3490	OHX	2	0
80	sR	1940	OHX	2	0
80	A	1912	OHX	1	0
80	AR	3598	OHX	1	0
84	1	4195	VDU	1	0
80	4	238	OHX	1	0
80	1	3614	OHX	1	0
80	sR	1972	OHX	1	0
80	1	4131	OHX	2	0
80	1	4137	OHX	2	0
80	A	2142	OHX	3	0
80	v	301	OHX	1	0
80	AR	3479	OHX	2	0
80	AR	3429	OHX	1	0
80	1	3560	OHX	1	0
80	A	1951	OHX	1	0
80	A	1947	OHX	1	0
80	1	3517	OHX	1	0
80	1	3564	OHX	1	0
80	AR	3577	OHX	2	0
80	sR	2020	OHX	1	0
80	AR	3557	OHX	1	0
80	AR	3605	OHX	3	0
80	4	237	OHX	2	0
80	AR	3523	OHX	1	0
80	AR	3554	OHX	1	0
80	S	201	OHX	1	0
80	sR	1928	OHX	1	0
80	AR	3627	OHX	3	0
80	sR	1946	OHX	2	0
80	3	220	OHX	1	0

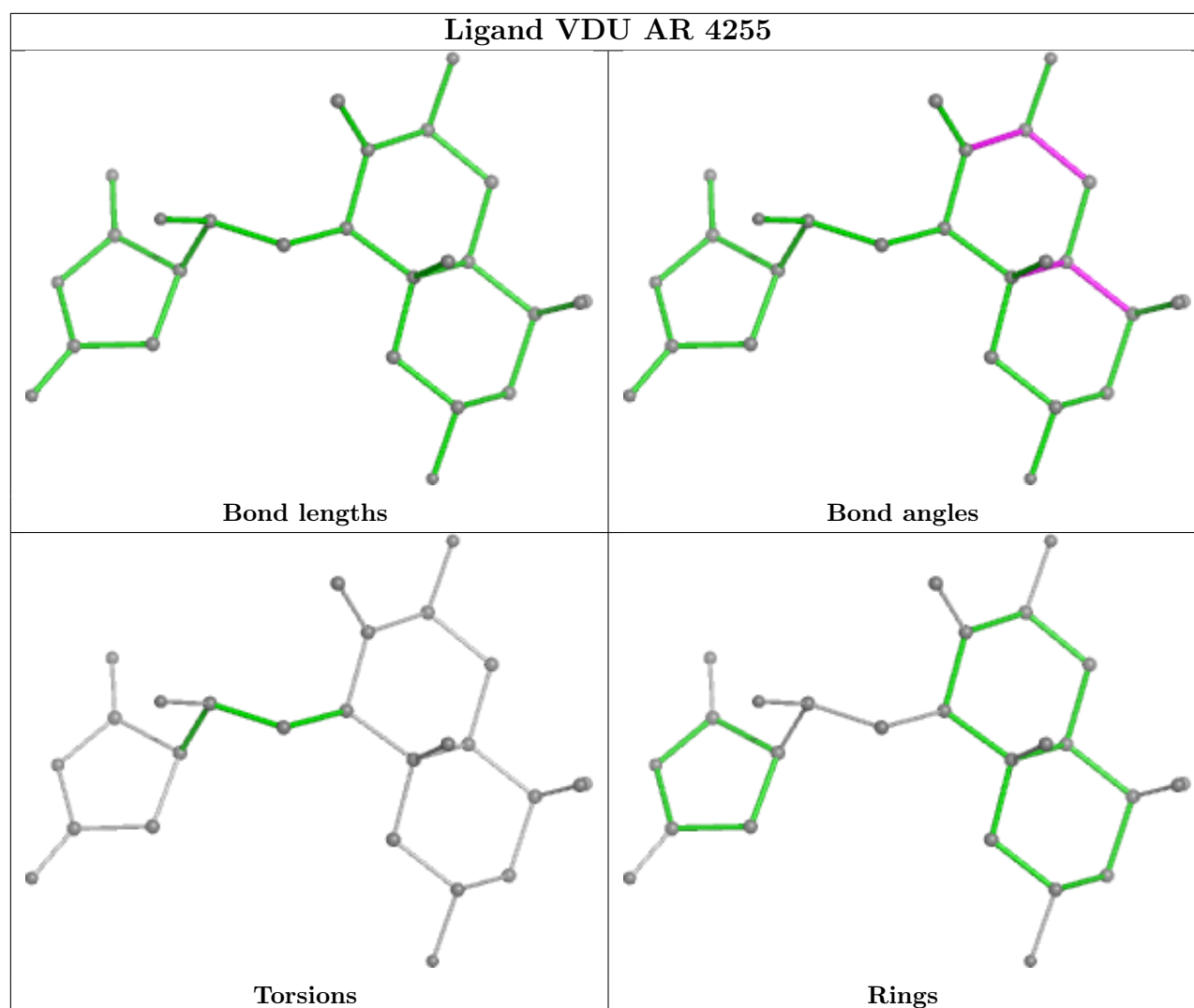
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	sR	2007	OHX	1	0
84	AR	4255	VDU	2	0
80	1	4179	OHX	1	0
80	1	4178	OHX	1	0
80	A	2132	OHX	1	0
80	AR	3622	OHX	1	0
80	AR	3497	OHX	1	0
80	A	1944	OHX	1	0
80	AR	3649	OHX	1	0
80	sR	1996	OHX	1	0
80	AR	3411	OHX	2	0
80	1	3436	OHX	1	0
80	1	3403	OHX	1	0
80	sR	2184	OHX	2	0
80	sR	1960	OHX	1	0
80	A	2138	OHX	1	0
80	AR	3449	OHX	2	0
80	AR	3458	OHX	2	0
80	AR	3407	OHX	2	0
80	1	3596	OHX	1	0
80	AR	3641	OHX	1	0
80	AS	202	OHX	1	0
80	sR	1932	OHX	1	0
80	1	3438	OHX	1	0
80	AR	3580	OHX	1	0
80	AR	3405	OHX	1	0
80	AR	3634	OHX	1	0
80	AR	3700[A]	OHX	1	0
80	AR	3442	OHX	1	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	A	1735/1800 (96%)	0.55	49 (2%)	55	49	61, 98, 201, 267	0
1	sR	1783/1800 (99%)	0.36	30 (1%)	69	63	52, 88, 204, 270	0
2	B	206/252 (81%)	1.42	50 (24%)	2	2	87, 122, 161, 176	0
2	s0	206/252 (81%)	1.16	35 (16%)	5	4	74, 108, 141, 180	0
3	C	214/255 (83%)	1.58	64 (29%)	1	1	84, 141, 177, 209	0
3	s1	216/255 (84%)	0.80	14 (6%)	26	22	63, 99, 132, 179	0
4	D	217/254 (85%)	1.28	46 (21%)	3	3	69, 103, 138, 180	0
4	s2	217/254 (85%)	0.76	20 (9%)	16	14	60, 88, 130, 162	0
5	E	223/240 (92%)	1.53	67 (30%)	1	1	74, 108, 146, 186	0
5	s3	223/240 (92%)	1.14	33 (14%)	7	6	80, 122, 161, 195	0
6	F	260/261 (99%)	1.54	76 (29%)	1	2	73, 104, 139, 161	0
6	s4	260/261 (99%)	0.69	19 (7%)	22	19	57, 85, 120, 175	0
7	G	200/225 (88%)	1.10	29 (14%)	7	6	79, 132, 166, 189	0
7	s5	199/225 (88%)	1.70	62 (31%)	1	1	83, 124, 161, 178	0
8	H	226/236 (95%)	1.39	59 (26%)	2	2	73, 112, 153, 172	0
8	s6	218/236 (92%)	1.02	29 (13%)	8	7	56, 92, 139, 168	0
9	I	184/190 (96%)	1.09	27 (14%)	7	6	80, 127, 170, 189	0
9	s7	186/190 (97%)	1.22	36 (19%)	4	3	72, 120, 170, 187	0
10	J	188/200 (94%)	0.98	25 (13%)	8	7	61, 90, 134, 163	0
10	s8	188/200 (94%)	1.36	40 (21%)	3	3	58, 86, 136, 184	0
11	K	179/197 (90%)	1.57	51 (28%)	1	2	82, 112, 149, 164	0
11	s9	185/197 (93%)	1.20	35 (18%)	4	3	59, 90, 140, 176	0
12	L	96/105 (91%)	1.66	30 (31%)	1	1	78, 119, 163, 179	0
12	c0	84/105 (80%)	1.17	18 (21%)	3	3	99, 137, 166, 179	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
13	M	143/156 (91%)	1.09	26 (18%)	4	4	60, 85, 133, 176	0
13	c1	146/156 (93%)	1.74	47 (32%)	1	1	56, 79, 151, 172	0
14	O	150/151 (99%)	1.10	24 (16%)	6	5	66, 103, 138, 151	0
14	c3	150/151 (99%)	1.03	16 (10%)	12	11	60, 91, 125, 165	0
15	P	127/138 (92%)	1.90	45 (35%)	1	1	78, 136, 171, 194	0
15	c4	128/138 (92%)	1.15	22 (17%)	5	4	61, 101, 137, 172	0
16	Q	117/142 (82%)	1.43	25 (21%)	3	3	77, 102, 159, 192	0
16	c5	127/142 (89%)	1.74	50 (39%)	1	1	83, 120, 168, 182	0
17	R	141/143 (98%)	1.50	38 (26%)	2	2	81, 119, 145, 177	0
17	c6	142/143 (99%)	1.86	58 (40%)	1	1	77, 111, 155, 176	0
18	S	115/136 (84%)	1.36	27 (23%)	2	2	78, 124, 179, 194	0
18	c7	117/136 (86%)	1.15	14 (11%)	10	9	82, 112, 160, 193	0
19	T	145/146 (99%)	0.71	13 (8%)	17	14	66, 117, 162, 200	0
19	c8	145/146 (99%)	1.15	27 (18%)	4	3	77, 110, 157, 178	0
20	U	143/144 (99%)	1.03	23 (16%)	5	5	90, 116, 153, 165	0
20	c9	143/144 (99%)	1.02	17 (11%)	10	9	69, 105, 133, 171	0
21	V	107/121 (88%)	2.12	51 (47%)	0	0	78, 121, 170, 192	0
21	d0	100/121 (82%)	1.80	38 (38%)	1	1	75, 125, 173, 186	0
22	W	87/87 (100%)	1.21	16 (18%)	4	4	83, 115, 147, 171	0
22	d1	87/87 (100%)	0.77	10 (11%)	11	9	68, 96, 127, 159	0
23	X	129/130 (99%)	1.61	42 (32%)	1	1	73, 98, 122, 141	0
23	d2	129/130 (99%)	0.83	9 (6%)	24	20	57, 78, 100, 119	0
24	Y	144/145 (99%)	1.43	40 (27%)	2	2	64, 87, 111, 144	0
24	d3	144/145 (99%)	0.86	13 (9%)	17	14	52, 71, 97, 142	0
25	Z	134/135 (99%)	1.20	25 (18%)	4	3	76, 116, 160, 192	0
25	d4	134/135 (99%)	0.80	13 (9%)	15	12	64, 94, 135, 165	0
26	AA	135/136 (99%)	0.98	13 (9%)	15	13	76, 105, 140, 170	0
26	DB	135/136 (99%)	0.98	20 (14%)	7	6	85, 111, 147, 171	0
27	9	126/127 (99%)	0.23	3 (2%)	59	53	49, 72, 103, 146	0
27	DA	124/127 (97%)	1.09	21 (16%)	5	4	53, 77, 103, 148	0
28	AB	148/149 (99%)	0.91	19 (12%)	9	7	44, 64, 94, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9
28	DC	148/149 (99%)	0.97	18 (12%)	10 8	43, 67, 100, 142	0
29	AC	58/59 (98%)	1.74	22 (37%)	1 1	48, 77, 142, 150	0
29	DD	58/59 (98%)	1.61	17 (29%)	1 1	49, 71, 107, 141	0
30	AD	97/105 (92%)	0.85	11 (11%)	11 10	73, 100, 131, 154	0
30	DE	97/105 (92%)	0.98	15 (15%)	6 5	64, 101, 141, 181	0
31	CD	252/254 (99%)	1.16	35 (13%)	7 6	45, 72, 101, 168	0
31	j	252/254 (99%)	1.02	30 (11%)	10 9	46, 68, 95, 141	0
32	AE	109/113 (96%)	1.27	18 (16%)	5 5	58, 83, 144, 178	0
32	DF	109/113 (96%)	1.05	17 (15%)	6 5	49, 70, 135, 167	0
33	CE	386/387 (99%)	0.62	28 (7%)	22 19	43, 59, 86, 127	0
33	k	386/387 (99%)	0.80	33 (8%)	18 15	47, 73, 105, 168	0
34	AF	127/130 (97%)	0.66	10 (7%)	20 17	46, 58, 82, 146	0
34	DG	127/130 (97%)	0.74	10 (7%)	20 17	44, 62, 89, 134	0
35	1	3134/3396 (92%)	0.25	37 (1%)	76 71	45, 68, 174, 261	0
35	AR	3147/3396 (92%)	0.19	45 (1%)	73 68	43, 66, 161, 267	0
36	3	121/121 (100%)	0.17	1 (0%)	82 78	51, 82, 105, 144	0
36	AS	121/121 (100%)	0.05	0	100 100	48, 69, 83, 133	0
37	4	158/158 (100%)	0.02	1 (0%)	85 82	52, 69, 130, 210	0
37	AT	158/158 (100%)	0.25	3 (1%)	66 60	54, 76, 151, 210	0
38	CF	361/362 (99%)	0.62	24 (6%)	26 22	43, 69, 99, 136	0
38	l	361/362 (99%)	0.53	25 (6%)	24 20	44, 64, 99, 123	0
39	CG	296/297 (99%)	0.78	32 (10%)	12 11	52, 74, 124, 185	0
39	m	296/297 (99%)	0.81	28 (9%)	15 13	59, 91, 140, 180	0
40	CH	156/176 (88%)	0.40	8 (5%)	34 29	48, 70, 111, 143	0
40	n	156/176 (88%)	0.41	5 (3%)	50 44	52, 67, 106, 146	0
41	CI	222/244 (90%)	0.66	10 (4%)	39 32	46, 59, 101, 180	0
41	o	222/244 (90%)	0.59	11 (4%)	35 30	49, 63, 102, 172	0
42	CJ	233/256 (91%)	1.01	34 (14%)	7 6	76, 106, 151, 173	0
42	p	233/256 (91%)	1.11	34 (14%)	7 6	59, 92, 142, 186	0
43	CK	191/191 (100%)	0.43	11 (5%)	30 26	49, 67, 100, 180	0
43	q	191/191 (100%)	1.06	25 (13%)	8 7	57, 83, 120, 184	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	CL	211/221 (95%)	0.49	14 (6%)	26	22	46, 69, 115, 159	0
44	r	211/221 (95%)	0.80	24 (11%)	11	10	49, 74, 124, 162	0
45	CM	169/174 (97%)	0.78	13 (7%)	21	18	54, 78, 112, 135	0
45	s	169/174 (97%)	1.04	22 (13%)	9	7	66, 95, 128, 182	0
46	CN	193/199 (96%)	1.04	28 (14%)	7	6	45, 81, 138, 163	0
46	t	193/199 (96%)	0.76	17 (8%)	17	15	47, 74, 123, 166	0
47	CO	136/138 (98%)	0.70	16 (11%)	10	9	50, 64, 99, 141	0
47	u	136/138 (98%)	0.82	13 (9%)	15	13	54, 73, 103, 176	0
48	CP	203/204 (99%)	0.91	15 (7%)	22	19	48, 75, 95, 117	0
48	v	203/204 (99%)	1.02	19 (9%)	15	13	44, 66, 85, 102	0
49	CQ	197/199 (98%)	0.77	21 (10%)	12	11	44, 54, 97, 156	0
49	w	197/199 (98%)	0.82	19 (9%)	15	13	48, 62, 90, 145	0
50	CR	155/184 (84%)	0.48	5 (3%)	50	44	44, 60, 80, 147	0
50	x	176/184 (95%)	0.61	9 (5%)	34	29	46, 65, 110, 170	0
51	CS	185/186 (99%)	0.98	26 (14%)	7	6	46, 67, 93, 107	0
51	y	185/186 (99%)	0.68	14 (7%)	21	18	48, 63, 84, 97	0
52	CT	184/189 (97%)	0.97	25 (13%)	8	7	53, 82, 142, 163	0
52	z	183/189 (96%)	0.83	16 (8%)	17	15	61, 85, 144, 167	0
53	0	172/172 (100%)	0.93	23 (13%)	8	7	52, 69, 101, 165	0
53	CU	172/172 (100%)	0.61	6 (3%)	47	41	47, 60, 91, 133	0
54	2	159/160 (99%)	1.05	25 (15%)	6	5	49, 72, 117, 164	0
54	CV	159/160 (99%)	0.88	15 (9%)	15	13	47, 64, 120, 183	0
55	5	100/121 (82%)	0.78	6 (6%)	29	24	92, 119, 154, 171	0
55	CW	100/121 (82%)	1.11	15 (15%)	6	6	79, 109, 156, 167	0
56	6	136/137 (99%)	1.16	20 (14%)	7	6	51, 73, 107, 146	0
56	CX	136/137 (99%)	0.74	9 (6%)	26	22	45, 59, 89, 155	0
57	7	67/155 (43%)	1.24	14 (20%)	3	3	54, 76, 131, 166	0
57	CY	113/155 (72%)	1.28	28 (24%)	2	2	52, 82, 129, 151	0
58	8	121/142 (85%)	0.99	19 (15%)	6	5	53, 81, 120, 154	0
58	CZ	118/142 (83%)	1.47	33 (27%)	2	2	56, 86, 116, 137	0
59	AG	105/107 (98%)	0.64	9 (8%)	18	15	48, 60, 79, 105	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
59	DH	106/107 (99%)	0.64	5 (4%) 37 31	45, 57, 94, 132	0
60	AH	112/121 (92%)	1.34	23 (20%) 3 3	48, 85, 126, 164	0
60	DI	112/121 (92%)	1.22	22 (19%) 4 3	58, 87, 144, 170	0
61	AI	119/120 (99%)	0.68	7 (5%) 29 25	50, 80, 107, 126	0
61	DJ	119/120 (99%)	1.22	18 (15%) 6 5	68, 88, 117, 138	0
62	AJ	99/100 (99%)	0.90	13 (13%) 8 7	59, 83, 136, 166	0
62	DK	97/100 (97%)	0.96	13 (13%) 8 7	67, 95, 137, 152	0
63	AK	87/88 (98%)	0.87	11 (12%) 9 8	48, 62, 95, 147	0
63	DL	86/88 (97%)	0.97	11 (12%) 9 7	45, 67, 106, 144	0
64	AL	77/78 (98%)	1.05	10 (12%) 9 7	79, 108, 144, 160	0
64	DM	77/78 (98%)	1.02	12 (15%) 6 5	84, 107, 151, 177	0
65	AM	50/51 (98%)	1.23	9 (18%) 4 4	52, 70, 90, 109	0
65	DN	50/51 (98%)	1.51	13 (26%) 2 2	57, 72, 97, 115	0
66	AN	52/128 (40%)	0.70	6 (11%) 11 9	53, 75, 104, 138	0
66	DO	52/128 (40%)	0.49	3 (5%) 30 26	47, 58, 82, 132	0
67	AO	25/25 (100%)	1.77	12 (48%) 0 0	63, 78, 92, 102	0
67	DP	25/25 (100%)	1.73	9 (36%) 1 1	56, 68, 92, 113	0
68	AP	105/106 (99%)	0.74	12 (11%) 11 10	47, 71, 108, 157	0
68	DQ	105/106 (99%)	0.50	4 (3%) 44 38	46, 68, 111, 148	0
69	AQ	91/92 (98%)	0.99	10 (10%) 12 10	52, 76, 105, 140	0
69	DR	91/92 (98%)	1.05	12 (13%) 8 7	52, 75, 108, 129	0
70	i	126/273 (46%)	0.97	15 (11%) 10 9	67, 108, 154, 182	0
70	sM	63/273 (23%)	1.56	23 (36%) 1 1	56, 122, 164, 187	0
71	p0	123/312 (39%)	1.50	36 (29%) 1 1	86, 128, 156, 167	0
72	a	70/108 (64%)	0.78	8 (11%) 11 10	110, 148, 180, 193	0
72	d5	69/108 (63%)	1.54	18 (26%) 2 2	102, 137, 165, 189	0
73	b	93/119 (78%)	2.24	48 (51%) 0 0	81, 109, 168, 185	0
73	d6	97/119 (81%)	1.47	30 (30%) 1 1	57, 84, 134, 157	0
74	c	81/82 (98%)	0.81	10 (12%) 9 8	85, 117, 160, 184	0
74	d7	81/82 (98%)	0.71	6 (7%) 22 19	62, 102, 161, 203	0
75	d	63/67 (94%)	1.39	14 (22%) 3 2	101, 148, 173, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	d8	63/67 (94%)	2.27	37 (58%) 0 0	99, 140, 171, 191	0
76	d9	53/56 (94%)	1.88	21 (39%) 1 1	79, 100, 151, 185	0
76	e	53/56 (94%)	2.15	27 (50%) 0 0	72, 95, 132, 168	0
77	e0	62/63 (98%)	0.96	8 (12%) 9 7	61, 100, 154, 190	0
77	f	60/63 (95%)	1.13	13 (21%) 3 3	69, 115, 164, 187	0
78	e1	39/152 (25%)	1.36	6 (15%) 6 5	143, 172, 205, 217	0
78	g	71/152 (46%)	1.86	27 (38%) 1 1	94, 148, 182, 211	0
79	Rb	318/319 (99%)	1.18	61 (19%) 4 3	92, 136, 169, 197	0
79	h	312/319 (97%)	1.12	56 (17%) 4 4	90, 128, 169, 187	0
All	All	32476/35284 (92%)	0.80	3584 (11%) 12 10	43, 84, 156, 270	0

The worst 5 of 3584 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	CD	253	GLN	10.4
31	CD	246	LEU	9.3
54	CV	86	GLU	8.9
13	c1	4	GLU	8.6
49	CQ	182	ASN	8.3

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	2095	1/1	-0.16	0.35	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	5XU	c0	201	5/5	0.07	0.19	150,152,155,156	0
81	MG	A	2045	1/1	0.08	0.22	127,127,127,127	0
81	MG	A	2077	1/1	0.33	0.56	101,101,101,101	0
81	MG	1	3992	1/1	0.34	0.29	114,114,114,114	0
81	MG	d4	203	1/1	0.43	0.22	77,77,77,77	0
81	MG	A	2094	1/1	0.43	0.20	118,118,118,118	0
81	MG	A	2062	1/1	0.45	0.39	95,95,95,95	0
81	MG	A	2073	1/1	0.47	0.27	92,92,92,92	0
81	MG	1	4061	1/1	0.48	0.26	75,75,75,75	0
81	MG	A	2035	1/1	0.49	0.32	107,107,107,107	0
86	5XU	c0	202	5/5	0.50	0.15	140,141,142,144	0
81	MG	s	300	1/1	0.51	0.17	97,97,97,97	0
81	MG	1	3920	1/1	0.51	0.59	116,116,116,116	0
81	MG	A	2032	1/1	0.52	0.32	102,102,102,102	0
81	MG	6	202	1/1	0.53	0.31	113,113,113,113	0
81	MG	1	3966	1/1	0.53	0.32	83,83,83,83	0
81	MG	A	2096	1/1	0.54	0.32	91,91,91,91	0
86	5XU	s3	301	5/5	0.54	0.14	147,149,150,151	0
81	MG	AR	3781	1/1	0.56	0.44	108,108,108,108	0
81	MG	AS	223	1/1	0.56	0.40	93,93,93,93	0
81	MG	1	3728	1/1	0.56	0.26	94,94,94,94	0
81	MG	1	4096	1/1	0.58	0.31	86,86,86,86	0
81	MG	sR	2166	1/1	0.58	0.29	77,77,77,77	0
81	MG	AR	3979	1/1	0.58	0.39	86,86,86,86	0
81	MG	1	4025	1/1	0.59	0.25	109,109,109,109	0
81	MG	CS	201	1/1	0.59	0.50	119,119,119,119	0
82	K	CK	204	1/1	0.59	0.25	131,131,131,131	0
81	MG	AR	4145	1/1	0.60	0.35	101,101,101,101	0
81	MG	1	3981	1/1	0.60	0.33	88,88,88,88	0
81	MG	AR	4074	1/1	0.60	0.24	80,80,80,80	0
81	MG	1	4016	1/1	0.61	0.27	59,59,59,59	0
81	MG	3	215	1/1	0.61	0.26	83,83,83,83	0
81	MG	A	2015	1/1	0.61	0.37	91,91,91,91	0
81	MG	1	3852	1/1	0.61	0.18	98,98,98,98	0
81	MG	AR	3892	1/1	0.62	0.27	77,77,77,77	0
81	MG	AR	4014	1/1	0.62	0.20	81,81,81,81	0
81	MG	DC	202	1/1	0.63	0.25	78,78,78,78	0
80	OHX	4	238	7/7	0.63	0.16	180,196,203,286	0
80	OHX	A	2132	7/7	0.63	0.21	209,218,225,303	0
81	MG	A	2025	1/1	0.63	0.31	85,85,85,85	0
80	OHX	A	2159[B]	7/7	0.64	0.23	149,152,154,184	7
81	MG	A	2049	1/1	0.64	0.30	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	A	2159[A]	7/7	0.64	0.23	150,152,154,178	7
81	MG	sR	2168	1/1	0.64	0.43	87,87,87,87	0
80	OHX	sR	2026	7/7	0.64	0.17	207,214,222,304	0
81	MG	A	2000	1/1	0.64	0.19	66,66,66,66	0
81	MG	AR	4098	1/1	0.64	0.17	80,80,80,80	0
81	MG	AR	4099	1/1	0.64	0.35	87,87,87,87	0
81	MG	1	3851	1/1	0.64	0.23	73,73,73,73	0
80	OHX	AR	4227	7/7	0.65	0.19	215,220,224,311	0
81	MG	A	2081	1/1	0.65	0.34	104,104,104,104	0
81	MG	1	3950	1/1	0.65	0.18	79,79,79,79	0
80	OHX	sR	2019	7/7	0.65	0.18	225,230,240,317	0
80	OHX	4	214	7/7	0.65	0.13	216,225,228,328	0
81	MG	AR	4092	1/1	0.66	0.29	81,81,81,81	0
81	MG	AR	3947	1/1	0.66	0.36	60,60,60,60	0
81	MG	AR	3745	1/1	0.66	0.19	82,82,82,82	0
81	MG	AR	4003	1/1	0.66	0.46	107,107,107,107	0
81	MG	AR	4146	1/1	0.66	0.25	86,86,86,86	0
80	OHX	1	3637	7/7	0.66	0.20	215,224,239,322	0
80	OHX	sR	2029	7/7	0.66	0.18	210,224,235,309	0
81	MG	sR	2108	1/1	0.67	0.24	83,83,83,83	0
81	MG	AR	3786	1/1	0.67	0.27	74,74,74,74	0
81	MG	1	3730	1/1	0.67	0.37	86,86,86,86	0
81	MG	1	4041	1/1	0.67	0.20	107,107,107,107	0
81	MG	1	4049	1/1	0.67	0.30	107,107,107,107	0
81	MG	A	2019	1/1	0.67	0.30	63,63,63,63	0
81	MG	1	3977	1/1	0.67	0.21	95,95,95,95	0
81	MG	AR	3783	1/1	0.67	0.44	87,87,87,87	0
81	MG	sR	2146	1/1	0.68	0.22	81,81,81,81	0
81	MG	1	3866	1/1	0.68	0.29	88,88,88,88	0
81	MG	AR	3976	1/1	0.68	0.32	79,79,79,79	0
80	OHX	AT	213	7/7	0.68	0.16	193,201,208,304	0
81	MG	1	3944	1/1	0.68	0.41	81,81,81,81	0
81	MG	3	217	1/1	0.68	0.13	120,120,120,120	0
81	MG	4	225	1/1	0.68	0.20	80,80,80,80	0
80	OHX	1	3590	7/7	0.68	0.13	250,257,267,342	0
81	MG	AS	221	1/1	0.69	0.27	83,83,83,83	0
81	MG	A	2028	1/1	0.69	0.24	77,77,77,77	0
81	MG	AR	4031	1/1	0.69	0.30	55,55,55,55	0
81	MG	1	3868	1/1	0.69	0.29	78,78,78,78	0
81	MG	sR	2109	1/1	0.69	0.26	79,79,79,79	0
81	MG	sR	2126	1/1	0.69	0.15	109,109,109,109	0
81	MG	sR	2143	1/1	0.69	0.23	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	4079	1/1	0.69	0.35	74,74,74,74	0
81	MG	sR	2157	1/1	0.69	0.19	78,78,78,78	0
81	MG	sR	2160	1/1	0.69	0.31	100,100,100,100	0
81	MG	t	202	1/1	0.69	0.23	91,91,91,91	0
81	MG	1	3654	1/1	0.69	0.17	82,82,82,82	0
81	MG	1	4032	1/1	0.69	0.22	79,79,79,79	0
81	MG	AR	3769	1/1	0.69	0.24	67,67,67,67	0
80	OHX	AR	3642	7/7	0.69	0.23	111,124,139,232	0
81	MG	AR	4156	1/1	0.69	0.24	77,77,77,77	0
81	MG	AR	4172	1/1	0.69	0.35	69,69,69,69	0
80	OHX	AR	3657	7/7	0.70	0.19	212,218,225,304	0
80	OHX	AR	3680	7/7	0.70	0.21	201,215,228,313	0
81	MG	1	3978	1/1	0.70	0.32	78,78,78,78	0
81	MG	sR	2138	1/1	0.70	0.34	87,87,87,87	0
80	OHX	AR	3687	7/7	0.70	0.17	206,208,217,309	0
81	MG	A	2097	1/1	0.70	0.47	74,74,74,74	0
81	MG	sR	2155	1/1	0.70	0.24	62,62,62,62	0
81	MG	AR	3974	1/1	0.70	0.47	76,76,76,76	0
80	OHX	AR	4224	7/7	0.70	0.14	228,236,238,320	0
81	MG	1	3871	1/1	0.70	0.25	76,76,76,76	0
81	MG	AR	3996	1/1	0.70	0.32	63,63,63,63	0
81	MG	1	3649	1/1	0.70	0.28	58,58,58,58	0
80	OHX	1	4175	7/7	0.70	0.15	231,235,237,306	0
81	MG	AS	224	1/1	0.70	0.23	76,76,76,76	0
81	MG	A	2008	1/1	0.70	0.42	70,70,70,70	0
81	MG	DR	502	1/1	0.70	0.20	90,90,90,90	0
81	MG	1	4004	1/1	0.71	0.31	83,83,83,83	0
81	MG	AR	3829	1/1	0.71	0.29	54,54,54,54	0
81	MG	AR	4087	1/1	0.71	0.22	80,80,80,80	0
81	MG	1	3947	1/1	0.71	0.36	73,73,73,73	0
81	MG	AR	3904	1/1	0.71	0.33	72,72,72,72	0
80	OHX	sR	2001	7/7	0.71	0.19	200,204,216,293	0
81	MG	AR	4141	1/1	0.71	0.23	97,97,97,97	0
81	MG	1	3964	1/1	0.71	0.30	74,74,74,74	0
81	MG	A	2072	1/1	0.71	0.31	63,63,63,63	0
81	MG	AR	3702	1/1	0.71	0.34	103,103,103,103	0
81	MG	AR	4166	1/1	0.71	0.21	61,61,61,61	0
81	MG	AR	3989	1/1	0.71	0.12	92,92,92,92	0
81	MG	AR	4186	1/1	0.71	0.34	68,68,68,68	0
81	MG	1	3725	1/1	0.71	0.30	80,80,80,80	0
80	OHX	1	3597	7/7	0.71	0.16	197,213,217,301	0
81	MG	A	2051	1/1	0.71	0.12	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	A	2060	1/1	0.71	0.33	100,100,100,100	0
81	MG	1	3822	1/1	0.72	0.23	53,53,53,53	0
81	MG	A	1985	1/1	0.72	0.21	78,78,78,78	0
81	MG	1	4120	1/1	0.72	0.22	93,93,93,93	0
81	MG	1	3700	1/1	0.72	0.19	67,67,67,67	0
81	MG	A	2112	1/1	0.72	0.30	78,78,78,78	0
81	MG	AR	4119	1/1	0.72	0.38	97,97,97,97	0
80	OHX	sR	2033	7/7	0.72	0.16	210,217,223,306	0
81	MG	c6	201	1/1	0.72	0.35	83,83,83,83	0
81	MG	1	3975	1/1	0.72	0.20	75,75,75,75	0
82	K	A	2161	1/1	0.72	0.42	134,134,134,134	0
80	OHX	sR	2182	7/7	0.72	0.17	156,169,178,217	7
81	MG	sR	2112	1/1	0.72	0.20	61,61,61,61	0
86	5XU	s3	302	4/5	0.72	0.10	85,86,89,99	0
81	MG	1	3742	1/1	0.72	0.41	51,51,51,51	0
81	MG	AR	3931	1/1	0.72	0.30	57,57,57,57	0
81	MG	A	2044	1/1	0.73	0.33	86,86,86,86	0
81	MG	A	2067	1/1	0.73	0.21	80,80,80,80	0
81	MG	1	4002	1/1	0.73	0.29	82,82,82,82	0
81	MG	1	3922	1/1	0.73	0.13	90,90,90,90	0
81	MG	1	4008	1/1	0.73	0.37	90,90,90,90	0
81	MG	A	2011	1/1	0.73	0.24	76,76,76,76	0
81	MG	8	202	1/1	0.73	0.19	62,62,62,62	0
81	MG	AR	3995	1/1	0.73	0.18	94,94,94,94	0
81	MG	A	2098	1/1	0.73	0.11	78,78,78,78	0
81	MG	A	2108	1/1	0.73	0.26	86,86,86,86	0
81	MG	d2	201	1/1	0.73	0.18	56,56,56,56	0
80	OHX	sR	2186	7/7	0.73	0.13	183,188,190,244	7
81	MG	A	2113	1/1	0.73	0.23	82,82,82,82	0
80	OHX	AR	4232	7/7	0.73	0.13	188,196,205,298	0
81	MG	1	4087	1/1	0.73	0.27	58,58,58,58	0
81	MG	A	2054	1/1	0.73	0.27	85,85,85,85	0
81	MG	AR	3860	1/1	0.73	0.33	52,52,52,52	0
81	MG	A	2023	1/1	0.73	0.28	74,74,74,74	0
80	OHX	AR	3638	7/7	0.74	0.13	170,188,194,273	0
81	MG	AR	4072	1/1	0.74	0.23	74,74,74,74	0
81	MG	1	3884	1/1	0.74	0.35	70,70,70,70	0
80	OHX	1	3629	7/7	0.74	0.12	259,263,276,359	0
81	MG	sR	2120	1/1	0.74	0.26	75,75,75,75	0
81	MG	AR	3790	1/1	0.74	0.29	48,48,48,48	0
81	MG	1	4097	1/1	0.74	0.34	80,80,80,80	0
81	MG	1	4107	1/1	0.74	0.31	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	4001	1/1	0.74	0.14	76,76,76,76	0
80	OHX	sR	2177	7/7	0.74	0.16	208,216,221,305	0
80	OHX	1	3614	7/7	0.74	0.15	191,197,215,297	0
81	MG	1	3759	1/1	0.74	0.28	57,57,57,57	0
80	OHX	1	4172	7/7	0.74	0.21	176,181,191,269	0
81	MG	1	4019	1/1	0.74	0.29	89,89,89,89	0
81	MG	c4	2201	1/1	0.74	0.17	84,84,84,84	0
81	MG	AR	4159	1/1	0.74	0.14	82,82,82,82	0
81	MG	1	4020	1/1	0.74	0.29	81,81,81,81	0
81	MG	1	3644	1/1	0.74	0.28	80,80,80,80	0
80	OHX	AR	3597	7/7	0.74	0.18	162,168,177,256	0
81	MG	AR	4191	1/1	0.74	0.35	85,85,85,85	0
81	MG	AR	3730	1/1	0.74	0.28	69,69,69,69	0
80	OHX	AR	3688	7/7	0.74	0.13	218,221,239,311	0
80	OHX	AR	3691	7/7	0.74	0.14	221,233,244,322	0
81	MG	AR	4026	1/1	0.74	0.27	66,66,66,66	0
81	MG	sR	2037	1/1	0.75	0.29	53,53,53,53	0
81	MG	sR	2049	1/1	0.75	0.30	70,70,70,70	0
81	MG	sR	2059	1/1	0.75	0.28	80,80,80,80	0
81	MG	sR	2098	1/1	0.75	0.26	75,75,75,75	0
81	MG	A	2105	1/1	0.75	0.42	84,84,84,84	0
81	MG	1	3897	1/1	0.75	0.42	67,67,67,67	0
81	MG	1	3900	1/1	0.75	0.41	72,72,72,72	0
80	OHX	sR	2184	7/7	0.75	0.21	127,131,134,154	7
81	MG	AR	3935	1/1	0.75	0.17	92,92,92,92	0
81	MG	sR	2129	1/1	0.75	0.12	81,81,81,81	0
81	MG	AR	3943	1/1	0.75	0.40	84,84,84,84	0
81	MG	A	2085	1/1	0.75	0.28	74,74,74,74	0
81	MG	A	2086	1/1	0.75	0.27	84,84,84,84	0
81	MG	1	3946	1/1	0.75	0.22	66,66,66,66	0
80	OHX	x	209	7/7	0.75	0.12	220,222,228,314	0
81	MG	AR	3983	1/1	0.75	0.19	68,68,68,68	0
81	MG	1	3948	1/1	0.75	0.15	52,52,52,52	0
81	MG	1	3771	1/1	0.75	0.34	84,84,84,84	0
80	OHX	1	3630	7/7	0.75	0.14	182,186,203,285	0
81	MG	AR	4189	1/1	0.75	0.31	68,68,68,68	0
80	OHX	A	1978	7/7	0.75	0.13	209,223,226,308	0
81	MG	1	3971	1/1	0.75	0.28	55,55,55,55	0
80	OHX	sR	2178	7/7	0.75	0.18	148,158,166,253	0
81	MG	1	3656	1/1	0.75	0.28	50,50,50,50	0
81	MG	AT	227	1/1	0.75	0.21	63,63,63,63	0
81	MG	AT	228	1/1	0.75	0.33	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	3677	1/1	0.75	0.29	77,77,77,77	0
80	OHX	A	1967	7/7	0.75	0.15	190,192,205,281	0
81	MG	AR	3972	1/1	0.76	0.19	55,55,55,55	0
80	OHX	AR	3690	7/7	0.76	0.13	195,198,211,294	0
81	MG	m	301	1/1	0.76	0.24	82,82,82,82	0
80	OHX	1	3603	7/7	0.76	0.20	158,164,170,261	0
81	MG	1	3986	1/1	0.76	0.21	97,97,97,97	0
81	MG	1	4037	1/1	0.76	0.19	65,65,65,65	0
81	MG	sR	2162	1/1	0.76	0.32	77,77,77,77	0
81	MG	1	4101	1/1	0.76	0.12	48,48,48,48	0
80	OHX	1	3560	7/7	0.76	0.20	126,141,151,236	0
81	MG	AR	3913	1/1	0.76	0.15	69,69,69,69	0
81	MG	AR	4154	1/1	0.76	0.23	85,85,85,85	0
81	MG	1	4110	1/1	0.76	0.19	81,81,81,81	0
81	MG	AR	4016	1/1	0.76	0.17	77,77,77,77	0
81	MG	d5	201	1/1	0.76	0.18	94,94,94,94	0
80	OHX	AR	3667	7/7	0.76	0.13	190,195,207,287	0
81	MG	AR	3936	1/1	0.76	0.29	75,75,75,75	0
81	MG	AR	4046	1/1	0.76	0.29	82,82,82,82	0
81	MG	1	4053	1/1	0.76	0.31	84,84,84,84	0
81	MG	sR	2128	1/1	0.76	0.27	97,97,97,97	0
81	MG	1	4056	1/1	0.76	0.42	85,85,85,85	0
81	MG	AR	3928	1/1	0.77	0.25	77,77,77,77	0
81	MG	sR	2055	1/1	0.77	0.19	59,59,59,59	0
81	MG	AR	3929	1/1	0.77	0.40	60,60,60,60	0
81	MG	sR	2064	1/1	0.77	0.42	90,90,90,90	0
81	MG	sR	2072	1/1	0.77	0.25	59,59,59,59	0
81	MG	sR	2096	1/1	0.77	0.18	81,81,81,81	0
81	MG	AR	4086	1/1	0.77	0.22	60,60,60,60	0
81	MG	1	4050	1/1	0.77	0.21	76,76,76,76	0
81	MG	1	3990	1/1	0.77	0.34	73,73,73,73	0
80	OHX	sR	2181	7/7	0.77	0.12	206,209,218,280	0
81	MG	1	3795	1/1	0.77	0.24	60,60,60,60	0
81	MG	AR	4108	1/1	0.77	0.38	92,92,92,92	0
81	MG	AR	3720	1/1	0.77	0.35	59,59,59,59	0
80	OHX	1	3564	7/7	0.77	0.15	167,174,180,271	0
81	MG	AR	3973	1/1	0.77	0.29	70,70,70,70	0
80	OHX	AR	4231	7/7	0.77	0.14	182,187,198,290	0
81	MG	1	3690	1/1	0.77	0.25	65,65,65,65	0
81	MG	sR	2154	1/1	0.77	0.24	89,89,89,89	0
81	MG	AR	3775	1/1	0.77	0.20	68,68,68,68	0
81	MG	AR	3980	1/1	0.77	0.15	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	A	2158	7/7	0.77	0.18	167,181,186,263	0
80	OHX	d6	201	7/7	0.77	0.17	184,189,196,270	0
81	MG	sR	2163	1/1	0.77	0.21	87,87,87,87	0
81	MG	AR	4174	1/1	0.77	0.29	64,64,64,64	0
80	OHX	AR	4238	7/7	0.77	0.17	182,190,198,297	0
80	OHX	AR	3695	7/7	0.77	0.19	205,217,229,324	0
81	MG	1	3735	1/1	0.77	0.28	78,78,78,78	0
81	MG	AR	3843	1/1	0.77	0.45	58,58,58,58	0
81	MG	AR	3844	1/1	0.77	0.22	64,64,64,64	0
80	OHX	AR	3679	7/7	0.77	0.12	194,196,206,288	0
81	MG	AT	218	1/1	0.77	0.19	73,73,73,73	0
81	MG	A	2070	1/1	0.77	0.25	87,87,87,87	0
81	MG	AR	4043	1/1	0.77	0.24	88,88,88,88	0
81	MG	1	4045	1/1	0.77	0.38	97,97,97,97	0
81	MG	AR	4054	1/1	0.77	0.21	66,66,66,66	0
81	MG	1	3769	1/1	0.77	0.28	65,65,65,65	0
81	MG	AR	4006	1/1	0.78	0.20	60,60,60,60	0
80	OHX	AR	4228	7/7	0.78	0.13	165,173,179,269	0
81	MG	1	4085	1/1	0.78	0.27	58,58,58,58	0
81	MG	AR	3792	1/1	0.78	0.44	81,81,81,81	0
81	MG	sR	2044	1/1	0.78	0.20	76,76,76,76	0
81	MG	A	2080	1/1	0.78	0.10	96,96,96,96	0
81	MG	AR	4034	1/1	0.78	0.40	75,75,75,75	0
81	MG	A	2034	1/1	0.78	0.12	97,97,97,97	0
80	OHX	sR	2030	7/7	0.78	0.14	185,199,205,280	0
81	MG	sR	2069	1/1	0.78	0.32	60,60,60,60	0
81	MG	1	3991	1/1	0.78	0.34	78,78,78,78	0
81	MG	AR	4067	1/1	0.78	0.27	84,84,84,84	0
81	MG	AR	3878	1/1	0.78	0.34	68,68,68,68	0
81	MG	sR	2101	1/1	0.78	0.20	73,73,73,73	0
81	MG	1	3872	1/1	0.78	0.19	56,56,56,56	0
81	MG	1	3876	1/1	0.78	0.30	81,81,81,81	0
81	MG	AR	3905	1/1	0.78	0.21	83,83,83,83	0
81	MG	1	3688	1/1	0.78	0.20	63,63,63,63	0
81	MG	AR	3924	1/1	0.78	0.40	70,70,70,70	0
81	MG	A	1988	1/1	0.78	0.30	59,59,59,59	0
80	OHX	3	223	7/7	0.78	0.11	207,216,224,300	0
81	MG	AR	4105	1/1	0.78	0.17	63,63,63,63	0
81	MG	A	2048	1/1	0.78	0.15	81,81,81,81	0
80	OHX	sR	2035	7/7	0.78	0.14	213,216,227,288	0
81	MG	A	2009	1/1	0.78	0.33	72,72,72,72	0
81	MG	1	4024	1/1	0.78	0.16	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	AR	3945	1/1	0.78	0.40	81,81,81,81	0
80	OHX	AR	3669	7/7	0.78	0.12	208,230,232,313	0
81	MG	AR	3955	1/1	0.78	0.18	48,48,48,48	0
80	OHX	AR	3673	7/7	0.78	0.18	166,167,177,266	0
80	OHX	A	1972	7/7	0.78	0.13	199,207,220,289	0
81	MG	1	4039	1/1	0.78	0.52	82,82,82,82	0
81	MG	AR	3722	1/1	0.78	0.28	68,68,68,68	0
81	MG	AR	4175	1/1	0.78	0.27	84,84,84,84	0
81	MG	c6	202	1/1	0.78	0.25	89,89,89,89	0
80	OHX	1	3615	7/7	0.78	0.21	201,205,216,303	0
80	OHX	AR	4226	7/7	0.78	0.11	203,210,218,285	0
81	MG	AR	3761	1/1	0.78	0.33	69,69,69,69	0
81	MG	AR	4196	1/1	0.78	0.21	64,64,64,64	0
81	MG	AR	3985	1/1	0.78	0.16	53,53,53,53	0
80	OHX	1	3632	7/7	0.78	0.15	196,209,215,304	0
81	MG	CE	404	1/1	0.78	0.32	62,62,62,62	0
81	MG	1	3838	1/1	0.78	0.25	79,79,79,79	0
81	MG	A	2031	1/1	0.78	0.17	62,62,62,62	0
81	MG	AR	3901	1/1	0.79	0.23	77,77,77,77	0
80	OHX	AR	3698	7/7	0.79	0.15	144,149,166,226	0
81	MG	sR	2110	1/1	0.79	0.15	92,92,92,92	0
81	MG	AR	4012	1/1	0.79	0.28	70,70,70,70	0
81	MG	sR	2118	1/1	0.79	0.17	83,83,83,83	0
80	OHX	sR	2187	7/7	0.79	0.13	188,191,195,282	0
81	MG	A	2065	1/1	0.79	0.13	83,83,83,83	0
81	MG	AR	4020	1/1	0.79	0.34	90,90,90,90	0
81	MG	AR	4178	1/1	0.79	0.29	59,59,59,59	0
81	MG	sR	2131	1/1	0.79	0.34	81,81,81,81	0
81	MG	A	2039	1/1	0.79	0.22	69,69,69,69	0
81	MG	1	3983	1/1	0.79	0.35	71,71,71,71	0
81	MG	sR	2144	1/1	0.79	0.16	75,75,75,75	0
81	MG	sR	2145	1/1	0.79	0.36	94,94,94,94	0
80	OHX	sR	2011	7/7	0.79	0.14	167,170,182,261	0
81	MG	AR	3724	1/1	0.79	0.20	63,63,63,63	0
81	MG	1	3988	1/1	0.79	0.12	55,55,55,55	0
81	MG	1	3761	1/1	0.79	0.25	69,69,69,69	0
81	MG	AR	3747	1/1	0.79	0.16	64,64,64,64	0
81	MG	1	3651	1/1	0.79	0.38	69,69,69,69	0
80	OHX	AR	3685	7/7	0.79	0.12	189,197,209,291	0
80	OHX	sR	2025	7/7	0.79	0.14	194,197,212,288	0
81	MG	AR	4081	1/1	0.79	0.39	73,73,73,73	0
81	MG	s4	303	1/1	0.79	0.27	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	s8	301	1/1	0.79	0.46	107,107,107,107	0
81	MG	1	3943	1/1	0.79	0.24	93,93,93,93	0
81	MG	1	3805	1/1	0.79	0.38	57,57,57,57	0
80	OHX	AR	4225	7/7	0.79	0.18	146,157,174,262	0
81	MG	1	4009	1/1	0.79	0.24	74,74,74,74	0
81	MG	1	4012	1/1	0.79	0.15	60,60,60,60	0
81	MG	A	2106	1/1	0.79	0.36	79,79,79,79	0
80	OHX	1	3628	7/7	0.79	0.10	223,234,248,332	0
81	MG	A	2111	1/1	0.79	0.12	58,58,58,58	0
85	ZN	d7	101	1/1	0.79	0.11	220,220,220,220	0
81	MG	1	3862	1/1	0.79	0.20	57,57,57,57	0
81	MG	AR	3990	1/1	0.79	0.33	83,83,83,83	0
81	MG	1	3865	1/1	0.79	0.32	88,88,88,88	0
80	OHX	1	3586	7/7	0.79	0.14	162,172,185,262	0
81	MG	1	3704	1/1	0.80	0.20	62,62,62,62	0
80	OHX	1	3609	7/7	0.80	0.12	201,217,225,294	0
81	MG	1	4048	1/1	0.80	0.26	72,72,72,72	0
80	OHX	AR	3648	7/7	0.80	0.19	148,157,168,258	0
81	MG	1	3982	1/1	0.80	0.31	63,63,63,63	0
80	OHX	e	102	7/7	0.80	0.12	234,236,247,320	0
81	MG	1	3734	1/1	0.80	0.24	71,71,71,71	0
81	MG	1	3877	1/1	0.80	0.27	89,89,89,89	0
81	MG	AR	3771	1/1	0.80	0.39	69,69,69,69	0
81	MG	1	4065	1/1	0.80	0.33	73,73,73,73	0
81	MG	1	4077	1/1	0.80	0.33	51,51,51,51	0
80	OHX	A	1976	7/7	0.80	0.11	184,191,201,266	0
81	MG	AR	4162	1/1	0.80	0.32	69,69,69,69	0
81	MG	1	3896	1/1	0.80	0.33	66,66,66,66	0
81	MG	1	4092	1/1	0.80	0.31	53,53,53,53	0
80	OHX	A	2143	7/7	0.80	0.16	180,186,192,262	0
81	MG	AR	3799	1/1	0.80	0.40	53,53,53,53	0
81	MG	AR	3999	1/1	0.80	0.33	90,90,90,90	0
80	OHX	sR	2018	7/7	0.80	0.12	200,207,214,274	0
81	MG	AR	3831	1/1	0.80	0.26	58,58,58,58	0
80	OHX	A	2154	7/7	0.80	0.11	238,241,243,304	0
81	MG	A	2087	1/1	0.80	0.10	61,61,61,61	0
81	MG	AR	4207	1/1	0.80	0.30	69,69,69,69	0
81	MG	AS	217	1/1	0.80	0.22	80,80,80,80	0
81	MG	1	3928	1/1	0.80	0.41	65,65,65,65	0
80	OHX	sR	2021	7/7	0.80	0.16	139,146,166,244	0
81	MG	AR	3891	1/1	0.80	0.12	48,48,48,48	0
80	OHX	A	1949	7/7	0.80	0.14	187,189,193,266	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	3	222	7/7	0.80	0.15	201,206,212,296	0
80	OHX	sR	2189	7/7	0.80	0.15	184,188,190,239	7
80	OHX	sR	2027	7/7	0.80	0.18	182,187,204,283	0
81	MG	A	2099	1/1	0.80	0.17	64,64,64,64	0
81	MG	d3	201	1/1	0.80	0.24	65,65,65,65	0
81	MG	A	2104	1/1	0.80	0.33	60,60,60,60	0
81	MG	z	202	1/1	0.80	0.18	111,111,111,111	0
81	MG	1	3859	1/1	0.80	0.30	81,81,81,81	0
80	OHX	AR	3696	7/7	0.80	0.12	187,199,201,292	0
81	MG	AR	3932	1/1	0.80	0.45	76,76,76,76	0
85	ZN	e1	501	1/1	0.80	0.11	181,181,181,181	0
81	MG	AR	4085	1/1	0.80	0.17	54,54,54,54	0
81	MG	1	3701	1/1	0.80	0.24	66,66,66,66	0
81	MG	AR	3708	1/1	0.80	0.23	56,56,56,56	0
81	MG	sR	2083	1/1	0.80	0.19	64,64,64,64	0
81	MG	AR	3918	1/1	0.81	0.23	77,77,77,77	0
81	MG	1	3659	1/1	0.81	0.25	64,64,64,64	0
81	MG	A	1995	1/1	0.81	0.23	69,69,69,69	0
80	OHX	AR	3694	7/7	0.81	0.13	197,201,210,283	0
81	MG	sR	2075	1/1	0.81	0.25	68,68,68,68	0
81	MG	sR	2078	1/1	0.81	0.19	56,56,56,56	0
81	MG	AR	4082	1/1	0.81	0.28	76,76,76,76	0
81	MG	AR	3930	1/1	0.81	0.36	72,72,72,72	0
81	MG	1	4051	1/1	0.81	0.28	79,79,79,79	0
80	OHX	AS	209	7/7	0.81	0.16	151,156,167,246	0
81	MG	AR	4091	1/1	0.81	0.19	71,71,71,71	0
80	OHX	AR	3635	7/7	0.81	0.16	179,190,202,287	0
80	OHX	AR	3675	7/7	0.81	0.15	155,165,174,261	0
81	MG	AR	3939	1/1	0.81	0.32	78,78,78,78	0
81	MG	AR	3760	1/1	0.81	0.17	63,63,63,63	0
81	MG	A	2012	1/1	0.81	0.36	91,91,91,91	0
81	MG	sR	2122	1/1	0.81	0.17	83,83,83,83	0
81	MG	AR	3762	1/1	0.81	0.29	72,72,72,72	0
81	MG	AR	4125	1/1	0.81	0.17	45,45,45,45	0
81	MG	AR	4128	1/1	0.81	0.27	101,101,101,101	0
81	MG	AR	3766	1/1	0.81	0.15	101,101,101,101	0
81	MG	sR	2136	1/1	0.81	0.44	84,84,84,84	0
81	MG	AR	3958	1/1	0.81	0.15	53,53,53,53	0
81	MG	1	4069	1/1	0.81	0.30	67,67,67,67	0
81	MG	A	2056	1/1	0.81	0.28	92,92,92,92	0
80	OHX	1	3636	7/7	0.81	0.14	170,175,190,268	0
81	MG	AR	3780	1/1	0.81	0.29	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	sR	2148	1/1	0.81	0.10	69,69,69,69	0
81	MG	A	2061	1/1	0.81	0.28	69,69,69,69	0
80	OHX	1	3574	7/7	0.81	0.14	153,160,175,255	0
81	MG	A	2064	1/1	0.81	0.15	82,82,82,82	0
81	MG	1	3905	1/1	0.81	0.31	80,80,80,80	0
81	MG	AR	3791	1/1	0.81	0.36	50,50,50,50	0
80	OHX	sR	2016	7/7	0.81	0.11	222,235,243,311	0
81	MG	A	2066	1/1	0.81	0.21	67,67,67,67	0
81	MG	AR	3810	1/1	0.81	0.20	53,53,53,53	0
81	MG	AR	3998	1/1	0.81	0.26	80,80,80,80	0
80	OHX	A	2110	7/7	0.81	0.14	165,171,179,253	0
81	MG	1	3929	1/1	0.81	0.32	72,72,72,72	0
81	MG	A	2069	1/1	0.81	0.21	96,96,96,96	0
80	OHX	AR	3653	7/7	0.81	0.14	162,174,180,269	0
81	MG	AR	3854	1/1	0.81	0.20	62,62,62,62	0
80	OHX	A	1957	7/7	0.81	0.11	203,205,213,283	0
80	OHX	AR	3689	7/7	0.81	0.09	249,257,263,339	0
80	OHX	AR	3591	7/7	0.81	0.17	146,148,156,256	0
80	OHX	A	1965	7/7	0.81	0.12	191,197,214,283	0
81	MG	1	3956	1/1	0.81	0.23	81,81,81,81	0
81	MG	DQ	201	1/1	0.81	0.28	69,69,69,69	0
81	MG	AR	4041	1/1	0.81	0.32	87,87,87,87	0
81	MG	1	3653	1/1	0.81	0.34	49,49,49,49	0
80	OHX	AR	4233	7/7	0.81	0.20	157,165,175,270	0
81	MG	AR	3907	1/1	0.81	0.34	64,64,64,64	0
81	MG	A	2042	1/1	0.81	0.24	82,82,82,82	0
80	OHX	sR	2008	7/7	0.82	0.15	192,197,207,294	0
81	MG	AR	4019	1/1	0.82	0.24	75,75,75,75	0
81	MG	A	2002	1/1	0.82	0.29	65,65,65,65	0
81	MG	1	4188	1/1	0.82	0.12	96,96,96,96	0
81	MG	sR	2042	1/1	0.82	0.23	78,78,78,78	0
81	MG	AR	4030	1/1	0.82	0.24	99,99,99,99	0
81	MG	1	3740	1/1	0.82	0.20	55,55,55,55	0
81	MG	sR	2050	1/1	0.82	0.22	70,70,70,70	0
81	MG	sR	2052	1/1	0.82	0.20	72,72,72,72	0
81	MG	AR	3846	1/1	0.82	0.25	50,50,50,50	0
81	MG	AR	3850	1/1	0.82	0.21	69,69,69,69	0
81	MG	1	3901	1/1	0.82	0.50	75,75,75,75	0
81	MG	sR	2066	1/1	0.82	0.19	71,71,71,71	0
81	MG	4	219	1/1	0.82	0.28	64,64,64,64	0
80	OHX	AR	3645	7/7	0.82	0.17	180,181,192,280	0
81	MG	sR	2074	1/1	0.82	0.26	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	AR	4057	1/1	0.82	0.15	85,85,85,85	0
81	MG	4	232	1/1	0.82	0.13	68,68,68,68	0
80	OHX	sR	2013	7/7	0.82	0.16	136,144,148,237	0
80	OHX	A	1968	7/7	0.82	0.11	221,224,231,300	0
80	OHX	1	3554	7/7	0.82	0.11	202,204,216,292	0
81	MG	AR	4080	1/1	0.82	0.28	70,70,70,70	0
81	MG	v	303	1/1	0.82	0.15	69,69,69,69	0
81	MG	A	2052	1/1	0.82	0.15	70,70,70,70	0
81	MG	1	3942	1/1	0.82	0.20	61,61,61,61	0
81	MG	AR	3915	1/1	0.82	0.33	70,70,70,70	0
81	MG	1	3775	1/1	0.82	0.09	44,44,44,44	0
81	MG	sR	2119	1/1	0.82	0.22	134,134,134,134	0
81	MG	1	4026	1/1	0.82	0.26	81,81,81,81	0
81	MG	1	3789	1/1	0.82	0.33	63,63,63,63	0
81	MG	AR	4096	1/1	0.82	0.12	75,75,75,75	0
81	MG	AR	3717	1/1	0.82	0.38	42,42,42,42	0
80	OHX	1	3623	7/7	0.82	0.13	181,195,205,290	0
81	MG	A	2090	1/1	0.82	0.19	73,73,73,73	0
81	MG	AR	4107	1/1	0.82	0.24	69,69,69,69	0
81	MG	1	3820	1/1	0.82	0.29	48,48,48,48	0
81	MG	1	3949	1/1	0.82	0.31	62,62,62,62	0
81	MG	AR	3735	1/1	0.82	0.24	69,69,69,69	0
81	MG	1	4046	1/1	0.82	0.18	71,71,71,71	0
81	MG	A	2092	1/1	0.82	0.36	53,53,53,53	0
81	MG	1	3955	1/1	0.82	0.38	78,78,78,78	0
81	MG	1	3828	1/1	0.82	0.41	48,48,48,48	0
81	MG	AR	4151	1/1	0.82	0.16	67,67,67,67	0
81	MG	sR	2156	1/1	0.82	0.20	64,64,64,64	0
80	OHX	CG	304	7/7	0.82	0.12	180,189,197,275	0
81	MG	AR	3763	1/1	0.82	0.26	77,77,77,77	0
81	MG	AR	3968	1/1	0.82	0.15	48,48,48,48	0
81	MG	A	2020	1/1	0.82	0.25	71,71,71,71	0
81	MG	sR	2164	1/1	0.82	0.25	62,62,62,62	0
81	MG	1	3660	1/1	0.82	0.44	58,58,58,58	0
81	MG	AR	3770	1/1	0.82	0.32	72,72,72,72	0
81	MG	sR	2169	1/1	0.82	0.33	75,75,75,75	0
81	MG	sR	2173	1/1	0.82	0.24	72,72,72,72	0
81	MG	1	3856	1/1	0.82	0.23	71,71,71,71	0
80	OHX	AR	3701	7/7	0.82	0.16	175,183,189,284	0
81	MG	s8	303	1/1	0.82	0.16	61,61,61,61	0
81	MG	AR	3776	1/1	0.82	0.27	66,66,66,66	0
80	OHX	sR	1973	7/7	0.82	0.12	193,198,202,277	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	sR	1982	7/7	0.82	0.14	205,210,221,290	0
80	OHX	sR	1990	7/7	0.82	0.14	136,139,144,234	0
81	MG	AR	4194	1/1	0.82	0.15	68,68,68,68	0
81	MG	A	2100	1/1	0.82	0.29	67,67,67,67	0
81	MG	AR	3787	1/1	0.82	0.33	79,79,79,79	0
80	OHX	AR	3693	7/7	0.82	0.10	179,183,199,279	0
81	MG	1	3712	1/1	0.82	0.42	84,84,84,84	0
81	MG	A	1989	1/1	0.82	0.20	64,64,64,64	0
81	MG	AR	3795	1/1	0.82	0.33	44,44,44,44	0
80	OHX	sR	2003	7/7	0.82	0.14	197,201,215,282	0
81	MG	A	1996	1/1	0.82	0.26	68,68,68,68	0
81	MG	AR	3815	1/1	0.82	0.25	48,48,48,48	0
81	MG	CG	301	1/1	0.82	0.32	79,79,79,79	0
86	5XU	c0	203	5/5	0.82	0.14	131,132,133,134	0
81	MG	x	207	1/1	0.83	0.25	89,89,89,89	0
81	MG	x	208	1/1	0.83	0.25	56,56,56,56	0
80	OHX	AR	3644	7/7	0.83	0.15	172,179,190,270	0
81	MG	AR	4114	1/1	0.83	0.23	59,59,59,59	0
81	MG	AR	3821	1/1	0.83	0.22	72,72,72,72	0
81	MG	sR	2091	1/1	0.83	0.25	64,64,64,64	0
81	MG	AR	3981	1/1	0.83	0.28	86,86,86,86	0
81	MG	1	3914	1/1	0.83	0.14	54,54,54,54	0
81	MG	sR	2100	1/1	0.83	0.14	83,83,83,83	0
81	MG	AR	4129	1/1	0.83	0.16	89,89,89,89	0
80	OHX	AR	3602	7/7	0.83	0.16	147,162,172,253	0
81	MG	AR	3842	1/1	0.83	0.35	53,53,53,53	0
81	MG	AN	201	1/1	0.83	0.23	76,76,76,76	0
81	MG	AR	4150	1/1	0.83	0.21	102,102,102,102	0
81	MG	AR	3994	1/1	0.83	0.34	63,63,63,63	0
81	MG	1	3732	1/1	0.83	0.28	48,48,48,48	0
81	MG	1	3839	1/1	0.83	0.38	74,74,74,74	0
81	MG	AR	4157	1/1	0.83	0.26	60,60,60,60	0
81	MG	AR	3714	1/1	0.83	0.28	65,65,65,65	0
80	OHX	AR	3670	7/7	0.83	0.12	162,169,185,266	0
81	MG	1	3934	1/1	0.83	0.11	89,89,89,89	0
81	MG	1	4070	1/1	0.83	0.40	50,50,50,50	0
81	MG	1	4076	1/1	0.83	0.33	45,45,45,45	0
80	OHX	sR	2023	7/7	0.83	0.14	200,202,212,301	0
80	OHX	A	1952	7/7	0.83	0.17	201,205,219,292	0
81	MG	AR	4183	1/1	0.83	0.31	66,66,66,66	0
81	MG	AR	3744	1/1	0.83	0.12	66,66,66,66	0
80	OHX	AT	201	7/7	0.83	0.14	182,186,192,275	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	3683	1/1	0.83	0.21	63,63,63,63	0
81	MG	sR	2150	1/1	0.83	0.38	65,65,65,65	0
81	MG	AR	3908	1/1	0.83	0.43	78,78,78,78	0
80	OHX	O	201	7/7	0.83	0.11	211,216,228,293	0
81	MG	DA	202	1/1	0.83	0.29	56,56,56,56	0
81	MG	AR	4212	1/1	0.83	0.24	71,71,71,71	0
81	MG	AR	4217	1/1	0.83	0.19	50,50,50,50	0
81	MG	AR	4218	1/1	0.83	0.23	68,68,68,68	0
81	MG	AR	4219	1/1	0.83	0.23	65,65,65,65	0
81	MG	AS	201	1/1	0.83	0.17	79,79,79,79	0
81	MG	AR	4039	1/1	0.83	0.14	68,68,68,68	0
81	MG	1	3692	1/1	0.83	0.53	72,72,72,72	0
81	MG	A	2030	1/1	0.83	0.13	79,79,79,79	0
81	MG	1	3777	1/1	0.83	0.24	70,70,70,70	0
81	MG	1	4119	1/1	0.83	0.34	83,83,83,83	0
81	MG	A	2006	1/1	0.83	0.30	68,68,68,68	0
81	MG	AR	4061	1/1	0.83	0.14	52,52,52,52	0
81	MG	1	3960	1/1	0.83	0.21	93,93,93,93	0
80	OHX	k	404	7/7	0.83	0.11	185,191,196,275	0
81	MG	1	3881	1/1	0.83	0.23	79,79,79,79	0
81	MG	c8	203	1/1	0.83	0.47	81,81,81,81	0
80	OHX	AR	3699	7/7	0.83	0.13	173,183,192,283	0
81	MG	1	3807	1/1	0.83	0.30	45,45,45,45	0
81	MG	1	3811	1/1	0.83	0.23	50,50,50,50	0
81	MG	l	401	1/1	0.83	0.29	74,74,74,74	0
81	MG	1	3815	1/1	0.83	0.28	61,61,61,61	0
81	MG	AR	3788	1/1	0.83	0.12	49,49,49,49	0
81	MG	AR	3956	1/1	0.83	0.11	66,66,66,66	0
81	MG	sR	2054	1/1	0.83	0.29	61,61,61,61	0
81	MG	1	4047	1/1	0.83	0.26	68,68,68,68	0
81	MG	AR	3964	1/1	0.83	0.23	76,76,76,76	0
80	OHX	sR	1963	7/7	0.83	0.16	142,149,152,239	0
81	MG	1	3904	1/1	0.83	0.18	59,59,59,59	0
81	MG	w	201	1/1	0.83	0.30	84,84,84,84	0
81	MG	A	2088	1/1	0.84	0.43	54,54,54,54	0
81	MG	1	3967	1/1	0.84	0.26	76,76,76,76	0
81	MG	AR	3778	1/1	0.84	0.27	56,56,56,56	0
81	MG	1	3968	1/1	0.84	0.32	65,65,65,65	0
81	MG	AS	218	1/1	0.84	0.25	59,59,59,59	0
81	MG	1	3686	1/1	0.84	0.24	72,72,72,72	0
81	MG	1	3855	1/1	0.84	0.34	74,74,74,74	0
80	OHX	A	1975	7/7	0.84	0.12	225,236,241,296	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	1	3631	7/7	0.84	0.11	181,185,192,278	0
81	MG	AR	4004	1/1	0.84	0.22	65,65,65,65	0
80	OHX	l	403	7/7	0.84	0.10	213,225,237,312	0
81	MG	1	4103	1/1	0.84	0.34	55,55,55,55	0
81	MG	CK	201	1/1	0.84	0.15	76,76,76,76	0
81	MG	CM	202	1/1	0.84	0.29	70,70,70,70	0
81	MG	1	3696	1/1	0.84	0.37	49,49,49,49	0
80	OHX	AR	3678	7/7	0.84	0.17	147,154,160,251	0
80	OHX	1	3598	7/7	0.84	0.11	232,239,243,302	0
81	MG	b	202	1/1	0.84	0.27	84,84,84,84	0
81	MG	AR	3796	1/1	0.84	0.20	63,63,63,63	0
81	MG	AR	4022	1/1	0.84	0.16	66,66,66,66	0
81	MG	sR	2043	1/1	0.84	0.20	60,60,60,60	0
81	MG	A	1999	1/1	0.84	0.33	55,55,55,55	0
80	OHX	z	204	7/7	0.84	0.10	142,146,151,198	7
81	MG	1	3874	1/1	0.84	0.23	63,63,63,63	0
81	MG	1	3718	1/1	0.84	0.16	61,61,61,61	0
81	MG	3	218	1/1	0.84	0.25	73,73,73,73	0
81	MG	1	3993	1/1	0.84	0.13	65,65,65,65	0
81	MG	AR	3835	1/1	0.84	0.26	46,46,46,46	0
81	MG	sR	2061	1/1	0.84	0.12	61,61,61,61	0
81	MG	4	224	1/1	0.84	0.12	61,61,61,61	0
81	MG	sR	2065	1/1	0.84	0.15	89,89,89,89	0
81	MG	1	3996	1/1	0.84	0.24	77,77,77,77	0
81	MG	1	3997	1/1	0.84	0.30	86,86,86,86	0
81	MG	1	3721	1/1	0.84	0.42	60,60,60,60	0
81	MG	AR	4064	1/1	0.84	0.23	68,68,68,68	0
81	MG	l	402	1/1	0.84	0.38	46,46,46,46	0
81	MG	A	2053	1/1	0.84	0.20	83,83,83,83	0
81	MG	AR	3858	1/1	0.84	0.28	44,44,44,44	0
81	MG	AR	4076	1/1	0.84	0.13	84,84,84,84	0
81	MG	sR	2095	1/1	0.84	0.09	66,66,66,66	0
81	MG	r	301	1/1	0.84	0.22	51,51,51,51	0
81	MG	AR	3868	1/1	0.84	0.19	43,43,43,43	0
81	MG	r	303	1/1	0.84	0.12	67,67,67,67	0
81	MG	1	3727	1/1	0.84	0.17	61,61,61,61	0
80	OHX	AR	3683	7/7	0.84	0.15	159,165,174,263	0
80	OHX	AR	3573	7/7	0.84	0.15	136,139,153,245	0
81	MG	AR	3903	1/1	0.84	0.34	71,71,71,71	0
81	MG	sR	2111	1/1	0.84	0.21	74,74,74,74	0
81	MG	v	305	1/1	0.84	0.38	68,68,68,68	0
80	OHX	1	3634	7/7	0.84	0.11	196,212,215,299	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	x	205	1/1	0.84	0.29	55,55,55,55	0
80	OHX	AS	210	7/7	0.84	0.12	179,183,198,274	0
81	MG	1	4018	1/1	0.84	0.28	73,73,73,73	0
81	MG	AR	4100	1/1	0.84	0.14	84,84,84,84	0
81	MG	sR	2127	1/1	0.84	0.24	73,73,73,73	0
80	OHX	A	2145	7/7	0.84	0.14	204,207,216,278	0
81	MG	A	2109	1/1	0.84	0.23	99,99,99,99	0
81	MG	AR	3919	1/1	0.84	0.15	65,65,65,65	0
81	MG	sR	2134	1/1	0.84	0.19	70,70,70,70	0
81	MG	AR	3923	1/1	0.84	0.15	57,57,57,57	0
80	OHX	sR	2032	7/7	0.84	0.12	192,198,209,289	0
81	MG	AR	4122	1/1	0.84	0.18	76,76,76,76	0
81	MG	AH	201	1/1	0.84	0.37	76,76,76,76	0
81	MG	AK	101	1/1	0.84	0.09	62,62,62,62	0
80	OHX	A	1980	7/7	0.84	0.11	241,244,251,321	0
81	MG	AR	4131	1/1	0.84	0.19	79,79,79,79	0
81	MG	AR	4132	1/1	0.84	0.22	58,58,58,58	0
81	MG	sR	2152	1/1	0.84	0.16	88,88,88,88	0
81	MG	AR	4136	1/1	0.84	0.26	50,50,50,50	0
81	MG	1	3921	1/1	0.84	0.22	81,81,81,81	0
81	MG	AR	3707	1/1	0.84	0.23	62,62,62,62	0
81	MG	1	4028	1/1	0.84	0.36	53,53,53,53	0
81	MG	1	4029	1/1	0.84	0.31	79,79,79,79	0
80	OHX	1	4150	7/7	0.84	0.13	168,173,189,277	0
81	MG	AR	4153	1/1	0.84	0.32	72,72,72,72	0
80	OHX	1	4168	7/7	0.84	0.14	155,158,169,255	0
81	MG	AC	101	1/1	0.84	0.14	55,55,55,55	0
81	MG	1	3930	1/1	0.84	0.32	66,66,66,66	0
80	OHX	A	2155	7/7	0.84	0.20	155,160,167,211	7
81	MG	AR	3734	1/1	0.84	0.20	58,58,58,58	0
81	MG	AR	4165	1/1	0.84	0.32	50,50,50,50	0
81	MG	CD	301	1/1	0.84	0.32	51,51,51,51	0
81	MG	AR	4169	1/1	0.84	0.24	43,43,43,43	0
81	MG	s8	304	1/1	0.84	0.24	63,63,63,63	0
80	OHX	1	4173	7/7	0.84	0.11	168,175,184,261	0
81	MG	A	2027	1/1	0.84	0.23	93,93,93,93	0
81	MG	AR	3971	1/1	0.84	0.14	79,79,79,79	0
81	MG	AR	4177	1/1	0.84	0.39	59,59,59,59	0
80	OHX	A	1943	7/7	0.84	0.14	190,199,204,281	0
81	MG	AR	4180	1/1	0.84	0.26	70,70,70,70	0
81	MG	1	3650	1/1	0.84	0.33	59,59,59,59	0
81	MG	A	2075	1/1	0.84	0.29	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	AR	4187	1/1	0.84	0.24	75,75,75,75	0
80	OHX	1	4177	7/7	0.84	0.24	134,140,142,171	7
81	MG	AR	3977	1/1	0.84	0.22	59,59,59,59	0
80	OHX	1	4180	6/7	0.84	0.11	185,189,193,281	0
80	OHX	1	3575	7/7	0.84	0.14	152,155,161,233	0
81	MG	AR	4198	1/1	0.84	0.24	55,55,55,55	0
80	OHX	A	1977	7/7	0.84	0.12	192,195,204,288	0
80	OHX	sR	2190	7/7	0.84	0.09	210,217,220,309	0
80	OHX	A	2141	7/7	0.84	0.13	165,167,178,250	0
81	MG	AR	4023	1/1	0.85	0.18	89,89,89,89	0
81	MG	1	3818	1/1	0.85	0.38	49,49,49,49	0
80	OHX	1	3638	7/7	0.85	0.14	156,162,169,250	0
81	MG	4	218	1/1	0.85	0.24	60,60,60,60	0
80	OHX	1	3616	7/7	0.85	0.10	169,176,185,268	0
81	MG	CM	201	1/1	0.85	0.25	69,69,69,69	0
81	MG	4	221	1/1	0.85	0.31	53,53,53,53	0
81	MG	CP	304	1/1	0.85	0.20	80,80,80,80	0
81	MG	AR	4040	1/1	0.85	0.23	81,81,81,81	0
80	OHX	1	4158	7/7	0.85	0.16	105,115,133,207	0
80	OHX	AR	3677	7/7	0.85	0.10	194,199,214,304	0
80	OHX	sR	2188	7/7	0.85	0.11	221,228,234,314	0
80	OHX	AR	3504	7/7	0.85	0.19	93,97,104,196	0
80	OHX	AR	3529	7/7	0.85	0.18	115,125,134,224	0
81	MG	1	3655	1/1	0.85	0.24	60,60,60,60	0
80	OHX	DK	201	7/7	0.85	0.12	222,225,245,328	0
80	OHX	1	4161	7/7	0.85	0.12	164,173,183,263	0
81	MG	AR	4069	1/1	0.85	0.27	82,82,82,82	0
80	OHX	AR	3578	7/7	0.85	0.16	135,139,143,242	0
81	MG	AR	3888	1/1	0.85	0.44	64,64,64,64	0
81	MG	1	3667	1/1	0.85	0.38	63,63,63,63	0
81	MG	1	3672	1/1	0.85	0.20	55,55,55,55	0
80	OHX	1	3619	7/7	0.85	0.11	180,184,194,271	0
81	MG	sR	2062	1/1	0.85	0.21	66,66,66,66	0
80	OHX	sR	1980	7/7	0.85	0.12	169,176,184,261	0
80	OHX	AR	3593	7/7	0.85	0.20	135,143,151,236	0
81	MG	A	1997	1/1	0.85	0.24	62,62,62,62	0
80	OHX	1	4170	7/7	0.85	0.11	179,188,198,280	0
81	MG	sR	2071	1/1	0.85	0.21	68,68,68,68	0
80	OHX	sR	1998	7/7	0.85	0.11	155,159,174,247	0
81	MG	1	3693	1/1	0.85	0.17	44,44,44,44	0
81	MG	1	3694	1/1	0.85	0.24	57,57,57,57	0
81	MG	AR	4093	1/1	0.85	0.25	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	3894	1/1	0.85	0.09	93,93,93,93	0
81	MG	sR	2088	1/1	0.85	0.22	61,61,61,61	0
81	MG	sR	2089	1/1	0.85	0.37	70,70,70,70	0
81	MG	1	3895	1/1	0.85	0.35	71,71,71,71	0
81	MG	AR	3920	1/1	0.85	0.30	76,76,76,76	0
81	MG	AK	102	1/1	0.85	0.40	66,66,66,66	0
80	OHX	1	3556	7/7	0.85	0.14	162,165,169,267	0
80	OHX	AR	3606	7/7	0.85	0.12	160,163,178,242	0
81	MG	A	2007	1/1	0.85	0.18	75,75,75,75	0
80	OHX	sR	2005	7/7	0.85	0.15	150,155,161,242	0
80	OHX	AR	3618	7/7	0.85	0.12	177,182,192,259	0
81	MG	A	2010	1/1	0.85	0.26	68,68,68,68	0
81	MG	1	3913	1/1	0.85	0.20	81,81,81,81	0
80	OHX	sR	2009	7/7	0.85	0.14	185,192,205,276	0
81	MG	sR	2113	1/1	0.85	0.13	65,65,65,65	0
81	MG	sR	2116	1/1	0.85	0.11	72,72,72,72	0
81	MG	AR	3938	1/1	0.85	0.18	55,55,55,55	0
80	OHX	A	1966	7/7	0.85	0.14	164,167,183,244	0
81	MG	AR	3728	1/1	0.85	0.17	52,52,52,52	0
81	MG	AR	4134	1/1	0.85	0.21	78,78,78,78	0
80	OHX	AR	3636	7/7	0.85	0.11	163,171,186,263	0
80	OHX	A	1962	7/7	0.85	0.10	173,180,190,262	0
81	MG	AR	4142	1/1	0.85	0.12	71,71,71,71	0
80	OHX	AR	3641	7/7	0.85	0.15	163,170,182,261	0
81	MG	AR	3738	1/1	0.85	0.34	61,61,61,61	0
80	OHX	A	2157	7/7	0.85	0.11	179,182,185,254	0
81	MG	AR	3962	1/1	0.85	0.24	69,69,69,69	0
81	MG	sR	2137	1/1	0.85	0.15	66,66,66,66	0
80	OHX	sR	2020	7/7	0.85	0.11	195,204,209,278	0
81	MG	1	3931	1/1	0.85	0.18	79,79,79,79	0
81	MG	AR	3758	1/1	0.85	0.16	60,60,60,60	0
81	MG	1	4052	1/1	0.85	0.13	57,57,57,57	0
80	OHX	1	3602	7/7	0.85	0.11	156,164,169,252	0
81	MG	1	3939	1/1	0.85	0.22	67,67,67,67	0
80	OHX	3	206	7/7	0.85	0.14	172,174,178,254	0
80	OHX	A	2147	7/7	0.85	0.10	198,206,217,280	0
81	MG	AR	4167	1/1	0.85	0.18	49,49,49,49	0
81	MG	AR	3978	1/1	0.85	0.15	80,80,80,80	0
80	OHX	AR	3651	7/7	0.85	0.13	158,165,170,256	0
80	OHX	1	3633	7/7	0.85	0.10	225,232,239,318	0
81	MG	1	4074	1/1	0.85	0.12	54,54,54,54	0
81	MG	AR	3982	1/1	0.85	0.21	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	AR	3654	7/7	0.85	0.11	177,182,199,278	0
80	OHX	AR	3656	7/7	0.85	0.12	185,190,199,285	0
81	MG	AR	3777	1/1	0.85	0.15	72,72,72,72	0
81	MG	1	4079	1/1	0.85	0.28	60,60,60,60	0
81	MG	AR	3992	1/1	0.85	0.18	47,47,47,47	0
81	MG	AR	4188	1/1	0.85	0.19	61,61,61,61	0
81	MG	s2	301	1/1	0.85	0.17	88,88,88,88	0
80	OHX	AR	4230	7/7	0.85	0.14	179,183,193,288	0
80	OHX	1	3578	7/7	0.85	0.15	158,164,172,256	0
81	MG	1	3784	1/1	0.85	0.22	68,68,68,68	0
81	MG	AR	3997	1/1	0.85	0.26	79,79,79,79	0
80	OHX	1	3580	7/7	0.85	0.13	171,175,186,263	0
81	MG	AR	4201	1/1	0.85	0.33	74,74,74,74	0
81	MG	AR	4205	1/1	0.85	0.11	59,59,59,59	0
81	MG	1	3791	1/1	0.85	0.40	55,55,55,55	0
81	MG	AR	4210	1/1	0.85	0.27	67,67,67,67	0
81	MG	AR	4211	1/1	0.85	0.16	74,74,74,74	0
81	MG	AR	4000	1/1	0.85	0.27	75,75,75,75	0
81	MG	1	3961	1/1	0.85	0.16	88,88,88,88	0
80	OHX	1	3585	7/7	0.85	0.12	154,156,173,250	0
81	MG	1	4105	1/1	0.85	0.15	65,65,65,65	0
81	MG	AR	4221	1/1	0.85	0.14	81,81,81,81	0
81	MG	1	3802	1/1	0.85	0.38	57,57,57,57	0
81	MG	A	2047	1/1	0.85	0.26	74,74,74,74	0
80	OHX	AR	4235	7/7	0.85	0.14	158,175,182,268	0
80	OHX	sR	2180	7/7	0.85	0.14	154,158,168,250	0
81	MG	1	3972	1/1	0.85	0.23	60,60,60,60	0
80	OHX	AR	4236	7/7	0.85	0.34	140,148,150,187	7
80	OHX	1	3611	7/7	0.86	0.15	112,118,131,219	0
81	MG	1	4059	1/1	0.86	0.31	95,95,95,95	0
81	MG	1	4060	1/1	0.86	0.32	79,79,79,79	0
80	OHX	AR	3620	7/7	0.86	0.11	186,195,207,282	0
80	OHX	sR	2179	7/7	0.86	0.14	140,154,157,234	0
81	MG	AR	3862	1/1	0.86	0.20	43,43,43,43	0
81	MG	AR	3863	1/1	0.86	0.36	45,45,45,45	0
80	OHX	AR	3672	7/7	0.86	0.12	159,168,187,259	0
80	OHX	AR	3626	7/7	0.86	0.11	183,184,190,265	0
81	MG	AR	3881	1/1	0.86	0.32	53,53,53,53	0
81	MG	A	2026	1/1	0.86	0.10	65,65,65,65	0
80	OHX	A	2146	7/7	0.86	0.13	202,205,217,290	0
81	MG	1	3891	1/1	0.86	0.31	78,78,78,78	0
81	MG	sR	2099	1/1	0.86	0.20	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	AR	4170	1/1	0.86	0.23	59,59,59,59	0
81	MG	AR	3895	1/1	0.86	0.22	49,49,49,49	0
81	MG	sR	2107	1/1	0.86	0.21	49,49,49,49	0
81	MG	AR	3899	1/1	0.86	0.14	51,51,51,51	0
81	MG	1	3748	1/1	0.86	0.30	44,44,44,44	0
81	MG	1	3987	1/1	0.86	0.18	70,70,70,70	0
80	OHX	1	3587	7/7	0.86	0.11	178,181,192,264	0
81	MG	1	3652	1/1	0.86	0.24	66,66,66,66	0
81	MG	1	4094	1/1	0.86	0.27	64,64,64,64	0
81	MG	1	3766	1/1	0.86	0.23	58,58,58,58	0
80	OHX	AR	3637	7/7	0.86	0.14	132,139,147,232	0
80	OHX	1	3589	7/7	0.86	0.12	152,155,162,243	0
81	MG	1	3994	1/1	0.86	0.27	70,70,70,70	0
80	OHX	A	2137	7/7	0.86	0.12	155,158,167,242	0
81	MG	AR	3752	1/1	0.86	0.24	59,59,59,59	0
81	MG	AR	4048	1/1	0.86	0.13	55,55,55,55	0
80	OHX	AR	3538	7/7	0.86	0.14	85,94,102,187	0
81	MG	1	3909	1/1	0.86	0.42	73,73,73,73	0
81	MG	1	4112	1/1	0.86	0.20	71,71,71,71	0
81	MG	sR	2132	1/1	0.86	0.10	71,71,71,71	0
81	MG	1	3780	1/1	0.86	0.25	55,55,55,55	0
81	MG	AR	4066	1/1	0.86	0.19	88,88,88,88	0
81	MG	1	3782	1/1	0.86	0.33	45,45,45,45	0
81	MG	AR	3764	1/1	0.86	0.16	50,50,50,50	0
81	MG	1	3783	1/1	0.86	0.36	44,44,44,44	0
80	OHX	A	2138	7/7	0.86	0.12	188,190,200,274	0
81	MG	AR	4075	1/1	0.86	0.21	61,61,61,61	0
80	OHX	1	3641	7/7	0.86	0.14	165,177,185,258	0
81	MG	AR	4223	1/1	0.86	0.16	69,69,69,69	0
81	MG	sR	2149	1/1	0.86	0.17	99,99,99,99	0
81	MG	1	3664	1/1	0.86	0.12	66,66,66,66	0
81	MG	4	217	1/1	0.86	0.35	69,69,69,69	0
81	MG	AR	3942	1/1	0.86	0.19	65,65,65,65	0
81	MG	AS	219	1/1	0.86	0.27	52,52,52,52	0
81	MG	A	2089	1/1	0.86	0.39	60,60,60,60	0
81	MG	A	2041	1/1	0.86	0.31	79,79,79,79	0
81	MG	sR	2159	1/1	0.86	0.25	75,75,75,75	0
81	MG	1	3676	1/1	0.86	0.45	74,74,74,74	0
80	OHX	AR	3647	7/7	0.86	0.11	161,167,181,255	0
80	OHX	AR	4237	6/7	0.86	0.14	177,180,184,267	0
81	MG	4	230	1/1	0.86	0.27	86,86,86,86	0
80	OHX	AR	3582	7/7	0.86	0.12	136,142,154,237	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	CI	301	1/1	0.86	0.20	67,67,67,67	0
81	MG	AR	4095	1/1	0.86	0.32	64,64,64,64	0
80	OHX	1	4129	7/7	0.86	0.39	144,144,152,167	7
80	OHX	AR	3652	7/7	0.86	0.12	175,176,185,274	0
80	OHX	sR	2024	7/7	0.86	0.10	206,211,220,297	0
81	MG	1	4033	1/1	0.86	0.17	92,92,92,92	0
80	OHX	AS	228	7/7	0.86	0.15	171,178,181,280	0
80	OHX	AR	3692	7/7	0.86	0.10	203,206,212,293	0
80	OHX	1	3577	7/7	0.86	0.14	163,164,177,254	0
80	OHX	sR	2028	7/7	0.86	0.12	205,208,219,290	0
81	MG	AR	3809	1/1	0.86	0.38	44,44,44,44	0
81	MG	AR	4120	1/1	0.86	0.24	64,64,64,64	0
81	MG	v	304	1/1	0.86	0.49	68,68,68,68	0
80	OHX	A	1981	7/7	0.86	0.12	160,166,172,243	0
81	MG	A	2057	1/1	0.86	0.24	76,76,76,76	0
80	OHX	A	1944	7/7	0.86	0.15	175,178,181,252	0
81	MG	d6	204	1/1	0.86	0.42	73,73,73,73	0
81	MG	1	3713	1/1	0.86	0.30	68,68,68,68	0
80	OHX	AR	3604	7/7	0.86	0.14	139,143,155,226	0
81	MG	AR	3988	1/1	0.86	0.20	68,68,68,68	0
80	OHX	AR	3697	7/7	0.86	0.11	175,183,187,258	0
80	OHX	sR	2034	7/7	0.86	0.11	240,246,252,326	0
81	MG	AR	3991	1/1	0.86	0.28	66,66,66,66	0
81	MG	AR	4143	1/1	0.86	0.33	68,68,68,68	0
80	OHX	A	1955	7/7	0.86	0.16	124,135,143,204	0
81	MG	sR	2067	1/1	0.86	0.28	89,89,89,89	0
80	OHX	A	1936	7/7	0.87	0.11	226,232,241,299	0
81	MG	AR	4037	1/1	0.87	0.43	73,73,73,73	0
81	MG	AR	4038	1/1	0.87	0.17	75,75,75,75	0
80	OHX	sR	2012	7/7	0.87	0.12	164,173,182,258	0
81	MG	1	3733	1/1	0.87	0.20	45,45,45,45	0
80	OHX	1	3624	7/7	0.87	0.15	195,200,210,292	0
80	OHX	sR	2014	7/7	0.87	0.12	138,149,161,243	0
81	MG	1	3736	1/1	0.87	0.31	47,47,47,47	0
80	OHX	AR	3659	7/7	0.87	0.12	145,152,165,248	0
81	MG	AR	3866	1/1	0.87	0.27	46,46,46,46	0
81	MG	CX	202	1/1	0.87	0.27	43,43,43,43	0
81	MG	DO	202	1/1	0.87	0.28	84,84,84,84	0
81	MG	A	2074	1/1	0.87	0.07	80,80,80,80	0
81	MG	AR	3877	1/1	0.87	0.32	44,44,44,44	0
81	MG	sM	301	1/1	0.87	0.10	53,53,53,53	0
81	MG	AR	4062	1/1	0.87	0.18	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	3743	1/1	0.87	0.46	44,44,44,44	0
81	MG	sR	2038	1/1	0.87	0.21	56,56,56,56	0
81	MG	AR	3879	1/1	0.87	0.41	48,48,48,48	0
81	MG	t	203	1/1	0.87	0.24	61,61,61,61	0
81	MG	v	302	1/1	0.87	0.15	48,48,48,48	0
81	MG	sR	2047	1/1	0.87	0.28	65,65,65,65	0
81	MG	AR	4070	1/1	0.87	0.26	89,89,89,89	0
81	MG	1	3747	1/1	0.87	0.29	43,43,43,43	0
80	OHX	AR	3661	7/7	0.87	0.10	202,206,210,276	0
81	MG	1	3906	1/1	0.87	0.15	65,65,65,65	0
81	MG	v	306	1/1	0.87	0.33	69,69,69,69	0
81	MG	1	3907	1/1	0.87	0.22	64,64,64,64	0
80	OHX	1	3610	7/7	0.87	0.14	202,204,215,292	0
81	MG	1	3912	1/1	0.87	0.18	60,60,60,60	0
80	OHX	AR	3668	7/7	0.87	0.10	192,200,207,285	0
80	OHX	1	3639	7/7	0.87	0.10	182,190,202,287	0
81	MG	z	203	1/1	0.87	0.19	74,74,74,74	0
81	MG	1	4036	1/1	0.87	0.23	75,75,75,75	0
81	MG	1	3916	1/1	0.87	0.09	71,71,71,71	0
81	MG	1	3919	1/1	0.87	0.30	68,68,68,68	0
81	MG	1	3767	1/1	0.87	0.35	55,55,55,55	0
81	MG	A	1987	1/1	0.87	0.17	54,54,54,54	0
81	MG	AR	3922	1/1	0.87	0.23	61,61,61,61	0
81	MG	A	2036	1/1	0.87	0.07	105,105,105,105	0
81	MG	1	3774	1/1	0.87	0.27	48,48,48,48	0
81	MG	AR	3925	1/1	0.87	0.13	50,50,50,50	0
80	OHX	1	3540	7/7	0.87	0.12	141,147,164,239	0
81	MG	A	2040	1/1	0.87	0.25	65,65,65,65	0
81	MG	1	3665	1/1	0.87	0.18	50,50,50,50	0
81	MG	1	3666	1/1	0.87	0.21	74,74,74,74	0
80	OHX	CL	304	6/7	0.87	0.12	201,209,217,305	0
81	MG	1	3941	1/1	0.87	0.15	70,70,70,70	0
80	OHX	A	2142	7/7	0.87	0.10	251,253,256,315	0
81	MG	1	3785	1/1	0.87	0.24	61,61,61,61	0
81	MG	sR	2102	1/1	0.87	0.15	74,74,74,74	0
81	MG	AR	3729	1/1	0.87	0.27	64,64,64,64	0
81	MG	AR	3941	1/1	0.87	0.10	55,55,55,55	0
81	MG	1	3673	1/1	0.87	0.26	48,48,48,48	0
81	MG	1	3675	1/1	0.87	0.37	57,57,57,57	0
81	MG	AR	4133	1/1	0.87	0.33	68,68,68,68	0
80	OHX	1	4182	7/7	0.87	0.11	166,181,193,274	0
81	MG	1	4067	1/1	0.87	0.27	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	AR	3950	1/1	0.87	0.09	45,45,45,45	0
81	MG	AR	3951	1/1	0.87	0.14	47,47,47,47	0
81	MG	AR	3954	1/1	0.87	0.32	66,66,66,66	0
81	MG	AR	4144	1/1	0.87	0.20	72,72,72,72	0
81	MG	AR	3742	1/1	0.87	0.35	44,44,44,44	0
81	MG	sR	2125	1/1	0.87	0.21	77,77,77,77	0
80	OHX	AR	3639	7/7	0.87	0.13	168,180,188,268	0
81	MG	AR	4149	1/1	0.87	0.27	99,99,99,99	0
81	MG	1	3681	1/1	0.87	0.28	50,50,50,50	0
81	MG	A	2046	1/1	0.87	0.21	83,83,83,83	0
81	MG	AR	3963	1/1	0.87	0.12	51,51,51,51	0
81	MG	1	3685	1/1	0.87	0.20	62,62,62,62	0
81	MG	AR	3967	1/1	0.87	0.11	73,73,73,73	0
80	OHX	A	1940	7/7	0.87	0.15	160,164,170,240	0
81	MG	AR	4158	1/1	0.87	0.23	58,58,58,58	0
80	OHX	1	3605	7/7	0.87	0.10	174,187,197,271	0
81	MG	sR	2139	1/1	0.87	0.28	73,73,73,73	0
81	MG	sR	2142	1/1	0.87	0.27	65,65,65,65	0
81	MG	1	4083	1/1	0.87	0.25	69,69,69,69	0
81	MG	1	3689	1/1	0.87	0.24	65,65,65,65	0
81	MG	1	3962	1/1	0.87	0.29	75,75,75,75	0
81	MG	1	4088	1/1	0.87	0.37	75,75,75,75	0
81	MG	1	4089	1/1	0.87	0.28	59,59,59,59	0
80	OHX	1	4160	7/7	0.87	0.15	141,145,156,229	0
81	MG	A	2050	1/1	0.87	0.29	91,91,91,91	0
81	MG	A	2005	1/1	0.87	0.27	75,75,75,75	0
81	MG	AR	3773	1/1	0.87	0.25	45,45,45,45	0
80	OHX	AR	3592	7/7	0.87	0.16	156,160,166,259	0
81	MG	1	3840	1/1	0.87	0.10	49,49,49,49	0
81	MG	AR	4179	1/1	0.87	0.33	78,78,78,78	0
81	MG	1	4102	1/1	0.87	0.33	65,65,65,65	0
80	OHX	sR	1994	7/7	0.87	0.10	176,180,194,269	0
81	MG	1	3699	1/1	0.87	0.21	47,47,47,47	0
80	OHX	4	213	7/7	0.87	0.13	133,137,149,243	0
81	MG	A	2107	1/1	0.87	0.18	102,102,102,102	0
81	MG	1	3857	1/1	0.87	0.27	46,46,46,46	0
81	MG	1	4116	1/1	0.87	0.28	57,57,57,57	0
81	MG	1	4117	1/1	0.87	0.17	59,59,59,59	0
80	OHX	1	3617	7/7	0.87	0.14	136,143,154,249	0
80	OHX	sR	2174	7/7	0.87	0.14	182,188,190,270	0
81	MG	1	4121	1/1	0.87	0.21	68,68,68,68	0
80	OHX	4	215	7/7	0.87	0.13	149,153,165,254	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	3	213	1/1	0.87	0.12	73,73,73,73	0
81	MG	1	3715	1/1	0.87	0.43	71,71,71,71	0
81	MG	AR	3800	1/1	0.87	0.19	65,65,65,65	0
80	OHX	AR	3603	7/7	0.87	0.12	149,151,168,255	0
81	MG	AR	4215	1/1	0.87	0.11	73,73,73,73	0
81	MG	AR	4216	1/1	0.87	0.16	70,70,70,70	0
81	MG	1	3719	1/1	0.87	0.29	61,61,61,61	0
81	MG	4	216	1/1	0.87	0.37	78,78,78,78	0
81	MG	A	2014	1/1	0.87	0.27	68,68,68,68	0
81	MG	AR	4220	1/1	0.87	0.10	78,78,78,78	0
81	MG	AR	4018	1/1	0.87	0.29	69,69,69,69	0
80	OHX	sR	2006	7/7	0.87	0.12	182,185,191,264	0
82	K	AR	4239	1/1	0.87	0.10	79,79,79,79	0
80	OHX	1	4164	7/7	0.87	0.12	199,202,210,282	0
83	SPD	1	4106	10/10	0.87	0.20	45,45,45,46	0
83	SPD	AR	4200	10/10	0.87	0.18	47,50,53,53	0
81	MG	AS	216	1/1	0.87	0.12	68,68,68,68	0
81	MG	AR	4021	1/1	0.87	0.13	49,49,49,49	0
81	MG	AR	3834	1/1	0.87	0.23	46,46,46,46	0
80	OHX	1	3608	7/7	0.87	0.10	182,185,195,276	0
81	MG	4	223	1/1	0.87	0.24	54,54,54,54	0
81	MG	1	3878	1/1	0.87	0.13	91,91,91,91	0
81	MG	1	3879	1/1	0.87	0.19	52,52,52,52	0
81	MG	AT	221	1/1	0.88	0.26	60,60,60,60	0
81	MG	AR	3847	1/1	0.88	0.41	56,56,56,56	0
81	MG	AR	3849	1/1	0.88	0.30	43,43,43,43	0
81	MG	1	3756	1/1	0.88	0.28	46,46,46,46	0
80	OHX	1	3523	7/7	0.88	0.09	150,154,171,251	0
81	MG	1	4021	1/1	0.88	0.23	78,78,78,78	0
81	MG	CK	203	1/1	0.88	0.28	80,80,80,80	0
81	MG	1	3661	1/1	0.88	0.17	60,60,60,60	0
81	MG	AR	4044	1/1	0.88	0.14	59,59,59,59	0
81	MG	CO	201	1/1	0.88	0.20	71,71,71,71	0
81	MG	CP	303	1/1	0.88	0.13	63,63,63,63	0
81	MG	1	3762	1/1	0.88	0.23	42,42,42,42	0
81	MG	CR	206	1/1	0.88	0.31	76,76,76,76	0
81	MG	1	3662	1/1	0.88	0.33	69,69,69,69	0
81	MG	CU	201	1/1	0.88	0.32	76,76,76,76	0
80	OHX	sR	1981	7/7	0.88	0.12	139,142,157,250	0
80	OHX	AR	3600	7/7	0.88	0.13	148,151,156,243	0
81	MG	AR	4058	1/1	0.88	0.14	74,74,74,74	0
81	MG	AR	3870	1/1	0.88	0.29	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	4031	1/1	0.88	0.18	67,67,67,67	0
80	OHX	sR	1985	7/7	0.88	0.11	172,184,190,264	0
81	MG	A	2083	1/1	0.88	0.21	93,93,93,93	0
81	MG	1	4034	1/1	0.88	0.15	130,130,130,130	0
81	MG	sR	2039	1/1	0.88	0.18	74,74,74,74	0
81	MG	sR	2041	1/1	0.88	0.28	61,61,61,61	0
81	MG	AR	3882	1/1	0.88	0.35	50,50,50,50	0
81	MG	AR	3883	1/1	0.88	0.33	48,48,48,48	0
81	MG	A	2084	1/1	0.88	0.31	60,60,60,60	0
81	MG	x	203	1/1	0.88	0.34	85,85,85,85	0
81	MG	sR	2048	1/1	0.88	0.24	48,48,48,48	0
81	MG	1	3776	1/1	0.88	0.18	54,54,54,54	0
81	MG	AR	3894	1/1	0.88	0.22	42,42,42,42	0
80	OHX	1	3527	7/7	0.88	0.15	142,151,164,247	0
80	OHX	A	2144	7/7	0.88	0.12	154,166,173,250	0
81	MG	1	4043	1/1	0.88	0.17	60,60,60,60	0
81	MG	1	3926	1/1	0.88	0.32	87,87,87,87	0
81	MG	sR	2060	1/1	0.88	0.23	65,65,65,65	0
80	OHX	1	3548	7/7	0.88	0.16	123,135,140,234	0
80	OHX	AR	3662	7/7	0.88	0.11	180,188,199,273	0
81	MG	1	3678	1/1	0.88	0.25	46,46,46,46	0
81	MG	1	3679	1/1	0.88	0.13	88,88,88,88	0
80	OHX	AR	3663	7/7	0.88	0.14	142,144,150,247	0
81	MG	1	3935	1/1	0.88	0.47	73,73,73,73	0
81	MG	AR	3917	1/1	0.88	0.30	87,87,87,87	0
80	OHX	1	3550	7/7	0.88	0.12	168,173,178,258	0
81	MG	AR	3705	1/1	0.88	0.08	48,48,48,48	0
81	MG	AR	3706	1/1	0.88	0.16	60,60,60,60	0
81	MG	A	2091	1/1	0.88	0.38	52,52,52,52	0
81	MG	1	3799	1/1	0.88	0.22	47,47,47,47	0
80	OHX	AR	3616	7/7	0.88	0.13	133,143,159,245	0
80	OHX	1	4152	7/7	0.88	0.13	128,135,145,216	0
81	MG	AR	4109	1/1	0.88	0.22	60,60,60,60	0
80	OHX	A	2139	7/7	0.88	0.12	163,170,172,255	0
81	MG	AR	4116	1/1	0.88	0.16	69,69,69,69	0
81	MG	AR	4117	1/1	0.88	0.15	80,80,80,80	0
81	MG	AR	4118	1/1	0.88	0.24	63,63,63,63	0
80	OHX	c3	201	7/7	0.88	0.11	178,184,193,262	0
80	OHX	AR	3621	7/7	0.88	0.12	135,137,150,235	0
80	OHX	1	3592	7/7	0.88	0.13	146,153,160,241	0
80	OHX	AR	3630	7/7	0.88	0.11	155,162,173,263	0
81	MG	sR	2103	1/1	0.88	0.27	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	sR	2105	1/1	0.88	0.14	67,67,67,67	0
81	MG	sR	2106	1/1	0.88	0.16	54,54,54,54	0
81	MG	1	4073	1/1	0.88	0.25	56,56,56,56	0
81	MG	1	3951	1/1	0.88	0.12	60,60,60,60	0
81	MG	1	3954	1/1	0.88	0.18	92,92,92,92	0
81	MG	1	3821	1/1	0.88	0.27	64,64,64,64	0
81	MG	AR	3940	1/1	0.88	0.20	81,81,81,81	0
81	MG	AR	3740	1/1	0.88	0.22	61,61,61,61	0
80	OHX	1	3627	7/7	0.88	0.12	170,178,186,264	0
80	OHX	A	1970	7/7	0.88	0.11	216,219,227,283	0
81	MG	AR	3944	1/1	0.88	0.17	44,44,44,44	0
80	OHX	sR	2017	7/7	0.88	0.11	149,153,160,230	0
81	MG	AR	3746	1/1	0.88	0.24	65,65,65,65	0
81	MG	sR	2121	1/1	0.88	0.36	69,69,69,69	0
80	OHX	1	3559	7/7	0.88	0.13	109,119,135,217	0
81	MG	1	3703	1/1	0.88	0.20	67,67,67,67	0
81	MG	AR	3952	1/1	0.88	0.19	56,56,56,56	0
81	MG	AR	3753	1/1	0.88	0.25	71,71,71,71	0
81	MG	AR	3756	1/1	0.88	0.15	46,46,46,46	0
81	MG	AR	3757	1/1	0.88	0.25	58,58,58,58	0
81	MG	sR	2130	1/1	0.88	0.11	88,88,88,88	0
81	MG	1	3843	1/1	0.88	0.34	57,57,57,57	0
81	MG	1	3845	1/1	0.88	0.16	53,53,53,53	0
81	MG	1	4093	1/1	0.88	0.21	58,58,58,58	0
81	MG	1	3847	1/1	0.88	0.10	65,65,65,65	0
80	OHX	AG	201	7/7	0.88	0.12	123,127,137,227	0
81	MG	1	3706	1/1	0.88	0.40	68,68,68,68	0
81	MG	AR	4164	1/1	0.88	0.36	67,67,67,67	0
81	MG	1	4099	1/1	0.88	0.30	60,60,60,60	0
80	OHX	AR	3682	7/7	0.88	0.16	182,185,195,290	0
80	OHX	AR	3495	7/7	0.88	0.11	115,120,131,216	0
81	MG	A	2001	1/1	0.88	0.14	60,60,60,60	0
81	MG	AR	3975	1/1	0.88	0.42	62,62,62,62	0
80	OHX	AR	3684	7/7	0.88	0.11	145,151,162,250	0
81	MG	A	2003	1/1	0.88	0.40	77,77,77,77	0
80	OHX	A	1939	7/7	0.88	0.15	126,131,135,213	0
81	MG	1	3723	1/1	0.88	0.31	61,61,61,61	0
81	MG	1	4113	1/1	0.88	0.28	71,71,71,71	0
81	MG	1	3724	1/1	0.88	0.21	47,47,47,47	0
81	MG	A	2059	1/1	0.88	0.21	84,84,84,84	0
80	OHX	1	4171	5/7	0.88	0.13	141,142,146,234	0
81	MG	sR	2158	1/1	0.88	0.35	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	AT	211	7/7	0.88	0.12	138,144,152,234	0
80	OHX	A	2153	7/7	0.88	0.14	141,146,151,233	0
80	OHX	AT	215	7/7	0.88	0.11	160,168,176,267	0
80	OHX	1	3567	7/7	0.88	0.11	136,140,153,236	0
80	OHX	J	301	7/7	0.88	0.09	204,208,219,291	0
81	MG	3	216	1/1	0.88	0.09	72,72,72,72	0
81	MG	AR	4195	1/1	0.88	0.20	67,67,67,67	0
80	OHX	sR	2031	7/7	0.88	0.10	176,186,194,269	0
81	MG	sR	2171	1/1	0.88	0.38	73,73,73,73	0
81	MG	1	3998	1/1	0.88	0.15	98,98,98,98	0
81	MG	AR	3797	1/1	0.88	0.21	66,66,66,66	0
81	MG	AR	4202	1/1	0.88	0.31	48,48,48,48	0
81	MG	A	2013	1/1	0.88	0.32	57,57,57,57	0
80	OHX	A	1963	7/7	0.88	0.15	149,154,159,228	0
81	MG	AR	3801	1/1	0.88	0.22	45,45,45,45	0
81	MG	AR	3804	1/1	0.88	0.26	47,47,47,47	0
81	MG	1	4003	1/1	0.88	0.32	74,74,74,74	0
81	MG	A	2071	1/1	0.88	0.26	76,76,76,76	0
81	MG	AR	4005	1/1	0.88	0.12	69,69,69,69	0
81	MG	1	4007	1/1	0.88	0.24	51,51,51,51	0
81	MG	AR	4010	1/1	0.88	0.08	69,69,69,69	0
81	MG	d4	202	1/1	0.88	0.12	60,60,60,60	0
81	MG	AR	3816	1/1	0.88	0.36	56,56,56,56	0
81	MG	AR	3820	1/1	0.88	0.36	45,45,45,45	0
80	OHX	1	4178	7/7	0.88	0.15	116,118,124,173	7
80	OHX	AE	201	7/7	0.88	0.13	146,158,168,240	0
81	MG	1	4010	1/1	0.88	0.17	62,62,62,62	0
81	MG	AR	3833	1/1	0.88	0.29	42,42,42,42	0
81	MG	4	227	1/1	0.88	0.20	58,58,58,58	0
81	MG	4	228	1/1	0.88	0.17	64,64,64,64	0
81	MG	AR	3836	1/1	0.88	0.29	81,81,81,81	0
81	MG	AS	220	1/1	0.88	0.19	96,96,96,96	0
80	OHX	1	3521	7/7	0.88	0.14	140,143,151,231	0
81	MG	1	3749	1/1	0.88	0.32	49,49,49,49	0
81	MG	j	303	1/1	0.88	0.18	56,56,56,56	0
81	MG	1	3754	1/1	0.88	0.44	49,49,49,49	0
81	MG	AT	219	1/1	0.88	0.46	67,67,67,67	0
81	MG	k	401	1/1	0.89	0.20	53,53,53,53	0
80	OHX	AR	3577	7/7	0.89	0.13	137,139,143,229	0
80	OHX	AR	3676	7/7	0.89	0.10	152,168,179,259	0
81	MG	1	3842	1/1	0.89	0.07	53,53,53,53	0
81	MG	sR	2045	1/1	0.89	0.30	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	1	3618[A]	7/7	0.89	0.15	133,139,147,184	7
81	MG	1	3726	1/1	0.89	0.30	60,60,60,60	0
80	OHX	1	3618[B]	7/7	0.89	0.15	131,135,140,170	7
81	MG	AR	4127	1/1	0.89	0.15	72,72,72,72	0
81	MG	AR	3802	1/1	0.89	0.39	52,52,52,52	0
81	MG	1	3952	1/1	0.89	0.25	56,56,56,56	0
80	OHX	AR	3589	7/7	0.89	0.12	135,145,153,237	0
81	MG	sR	2057	1/1	0.89	0.32	77,77,77,77	0
80	OHX	sR	2007	7/7	0.89	0.12	173,178,184,260	0
81	MG	AR	3813	1/1	0.89	0.38	42,42,42,42	0
81	MG	AR	3814	1/1	0.89	0.26	43,43,43,43	0
81	MG	A	2029	1/1	0.89	0.26	63,63,63,63	0
81	MG	AR	4137	1/1	0.89	0.20	58,58,58,58	0
81	MG	1	4057	1/1	0.89	0.13	76,76,76,76	0
81	MG	1	3658	1/1	0.89	0.09	55,55,55,55	0
80	OHX	AR	4234	7/7	0.89	0.27	90,91,94,119	7
80	OHX	1	4141	7/7	0.89	0.17	85,88,99,175	0
81	MG	AR	3830	1/1	0.89	0.33	46,46,46,46	0
81	MG	1	3860	1/1	0.89	0.07	72,72,72,72	0
80	OHX	1	3596	7/7	0.89	0.10	169,180,185,268	0
80	OHX	s8	302	7/7	0.89	0.10	204,208,219,295	0
80	OHX	1	3518	7/7	0.89	0.11	123,129,140,220	0
81	MG	AR	4152	1/1	0.89	0.33	75,75,75,75	0
81	MG	sR	2087	1/1	0.89	0.35	65,65,65,65	0
81	MG	1	4071	1/1	0.89	0.30	45,45,45,45	0
81	MG	1	4072	1/1	0.89	0.31	48,48,48,48	0
80	OHX	A	1938	7/7	0.89	0.13	112,117,124,205	0
81	MG	1	3746	1/1	0.89	0.33	51,51,51,51	0
81	MG	A	2038	1/1	0.89	0.33	67,67,67,67	0
80	OHX	1	3555	7/7	0.89	0.10	150,163,168,254	0
81	MG	1	3669	1/1	0.89	0.36	68,68,68,68	0
81	MG	1	4081	1/1	0.89	0.21	54,54,54,54	0
81	MG	AR	3852	1/1	0.89	0.26	54,54,54,54	0
80	OHX	A	1960	7/7	0.89	0.09	171,176,186,255	0
81	MG	AR	4001	1/1	0.89	0.20	75,75,75,75	0
81	MG	AR	3703	1/1	0.89	0.18	45,45,45,45	0
81	MG	1	4084	1/1	0.89	0.25	51,51,51,51	0
81	MG	1	3755	1/1	0.89	0.27	43,43,43,43	0
80	OHX	1	3582	7/7	0.89	0.13	139,145,160,243	0
81	MG	1	3880	1/1	0.89	0.16	44,44,44,44	0
81	MG	AR	3711	1/1	0.89	0.21	47,47,47,47	0
80	OHX	1	3583	7/7	0.89	0.11	142,155,163,239	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	AR	4015	1/1	0.89	0.18	63,63,63,63	0
81	MG	AR	3875	1/1	0.89	0.23	47,47,47,47	0
81	MG	AR	3876	1/1	0.89	0.29	43,43,43,43	0
81	MG	sR	2117	1/1	0.89	0.20	70,70,70,70	0
81	MG	1	4091	1/1	0.89	0.35	61,61,61,61	0
81	MG	A	2093	1/1	0.89	0.31	60,60,60,60	0
81	MG	A	1994	1/1	0.89	0.19	78,78,78,78	0
81	MG	AR	3723	1/1	0.89	0.19	62,62,62,62	0
81	MG	1	3893	1/1	0.89	0.17	59,59,59,59	0
81	MG	sR	2123	1/1	0.89	0.17	79,79,79,79	0
80	OHX	AR	3605	7/7	0.89	0.11	107,114,123,223	0
81	MG	AR	4027	1/1	0.89	0.18	55,55,55,55	0
81	MG	AR	4028	1/1	0.89	0.28	68,68,68,68	0
81	MG	AR	4029	1/1	0.89	0.10	72,72,72,72	0
80	OHX	1	3584	7/7	0.89	0.10	136,139,152,232	0
81	MG	AR	3889	1/1	0.89	0.35	62,62,62,62	0
80	OHX	AR	3608	7/7	0.89	0.12	127,132,140,231	0
81	MG	AR	3731	1/1	0.89	0.25	62,62,62,62	0
81	MG	1	4100	1/1	0.89	0.18	65,65,65,65	0
81	MG	1	3770	1/1	0.89	0.24	46,46,46,46	0
81	MG	AR	3896	1/1	0.89	0.19	63,63,63,63	0
80	OHX	AR	3609	7/7	0.89	0.10	150,156,164,247	0
80	OHX	CK	202	7/7	0.89	0.10	166,171,179,257	0
81	MG	1	3903	1/1	0.89	0.14	54,54,54,54	0
81	MG	AR	3743	1/1	0.89	0.28	55,55,55,55	0
80	OHX	AR	3613	7/7	0.89	0.15	134,138,143,241	0
80	OHX	A	2127	7/7	0.89	0.12	162,169,178,245	0
80	OHX	1	3528	7/7	0.89	0.12	127,130,142,226	0
81	MG	AR	4222	1/1	0.89	0.23	50,50,50,50	0
80	OHX	sR	1952	7/7	0.89	0.09	190,195,203,270	0
81	MG	AR	4059	1/1	0.89	0.23	67,67,67,67	0
81	MG	sR	2151	1/1	0.89	0.29	83,83,83,83	0
81	MG	AS	215	1/1	0.89	0.14	66,66,66,66	0
81	MG	1	4114	1/1	0.89	0.51	67,67,67,67	0
80	OHX	1	3613	7/7	0.89	0.12	157,160,175,254	0
81	MG	1	3910	1/1	0.89	0.10	68,68,68,68	0
80	OHX	AR	3664	7/7	0.89	0.11	152,154,160,246	0
80	OHX	A	1950	7/7	0.89	0.12	172,183,183,255	0
81	MG	AR	4068	1/1	0.89	0.12	44,44,44,44	0
80	OHX	AR	3622	7/7	0.89	0.11	132,132,143,220	0
81	MG	1	3788	1/1	0.89	0.36	89,89,89,89	0
81	MG	AS	227	1/1	0.89	0.26	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
80	OHX	1	3544	7/7	0.89	0.15	137,140,143,228	0
80	OHX	1	3572	7/7	0.89	0.11	181,187,199,274	0
81	MG	AT	220	1/1	0.89	0.18	58,58,58,58	0
81	MG	D	301	1/1	0.89	0.25	71,71,71,71	0
80	OHX	sR	1986	7/7	0.89	0.13	149,157,169,239	0
81	MG	AR	3768	1/1	0.89	0.33	70,70,70,70	0
81	MG	CF	401	1/1	0.89	0.19	72,72,72,72	0
81	MG	1	3923	1/1	0.89	0.21	50,50,50,50	0
80	OHX	AR	3634	7/7	0.89	0.13	177,183,191,276	0
80	OHX	1	3507	7/7	0.89	0.15	103,111,115,204	0
81	MG	1	3711	1/1	0.89	0.17	73,73,73,73	0
81	MG	c1	201	1/1	0.89	0.28	83,83,83,83	0
81	MG	1	4030	1/1	0.89	0.16	59,59,59,59	0
80	OHX	sR	1995	7/7	0.89	0.10	172,174,177,256	0
81	MG	1	3813	1/1	0.89	0.29	49,49,49,49	0
81	MG	c8	201	1/1	0.89	0.12	70,70,70,70	0
81	MG	A	2016	1/1	0.89	0.29	56,56,56,56	0
81	MG	A	2017	1/1	0.89	0.28	60,60,60,60	0
81	MG	CQ	203	1/1	0.89	0.32	84,84,84,84	0
81	MG	CR	201	1/1	0.89	0.27	56,56,56,56	0
81	MG	CR	204	1/1	0.89	0.37	48,48,48,48	0
81	MG	1	3645	1/1	0.89	0.22	60,60,60,60	0
81	MG	1	3646	1/1	0.89	0.11	55,55,55,55	0
81	MG	d9	102	1/1	0.89	0.10	92,92,92,92	0
82	K	A	2160	1/1	0.89	0.23	103,103,103,103	0
81	MG	AR	4097	1/1	0.89	0.16	85,85,85,85	0
81	MG	AR	3785	1/1	0.89	0.33	66,66,66,66	0
81	MG	AR	3946	1/1	0.89	0.24	47,47,47,47	0
81	MG	1	3720	1/1	0.89	0.17	55,55,55,55	0
81	MG	DQ	205	1/1	0.89	0.19	53,53,53,53	0
80	OHX	sR	1997	7/7	0.89	0.10	218,222,230,297	0
81	MG	4	234	1/1	0.89	0.35	62,62,62,62	0
81	MG	AR	3789	1/1	0.89	0.14	55,55,55,55	0
81	MG	j	301	1/1	0.89	0.30	52,52,52,52	0
81	MG	AR	4111	1/1	0.89	0.19	54,54,54,54	0
81	MG	1	3722	1/1	0.89	0.17	58,58,58,58	0
81	MG	sR	2040	1/1	0.89	0.42	66,66,66,66	0
80	OHX	1	4169	7/7	0.90	0.09	195,201,204,268	0
80	OHX	sR	1972	7/7	0.90	0.11	122,134,139,211	0
81	MG	x	204	1/1	0.90	0.28	43,43,43,43	0
81	MG	1	3642	1/1	0.90	0.29	57,57,57,57	0
81	MG	CQ	201	1/1	0.90	0.18	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	3643	1/1	0.90	0.17	50,50,50,50	0
80	OHX	1	3551	7/7	0.90	0.11	194,196,198,260	0
80	OHX	sR	1974	7/7	0.90	0.12	123,129,133,209	0
81	MG	CR	205	1/1	0.90	0.17	41,41,41,41	0
80	OHX	sR	1977	7/7	0.90	0.11	143,147,160,220	0
80	OHX	A	1971	7/7	0.90	0.13	129,130,140,204	0
81	MG	1	3750	1/1	0.90	0.29	52,52,52,52	0
81	MG	1	3752	1/1	0.90	0.28	55,55,55,55	0
81	MG	DI	201	1/1	0.90	0.24	55,55,55,55	0
80	OHX	AR	3557	7/7	0.90	0.14	102,104,114,197	0
81	MG	DP	101	1/1	0.90	0.41	59,59,59,59	0
80	OHX	s4	301	7/7	0.90	0.11	154,162,171,245	0
80	OHX	AR	3566	7/7	0.90	0.13	122,131,146,210	0
81	MG	AR	3893	1/1	0.90	0.33	44,44,44,44	0
81	MG	1	3911	1/1	0.90	0.20	63,63,63,63	0
80	OHX	sR	1983	7/7	0.90	0.11	140,143,151,227	0
80	OHX	d4	201	7/7	0.90	0.10	170,172,175,257	0
81	MG	AR	4083	1/1	0.90	0.30	74,74,74,74	0
81	MG	AR	4084	1/1	0.90	0.11	71,71,71,71	0
80	OHX	AR	3571	7/7	0.90	0.11	106,110,118,207	0
81	MG	1	4054	1/1	0.90	0.12	73,73,73,73	0
81	MG	1	4055	1/1	0.90	0.10	63,63,63,63	0
81	MG	AR	4088	1/1	0.90	0.20	63,63,63,63	0
81	MG	AR	3710	1/1	0.90	0.26	58,58,58,58	0
81	MG	1	3764	1/1	0.90	0.13	49,49,49,49	0
81	MG	1	3917	1/1	0.90	0.17	69,69,69,69	0
81	MG	AR	3715	1/1	0.90	0.23	56,56,56,56	0
81	MG	AR	3716	1/1	0.90	0.11	44,44,44,44	0
81	MG	1	4058	1/1	0.90	0.21	63,63,63,63	0
81	MG	1	3918	1/1	0.90	0.30	60,60,60,60	0
81	MG	A	1984	1/1	0.90	0.17	63,63,63,63	0
81	MG	1	3657	1/1	0.90	0.34	63,63,63,63	0
80	OHX	A	2135	7/7	0.90	0.10	171,176,188,248	0
81	MG	1	4066	1/1	0.90	0.11	48,48,48,48	0
80	OHX	sR	1987	7/7	0.90	0.11	150,159,166,242	0
80	OHX	Q	201	7/7	0.90	0.10	190,194,196,261	0
80	OHX	sR	1993	7/7	0.90	0.11	138,143,154,226	0
81	MG	1	3927	1/1	0.90	0.30	88,88,88,88	0
81	MG	AR	4115	1/1	0.90	0.08	96,96,96,96	0
81	MG	A	2063	1/1	0.90	0.28	63,63,63,63	0
81	MG	A	1991	1/1	0.90	0.42	60,60,60,60	0
81	MG	AR	3739	1/1	0.90	0.24	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	sR	2070	1/1	0.90	0.16	68,68,68,68	0
80	OHX	1	4174	7/7	0.90	0.09	141,146,163,234	0
81	MG	AR	3934	1/1	0.90	0.21	65,65,65,65	0
81	MG	1	4075	1/1	0.90	0.37	69,69,69,69	0
81	MG	1	3779	1/1	0.90	0.35	61,61,61,61	0
81	MG	AR	4126	1/1	0.90	0.17	50,50,50,50	0
81	MG	sR	2080	1/1	0.90	0.29	62,62,62,62	0
80	OHX	1	3524	7/7	0.90	0.09	165,172,176,250	0
81	MG	sR	2086	1/1	0.90	0.39	57,57,57,57	0
80	OHX	1	4176	7/7	0.90	0.11	151,152,154,220	7
81	MG	1	3937	1/1	0.90	0.10	59,59,59,59	0
81	MG	A	2068	1/1	0.90	0.07	64,64,64,64	0
81	MG	sR	2090	1/1	0.90	0.30	53,53,53,53	0
81	MG	1	3670	1/1	0.90	0.12	61,61,61,61	0
81	MG	sR	2092	1/1	0.90	0.22	54,54,54,54	0
81	MG	sR	2093	1/1	0.90	0.20	100,100,100,100	0
81	MG	sR	2094	1/1	0.90	0.20	61,61,61,61	0
80	OHX	AR	3650	7/7	0.90	0.10	180,184,191,277	0
81	MG	AR	3754	1/1	0.90	0.31	45,45,45,45	0
81	MG	1	4086	1/1	0.90	0.23	68,68,68,68	0
81	MG	1	3787	1/1	0.90	0.34	45,45,45,45	0
81	MG	AR	4139	1/1	0.90	0.28	62,62,62,62	0
80	OHX	A	2136	7/7	0.90	0.12	147,150,153,231	0
81	MG	1	3674	1/1	0.90	0.18	50,50,50,50	0
80	OHX	1	3563	7/7	0.90	0.11	164,168,182,261	0
81	MG	1	3794	1/1	0.90	0.13	59,59,59,59	0
80	OHX	sR	2004	7/7	0.90	0.12	144,147,154,241	0
81	MG	1	3796	1/1	0.90	0.22	57,57,57,57	0
80	OHX	1	4179	7/7	0.90	0.09	199,203,215,280	0
81	MG	AR	3957	1/1	0.90	0.19	45,45,45,45	0
81	MG	AR	3767	1/1	0.90	0.20	46,46,46,46	0
81	MG	AR	3959	1/1	0.90	0.20	59,59,59,59	0
81	MG	1	3801	1/1	0.90	0.19	44,44,44,44	0
80	OHX	AR	3596	7/7	0.90	0.12	156,157,164,247	0
80	OHX	AR	3655	7/7	0.90	0.14	116,123,132,226	0
81	MG	A	2076	1/1	0.90	0.17	64,64,64,64	0
80	OHX	1	3477	7/7	0.90	0.12	201,208,214,305	0
81	MG	AR	3969	1/1	0.90	0.13	57,57,57,57	0
81	MG	AR	4160	1/1	0.90	0.38	63,63,63,63	0
81	MG	AR	4161	1/1	0.90	0.24	45,45,45,45	0
81	MG	AR	3970	1/1	0.90	0.38	75,75,75,75	0
80	OHX	AR	3599	7/7	0.90	0.09	158,166,176,250	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	1	4181	7/7	0.90	0.15	135,137,149,230	0
81	MG	1	3816	1/1	0.90	0.38	53,53,53,53	0
80	OHX	AR	3660	7/7	0.90	0.08	174,186,191,259	0
80	OHX	1	3491	7/7	0.90	0.12	118,121,125,208	0
80	OHX	3	204	7/7	0.90	0.12	143,145,149,222	0
81	MG	AR	4171	1/1	0.90	0.21	44,44,44,44	0
80	OHX	1	3569	7/7	0.90	0.11	131,132,138,228	0
81	MG	AR	3784	1/1	0.90	0.26	47,47,47,47	0
81	MG	sR	2133	1/1	0.90	0.18	71,71,71,71	0
81	MG	1	4115	1/1	0.90	0.19	53,53,53,53	0
80	OHX	1	3591	7/7	0.90	0.13	142,150,156,234	0
81	MG	1	3833	1/1	0.90	0.10	52,52,52,52	0
80	OHX	AR	3666	7/7	0.90	0.09	199,203,204,272	0
80	OHX	1	4139	7/7	0.90	0.14	97,102,111,190	0
81	MG	sR	2141	1/1	0.90	0.10	57,57,57,57	0
80	OHX	4	210	7/7	0.90	0.12	112,118,124,222	0
80	OHX	1	3571	7/7	0.90	0.13	161,163,170,260	0
81	MG	A	2018	1/1	0.90	0.28	55,55,55,55	0
81	MG	AR	3794	1/1	0.90	0.37	76,76,76,76	0
81	MG	3	214	1/1	0.90	0.16	61,61,61,61	0
81	MG	1	3844	1/1	0.90	0.25	44,44,44,44	0
81	MG	1	3702	1/1	0.90	0.19	63,63,63,63	0
80	OHX	AR	3612	7/7	0.90	0.16	116,120,128,220	0
81	MG	1	3849	1/1	0.90	0.29	63,63,63,63	0
80	OHX	AS	208	7/7	0.90	0.12	113,117,119,196	0
81	MG	sR	2153	1/1	0.90	0.20	83,83,83,83	0
81	MG	A	2022	1/1	0.90	0.23	66,66,66,66	0
81	MG	AR	3803	1/1	0.90	0.31	41,41,41,41	0
80	OHX	AR	3671	7/7	0.90	0.10	151,158,167,246	0
81	MG	AR	3808	1/1	0.90	0.15	52,52,52,52	0
80	OHX	1	3501	7/7	0.90	0.10	120,131,141,235	0
80	OHX	1	3622	7/7	0.90	0.15	141,144,149,232	0
81	MG	AR	3812	1/1	0.90	0.17	52,52,52,52	0
80	OHX	AR	3674	7/7	0.90	0.09	221,231,236,302	0
81	MG	1	3716	1/1	0.90	0.20	48,48,48,48	0
81	MG	1	3861	1/1	0.90	0.13	57,57,57,57	0
80	OHX	1	3573	7/7	0.90	0.11	137,139,146,218	0
81	MG	1	3864	1/1	0.90	0.32	89,89,89,89	0
81	MG	4	229	1/1	0.90	0.24	62,62,62,62	0
81	MG	sR	2170	1/1	0.90	0.17	48,48,48,48	0
81	MG	AR	3827	1/1	0.90	0.33	58,58,58,58	0
81	MG	sR	2172	1/1	0.90	0.17	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	A	2101	1/1	0.90	0.24	72,72,72,72	0
81	MG	1	4006	1/1	0.90	0.27	62,62,62,62	0
81	MG	4	233	1/1	0.90	0.11	56,56,56,56	0
81	MG	AS	214	1/1	0.90	0.39	45,45,45,45	0
80	OHX	1	3547	7/7	0.90	0.14	133,143,159,227	0
80	OHX	A	1964	7/7	0.90	0.09	149,157,163,232	0
81	MG	1	3869	1/1	0.90	0.23	64,64,64,64	0
80	OHX	CG	302	7/7	0.90	0.09	160,163,174,248	0
80	OHX	1	4162	7/7	0.90	0.12	109,118,135,226	0
80	OHX	AR	3623	7/7	0.90	0.09	167,181,184,248	0
80	OHX	CL	302	7/7	0.90	0.11	133,140,150,237	0
80	OHX	1	3517	7/7	0.90	0.10	163,170,175,242	0
80	OHX	AR	3681	7/7	0.90	0.10	179,182,192,267	0
81	MG	AR	4035	1/1	0.90	0.19	62,62,62,62	0
81	MG	AT	216	1/1	0.90	0.20	61,61,61,61	0
81	MG	AT	217	1/1	0.90	0.22	51,51,51,51	0
80	OHX	1	4166	7/7	0.90	0.10	147,159,171,247	0
81	MG	t	201	1/1	0.90	0.12	65,65,65,65	0
80	OHX	sR	1951	7/7	0.90	0.13	117,124,127,196	0
81	MG	DA	201	1/1	0.90	0.18	71,71,71,71	0
81	MG	AT	222	1/1	0.90	0.14	86,86,86,86	0
81	MG	AT	225	1/1	0.90	0.11	52,52,52,52	0
81	MG	AT	226	1/1	0.90	0.31	78,78,78,78	0
81	MG	AR	3857	1/1	0.90	0.34	45,45,45,45	0
80	OHX	1	3604	7/7	0.90	0.12	136,139,153,235	0
85	ZN	c	101	1/1	0.90	0.07	188,188,188,188	0
81	MG	1	3889	1/1	0.90	0.17	79,79,79,79	0
81	MG	CF	402	1/1	0.90	0.20	64,64,64,64	0
81	MG	1	3890	1/1	0.90	0.29	65,65,65,65	0
80	OHX	sR	1961	7/7	0.90	0.15	111,118,132,209	0
81	MG	AR	4050	1/1	0.90	0.17	65,65,65,65	0
81	MG	A	2043	1/1	0.90	0.17	57,57,57,57	0
81	MG	AR	3867	1/1	0.90	0.36	48,48,48,48	0
81	MG	AR	3987	1/1	0.91	0.18	51,51,51,51	0
80	OHX	1	3601	7/7	0.91	0.10	143,151,161,251	0
81	MG	AR	4148	1/1	0.91	0.23	63,63,63,63	0
81	MG	sR	2053	1/1	0.91	0.28	52,52,52,52	0
81	MG	1	3959	1/1	0.91	0.09	55,55,55,55	0
81	MG	1	3858	1/1	0.91	0.21	56,56,56,56	0
80	OHX	sR	2022	7/7	0.91	0.10	145,148,156,245	0
80	OHX	1	3508	7/7	0.91	0.11	114,116,123,202	0
80	OHX	h	401	7/7	0.91	0.09	175,176,182,249	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	4078	1/1	0.91	0.38	54,54,54,54	0
80	OHX	1	3516	7/7	0.91	0.11	115,122,134,216	0
81	MG	sR	2063	1/1	0.91	0.20	60,60,60,60	0
81	MG	1	4080	1/1	0.91	0.22	56,56,56,56	0
80	OHX	S	201	7/7	0.91	0.11	161,163,165,233	0
80	OHX	sR	1959	7/7	0.91	0.10	125,133,142,228	0
80	OHX	AR	3601	7/7	0.91	0.12	119,128,136,223	0
81	MG	AR	3709	1/1	0.91	0.23	65,65,65,65	0
80	OHX	A	1969	7/7	0.91	0.10	155,157,167,235	0
81	MG	AR	3855	1/1	0.91	0.29	42,42,42,42	0
80	OHX	sR	1966	7/7	0.91	0.09	98,102,117,190	0
80	OHX	1	3606	7/7	0.91	0.11	152,154,160,238	0
81	MG	AR	4009	1/1	0.91	0.20	64,64,64,64	0
81	MG	sR	2076	1/1	0.91	0.31	58,58,58,58	0
81	MG	AR	4168	1/1	0.91	0.20	59,59,59,59	0
80	OHX	1	3607	7/7	0.91	0.13	151,153,164,243	0
81	MG	1	3873	1/1	0.91	0.17	67,67,67,67	0
81	MG	sR	2085	1/1	0.91	0.21	52,52,52,52	0
81	MG	1	4090	1/1	0.91	0.18	74,74,74,74	0
81	MG	AR	3718	1/1	0.91	0.15	52,52,52,52	0
81	MG	1	3758	1/1	0.91	0.28	45,45,45,45	0
81	MG	1	3668	1/1	0.91	0.24	53,53,53,53	0
80	OHX	1	3519	7/7	0.91	0.12	117,121,128,206	0
80	OHX	AR	3658	7/7	0.91	0.11	146,152,164,250	0
80	OHX	sR	1978	7/7	0.91	0.13	137,140,150,226	0
81	MG	1	3989	1/1	0.91	0.11	100,100,100,100	0
81	MG	AR	4181	1/1	0.91	0.16	62,62,62,62	0
81	MG	1	3765	1/1	0.91	0.31	46,46,46,46	0
80	OHX	CE	402	7/7	0.91	0.10	150,157,168,244	0
81	MG	AR	3733	1/1	0.91	0.20	43,43,43,43	0
81	MG	1	3882	1/1	0.91	0.11	45,45,45,45	0
80	OHX	A	1937	7/7	0.91	0.11	143,147,152,220	0
81	MG	AR	3884	1/1	0.91	0.08	44,44,44,44	0
81	MG	AR	3886	1/1	0.91	0.08	50,50,50,50	0
81	MG	AR	3736	1/1	0.91	0.26	48,48,48,48	0
81	MG	sR	2104	1/1	0.91	0.23	70,70,70,70	0
81	MG	1	3885	1/1	0.91	0.27	61,61,61,61	0
81	MG	AR	4197	1/1	0.91	0.12	61,61,61,61	0
81	MG	1	3995	1/1	0.91	0.39	60,60,60,60	0
81	MG	AR	4199	1/1	0.91	0.22	52,52,52,52	0
81	MG	1	3888	1/1	0.91	0.10	68,68,68,68	0
80	OHX	AR	3494	7/7	0.91	0.14	96,106,111,202	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	1	3635	7/7	0.91	0.07	233,239,246,309	0
80	OHX	1	3479	7/7	0.91	0.12	94,98,109,178	0
81	MG	AR	4208	1/1	0.91	0.28	85,85,85,85	0
81	MG	AR	4209	1/1	0.91	0.15	64,64,64,64	0
80	OHX	AR	3615	7/7	0.91	0.09	140,156,161,232	0
81	MG	AR	3897	1/1	0.91	0.24	58,58,58,58	0
80	OHX	AR	3665	7/7	0.91	0.10	158,162,176,252	0
80	OHX	sR	1989	7/7	0.91	0.12	136,151,153,225	0
81	MG	AR	3748	1/1	0.91	0.16	44,44,44,44	0
81	MG	AR	4051	1/1	0.91	0.13	51,51,51,51	0
80	OHX	sR	2185	6/7	0.91	0.09	150,154,156,253	0
80	OHX	AR	3523	7/7	0.91	0.11	73,82,109,172	0
81	MG	1	3899	1/1	0.91	0.14	88,88,88,88	0
80	OHX	sR	1992	7/7	0.91	0.11	125,129,133,208	0
81	MG	AR	3909	1/1	0.91	0.19	67,67,67,67	0
80	OHX	1	3482	7/7	0.91	0.12	121,125,138,208	0
81	MG	AR	4063	1/1	0.91	0.34	76,76,76,76	0
81	MG	3	208	1/1	0.91	0.17	70,70,70,70	0
81	MG	3	212	1/1	0.91	0.22	61,61,61,61	0
80	OHX	AR	3619	7/7	0.91	0.11	146,151,156,234	0
81	MG	1	4013	1/1	0.91	0.19	56,56,56,56	0
80	OHX	AR	3535	7/7	0.91	0.13	98,102,109,199	0
81	MG	AR	3921	1/1	0.91	0.21	45,45,45,45	0
81	MG	1	3691	1/1	0.91	0.14	64,64,64,64	0
80	OHX	Rb	401	7/7	0.91	0.09	223,226,233,295	0
81	MG	sR	2140	1/1	0.91	0.11	76,76,76,76	0
81	MG	AS	222	1/1	0.91	0.12	66,66,66,66	0
81	MG	A	2102	1/1	0.91	0.44	67,67,67,67	0
81	MG	1	3908	1/1	0.91	0.11	72,72,72,72	0
81	MG	AS	226	1/1	0.91	0.21	54,54,54,54	0
80	OHX	1	3487	7/7	0.91	0.14	98,105,111,183	0
81	MG	1	3790	1/1	0.91	0.38	45,45,45,45	0
80	OHX	AR	3545	7/7	0.91	0.11	125,129,136,222	0
81	MG	1	3697	1/1	0.91	0.26	44,44,44,44	0
81	MG	1	3698	1/1	0.91	0.24	48,48,48,48	0
80	OHX	sR	2000	7/7	0.91	0.09	131,134,139,217	0
81	MG	1	3915	1/1	0.91	0.32	51,51,51,51	0
80	OHX	AR	3554	7/7	0.91	0.09	116,119,127,220	0
81	MG	AT	223	1/1	0.91	0.11	62,62,62,62	0
81	MG	1	3800	1/1	0.91	0.29	46,46,46,46	0
80	OHX	AR	3555	7/7	0.91	0.12	103,112,116,201	0
81	MG	AR	3782	1/1	0.91	0.43	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	4035	1/1	0.91	0.21	125,125,125,125	0
81	MG	4	231	1/1	0.91	0.08	71,71,71,71	0
81	MG	A	1983	1/1	0.91	0.28	54,54,54,54	0
80	OHX	1	3568	7/7	0.91	0.10	132,134,148,217	0
80	OHX	AR	3631	7/7	0.91	0.10	110,111,123,205	0
80	OHX	1	3529	7/7	0.91	0.12	124,130,135,222	0
80	OHX	1	3570	7/7	0.91	0.13	107,114,121,196	0
80	OHX	A	2140	7/7	0.91	0.10	150,158,169,240	0
81	MG	AR	4104	1/1	0.91	0.20	71,71,71,71	0
81	MG	A	1990	1/1	0.91	0.11	59,59,59,59	0
81	MG	CP	301	1/1	0.91	0.09	56,56,56,56	0
81	MG	AB	201	1/1	0.91	0.16	61,61,61,61	0
81	MG	AR	3793	1/1	0.91	0.12	44,44,44,44	0
81	MG	AB	203	1/1	0.91	0.22	70,70,70,70	0
81	MG	o	301	1/1	0.91	0.09	59,59,59,59	0
80	OHX	A	1961	7/7	0.91	0.10	198,203,209,275	0
81	MG	CR	203	1/1	0.91	0.26	60,60,60,60	0
81	MG	A	1992	1/1	0.91	0.19	58,58,58,58	0
81	MG	AR	3798	1/1	0.91	0.19	49,49,49,49	0
81	MG	1	3824	1/1	0.91	0.28	44,44,44,44	0
81	MG	A	2055	1/1	0.91	0.09	79,79,79,79	0
81	MG	CE	403	1/1	0.91	0.38	43,43,43,43	0
80	OHX	sR	2010	7/7	0.91	0.11	152,162,171,238	0
80	OHX	1	4143	7/7	0.91	0.12	100,102,110,173	0
81	MG	c9	201	1/1	0.91	0.14	78,78,78,78	0
81	MG	DL	101	1/1	0.91	0.28	63,63,63,63	0
81	MG	AR	4124	1/1	0.91	0.36	104,104,104,104	0
81	MG	d3	203	1/1	0.91	0.22	52,52,52,52	0
80	OHX	1	3506	7/7	0.91	0.12	88,102,123,192	0
80	OHX	3	205	7/7	0.91	0.11	134,140,144,214	0
81	MG	A	1998	1/1	0.91	0.26	60,60,60,60	0
80	OHX	1	3620	7/7	0.91	0.10	191,194,202,277	0
81	MG	DR	503	1/1	0.91	0.18	84,84,84,84	0
81	MG	1	3647	1/1	0.91	0.16	48,48,48,48	0
81	MG	sM	302	1/1	0.91	0.10	66,66,66,66	0
81	MG	x	201	1/1	0.91	0.30	66,66,66,66	0
81	MG	x	202	1/1	0.91	0.30	55,55,55,55	0
80	OHX	sR	2015	7/7	0.91	0.09	199,205,206,265	0
81	MG	1	3848	1/1	0.91	0.18	69,69,69,69	0
81	MG	AR	3817	1/1	0.91	0.25	43,43,43,43	0
80	OHX	1	4154	7/7	0.91	0.12	119,129,131,211	0
80	OHX	A	1954	7/7	0.91	0.11	134,141,151,226	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	AR	4140	1/1	0.91	0.13	66,66,66,66	0
81	MG	AR	3826	1/1	0.91	0.16	54,54,54,54	0
80	OHX	AR	3646	7/7	0.91	0.12	129,137,143,238	0
80	OHX	AR	3595	7/7	0.91	0.11	111,118,125,220	0
80	OHX	CS	202	7/7	0.91	0.11	115,118,120,214	0
81	MG	x	206	1/1	0.92	0.27	62,62,62,62	0
80	OHX	AR	3572	7/7	0.92	0.08	133,134,146,237	0
81	MG	AR	3818	1/1	0.92	0.32	50,50,50,50	0
81	MG	sR	2051	1/1	0.92	0.19	59,59,59,59	0
81	MG	AR	4147	1/1	0.92	0.23	67,67,67,67	0
80	OHX	sR	1967	7/7	0.92	0.12	121,127,130,195	0
80	OHX	A	1932	7/7	0.92	0.10	131,138,144,207	0
81	MG	AR	3984	1/1	0.92	0.26	69,69,69,69	0
81	MG	AR	3823	1/1	0.92	0.16	44,44,44,44	0
80	OHX	AR	3640	7/7	0.92	0.10	132,145,152,221	0
81	MG	6	201	1/1	0.92	0.31	52,52,52,52	0
80	OHX	1	3509	7/7	0.92	0.13	127,129,132,220	0
81	MG	6	203	1/1	0.92	0.22	56,56,56,56	0
81	MG	1	3867	1/1	0.92	0.14	56,56,56,56	0
80	OHX	1	4157	7/7	0.92	0.10	141,147,156,217	0
81	MG	1	3963	1/1	0.92	0.29	61,61,61,61	0
80	OHX	AR	3643	7/7	0.92	0.10	125,127,132,234	0
81	MG	1	3870	1/1	0.92	0.32	69,69,69,69	0
81	MG	AR	3837	1/1	0.92	0.19	51,51,51,51	0
80	OHX	A	2134	7/7	0.92	0.10	139,143,147,223	0
80	OHX	1	3626	7/7	0.92	0.10	136,142,151,224	0
81	MG	1	3969	1/1	0.92	0.14	61,61,61,61	0
81	MG	1	4082	1/1	0.92	0.25	45,45,45,45	0
81	MG	AR	4002	1/1	0.92	0.11	59,59,59,59	0
80	OHX	A	1935	7/7	0.92	0.10	144,148,159,224	0
80	OHX	A	1953	7/7	0.92	0.09	199,202,208,257	0
81	MG	1	3973	1/1	0.92	0.16	45,45,45,45	0
80	OHX	A	2148	7/7	0.92	0.11	152,157,161,236	0
81	MG	AR	4007	1/1	0.92	0.19	58,58,58,58	0
81	MG	1	3684	1/1	0.92	0.23	50,50,50,50	0
81	MG	AR	4176	1/1	0.92	0.20	49,49,49,49	0
81	MG	AR	3712	1/1	0.92	0.31	50,50,50,50	0
81	MG	AR	3856	1/1	0.92	0.33	60,60,60,60	0
81	MG	AR	4013	1/1	0.92	0.15	66,66,66,66	0
81	MG	AR	3713	1/1	0.92	0.26	47,47,47,47	0
80	OHX	1	4165	7/7	0.92	0.11	124,134,141,228	0
81	MG	1	3979	1/1	0.92	0.17	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	AR	3861	1/1	0.92	0.30	50,50,50,50	0
80	OHX	1	3581	7/7	0.92	0.08	172,178,182,250	0
80	OHX	sR	1988	7/7	0.92	0.08	142,148,158,230	0
81	MG	A	2103	1/1	0.92	0.37	78,78,78,78	0
81	MG	1	3984	1/1	0.92	0.16	53,53,53,53	0
80	OHX	A	2151	7/7	0.92	0.11	109,109,115,188	0
81	MG	AR	4024	1/1	0.92	0.28	66,66,66,66	0
80	OHX	AR	3598	7/7	0.92	0.09	115,119,120,203	0
81	MG	AR	3872	1/1	0.92	0.42	55,55,55,55	0
80	OHX	A	1979	7/7	0.92	0.11	123,126,134,199	0
80	OHX	y	201	7/7	0.92	0.10	104,109,116,191	0
80	OHX	1	3562	7/7	0.92	0.13	148,153,161,236	0
80	OHX	c8	202	7/7	0.92	0.09	137,139,147,219	0
81	MG	AR	4203	1/1	0.92	0.28	63,63,63,63	0
80	OHX	A	1914	7/7	0.92	0.14	116,119,122,179	0
81	MG	1	3892	1/1	0.92	0.25	66,66,66,66	0
80	OHX	sR	1996	7/7	0.92	0.11	137,144,148,221	0
81	MG	A	1982	1/1	0.92	0.19	65,65,65,65	0
80	OHX	AP	502	7/7	0.92	0.15	113,119,123,219	0
81	MG	F	301	1/1	0.92	0.16	71,71,71,71	0
81	MG	O	202	1/1	0.92	0.32	71,71,71,71	0
81	MG	AR	4214	1/1	0.92	0.28	80,80,80,80	0
81	MG	1	3898	1/1	0.92	0.11	45,45,45,45	0
81	MG	AR	3890	1/1	0.92	0.08	49,49,49,49	0
81	MG	AR	3741	1/1	0.92	0.24	43,43,43,43	0
81	MG	1	3793	1/1	0.92	0.35	46,46,46,46	0
80	OHX	A	1917	7/7	0.92	0.12	104,109,118,181	0
80	OHX	1	3566	7/7	0.92	0.10	139,145,151,225	0
81	MG	1	4118	1/1	0.92	0.12	69,69,69,69	0
81	MG	AR	4056	1/1	0.92	0.12	72,72,72,72	0
81	MG	1	3902	1/1	0.92	0.14	64,64,64,64	0
80	OHX	1	3588	7/7	0.92	0.11	121,128,143,232	0
81	MG	AS	211	1/1	0.92	0.34	53,53,53,53	0
81	MG	AR	3898	1/1	0.92	0.10	55,55,55,55	0
80	OHX	AR	3508	7/7	0.92	0.13	92,99,103,182	0
81	MG	AR	3751	1/1	0.92	0.27	53,53,53,53	0
80	OHX	A	2156	6/7	0.92	0.10	148,153,160,224	0
81	MG	1	4190	1/1	0.92	0.14	46,46,46,46	0
81	MG	3	207	1/1	0.92	0.11	58,58,58,58	0
80	OHX	AR	3611	7/7	0.92	0.12	124,132,136,234	0
81	MG	3	210	1/1	0.92	0.18	51,51,51,51	0
81	MG	3	211	1/1	0.92	0.34	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	AR	3759	1/1	0.92	0.21	42,42,42,42	0
81	MG	1	4011	1/1	0.92	0.23	104,104,104,104	0
81	MG	AS	225	1/1	0.92	0.37	54,54,54,54	0
80	OHX	A	1923	7/7	0.92	0.11	121,123,130,200	0
80	OHX	AR	3533	7/7	0.92	0.14	99,107,112,196	0
81	MG	1	4014	1/1	0.92	0.12	53,53,53,53	0
81	MG	AR	4077	1/1	0.92	0.17	54,54,54,54	0
80	OHX	AR	3614	7/7	0.92	0.14	106,115,119,216	0
81	MG	AR	3765	1/1	0.92	0.14	61,61,61,61	0
81	MG	1	3808	1/1	0.92	0.16	43,43,43,43	0
80	OHX	1	3640	7/7	0.92	0.11	116,117,123,199	0
81	MG	1	3812	1/1	0.92	0.09	54,54,54,54	0
80	OHX	1	3538	7/7	0.92	0.10	117,118,137,217	0
81	MG	AR	3926	1/1	0.92	0.21	60,60,60,60	0
81	MG	1	4022	1/1	0.92	0.17	58,58,58,58	0
80	OHX	AR	3617	7/7	0.92	0.11	123,127,133,229	0
80	OHX	AT	209	7/7	0.92	0.11	117,129,131,219	0
80	OHX	A	2118	7/7	0.92	0.13	102,109,115,156	0
80	OHX	AR	3546	7/7	0.92	0.13	86,91,100,170	0
80	OHX	AR	3549	7/7	0.92	0.11	105,115,127,220	0
80	OHX	1	3595	7/7	0.92	0.10	107,114,127,200	0
80	OHX	A	1958	7/7	0.92	0.11	161,162,166,238	0
80	OHX	A	2131	7/7	0.92	0.10	148,152,156,217	0
81	MG	sR	2167	1/1	0.92	0.19	65,65,65,65	0
81	MG	1	3830	1/1	0.92	0.10	48,48,48,48	0
81	MG	1	3729	1/1	0.92	0.13	47,47,47,47	0
81	MG	1	3925	1/1	0.92	0.31	57,57,57,57	0
81	MG	1	3835	1/1	0.92	0.15	49,49,49,49	0
80	OHX	AR	3625	7/7	0.92	0.10	129,136,146,231	0
81	MG	1	3731	1/1	0.92	0.18	46,46,46,46	0
81	MG	sR	2175	1/1	0.92	0.32	75,75,75,75	0
81	MG	s1	302	1/1	0.92	0.12	93,93,93,93	0
80	OHX	AR	3560	7/7	0.92	0.11	132,137,143,216	0
81	MG	CQ	202	1/1	0.92	0.21	66,66,66,66	0
81	MG	1	3841	1/1	0.92	0.08	51,51,51,51	0
81	MG	AR	4110	1/1	0.92	0.10	67,67,67,67	0
80	OHX	AR	3629	7/7	0.92	0.10	165,169,178,249	0
81	MG	AR	4113	1/1	0.92	0.16	73,73,73,73	0
81	MG	1	3933	1/1	0.92	0.08	79,79,79,79	0
81	MG	1	404	1/1	0.92	0.14	62,62,62,62	0
80	OHX	AR	3564	7/7	0.92	0.14	98,104,115,204	0
80	OHX	3	203	7/7	0.92	0.12	120,127,138,207	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	CU	202	1/1	0.92	0.20	52,52,52,52	0
80	OHX	AR	3632	7/7	0.92	0.10	119,120,130,221	0
81	MG	DH	203	1/1	0.92	0.10	59,59,59,59	0
81	MG	1	3938	1/1	0.92	0.27	58,58,58,58	0
81	MG	d3	202	1/1	0.92	0.30	60,60,60,60	0
80	OHX	sR	1902	7/7	0.92	0.10	106,113,115,207	0
81	MG	1	3940	1/1	0.92	0.32	66,66,66,66	0
80	OHX	sR	1920	7/7	0.92	0.15	73,81,96,138	0
81	MG	AR	3961	1/1	0.92	0.22	58,58,58,58	0
80	OHX	sR	1941	7/7	0.92	0.11	115,116,123,186	0
81	MG	1	3850	1/1	0.92	0.20	95,95,95,95	0
81	MG	1	3745	1/1	0.92	0.22	45,45,45,45	0
80	OHX	AR	3567	7/7	0.92	0.09	137,141,143,222	0
80	OHX	AR	3568	7/7	0.92	0.10	124,126,133,222	0
81	MG	AR	3805	1/1	0.92	0.33	43,43,43,43	0
81	MG	AR	3807	1/1	0.92	0.16	41,41,41,41	0
80	OHX	sR	1956	7/7	0.92	0.11	137,140,149,206	0
84	VDU	AR	4255	26/26	0.92	0.13	55,59,60,63	0
81	MG	AR	4135	1/1	0.92	0.47	66,66,66,66	0
80	OHX	AR	3570	7/7	0.92	0.09	121,124,129,219	0
80	OHX	AR	3686	7/7	0.92	0.08	203,207,211,278	0
81	MG	AR	3811	1/1	0.92	0.20	42,42,42,42	0
81	MG	1	4062	1/1	0.92	0.11	63,63,63,63	0
81	MG	1	3751	1/1	0.92	0.26	44,44,44,44	0
80	OHX	1	3621	7/7	0.92	0.11	147,162,174,255	0
81	MG	1	3953	1/1	0.92	0.10	69,69,69,69	0
81	MG	1	3648	1/1	0.93	0.20	46,46,46,46	0
80	OHX	sR	1971	7/7	0.93	0.09	126,132,138,213	0
81	MG	1	4098	1/1	0.93	0.34	61,61,61,61	0
80	OHX	1	3511	7/7	0.93	0.10	115,120,125,213	0
81	MG	sR	2056	1/1	0.93	0.15	66,66,66,66	0
81	MG	1	3875	1/1	0.93	0.25	51,51,51,51	0
81	MG	AR	3727	1/1	0.93	0.13	54,54,54,54	0
80	OHX	AR	3548	7/7	0.93	0.10	101,106,116,198	0
80	OHX	1	3513	7/7	0.93	0.11	94,96,102,179	0
80	OHX	sR	1976	7/7	0.93	0.12	102,116,122,196	0
81	MG	1	4104	1/1	0.93	0.37	47,47,47,47	0
80	OHX	A	1908	7/7	0.93	0.14	76,88,98,141	0
80	OHX	1	3599	7/7	0.93	0.08	152,161,181,256	0
81	MG	AR	4017	1/1	0.93	0.28	73,73,73,73	0
80	OHX	sR	1979	7/7	0.93	0.12	96,98,106,188	0
81	MG	sR	2068	1/1	0.93	0.24	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	4111	1/1	0.93	0.24	48,48,48,48	0
80	OHX	AR	3556	7/7	0.93	0.12	96,98,112,208	0
81	MG	1	3883	1/1	0.93	0.35	57,57,57,57	0
80	OHX	1	3600	7/7	0.93	0.09	135,137,147,228	0
80	OHX	A	2150	7/7	0.93	0.11	131,132,136,208	0
81	MG	1	3887	1/1	0.93	0.20	69,69,69,69	0
80	OHX	AR	3561	7/7	0.93	0.11	131,135,139,223	0
80	OHX	AR	3633	7/7	0.93	0.11	124,127,131,216	0
81	MG	1	3999	1/1	0.93	0.12	69,69,69,69	0
81	MG	sR	2081	1/1	0.93	0.16	49,49,49,49	0
81	MG	sR	2082	1/1	0.93	0.22	60,60,60,60	0
81	MG	AR	4184	1/1	0.93	0.11	44,44,44,44	0
80	OHX	AR	3563	7/7	0.93	0.09	128,131,137,223	0
81	MG	A	1986	1/1	0.93	0.34	72,72,72,72	0
80	OHX	A	1925	7/7	0.93	0.11	134,138,141,203	0
81	MG	AR	3750	1/1	0.93	0.23	48,48,48,48	0
80	OHX	AR	3565	7/7	0.93	0.11	103,107,118,198	0
81	MG	AR	4192	1/1	0.93	0.28	51,51,51,51	0
81	MG	AR	4036	1/1	0.93	0.25	63,63,63,63	0
80	OHX	3	202	7/7	0.93	0.11	113,117,122,193	0
81	MG	1	3773	1/1	0.93	0.17	63,63,63,63	0
81	MG	3	209	1/1	0.93	0.33	57,57,57,57	0
80	OHX	A	2152	7/7	0.93	0.08	137,140,145,227	0
80	OHX	sR	1991	7/7	0.93	0.10	154,160,166,232	0
81	MG	AR	4042	1/1	0.93	0.29	80,80,80,80	0
80	OHX	1	3463	7/7	0.93	0.12	75,85,87,154	0
81	MG	1	3671	1/1	0.93	0.20	56,56,56,56	0
81	MG	AR	4204	1/1	0.93	0.23	58,58,58,58	0
80	OHX	AR	3700[A]	7/7	0.93	0.16	129,131,135,157	7
81	MG	AR	3902	1/1	0.93	0.16	63,63,63,63	0
80	OHX	AR	3700[B]	7/7	0.93	0.16	127,130,136,157	7
80	OHX	1	3467	7/7	0.93	0.13	96,105,108,179	0
81	MG	AR	4052	1/1	0.93	0.28	95,95,95,95	0
80	OHX	1	3468	7/7	0.93	0.11	64,80,91,152	0
81	MG	AR	4055	1/1	0.93	0.12	57,57,57,57	0
81	MG	AR	3906	1/1	0.93	0.22	64,64,64,64	0
81	MG	1	4017	1/1	0.93	0.25	66,66,66,66	0
81	MG	4	202	1/1	0.93	0.12	70,70,70,70	0
81	MG	A	2078	1/1	0.93	0.26	67,67,67,67	0
81	MG	AR	4060	1/1	0.93	0.11	53,53,53,53	0
80	OHX	A	1926	7/7	0.93	0.10	159,160,164,234	0
80	OHX	A	1927	7/7	0.93	0.11	100,106,111,186	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	A	2082	1/1	0.93	0.09	60,60,60,60	0
81	MG	1	3680	1/1	0.93	0.26	61,61,61,61	0
81	MG	AR	4065	1/1	0.93	0.12	67,67,67,67	0
81	MG	AR	4253	1/1	0.93	0.12	105,105,105,105	0
80	OHX	AR	3574	7/7	0.93	0.11	107,111,118,206	0
80	OHX	AR	3575	7/7	0.93	0.12	105,107,115,192	0
80	OHX	A	1928	7/7	0.93	0.11	124,129,131,197	0
81	MG	4	226	1/1	0.93	0.11	56,56,56,56	0
80	OHX	1	3531	7/7	0.93	0.10	106,115,119,204	0
80	OHX	AR	3579	7/7	0.93	0.10	151,153,158,245	0
81	MG	AR	4073	1/1	0.93	0.20	50,50,50,50	0
81	MG	1	3687	1/1	0.93	0.32	63,63,63,63	0
81	MG	1	3797	1/1	0.93	0.32	48,48,48,48	0
80	OHX	AR	3649	7/7	0.93	0.09	105,107,123,211	0
80	OHX	AR	3580	7/7	0.93	0.10	117,123,126,198	0
80	OHX	1	3535	7/7	0.93	0.13	93,100,106,193	0
81	MG	sR	2135	1/1	0.93	0.28	51,51,51,51	0
80	OHX	AR	3583	7/7	0.93	0.10	93,95,102,186	0
81	MG	4	235	1/1	0.93	0.31	51,51,51,51	0
80	OHX	1	3536	7/7	0.93	0.10	130,135,141,220	0
80	OHX	AR	3590	7/7	0.93	0.10	104,111,116,200	0
81	MG	AT	202	1/1	0.93	0.14	80,80,80,80	0
80	OHX	1	3537	7/7	0.93	0.13	118,122,123,206	0
81	MG	1	3695	1/1	0.93	0.34	73,73,73,73	0
80	OHX	A	1911	7/7	0.93	0.12	88,92,101,141	0
80	OHX	1	3539	7/7	0.93	0.11	92,98,107,192	0
80	OHX	AR	3594	7/7	0.93	0.12	108,113,119,196	0
80	OHX	1	3488	7/7	0.93	0.13	87,93,99,163	0
80	OHX	AT	205	7/7	0.93	0.13	94,100,106,175	0
80	OHX	1	3542	7/7	0.93	0.09	119,120,131,204	0
81	MG	AT	224	1/1	0.93	0.12	78,78,78,78	0
80	OHX	AT	210	7/7	0.93	0.10	109,113,127,204	0
80	OHX	A	1959	7/7	0.93	0.11	125,136,139,203	0
80	OHX	1	4163	7/7	0.93	0.08	164,172,184,254	0
81	MG	1	3827	1/1	0.93	0.31	42,42,42,42	0
80	OHX	AK	104	7/7	0.93	0.13	83,85,90,153	0
81	MG	1	3709	1/1	0.93	0.36	44,44,44,44	0
81	MG	A	2024	1/1	0.93	0.24	60,60,60,60	0
80	OHX	1	3499	7/7	0.93	0.10	126,136,137,202	0
81	MG	1	3837	1/1	0.93	0.62	81,81,81,81	0
81	MG	AR	3806	1/1	0.93	0.35	44,44,44,44	0
81	MG	sR	2161	1/1	0.93	0.37	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	CG	303	7/7	0.93	0.08	204,205,214,286	0
80	OHX	A	1933	7/7	0.93	0.10	133,136,141,220	0
81	MG	AR	3960	1/1	0.93	0.06	69,69,69,69	0
80	OHX	1	3549	7/7	0.93	0.09	148,149,162,227	0
80	OHX	AR	3500	7/7	0.93	0.11	73,84,96,151	0
81	MG	1	4064	1/1	0.93	0.14	44,44,44,44	0
80	OHX	AR	3503	7/7	0.93	0.13	119,121,126,213	0
81	MG	AR	3965	1/1	0.93	0.29	60,60,60,60	0
81	MG	AR	3966	1/1	0.93	0.16	72,72,72,72	0
80	OHX	1	3503	7/7	0.93	0.09	114,123,133,226	0
81	MG	CR	202	1/1	0.93	0.34	61,61,61,61	0
80	OHX	A	1947	7/7	0.93	0.10	141,146,151,214	0
80	OHX	DQ	203	7/7	0.93	0.14	118,125,138,230	0
80	OHX	AR	3607	7/7	0.93	0.11	99,112,121,213	0
80	OHX	AR	3514	7/7	0.93	0.11	98,100,110,192	0
80	OHX	AR	3516	7/7	0.93	0.12	81,91,95,186	0
80	OHX	sR	1915	7/7	0.93	0.10	121,122,129,200	0
81	MG	AB	202	1/1	0.93	0.12	59,59,59,59	0
80	OHX	AR	3519	7/7	0.93	0.12	103,115,124,198	0
81	MG	DH	201	1/1	0.93	0.13	58,58,58,58	0
81	MG	AR	4130	1/1	0.93	0.15	60,60,60,60	0
81	MG	1	3958	1/1	0.93	0.28	69,69,69,69	0
80	OHX	sR	2176	7/7	0.93	0.11	134,139,142,220	0
80	OHX	1	3553	7/7	0.93	0.10	128,139,145,211	0
81	MG	AK	105	1/1	0.93	0.16	88,88,88,88	0
80	OHX	AR	3526	7/7	0.93	0.10	118,124,132,206	0
81	MG	DQ	204	1/1	0.93	0.22	74,74,74,74	0
81	MG	CD	302	1/1	0.93	0.12	64,64,64,64	0
80	OHX	A	1974	7/7	0.93	0.08	171,173,180,255	0
80	OHX	A	1934	7/7	0.93	0.09	156,157,162,228	0
81	MG	1	3965	1/1	0.93	0.09	47,47,47,47	0
81	MG	CE	405	1/1	0.93	0.24	71,71,71,71	0
81	MG	d6	202	1/1	0.93	0.37	53,53,53,53	0
81	MG	AR	3839	1/1	0.93	0.46	67,67,67,67	0
81	MG	sR	2036	1/1	0.93	0.32	55,55,55,55	0
81	MG	AR	3840	1/1	0.93	0.24	54,54,54,54	0
81	MG	AF	201	1/1	0.93	0.27	66,66,66,66	0
81	MG	1	3863	1/1	0.93	0.25	56,56,56,56	0
81	MG	1	3737	1/1	0.93	0.15	50,50,50,50	0
81	MG	AR	3845	1/1	0.93	0.39	58,58,58,58	0
81	MG	1	3739	1/1	0.93	0.38	57,57,57,57	0
80	OHX	A	1922	7/7	0.93	0.10	126,131,141,205	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	AR	3848	1/1	0.93	0.34	53,53,53,53	0
80	OHX	AR	3536	7/7	0.93	0.11	114,121,129,219	0
81	MG	sR	2046	1/1	0.93	0.19	76,76,76,76	0
80	OHX	sR	1962	7/7	0.93	0.12	98,105,113,190	0
80	OHX	1	3594	7/7	0.93	0.11	131,131,138,195	0
81	MG	AR	3853	1/1	0.93	0.36	44,44,44,44	0
80	OHX	AR	3544	7/7	0.93	0.10	129,135,141,193	0
80	OHX	1	3557	7/7	0.93	0.12	89,96,101,181	0
81	MG	AR	3749	1/1	0.94	0.23	53,53,53,53	0
81	MG	1	4191	1/1	0.94	0.10	84,84,84,84	0
81	MG	1	4193	1/1	0.94	0.07	98,98,98,98	0
80	OHX	AR	3624	7/7	0.94	0.08	136,143,148,231	0
80	OHX	sR	1975	7/7	0.94	0.10	113,118,125,200	0
80	OHX	1	3476	7/7	0.94	0.11	80,90,93,157	0
80	OHX	A	1942	7/7	0.94	0.10	113,118,126,211	0
80	OHX	AR	3628	7/7	0.94	0.09	116,121,128,204	0
80	OHX	4	208	7/7	0.94	0.09	94,100,113,207	0
80	OHX	4	209	7/7	0.94	0.09	101,107,115,200	0
80	OHX	1	3552	7/7	0.94	0.08	123,126,139,217	0
81	MG	sR	2077	1/1	0.94	0.18	61,61,61,61	0
81	MG	A	2079	1/1	0.94	0.08	68,68,68,68	0
81	MG	sR	2079	1/1	0.94	0.18	53,53,53,53	0
80	OHX	1	4156	6/7	0.94	0.12	119,125,131,202	0
80	OHX	A	1973	7/7	0.94	0.13	89,93,102,132	0
80	OHX	A	1916	7/7	0.94	0.10	111,117,125,180	0
80	OHX	1	4159	7/7	0.94	0.09	159,165,170,242	0
81	MG	sR	2084	1/1	0.94	0.29	64,64,64,64	0
81	MG	AR	4049	1/1	0.94	0.11	63,63,63,63	0
80	OHX	k	402	7/7	0.94	0.10	101,105,108,190	0
80	OHX	k	403	7/7	0.94	0.11	107,108,121,189	0
80	OHX	A	1918	7/7	0.94	0.10	108,110,117,180	0
81	MG	1	4027	1/1	0.94	0.17	44,44,44,44	0
80	OHX	A	1946	7/7	0.94	0.10	160,162,165,221	0
81	MG	AR	3912	1/1	0.94	0.13	47,47,47,47	0
80	OHX	r	304	7/7	0.94	0.12	77,86,94,146	0
81	MG	AR	3914	1/1	0.94	0.09	59,59,59,59	0
80	OHX	1	3490	7/7	0.94	0.13	91,97,103,183	0
81	MG	AR	3774	1/1	0.94	0.15	44,44,44,44	0
80	OHX	1	3558	7/7	0.94	0.08	146,151,156,222	0
81	MG	1	3803	1/1	0.94	0.24	48,48,48,48	0
80	OHX	1	3525	7/7	0.94	0.09	124,133,135,201	0
80	OHX	A	1930	7/7	0.94	0.11	114,118,127,199	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	AR	3779	1/1	0.94	0.43	59,59,59,59	0
80	OHX	AR	3576	7/7	0.94	0.08	132,137,144,224	0
81	MG	1	3809	1/1	0.94	0.31	44,44,44,44	0
80	OHX	A	1924	7/7	0.94	0.12	103,107,114,189	0
81	MG	1	4038	1/1	0.94	0.11	67,67,67,67	0
81	MG	AR	4252	1/1	0.94	0.08	89,89,89,89	0
81	MG	1	3924	1/1	0.94	0.05	87,87,87,87	0
80	OHX	1	4167	7/7	0.94	0.10	153,159,161,214	0
81	MG	1	4042	1/1	0.94	0.12	47,47,47,47	0
81	MG	AS	212	1/1	0.94	0.25	45,45,45,45	0
81	MG	AS	213	1/1	0.94	0.20	61,61,61,61	0
80	OHX	sR	1999	7/7	0.94	0.12	120,126,135,203	0
81	MG	1	4044	1/1	0.94	0.10	68,68,68,68	0
81	MG	1	3814	1/1	0.94	0.23	45,45,45,45	0
80	OHX	AR	3441	7/7	0.94	0.12	68,77,86,133	0
80	OHX	AR	3443	7/7	0.94	0.17	55,76,91,116	0
80	OHX	AR	3475	7/7	0.94	0.11	60,80,83,142	0
80	OHX	AR	3488	7/7	0.94	0.11	75,82,90,153	0
80	OHX	AS	204	7/7	0.94	0.12	72,86,101,161	0
80	OHX	AS	205	7/7	0.94	0.12	95,99,109,186	0
80	OHX	AR	3585	7/7	0.94	0.10	114,121,130,209	0
81	MG	1	3707	1/1	0.94	0.21	53,53,53,53	0
81	MG	1	3708	1/1	0.94	0.16	44,44,44,44	0
80	OHX	AR	3586	7/7	0.94	0.11	87,93,99,180	0
80	OHX	AR	3587	7/7	0.94	0.09	135,138,144,213	0
81	MG	AR	4089	1/1	0.94	0.33	76,76,76,76	0
80	OHX	AR	3588	7/7	0.94	0.08	109,112,127,212	0
81	MG	AR	3949	1/1	0.94	0.29	53,53,53,53	0
80	OHX	AR	3493	7/7	0.94	0.12	76,79,93,152	0
80	OHX	1	3434	7/7	0.94	0.17	66,77,86,118	0
80	OHX	AT	206	7/7	0.94	0.11	87,88,95,175	0
80	OHX	AT	208	7/7	0.94	0.10	98,100,111,190	0
80	OHX	1	3451	7/7	0.94	0.12	86,95,98,155	0
81	MG	1	4063	1/1	0.94	0.12	64,64,64,64	0
80	OHX	AR	3496	7/7	0.94	0.11	81,92,97,184	0
81	MG	A	2166	1/1	0.94	0.10	98,98,98,98	0
80	OHX	1	3565	7/7	0.94	0.09	113,116,130,199	0
80	OHX	AR	3502	7/7	0.94	0.14	80,92,96,156	0
80	OHX	AT	214	7/7	0.94	0.08	144,151,159,238	0
80	OHX	1	3534	7/7	0.94	0.09	147,148,154,228	0
80	OHX	1	3504	7/7	0.94	0.11	89,94,100,195	0
80	OHX	1	3505	7/7	0.94	0.09	118,122,129,209	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	AR	3509	7/7	0.94	0.10	118,125,128,183	0
81	MG	A	2033	1/1	0.94	0.20	72,72,72,72	0
81	MG	1	3853	1/1	0.94	0.09	57,57,57,57	0
81	MG	CL	303	1/1	0.94	0.25	47,47,47,47	0
80	OHX	AR	3511	7/7	0.94	0.12	74,88,100,192	0
80	OHX	A	1919	7/7	0.94	0.10	131,137,141,211	0
81	MG	8	203	1/1	0.94	0.08	112,112,112,112	0
81	MG	AR	3824	1/1	0.94	0.23	51,51,51,51	0
81	MG	AR	3825	1/1	0.94	0.37	42,42,42,42	0
81	MG	9	201	1/1	0.94	0.13	59,59,59,59	0
81	MG	AR	4123	1/1	0.94	0.12	48,48,48,48	0
80	OHX	1	3464	7/7	0.94	0.15	67,84,88,142	0
81	MG	A	2037	1/1	0.94	0.15	55,55,55,55	0
80	OHX	A	1951	7/7	0.94	0.08	138,140,151,221	0
80	OHX	A	1920	7/7	0.94	0.11	115,115,120,179	0
81	MG	AR	3832	1/1	0.94	0.30	42,42,42,42	0
80	OHX	1	3541	7/7	0.94	0.10	97,99,102,179	0
80	OHX	AR	3528	7/7	0.94	0.09	87,98,103,171	0
81	MG	sR	2165	1/1	0.94	0.12	81,81,81,81	0
81	MG	AF	202	1/1	0.94	0.09	59,59,59,59	0
80	OHX	1	3510	7/7	0.94	0.12	126,128,136,212	0
80	OHX	sR	1901	7/7	0.94	0.12	122,126,134,226	0
81	MG	AR	3838	1/1	0.94	0.30	51,51,51,51	0
80	OHX	AR	3530	7/7	0.94	0.10	72,81,95,174	0
81	MG	AR	3986	1/1	0.94	0.13	95,95,95,95	0
81	MG	1	3744	1/1	0.94	0.13	45,45,45,45	0
81	MG	1	3974	1/1	0.94	0.07	56,56,56,56	0
80	OHX	1	3543	7/7	0.94	0.08	154,157,164,235	0
80	OHX	1	3469	7/7	0.94	0.13	73,76,85,144	0
80	OHX	sR	1929	7/7	0.94	0.12	102,103,107,160	0
80	OHX	sR	1933	7/7	0.94	0.12	86,95,100,143	0
81	MG	AR	3993	1/1	0.94	0.09	78,78,78,78	0
80	OHX	1	3546	7/7	0.94	0.08	126,135,144,215	0
81	MG	1	4095	1/1	0.94	0.20	46,46,46,46	0
80	OHX	sR	1944	7/7	0.94	0.10	96,101,105,164	0
80	OHX	sR	1950	7/7	0.94	0.08	114,121,126,204	0
81	MG	c4	2202	1/1	0.94	0.14	51,51,51,51	0
80	OHX	1	3473	7/7	0.94	0.11	90,91,95,156	0
80	OHX	AR	3539	7/7	0.94	0.08	95,100,111,177	0
80	OHX	sR	1954	7/7	0.94	0.10	86,97,100,171	0
80	OHX	sR	1955	7/7	0.94	0.09	155,157,160,228	0
81	MG	1	3757	1/1	0.94	0.23	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	AR	3725	1/1	0.94	0.27	54,54,54,54	0
80	OHX	AR	3540	7/7	0.94	0.10	102,108,118,186	0
80	OHX	AR	3541	7/7	0.94	0.09	110,115,121,194	0
81	MG	A	2058	1/1	0.94	0.13	61,61,61,61	0
80	OHX	AR	3542	7/7	0.94	0.12	89,96,98,190	0
80	OHX	1	3612	7/7	0.94	0.12	75,85,91,168	0
80	OHX	1	3514	7/7	0.94	0.10	122,126,131,208	0
81	MG	AR	4011	1/1	0.94	0.15	46,46,46,46	0
80	OHX	sR	1964	7/7	0.94	0.10	130,137,141,228	0
81	MG	1	3663	1/1	0.94	0.17	54,54,54,54	0
81	MG	1	3768	1/1	0.94	0.49	46,46,46,46	0
80	OHX	1	3515	7/7	0.94	0.11	130,137,146,221	0
81	MG	AR	3873	1/1	0.94	0.38	47,47,47,47	0
81	MG	1	4000	1/1	0.94	0.11	66,66,66,66	0
80	OHX	1	4149	7/7	0.94	0.09	92,96,105,179	0
80	OHX	sR	1969	7/7	0.94	0.11	96,104,109,190	0
84	VDU	1	4195	26/26	0.94	0.11	55,57,59,64	0
80	OHX	sR	1970	7/7	0.94	0.12	114,115,130,191	0
81	MG	AR	4173	1/1	0.94	0.10	71,71,71,71	0
80	OHX	c5	201	7/7	0.94	0.08	172,174,183,246	0
80	OHX	3	219	7/7	0.94	0.12	109,114,123,194	0
81	MG	1	4184	1/1	0.94	0.16	55,55,55,55	0
81	MG	1	4185	1/1	0.94	0.17	71,71,71,71	0
80	OHX	AR	3550	7/7	0.94	0.10	109,113,120,207	0
80	OHX	AR	3551	7/7	0.94	0.11	103,112,115,193	0
81	MG	AR	3887	1/1	0.94	0.09	80,80,80,80	0
80	OHX	A	2124	7/7	0.95	0.10	96,99,108,179	0
81	MG	1	4005	1/1	0.95	0.08	66,66,66,66	0
80	OHX	sR	1922	7/7	0.95	0.13	95,98,104,137	0
81	MG	AR	4032	1/1	0.95	0.26	71,71,71,71	0
81	MG	AR	4185	1/1	0.95	0.41	66,66,66,66	0
81	MG	AR	4033	1/1	0.95	0.13	63,63,63,63	0
80	OHX	sR	1925	7/7	0.95	0.11	91,94,104,144	0
81	MG	sR	2073	1/1	0.95	0.20	45,45,45,45	0
80	OHX	AR	3517	7/7	0.95	0.09	88,98,100,182	0
80	OHX	A	2125	7/7	0.95	0.14	82,91,95,145	0
80	OHX	sR	1940	7/7	0.95	0.10	95,101,110,172	0
80	OHX	AR	3521	7/7	0.95	0.11	80,90,96,173	0
80	OHX	sR	1942	7/7	0.95	0.13	66,79,85,153	0
81	MG	AR	3900	1/1	0.95	0.06	59,59,59,59	0
80	OHX	sR	1943	7/7	0.95	0.10	106,110,110,170	0
80	OHX	AR	3522	7/7	0.95	0.09	94,98,106,189	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	sR	1947	7/7	0.95	0.09	102,106,110,198	0
80	OHX	1	3475	7/7	0.95	0.09	95,100,109,169	0
80	OHX	AR	3524	7/7	0.95	0.10	83,87,101,164	0
80	OHX	sR	2183	7/7	0.95	0.22	97,99,100,132	7
80	OHX	AR	3525	7/7	0.95	0.09	91,94,99,188	0
80	OHX	sR	1953	7/7	0.95	0.08	132,134,138,203	0
81	MG	4	220	1/1	0.95	0.11	43,43,43,43	0
80	OHX	A	1931	7/7	0.95	0.10	97,101,109,166	0
80	OHX	A	1945	7/7	0.95	0.10	119,123,125,192	0
80	OHX	A	1915	7/7	0.95	0.10	96,103,110,172	0
80	OHX	sR	1958	7/7	0.95	0.10	98,102,109,169	0
81	MG	AR	3916	1/1	0.95	0.19	50,50,50,50	0
80	OHX	AR	3610	7/7	0.95	0.11	92,99,103,190	0
80	OHX	sR	1960	7/7	0.95	0.09	112,113,121,178	0
81	MG	1	3786	1/1	0.95	0.40	45,45,45,45	0
80	OHX	1	3520[A]	7/7	0.95	0.14	92,97,103,130	7
80	OHX	AR	3532	7/7	0.95	0.10	72,81,88,180	0
80	OHX	1	3520[B]	7/7	0.95	0.14	88,92,97,109	7
80	OHX	1	3561	7/7	0.95	0.12	122,129,134,221	0
80	OHX	sR	1965	7/7	0.95	0.10	114,117,125,195	0
80	OHX	1	4109	7/7	0.95	0.12	93,95,99,171	0
80	OHX	3	220	7/7	0.95	0.12	93,98,111,160	0
81	MG	AR	3927	1/1	0.95	0.18	77,77,77,77	0
81	MG	AR	4251	1/1	0.95	0.04	98,98,98,98	0
80	OHX	sR	1968	7/7	0.95	0.09	103,111,114,193	0
80	OHX	1	3480	7/7	0.95	0.10	89,94,97,173	0
80	OHX	1	4137	7/7	0.95	0.10	105,108,111,169	0
80	OHX	1	3522	7/7	0.95	0.09	105,107,120,195	0
80	OHX	1	4140	7/7	0.95	0.13	84,88,92,156	0
80	OHX	1	3417	7/7	0.95	0.18	78,88,96,110	0
81	MG	l	405	1/1	0.95	0.09	53,53,53,53	0
81	MG	sR	2115	1/1	0.95	0.08	70,70,70,70	0
80	OHX	4	211	7/7	0.95	0.07	140,145,157,230	0
80	OHX	4	212	7/7	0.95	0.08	132,138,144,226	0
81	MG	1	3804	1/1	0.95	0.34	49,49,49,49	0
80	OHX	AR	3547	7/7	0.95	0.10	95,97,107,195	0
80	OHX	1	4142	7/7	0.95	0.16	69,74,87,114	0
80	OHX	1	3484	7/7	0.95	0.11	92,98,108,166	0
81	MG	A	1993	1/1	0.95	0.08	58,58,58,58	0
80	OHX	AR	3627	7/7	0.95	0.08	155,160,167,237	0
81	MG	sR	2124	1/1	0.95	0.06	61,61,61,61	0
80	OHX	1	4144	7/7	0.95	0.08	86,94,100,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	1	3486	7/7	0.95	0.11	94,102,107,189	0
80	OHX	AR	3552	7/7	0.95	0.11	93,99,106,195	0
81	MG	AR	3948	1/1	0.95	0.37	72,72,72,72	0
81	MG	1	3932	1/1	0.95	0.15	57,57,57,57	0
80	OHX	A	2133	7/7	0.95	0.10	124,127,132,198	0
80	OHX	sR	1984	7/7	0.95	0.09	106,112,116,181	0
81	MG	1	3817	1/1	0.95	0.25	63,63,63,63	0
81	MG	AR	3953	1/1	0.95	0.14	53,53,53,53	0
80	OHX	1	3440	7/7	0.95	0.11	73,76,82,133	0
80	OHX	1	4153	7/7	0.95	0.11	90,92,106,169	0
80	OHX	1	3441	7/7	0.95	0.11	93,95,107,146	0
81	MG	1	3705	1/1	0.95	0.21	64,64,64,64	0
81	MG	AR	4102	1/1	0.95	0.23	45,45,45,45	0
81	MG	AR	4103	1/1	0.95	0.14	80,80,80,80	0
81	MG	1	3823	1/1	0.95	0.08	64,64,64,64	0
80	OHX	AR	3558	7/7	0.95	0.10	93,97,102,163	0
81	MG	1	3825	1/1	0.95	0.33	43,43,43,43	0
81	MG	A	2004	1/1	0.95	0.24	55,55,55,55	0
80	OHX	AR	3559	7/7	0.95	0.10	85,87,96,178	0
80	OHX	1	3530	7/7	0.95	0.09	99,100,102,183	0
81	MG	1	3831	1/1	0.95	0.11	44,44,44,44	0
81	MG	sR	2147	1/1	0.95	0.22	57,57,57,57	0
81	MG	1	3832	1/1	0.95	0.19	45,45,45,45	0
81	MG	CI	302	1/1	0.95	0.10	57,57,57,57	0
81	MG	8	201	1/1	0.95	0.19	80,80,80,80	0
81	MG	1	3710	1/1	0.95	0.13	46,46,46,46	0
80	OHX	v	301	7/7	0.95	0.09	102,109,116,203	0
80	OHX	1	3443	7/7	0.95	0.12	91,101,105,163	0
80	OHX	1	3532	7/7	0.95	0.10	94,96,102,165	0
81	MG	1	3714	1/1	0.95	0.08	68,68,68,68	0
80	OHX	z	201	7/7	0.95	0.14	114,119,122,203	0
80	OHX	1	3492	7/7	0.95	0.11	107,110,119,193	0
81	MG	1	3957	1/1	0.95	0.17	63,63,63,63	0
81	MG	1	3717	1/1	0.95	0.09	47,47,47,47	0
80	OHX	1	3493	7/7	0.95	0.10	110,112,119,190	0
80	OHX	1	3494	7/7	0.95	0.10	93,99,109,160	0
80	OHX	AR	3569	7/7	0.95	0.10	109,117,123,201	0
81	MG	1	3846	1/1	0.95	0.08	45,45,45,45	0
80	OHX	1	3495	7/7	0.95	0.09	83,98,103,176	0
80	OHX	1	3450	7/7	0.95	0.14	66,88,94,133	0
80	OHX	1	3500	7/7	0.95	0.09	139,144,149,216	0
81	MG	A	2165	1/1	0.95	0.07	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	sR	2002	7/7	0.95	0.10	103,108,117,199	0
80	OHX	AR	3450	7/7	0.95	0.11	77,93,99,148	0
80	OHX	AR	3468	7/7	0.95	0.14	68,73,83,139	0
81	MG	1	3854	1/1	0.95	0.11	62,62,62,62	0
81	MG	A	2021	1/1	0.95	0.09	69,69,69,69	0
81	MG	AR	4138	1/1	0.95	0.16	61,61,61,61	0
80	OHX	AR	3473	7/7	0.95	0.13	81,88,93,161	0
80	OHX	AT	207	7/7	0.95	0.09	118,119,131,202	0
81	MG	AR	3719	1/1	0.95	0.08	60,60,60,60	0
81	MG	AR	3851	1/1	0.95	0.19	42,42,42,42	0
80	OHX	A	1913	7/7	0.95	0.09	103,110,115,173	0
81	MG	AR	3721	1/1	0.95	0.08	49,49,49,49	0
81	MG	1	3976	1/1	0.95	0.19	65,65,65,65	0
80	OHX	AR	3476	7/7	0.95	0.12	70,91,97,143	0
80	OHX	AR	3484	7/7	0.95	0.09	83,92,102,186	0
80	OHX	1	3455	7/7	0.95	0.12	86,91,109,154	0
81	MG	1	3980	1/1	0.95	0.10	69,69,69,69	0
81	MG	DC	201	1/1	0.95	0.17	56,56,56,56	0
80	OHX	AR	3489	7/7	0.95	0.10	88,97,103,167	0
80	OHX	1	3456	7/7	0.95	0.13	85,86,89,138	0
80	OHX	1	3458	7/7	0.95	0.10	81,84,95,140	0
81	MG	AR	3865	1/1	0.95	0.25	50,50,50,50	0
81	MG	AR	4155	1/1	0.95	0.12	61,61,61,61	0
81	MG	AR	3732	1/1	0.95	0.12	76,76,76,76	0
81	MG	1	3985	1/1	0.95	0.09	45,45,45,45	0
80	OHX	1	3462	7/7	0.95	0.10	80,82,90,134	0
81	MG	AR	4008	1/1	0.95	0.15	67,67,67,67	0
81	MG	AR	3869	1/1	0.95	0.29	48,48,48,48	0
81	MG	1	3741	1/1	0.95	0.38	51,51,51,51	0
81	MG	AR	3871	1/1	0.95	0.34	48,48,48,48	0
81	MG	AR	4163	1/1	0.95	0.15	46,46,46,46	0
80	OHX	A	1956	7/7	0.95	0.10	123,128,132,184	0
80	OHX	AR	3497	7/7	0.95	0.12	77,80,85,159	0
80	OHX	1	3625	7/7	0.95	0.08	122,126,129,221	0
80	OHX	CL	301	7/7	0.95	0.09	108,115,121,184	0
80	OHX	A	1901	7/7	0.95	0.17	90,97,99,112	0
80	OHX	1	3465	7/7	0.95	0.10	75,81,90,148	0
80	OHX	CP	302	7/7	0.95	0.10	127,134,139,217	0
80	OHX	1	3466	6/7	0.95	0.13	78,82,85,121	0
85	ZN	DI	202	1/1	0.95	0.32	20,20,20,20	0
80	OHX	DH	202	7/7	0.95	0.10	100,105,110,187	0
80	OHX	AR	3505	7/7	0.95	0.09	72,86,93,171	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	0.95	0.12	71,81,86,147	0
80	OHX	A	1929	7/7	0.95	0.10	109,112,117,180	0
80	OHX	1	3512	7/7	0.95	0.10	118,123,126,208	0
80	OHX	A	1921	7/7	0.95	0.10	109,111,113,178	0
80	OHX	1	3593	7/7	0.95	0.09	128,135,142,216	0
80	OHX	AR	3515	7/7	0.95	0.08	138,141,145,195	0
80	OHX	AR	3498	7/7	0.96	0.08	111,115,118,171	0
80	OHX	1	3579	7/7	0.96	0.10	93,94,100,176	0
81	MG	A	2167	1/1	0.96	0.06	87,87,87,87	0
81	MG	A	2168	1/1	0.96	0.09	100,100,100,100	0
81	MG	A	2169	1/1	0.96	0.06	89,89,89,89	0
81	MG	1	4068	1/1	0.96	0.34	62,62,62,62	0
80	OHX	AT	212	7/7	0.96	0.07	138,143,148,226	0
80	OHX	AR	3501	7/7	0.96	0.10	84,86,100,161	0
80	OHX	1	3545	7/7	0.96	0.08	102,107,114,193	0
80	OHX	A	2126	7/7	0.96	0.08	120,122,131,196	0
81	MG	AR	3937	1/1	0.96	0.08	43,43,43,43	0
80	OHX	1	4145	7/7	0.96	0.11	75,78,88,162	0
80	OHX	1	4147	7/7	0.96	0.10	111,116,119,185	0
80	OHX	1	4148	7/7	0.96	0.10	99,100,112,188	0
80	OHX	4	205	7/7	0.96	0.10	80,82,91,158	0
80	OHX	4	206	7/7	0.96	0.08	92,94,104,178	0
80	OHX	4	207	7/7	0.96	0.09	119,122,133,204	0
80	OHX	A	1907	7/7	0.96	0.10	99,109,113,160	0
80	OHX	A	2130	7/7	0.96	0.08	111,117,122,205	0
81	MG	AR	4078	1/1	0.96	0.28	59,59,59,59	0
80	OHX	1	4151	7/7	0.96	0.09	108,115,118,195	0
81	MG	1	3738	1/1	0.96	0.26	44,44,44,44	0
80	OHX	1	3445	7/7	0.96	0.10	73,80,85,132	0
81	MG	AR	4241	1/1	0.96	0.09	68,68,68,68	0
81	MG	AR	4243	1/1	0.96	0.07	77,77,77,77	0
81	MG	AR	3819	1/1	0.96	0.26	44,44,44,44	0
80	OHX	AR	3518	7/7	0.96	0.10	78,87,97,165	0
80	OHX	DL	102	7/7	0.96	0.09	85,88,90,165	0
81	MG	AR	3822	1/1	0.96	0.37	52,52,52,52	0
80	OHX	A	1903	7/7	0.96	0.12	77,79,90,120	0
80	OHX	A	1909	7/7	0.96	0.12	83,89,93,133	0
80	OHX	1	4155	7/7	0.96	0.07	118,125,131,199	0
81	MG	AR	3704	1/1	0.96	0.05	46,46,46,46	0
81	MG	AR	4090	1/1	0.96	0.04	110,110,110,110	0
80	OHX	A	1941	7/7	0.96	0.10	138,139,148,217	0
81	MG	AR	3828	1/1	0.96	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	4	236	7/7	0.96	0.10	80,80,95,158	0
81	MG	AR	4094	1/1	0.96	0.18	51,51,51,51	0
81	MG	sR	2114	1/1	0.96	0.12	78,78,78,78	0
80	OHX	sR	1904	7/7	0.96	0.16	80,85,91,100	0
80	OHX	sR	1911	7/7	0.96	0.12	77,86,93,121	0
80	OHX	1	3489	7/7	0.96	0.10	74,80,93,157	0
80	OHX	T	201	7/7	0.96	0.10	100,106,111,137	0
80	OHX	sR	1921	7/7	0.96	0.09	73,76,86,148	0
80	OHX	AR	3527	7/7	0.96	0.08	99,102,108,174	0
81	MG	AR	4101	1/1	0.96	0.07	92,92,92,92	0
80	OHX	sR	1923	7/7	0.96	0.10	85,89,100,159	0
80	OHX	sR	1924	7/7	0.96	0.13	73,77,83,119	0
80	OHX	A	1948	7/7	0.96	0.10	97,98,109,157	0
80	OHX	sR	1926	7/7	0.96	0.11	79,82,88,137	0
80	OHX	sR	1927	7/7	0.96	0.09	83,91,93,151	0
81	MG	AR	3841	1/1	0.96	0.30	51,51,51,51	0
80	OHX	1	3459	7/7	0.96	0.12	79,81,91,136	0
81	MG	1	3760	1/1	0.96	0.30	47,47,47,47	0
80	OHX	sR	1932	7/7	0.96	0.12	79,84,92,153	0
81	MG	AR	4112	1/1	0.96	0.09	62,62,62,62	0
80	OHX	1	3460	7/7	0.96	0.09	83,86,89,163	0
81	MG	1	3763	1/1	0.96	0.28	49,49,49,49	0
80	OHX	sR	1934	7/7	0.96	0.12	67,73,80,138	0
80	OHX	sR	1935	7/7	0.96	0.08	96,97,99,158	0
80	OHX	sR	1936	7/7	0.96	0.10	87,89,98,157	0
80	OHX	sR	1937	7/7	0.96	0.11	79,83,89,138	0
80	OHX	sR	1939	7/7	0.96	0.09	92,95,101,155	0
80	OHX	AR	3531	7/7	0.96	0.10	67,79,87,173	0
81	MG	AR	4121	1/1	0.96	0.17	63,63,63,63	0
81	MG	1	3886	1/1	0.96	0.06	48,48,48,48	0
80	OHX	CE	401	7/7	0.96	0.09	74,82,93,157	0
80	OHX	1	3526	7/7	0.96	0.07	114,116,127,199	0
81	MG	1	3772	1/1	0.96	0.12	43,43,43,43	0
80	OHX	AR	3534	7/7	0.96	0.08	124,125,132,193	0
80	OHX	A	2121	7/7	0.96	0.10	82,85,88,133	0
81	MG	AR	3859	1/1	0.96	0.17	46,46,46,46	0
80	OHX	sR	1945	7/7	0.96	0.09	107,113,115,167	0
80	OHX	sR	1946	7/7	0.96	0.09	93,95,97,175	0
80	OHX	1	3496	7/7	0.96	0.08	98,104,113,181	0
81	MG	1	3778	1/1	0.96	0.18	71,71,71,71	0
80	OHX	sR	1949	7/7	0.96	0.09	81,85,95,155	0
80	OHX	1	3497	7/7	0.96	0.09	96,100,110,178	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
80	OHX	A	1906	7/7	0.96	0.10	90,94,103,138	0
80	OHX	1	3420	7/7	0.96	0.13	77,80,89,109	0
80	OHX	1	3421	7/7	0.96	0.15	70,76,80,107	0
80	OHX	1	3533	7/7	0.96	0.10	90,90,95,168	0
80	OHX	AR	3543	7/7	0.96	0.10	101,104,112,198	0
80	OHX	AR	3428	7/7	0.96	0.15	62,81,87,98	0
80	OHX	AR	3433	7/7	0.96	0.13	72,83,86,106	0
81	MG	AR	3874	1/1	0.96	0.43	43,43,43,43	0
80	OHX	1	3423	7/7	0.96	0.13	75,79,96,106	0
81	MG	1	3682	1/1	0.96	0.07	51,51,51,51	0
80	OHX	AR	3442	7/7	0.96	0.12	66,73,76,122	0
80	OHX	1	3430	7/7	0.96	0.11	69,74,91,109	0
80	OHX	AR	3444	7/7	0.96	0.12	66,76,83,114	0
81	MG	AR	3880	1/1	0.96	0.29	43,43,43,43	0
80	OHX	AR	3448	7/7	0.96	0.12	72,77,87,123	0
80	OHX	1	3432	7/7	0.96	0.13	77,78,88,116	0
80	OHX	AR	3452	7/7	0.96	0.10	92,96,103,131	0
80	OHX	AR	4213	7/7	0.96	0.11	75,85,90,150	0
80	OHX	AR	3553	7/7	0.96	0.08	109,112,118,185	0
80	OHX	AR	3460	7/7	0.96	0.12	66,76,90,106	0
80	OHX	AR	3461	7/7	0.96	0.12	55,70,81,119	0
81	MG	sR	2191	1/1	0.96	0.11	57,57,57,57	0
81	MG	sR	2194	1/1	0.96	0.06	96,96,96,96	0
81	MG	4	222	1/1	0.96	0.09	42,42,42,42	0
80	OHX	AR	3467	7/7	0.96	0.10	82,84,89,143	0
81	MG	s4	302	1/1	0.96	0.18	60,60,60,60	0
80	OHX	1	3470	7/7	0.96	0.10	85,86,91,148	0
80	OHX	AR	4229	7/7	0.96	0.10	85,95,100,184	0
80	OHX	AR	3472	7/7	0.96	0.12	77,79,84,154	0
80	OHX	1	3471	7/7	0.96	0.11	79,82,93,145	0
80	OHX	1	3472	7/7	0.96	0.10	98,102,108,165	0
81	MG	1	3810	1/1	0.96	0.31	49,49,49,49	0
80	OHX	A	1912	7/7	0.96	0.09	106,107,110,162	0
81	MG	AR	3772	1/1	0.96	0.09	69,69,69,69	0
80	OHX	AR	3562	7/7	0.96	0.07	87,91,104,181	0
81	MG	1	4040	1/1	0.96	0.17	82,82,82,82	0
80	OHX	AR	3477	7/7	0.96	0.11	78,84,90,148	0
80	OHX	AR	3478	7/7	0.96	0.11	82,83,86,159	0
80	OHX	AR	3479	7/7	0.96	0.11	74,83,89,126	0
80	OHX	AR	3480	7/7	0.96	0.11	75,77,93,141	0
81	MG	j	302	1/1	0.96	0.07	45,45,45,45	0
80	OHX	AS	203	7/7	0.96	0.11	72,79,84,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	AR	3481	7/7	0.96	0.09	70,78,88,155	0
81	MG	1	3819	1/1	0.96	0.37	48,48,48,48	0
80	OHX	AR	3482	7/7	0.96	0.10	71,76,89,146	0
81	MG	AR	3910	1/1	0.96	0.15	51,51,51,51	0
81	MG	AR	3911	1/1	0.96	0.24	54,54,54,54	0
80	OHX	AS	206	7/7	0.96	0.10	80,83,85,159	0
80	OHX	AS	207	7/7	0.96	0.09	90,94,101,169	0
81	MG	1	3936	1/1	0.96	0.45	56,56,56,56	0
81	MG	AR	4182	1/1	0.96	0.34	43,43,43,43	0
80	OHX	1	3474	7/7	0.96	0.10	78,80,93,150	0
80	OHX	AR	3485	7/7	0.96	0.10	76,78,90,145	0
81	MG	AR	4047	1/1	0.96	0.07	56,56,56,56	0
80	OHX	1	4133	7/7	0.96	0.13	74,78,85,119	0
80	OHX	1	4136	7/7	0.96	0.13	65,78,81,126	0
80	OHX	AR	3491	7/7	0.96	0.10	78,84,90,170	0
80	OHX	1	3435	7/7	0.96	0.11	79,83,93,134	0
80	OHX	1	4138	7/7	0.96	0.10	100,107,112,164	0
81	MG	AR	4053	1/1	0.96	0.17	72,72,72,72	0
81	MG	AR	4193	1/1	0.96	0.22	42,42,42,42	0
80	OHX	1	3576	7/7	0.96	0.07	162,162,167,222	0
81	MG	1	3945	1/1	0.96	0.11	60,60,60,60	0
80	OHX	1	3436	7/7	0.96	0.10	62,71,79,116	0
80	OHX	1	3439	7/7	0.96	0.12	67,74,82,136	0
80	OHX	AR	3513[B]	7/7	0.97	0.14	86,87,88,120	7
80	OHX	sR	1912	7/7	0.97	0.14	76,82,86,96	0
80	OHX	sR	1914	7/7	0.97	0.09	80,82,85,121	0
80	OHX	1	3498	7/7	0.97	0.07	89,94,103,168	0
80	OHX	sR	1916[A]	7/7	0.97	0.15	72,72,77,85	7
80	OHX	sR	1916[B]	7/7	0.97	0.15	74,75,78,88	7
80	OHX	sR	1917	7/7	0.97	0.09	71,76,82,115	0
80	OHX	sR	1918	7/7	0.97	0.12	76,83,88,120	0
80	OHX	AR	3411	7/7	0.97	0.17	78,83,90,98	0
80	OHX	AR	3416	7/7	0.97	0.15	68,82,87,91	0
80	OHX	1	3425	7/7	0.97	0.11	78,83,94,117	0
81	MG	r	302	1/1	0.97	0.05	50,50,50,50	0
80	OHX	AR	3430	7/7	0.97	0.11	69,77,88,104	0
80	OHX	1	3426	7/7	0.97	0.11	72,77,86,128	0
80	OHX	AR	3520	7/7	0.97	0.07	98,102,107,171	0
80	OHX	AR	3434	7/7	0.97	0.11	75,87,96,119	0
80	OHX	AR	3436	7/7	0.97	0.10	69,75,86,110	0
80	OHX	sR	1928	7/7	0.97	0.07	73,77,87,148	0
80	OHX	AR	3437	7/7	0.97	0.11	70,78,84,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	sR	1930	7/7	0.97	0.08	119,121,128,170	0
80	OHX	sR	1931	7/7	0.97	0.10	76,84,89,128	0
80	OHX	AR	3438	7/7	0.97	0.12	71,79,86,97	0
80	OHX	AR	3439	7/7	0.97	0.12	73,78,84,107	0
81	MG	AR	4025	1/1	0.97	0.12	44,44,44,44	0
80	OHX	AR	3440	7/7	0.97	0.09	78,86,91,125	0
80	OHX	1	3428	7/7	0.97	0.12	81,84,96,111	0
80	OHX	1	3502	7/7	0.97	0.11	78,87,96,159	0
80	OHX	1	3429	7/7	0.97	0.13	78,86,91,97	0
80	OHX	sR	1938	7/7	0.97	0.08	82,86,93,149	0
80	OHX	A	2119	7/7	0.97	0.11	79,81,90,133	0
81	MG	1	3970	1/1	0.97	0.04	60,60,60,60	0
80	OHX	AR	3445	7/7	0.97	0.10	64,69,86,114	0
80	OHX	AR	3446	7/7	0.97	0.11	61,62,75,116	0
80	OHX	AR	3447	7/7	0.97	0.11	69,78,84,106	0
80	OHX	3	201	7/7	0.97	0.10	80,89,96,138	0
80	OHX	A	2120	7/7	0.97	0.12	87,91,96,131	0
80	OHX	AR	3451	7/7	0.97	0.11	68,72,78,120	0
80	OHX	AR	3537	7/7	0.97	0.10	78,80,84,135	0
80	OHX	A	1905	7/7	0.97	0.09	88,92,99,148	0
80	OHX	sR	1948	7/7	0.97	0.08	83,89,94,164	0
80	OHX	AR	3453	7/7	0.97	0.09	80,84,90,142	0
80	OHX	AR	3454	7/7	0.97	0.13	72,77,84,107	0
80	OHX	AR	3456	7/7	0.97	0.12	70,76,79,123	0
81	MG	AR	4045	1/1	0.97	0.04	60,60,60,60	0
81	MG	CY	201	1/1	0.97	0.07	102,102,102,102	0
80	OHX	AR	3457	7/7	0.97	0.11	74,86,98,131	0
80	OHX	AR	3459	7/7	0.97	0.11	70,78,86,137	0
80	OHX	A	2122	7/7	0.97	0.11	82,84,90,141	0
80	OHX	AC	102	7/7	0.97	0.15	61,73,86,89	0
80	OHX	s1	301	7/7	0.97	0.11	78,83,95,108	0
81	MG	AR	3933	1/1	0.97	0.13	103,103,103,103	0
80	OHX	AR	3463	7/7	0.97	0.09	84,85,92,144	0
80	OHX	AR	3464	7/7	0.97	0.11	72,75,86,124	0
80	OHX	AR	3465	7/7	0.97	0.11	68,72,78,118	0
80	OHX	AR	3466	7/7	0.97	0.12	83,87,97,123	0
80	OHX	1	4146	7/7	0.97	0.10	98,101,104,164	0
80	OHX	1	3438	7/7	0.97	0.10	88,89,96,143	0
81	MG	1	3781	1/1	0.97	0.15	45,45,45,45	0
80	OHX	AR	3469	7/7	0.97	0.08	73,77,82,121	0
80	OHX	AR	3470	7/7	0.97	0.09	82,85,89,145	0
80	OHX	A	2115	7/7	0.97	0.16	84,88,89,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	3	221	7/7	0.97	0.10	83,93,108,169	0
80	OHX	AR	3474	7/7	0.97	0.14	70,81,92,126	0
80	OHX	A	2116	7/7	0.97	0.12	85,86,95,105	0
80	OHX	A	2117	7/7	0.97	0.12	82,90,94,118	0
80	OHX	4	204	7/7	0.97	0.11	66,75,78,121	0
80	OHX	1	3442	7/7	0.97	0.10	70,73,81,133	0
80	OHX	1	3406	7/7	0.97	0.14	73,82,88,91	0
81	MG	1	3792	1/1	0.97	0.32	44,44,44,44	0
80	OHX	1	3444	7/7	0.97	0.10	79,83,85,135	0
80	OHX	1	3478	7/7	0.97	0.09	87,98,110,188	0
80	OHX	1	3415	7/7	0.97	0.12	78,81,90,98	0
80	OHX	AT	204	7/7	0.97	0.11	64,73,78,116	0
80	OHX	AR	3483	7/7	0.97	0.11	69,72,79,130	0
81	MG	1	4183	1/1	0.97	0.08	60,60,60,60	0
81	MG	1	3798	1/1	0.97	0.23	55,55,55,55	0
80	OHX	1	3446	7/7	0.97	0.14	69,78,88,113	0
80	OHX	1	3481	7/7	0.97	0.07	86,92,97,150	0
80	OHX	AR	3486	7/7	0.97	0.08	75,80,85,141	0
81	MG	1	4015	1/1	0.97	0.06	64,64,64,64	0
80	OHX	AR	3487	7/7	0.97	0.12	69,75,81,132	0
81	MG	sR	2058	1/1	0.97	0.25	53,53,53,53	0
81	MG	1	4194	1/1	0.97	0.05	93,93,93,93	0
80	OHX	1	3447	7/7	0.97	0.13	69,76,83,121	0
81	MG	AR	3737	1/1	0.97	0.49	53,53,53,53	0
80	OHX	1	3483	7/7	0.97	0.08	99,102,109,180	0
80	OHX	1	3448	7/7	0.97	0.09	89,92,98,148	0
81	MG	1	3806	1/1	0.97	0.36	44,44,44,44	0
80	OHX	1	3449	7/7	0.97	0.10	74,80,83,126	0
80	OHX	A	1904	7/7	0.97	0.09	83,87,91,123	0
81	MG	1	4023	1/1	0.97	0.07	54,54,54,54	0
80	OHX	4	237	7/7	0.97	0.10	72,78,81,140	0
80	OHX	1	3418	7/7	0.97	0.12	76,81,97,101	0
80	OHX	1	3452	7/7	0.97	0.10	72,84,93,124	0
80	OHX	1	3453	7/7	0.97	0.11	74,82,88,139	0
80	OHX	AR	3499	7/7	0.97	0.08	92,96,100,156	0
80	OHX	A	2128	7/7	0.97	0.09	92,95,104,163	0
80	OHX	A	2149	7/7	0.97	0.10	79,83,89,140	0
81	MG	AR	3864	1/1	0.97	0.28	44,44,44,44	0
80	OHX	1	3457	7/7	0.97	0.12	78,84,91,147	0
80	OHX	1	3422	7/7	0.97	0.13	61,79,85,107	0
80	OHX	A	2129	7/7	0.97	0.08	99,100,103,168	0
80	OHX	CX	201	7/7	0.97	0.12	70,74,87,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	AR	3755	1/1	0.97	0.31	43,43,43,43	0
81	MG	A	2164	1/1	0.97	0.06	62,62,62,62	0
80	OHX	1	3424	7/7	0.97	0.13	81,82,86,104	0
80	OHX	1	4122	7/7	0.97	0.18	74,76,82,82	0
80	OHX	AR	3507	7/7	0.97	0.09	84,89,96,171	0
80	OHX	1	4127	7/7	0.97	0.14	75,82,85,94	0
80	OHX	1	3461	7/7	0.97	0.09	90,93,96,152	0
81	MG	1	3826	1/1	0.97	0.51	45,45,45,45	0
80	OHX	AR	3510	7/7	0.97	0.11	68,71,79,115	0
85	ZN	AP	501	1/1	0.97	0.04	114,114,114,114	0
80	OHX	1	4132	7/7	0.97	0.10	76,81,84,122	0
80	OHX	AR	3512	7/7	0.97	0.07	89,91,100,157	0
81	MG	P	201	1/1	0.97	0.07	66,66,66,66	0
80	OHX	AR	3513[A]	7/7	0.97	0.14	80,83,86,98	7
80	OHX	sR	1907	7/7	0.97	0.12	72,86,98,102	0
81	MG	1	3834	1/1	0.97	0.11	47,47,47,47	0
80	OHX	sR	1909	7/7	0.97	0.13	68,81,87,98	0
81	MG	AR	3885	1/1	0.97	0.05	51,51,51,51	0
81	MG	sR	2097	1/1	0.97	0.07	61,61,61,61	0
80	OHX	AR	3417	7/7	0.98	0.12	82,83,92,97	0
81	MG	1	4186	1/1	0.98	0.06	65,65,65,65	0
81	MG	1	4187	1/1	0.98	0.05	71,71,71,71	0
80	OHX	sR	1903	7/7	0.98	0.14	62,67,71,80	0
81	MG	1	4189	1/1	0.98	0.06	75,75,75,75	0
80	OHX	AR	3418	7/7	0.98	0.12	67,84,90,92	0
80	OHX	sR	1906	7/7	0.98	0.10	77,84,90,99	0
80	OHX	AR	3419	7/7	0.98	0.11	76,79,87,88	0
80	OHX	AR	3420	7/7	0.98	0.11	79,81,88,96	0
81	MG	AR	4246	1/1	0.98	0.04	48,48,48,48	0
81	MG	AR	4247	1/1	0.98	0.06	52,52,52,52	0
80	OHX	sR	1910	7/7	0.98	0.14	74,81,87,103	0
80	OHX	AR	3421	7/7	0.98	0.12	83,87,90,97	0
80	OHX	AR	3490	7/7	0.98	0.10	72,76,79,110	0
80	OHX	sR	1913	7/7	0.98	0.10	78,80,84,104	0
80	OHX	AR	3422	7/7	0.98	0.11	78,89,92,94	0
80	OHX	AR	3492	7/7	0.98	0.08	81,85,89,154	0
80	OHX	AR	3423	7/7	0.98	0.12	81,83,87,88	0
80	OHX	AR	3425	7/7	0.98	0.18	76,89,92,97	0
80	OHX	AR	3426	7/7	0.98	0.11	77,79,87,97	0
80	OHX	1	4128	7/7	0.98	0.12	76,77,85,96	0
80	OHX	sR	1919	7/7	0.98	0.10	71,75,81,113	0
80	OHX	AR	3429	7/7	0.98	0.10	73,75,83,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	1	3413	7/7	0.98	0.12	76,80,90,97	0
80	OHX	AR	4206	7/7	0.98	0.12	56,63,68,74	0
80	OHX	AR	3431	7/7	0.98	0.11	78,81,86,98	0
80	OHX	4	201	7/7	0.98	0.12	78,83,86,89	0
80	OHX	4	203	7/7	0.98	0.14	79,83,88,89	0
80	OHX	AR	3435	7/7	0.98	0.11	75,76,95,106	0
81	MG	AR	3726	1/1	0.98	0.23	45,45,45,45	0
80	OHX	1	4130	7/7	0.98	0.12	78,84,89,98	0
80	OHX	1	4131	7/7	0.98	0.11	71,78,85,105	0
80	OHX	1	3431	7/7	0.98	0.10	82,82,90,125	0
80	OHX	1	3414	7/7	0.98	0.12	78,82,88,96	0
81	MG	AR	4071	1/1	0.98	0.05	55,55,55,55	0
80	OHX	1	4134	7/7	0.98	0.10	79,80,85,126	0
80	OHX	1	4135	7/7	0.98	0.11	74,81,87,97	0
80	OHX	1	3433	7/7	0.98	0.09	76,83,85,115	0
80	OHX	1	3454	7/7	0.98	0.10	86,94,100,133	0
81	MG	1	3829	1/1	0.98	0.32	44,44,44,44	0
80	OHX	DD	101	7/7	0.98	0.13	73,82,94,100	0
80	OHX	1	3416	7/7	0.98	0.11	77,83,84,105	0
80	OHX	A	2123	7/7	0.98	0.07	104,107,110,155	0
81	MG	1	3753	1/1	0.98	0.06	54,54,54,54	0
80	OHX	1	3437	7/7	0.98	0.10	76,85,89,128	0
80	OHX	AS	202	7/7	0.98	0.10	74,82,85,116	0
81	MG	AT	229	1/1	0.98	0.08	90,90,90,90	0
81	MG	sR	2192	1/1	0.98	0.04	89,89,89,89	0
81	MG	sR	2193	1/1	0.98	0.03	93,93,93,93	0
81	MG	1	3836	1/1	0.98	0.06	62,62,62,62	0
80	OHX	AR	3581	7/7	0.98	0.07	73,76,83,158	0
80	OHX	A	2114	7/7	0.98	0.15	77,85,88,96	0
80	OHX	AR	3449	7/7	0.98	0.09	83,88,94,126	0
80	OHX	AR	3584	7/7	0.98	0.08	82,84,88,135	0
80	OHX	1	3419	7/7	0.98	0.10	79,80,87,95	0
80	OHX	A	1902	7/7	0.98	0.12	79,83,85,108	0
80	OHX	1	3401	7/7	0.98	0.13	49,53,63,67	0
80	OHX	1	3405	7/7	0.98	0.15	73,77,91,95	0
80	OHX	1	3485	7/7	0.98	0.08	87,89,92,136	0
80	OHX	AR	3455	6/7	0.98	0.08	78,83,88,131	0
80	OHX	AT	203	7/7	0.98	0.14	77,79,83,93	0
80	OHX	A	1910	7/7	0.98	0.09	88,91,96,141	0
80	OHX	n	201	7/7	0.98	0.11	70,77,80,82	0
80	OHX	AR	3458	7/7	0.98	0.08	70,76,80,117	0
80	OHX	1	3407	7/7	0.98	0.12	77,79,85,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	1	3409	7/7	0.98	0.10	77,79,87,97	0
80	OHX	1	3410	7/7	0.98	0.13	71,75,83,88	0
80	OHX	sR	1957	7/7	0.98	0.07	129,131,132,188	0
80	OHX	AR	3462	7/7	0.98	0.09	75,82,85,141	0
81	MG	AR	4190	1/1	0.98	0.18	49,49,49,49	0
80	OHX	1	4108	7/7	0.98	0.13	79,81,86,88	0
80	OHX	1	3427	7/7	0.98	0.10	76,81,85,103	0
80	OHX	1	3411	7/7	0.98	0.11	73,76,87,91	0
81	MG	AR	4106	1/1	0.98	0.09	56,56,56,56	0
80	OHX	2	201	7/7	0.98	0.11	78,81,91,99	0
80	OHX	1	4123	7/7	0.98	0.13	58,62,73,77	0
80	OHX	1	4124	7/7	0.98	0.12	76,78,85,86	0
80	OHX	1	4125	7/7	0.98	0.12	85,86,98,103	0
80	OHX	AR	3401	7/7	0.98	0.14	53,61,67,73	0
80	OHX	AR	3471	7/7	0.98	0.07	79,79,85,142	0
80	OHX	AR	3402	7/7	0.98	0.16	59,61,70,72	0
80	OHX	AR	3403	7/7	0.98	0.14	67,67,73,73	0
80	OHX	AR	3404	7/7	0.98	0.13	72,75,78,78	0
85	ZN	AK	103	1/1	0.98	0.04	58,58,58,58	0
80	OHX	AR	3405	7/7	0.98	0.14	73,76,79,82	0
80	OHX	AR	3406	7/7	0.98	0.12	83,84,87,89	0
85	ZN	DQ	202	1/1	0.98	0.04	114,114,114,114	0
85	ZN	b	201	1/1	0.98	0.05	95,95,95,95	0
80	OHX	AR	3407	7/7	0.98	0.17	74,79,84,85	0
85	ZN	e	101	1/1	0.98	0.04	93,93,93,93	0
85	ZN	g	501	1/1	0.98	0.04	130,130,130,130	0
80	OHX	AR	3409	7/7	0.98	0.13	64,67,76,80	0
85	ZN	d9	101	1/1	0.98	0.05	96,96,96,96	0
80	OHX	1	4126	7/7	0.98	0.13	80,85,90,91	0
80	OHX	AR	3412	7/7	0.98	0.12	76,80,84,86	0
80	OHX	AR	3413	7/7	0.98	0.12	83,84,93,95	0
80	OHX	AR	3414	7/7	0.98	0.14	79,82,90,95	0
80	OHX	AR	3415	7/7	0.98	0.12	77,82,86,94	0
80	OHX	1	3412	7/7	0.98	0.12	77,78,89,96	0
81	MG	A	2162	1/1	0.99	0.14	54,54,54,54	0
81	MG	A	2163	1/1	0.99	0.07	67,67,67,67	0
80	OHX	AR	3424	7/7	0.99	0.09	82,85,94,94	0
80	OHX	sR	1908	7/7	0.99	0.10	81,81,86,96	0
81	MG	AR	4240	1/1	0.99	0.04	43,43,43,43	0
80	OHX	1	3404	7/7	0.99	0.12	72,81,84,85	0
81	MG	AR	4242	1/1	0.99	0.06	59,59,59,59	0
85	ZN	AN	202	1/1	0.99	0.03	66,66,66,66	0

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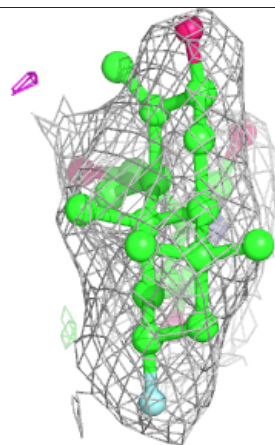
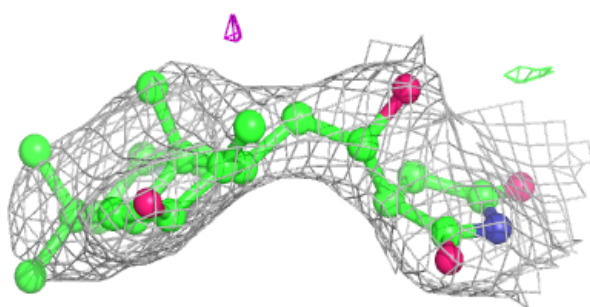
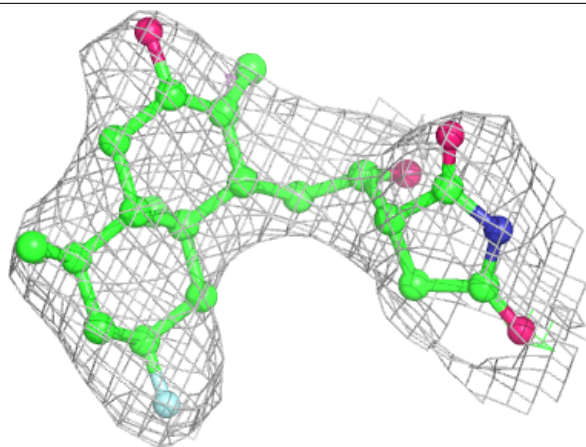
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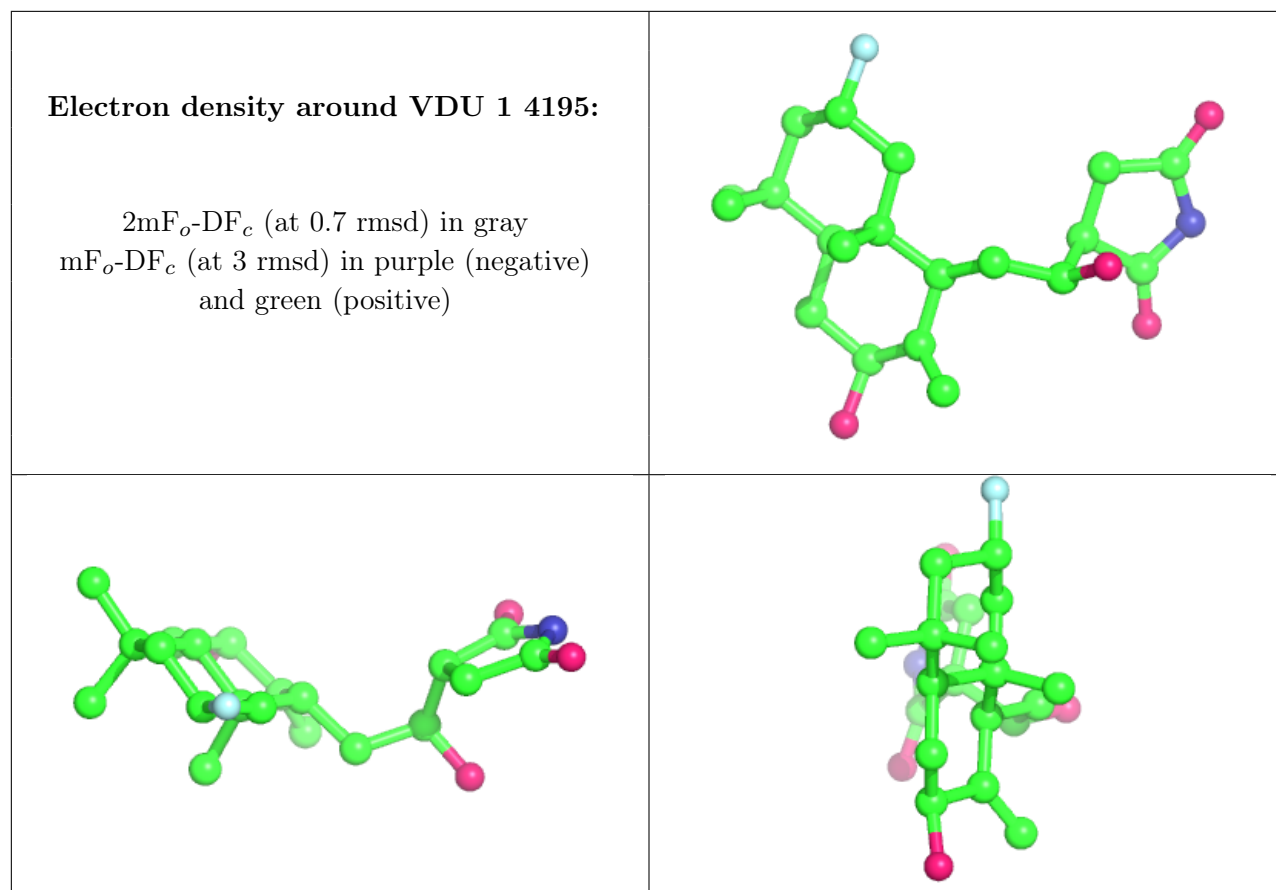
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	OHX	1	3408	7/7	0.99	0.10	77,83,89,92	0
85	ZN	AQ	501	1/1	0.99	0.04	88,88,88,88	0
81	MG	AR	4244	1/1	0.99	0.09	86,86,86,86	0
85	ZN	DL	103	1/1	0.99	0.04	64,64,64,64	0
85	ZN	DO	201	1/1	0.99	0.03	48,48,48,48	0
81	MG	AR	4245	1/1	0.99	0.05	45,45,45,45	0
85	ZN	DR	501	1/1	0.99	0.04	88,88,88,88	0
81	MG	1	4192	1/1	0.99	0.05	88,88,88,88	0
80	OHX	AR	3427	7/7	0.99	0.10	80,82,90,91	0
81	MG	AR	4248	1/1	0.99	0.12	42,42,42,42	0
81	MG	AR	4249	1/1	0.99	0.09	49,49,49,49	0
85	ZN	d6	203	1/1	0.99	0.04	70,70,70,70	0
81	MG	AR	4250	1/1	0.99	0.08	48,48,48,48	0
80	OHX	AR	3408	7/7	0.99	0.12	78,88,92,93	0
80	OHX	1	3402	7/7	0.99	0.10	48,49,52,70	0
80	OHX	AR	3410	7/7	0.99	0.10	51,52,54,72	0
81	MG	AR	4254	1/1	0.99	0.08	46,46,46,46	0
80	OHX	1	3403	7/7	0.99	0.12	53,56,62,70	0
80	OHX	sR	1905	7/7	0.99	0.13	78,83,87,90	0
80	OHX	AR	3432	7/7	0.99	0.13	85,90,97,99	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 VDU AR 4255:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.