



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 01:10 AM UTC

PDB ID : 8P4V / pdb_00008p4v
Title : 80S yeast ribosome in complex with HaterumaimideQ
Authors : Terrosu, S.; Yusupov, M.
Deposited on : 2023-05-23
Resolution : 3.16 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 Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

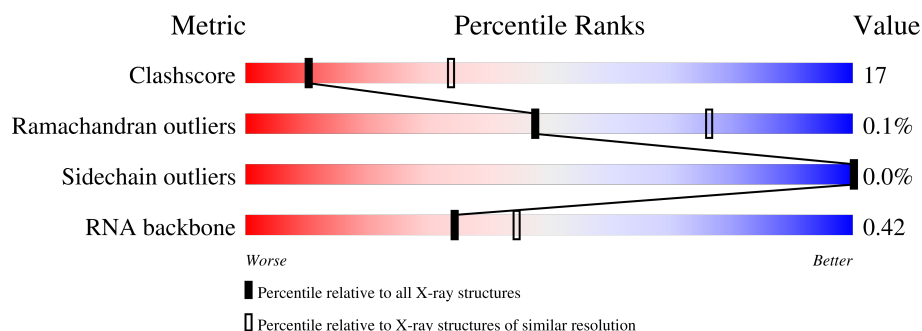
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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))
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RNA backbone	3983	1113 (3.42-2.90)

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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1	3396	42% 41% 10% 7%
1	AR	3396	43% 39% 10% 7%
2	3	121	52% 39% 9%
2	AS	121	46% 46% 7%
3	4	158	42% 45% 13%
3	AT	158	55% 37% 8%

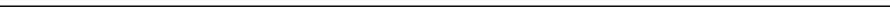
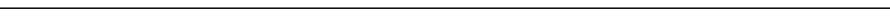
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Mol	Chain	Length	Quality of chain
4	CD	254	
4	j	254	
5	CE	387	
5	k	387	
6	CF	362	
6	l	362	
7	CG	297	
7	m	297	
8	CH	176	
8	n	176	
9	CI	244	
9	o	244	
10	CJ	256	
10	p	256	
11	CK	191	
11	q	191	
12	CL	221	
12	r	221	
13	CM	174	
13	s	174	
14	CN	199	
14	t	199	
15	CO	138	
15	u	138	
16	CP	204	

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Mol	Chain	Length	Quality of chain
16	v	204	
17	CQ	199	
17	w	199	
18	CR	184	
18	x	184	
19	CS	186	
19	y	186	
20	CT	189	
20	z	189	
21	0	172	
21	CU	172	
22	2	160	
22	CV	160	
23	5	121	
23	CW	121	
24	6	137	
24	CX	137	
25	7	155	
25	CY	155	
26	8	142	
26	CZ	142	
27	9	127	
27	DA	127	
28	AA	136	
28	DB	136	

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Mol	Chain	Length	Quality of chain
29	AB	149	
29	DC	149	
30	AC	59	
30	DD	59	
31	AD	105	
31	DE	105	
32	AE	113	
32	DF	113	
33	AF	130	
33	DG	130	
34	AG	107	
34	DH	107	
35	AH	121	
35	DI	121	
36	AI	120	
36	DJ	120	
37	AJ	100	
37	DK	100	
38	AK	88	
38	DL	88	
39	AL	78	
39	DM	78	
40	AM	51	
40	DN	51	
41	AN	128	

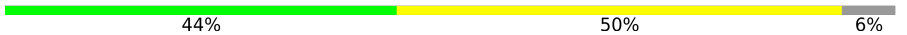
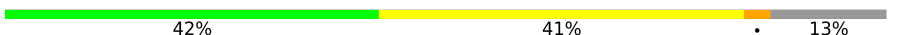
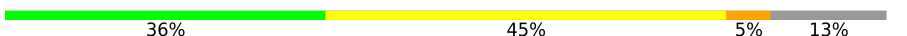
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Mol	Chain	Length	Quality of chain
41	DO	128	
42	AO	25	
42	DP	25	
43	AP	106	
43	DQ	106	
44	AQ	92	
44	DR	92	
45	i	273	
45	sM	273	
46	p0	311	
47	A	1800	
47	sR	1800	
48	B	252	
48	s0	252	
49	C	255	
49	s1	255	
50	D	254	
50	s2	254	
51	E	240	
51	s3	240	
52	F	261	
52	s4	261	
53	G	225	
53	s5	225	
54	H	236	

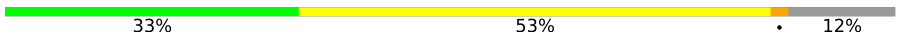
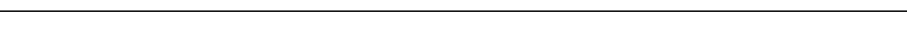
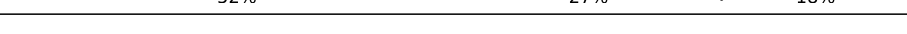
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Mol	Chain	Length	Quality of chain
54	s6	236	
55	I	190	
55	s7	190	
56	J	200	
56	s8	200	
57	K	197	
57	s9	197	
58	L	105	
58	c0	105	
59	M	156	
59	c1	156	
60	N	143	
60	c2	143	
61	O	151	
61	c3	151	
62	P	138	
62	c4	138	
63	Q	142	
63	c5	142	
64	R	143	
64	c6	143	
65	S	136	
66	T	146	
66	c8	146	
67	U	144	

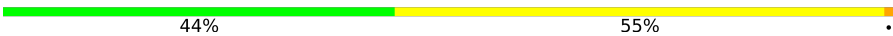
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Mol	Chain	Length	Quality of chain
67	c9	144	
68	V	121	
68	d0	121	
69	W	87	
69	d1	87	
70	X	130	
70	d2	130	
71	Y	145	
71	d3	145	
72	Z	135	
72	d4	135	
73	a	108	
73	d5	108	
74	b	119	
74	d6	119	
75	c	82	
75	d7	82	
76	d	67	
76	d8	67	
77	d9	56	
77	e	56	
78	e0	63	
78	f	63	
79	e1	152	
79	g	152	

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Mol	Chain	Length	Quality of chain
80	Rb	319	 45% 54%
80	h	319	 44% 55%
81	c7	136	 46% 40% 14%

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
82	OHX	1	3455	-	-	X	-
82	OHX	1	4080	-	-	X	-
82	OHX	A	2121	-	-	X	-
82	OHX	A	2127	-	-	X	-
82	OHX	AK	102	-	-	X	-
82	OHX	AR	3401	-	-	X	-
82	OHX	AR	3604	-	-	X	-
82	OHX	AR	3642	-	-	X	-
82	OHX	AR	4160	-	-	X	-
82	OHX	sR	1990	-	-	X	-

2 Entry composition [i](#)

There are 89 unique types of molecules in this entry. The entry contains 409267 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 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			
1	AR	3147	Total	C	N	O	P	0	0	0
			67313	30067	12134	21965	3147			

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
2	AS	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			
3	AT	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

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

- Molecule 5 is a protein called 60S ribosomal protein L3.

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

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

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

- Molecule 7 is a protein called 60S ribosomal protein L5.

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

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

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

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

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

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

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

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

- Molecule 12 is a protein called 60S ribosomal protein L10.

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

- Molecule 13 is a protein called Large ribosomal subunit protein uL5B.

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

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

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

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	x	183	Total	C	N	O	S	0	0	0
			1420	882	281	257				
18	CR	183	Total	C	N	O	S	0	0	0
			1420	882	281	257				

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	z	188	Total	C	N	O	S	0	0	0
			1521	935	326	260				
20	CT	188	Total	C	N	O	S	0	0	0
			1521	935	326	260				

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
21	CU	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	2	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			
22	CV	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	5	100	Total	C	N	O	0	0	0
			796	516	131	149			
23	CW	100	Total	C	N	O	0	0	0
			796	516	131	149			

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	6	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
24	CX	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	7	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			
25	CY	124	Total	C	N	O	S	0	0	0
			836	525	166	144	1			

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	8	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	CZ	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			

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

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

- Molecule 28 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	AA	135	Total	C	N	O		0	0	0
			1092	710	202	180				
28	DB	135	Total	C	N	O		0	0	0
			1087	706	201	180				

- Molecule 29 is a protein called 60S ribosomal protein L28.

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

- Molecule 30 is a protein called 60S ribosomal protein L29.

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

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	AD	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			
31	DE	97	Total	C	N	O	S	0	0	0
			743	479	124	139	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 L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 35 is a protein called 60S ribosomal protein L34-A.

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

- Molecule 36 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 37 is a protein called 60S ribosomal protein L36-A.

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

- Molecule 38 is a protein called 60S ribosomal protein L37-A.

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

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 42 is a protein called 60S ribosomal protein L41-A.

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

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

- Molecule 43 is a protein called 60S ribosomal protein L42-A.

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

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 45 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	i	159	Total	C	N	O		0	0	0
			1104	652	221	231				
45	sM	63	Total	C	N	O		0	0	0
			475	280	99	96				

- Molecule 46 is a protein called 60S acidic protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	p0	143	Total	C	N	O	S	0	0	0
			1076	686	192	195	3			

- Molecule 47 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	A	1781	Total	C	N	O	P	0	0	0
			37948	16965	6715	12487	1781			
47	sR	1783	Total	C	N	O	P	0	0	0
			37990	16984	6723	12500	1783			

- Molecule 48 is a protein called 40S ribosomal protein S0-A.

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

- Molecule 49 is a protein called 40S ribosomal protein S1-A.

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

- Molecule 50 is a protein called 40S ribosomal protein S2.

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

- Molecule 51 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 52 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 53 is a protein called 40S ribosomal protein S5.

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

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

- Molecule 54 is a protein called 40S ribosomal protein S6-A.

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

- Molecule 55 is a protein called 40S ribosomal protein S7-A.

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

- Molecule 56 is a protein called 40S ribosomal protein S8-A.

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

- Molecule 57 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	K	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			
57	s9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

- Molecule 58 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	L	96	Total	C	N	O	S	0	0	0
			772	499	126	145	2			
58	c0	96	Total	C	N	O	S	0	0	0
			761	490	125	144	2			

- Molecule 59 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	M	155	Total	C	N	O	S	0	0	0
			1213	774	230	206	3			
59	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

- Molecule 60 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	N	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			
60	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

- Molecule 61 is a protein called 40S ribosomal protein S13.

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

- Molecule 62 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
62	P	127	Total	C	N	O	S	0	0	0
			886	541	182	162	1			
62	c4	128	Total	C	N	O	S	0	0	0
			949	582	188	176	3			

- Molecule 63 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
63	Q	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			
63	c5	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	7			

- Molecule 64 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 65 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
65	S	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			

- Molecule 66 is a protein called 40S ribosomal protein S18-A.

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

- Molecule 67 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 68 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	V	107	Total	C	N	O	S	0	0	0
			855	539	156	159	1			
68	d0	110	Total	C	N	O	S	0	0	0
			882	554	161	166	1			

- Molecule 69 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 70 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 71 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 72 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 73 is a protein called 40S ribosomal protein S25-A.

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

- Molecule 74 is a protein called Small ribosomal subunit protein eS26B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
74	b	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			
74	d6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

- Molecule 75 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 76 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 77 is a protein called Small ribosomal subunit protein uS14A.

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

- Molecule 78 is a protein called 40S ribosomal protein S30-A.

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

- Molecule 79 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	g	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			
79	e1	51	Total	C	N	O	S	0	0	0
			397	249	73	71	4			

- Molecule 80 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	h	318	Total	C	N	O	S	0	0	0
			2437	1541	418	470	8			

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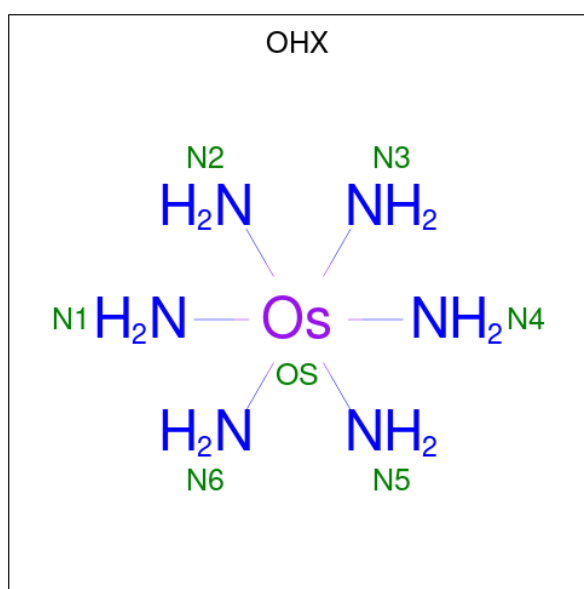
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	Rb	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 81 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

- Molecule 82 is osmium (III) hexammine (CCD ID: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
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82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
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			7	6	1		
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82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
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			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
82	1	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		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	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		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
			6	5	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	1
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
			7	6	1		
82	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
			6	5	1		
82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	1	1	Total	N	Os	0	0
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82	3	1	Total	N	Os	0	0
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82	3	1	Total	N	Os	0	0
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			7	6	1		
82	3	1	Total	N	Os	0	0
			7	6	1		
82	3	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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82	4	1	Total	N	Os	0	0
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82	4	1	Total	N	Os	0	0
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82	4	1	Total	N	Os	0	0
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82	k	1	Total	N	Os	0	0
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82	k	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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82	r	1	Total	N	Os	0	0
			7	6	1		
82	v	1	Total	N	Os	0	0
			7	6	1		
82	z	1	Total	N	Os	0	0
			7	6	1		
82	2	1	Total	N	Os	0	0
			7	6	1		
82	AC	1	Total	N	Os	0	0
			7	6	1		
82	AG	1	Total	N	Os	0	0
			7	6	1		
82	AK	1	Total	N	Os	0	0
			7	6	1		
82	AK	1	Total	N	Os	0	0
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82	AP	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
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			7	6	1		
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			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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82	AR	1	Total	N	Os	0	0
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			7	6	1		
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			7	6	1		
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82	AR	1	Total	N	Os	0	0
			7	6	1		
82	AR	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AS	1	Total	N	Os	0	0
			7	6	1		
82	AS	1	Total	N	Os	0	0
			7	6	1		
82	AS	1	Total	N	Os	0	0
			7	6	1		
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82	AS	1	Total	N	Os	0	0
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82	AT	1	Total	N	Os	0	0
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82	AT	1	Total	N	Os	0	0
			7	6	1		
82	AT	1	Total	N	Os	0	0
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82	AT	1	Total	N	Os	0	0
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82	AT	1	Total	N	Os	0	0
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82	AT	1	Total	N	Os	0	0
			7	6	1		
82	AT	1	Total	N	Os	0	0
			7	6	1		
82	AT	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	AT	1	Total	N	Os	0	0
			7	6	1		
82	CE	1	Total	N	Os	0	0
			7	6	1		
82	CE	1	Total	N	Os	0	0
			7	6	1		
82	CG	1	Total	N	Os	0	0
			7	6	1		
82	CG	1	Total	N	Os	0	0
			7	6	1		
82	CG	1	Total	N	Os	0	0
			7	6	1		
82	CH	1	Total	N	Os	0	0
			7	6	1		
82	CK	1	Total	N	Os	0	0
			7	6	1		
82	CL	1	Total	N	Os	0	0
			7	6	1		
82	CL	1	Total	N	Os	0	0
			7	6	1		
82	CP	1	Total	N	Os	0	0
			7	6	1		
82	CS	1	Total	N	Os	0	0
			7	6	1		
82	CV	1	Total	N	Os	0	0
			7	6	1		
82	CX	1	Total	N	Os	0	0
			7	6	1		
82	DD	1	Total	N	Os	0	0
			7	6	1		
82	DH	1	Total	N	Os	0	0
			7	6	1		
82	DL	1	Total	N	Os	0	0
			7	6	1		
82	DQ	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	A	1	Total	N	Os	0	0
			7	6	1		
82	J	1	Total	N	Os	0	0
			7	6	1		
82	O	1	Total	N	Os	0	0
			7	6	1		
82	Q	1	Total	N	Os	0	0
			7	6	1		
82	T	1	Total	N	Os	0	0
			7	6	1		
82	U	1	Total	N	Os	0	0
			7	6	1		
82	h	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	sR	1	Total	N	Os	0	0
			7	6	1		
82	Rb	1	Total	N	Os	0	0
			7	6	1		
82	s1	1	Total	N	Os	0	0
			7	6	1		
82	s4	1	Total	N	Os	0	0
			7	6	1		
82	s8	1	Total	N	Os	0	0
			7	6	1		
82	c3	1	Total	N	Os	0	0
			7	6	1		
82	c5	1	Total	N	Os	0	0
			7	6	1		
82	c7	1	Total	N	Os	0	0
			7	6	1		
82	c8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	d4	1	Total	N	Os	0	0
			7	6	1		

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	1	486	Total	Mg	0	0
			486	486		
83	3	12	Total	Mg	0	0
			12	12		
83	4	18	Total	Mg	0	0
			18	18		
83	j	2	Total	Mg	0	0
			2	2		
83	k	2	Total	Mg	0	0
			2	2		
83	l	4	Total	Mg	0	0
			4	4		
83	m	1	Total	Mg	0	0
			1	1		
83	o	3	Total	Mg	0	0
			3	3		
83	r	2	Total	Mg	0	0
			2	2		
83	s	1	Total	Mg	0	0
			1	1		
83	t	2	Total	Mg	0	0
			2	2		
83	u	1	Total	Mg	0	0
			1	1		
83	v	4	Total	Mg	0	0
			4	4		
83	w	1	Total	Mg	0	0
			1	1		
83	x	8	Total	Mg	0	0
			8	8		
83	y	1	Total	Mg	0	0
			1	1		
83	z	1	Total	Mg	0	0
			1	1		
83	6	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	9	1	Total 1	Mg 1	0	0
83	AB	5	Total 5	Mg 5	0	0
83	AC	1	Total 1	Mg 1	0	0
83	AF	2	Total 2	Mg 2	0	0
83	AG	1	Total 1	Mg 1	0	0
83	AH	2	Total 2	Mg 2	0	0
83	AI	1	Total 1	Mg 1	0	0
83	AP	1	Total 1	Mg 1	0	0
83	i	1	Total 1	Mg 1	0	0
83	AR	498	Total 498	Mg 498	0	0
83	AS	19	Total 19	Mg 19	0	0
83	AT	19	Total 19	Mg 19	0	0
83	CD	1	Total 1	Mg 1	0	0
83	CE	3	Total 3	Mg 3	0	0
83	CF	5	Total 5	Mg 5	0	0
83	CG	1	Total 1	Mg 1	0	0
83	CI	2	Total 2	Mg 2	0	0
83	CJ	1	Total 1	Mg 1	0	0
83	CK	1	Total 1	Mg 1	0	0
83	CL	2	Total 2	Mg 2	0	0
83	CM	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	CO	1	Total 1	Mg 1	0	0
83	CP	5	Total 5	Mg 5	0	0
83	CQ	3	Total 3	Mg 3	0	0
83	CR	8	Total 8	Mg 8	0	0
83	CU	1	Total 1	Mg 1	0	0
83	CX	1	Total 1	Mg 1	0	0
83	DA	2	Total 2	Mg 2	0	0
83	DC	2	Total 2	Mg 2	0	0
83	DD	1	Total 1	Mg 1	0	0
83	DH	2	Total 2	Mg 2	0	0
83	DI	3	Total 3	Mg 3	0	0
83	DL	2	Total 2	Mg 2	0	0
83	DO	2	Total 2	Mg 2	0	0
83	DP	1	Total 1	Mg 1	0	0
83	DQ	2	Total 2	Mg 2	0	0
83	sM	2	Total 2	Mg 2	0	0
83	A	135	Total 135	Mg 135	0	0
83	D	2	Total 2	Mg 2	0	0
83	F	1	Total 1	Mg 1	0	0
83	O	1	Total 1	Mg 1	0	0
83	P	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	S	1	Total 1	Mg 1	0	0
83	X	1	Total 1	Mg 1	0	0
83	Y	1	Total 1	Mg 1	0	0
83	b	1	Total 1	Mg 1	0	0
83	sR	149	Total 149	Mg 149	0	0
83	s1	1	Total 1	Mg 1	0	0
83	s2	1	Total 1	Mg 1	0	0
83	s4	1	Total 1	Mg 1	0	0
83	s6	1	Total 1	Mg 1	0	0
83	s8	2	Total 2	Mg 2	0	0
83	s9	1	Total 1	Mg 1	0	0
83	c1	1	Total 1	Mg 1	0	0
83	c3	1	Total 1	Mg 1	0	0
83	c4	2	Total 2	Mg 2	0	0
83	c6	1	Total 1	Mg 1	0	0
83	c8	1	Total 1	Mg 1	0	0
83	c9	2	Total 2	Mg 2	0	0
83	d3	3	Total 3	Mg 3	0	0
83	d4	3	Total 3	Mg 3	0	0
83	d5	1	Total 1	Mg 1	0	0
83	d6	2	Total 2	Mg 2	0	0

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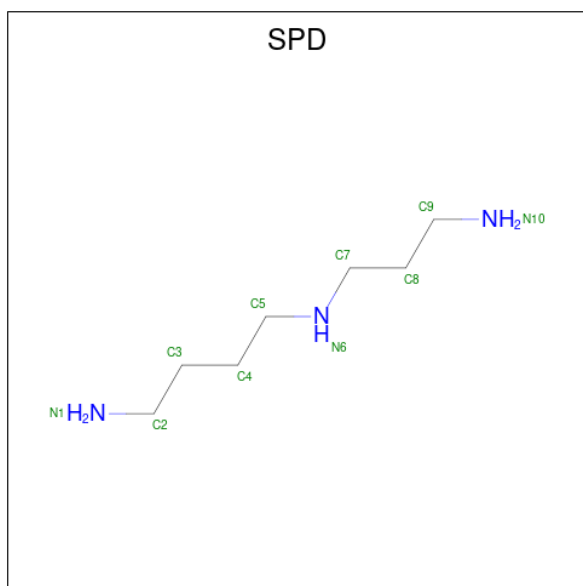
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	d9	1	Total	Mg	0	0
			1	1		

- Molecule 84 is POTASSIUM ION (CCD ID: K) (formula: K).

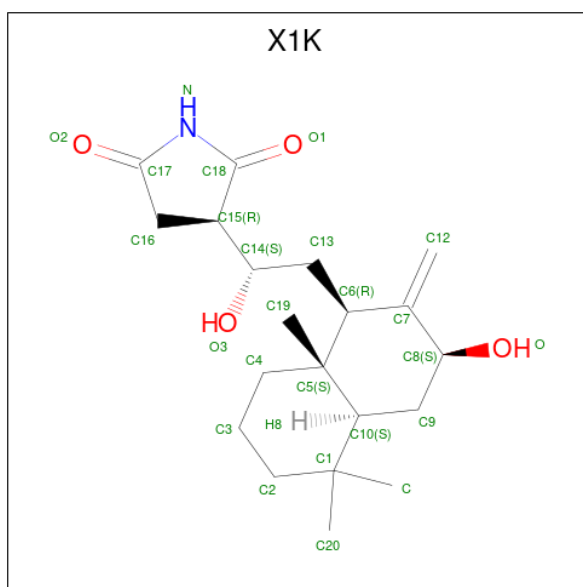
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	1	1	Total	K	0	0
			1	1		
84	j	1	Total	K	0	0
			1	1		
84	AR	4	Total	K	0	0
			4	4		
84	sR	1	Total	K	0	0
			1	1		

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



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

- Molecule 86 is (3 {R})-3-[(1 {S})-2-[(1 {R},3 {S},4 {a} {S},8 {a} {S})-5,5,8 {a}-trimethyl-2-methylidene-3-oxidanyl-3,4,4 {a},6,7,8-hexahydro-1 {H}-naphthalen-1-yl]-1-oxidanyl-ethyl]pyrrolidine-2,5-dione (CCD ID: X1K) (formula: C₂₀H₃₁NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
86	1	1	Total	C	N	O	0	0
			25	20	1	4		
86	AR	1	Total	C	N	O	0	0
			25	20	1	4		

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	e	1	Total 1	Zn 1	0	0
87	g	1	Total 1	Zn 1	0	0
87	d6	1	Total 1	Zn 1	0	0
87	d7	1	Total 1	Zn 1	0	0
87	d9	1	Total 1	Zn 1	0	0

- Molecule 88 is OSMIUM ION (CCD ID: OS) (formula: Os).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	A	1	Total 1	Os 1	0	0

- Molecule 89 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
89	1	148	Total 148	O 148	0	0
89	4	14	Total 14	O 14	0	0
89	j	1	Total 1	O 1	0	0
89	x	4	Total 4	O 4	0	0
89	AE	2	Total 2	O 2	0	0
89	AO	1	Total 1	O 1	0	0
89	AR	210	Total 210	O 210	0	0
89	CD	1	Total 1	O 1	0	0
89	CF	7	Total 7	O 7	0	0
89	CI	1	Total 1	O 1	0	0
89	CP	1	Total 1	O 1	0	0

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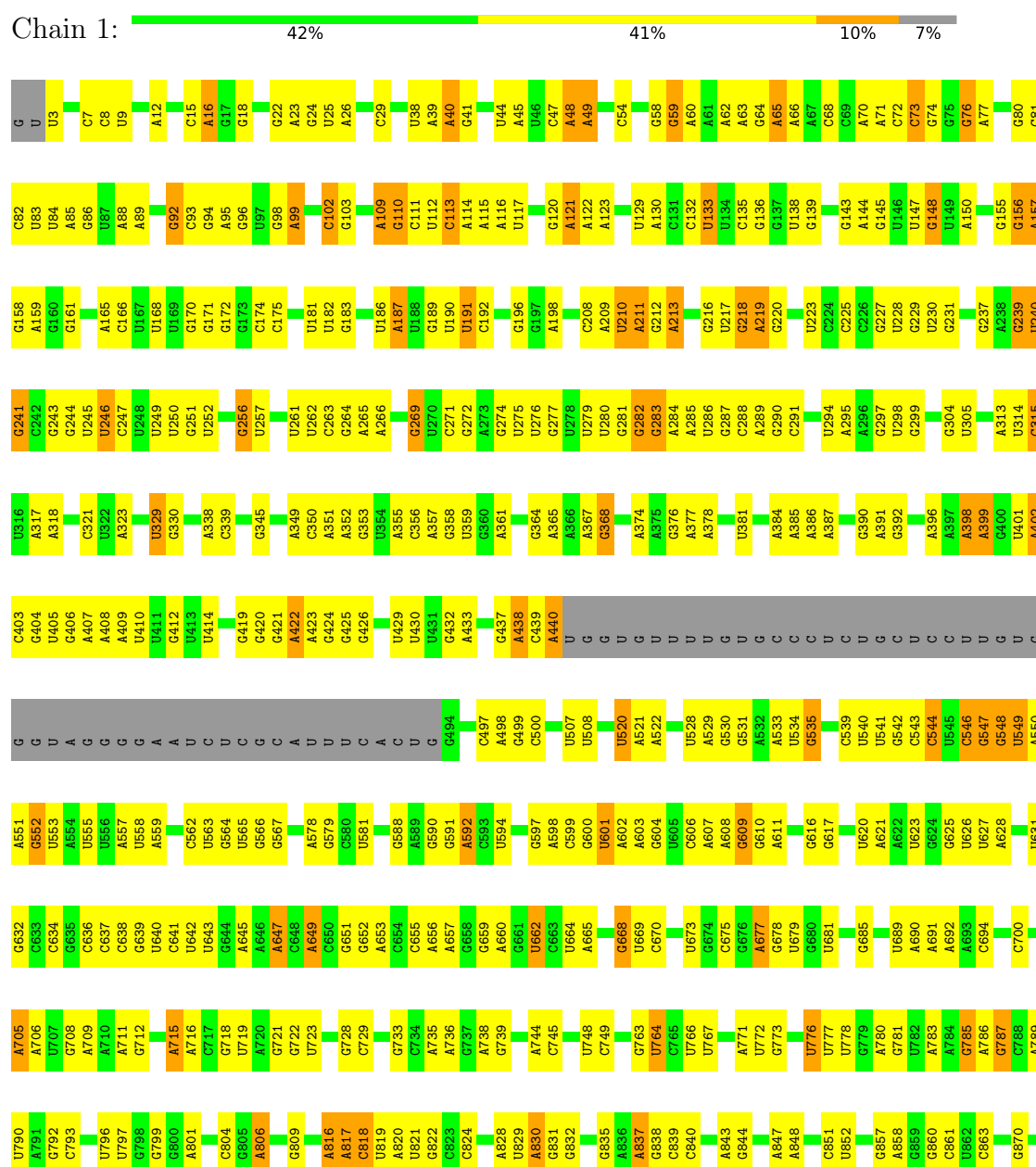
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
89	CR	1	Total 1	O 1	0	0
89	CT	1	Total 1	O 1	0	0
89	DG	1	Total 1	O 1	0	0
89	A	57	Total 57	O 57	0	0
89	R	1	Total 1	O 1	0	0
89	S	6	Total 6	O 6	0	0
89	Y	1	Total 1	O 1	0	0
89	sR	41	Total 41	O 41	0	0
89	s8	1	Total 1	O 1	0	0
89	c1	1	Total 1	O 1	0	0
89	c7	2	Total 2	O 2	0	0

3 Residue-property plots

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

Note EDS failed to run properly.

• Molecule 1: 25S ribosomal RNA

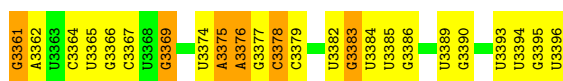




A3123	U3050	U2985	A2887	A2812	A2736	G2658	U2565	U	A2424	A2348	U2258	C2181	G2095	G
G3128	G3053	G2968	A2887	C2812	C2737	G2659	C2566	A	G2425	U2349	A2259	A2182	A2096	U
A3129	U3054	A2969	A2890	A2813	A2740	G2660	A2569	C	U2426	U2260	U2260	G2187	C2097	G
A3130	U3055	C2970	G2895	G2815	C2741	G2662	U2570	A	U2427	U2261	C2261	C2188	C2098	C
U3131	U3056	A2971	G2896	A2817	C2742	G2663	U2571	C	G2428	A2352	A2262	U2189	A2100	C
U3135	U3057	G2972	A2897	U2818	A2743	A2667	C2572	U	U2429	C2354	C2263	U2190	C2101	U
U3138	G3059	U2979	A2898	U2822	U2744	A2668	G2573	A	U2433	G2355	C2267	U2191	U2102	U
A3139	C3060	C2983	C2899	G2823	G2745	U2669	G2574	C	U2434	A2356	U2268	U2192	U2103	U
G3140	G3061	C2984	A2900	U2824	A2746	G2670	G2575	U	G2435	A2357	A2269	U2193	A2104	U
A3141	C3067	C2985	G2901	G2825	A2747	A2673	C2577	U	A2438	C2359	A2271	U2202	A2107	U
A3142	U3068	U2986	A2902	C2826	U2748	C2675	U2578	U	A2439	C2360	G2272	U2203	C2108	A
C3143	A2987	U2987	U2904	U2827	U2751	A2676	G2579	A	G2440	A2361	C2273	G2204		G
C3144	C2988	G2989	U2905	U2828	U2752	A2677		U2501	U2442	C2363	U2274	U2205		C
C3145	U2989	U2989	G2906	U2829	U2753	A2678	G2584	G2502	A2443	G2369	C2278	U2212	U2112	C
G3146	G2990	U2991	G2908	U2830	U2754	A2679	G2585	G2503	C2444	G2370	A2281	U2210	A2113	G
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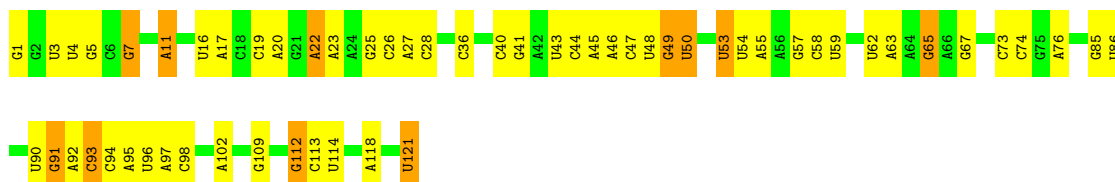


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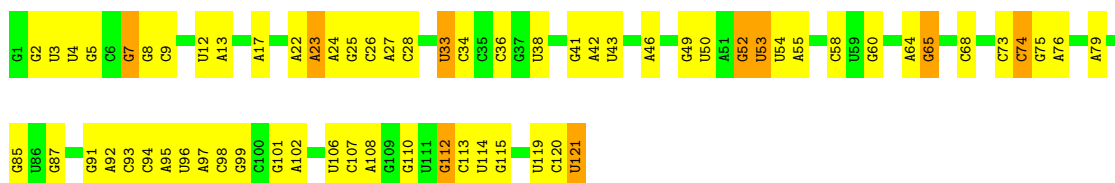
• Molecule 2: 5S ribosomal RNA

Chain 3: 52% 39% 9%



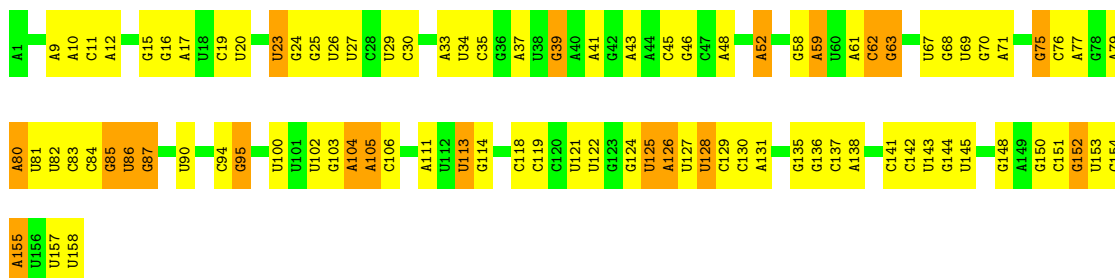
• Molecule 2: 5S ribosomal RNA

Chain AS: 46% 46% 7%



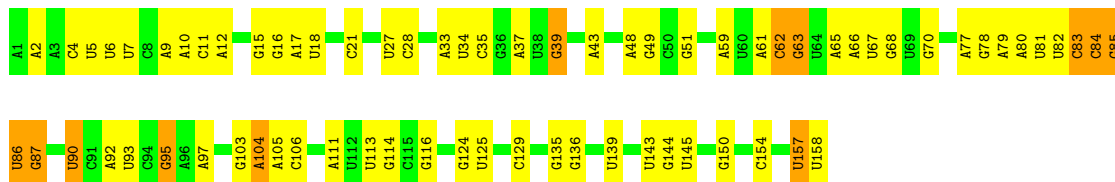
• Molecule 3: 5.8S ribosomal RNA

Chain 4: 42% 45% 13%



• Molecule 3: 5.8S ribosomal RNA

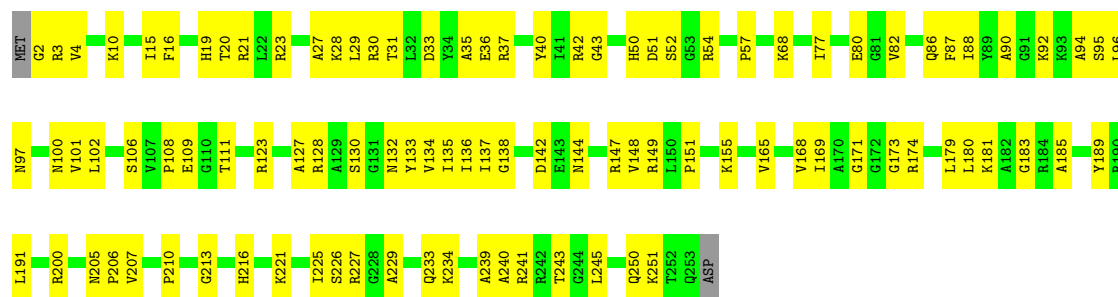
Chain AT: 55% 37% 8%



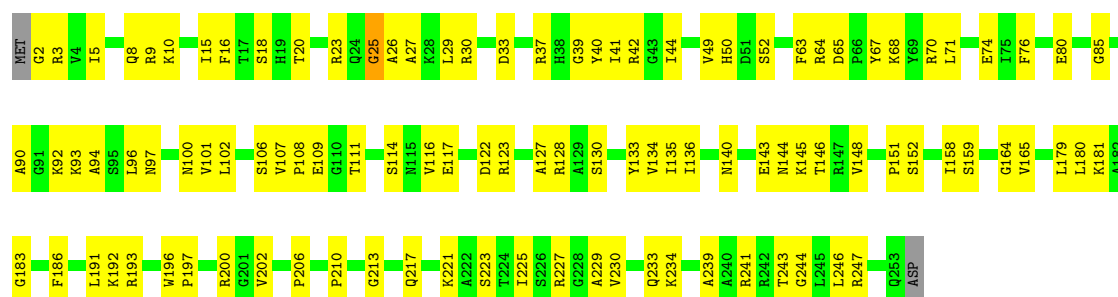
• Molecule 4: 60S ribosomal protein L2-A

Chain j: 60% 39%

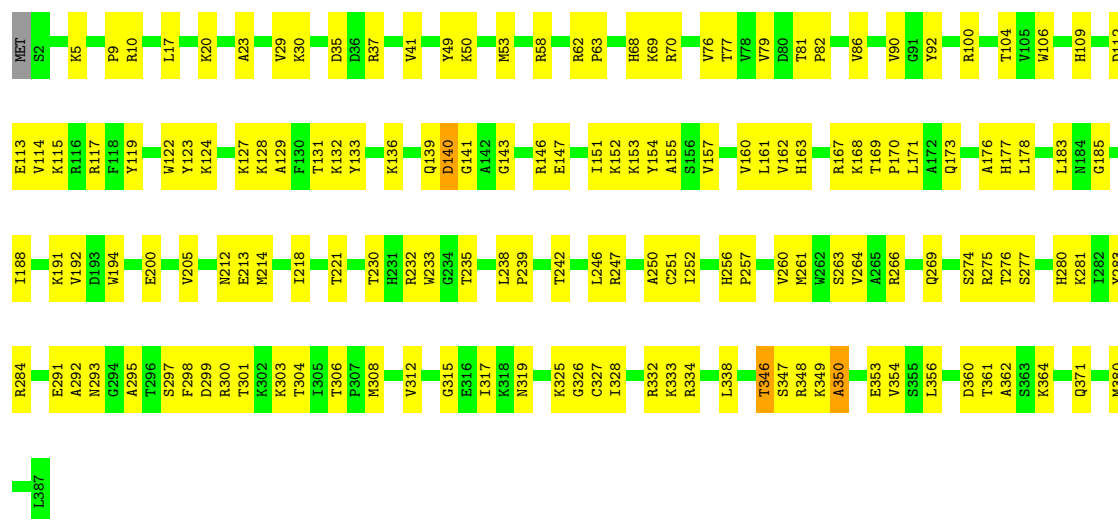




• Molecule 4: 60S ribosomal protein L2-A



• Molecule 5: 60S ribosomal protein L3

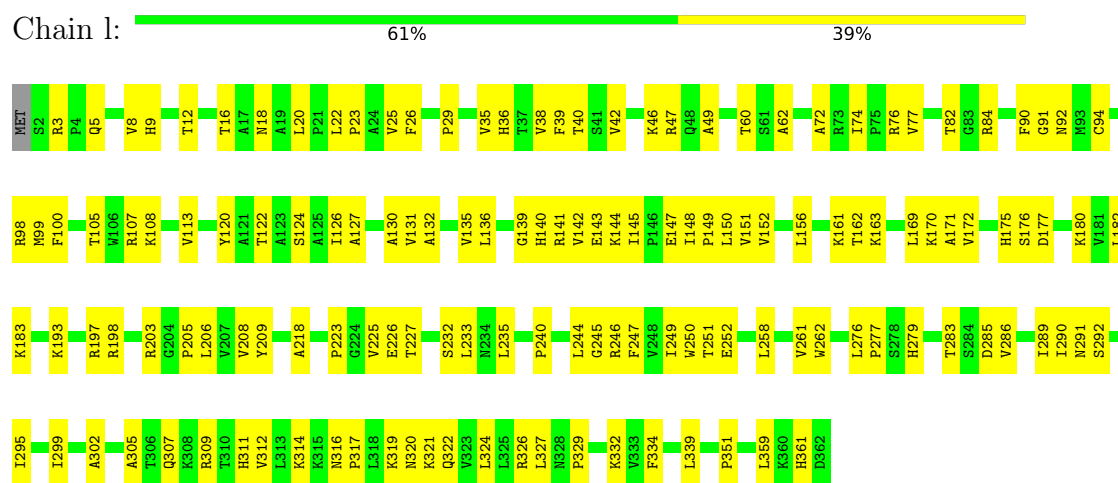


• Molecule 5: 60S ribosomal protein L3

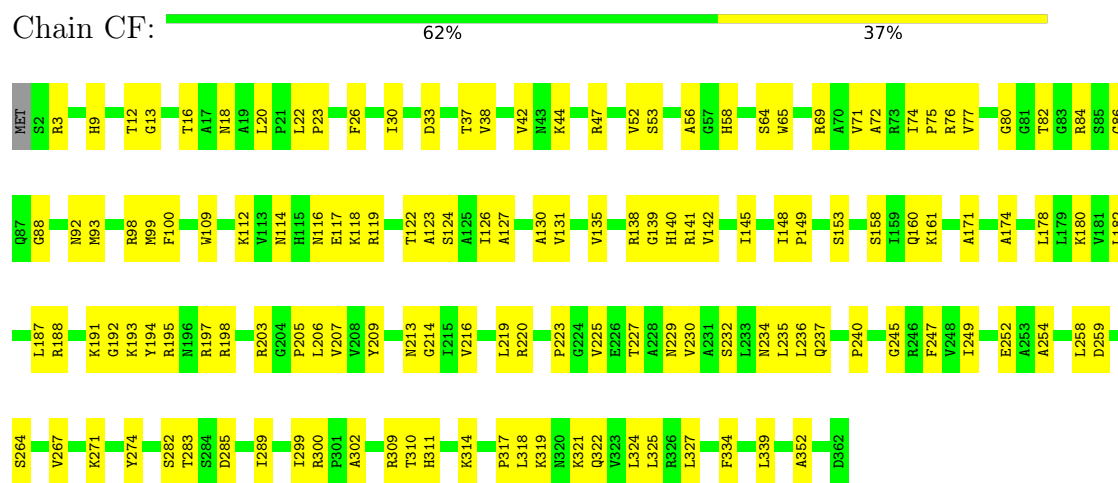




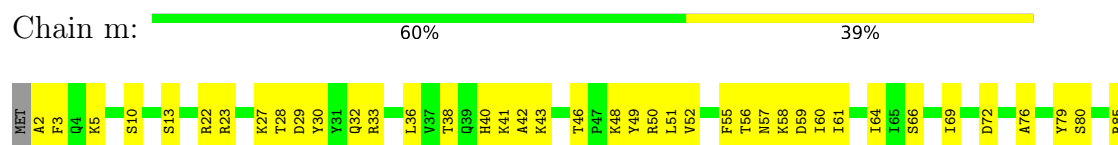
• Molecule 6: 60S ribosomal protein L4-A

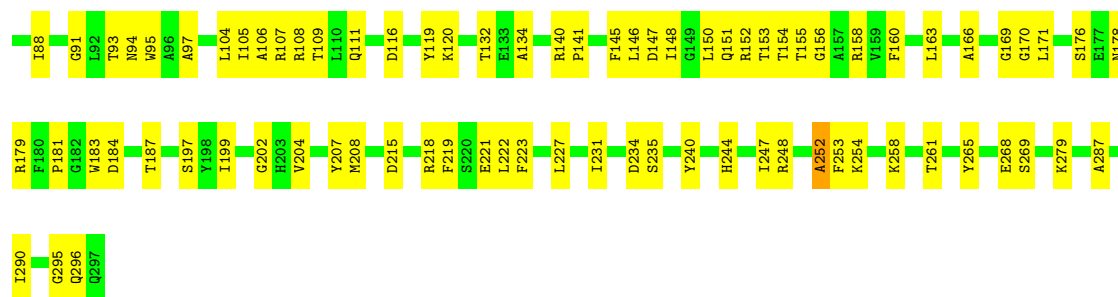


• Molecule 6: 60S ribosomal protein L4-A

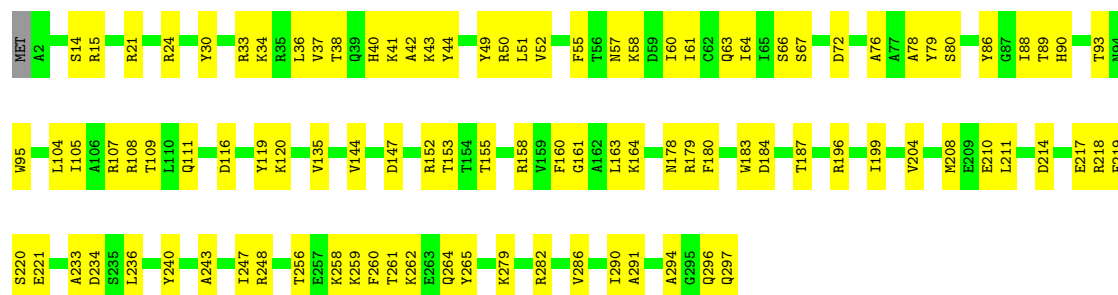


• Molecule 7: 60S ribosomal protein L5

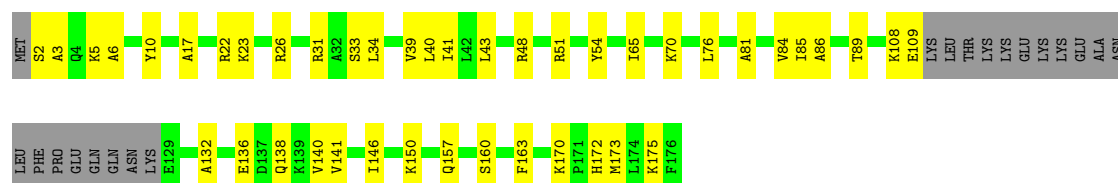




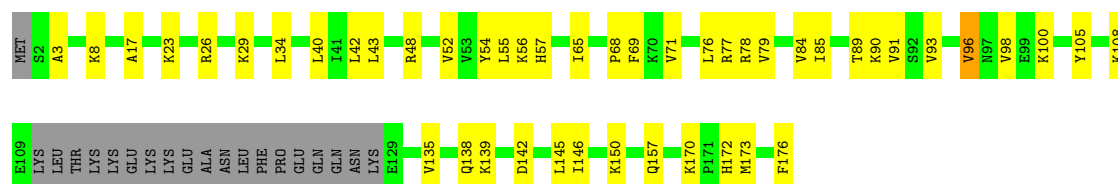
• Molecule 7: 60S ribosomal protein L5



• Molecule 8: 60S ribosomal protein L6-A

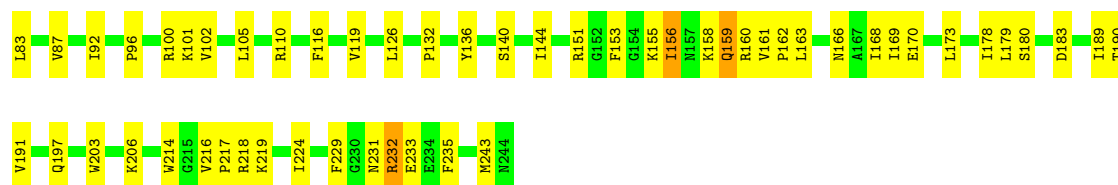


• Molecule 8: 60S ribosomal protein L6-A



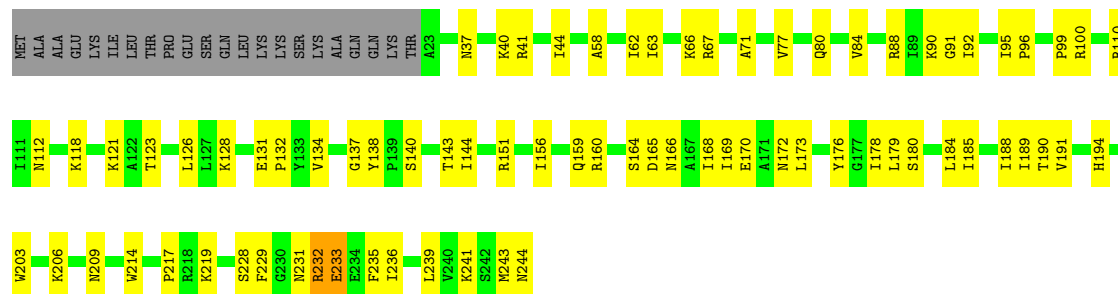
• Molecule 9: 60S ribosomal protein L7-A





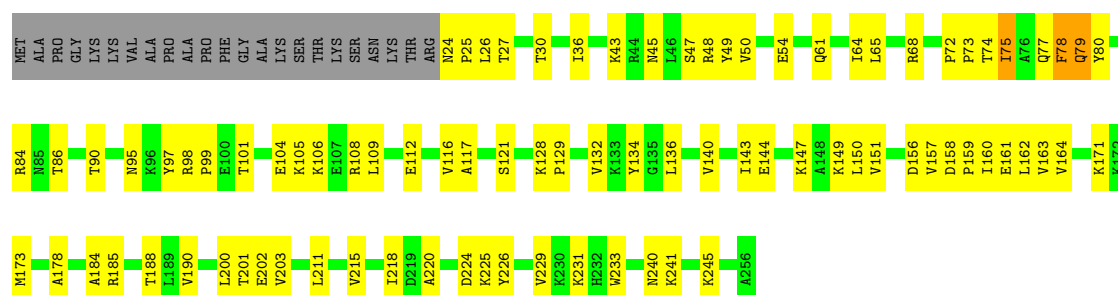
• Molecule 9: 60S ribosomal protein L7-A

Chain CI: 60% 30% 9%



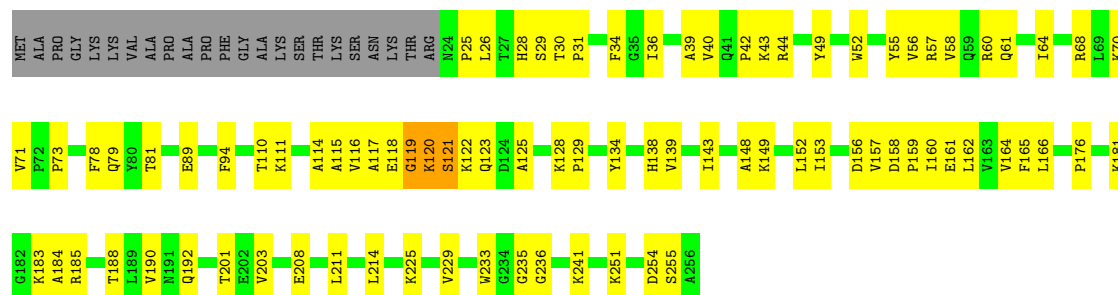
• Molecule 10: 60S ribosomal protein L8-A

Chain p: 57% 33% 9%



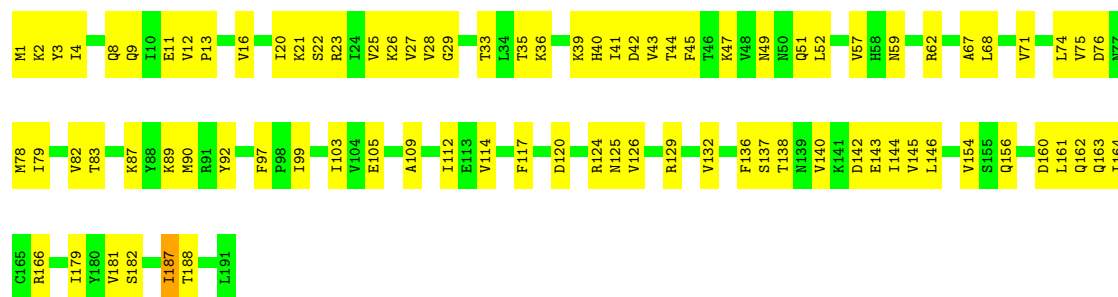
• Molecule 10: 60S ribosomal protein L8-A

Chain CJ: 57% 32% 9%

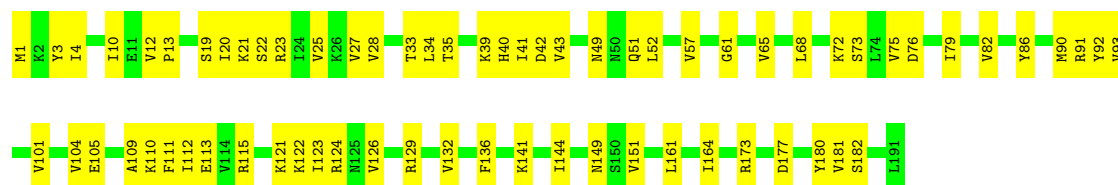


• Molecule 11: 60S ribosomal protein L9-A

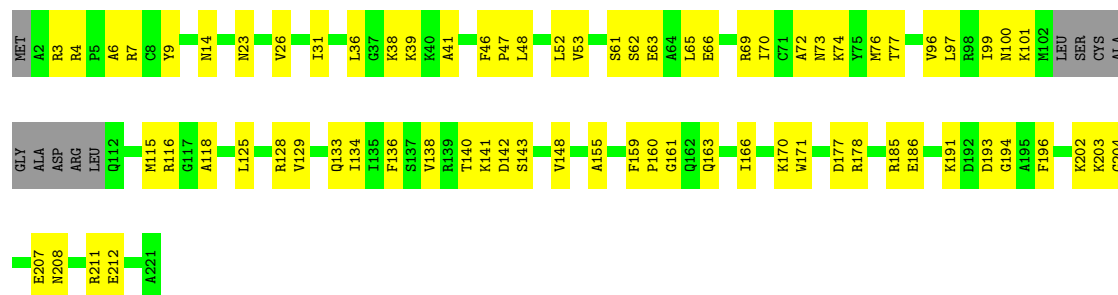
Chain q: 55% 45%



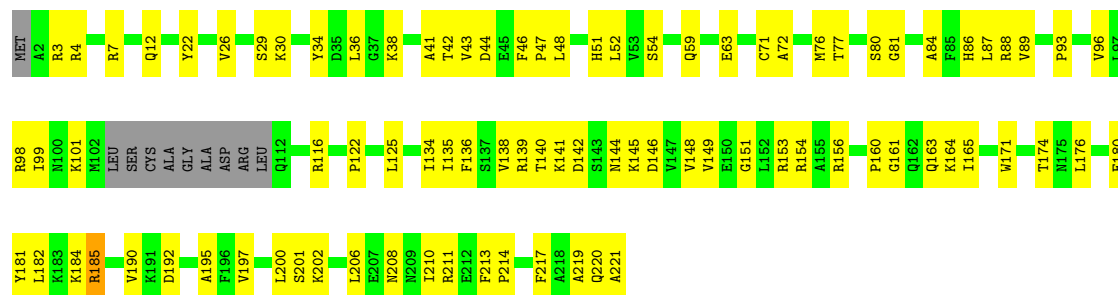
- Molecule 11: 60S ribosomal protein L9-A



- Molecule 12: 60S ribosomal protein L10

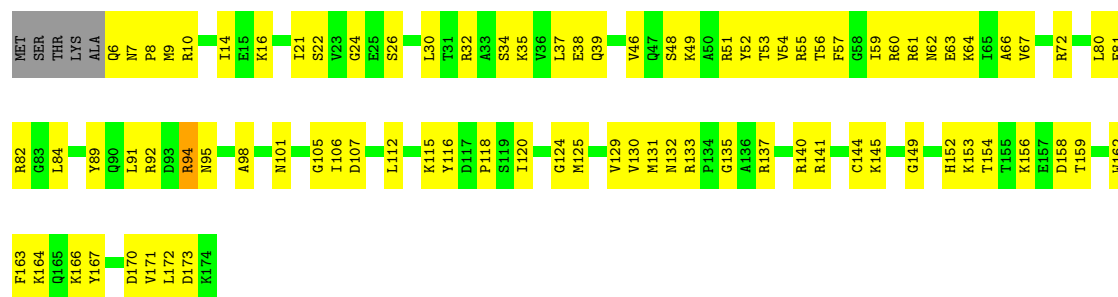


- Molecule 12: 60S ribosomal protein L10



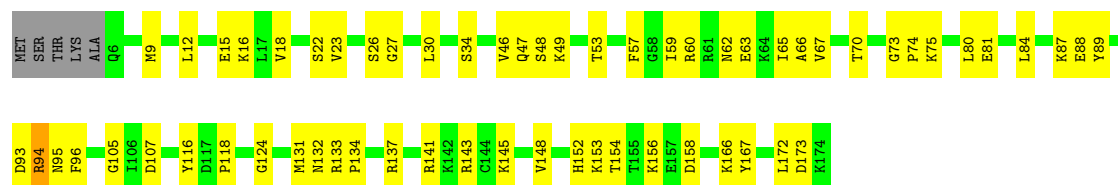
- Molecule 13: Large ribosomal subunit protein uL5B





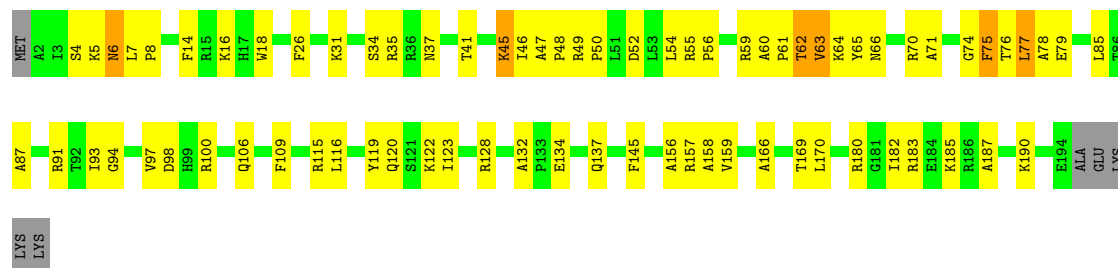
- Molecule 13: Large ribosomal subunit protein uL5B

Chain CM: 62% 34%



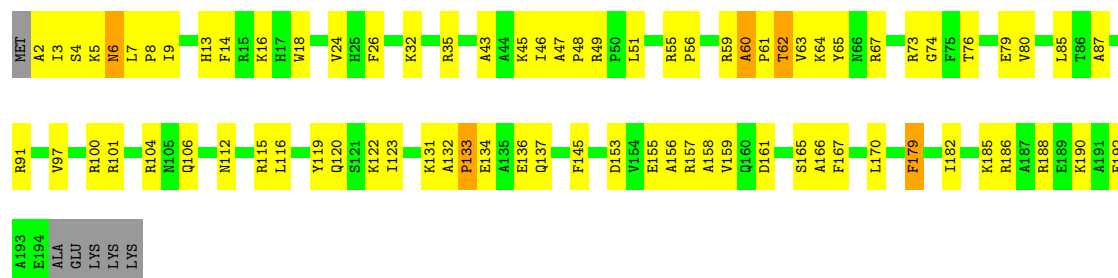
- Molecule 14: 60S ribosomal protein L13-A

Chain t: 60% 34%



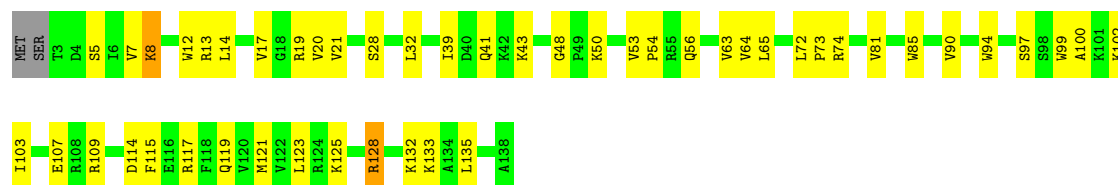
- Molecule 14: 60S ribosomal protein L13-A

Chain CN: 58% 37%



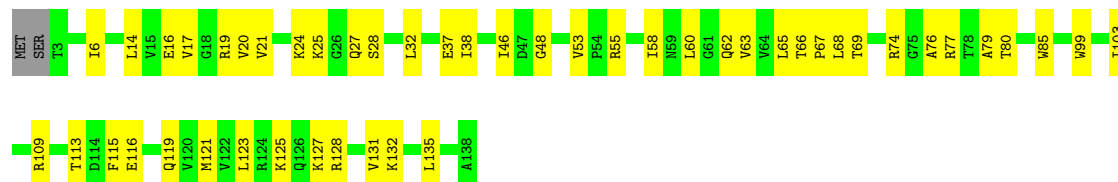
- Molecule 15: 60S ribosomal protein L14-A

Chain u: 64% 33%



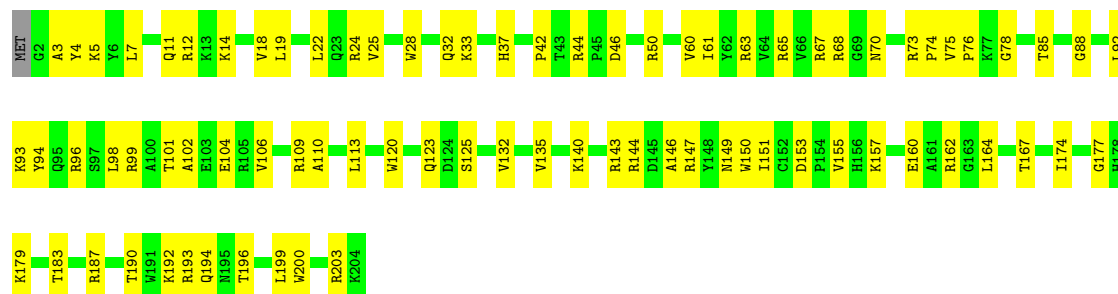
- Molecule 15: 60S ribosomal protein L14-A

Chain CO: 64% 35% .



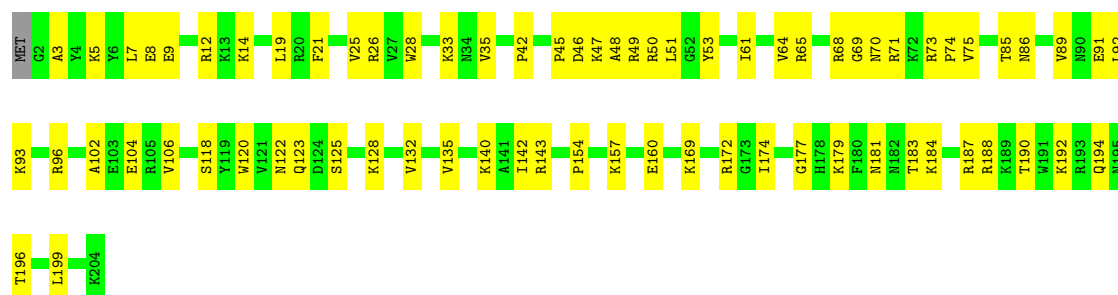
- Molecule 16: 60S ribosomal protein L15-A

Chain v: 60% 39%



- Molecule 16: 60S ribosomal protein L15-A

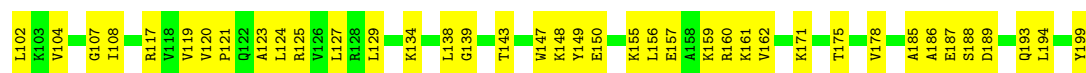
Chain CP: 64% 35%



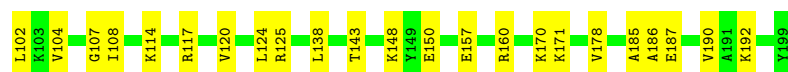
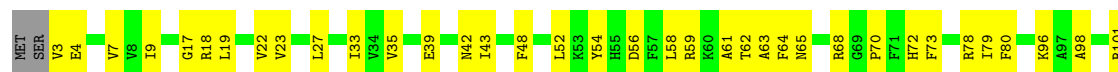
- Molecule 17: 60S ribosomal protein L16-A

Chain w: 63% 36% .





- Molecule 17: 60S ribosomal protein L16-A



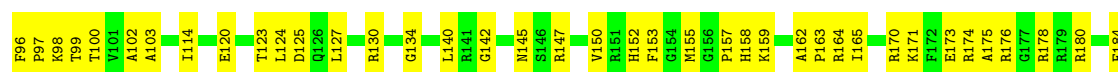
- Molecule 18: 60S ribosomal protein L17-A



- Molecule 18: 60S ribosomal protein L17-A

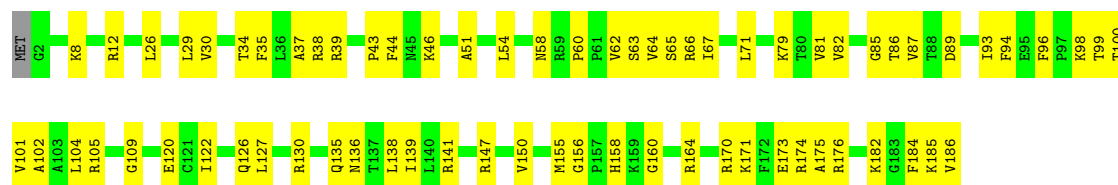


- Molecule 19: 60S ribosomal protein L18-A

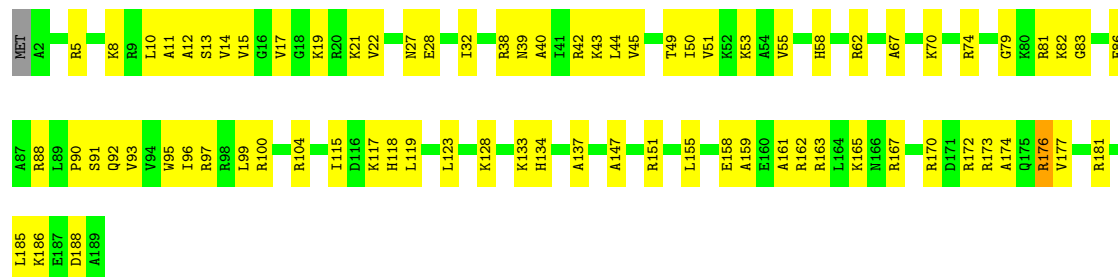


- Molecule 19: 60S ribosomal protein L18-A

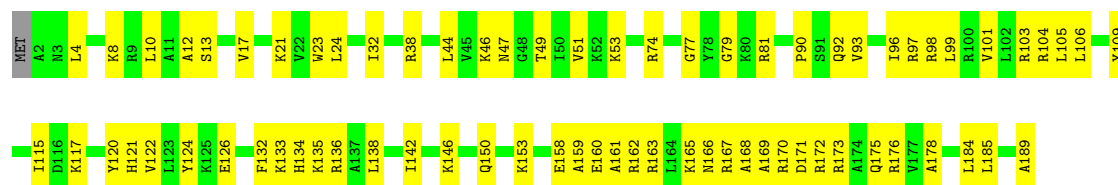




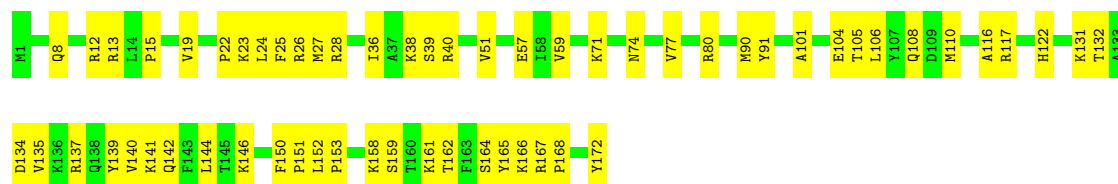
• Molecule 20: 60S ribosomal protein L19-A



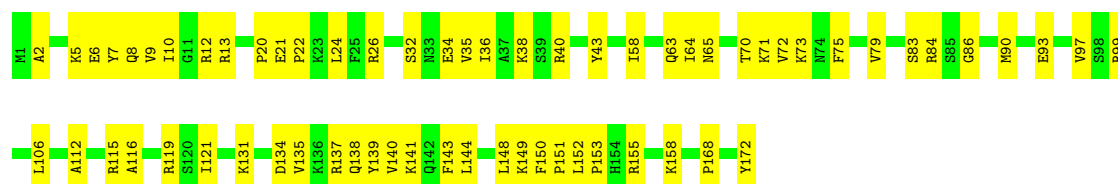
• Molecule 20: 60S ribosomal protein L19-A



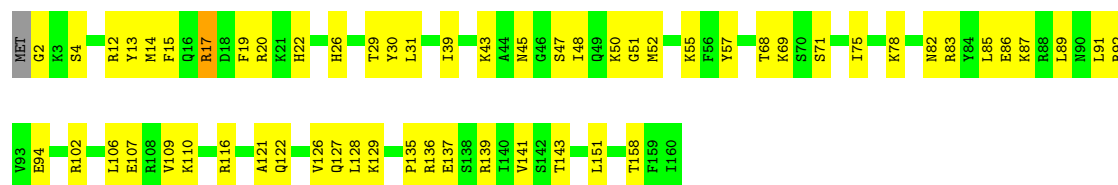
• Molecule 21: 60S ribosomal protein L20-A



• Molecule 21: 60S ribosomal protein L20-A



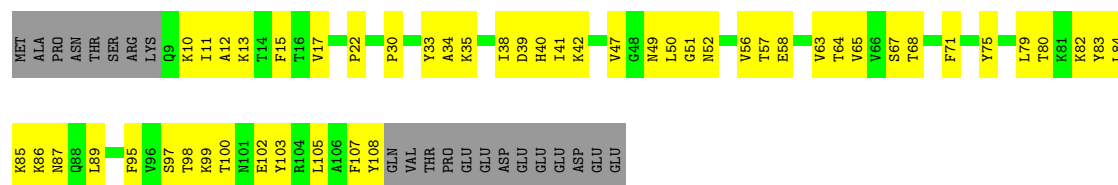
Chain 2: 63% 36% ..



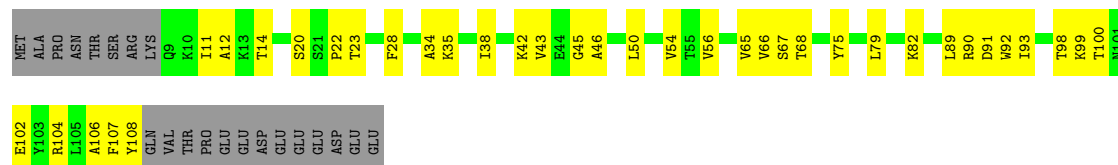
Chain CV: 69% 30%



Chain 5: 41% 41% 17%



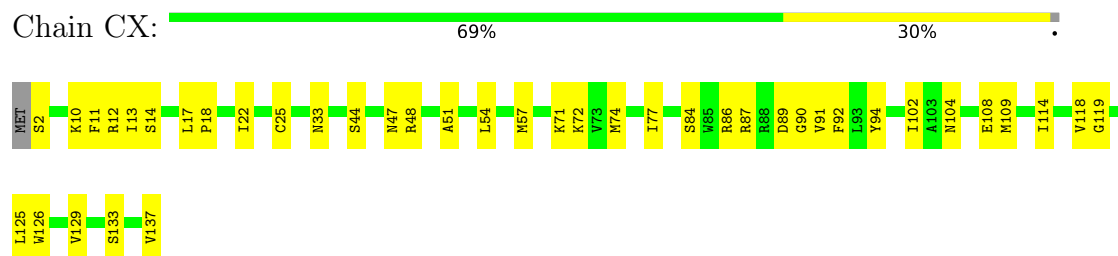
Chain CW:



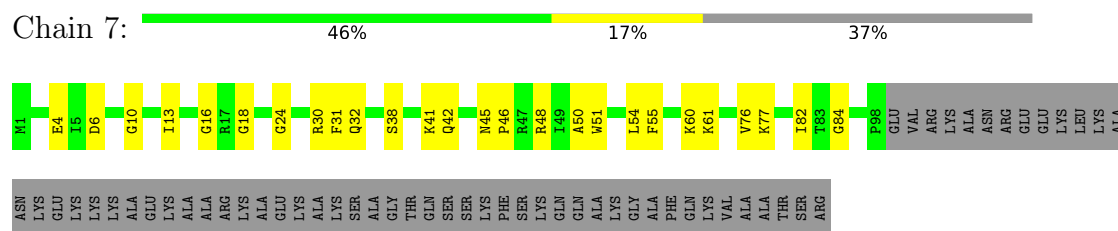
Chain 6: 60% 39%



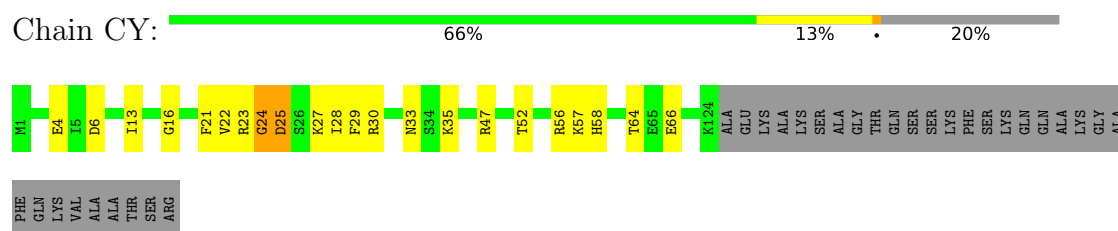
- Molecule 24: 60S ribosomal protein L23-A



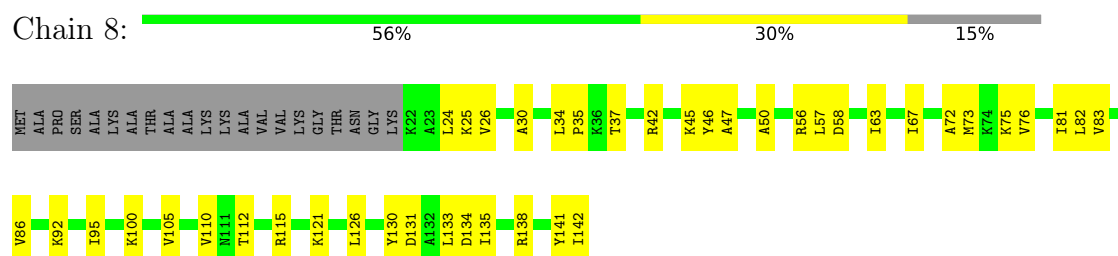
- Molecule 25: 60S ribosomal protein L24-A



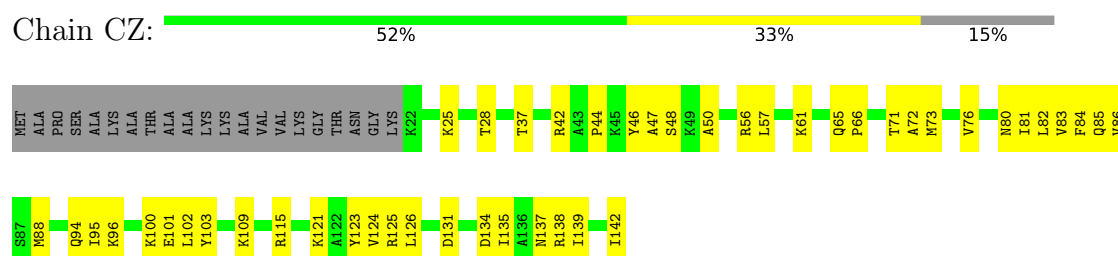
- Molecule 25: 60S ribosomal protein L24-A



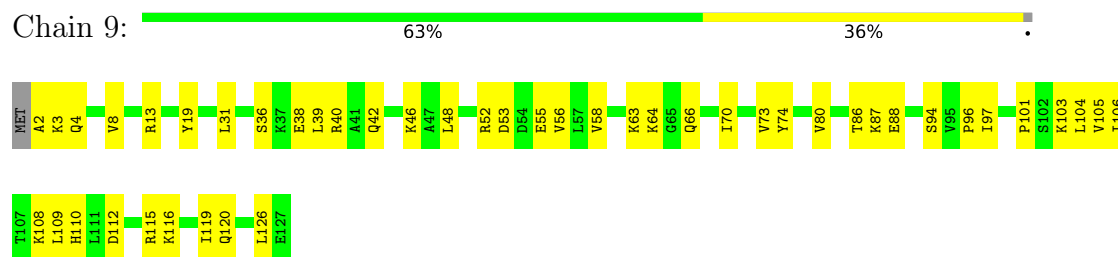
- Molecule 26: 60S ribosomal protein L25



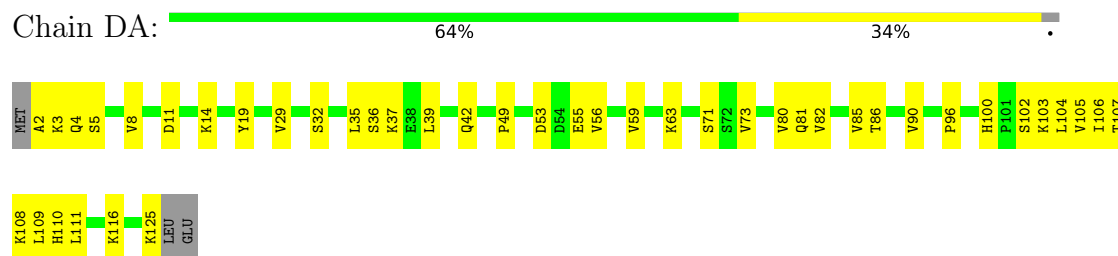
- Molecule 26: 60S ribosomal protein L25



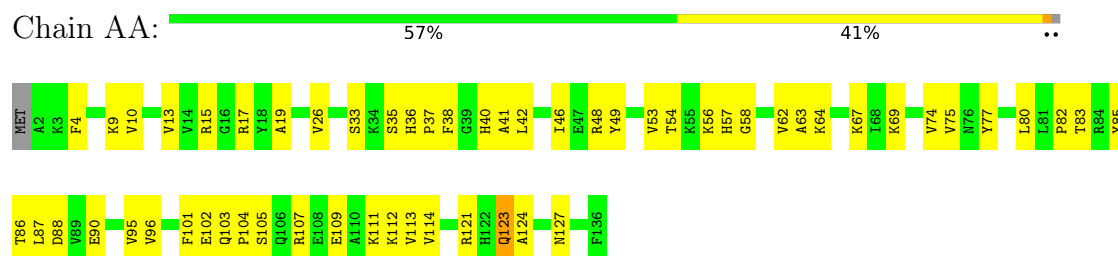
- Molecule 27: 60S ribosomal protein L26-A



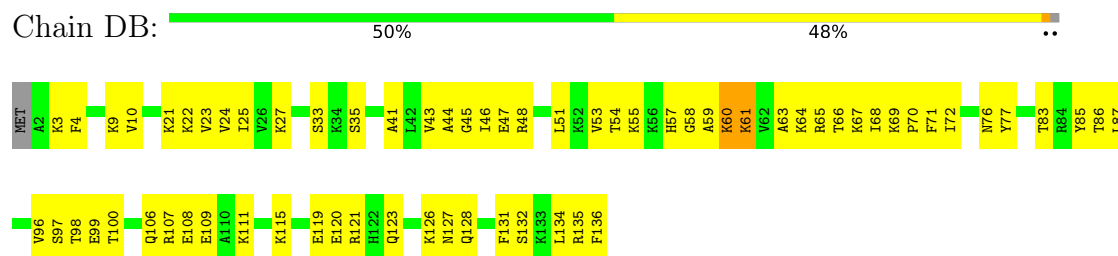
- Molecule 27: 60S ribosomal protein L26-A



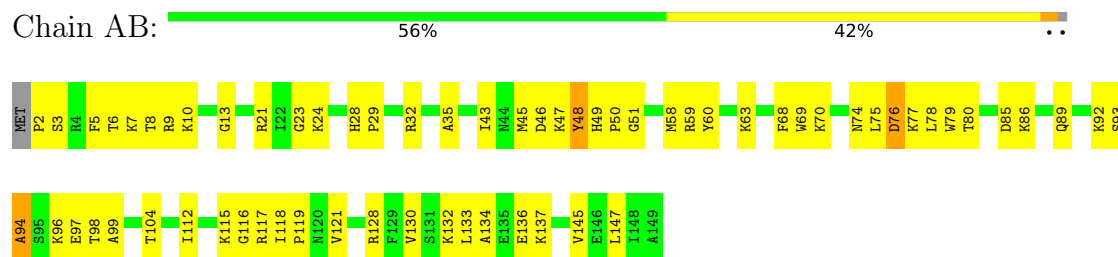
- Molecule 28: 60S ribosomal protein L27-A



- Molecule 28: 60S ribosomal protein L27-A

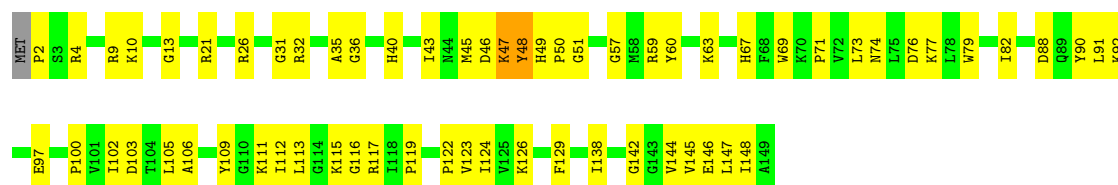


- Molecule 29: 60S ribosomal protein L28



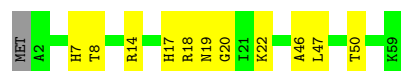
- Molecule 29: 60S ribosomal protein L28

Chain DC:  57% 41% ..



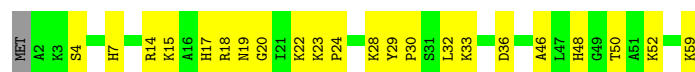
- Molecule 30: 60S ribosomal protein L29

Chain AC:  80% 19% .



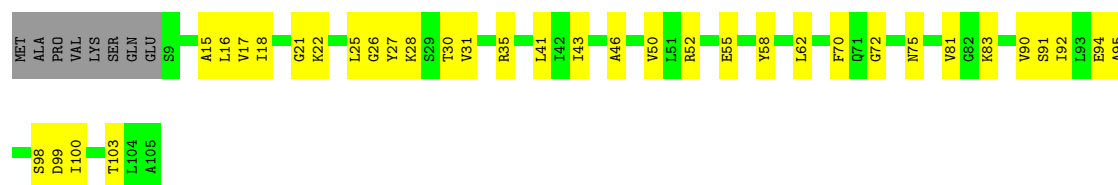
- Molecule 30: 60S ribosomal protein L29

Chain DD:  61% 37% .



- Molecule 31: 60S ribosomal protein L30

Chain AD:  59% 33% 8%



- Molecule 31: 60S ribosomal protein L30

Chain DE:  63% 30% 8%



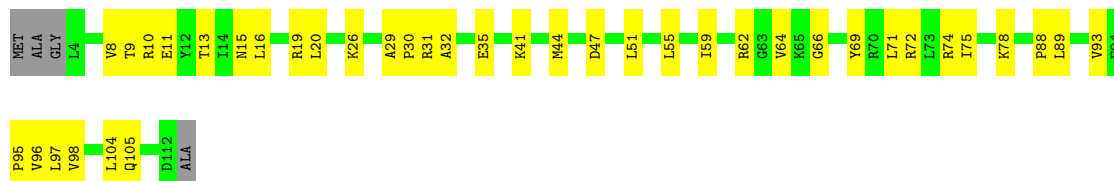
- Molecule 32: 60S ribosomal protein L31-A

Chain AE:  72% 25% .

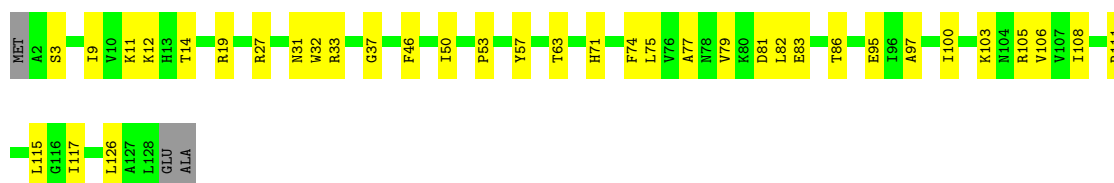


ALA

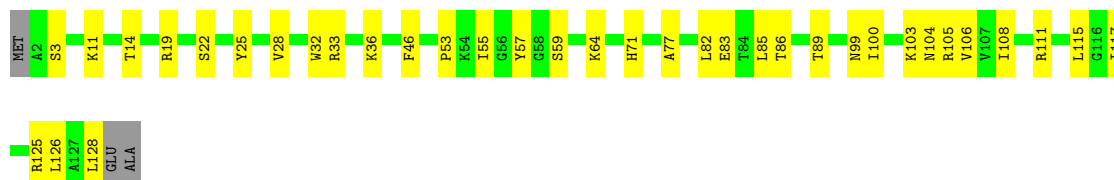
- Molecule 32: 60S ribosomal protein L31-A

Chain DF:  62% 35%

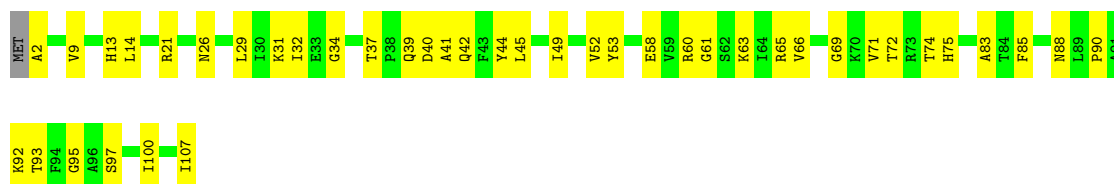
- Molecule 33: 60S ribosomal protein L32

Chain AF:  70% 28%

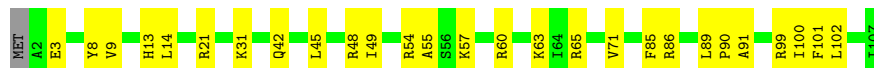
- Molecule 33: 60S ribosomal protein L32

Chain DG:  70% 28%

- Molecule 34: 60S ribosomal protein L33-A

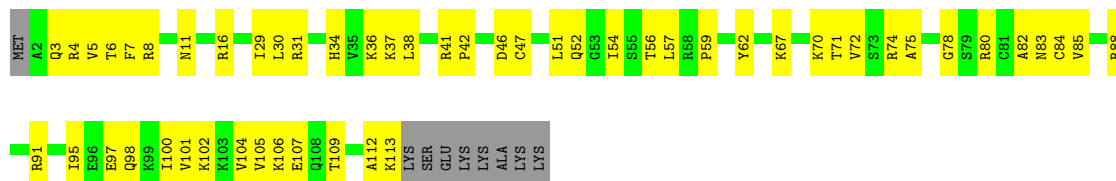
Chain AG:  61% 38%

- Molecule 34: 60S ribosomal protein L33-A

Chain DH:  74% 25%

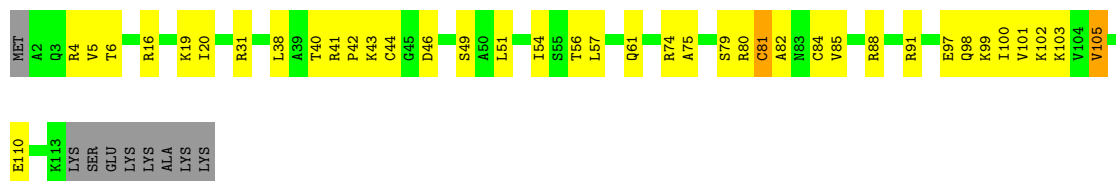
- Molecule 35: 60S ribosomal protein L34-A

Chain AH:  49% 44% 7%



- Molecule 35: 60S ribosomal protein L34-A

Chain DI:  60% 31% 7%



- Molecule 36: 60S ribosomal protein L35-A

Chain AI:  64% 34% ..



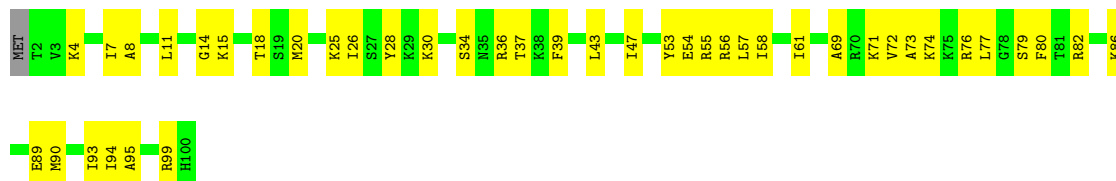
- Molecule 36: 60S ribosomal protein L35-A

Chain DJ:  73% 26% .



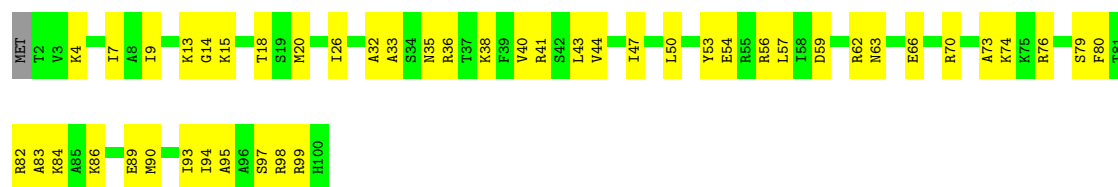
- Molecule 37: 60S ribosomal protein L36-A

Chain AJ:  57% 42% .



- Molecule 37: 60S ribosomal protein L36-A

Chain DK:  53% 46%



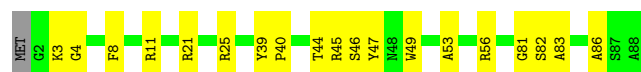
- Molecule 38: 60S ribosomal protein L37-A

Chain AK:  64% 35%



- Molecule 38: 60S ribosomal protein L37-A

Chain DL:  77% 22%



- Molecule 39: 60S ribosomal protein L38

Chain AL:  53% 46%



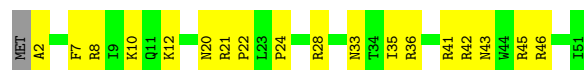
- Molecule 39: 60S ribosomal protein L38

Chain DM:  72% 26%



- Molecule 40: 60S ribosomal protein L39

Chain AM:  63% 35%



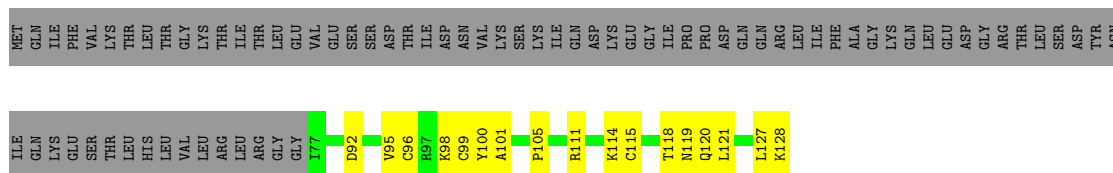
- Molecule 40: 60S ribosomal protein L39

Chain DN:  71% 27%



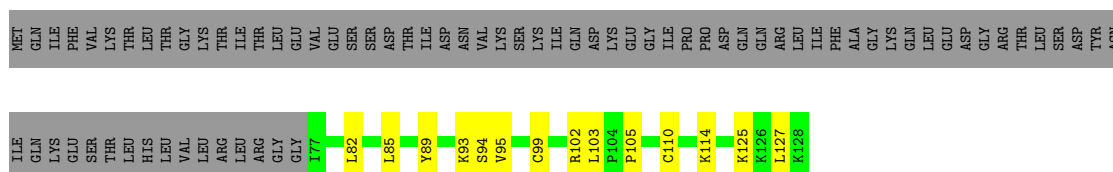
- Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain AN:  27% 13% 59%



- Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain DO:  30% 11% 59%



- Molecule 42: 60S ribosomal protein L41-A

Chain AO:  72% 28%



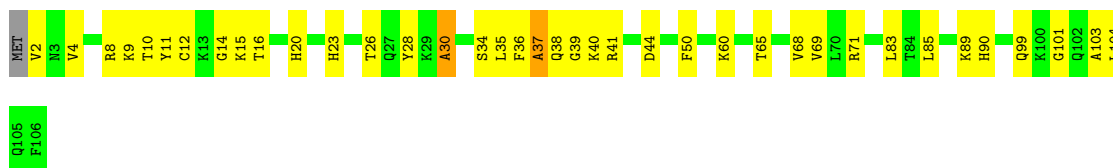
- Molecule 42: 60S ribosomal protein L41-A

Chain DP:  60% 40%



- Molecule 43: 60S ribosomal protein L42-A

Chain AP:  63% 34% ..



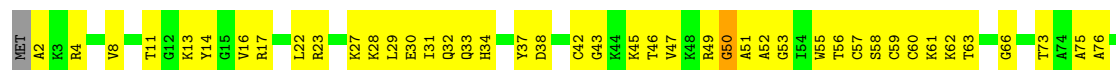
- Molecule 43: 60S ribosomal protein L42-A

Chain DQ:  52% 46% ..





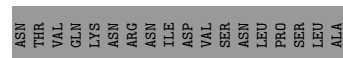
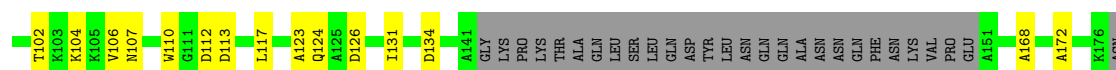
- Molecule 44: 60S ribosomal protein L43-A



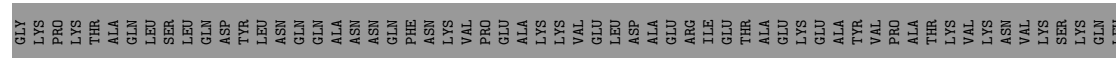
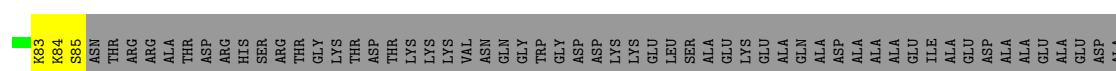
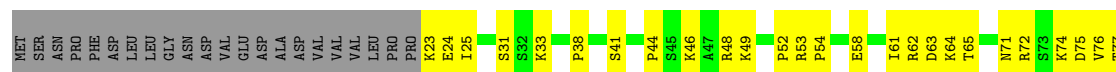
- Molecule 44: 60S ribosomal protein L43-A



- Molecule 45: Suppressor protein STM1



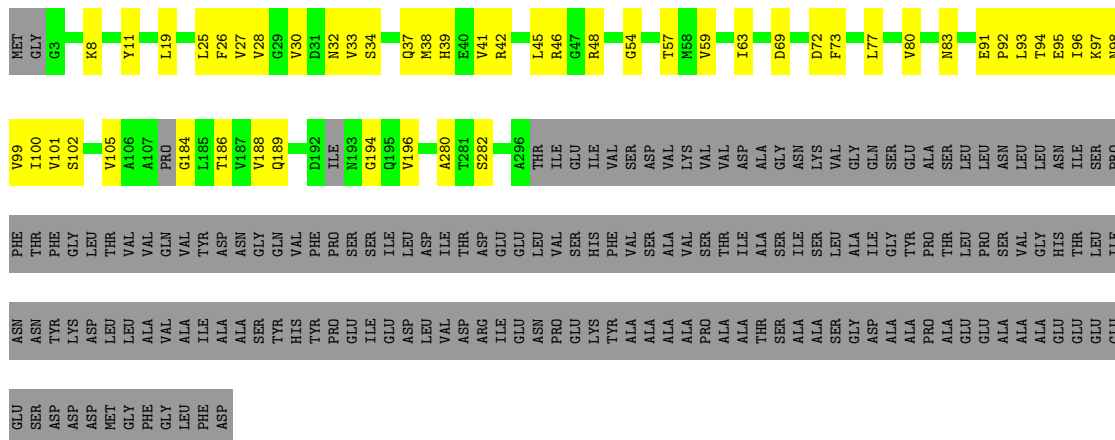
- Molecule 45: Suppressor protein STM1



ARG
ASN
ILE
ASP
VAL
SER
ASN
LEU
PRO
SER
LEU
ALA

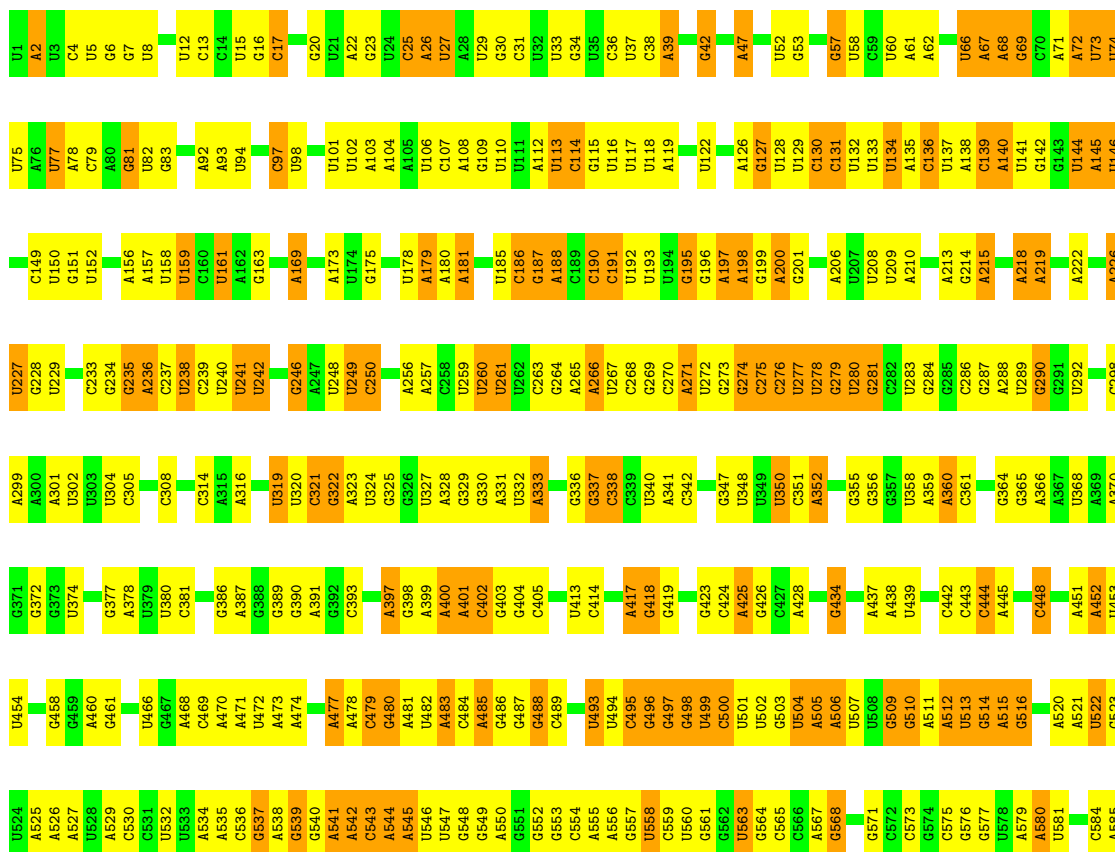
• Molecule 46: 60S acidic protein P0

Chain p0: 30% 16% 54%

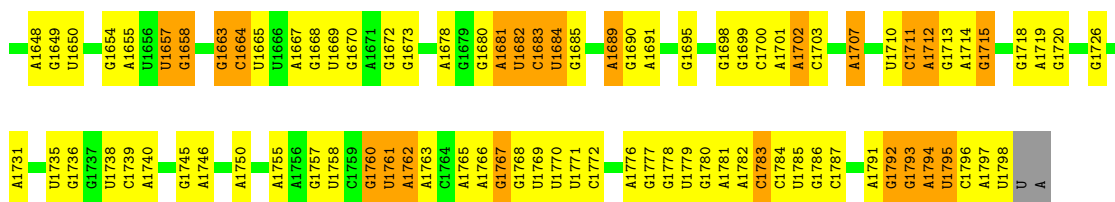


• Molecule 47: 18S ribosomal RNA

Chain A: 35% 47% 18%

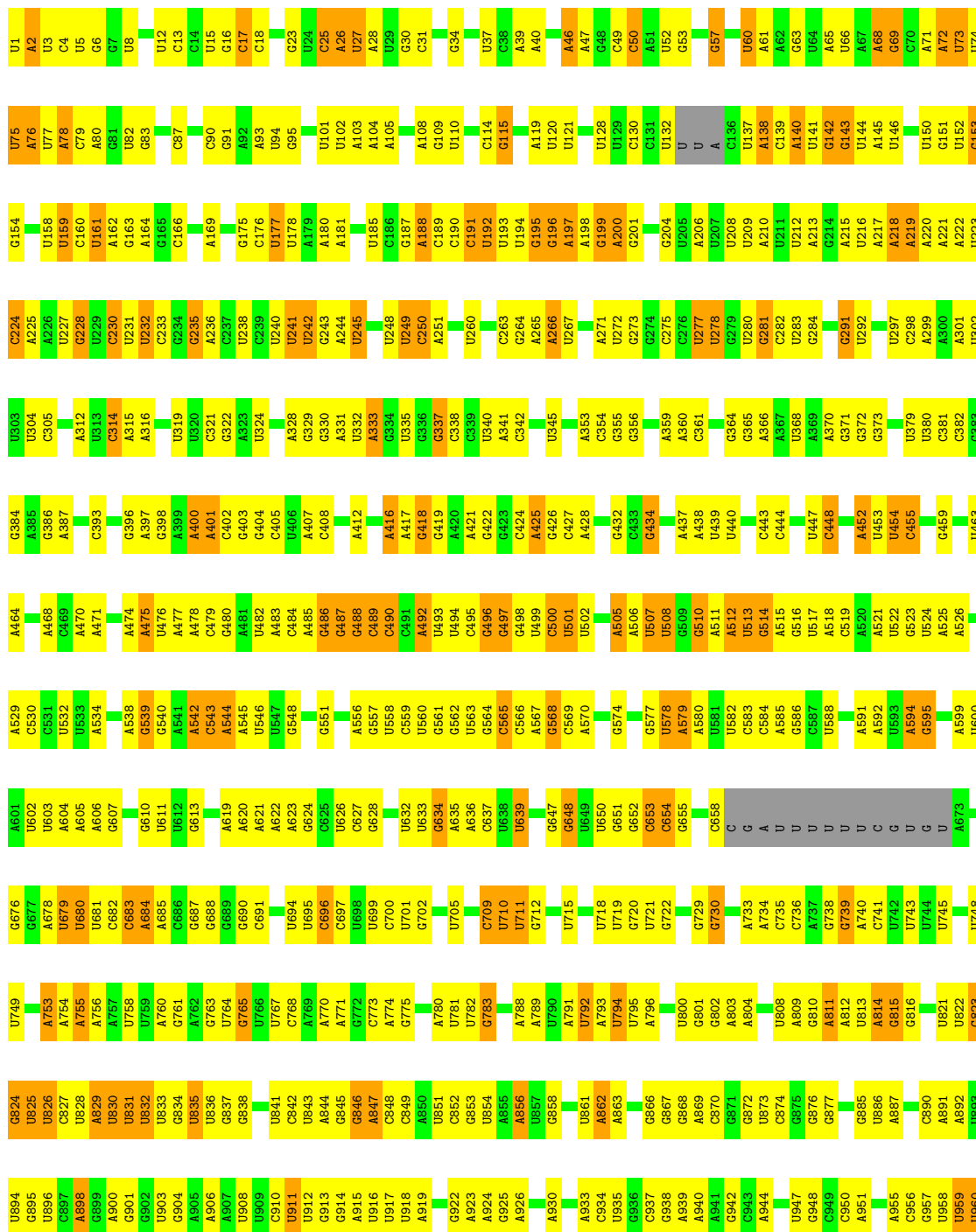


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C1580	U1517	U1450	G1297	A1143	U1071	A1001	A929	C853	A791	U725	U	A592
U1581	C1518	C1451	G1300	U1144	C1072	A1002	A930	U854	U792	U726	U	U593
A1583	U1520	U1452	A1301	U1145	G1073	A1003	C931	A855	A793	U727	U	A594
U1585	G1521	G1455	U1302	A1146	G1074	U1004	U932	A856	U794	U728	U	G595
A1586	U1522	C1456	A1303	A1147	C1077	A1005	A933	U857	U795	U729	U	C596
U1587	G1523	C1457	U1305	C1148	C1078	C1006	C934	C858	A796	G730	C	G597
A1588	U1524	G1458	C1306	G1149	U1079	G1007	U935	A859	G	C731	G	U598
C1589	A1525	A1459	U1307	G1150	U1080	U1008	A939	U860	U799	G732	U	A599
U1590	A1526	C1461	U1310	U1151	U1081	G1011	A940	U861	U800	A733	G	U600
C1591	G1464	G	U1314	A1157	U1082	U1012	A941	A862	G801	A734	U	A601
A1592	U1468	U	U1315	C1158	G1083	A1013	G942	U863	G802	C735	A	A602
U1593	G1531	U1469	G1316	C1159	A1084	G1014	C943	U864	A803	C736	C	U603
C1594	U1532	A1470	C1317	A1160	G1085	U1015	A944	A865	A804	A737	U	A604
U1595	G1533	C1534	G1318	C1162	U1087	C1016	U947	G866	U805	G738	G677	A605
C1596	C1534	U1471	G1319	A1163	A1088	U1017	G948	G867	A806	G739	A678	A606
U1599	U1535	A1472	U1320	G1164	U1091	A1019	A951	G871	U807	A740	U679	G607
C1600	G1536	U1473	A1321	G1165	A1092	C1022	A952	C872	C810	U742	U680	U608
G1601	U1537	C1474	G1322	A1166	U1096	A1026	A953	U873	A811	U743	U681	U609
U1602	U1538	A1475	G1324	G1167	C1096	U1027	G954	C874	U812	U744	C682	G610
U1603	G1539	C1476	G1325	U1168	U1098	A1028	G955	C875	U813	U745	C683	U611
C1606	U1540	G1477	U1326	G1169	U1099	C1032	A956	C876	U814	C747	A684	U612
G1607	G1541	U1478	C1327	U1170	U1098	G1034	A966	G877	G815	A752	G685	G613
U1608	G1542	A1479	G1328	A1171	U1099	G1035	U968	C878	C816	A753	G687	A619
C1609	A1545	G1480	A1329	C1172	G1100	A1039	C969	C879	A817	U754	G688	A620
G1610	U1546	C1481	G1330	C1173	G1101	U1031	A970	C880	C818	A755	C	A621
A1611	A1547	A1482	A1331	U1174	G1102	G1032	A971	U881	C692	A756	C692	A622
U1614	G1548	G1484	C1332	U1175	G1105	C1033	A967	U882	U820	A757	U693	A623
C1615	U1550	C1485	U1335	U1176	U1106	G1034	U968	U883	U821	U758	U694	G624
G1616	U1551	A1486	A1336	C1180	G1107	G1035	C969	G886	U822	U759	U695	C625
C1618	U1552	G1487	C1339	U1181	C	A1039	A970	A887	G823	U760	C696	U626
U1619	G1553	C1488	U1340	A1182	G1110	U1040	A971	U887	G824	A761	C697	C627
C1620	U1554	C1489	A1341	A1183	G1111	G1041	G972	C890	U825	G762	U698	U628
U1621	A1555	U1491	U1344	A1184	G1112	G1042	A973	C891	U826	G765	C700	U629
G1622	U1556	A1492	A1345	U1185	A1113	U1045	A974	A892	C827	U766	U701	U633
C1623	U1557	C1493	A1346	G1188	G1114	C1045	C975	U893	U830	U767	G702	A636
U1624	U1558	C1494	U1347	U1189	U1115	U1049	A976	U894	U831	C768	G703	C637
C1625	U1560	U1496	G1349	U1191	G1119	G1051	A977	C895	U832	A771	C704	U638
U1628	G1561	U1497	U1350	A1194	C1123	U1052	G980	U896	U833	G772	A706	U639
G1629	U1562	G1498	G1351	C1195	A1124	G1053	U981	A898	U835	C773	A707	U640
U1630	C1563	G1499	U1352	A1196	G1125	U1056	G984	U912	U836	A774	C708	G641
A1631	U1564	C1500	G1353	C1197	G1126	U1057	G985	G913	G837	G775	C709	G647
C1632	C1565	U1503	G1354	G1198	U1130	U1058	G986	G914	U838	G776	U710	G648
U1633	U1567	G1504	C1355	U1199	G1131	U1059	G987	A915	U840	G778	G712	U649
C1634	A1568	U1505	G1358	G1200	A1132	U1060	A988	U916	U841	U779	A713	U650
A1635	G1569	C1506	U1359	G1201	A1133	U1061	U989	U917	C842	A780	G714	G651
C1636	U1570	G1507	A1360	A1202	A1134	A1062	A992	U918	U843	U781	U715	C654
G1637	C1571	U1508	U1361	A1203	C1134	U1063	A993	A919	A844	G775	C716	G655
U1638	G1572	C1509	U1362	C1207	U1135	G1064	G994	G922	G845	G776	C717	C656
C1640	U1573	U1510	U1363	A1208	A1137	A1065	A995	A923	U847	U785	U718	U657
G1641	G1574	U1511	G1364	A1208	A1138	C1066	A996	A924	C848	C786	G720	C658
C1642	U1575	G1512	G1369	G1213	A1139	C1067	U996	G925	C849	G787	G721	C
U1643	A1576	U1512	U1370	U1291	G1140	U1068	G997	A926	A850	A788	G722	G
				U1292	G1141	A1069		C927	U851	A789	G723	A



• Molecule 47: 18S ribosomal RNA

Chain sR: 40% 45% 14%



U961	C962	G1042	A1043	G1119	A1196	G1264	A1345	G1418	G1504	C1571	U1643	A1728
A966	G1048	G1048	G1049	U1120	G1197	G1265	A1346	G1419	A1505	G1572	C1644	C1729
A967	U1049	G1048	U1049	C1122	G1198	U1272	U1347	A1427	G1507	A1574	G1649	A1730
U968	G1200	U1052	U1053	A1125	G1199	G1273	G1349	G1428	G1508	G1575	U1650	A1731
C969	A970	U1052	U1053	U1129	G1201	C1274	U1350	G1429	U1512	C1580	A1651	A1732
A971	G972	U1057	U1058	G1130	A1202	G1278	G1354	U1430	G1513	C1581	G1654	U1734
A974	A974	U1057	U1058	G1132	A1203	C1279	G1355	C1431	U1514	U1582	A1655	U1735
		U1059	U1060	A1137	C1208	G1281	U1356	G1432	A1516	A1583	U1656	
		U1060	U1061	A1138	C1209	G1282	A1357	G1433	A1515	G1584	U1657	U1742
		A1061	A1062	A1139	G1210	U1283	G1358	U1434	U1517	U1585	G1658	U1743
		U1062	U1063	A1142	C1211	G1284	C1359	A1444	C1518	A1586		A1744
		U1063	U1064	A1143	A1211	U1285	A1360	G1445	U1519	A1587	G1672	G1745
		A1065	A1066	G1150	G1212	U1286	U1361	A1446	U1520	C1588	G1673	G1746
		C1067	C1068	G1154	G1213	A1287	U1362	C1447	G1521	C1589	A1678	A1747
		U1068	U1069	G1155	G1214	G1288	G1363	G1448	U1522	C1590	A1679	
		G987	C1070	G1156	C1216	G1291	U1364	U1449	G1523	C1591	G1680	A1755
		U1071	U1072	C1157	G1217	G1292	C1365	U1450	A1524	A1592	A1681	A1756
		C1072	G1073	C1158	A1218	G1293	U1366	C1451	A1525	A1593	A1682	G1757
		G1073		C1159	G1219	U1298	U1367	G1452	U1527	U1596	A1683	U1758
				C1161	G1220	G1294	G1368	G1453	U1528			U1759
				G1162	A1221	G1295	U1370	G1454	U1529			G1760
				C1163	G1222	G1296	A1371	G1455	C1530			U1761
				A1166	G1223	G1297	G1379	G1456	G1531			U1762
				G1167	A1224	G1298	U1380	C1457	U1532			A1763
				G1170	G1225	U1300	U1381	G1458	U1533			
				A1171	U1226	U1301	A1382	C1459	G1534			A1766
				G1172	G1227	U1302	G1383	G1470	U1535			G1767
				C1173	G1228	U1305	U1388	C1471	G1536			U1768
				G1174	G1229	G1306	U1389	G1472	G1537			U1769
				U1175	A1230	U1307	U1390	G1473	U1538			U1770
				G1176	G1231	U1311	A1391	G1474	G1539			A1776
				C1177	G1232	U1312	A1392	G1475	G1540			G1777
				G1178	G1233	A1313	U1393	G1476	G1541			G1778
				U1179	G1234	U1314	C1398	G1477	G1542			U1779
				U1180	G1241	U1315	U1399	G1478	A1545			G1780
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				U1182	G1243	U1317	A1401	G1480	U1547			G1782
				A1183	G1244	U1318	G1402	C1481	A1550			C1783
				A1184	G1245	U1319	G1405	C1482	U1551			U1784
				U1185	C1246	U1320	A1406	C1483	U1552			U1785
				U1186	U1247	A1321	A1410	C1484	G1553			G1786
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							A1502	C1491	U1560			U1795
							A1503	C1492	U1561			C1796
								C1493	G1562			A1797
								C1494	U1563			G1798
								C1495	C1563			U1799
								C1496	U1564			A1800
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								C1498	U1566			
								C1499				
								C1500				
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GLU
GLN
ALA
GLU
GLU
ASN
ALA
ASP
ASN
VAL
GLU
TRP

• Molecule 48: 40S ribosomal protein S0-A

Chain s0: 39% 43% 18%

MET
S2
F7
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P11
E12
D13
A14
Q15
Q15
L16
L17
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S78
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A178
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VAL
GLU
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GLN
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THR
GLU
ALA

• Molecule 49: 40S ribosomal protein S1-A

Chain C: 33% 47% 16%

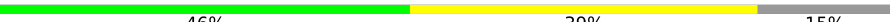
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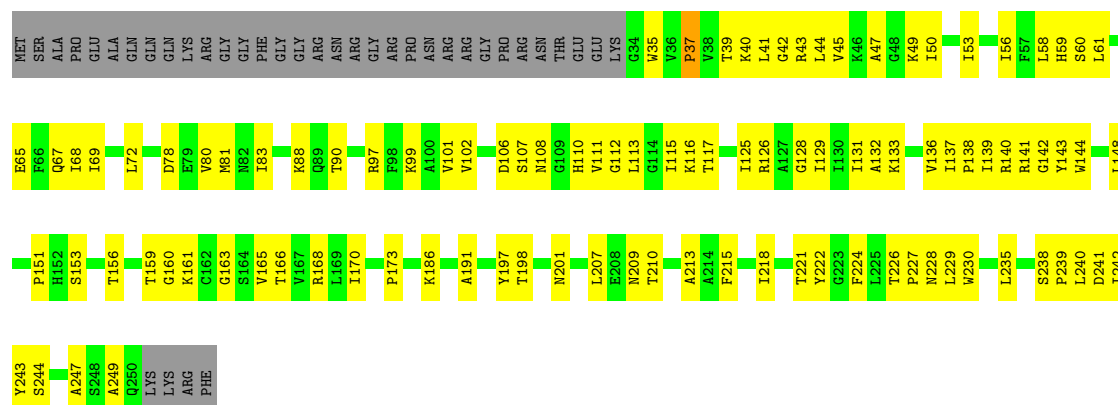
• Molecule 49: 40S ribosomal protein S1-A

Chain s1: 44% 40% 15%

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ARG
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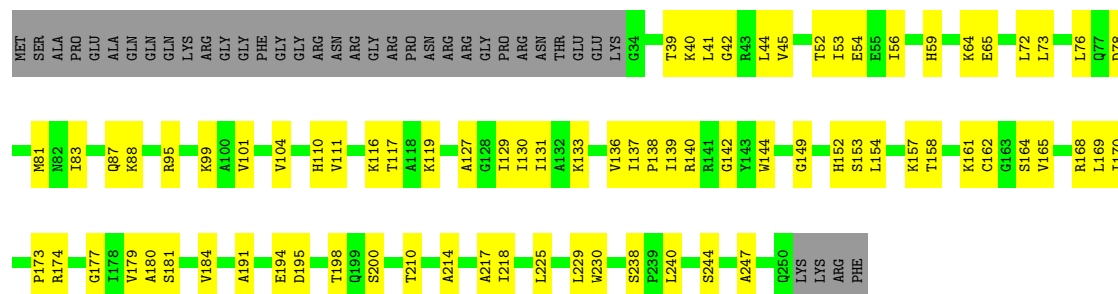
- Molecule 50: 40S ribosomal protein S2

Chain D:  46% 39% 15%



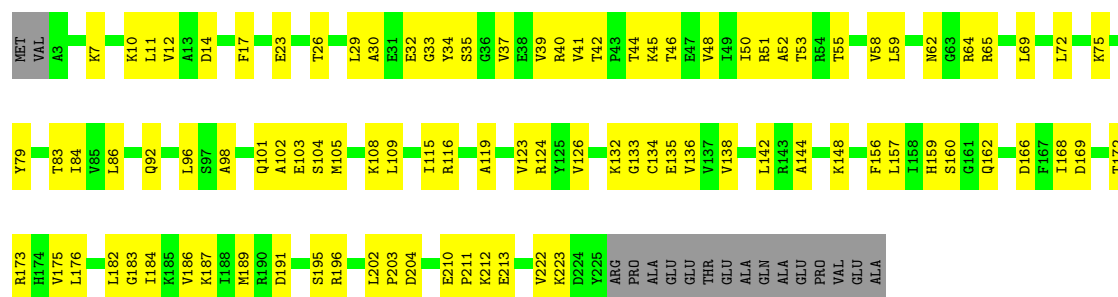
- Molecule 50: 40S ribosomal protein S2

Chain s2:  55% 31% 15%



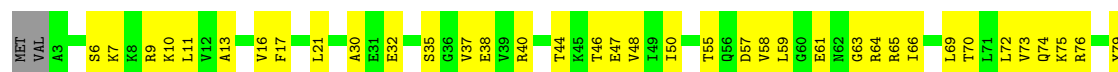
- Molecule 51: Small ribosomal subunit protein uS3

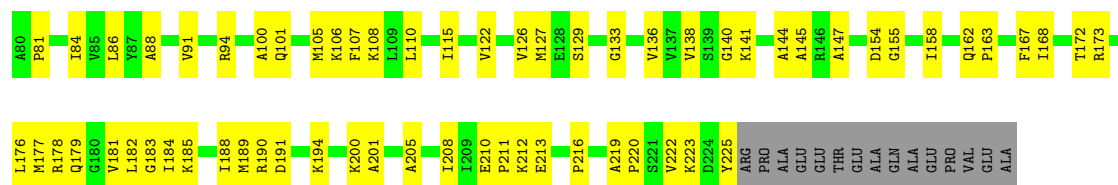
Chain E:  53% 40% 7%



- Molecule 51: Small ribosomal subunit protein uS3

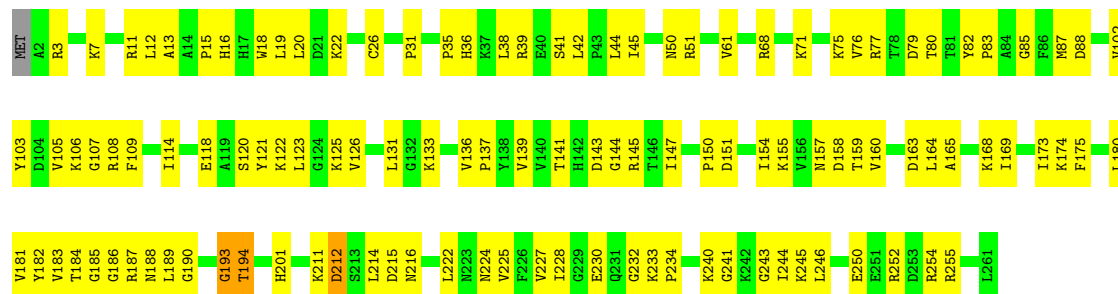
Chain s3:  51% 42% 7%





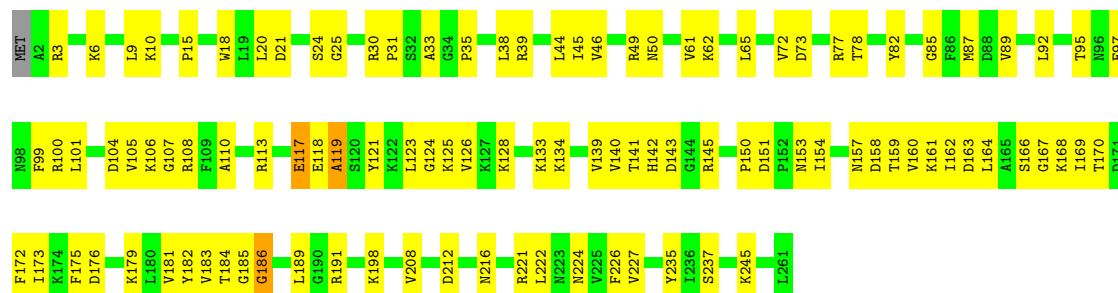
• Molecule 52: 40S ribosomal protein S4-A

Chain F: 56% 43%



• Molecule 52: 40S ribosomal protein S4-A

Chain s4: 60% 39%



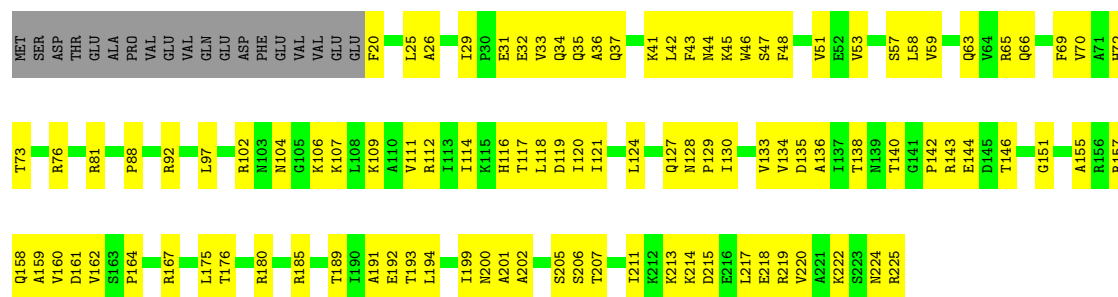
• Molecule 53: 40S ribosomal protein S5

Chain G: 41% 48% 8%



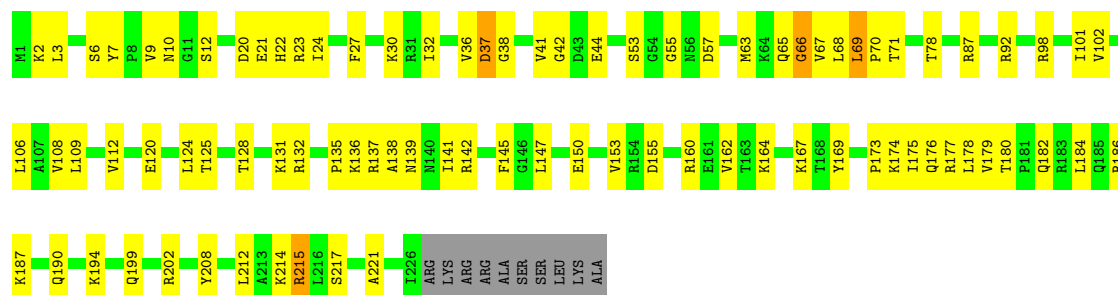
• Molecule 53: 40S ribosomal protein S5

Chain s5: 46% 45% 8%



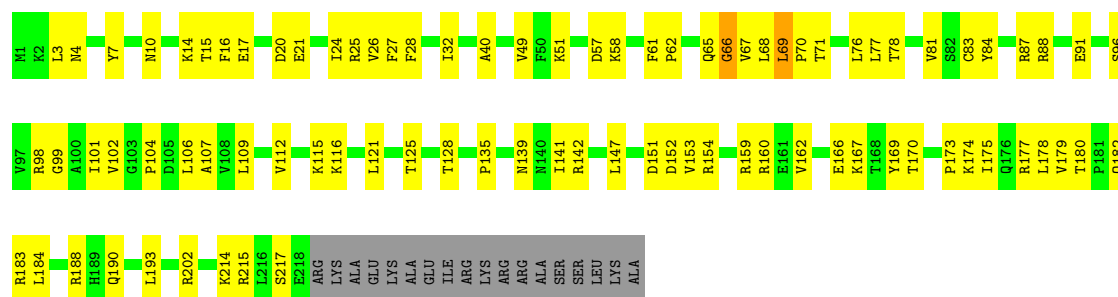
• Molecule 54: 40S ribosomal protein S6-A

Chain H: 59% 35%



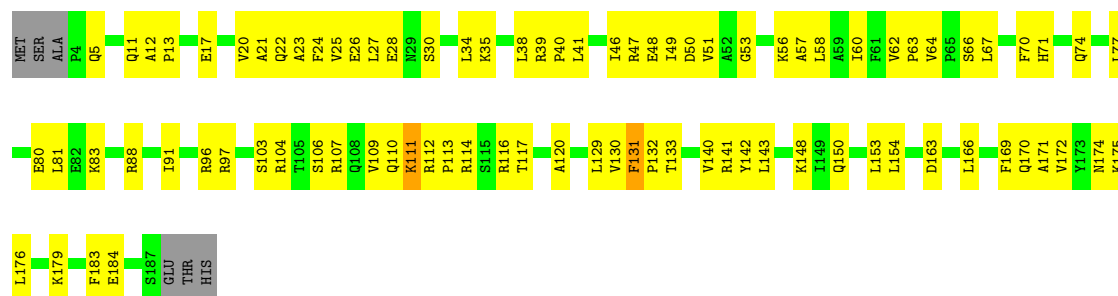
• Molecule 54: 40S ribosomal protein S6-A

Chain s6: 56% 36% 8%

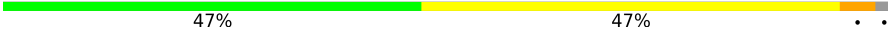


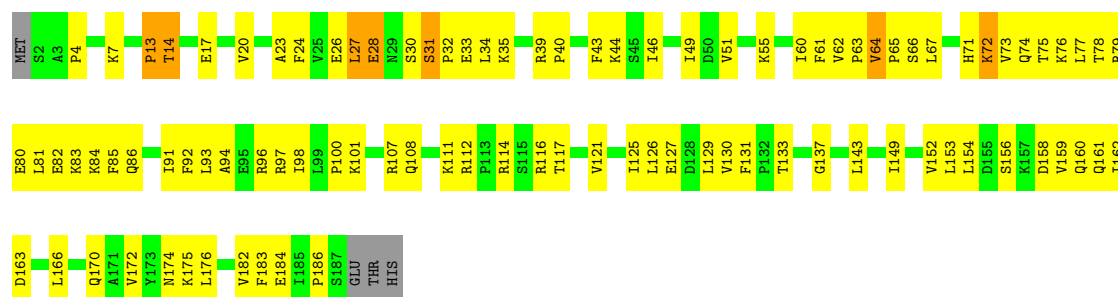
• Molecule 55: 40S ribosomal protein S7-A

Chain I: 52% 44%



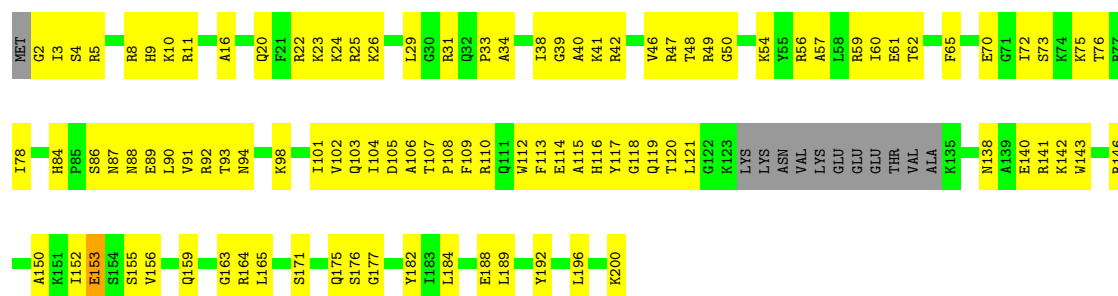
• Molecule 55: 40S ribosomal protein S7-A

Chain s7: 



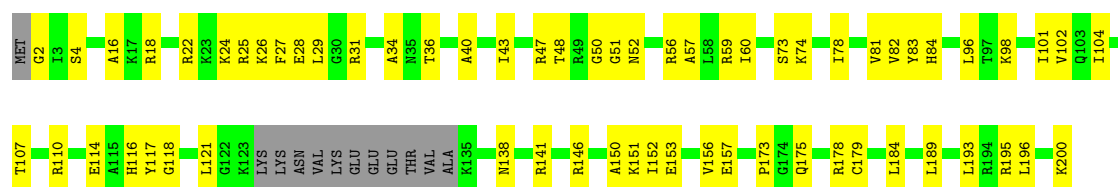
- Molecule 56: 40S ribosomal protein S8-A

Chain J: 



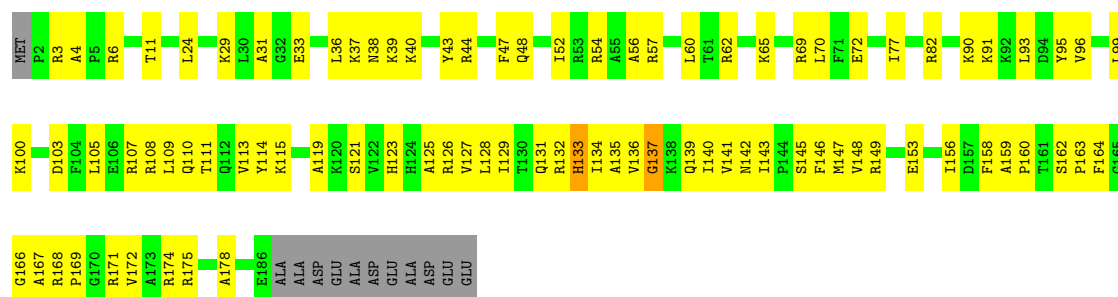
- Molecule 56: 40S ribosomal protein S8-A

Chain s8: 



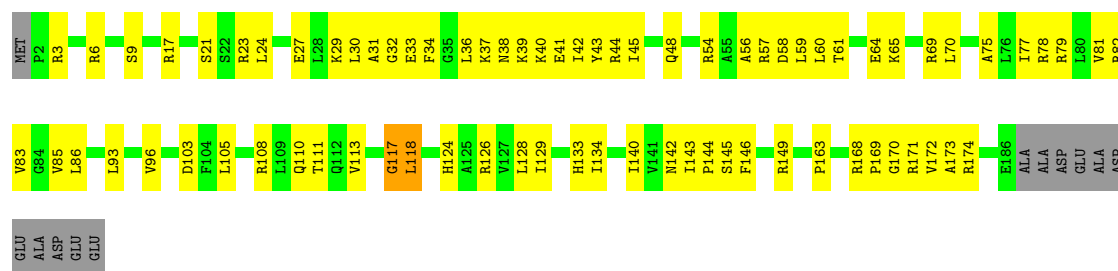
- Molecule 57: 40S ribosomal protein S9-A

Chain K: 



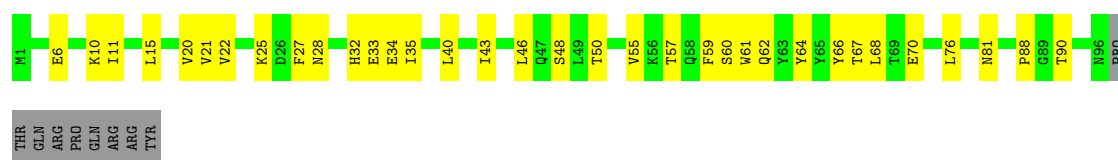
- Molecule 57: 40S ribosomal protein S9-A

Chain s9:  55% 38% • 6%



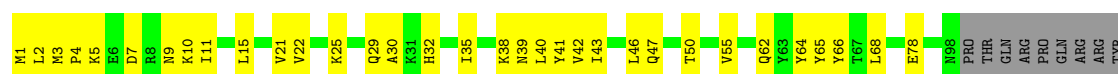
- Molecule 58: 40S ribosomal protein S10-A

Chain L:  59% 32% 9%



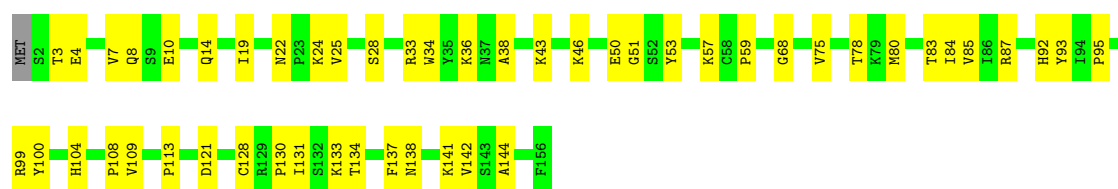
- Molecule 58: 40S ribosomal protein S10-A

Chain c0:  60% 31% 9%



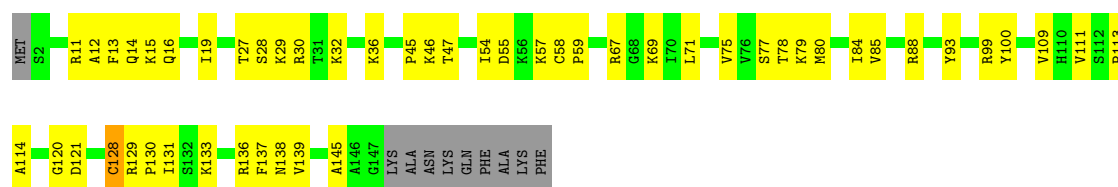
- Molecule 59: 40S ribosomal protein S11-A

Chain M:  67% 32% •

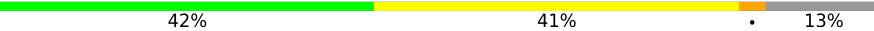


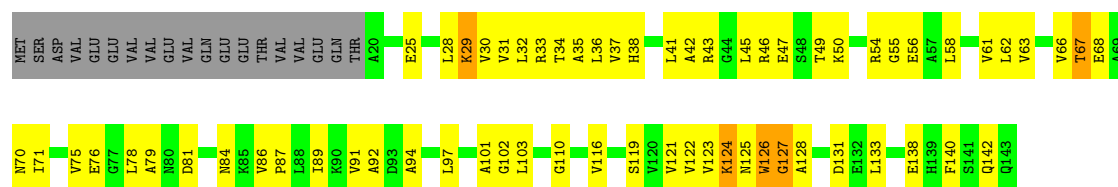
- Molecule 59: 40S ribosomal protein S11-A

Chain c1:  61% 32% • 6%

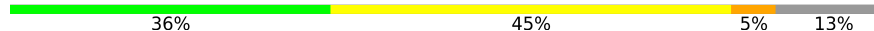


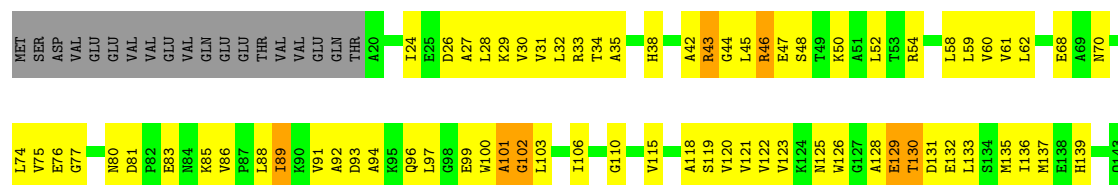
- Molecule 60: 40S ribosomal protein S12

Chain N: 



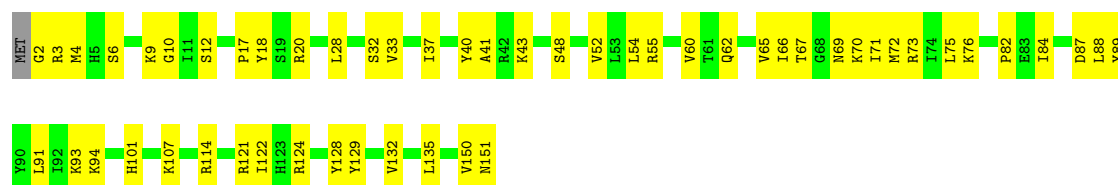
- Molecule 60: 40S ribosomal protein S12

Chain c2: 



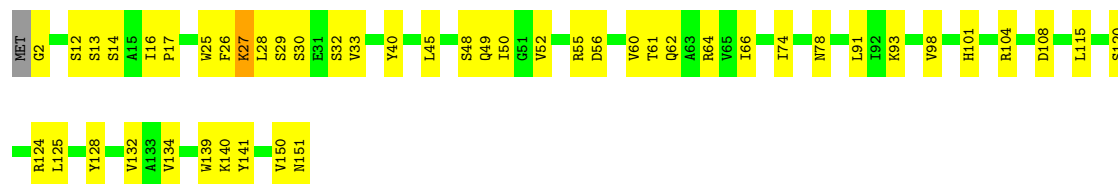
- Molecule 61: 40S ribosomal protein S13

Chain O: 



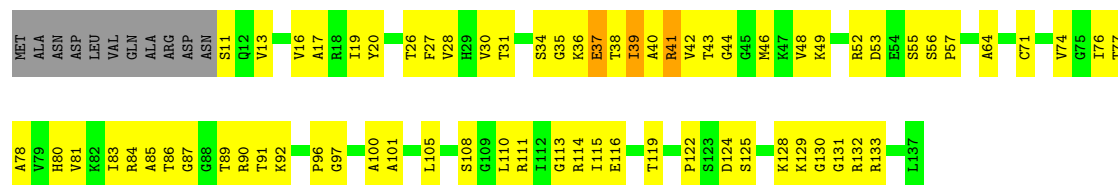
- Molecule 61: 40S ribosomal protein S13

Chain c3: 

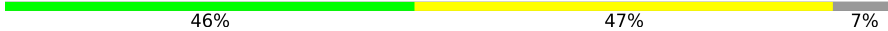


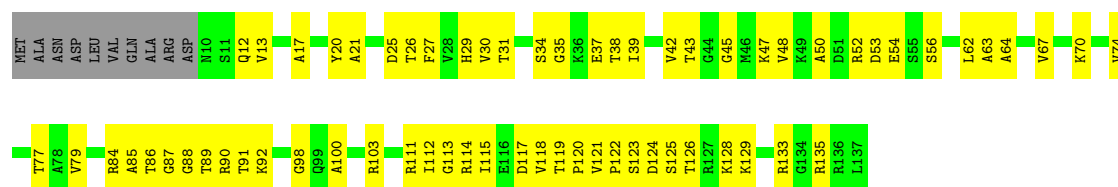
- Molecule 62: 40S ribosomal protein S14-B

Chain P: 

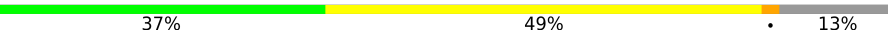


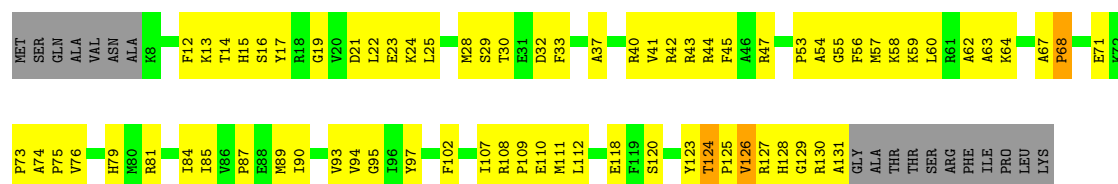
- Molecule 62: 40S ribosomal protein S14-B

Chain c4: 



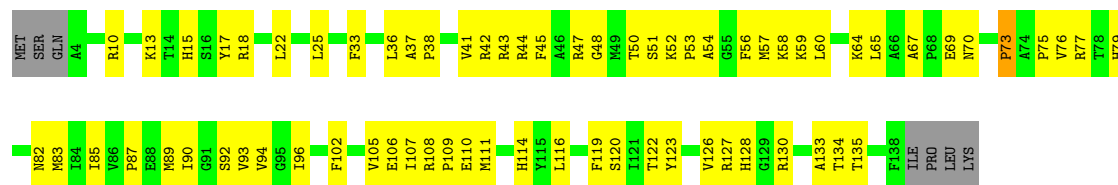
- Molecule 63: 40S ribosomal protein S15

Chain Q: 

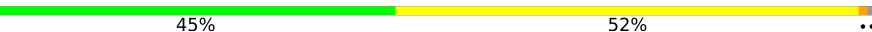


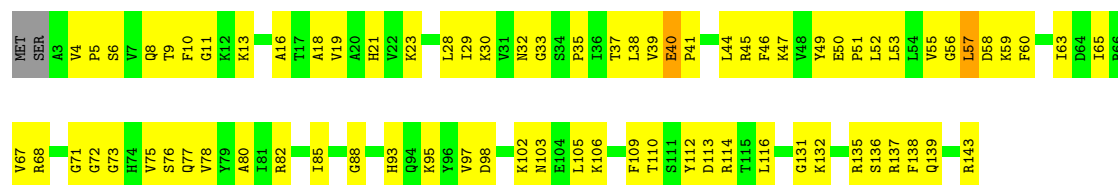
- Molecule 63: 40S ribosomal protein S15

Chain c5: 

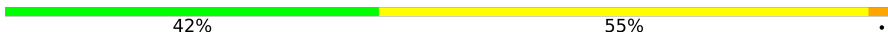


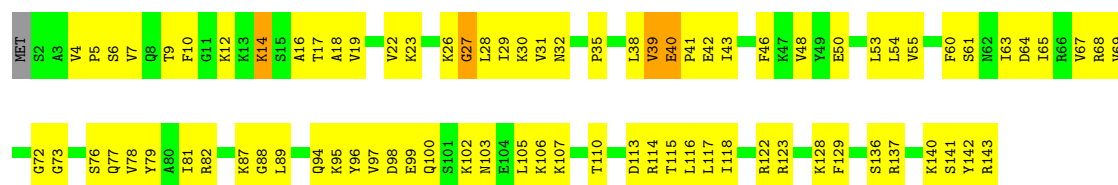
- Molecule 64: 40S ribosomal protein S16-A

Chain R: 

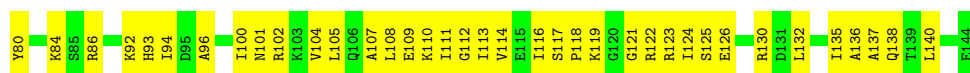


- Molecule 64: 40S ribosomal protein S16-A

Chain c6: 



- Molecule 65: 40S ribosomal protein S17-B



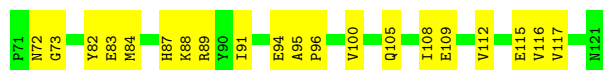
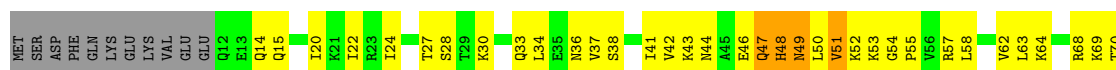
- Molecule 68: Small ribosomal subunit protein uS10

Chain V: 33% 53% 12%



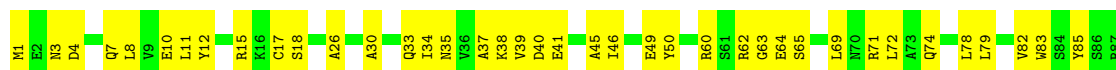
- Molecule 68: Small ribosomal subunit protein uS10

Chain d0: 45% 42% 9%



- Molecule 69: 40S ribosomal protein S21-A

Chain W: 55% 45%



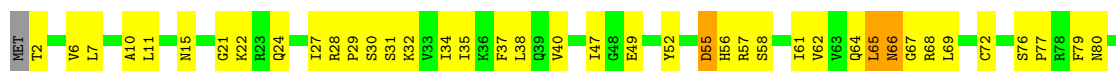
- Molecule 69: 40S ribosomal protein S21-A

Chain d1: 53% 47%



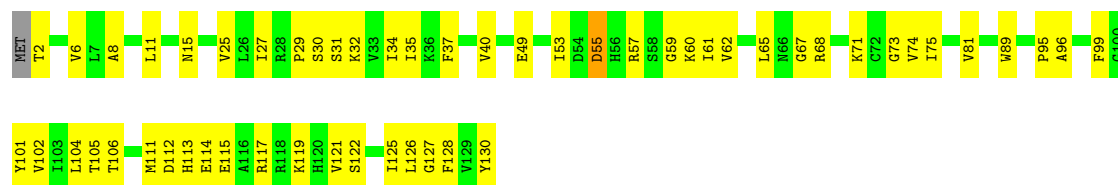
- Molecule 70: 40S ribosomal protein S22-A

Chain X: 58% 39%



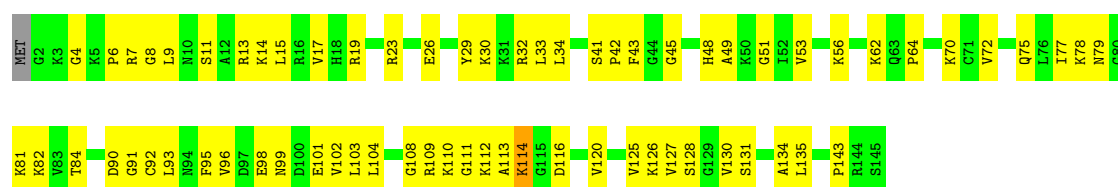
- Molecule 70: 40S ribosomal protein S22-A

Chain d2:  58% 41% ..



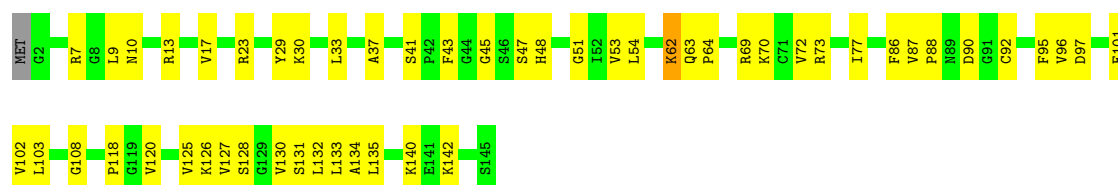
- Molecule 71: 40S ribosomal protein S23-A

Chain Y:  52% 46% ..



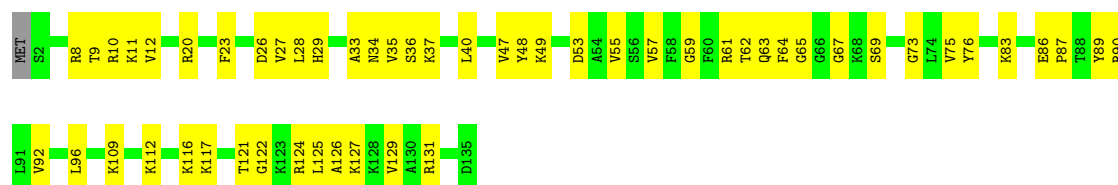
- Molecule 71: 40S ribosomal protein S23-A

Chain d3:  63% 35% ..



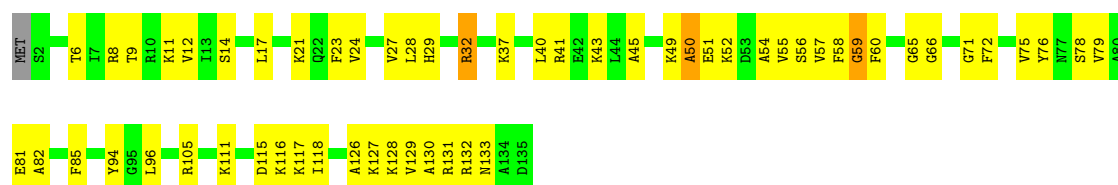
- Molecule 72: 40S ribosomal protein S24-A

Chain Z:  60% 39% .

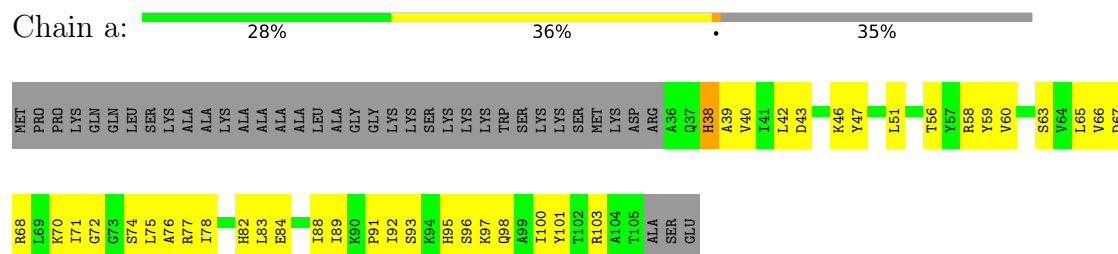


- Molecule 72: 40S ribosomal protein S24-A

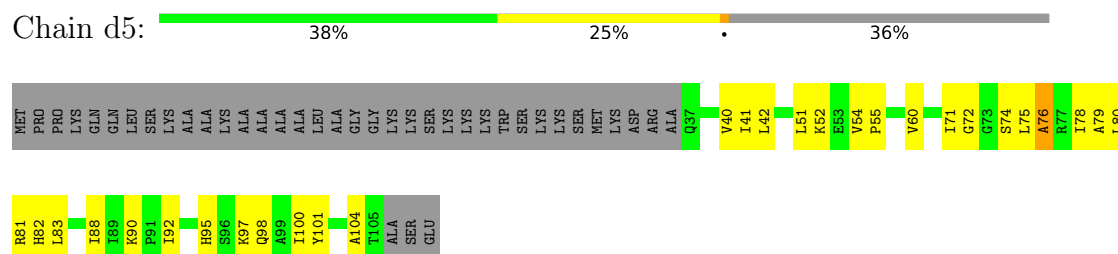
Chain d4:  57% 40% ..



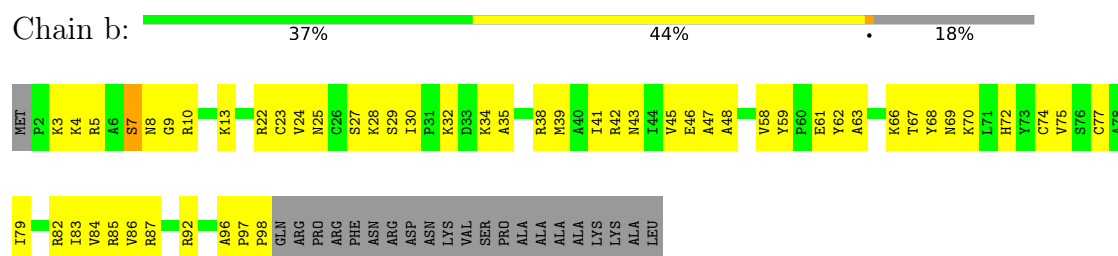
- Molecule 73: 40S ribosomal protein S25-A



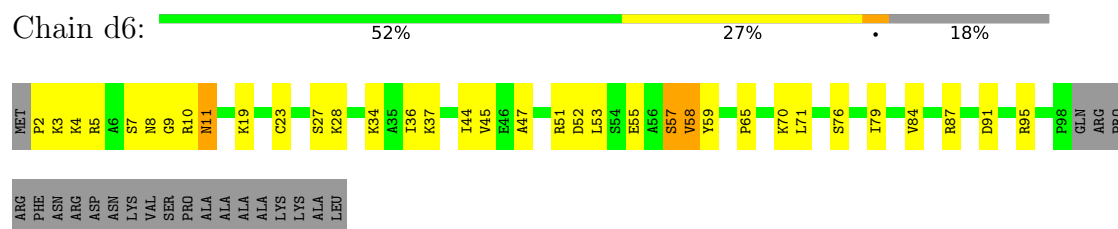
- Molecule 73: 40S ribosomal protein S25-A



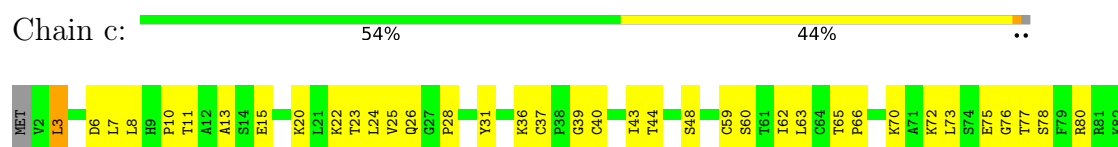
- Molecule 74: Small ribosomal subunit protein eS26B



- Molecule 74: Small ribosomal subunit protein eS26B

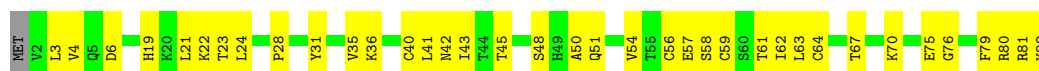


- Molecule 75: 40S ribosomal protein S27-A

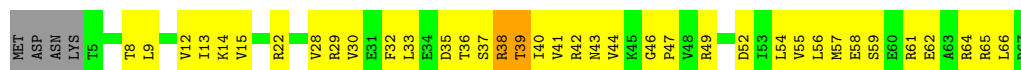


- Molecule 75: 40S ribosomal protein S27-A





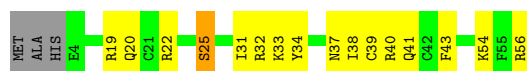
- Molecule 76: 40S ribosomal protein S28-A



- Molecule 76: 40S ribosomal protein S28-A



- Molecule 77: Small ribosomal subunit protein uS14A



- Molecule 77: Small ribosomal subunit protein uS14A



- Molecule 78: 40S ribosomal protein S30-A

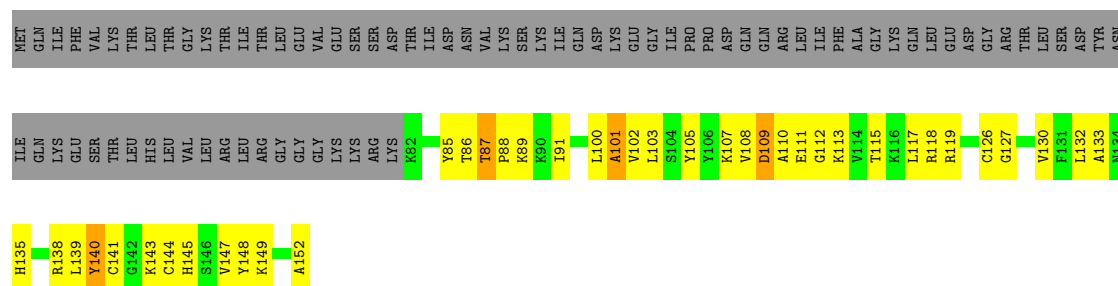


- Molecule 78: 40S ribosomal protein S30-A

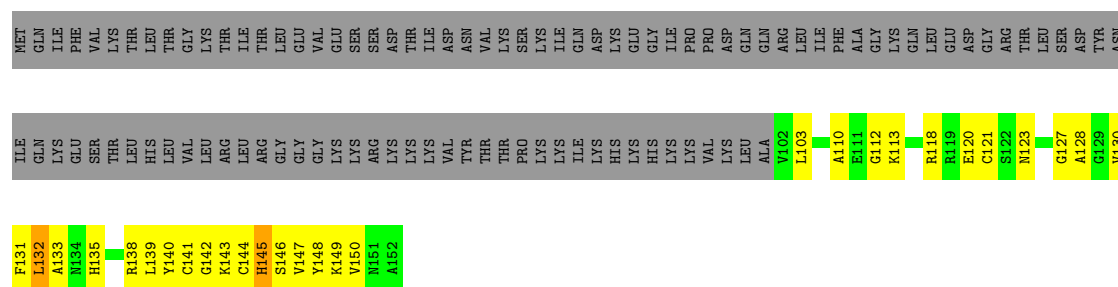


- Molecule 79: Ubiquitin

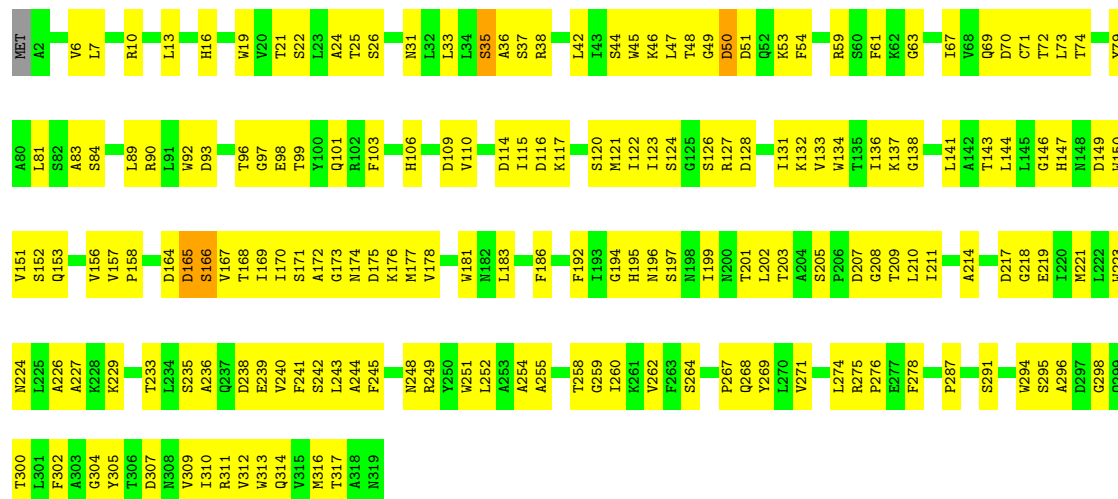




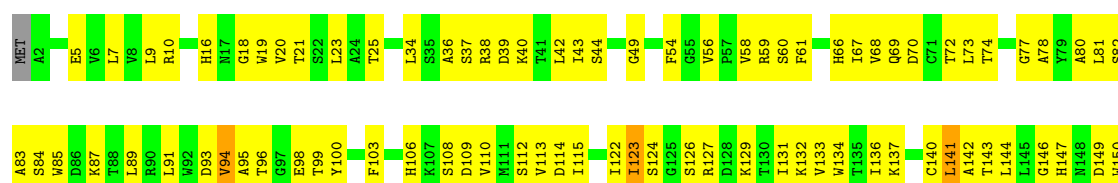
• Molecule 79: Ubiquitin

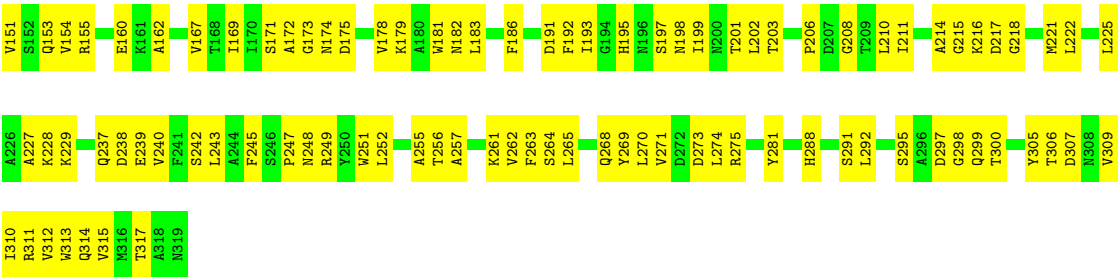


• Molecule 80: Guanine nucleotide-binding protein subunit beta-like protein

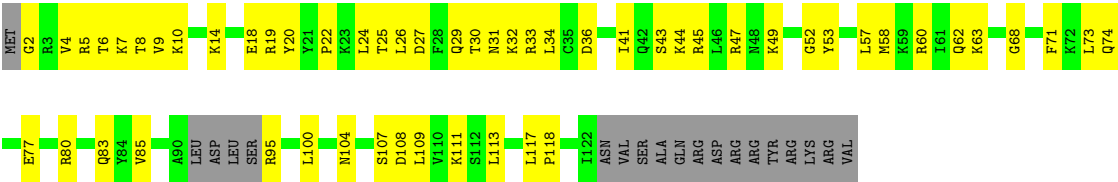


• Molecule 80: Guanine nucleotide-binding protein subunit beta-like protein





● Molecule 81: 40S ribosomal protein S17-A



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	302.58Å 285.05Å 433.72Å 90.00° 98.89° 90.00°	Depositor
Resolution (Å)	206.30 – 3.16	Depositor
% Data completeness (in resolution range)	98.1 (206.30-3.16)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.52 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.223 , 0.251	Depositor
Wilson B-factor (Å ²)	72.9	Xtriage
Anisotropy	0.178	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	409267	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, SPD, X1K, MG, ZN, OHX, OS

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	1	0.13	0/75394	0.36	0/117545
1	AR	0.13	0/75347	0.35	0/117472
2	3	0.13	0/2883	0.32	0/4491
2	AS	0.12	0/2883	0.33	0/4491
3	4	0.12	0/3746	0.33	0/5832
3	AT	0.12	0/3746	0.32	0/5832
4	CD	0.20	0/1948	0.70	1/2617 (0.0%)
4	j	0.17	0/1948	0.68	0/2617
5	CE	0.19	0/3146	0.69	2/4228 (0.0%)
5	k	0.20	0/3146	0.72	5/4228 (0.1%)
6	CF	0.19	0/2800	0.70	3/3790 (0.1%)
6	l	0.20	0/2800	0.73	4/3790 (0.1%)
7	CG	0.20	0/2425	0.76	2/3271 (0.1%)
7	m	0.19	0/2425	0.75	1/3271 (0.0%)
8	CH	0.17	0/1260	0.64	2/1694 (0.1%)
8	n	0.16	0/1260	0.63	0/1694
9	CI	0.17	0/1821	0.69	6/2451 (0.2%)
9	o	0.18	0/1821	0.81	6/2451 (0.2%)
10	CJ	0.21	0/1836	0.79	9/2481 (0.4%)
10	p	0.20	0/1836	0.78	9/2481 (0.4%)
11	CK	0.19	0/1539	0.69	0/2073
11	q	0.19	0/1539	0.70	1/2073 (0.0%)
12	CL	0.20	0/1741	0.69	0/2335
12	r	0.19	0/1741	0.63	2/2335 (0.1%)
13	CM	0.21	0/1374	0.74	2/1842 (0.1%)
13	s	0.23	0/1374	0.83	3/1842 (0.2%)
14	CN	0.24	0/1568	0.89	10/2106 (0.5%)
14	t	0.23	0/1568	0.85	9/2106 (0.4%)
15	CO	0.20	0/1068	0.60	0/1438
15	u	0.20	0/1068	0.62	0/1438
16	CP	0.17	0/1757	0.57	0/2354
16	v	0.17	0/1757	0.60	0/2354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	CQ	0.17	0/1585	0.62	0/2128
17	w	0.16	0/1585	0.59	0/2128
18	CR	0.23	0/1443	0.73	0/1944
18	x	0.17	0/1443	0.66	0/1944
19	CS	0.18	0/1465	0.70	2/1965 (0.1%)
19	y	0.18	0/1465	0.64	2/1965 (0.1%)
20	CT	0.19	0/1538	0.75	0/2050
20	z	0.16	0/1538	0.67	1/2050 (0.0%)
21	0	0.22	0/1481	0.71	0/1990
21	CU	0.18	0/1481	0.66	0/1990
22	2	0.23	0/1300	0.67	1/1743 (0.1%)
22	CV	0.19	0/1300	0.72	2/1743 (0.1%)
23	5	0.19	0/812	0.73	0/1099
23	CW	0.23	0/812	0.80	0/1099
24	6	0.18	0/1018	0.66	0/1369
24	CX	0.17	0/1018	0.60	0/1369
25	7	0.20	0/712	0.84	3/958 (0.3%)
25	CY	0.19	0/848	0.73	4/1146 (0.3%)
26	8	0.15	0/979	0.70	0/1321
26	CZ	0.18	0/979	0.64	0/1321
27	9	0.18	0/1004	0.64	0/1341
27	DA	0.18	0/987	0.61	0/1318
28	AA	0.25	0/1118	0.91	3/1497 (0.2%)
28	DB	0.21	0/1113	0.81	5/1491 (0.3%)
29	AB	0.25	0/1204	1.07	12/1612 (0.7%)
29	DC	0.24	0/1204	0.91	10/1612 (0.6%)
30	AC	0.17	0/473	0.68	0/629
30	DD	0.19	0/473	0.78	0/629
31	AD	0.17	0/751	0.54	0/1008
31	DE	0.17	0/751	0.61	0/1008
32	AE	0.17	0/890	0.63	0/1196
32	DF	0.17	0/890	0.66	0/1196
33	AF	0.15	0/1041	0.67	2/1394 (0.1%)
33	DG	0.15	0/1041	0.61	2/1394 (0.1%)
34	AG	0.20	0/868	0.75	0/1168
34	DH	0.22	0/868	0.79	1/1168 (0.1%)
35	AH	0.22	0/890	0.75	1/1189 (0.1%)
35	DI	0.32	0/890	0.87	2/1189 (0.2%)
36	AI	0.21	0/978	0.86	9/1301 (0.7%)
36	DJ	0.17	0/978	0.64	0/1301
37	AJ	0.19	0/778	0.62	0/1034
37	DK	0.18	0/778	0.69	0/1034
38	AK	0.19	0/696	0.67	0/923

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DL	0.16	0/696	0.59	0/923
39	AL	0.22	0/618	0.73	2/826 (0.2%)
39	DM	0.22	0/618	0.97	5/826 (0.6%)
40	AM	0.18	0/443	0.72	0/588
40	DN	0.18	0/443	0.70	0/588
41	AN	0.20	0/423	0.56	0/562
41	DO	0.21	0/423	0.59	0/562
42	AO	0.16	0/234	0.79	0/300
42	DP	0.19	0/234	0.70	0/300
43	AP	0.57	0/860	1.03	4/1136 (0.4%)
43	DQ	0.55	0/860	0.99	1/1136 (0.1%)
44	AQ	0.16	0/701	0.79	1/934 (0.1%)
44	DR	0.18	0/701	0.75	1/934 (0.1%)
45	i	0.24	0/1113	0.76	0/1502
45	sM	0.39	1/480 (0.2%)	1.06	3/642 (0.5%)
46	p0	0.19	0/1091	0.85	0/1472
47	A	0.14	0/42443	0.38	0/66134
47	sR	0.14	0/42490	0.37	0/66207
48	B	0.26	0/1617	1.04	7/2215 (0.3%)
48	s0	0.22	0/1623	0.84	3/2222 (0.1%)
49	C	0.30	0/1735	1.24	20/2335 (0.9%)
49	s1	0.18	0/1748	0.71	0/2352
50	D	0.22	0/1665	0.76	4/2263 (0.2%)
50	s2	0.20	0/1665	0.75	3/2263 (0.1%)
51	E	0.20	0/1759	0.78	1/2368 (0.0%)
51	s3	0.23	0/1759	0.91	3/2368 (0.1%)
52	F	0.29	0/2109	0.86	6/2839 (0.2%)
52	s4	0.21	0/2109	0.79	5/2839 (0.2%)
53	G	0.26	0/1629	1.06	9/2202 (0.4%)
53	s5	0.20	0/1629	0.80	0/2202
54	H	0.22	0/1823	0.94	6/2439 (0.2%)
54	s6	0.19	0/1779	0.77	3/2379 (0.1%)
55	I	0.26	0/1506	0.96	4/2028 (0.2%)
55	s7	0.26	0/1516	0.94	11/2043 (0.5%)
56	J	0.20	0/1514	0.91	5/2021 (0.2%)
56	s8	0.16	0/1514	0.70	1/2021 (0.0%)
57	K	0.23	0/1519	0.89	6/2035 (0.3%)
57	s9	0.20	0/1519	0.78	2/2035 (0.1%)
58	L	0.22	0/789	0.87	2/1067 (0.2%)
58	c0	0.26	0/776	0.98	3/1047 (0.3%)
59	M	0.19	0/1239	0.74	2/1673 (0.1%)
59	c1	0.20	0/1194	0.77	2/1610 (0.1%)
60	N	0.31	0/898	1.31	13/1220 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	c2	0.33	0/898	1.63	20/1220 (1.6%)
61	O	0.16	0/1215	0.58	0/1638
61	c3	0.19	0/1215	0.68	2/1638 (0.1%)
62	P	0.56	3/896 (0.3%)	1.24	10/1210 (0.8%)
62	c4	0.19	0/960	0.88	0/1290
63	Q	0.26	0/998	0.98	7/1341 (0.5%)
63	c5	0.24	0/1060	0.94	1/1426 (0.1%)
64	R	0.23	0/1125	0.84	3/1510 (0.2%)
64	c6	0.20	0/1131	0.93	6/1518 (0.4%)
65	S	0.27	0/935	0.91	5/1254 (0.4%)
66	T	0.23	0/1211	0.95	6/1628 (0.4%)
66	c8	0.25	0/1211	1.02	5/1628 (0.3%)
67	U	0.25	0/1130	0.95	6/1517 (0.4%)
67	c9	0.17	0/1130	0.64	0/1517
68	V	0.30	0/865	1.09	6/1169 (0.5%)
68	d0	0.23	0/892	1.05	10/1205 (0.8%)
69	W	0.20	0/693	0.87	2/935 (0.2%)
69	d1	0.20	0/693	0.91	3/935 (0.3%)
70	X	0.22	0/1038	0.92	6/1395 (0.4%)
70	d2	0.19	0/1038	0.72	1/1395 (0.1%)
71	Y	0.23	0/1139	0.97	5/1518 (0.3%)
71	d3	0.19	0/1139	0.75	2/1518 (0.1%)
72	Z	0.19	0/1087	0.78	0/1449
72	d4	0.25	0/1087	1.08	7/1449 (0.5%)
73	a	0.25	0/571	1.01	1/768 (0.1%)
73	d5	0.21	0/566	0.84	1/761 (0.1%)
74	b	0.27	0/782	0.98	2/1047 (0.2%)
74	d6	0.23	0/782	1.08	8/1047 (0.8%)
75	c	0.22	0/620	0.90	1/838 (0.1%)
75	d7	0.20	0/620	0.95	2/838 (0.2%)
76	d	0.20	0/499	1.29	5/670 (0.7%)
76	d8	0.29	0/499	1.10	4/670 (0.6%)
77	d9	0.18	0/452	0.74	0/600
77	e	0.18	0/452	0.71	0/600
78	e0	0.21	0/499	0.96	1/665 (0.2%)
78	f	0.19	0/483	0.79	0/643
79	e1	0.39	0/404	1.26	1/542 (0.2%)
79	g	0.36	0/577	1.36	8/770 (1.0%)
80	Rb	0.25	0/2495	0.96	12/3395 (0.4%)
80	h	0.22	0/2490	0.87	6/3389 (0.2%)
81	c7	0.18	0/914	0.80	2/1224 (0.2%)
All	All	0.18	4/430026 (0.0%)	0.58	444/631405 (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
15	u	0	1
49	C	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	P	38	THR	C-N	6.99	1.43	1.33
45	sM	38	PRO	CA-C	-6.50	1.48	1.51
62	P	40	ALA	CA-CB	5.51	1.62	1.53
62	P	39	ILE	CA-C	-5.01	1.46	1.52

The worst 5 of 444 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	G	120	ILE	CA-C-N	18.25	154.54	121.70
53	G	120	ILE	C-N-CA	18.25	154.54	121.70
49	C	129	THR	CA-C-N	16.98	153.97	121.54
49	C	129	THR	C-N-CA	16.98	153.97	121.54
72	d4	32	ARG	CA-C-N	16.86	152.05	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
49	C	129	THR	Peptide
15	u	128	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	1	67355	0	33847	1365	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AR	67313	0	33823	1348	1
2	3	2579	0	1303	59	0
2	AS	2579	0	1304	57	1
3	4	3353	0	1695	82	0
3	AT	3353	0	1695	56	0
4	CD	1914	0	1981	88	0
4	j	1914	0	1981	79	0
5	CE	3075	0	3142	120	0
5	k	3075	0	3142	124	0
6	CF	2748	0	2859	107	0
6	l	2748	0	2858	118	0
7	CG	2375	0	2325	85	0
7	m	2375	0	2325	105	0
8	CH	1239	0	1326	42	0
8	n	1239	0	1326	39	0
9	CI	1784	0	1862	64	0
9	o	1784	0	1862	69	0
10	CJ	1804	0	1877	65	1
10	p	1804	0	1877	76	0
11	CK	1518	0	1587	60	0
11	q	1518	0	1587	81	0
12	CL	1705	0	1736	67	0
12	r	1705	0	1736	69	0
13	CM	1353	0	1383	48	0
13	s	1353	0	1383	78	0
14	CN	1543	0	1608	87	0
14	t	1543	0	1608	90	0
15	CO	1053	0	1149	46	0
15	u	1053	0	1149	48	0
16	CP	1720	0	1779	63	0
16	v	1720	0	1779	74	0
17	CQ	1555	0	1659	47	0
17	w	1555	0	1659	60	0
18	CR	1420	0	1437	65	1
18	x	1420	0	1437	48	0
19	CS	1441	0	1543	62	0
19	y	1441	0	1543	72	0
20	CT	1521	0	1617	61	0
20	z	1521	0	1617	65	0
21	0	1445	0	1487	61	0
21	CU	1445	0	1487	55	0
22	2	1276	0	1323	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CV	1276	0	1323	48	0
23	5	796	0	812	40	0
23	CW	796	0	812	26	0
24	6	1003	0	1048	48	0
24	CX	1003	0	1048	38	0
25	7	699	0	640	21	0
25	CY	836	0	721	18	0
26	8	964	0	1025	37	0
26	CZ	964	0	1025	40	0
27	9	993	0	1081	38	0
27	DA	976	0	1064	36	0
28	AA	1092	0	1155	52	0
28	DB	1087	0	1143	54	0
29	AB	1173	0	1215	74	0
29	DC	1173	0	1215	66	0
30	AC	462	0	491	12	0
30	DD	462	0	491	23	0
31	AD	743	0	797	29	0
31	DE	743	0	797	30	0
32	AE	876	0	912	21	0
32	DF	876	0	912	30	0
33	AF	1020	0	1090	27	0
33	DG	1020	0	1090	26	0
34	AG	850	0	880	35	0
34	DH	850	0	880	20	0
35	AH	880	0	943	53	0
35	DI	880	0	942	37	0
36	AI	969	0	1078	41	0
36	DJ	969	0	1078	33	0
37	AJ	771	0	849	38	0
37	DK	771	0	849	39	0
38	AK	681	0	682	33	0
38	DL	681	0	683	16	0
39	AL	612	0	682	30	0
39	DM	612	0	682	18	0
40	AM	436	0	475	19	0
40	DN	436	0	475	13	0
41	AN	417	0	455	13	0
41	DO	417	0	455	12	0
42	AO	233	0	284	8	0
42	DP	233	0	284	8	0
43	AP	847	0	915	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DQ	847	0	915	42	0
44	AQ	694	0	735	37	0
44	DR	694	0	735	27	0
45	i	1104	0	1002	54	0
45	sM	475	0	492	30	0
46	p0	1076	0	1076	37	1
47	A	37948	0	19094	1099	1
47	sR	37990	0	19116	914	2
48	B	1577	0	1567	123	0
48	s0	1583	0	1578	102	0
49	C	1709	0	1784	142	0
49	s1	1722	0	1793	97	0
50	D	1635	0	1723	82	0
50	s2	1635	0	1723	67	0
51	E	1734	0	1817	87	0
51	s3	1734	0	1817	90	0
52	F	2068	0	2154	112	0
52	s4	2068	0	2154	95	0
53	G	1609	0	1674	129	0
53	s5	1609	0	1675	100	0
54	H	1799	0	1879	97	0
54	s6	1755	0	1846	76	0
55	I	1481	0	1572	82	0
55	s7	1491	0	1578	80	0
56	J	1489	0	1525	98	0
56	s8	1489	0	1525	53	0
57	K	1494	0	1573	85	0
57	s9	1494	0	1573	66	0
58	L	772	0	727	35	0
58	c0	761	0	698	29	0
59	M	1213	0	1257	36	0
59	c1	1168	0	1233	42	0
60	N	890	0	887	65	0
60	c2	890	0	887	67	0
61	O	1192	0	1255	52	0
61	c3	1192	0	1255	40	0
62	P	886	0	869	70	0
62	c4	949	0	985	59	0
63	Q	977	0	1002	66	0
63	c5	1039	0	1050	73	0
64	R	1105	0	1166	83	0
64	c6	1111	0	1171	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	S	926	0	930	49	0
66	T	1192	0	1222	87	0
66	c8	1192	0	1222	84	0
67	U	1112	0	1124	95	0
67	c9	1112	0	1124	70	0
68	V	855	0	917	74	0
68	d0	882	0	939	50	0
69	W	684	0	672	39	0
69	d1	684	0	672	39	0
70	X	1021	0	1060	55	0
70	d2	1021	0	1060	47	0
71	Y	1121	0	1196	61	0
71	d3	1121	0	1196	42	0
72	Z	1073	0	1132	53	0
72	d4	1073	0	1132	53	0
73	a	563	0	603	49	0
73	d5	558	0	598	36	0
74	b	769	0	814	64	0
74	d6	769	0	814	38	0
75	c	610	0	633	34	0
75	d7	610	0	632	34	0
76	d	497	0	535	36	0
76	d8	497	0	535	31	0
77	d9	442	0	429	21	0
77	e	442	0	428	16	0
78	e0	491	0	542	28	0
78	f	475	0	525	29	0
79	e1	397	0	399	38	0
79	g	566	0	603	40	0
80	Rb	2442	0	2392	184	0
80	h	2437	0	2386	160	0
81	c7	906	0	909	53	0
82	1	2078	0	0	220	0
82	2	7	0	0	1	0
82	3	70	0	0	4	0
82	4	98	0	0	11	0
82	A	874	0	0	113	0
82	AC	7	0	0	2	0
82	AG	7	0	0	1	0
82	AK	14	0	0	6	0
82	AP	7	0	0	3	0
82	AR	2111	0	0	206	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
82	AS	63	0	0	4	0
82	AT	112	0	0	11	0
82	CE	14	0	0	1	0
82	CG	21	0	0	1	1
82	CH	7	0	0	3	0
82	CK	7	0	0	0	0
82	CL	14	0	0	2	0
82	CP	7	0	0	0	0
82	CS	7	0	0	0	0
82	CV	7	0	0	1	0
82	CX	7	0	0	1	0
82	DD	7	0	0	1	0
82	DH	7	0	0	1	0
82	DL	7	0	0	0	0
82	DQ	7	0	0	3	0
82	J	7	0	0	1	0
82	O	7	0	0	0	0
82	Q	7	0	0	1	0
82	Rb	7	0	0	1	0
82	T	7	0	0	2	0
82	U	7	0	0	0	0
82	c3	7	0	0	1	0
82	c5	7	0	0	2	0
82	c7	7	0	0	1	0
82	c8	7	0	0	1	0
82	d4	7	0	0	0	0
82	h	7	0	0	0	0
82	k	14	0	0	3	0
82	l	7	0	0	1	0
82	r	7	0	0	1	0
82	s1	7	0	0	3	0
82	s4	7	0	0	0	0
82	s8	7	0	0	0	0
82	sR	980	0	0	118	0
82	v	7	0	0	0	0
82	z	7	0	0	2	0
83	1	486	0	0	0	0
83	3	12	0	0	0	0
83	4	18	0	0	0	0
83	6	3	0	0	0	0
83	9	1	0	0	0	0
83	A	135	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	AB	5	0	0	0	0
83	AC	1	0	0	0	0
83	AF	2	0	0	0	0
83	AG	1	0	0	0	0
83	AH	2	0	0	0	0
83	AI	1	0	0	0	0
83	AP	1	0	0	0	0
83	AR	498	0	0	0	0
83	AS	19	0	0	0	0
83	AT	19	0	0	0	0
83	CD	1	0	0	0	0
83	CE	3	0	0	0	0
83	CF	5	0	0	0	0
83	CG	1	0	0	0	0
83	CI	2	0	0	0	0
83	CJ	1	0	0	0	0
83	CK	1	0	0	0	0
83	CL	2	0	0	0	0
83	CM	2	0	0	0	0
83	CO	1	0	0	0	0
83	CP	5	0	0	0	0
83	CQ	3	0	0	0	0
83	CR	8	0	0	0	0
83	CU	1	0	0	0	0
83	CX	1	0	0	0	0
83	D	2	0	0	0	0
83	DA	2	0	0	0	0
83	DC	2	0	0	0	0
83	DD	1	0	0	0	0
83	DH	2	0	0	0	0
83	DI	3	0	0	0	0
83	DL	2	0	0	0	0
83	DO	2	0	0	0	0
83	DP	1	0	0	0	0
83	DQ	2	0	0	0	0
83	F	1	0	0	0	0
83	O	1	0	0	0	0
83	P	1	0	0	0	0
83	S	1	0	0	0	0
83	X	1	0	0	0	0
83	Y	1	0	0	0	0
83	b	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	c1	1	0	0	0	0
83	c3	1	0	0	0	0
83	c4	2	0	0	0	0
83	c6	1	0	0	0	0
83	c8	1	0	0	0	0
83	c9	2	0	0	0	0
83	d3	3	0	0	0	0
83	d4	3	0	0	0	0
83	d5	1	0	0	0	0
83	d6	2	0	0	0	0
83	d9	1	0	0	0	0
83	i	1	0	0	0	0
83	j	2	0	0	0	0
83	k	2	0	0	0	0
83	l	4	0	0	0	0
83	m	1	0	0	0	0
83	o	3	0	0	0	0
83	r	2	0	0	0	0
83	s	1	0	0	0	0
83	s1	1	0	0	0	0
83	s2	1	0	0	0	0
83	s4	1	0	0	0	0
83	s6	1	0	0	0	0
83	s8	2	0	0	0	0
83	s9	1	0	0	0	0
83	sM	2	0	0	0	0
83	sR	149	0	0	0	0
83	t	2	0	0	0	0
83	u	1	0	0	0	0
83	v	4	0	0	0	0
83	w	1	0	0	0	0
83	x	8	0	0	0	0
83	y	1	0	0	0	0
83	z	1	0	0	0	0
84	1	1	0	0	0	0
84	AR	4	0	0	0	0
84	j	1	0	0	0	0
84	sR	1	0	0	0	0
85	1	10	0	19	0	0
85	AR	10	0	19	0	0
86	1	25	0	0	1	0
86	AR	25	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	AK	1	0	0	0	0
87	AN	1	0	0	0	0
87	AP	1	0	0	0	0
87	AQ	1	0	0	0	0
87	DL	1	0	0	0	0
87	DO	1	0	0	0	0
87	DQ	1	0	0	0	0
87	DR	1	0	0	0	0
87	b	1	0	0	0	0
87	c	1	0	0	0	0
87	d6	1	0	0	0	0
87	d7	1	0	0	0	0
87	d9	1	0	0	0	0
87	e	1	0	0	0	0
87	g	1	0	0	0	0
88	A	1	0	0	0	0
89	1	148	0	0	9	0
89	4	14	0	0	0	0
89	A	57	0	0	3	0
89	AE	2	0	0	0	0
89	AO	1	0	0	0	0
89	AR	210	0	0	12	0
89	CD	1	0	0	0	0
89	CF	7	0	0	0	0
89	CI	1	0	0	0	0
89	CP	1	0	0	0	0
89	CR	1	0	0	1	0
89	CT	1	0	0	0	0
89	DG	1	0	0	0	0
89	R	1	0	0	1	0
89	S	6	0	0	0	0
89	Y	1	0	0	0	0
89	c1	1	0	0	0	0
89	c7	2	0	0	0	0
89	j	1	0	0	1	0
89	s8	1	0	0	0	0
89	sR	41	0	0	0	0
89	x	4	0	0	1	0
All	All	409267	0	296731	11547	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 11547 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)
47:sR:568:G:H4'	71:d3:90:ASP:HB2	1.23	1.18
47:A:568:G:H4'	71:Y:90:ASP:HB2	1.27	1.10
52:F:181:VAL:H	52:F:193:GLY:HA2	1.16	1.04
67:c9:117:SER:HB2	67:c9:123:ARG:HB2	1.39	1.04
1:1:2232:A:OP2	82:1:4102:OHX:N4	1.92	1.03

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:1269:U:OP2	82:CG:304:OHX:N4[2_746]	2.03	0.17
18:CR:181:ARG:NH1	47:A:1358:G:OP1[2_645]	2.12	0.08
2:AS:52:G:OP1	82:AR:3440:OHX:N2[2_756]	2.14	0.06
10:CJ:119:GLY:O	47:sR:851:U:O2'[2_656]	2.14	0.06
46:p0:48:ARG:NH1	47:sR:1700:C:OP2[2_756]	2.16	0.04

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	
4	CD	250/254 (98%)	248 (99%)	2 (1%)	0	100	100
4	j	250/254 (98%)	250 (100%)	0	0	100	100
5	CE	384/387 (99%)	382 (100%)	2 (0%)	0	100	100
5	k	384/387 (99%)	374 (97%)	10 (3%)	0	100	100
6	CF	359/362 (99%)	353 (98%)	6 (2%)	0	100	100
6	l	359/362 (99%)	350 (98%)	9 (2%)	0	100	100
7	CG	294/297 (99%)	289 (98%)	5 (2%)	0	100	100
7	m	294/297 (99%)	287 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	CH	152/176 (86%)	150 (99%)	2 (1%)	0	100	100
8	n	152/176 (86%)	152 (100%)	0	0	100	100
9	CI	220/244 (90%)	217 (99%)	3 (1%)	0	100	100
9	o	220/244 (90%)	210 (96%)	10 (4%)	0	100	100
10	CJ	231/256 (90%)	221 (96%)	10 (4%)	0	100	100
10	p	231/256 (90%)	226 (98%)	5 (2%)	0	100	100
11	CK	189/191 (99%)	185 (98%)	4 (2%)	0	100	100
11	q	189/191 (99%)	185 (98%)	4 (2%)	0	100	100
12	CL	207/221 (94%)	205 (99%)	2 (1%)	0	100	100
12	r	207/221 (94%)	205 (99%)	2 (1%)	0	100	100
13	CM	167/174 (96%)	162 (97%)	5 (3%)	0	100	100
13	s	167/174 (96%)	160 (96%)	7 (4%)	0	100	100
14	CN	191/199 (96%)	179 (94%)	11 (6%)	1 (0%)	24	55
14	t	191/199 (96%)	180 (94%)	9 (5%)	2 (1%)	12	41
15	CO	134/138 (97%)	134 (100%)	0	0	100	100
15	u	134/138 (97%)	131 (98%)	2 (2%)	1 (1%)	18	49
16	CP	201/204 (98%)	201 (100%)	0	0	100	100
16	v	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
17	CQ	195/199 (98%)	195 (100%)	0	0	100	100
17	w	195/199 (98%)	195 (100%)	0	0	100	100
18	CR	181/184 (98%)	181 (100%)	0	0	100	100
18	x	181/184 (98%)	180 (99%)	1 (1%)	0	100	100
19	CS	183/186 (98%)	181 (99%)	2 (1%)	0	100	100
19	y	183/186 (98%)	180 (98%)	3 (2%)	0	100	100
20	CT	186/189 (98%)	182 (98%)	4 (2%)	0	100	100
20	z	186/189 (98%)	183 (98%)	3 (2%)	0	100	100
21	0	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
21	CU	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
22	2	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
22	CV	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
23	5	98/121 (81%)	98 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	CW	98/121 (81%)	96 (98%)	2 (2%)	0	100	100
24	6	134/137 (98%)	131 (98%)	3 (2%)	0	100	100
24	CX	134/137 (98%)	134 (100%)	0	0	100	100
25	7	96/155 (62%)	94 (98%)	2 (2%)	0	100	100
25	CY	122/155 (79%)	118 (97%)	4 (3%)	0	100	100
26	8	119/142 (84%)	119 (100%)	0	0	100	100
26	CZ	119/142 (84%)	118 (99%)	1 (1%)	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	AA	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
28	DB	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
29	AB	146/149 (98%)	139 (95%)	7 (5%)	0	100	100
29	DC	146/149 (98%)	142 (97%)	4 (3%)	0	100	100
30	AC	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
30	DD	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
31	AD	95/105 (90%)	95 (100%)	0	0	100	100
31	DE	95/105 (90%)	95 (100%)	0	0	100	100
32	AE	107/113 (95%)	101 (94%)	6 (6%)	0	100	100
32	DF	107/113 (95%)	104 (97%)	3 (3%)	0	100	100
33	AF	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
33	DG	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
34	AG	104/107 (97%)	102 (98%)	2 (2%)	0	100	100
34	DH	104/107 (97%)	102 (98%)	2 (2%)	0	100	100
35	AH	110/121 (91%)	110 (100%)	0	0	100	100
35	DI	110/121 (91%)	109 (99%)	1 (1%)	0	100	100
36	AI	117/120 (98%)	110 (94%)	7 (6%)	0	100	100
36	DJ	117/120 (98%)	116 (99%)	1 (1%)	0	100	100
37	AJ	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
37	DK	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
38	AK	85/88 (97%)	85 (100%)	0	0	100	100
38	DL	85/88 (97%)	85 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	AL	75/78 (96%)	75 (100%)	0	0	100	100
39	DM	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
40	AM	48/51 (94%)	48 (100%)	0	0	100	100
40	DN	48/51 (94%)	48 (100%)	0	0	100	100
41	AN	50/128 (39%)	50 (100%)	0	0	100	100
41	DO	50/128 (39%)	48 (96%)	2 (4%)	0	100	100
42	AO	23/25 (92%)	23 (100%)	0	0	100	100
42	DP	23/25 (92%)	23 (100%)	0	0	100	100
43	AP	103/106 (97%)	94 (91%)	8 (8%)	1 (1%)	12	41
43	DQ	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
44	AQ	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
44	DR	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
45	i	155/273 (57%)	147 (95%)	8 (5%)	0	100	100
45	sM	61/273 (22%)	57 (93%)	4 (7%)	0	100	100
46	p0	139/311 (45%)	139 (100%)	0	0	100	100
48	B	204/252 (81%)	185 (91%)	19 (9%)	0	100	100
48	s0	204/252 (81%)	194 (95%)	10 (5%)	0	100	100
49	C	212/255 (83%)	200 (94%)	12 (6%)	0	100	100
49	s1	214/255 (84%)	213 (100%)	1 (0%)	0	100	100
50	D	215/254 (85%)	207 (96%)	7 (3%)	1 (0%)	24	55
50	s2	215/254 (85%)	210 (98%)	5 (2%)	0	100	100
51	E	221/240 (92%)	215 (97%)	6 (3%)	0	100	100
51	s3	221/240 (92%)	208 (94%)	13 (6%)	0	100	100
52	F	258/261 (99%)	253 (98%)	5 (2%)	0	100	100
52	s4	258/261 (99%)	253 (98%)	5 (2%)	0	100	100
53	G	204/225 (91%)	198 (97%)	6 (3%)	0	100	100
53	s5	204/225 (91%)	195 (96%)	9 (4%)	0	100	100
54	H	224/236 (95%)	216 (96%)	8 (4%)	0	100	100
54	s6	216/236 (92%)	209 (97%)	7 (3%)	0	100	100
55	I	182/190 (96%)	175 (96%)	7 (4%)	0	100	100
55	s7	184/190 (97%)	173 (94%)	9 (5%)	2 (1%)	11	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	J	184/200 (92%)	170 (92%)	14 (8%)	0	100	100
56	s8	184/200 (92%)	184 (100%)	0	0	100	100
57	K	183/197 (93%)	174 (95%)	9 (5%)	0	100	100
57	s9	183/197 (93%)	178 (97%)	5 (3%)	0	100	100
58	L	94/105 (90%)	86 (92%)	8 (8%)	0	100	100
58	c0	92/105 (88%)	80 (87%)	12 (13%)	0	100	100
59	M	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
59	c1	144/156 (92%)	139 (96%)	5 (4%)	0	100	100
60	N	122/143 (85%)	111 (91%)	11 (9%)	0	100	100
60	c2	122/143 (85%)	109 (89%)	12 (10%)	1 (1%)	16	46
61	O	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
61	c3	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
62	P	125/138 (91%)	116 (93%)	7 (6%)	2 (2%)	7	32
62	c4	126/138 (91%)	119 (94%)	7 (6%)	0	100	100
63	Q	122/142 (86%)	111 (91%)	11 (9%)	0	100	100
63	c5	133/142 (94%)	123 (92%)	10 (8%)	0	100	100
64	R	139/143 (97%)	133 (96%)	4 (3%)	2 (1%)	9	34
64	c6	140/143 (98%)	136 (97%)	3 (2%)	1 (1%)	18	49
65	S	116/136 (85%)	110 (95%)	6 (5%)	0	100	100
66	T	143/146 (98%)	132 (92%)	10 (7%)	1 (1%)	18	49
66	c8	143/146 (98%)	126 (88%)	17 (12%)	0	100	100
67	U	141/144 (98%)	137 (97%)	4 (3%)	0	100	100
67	c9	141/144 (98%)	139 (99%)	2 (1%)	0	100	100
68	V	105/121 (87%)	96 (91%)	9 (9%)	0	100	100
68	d0	108/121 (89%)	102 (94%)	6 (6%)	0	100	100
69	W	85/87 (98%)	80 (94%)	5 (6%)	0	100	100
69	d1	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
70	X	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
70	d2	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
71	Y	142/145 (98%)	128 (90%)	14 (10%)	0	100	100
71	d3	142/145 (98%)	134 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	Z	132/135 (98%)	132 (100%)	0	0	100	100
72	d4	132/135 (98%)	126 (96%)	6 (4%)	0	100	100
73	a	68/108 (63%)	62 (91%)	6 (9%)	0	100	100
73	d5	67/108 (62%)	67 (100%)	0	0	100	100
74	b	95/119 (80%)	86 (90%)	9 (10%)	0	100	100
74	d6	95/119 (80%)	89 (94%)	6 (6%)	0	100	100
75	c	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
75	d7	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
76	d	61/67 (91%)	58 (95%)	3 (5%)	0	100	100
76	d8	61/67 (91%)	56 (92%)	5 (8%)	0	100	100
77	d9	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
77	e	51/56 (91%)	50 (98%)	0	1 (2%)	6	27
78	e0	60/63 (95%)	58 (97%)	1 (2%)	1 (2%)	7	30
78	f	58/63 (92%)	58 (100%)	0	0	100	100
79	e1	49/152 (32%)	42 (86%)	5 (10%)	2 (4%)	2	14
79	g	69/152 (45%)	57 (83%)	12 (17%)	0	100	100
80	Rb	316/319 (99%)	307 (97%)	9 (3%)	0	100	100
80	h	316/319 (99%)	304 (96%)	12 (4%)	0	100	100
81	c7	113/136 (83%)	110 (97%)	3 (3%)	0	100	100
All	All	22284/24619 (90%)	21584 (97%)	681 (3%)	19 (0%)	48	76

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	u	8	LYS
50	D	107	SER
62	P	37	GLU
64	R	40	GLU
64	R	59	LYS

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	
4	CD	193/196 (98%)	193 (100%)	0	100	100
4	j	193/196 (98%)	193 (100%)	0	100	100
5	CE	319/323 (99%)	318 (100%)	1 (0%)	86	85
5	k	320/323 (99%)	318 (99%)	2 (1%)	78	81
6	CF	288/289 (100%)	288 (100%)	0	100	100
6	l	288/289 (100%)	288 (100%)	0	100	100
7	CG	244/245 (100%)	244 (100%)	0	100	100
7	m	244/245 (100%)	244 (100%)	0	100	100
8	CH	134/153 (88%)	134 (100%)	0	100	100
8	n	134/153 (88%)	134 (100%)	0	100	100
9	CI	186/205 (91%)	186 (100%)	0	100	100
9	o	186/205 (91%)	186 (100%)	0	100	100
10	CJ	187/208 (90%)	187 (100%)	0	100	100
10	p	187/208 (90%)	187 (100%)	0	100	100
11	CK	171/171 (100%)	171 (100%)	0	100	100
11	q	171/171 (100%)	171 (100%)	0	100	100
12	CL	177/187 (95%)	176 (99%)	1 (1%)	78	81
12	r	177/187 (95%)	177 (100%)	0	100	100
13	CM	147/151 (97%)	147 (100%)	0	100	100
13	s	147/151 (97%)	147 (100%)	0	100	100
14	CN	154/159 (97%)	154 (100%)	0	100	100
14	t	154/159 (97%)	154 (100%)	0	100	100
15	CO	107/109 (98%)	107 (100%)	0	100	100
15	u	107/109 (98%)	107 (100%)	0	100	100
16	CP	175/176 (99%)	175 (100%)	0	100	100
16	v	175/176 (99%)	175 (100%)	0	100	100
17	CQ	160/162 (99%)	160 (100%)	0	100	100
17	w	160/162 (99%)	160 (100%)	0	100	100
18	CR	140/146 (96%)	140 (100%)	0	100	100
18	x	140/146 (96%)	140 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	CS	150/151 (99%)	150 (100%)	0	100	100
19	y	150/151 (99%)	150 (100%)	0	100	100
20	CT	153/154 (99%)	153 (100%)	0	100	100
20	z	153/154 (99%)	153 (100%)	0	100	100
21	0	156/156 (100%)	156 (100%)	0	100	100
21	CU	156/156 (100%)	156 (100%)	0	100	100
22	2	136/137 (99%)	136 (100%)	0	100	100
22	CV	136/137 (99%)	136 (100%)	0	100	100
23	5	87/107 (81%)	87 (100%)	0	100	100
23	CW	87/107 (81%)	87 (100%)	0	100	100
24	6	104/105 (99%)	104 (100%)	0	100	100
24	CX	104/105 (99%)	104 (100%)	0	100	100
25	7	57/129 (44%)	57 (100%)	0	100	100
25	CY	58/129 (45%)	58 (100%)	0	100	100
26	8	104/118 (88%)	104 (100%)	0	100	100
26	CZ	104/118 (88%)	104 (100%)	0	100	100
27	9	109/110 (99%)	109 (100%)	0	100	100
27	DA	107/110 (97%)	107 (100%)	0	100	100
28	AA	115/116 (99%)	115 (100%)	0	100	100
28	DB	114/116 (98%)	114 (100%)	0	100	100
29	AB	118/119 (99%)	118 (100%)	0	100	100
29	DC	118/119 (99%)	118 (100%)	0	100	100
30	AC	46/47 (98%)	46 (100%)	0	100	100
30	DD	46/47 (98%)	46 (100%)	0	100	100
31	AD	81/88 (92%)	81 (100%)	0	100	100
31	DE	81/88 (92%)	81 (100%)	0	100	100
32	AE	92/97 (95%)	92 (100%)	0	100	100
32	DF	92/97 (95%)	92 (100%)	0	100	100
33	AF	109/111 (98%)	109 (100%)	0	100	100
33	DG	109/111 (98%)	109 (100%)	0	100	100
34	AG	90/91 (99%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	DH	90/91 (99%)	90 (100%)	0	100	100
35	AH	95/103 (92%)	94 (99%)	1 (1%)	65	75
35	DI	95/103 (92%)	95 (100%)	0	100	100
36	AI	104/105 (99%)	104 (100%)	0	100	100
36	DJ	104/105 (99%)	104 (100%)	0	100	100
37	AJ	81/82 (99%)	81 (100%)	0	100	100
37	DK	81/82 (99%)	81 (100%)	0	100	100
38	AK	70/71 (99%)	70 (100%)	0	100	100
38	DL	70/71 (99%)	70 (100%)	0	100	100
39	AL	68/69 (99%)	68 (100%)	0	100	100
39	DM	68/69 (99%)	68 (100%)	0	100	100
40	AM	45/46 (98%)	45 (100%)	0	100	100
40	DN	45/46 (98%)	45 (100%)	0	100	100
41	AN	47/116 (40%)	47 (100%)	0	100	100
41	DO	47/116 (40%)	47 (100%)	0	100	100
42	AO	23/23 (100%)	23 (100%)	0	100	100
42	DP	23/23 (100%)	23 (100%)	0	100	100
43	AP	90/91 (99%)	90 (100%)	0	100	100
43	DQ	90/91 (99%)	90 (100%)	0	100	100
44	AQ	71/72 (99%)	71 (100%)	0	100	100
44	DR	71/72 (99%)	71 (100%)	0	100	100
45	i	97/228 (42%)	97 (100%)	0	100	100
45	sM	54/228 (24%)	54 (100%)	0	100	100
46	p0	105/248 (42%)	105 (100%)	0	100	100
48	B	164/210 (78%)	164 (100%)	0	100	100
48	s0	165/210 (79%)	165 (100%)	0	100	100
49	C	191/224 (85%)	191 (100%)	0	100	100
49	s1	192/224 (86%)	192 (100%)	0	100	100
50	D	176/205 (86%)	176 (100%)	0	100	100
50	s2	176/205 (86%)	176 (100%)	0	100	100
51	E	182/195 (93%)	182 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	s3	182/195 (93%)	182 (100%)	0	100	100
52	F	221/222 (100%)	221 (100%)	0	100	100
52	s4	221/222 (100%)	221 (100%)	0	100	100
53	G	173/191 (91%)	173 (100%)	0	100	100
53	s5	173/191 (91%)	173 (100%)	0	100	100
54	H	188/201 (94%)	188 (100%)	0	100	100
54	s6	187/201 (93%)	187 (100%)	0	100	100
55	I	165/170 (97%)	165 (100%)	0	100	100
55	s7	165/170 (97%)	165 (100%)	0	100	100
56	J	150/161 (93%)	150 (100%)	0	100	100
56	s8	150/161 (93%)	150 (100%)	0	100	100
57	K	158/166 (95%)	158 (100%)	0	100	100
57	s9	158/166 (95%)	158 (100%)	0	100	100
58	L	77/98 (79%)	77 (100%)	0	100	100
58	c0	73/98 (74%)	73 (100%)	0	100	100
59	M	129/137 (94%)	129 (100%)	0	100	100
59	c1	129/137 (94%)	129 (100%)	0	100	100
60	N	88/119 (74%)	88 (100%)	0	100	100
60	c2	88/119 (74%)	88 (100%)	0	100	100
61	O	127/128 (99%)	127 (100%)	0	100	100
61	c3	127/128 (99%)	127 (100%)	0	100	100
62	P	79/105 (75%)	79 (100%)	0	100	100
62	c4	97/105 (92%)	97 (100%)	0	100	100
63	Q	101/118 (86%)	101 (100%)	0	100	100
63	c5	103/118 (87%)	103 (100%)	0	100	100
64	R	117/119 (98%)	117 (100%)	0	100	100
64	c6	118/119 (99%)	118 (100%)	0	100	100
65	S	94/124 (76%)	94 (100%)	0	100	100
66	T	128/129 (99%)	128 (100%)	0	100	100
66	c8	128/129 (99%)	128 (100%)	0	100	100
67	U	115/116 (99%)	115 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	c9	115/116 (99%)	115 (100%)	0	100	100
68	V	100/114 (88%)	100 (100%)	0	100	100
68	d0	103/114 (90%)	103 (100%)	0	100	100
69	W	74/74 (100%)	74 (100%)	0	100	100
69	d1	74/74 (100%)	74 (100%)	0	100	100
70	X	110/111 (99%)	110 (100%)	0	100	100
70	d2	110/111 (99%)	110 (100%)	0	100	100
71	Y	119/120 (99%)	119 (100%)	0	100	100
71	d3	119/120 (99%)	119 (100%)	0	100	100
72	Z	112/113 (99%)	112 (100%)	0	100	100
72	d4	112/113 (99%)	112 (100%)	0	100	100
73	a	61/89 (68%)	61 (100%)	0	100	100
73	d5	61/89 (68%)	61 (100%)	0	100	100
74	b	83/100 (83%)	83 (100%)	0	100	100
74	d6	83/100 (83%)	83 (100%)	0	100	100
75	c	70/71 (99%)	70 (100%)	0	100	100
75	d7	70/71 (99%)	70 (100%)	0	100	100
76	d	56/60 (93%)	56 (100%)	0	100	100
76	d8	56/60 (93%)	56 (100%)	0	100	100
77	d9	47/49 (96%)	47 (100%)	0	100	100
77	e	47/49 (96%)	47 (100%)	0	100	100
78	e0	53/54 (98%)	53 (100%)	0	100	100
78	f	51/54 (94%)	51 (100%)	0	100	100
79	e1	43/135 (32%)	43 (100%)	0	100	100
79	g	62/135 (46%)	61 (98%)	1 (2%)	55	71
80	Rb	260/262 (99%)	260 (100%)	0	100	100
80	h	259/262 (99%)	259 (100%)	0	100	100
81	c7	92/124 (74%)	92 (100%)	0	100	100
All	All	18678/20672 (90%)	18672 (100%)	6 (0%)	100	100

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	CE	104	THR
12	CL	185	ARG
79	g	140	TYR
5	k	104	THR
5	k	90	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 186 such sidechains are listed below:

Mol	Chain	Res	Type
53	G	66	GLN
80	h	4	ASN
54	H	139	ASN
66	T	13	HIS
49	s1	148	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3145/3396 (92%)	623 (19%)	49 (1%)
1	AR	3143/3396 (92%)	638 (20%)	46 (1%)
2	3	120/121 (99%)	17 (14%)	1 (0%)
2	AS	120/121 (99%)	20 (16%)	1 (0%)
3	4	157/158 (99%)	34 (21%)	2 (1%)
3	AT	157/158 (99%)	31 (19%)	1 (0%)
47	A	1778/1800 (98%)	490 (27%)	42 (2%)
47	sR	1780/1800 (98%)	453 (25%)	0
All	All	10400/10950 (94%)	2306 (22%)	142 (1%)

5 of 2306 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	16	A
1	1	26	A
1	1	40	A
1	1	48	A
1	1	49	A

5 of 142 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
47	A	555	A

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Mol	Chain	Res	Type
47	A	720	G
47	A	1250	U
1	1	3353	G
1	1	3351	U

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 2462 ligands modelled in this entry, 1 is modelled with single atom and 1500 are monoatomic - leaving 961 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	$\# Z > 2$
82	OHX	AR	3470	-	0,6,6	-	-	-		
82	OHX	AR	3510	-	0,6,6	-	-	-		
82	OHX	AR	3641	-	0,6,6	-	-	-		
82	OHX	CL	302	-	0,6,6	-	-	-		
82	OHX	sR	1901	-	0,6,6	-	-	-		
82	OHX	1	4106	-	0,6,6	-	-	-		
82	OHX	A	2145	-	0,6,6	-	-	-		
82	OHX	AR	3513	-	0,6,6	-	-	-		
82	OHX	A	1907	-	0,6,6	-	-	-		
82	OHX	1	3533	-	0,6,6	-	-	-		
82	OHX	1	4050	-	0,6,6	-	-	-		
82	OHX	AR	3413	-	0,6,6	-	-	-		
82	OHX	1	3502	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	AR	3558	-	0,6,6	-	-	-		
82	OHX	AR	3473	-	0,6,6	-	-	-		
82	OHX	AR	3608	-	0,6,6	-	-	-		
82	OHX	AR	3534	-	0,6,6	-	-	-		
82	OHX	AR	3580	-	0,6,6	-	-	-		
82	OHX	AR	3407	-	0,6,6	-	-	-		
82	OHX	A	2105	-	0,6,6	-	-	-		
82	OHX	sR	2016	-	0,6,6	-	-	-		
82	OHX	1	3539	-	0,6,6	-	-	-		
82	OHX	1	4088	-	0,6,6	-	-	-		
82	OHX	AR	4139	-	0,6,6	-	-	-		
82	OHX	1	4152	-	0,6,6	-	-	-		
82	OHX	1	3420	-	0,6,6	-	-	-		
82	OHX	1	3551	-	0,6,6	-	-	-		
82	OHX	AR	3486	-	0,6,6	-	-	-		
82	OHX	AR	3596	-	0,6,6	-	-	-		
82	OHX	AR	3437	-	0,6,6	-	-	-		
82	OHX	AR	3647	-	0,6,6	-	-	-		
82	OHX	AT	212	-	0,6,6	-	-	-		
82	OHX	CG	304	-	0,6,6	-	-	-		
82	OHX	A	1977	-	0,6,6	-	-	-		
82	OHX	1	3589	-	0,6,6	-	-	-		
82	OHX	AR	3560	-	0,6,6	-	-	-		
82	OHX	AR	3628	-	0,6,6	-	-	-		
82	OHX	AT	211	-	0,6,6	-	-	-		
82	OHX	3	221	-	0,6,6	-	-	-		
82	OHX	AR	3427	-	0,6,6	-	-	-		
82	OHX	1	4115	-	0,6,6	-	-	-		
82	OHX	AR	3562	-	0,6,6	-	-	-		
82	OHX	AR	3625	-	0,6,6	-	-	-		
82	OHX	A	1918	-	0,6,6	-	-	-		
82	OHX	AR	3526	-	0,6,6	-	-	-		
82	OHX	sR	1928	-	0,6,6	-	-	-		
82	OHX	AR	3425	-	0,6,6	-	-	-		
82	OHX	sR	1980	-	0,6,6	-	-	-		
82	OHX	1	3404	-	0,6,6	-	-	-		
82	OHX	AR	3402	-	0,6,6	-	-	-		
82	OHX	A	1940[A]	-	0,6,6	-	-	-		
82	OHX	1	4081	-	0,6,6	-	-	-		
82	OHX	A	1930	-	0,6,6	-	-	-		
82	OHX	A	2137	-	0,6,6	-	-	-		
82	OHX	O	201	-	0,6,6	-	-	-		
82	OHX	1	3442	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	sR	1957	-	0,6,6	-	-	-		
82	OHX	sR	1958	-	0,6,6	-	-	-		
82	OHX	4	208	-	0,6,6	-	-	-		
82	OHX	sR	1941	-	0,6,6	-	-	-		
82	OHX	AT	214	-	0,6,6	-	-	-		
82	OHX	AR	3496	-	0,6,6	-	-	-		
82	OHX	AR	3448	-	0,6,6	-	-	-		
82	OHX	A	2123	-	0,6,6	-	-	-		
82	OHX	AR	3483	-	0,6,6	-	-	-		
82	OHX	AK	103	-	0,6,6	-	-	-		
82	OHX	1	4109	-	0,6,6	-	-	-		
82	OHX	AR	3642	-	0,6,6	-	-	-		
82	OHX	AT	206	-	0,6,6	-	-	-		
82	OHX	AR	3547	-	0,6,6	-	-	-		
82	OHX	AS	203	-	0,6,6	-	-	-		
82	OHX	1	3552	-	0,6,6	-	-	-		
82	OHX	AR	3531	-	0,6,6	-	-	-		
82	OHX	1	3503	-	0,6,6	-	-	-		
82	OHX	4	212	-	0,6,6	-	-	-		
82	OHX	AR	3587	-	0,6,6	-	-	-		
82	OHX	AR	4144	-	0,6,6	-	-	-		
82	OHX	AR	3490	-	0,6,6	-	-	-		
82	OHX	sR	1968	-	0,6,6	-	-	-		
82	OHX	A	2104	-	0,6,6	-	-	-		
82	OHX	U	201	-	0,6,6	-	-	-		
82	OHX	AR	3557	-	0,6,6	-	-	-		
82	OHX	AR	3595	-	0,6,6	-	-	-		
82	OHX	sR	2017	-	0,6,6	-	-	-		
82	OHX	sR	1951	-	0,6,6	-	-	-		
82	OHX	1	3411	-	0,6,6	-	-	-		
82	OHX	sR	1932	-	0,6,6	-	-	-		
82	OHX	1	4146	-	0,6,6	-	-	-		
82	OHX	1	3412	-	0,6,6	-	-	-		
82	OHX	AR	4126	-	0,6,6	-	-	-		
82	OHX	1	3500	-	0,6,6	-	-	-		
82	OHX	AR	3571	-	0,6,6	-	-	-		
82	OHX	3	205	-	0,6,6	-	-	-		
82	OHX	1	4105	-	0,6,6	-	-	-		
82	OHX	AR	3423	-	0,6,6	-	-	-		
82	OHX	1	4140	-	0,6,6	-	-	-		
82	OHX	A	1904	-	0,6,6	-	-	-		
82	OHX	1	3570	-	0,6,6	-	-	-		
82	OHX	1	3548	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	AR	3506	-	0,6,6	-	-	-		
82	OHX	CG	303	-	0,6,6	-	-	-		
82	OHX	1	3476	-	0,6,6	-	-	-		
82	OHX	sR	1964	-	0,6,6	-	-	-		
82	OHX	1	3580	-	0,6,6	-	-	-		
82	OHX	AR	3430	-	0,6,6	-	-	-		
82	OHX	A	2117	-	0,6,6	-	-	-		
82	OHX	sR	1990	-	0,6,6	-	-	-		
82	OHX	1	3600	-	0,6,6	-	-	-		
82	OHX	A	2109	-	0,6,6	-	-	-		
82	OHX	1	3409	-	0,6,6	-	-	-		
82	OHX	sR	1965	-	0,6,6	-	-	-		
82	OHX	sR	1995	-	0,6,6	-	-	-		
82	OHX	A	2130	-	0,6,6	-	-	-		
82	OHX	1	3484	-	0,6,6	-	-	-		
82	OHX	AR	3410	-	0,6,6	-	-	-		
82	OHX	AR	3414	-	0,6,6	-	-	-		
82	OHX	1	4134	-	0,6,6	-	-	-		
82	OHX	A	1949	-	0,6,6	-	-	-		
82	OHX	J	301	-	0,6,6	-	-	-		
82	OHX	1	3592	-	0,6,6	-	-	-		
82	OHX	AR	3478	-	0,6,6	-	-	-		
82	OHX	AR	3507	-	0,6,6	-	-	-		
82	OHX	1	3532	-	0,6,6	-	-	-		
82	OHX	AR	3543	-	0,6,6	-	-	-		
82	OHX	sR	2003	-	0,6,6	-	-	-		
82	OHX	A	1968	-	0,6,6	-	-	-		
82	OHX	A	2120	-	0,6,6	-	-	-		
82	OHX	1	4091	-	0,6,6	-	-	-		
82	OHX	1	3598	-	0,6,6	-	-	-		
82	OHX	AR	3434	-	0,6,6	-	-	-		
82	OHX	AR	3671	-	0,6,6	-	-	-		
82	OHX	AR	4148	-	0,6,6	-	-	-		
82	OHX	1	3436	-	0,6,6	-	-	-		
82	OHX	sR	1919	-	0,6,6	-	-	-		
82	OHX	A	1922	-	0,6,6	-	-	-		
82	OHX	sR	1993	-	0,6,6	-	-	-		
82	OHX	AR	3622	-	0,6,6	-	-	-		
82	OHX	1	3602	-	0,6,6	-	-	-		
82	OHX	AR	3533	-	0,6,6	-	-	-		
82	OHX	AR	4161	-	0,6,6	-	-	-		
82	OHX	1	3507	-	0,6,6	-	-	-		
82	OHX	A	1959	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	sR	2175	-	0,6,6	-	-	-		
82	OHX	1	3448	-	0,6,6	-	-	-		
82	OHX	DQ	502	-	0,6,6	-	-	-		
82	OHX	AR	3415	-	0,6,6	-	-	-		
82	OHX	1	4077	-	0,6,6	-	-	-		
82	OHX	AR	4156	-	0,6,6	-	-	-		
82	OHX	1	3424	-	0,6,6	-	-	-		
82	OHX	AR	4150	-	0,6,6	-	-	-		
82	OHX	1	4098	-	0,6,6	-	-	-		
82	OHX	AR	3576	-	0,6,6	-	-	-		
82	OHX	A	1934	-	0,6,6	-	-	-		
82	OHX	AS	207	-	0,6,6	-	-	-		
82	OHX	A	2141	-	0,6,6	-	-	-		
82	OHX	1	3567	-	0,6,6	-	-	-		
82	OHX	sR	2026	-	0,6,6	-	-	-		
82	OHX	A	1960	-	0,6,6	-	-	-		
82	OHX	AT	216	-	0,6,6	-	-	-		
82	OHX	AR	3472	-	0,6,6	-	-	-		
82	OHX	sR	1933	-	0,6,6	-	-	-		
82	OHX	1	3561	-	0,6,6	-	-	-		
82	OHX	1	3438	-	0,6,6	-	-	-		
82	OHX	AR	3515	-	0,6,6	-	-	-		
82	OHX	1	3582	-	0,6,6	-	-	-		
82	OHX	sR	1915	-	0,6,6	-	-	-		
82	OHX	sR	1908	-	0,6,6	-	-	-		
82	OHX	AR	3528	-	0,6,6	-	-	-		
82	OHX	1	3456	-	0,6,6	-	-	-		
82	OHX	AR	3636	-	0,6,6	-	-	-		
82	OHX	A	1941	-	0,6,6	-	-	-		
82	OHX	AS	201	-	0,6,6	-	-	-		
82	OHX	sR	1937	-	0,6,6	-	-	-		
82	OHX	DH	202	-	0,6,6	-	-	-		
82	OHX	AR	3447	-	0,6,6	-	-	-		
82	OHX	A	2144	-	0,6,6	-	-	-		
82	OHX	CE	402	-	0,6,6	-	-	-		
82	OHX	1	3437	-	0,6,6	-	-	-		
82	OHX	A	1973	-	0,6,6	-	-	-		
82	OHX	1	3581	-	0,6,6	-	-	-		
82	OHX	A	2138	-	0,6,6	-	-	-		
82	OHX	1	3485	-	0,6,6	-	-	-		
82	OHX	AR	3668	-	0,6,6	-	-	-		
82	OHX	4	204	-	0,6,6	-	-	-		
82	OHX	AR	3419	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	A	2121	-	0,6,6	-	-	-		
82	OHX	A	2127	-	0,6,6	-	-	-		
82	OHX	sR	1975	-	0,6,6	-	-	-		
82	OHX	sR	2176	-	0,6,6	-	-	-		
82	OHX	sR	1986	-	0,6,6	-	-	-		
82	OHX	1	4119	-	0,6,6	-	-	-		
82	OHX	1	3593	-	0,6,6	-	-	-		
82	OHX	1	4148	-	0,6,6	-	-	-		
82	OHX	AR	3572	-	0,6,6	-	-	-		
82	OHX	AR	3535	-	0,6,6	-	-	-		
82	OHX	sR	1903	-	0,6,6	-	-	-		
82	OHX	AR	3603	-	0,6,6	-	-	-		
82	OHX	1	4149	-	0,6,6	-	-	-		
82	OHX	A	1964	-	0,6,6	-	-	-		
82	OHX	AR	3548	-	0,6,6	-	-	-		
82	OHX	A	2143	-	0,6,6	-	-	-		
82	OHX	1	3547	-	0,6,6	-	-	-		
82	OHX	AR	3428	-	0,6,6	-	-	-		
82	OHX	A	2136	-	0,6,6	-	-	-		
82	OHX	AR	3563	-	0,6,6	-	-	-		
82	OHX	sR	1988	-	0,6,6	-	-	-		
82	OHX	sR	1931	-	0,6,6	-	-	-		
82	OHX	AR	3590	-	0,6,6	-	-	-		
82	OHX	AR	3453	-	0,6,6	-	-	-		
82	OHX	1	3599	-	0,6,6	-	-	-		
82	OHX	AR	4154	-	0,6,6	-	-	-		
82	OHX	A	2140	-	0,6,6	-	-	-		
82	OHX	1	3446	-	0,6,6	-	-	-		
82	OHX	AR	3420	-	0,6,6	-	-	-		
82	OHX	1	4103	-	0,6,6	-	-	-		
82	OHX	1	3521	-	0,6,6	-	-	-		
82	OHX	A	1926	-	0,6,6	-	-	-		
82	OHX	1	3524	-	0,6,6	-	-	-		
82	OHX	1	4139	-	0,6,6	-	-	-		
82	OHX	A	2132	-	0,6,6	-	-	-		
82	OHX	1	3406	-	0,6,6	-	-	-		
82	OHX	AR	3634	-	0,6,6	-	-	-		
82	OHX	AR	4138	-	0,6,6	-	-	-		
82	OHX	sR	1927	-	0,6,6	-	-	-		
82	OHX	AR	3421	-	0,6,6	-	-	-		
82	OHX	AR	4120	-	0,6,6	-	-	-		
82	OHX	AR	4160	-	0,6,6	-	-	-		
82	OHX	A	2108	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	sR	2000	-	0,6,6	-	-	-		
82	OHX	A	1921	-	0,6,6	-	-	-		
82	OHX	1	4133	-	0,6,6	-	-	-		
82	OHX	4	210	-	0,6,6	-	-	-		
82	OHX	AR	3444	-	0,6,6	-	-	-		
82	OHX	1	3525	-	0,6,6	-	-	-		
82	OHX	AR	4116	-	0,6,6	-	-	-		
82	OHX	A	2118	-	0,6,6	-	-	-		
82	OHX	AR	3643	-	0,6,6	-	-	-		
82	OHX	1	3418	-	0,6,6	-	-	-		
82	OHX	AR	3602	-	0,6,6	-	-	-		
82	OHX	A	2114	-	0,6,6	-	-	-		
82	OHX	AR	3662	-	0,6,6	-	-	-		
82	OHX	1	4092	-	0,6,6	-	-	-		
82	OHX	1	3495	-	0,6,6	-	-	-		
82	OHX	1	4147	-	0,6,6	-	-	-		
82	OHX	AR	3450	-	0,6,6	-	-	-		
82	OHX	1	3457	-	0,6,6	-	-	-		
82	OHX	AR	3585	-	0,6,6	-	-	-		
82	OHX	1	3497	-	0,6,6	-	-	-		
82	OHX	AR	3629	-	0,6,6	-	-	-		
82	OHX	AR	3441	-	0,6,6	-	-	-		
82	OHX	1	3482	-	0,6,6	-	-	-		
82	OHX	AS	205	-	0,6,6	-	-	-		
82	OHX	1	3441	-	0,6,6	-	-	-		
82	OHX	1	3579	-	0,6,6	-	-	-		
82	OHX	sR	1940	-	0,6,6	-	-	-		
82	OHX	sR	1992	-	0,6,6	-	-	-		
82	OHX	A	1901	-	0,6,6	-	-	-		
82	OHX	1	4155	-	0,6,6	-	-	-		
82	OHX	1	3445	-	0,6,6	-	-	-		
82	OHX	AR	3609	-	0,6,6	-	-	-		
82	OHX	AR	3644	-	0,6,6	-	-	-		
82	OHX	AR	3648	-	0,6,6	-	-	-		
82	OHX	AR	3604	-	0,6,6	-	-	-		
82	OHX	1	3518	-	0,6,6	-	-	-		
82	OHX	AR	4136	-	0,6,6	-	-	-		
82	OHX	AR	3464	-	0,6,6	-	-	-		
82	OHX	AR	3655	-	0,6,6	-	-	-		
82	OHX	AR	3459	-	0,6,6	-	-	-		
82	OHX	AR	3656	-	0,6,6	-	-	-		
82	OHX	sR	2181	-	0,6,6	-	-	-		
82	OHX	A	1970	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3566	-	0,6,6	-	-	-		
82	OHX	A	1974	-	0,6,6	-	-	-		
82	OHX	1	3585	-	0,6,6	-	-	-		
82	OHX	1	3577	-	0,6,6	-	-	-		
82	OHX	1	3583	-	0,6,6	-	-	-		
82	OHX	sR	1952	-	0,6,6	-	-	-		
82	OHX	AR	3479	-	0,6,6	-	-	-		
82	OHX	CS	201	-	0,6,6	-	-	-		
82	OHX	1	3435	-	0,6,6	-	-	-		
82	OHX	1	4058	-	0,6,6	-	-	-		
82	OHX	AR	4143	-	0,6,6	-	-	-		
82	OHX	A	2116	-	0,6,6	-	-	-		
82	OHX	AR	3618	-	0,6,6	-	-	-		
82	OHX	AR	3651	-	0,6,6	-	-	-		
82	OHX	4	228	-	0,6,6	-	-	-		
82	OHX	AR	3480	-	0,6,6	-	-	-		
82	OHX	1	4121	-	0,6,6	-	-	-		
82	OHX	1	4129	-	0,6,6	-	-	-		
82	OHX	k	404	-	0,6,6	-	-	-		
82	OHX	AR	3638	-	0,6,6	-	-	-		
82	OHX	c3	202	-	0,6,6	-	-	-		
82	OHX	sR	2169	-	0,6,6	-	-	-		
82	OHX	AR	3551	-	0,6,6	-	-	-		
82	OHX	AR	3659	-	0,6,6	-	-	-		
82	OHX	1	3421	-	0,6,6	-	-	-		
82	OHX	1	4120	-	0,6,6	-	-	-		
82	OHX	AR	3598	-	0,6,6	-	-	-		
82	OHX	sR	1972	-	0,6,6	-	-	-		
82	OHX	sR	2005	-	0,6,6	-	-	-		
82	OHX	1	4151	-	0,6,6	-	-	-		
82	OHX	1	4097	-	0,6,6	-	-	-		
82	OHX	1	3527	-	0,6,6	-	-	-		
82	OHX	AR	4149	-	0,6,6	-	-	-		
82	OHX	sR	2002	-	0,6,6	-	-	-		
82	OHX	1	3401	-	0,6,6	-	-	-		
82	OHX	1	3468	-	0,6,6	-	-	-		
82	OHX	1	3540	-	0,6,6	-	-	-		
82	OHX	sR	2172	-	0,6,6	-	-	-		
82	OHX	1	3433	-	0,6,6	-	-	-		
82	OHX	1	3471	-	0,6,6	-	-	-		
82	OHX	1	3494	-	0,6,6	-	-	-		
82	OHX	1	3597	-	0,6,6	-	-	-		
82	OHX	AT	209	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3449	-	0,6,6	-	-	-		
82	OHX	AR	3501	-	0,6,6	-	-	-		
82	OHX	AR	3567	-	0,6,6	-	-	-		
82	OHX	1	3467	-	0,6,6	-	-	-		
82	OHX	AR	3458	-	0,6,6	-	-	-		
82	OHX	sR	2021	-	0,6,6	-	-	-		
82	OHX	AR	3503	-	0,6,6	-	-	-		
82	OHX	AR	3530	-	0,6,6	-	-	-		
82	OHX	1	3465	-	0,6,6	-	-	-		
82	OHX	AR	3620	-	0,6,6	-	-	-		
82	OHX	A	2119	-	0,6,6	-	-	-		
82	OHX	1	4101	-	0,6,6	-	-	-		
82	OHX	1	4114[B]	-	0,6,6	-	-	-		
82	OHX	AR	3615	-	0,6,6	-	-	-		
82	OHX	sR	2014	-	0,6,6	-	-	-		
82	OHX	A	1946	-	0,6,6	-	-	-		
82	OHX	3	220	-	0,6,6	-	-	-		
82	OHX	sR	2015	-	0,6,6	-	-	-		
82	OHX	AT	208	-	0,6,6	-	-	-		
82	OHX	A	1962	-	0,6,6	-	-	-		
82	OHX	1	4094	-	0,6,6	-	-	-		
82	OHX	AR	3555	-	0,6,6	-	-	-		
82	OHX	AR	3568	-	0,6,6	-	-	-		
82	OHX	A	1954	-	0,5,6	-	-	-		
82	OHX	AR	3469	-	0,6,6	-	-	-		
82	OHX	1	3488	-	0,6,6	-	-	-		
82	OHX	1	3425	-	0,6,6	-	-	-		
82	OHX	A	1971	-	0,6,6	-	-	-		
82	OHX	A	1920	-	0,6,6	-	-	-		
82	OHX	sR	1936	-	0,6,6	-	-	-		
82	OHX	sR	2025	-	0,6,6	-	-	-		
82	OHX	4	202	-	0,6,6	-	-	-		
82	OHX	1	4123	-	0,6,6	-	-	-		
82	OHX	AR	3409	-	0,6,6	-	-	-		
82	OHX	1	3487	-	0,6,6	-	-	-		
82	OHX	AR	3485	-	0,6,6	-	-	-		
82	OHX	A	1948	-	0,6,6	-	-	-		
82	OHX	AR	3623	-	0,6,6	-	-	-		
82	OHX	1	4111	-	0,6,6	-	-	-		
82	OHX	sR	2024	-	0,6,6	-	-	-		
82	OHX	d4	201	-	0,6,6	-	-	-		
82	OHX	AR	3617	-	0,6,6	-	-	-		
82	OHX	v	301	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	AR	3520	-	0,6,6	-	-	-		
82	OHX	AR	3635	-	0,6,6	-	-	-		
82	OHX	1	3550	-	0,6,6	-	-	-		
82	OHX	AR	3508	-	0,6,6	-	-	-		
82	OHX	sR	1921	-	0,6,6	-	-	-		
82	OHX	AR	3462	-	0,6,6	-	-	-		
82	OHX	4	211	-	0,6,6	-	-	-		
82	OHX	1	4051	-	0,6,6	-	-	-		
82	OHX	4	205	-	0,6,6	-	-	-		
82	OHX	sR	1922	-	0,6,6	-	-	-		
82	OHX	A	1938	-	0,6,6	-	-	-		
82	OHX	sR	1999	-	0,6,6	-	-	-		
82	OHX	sR	2170	-	0,6,6	-	-	-		
82	OHX	1	4132	-	0,6,6	-	-	-		
82	OHX	sR	1914	-	0,6,6	-	-	-		
82	OHX	1	3461	-	0,6,6	-	-	-		
82	OHX	1	3545	-	0,6,6	-	-	-		
82	OHX	AR	3583	-	0,6,6	-	-	-		
82	OHX	AR	3653	-	0,6,6	-	-	-		
82	OHX	1	4078	-	0,6,6	-	-	-		
82	OHX	AR	3522	-	0,6,6	-	-	-		
82	OHX	AR	4146	-	0,6,6	-	-	-		
82	OHX	AR	3509	-	0,6,6	-	-	-		
82	OHX	AR	3500	-	0,6,6	-	-	-		
82	OHX	1	3520	-	0,6,6	-	-	-		
82	OHX	3	206	-	0,6,6	-	-	-		
82	OHX	1	3477	-	0,6,6	-	-	-		
82	OHX	AR	3504	-	0,6,6	-	-	-		
82	OHX	AR	3552	-	0,6,6	-	-	-		
82	OHX	AR	3574	-	0,6,6	-	-	-		
82	OHX	A	1942	-	0,6,6	-	-	-		
82	OHX	c5	201	-	0,6,6	-	-	-		
82	OHX	AR	3664	-	0,6,6	-	-	-		
82	OHX	1	4125	-	0,6,6	-	-	-		
82	OHX	1	3557	-	0,6,6	-	-	-		
82	OHX	sR	1943	-	0,6,6	-	-	-		
82	OHX	A	1909	-	0,6,6	-	-	-		
82	OHX	AR	3416	-	0,6,6	-	-	-		
82	OHX	AT	213	-	0,6,6	-	-	-		
82	OHX	1	4100	-	0,6,6	-	-	-		
82	OHX	sR	1950	-	0,6,6	-	-	-		
82	OHX	A	1940[B]	-	0,6,6	-	-	-		
82	OHX	s4	301	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	AR	4152	-	0,6,6	-	-	-		
82	OHX	A	2125	-	0,6,6	-	-	-		
82	OHX	1	3571	-	0,6,6	-	-	-		
82	OHX	1	4131	-	0,6,6	-	-	-		
82	OHX	AR	3553	-	0,6,6	-	-	-		
82	OHX	sR	2178	-	0,6,6	-	-	-		
82	OHX	AR	3554	-	0,6,6	-	-	-		
82	OHX	AR	4140	-	0,6,6	-	-	-		
82	OHX	A	1937	-	0,6,6	-	-	-		
82	OHX	1	3555	-	0,6,6	-	-	-		
82	OHX	1	4060	-	0,6,6	-	-	-		
82	OHX	1	4107	-	0,6,6	-	-	-		
82	OHX	1	4075	-	0,6,6	-	-	-		
82	OHX	AR	3616	-	0,6,6	-	-	-		
82	OHX	AR	4147	-	0,6,6	-	-	-		
82	OHX	AR	3404	-	0,6,6	-	-	-		
82	OHX	1	3480	-	0,6,6	-	-	-		
82	OHX	sR	1994	-	0,6,6	-	-	-		
82	OHX	AR	3442	-	0,6,6	-	-	-		
82	OHX	AR	3482	-	0,6,6	-	-	-		
82	OHX	A	2107	-	0,6,6	-	-	-		
82	OHX	sR	1926	-	0,6,6	-	-	-		
82	OHX	1	4090	-	0,6,6	-	-	-		
82	OHX	sR	1929	-	0,6,6	-	-	-		
82	OHX	sR	1984	-	0,6,6	-	-	-		
82	OHX	4	229	-	0,6,6	-	-	-		
82	OHX	1	3463	-	0,6,6	-	-	-		
82	OHX	1	3499	-	0,6,6	-	-	-		
82	OHX	1	3554	-	0,6,6	-	-	-		
82	OHX	sR	1944	-	0,6,6	-	-	-		
82	OHX	1	3546	-	0,6,6	-	-	-		
82	OHX	CP	302	-	0,6,6	-	-	-		
82	OHX	AR	3612	-	0,6,6	-	-	-		
82	OHX	A	2113	-	0,6,6	-	-	-		
82	OHX	AG	202	-	0,6,6	-	-	-		
82	OHX	A	1951	-	0,6,6	-	-	-		
82	OHX	1	3462	-	0,6,6	-	-	-		
82	OHX	AC	102	-	0,6,6	-	-	-		
82	OHX	AR	3627	-	0,6,6	-	-	-		
82	OHX	AR	4141	-	0,6,6	-	-	-		
82	OHX	1	3452	-	0,6,6	-	-	-		
82	OHX	1	3511	-	0,6,6	-	-	-		
82	OHX	1	3517	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	A	1906	-	0,6,6	-	-	-		
82	OHX	A	2106	-	0,6,6	-	-	-		
82	OHX	1	3475	-	0,6,6	-	-	-		
82	OHX	CG	302	-	0,6,6	-	-	-		
82	OHX	1	3594	-	0,6,6	-	-	-		
82	OHX	1	3534	-	0,6,6	-	-	-		
82	OHX	z	202	-	0,6,6	-	-	-		
82	OHX	AR	3412	-	0,6,6	-	-	-		
82	OHX	A	1957	-	0,6,6	-	-	-		
82	OHX	A	2122	-	0,6,6	-	-	-		
82	OHX	AR	3426	-	0,6,6	-	-	-		
82	OHX	A	1924	-	0,6,6	-	-	-		
82	OHX	AR	3666	-	0,6,6	-	-	-		
82	OHX	1	4150	-	0,6,6	-	-	-		
82	OHX	1	3460	-	0,6,6	-	-	-		
82	OHX	AR	3631	-	0,6,6	-	-	-		
82	OHX	sR	1924	-	0,6,6	-	-	-		
82	OHX	1	4062	-	0,6,6	-	-	-		
82	OHX	AR	3476	-	0,6,6	-	-	-		
82	OHX	AR	3607	-	0,6,6	-	-	-		
82	OHX	sR	1981	-	0,6,6	-	-	-		
82	OHX	l	405	-	0,6,6	-	-	-		
82	OHX	1	3416	-	0,6,6	-	-	-		
82	OHX	1	3474	-	0,6,6	-	-	-		
82	OHX	1	4072	-	0,6,6	-	-	-		
82	OHX	AR	3600	-	0,6,6	-	-	-		
82	OHX	A	1908	-	0,6,6	-	-	-		
82	OHX	1	4141	-	0,6,6	-	-	-		
82	OHX	1	4084	-	0,6,6	-	-	-		
82	OHX	1	4085	-	0,6,6	-	-	-		
82	OHX	A	1910	-	0,6,6	-	-	-		
86	X1K	AR	4205	-	27,27,27	0.71	2 (7%)	37,43,43	1.90	8 (21%)
82	OHX	AR	3633	-	0,6,6	-	-	-		
82	OHX	AR	3497	-	0,6,6	-	-	-		
82	OHX	sR	2006	-	0,6,6	-	-	-		
82	OHX	sR	1955	-	0,6,6	-	-	-		
82	OHX	AR	3650	-	0,6,6	-	-	-		
82	OHX	AR	3438	-	0,6,6	-	-	-		
82	OHX	sR	1949	-	0,6,6	-	-	-		
82	OHX	AR	3581	-	0,6,6	-	-	-		
82	OHX	Q	201	-	0,6,6	-	-	-		
82	OHX	AR	3578	-	0,6,6	-	-	-		
82	OHX	AR	3451	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	sR	1997	-	0,6,6	-	-	-		
82	OHX	A	1932	-	0,6,6	-	-	-		
82	OHX	AR	3481	-	0,6,6	-	-	-		
82	OHX	sR	2022	-	0,6,6	-	-	-		
82	OHX	AR	3593	-	0,6,6	-	-	-		
82	OHX	AR	3456	-	0,6,6	-	-	-		
82	OHX	A	1975	-	0,6,6	-	-	-		
82	OHX	1	3544	-	0,6,6	-	-	-		
82	OHX	1	3447	-	0,6,6	-	-	-		
82	OHX	1	3516	-	0,6,6	-	-	-		
82	OHX	1	3417	-	0,6,6	-	-	-		
82	OHX	1	4079	-	0,6,6	-	-	-		
82	OHX	AR	3465	-	0,6,6	-	-	-		
82	OHX	1	3529	-	0,6,6	-	-	-		
82	OHX	AR	3518	-	0,6,6	-	-	-		
82	OHX	AR	3539	-	0,6,6	-	-	-		
82	OHX	AR	3637	-	0,6,6	-	-	-		
82	OHX	A	1966	-	0,6,6	-	-	-		
82	OHX	sR	1961	-	0,6,6	-	-	-		
82	OHX	AR	3640	-	0,6,6	-	-	-		
82	OHX	AR	3646	-	0,6,6	-	-	-		
82	OHX	1	3541	-	0,6,6	-	-	-		
82	OHX	1	3513	-	0,6,6	-	-	-		
82	OHX	AR	3670	-	0,6,6	-	-	-		
82	OHX	A	2111	-	0,6,6	-	-	-		
82	OHX	sR	1996	-	0,6,6	-	-	-		
82	OHX	AR	4157	-	0,6,6	-	-	-		
82	OHX	sR	2011	-	0,6,6	-	-	-		
82	OHX	AR	3457	-	0,6,6	-	-	-		
82	OHX	A	1912	-	0,6,6	-	-	-		
82	OHX	sR	1966	-	0,6,6	-	-	-		
82	OHX	sR	1953	-	0,6,6	-	-	-		
82	OHX	A	1943	-	0,6,6	-	-	-		
82	OHX	AR	3660	-	0,6,6	-	-	-		
82	OHX	sR	1911	-	0,6,6	-	-	-		
85	SPD	AR	4204	-	9,9,9	0.33	0	8,8,8	0.88	0
82	OHX	1	3489	-	0,6,6	-	-	-		
82	OHX	sR	1998	-	0,6,6	-	-	-		
82	OHX	AR	3579	-	0,6,6	-	-	-		
82	OHX	AT	201	-	0,6,6	-	-	-		
82	OHX	k	403	-	0,6,6	-	-	-		
82	OHX	AR	3429	-	0,6,6	-	-	-		
82	OHX	1	3535[A]	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3586	-	0,6,6	-	-	-		
82	OHX	1	4126	-	0,6,6	-	-	-		
82	OHX	AR	3556	-	0,6,6	-	-	-		
82	OHX	1	3572	-	0,6,6	-	-	-		
82	OHX	3	222	-	0,6,6	-	-	-		
82	OHX	AR	3424	-	0,6,6	-	-	-		
82	OHX	1	4142	-	0,6,6	-	-	-		
82	OHX	sR	2171	-	0,6,6	-	-	-		
82	OHX	AR	3566	-	0,6,6	-	-	-		
82	OHX	A	1919	-	0,6,6	-	-	-		
82	OHX	1	4086	-	0,6,6	-	-	-		
82	OHX	3	204	-	0,6,6	-	-	-		
82	OHX	sR	1989	-	0,6,6	-	-	-		
82	OHX	1	3426	-	0,6,6	-	-	-		
82	OHX	1	3537	-	0,6,6	-	-	-		
82	OHX	A	1913	-	0,6,6	-	-	-		
82	OHX	AR	3454	-	0,6,6	-	-	-		
82	OHX	1	3472	-	0,6,6	-	-	-		
82	OHX	AR	3468	-	0,6,6	-	-	-		
82	OHX	1	3565	-	0,6,6	-	-	-		
82	OHX	AR	3525	-	0,6,6	-	-	-		
82	OHX	1	3410	-	0,6,6	-	-	-		
82	OHX	A	1902	-	0,6,6	-	-	-		
82	OHX	AR	3575	-	0,5,6	-	-	-		
82	OHX	A	1929	-	0,6,6	-	-	-		
82	OHX	sR	1913	-	0,6,6	-	-	-		
82	OHX	sR	1942	-	0,6,6	-	-	-		
82	OHX	sR	1947	-	0,6,6	-	-	-		
82	OHX	AR	3406	-	0,6,6	-	-	-		
82	OHX	AR	3439	-	0,6,6	-	-	-		
82	OHX	A	1944	-	0,6,6	-	-	-		
82	OHX	3	203	-	0,6,6	-	-	-		
82	OHX	CL	303	-	0,6,6	-	-	-		
82	OHX	1	3403	-	0,6,6	-	-	-		
82	OHX	AR	4158	-	0,6,6	-	-	-		
82	OHX	sR	1905	-	0,6,6	-	-	-		
82	OHX	AR	3452	-	0,6,6	-	-	-		
82	OHX	sR	1904	-	0,6,6	-	-	-		
82	OHX	AR	3527	-	0,6,6	-	-	-		
82	OHX	1	3454	-	0,6,6	-	-	-		
82	OHX	1	3523	-	0,6,6	-	-	-		
82	OHX	AR	3422	-	0,6,6	-	-	-		
82	OHX	AR	3495	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	AR	4162	-	0,6,6	-	-	-		
82	OHX	sR	2012	-	0,6,6	-	-	-		
82	OHX	AR	3540	-	0,6,6	-	-	-		
82	OHX	1	3408	-	0,6,6	-	-	-		
82	OHX	1	3535[B]	-	0,6,6	-	-	-		
82	OHX	AR	3433	-	0,6,6	-	-	-		
82	OHX	AR	3588	-	0,6,6	-	-	-		
82	OHX	sR	1970	-	0,6,6	-	-	-		
82	OHX	AR	3432	-	0,6,6	-	-	-		
82	OHX	s8	301	-	0,6,6	-	-	-		
82	OHX	AR	3584	-	0,6,6	-	-	-		
82	OHX	AR	3467	-	0,6,6	-	-	-		
82	OHX	1	3514	-	0,6,6	-	-	-		
82	OHX	sR	1956	-	0,6,6	-	-	-		
82	OHX	CH	201	-	0,6,6	-	-	-		
82	OHX	sR	1985	-	0,6,6	-	-	-		
82	OHX	sR	2180	-	0,6,6	-	-	-		
82	OHX	A	2126[A]	-	0,6,6	-	-	-		
82	OHX	1	3505	-	0,6,6	-	-	-		
82	OHX	4	209	-	0,6,6	-	-	-		
82	OHX	AR	3564	-	0,6,6	-	-	-		
82	OHX	sR	2010	-	0,6,6	-	-	-		
82	OHX	1	3413	-	0,6,6	-	-	-		
82	OHX	AR	3512	-	0,6,6	-	-	-		
82	OHX	1	3519	-	0,6,6	-	-	-		
82	OHX	1	3573	-	0,6,6	-	-	-		
82	OHX	1	3407	-	0,6,6	-	-	-		
82	OHX	sR	1974	-	0,6,6	-	-	-		
82	OHX	1	3590	-	0,6,6	-	-	-		
82	OHX	1	4073	-	0,6,6	-	-	-		
82	OHX	sR	1978	-	0,6,6	-	-	-		
82	OHX	1	3479	-	0,6,6	-	-	-		
82	OHX	AR	3577	-	0,6,6	-	-	-		
82	OHX	AR	3544	-	0,6,6	-	-	-		
82	OHX	AR	3516	-	0,6,6	-	-	-		
82	OHX	AR	3435	-	0,6,6	-	-	-		
82	OHX	1	3493	-	0,6,6	-	-	-		
82	OHX	CK	201	-	0,6,6	-	-	-		
82	OHX	AT	234	-	0,6,6	-	-	-		
82	OHX	AR	3569	-	0,6,6	-	-	-		
85	SPD	1	4180	-	9,9,9	0.32	0	8,8,8	0.92	0
82	OHX	A	2135	-	0,6,6	-	-	-		
82	OHX	A	1953	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	AR	3665	-	0,6,6	-	-	-		
82	OHX	1	4087	-	0,6,6	-	-	-		
82	OHX	AR	3538	-	0,6,6	-	-	-		
82	OHX	AR	3645	-	0,6,6	-	-	-		
82	OHX	1	4110	-	0,6,6	-	-	-		
82	OHX	1	3564	-	0,6,6	-	-	-		
82	OHX	AR	3632	-	0,6,6	-	-	-		
82	OHX	AR	3401	-	0,6,6	-	-	-		
82	OHX	sR	1973	-	0,6,6	-	-	-		
82	OHX	1	3469	-	0,6,6	-	-	-		
82	OHX	1	3578	-	0,6,6	-	-	-		
82	OHX	AR	3455	-	0,6,6	-	-	-		
82	OHX	AR	3586	-	0,6,6	-	-	-		
82	OHX	1	3440	-	0,6,6	-	-	-		
82	OHX	AR	3542	-	0,6,6	-	-	-		
82	OHX	A	1923	-	0,6,6	-	-	-		
82	OHX	1	3559	-	0,6,6	-	-	-		
82	OHX	AS	206	-	0,6,6	-	-	-		
82	OHX	1	4096	-	0,6,6	-	-	-		
82	OHX	1	3509	-	0,6,6	-	-	-		
82	OHX	AR	3449	-	0,6,6	-	-	-		
82	OHX	r	303	-	0,6,6	-	-	-		
82	OHX	AR	3475	-	0,6,6	-	-	-		
82	OHX	1	3496	-	0,6,6	-	-	-		
82	OHX	AR	4155	-	0,6,6	-	-	-		
82	OHX	AR	3445	-	0,6,6	-	-	-		
82	OHX	A	2142	-	0,6,6	-	-	-		
82	OHX	A	2112	-	0,6,6	-	-	-		
82	OHX	AR	3466	-	0,6,6	-	-	-		
82	OHX	AR	4142	-	0,6,6	-	-	-		
82	OHX	AR	3491	-	0,6,6	-	-	-		
86	X1K	1	4181	-	27,27,27	0.50	1 (3%)	37,43,43	2.31	8 (21%)
82	OHX	1	4117	-	0,6,6	-	-	-		
82	OHX	AR	3471	-	0,6,6	-	-	-		
82	OHX	1	4116	-	0,6,6	-	-	-		
82	OHX	A	2126[B]	-	0,6,6	-	-	-		
82	OHX	1	3530	-	0,6,6	-	-	-		
82	OHX	sR	2167	-	0,6,6	-	-	-		
82	OHX	A	1917	-	0,6,6	-	-	-		
82	OHX	1	4122	-	0,6,6	-	-	-		
82	OHX	A	1933	-	0,6,6	-	-	-		
82	OHX	1	3510	-	0,6,6	-	-	-		
82	OHX	sR	2009	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3596	-	0,6,6	-	-	-		
82	OHX	AT	202	-	0,6,6	-	-	-		
82	OHX	AR	3550	-	0,6,6	-	-	-		
82	OHX	1	3427	-	0,6,6	-	-	-		
82	OHX	1	3512	-	0,6,6	-	-	-		
82	OHX	1	4130	-	0,6,6	-	-	-		
82	OHX	AR	3614	-	0,6,6	-	-	-		
82	OHX	AR	3405	-	0,6,6	-	-	-		
82	OHX	A	2110	-	0,6,6	-	-	-		
82	OHX	AR	3488	-	0,6,6	-	-	-		
82	OHX	A	2124	-	0,6,6	-	-	-		
82	OHX	AR	3613	-	0,6,6	-	-	-		
82	OHX	AT	210	-	0,6,6	-	-	-		
82	OHX	1	3605	-	0,6,6	-	-	-		
82	OHX	AR	4159	-	0,6,6	-	-	-		
82	OHX	A	1903	-	0,6,6	-	-	-		
82	OHX	AR	3667	-	0,6,6	-	-	-		
82	OHX	1	3431	-	0,6,6	-	-	-		
82	OHX	A	1931	-	0,6,6	-	-	-		
82	OHX	sR	1979	-	0,6,6	-	-	-		
82	OHX	sR	2004	-	0,6,6	-	-	-		
82	OHX	A	1928	-	0,6,6	-	-	-		
82	OHX	AT	233	-	0,6,6	-	-	-		
82	OHX	sR	1963	-	0,6,6	-	-	-		
82	OHX	sR	1910	-	0,6,6	-	-	-		
82	OHX	AR	4153	-	0,6,6	-	-	-		
82	OHX	sR	1960	-	0,6,6	-	-	-		
82	OHX	4	206	-	0,6,6	-	-	-		
82	OHX	sR	1945	-	0,6,6	-	-	-		
82	OHX	sR	1977	-	0,6,6	-	-	-		
82	OHX	1	3508	-	0,6,6	-	-	-		
82	OHX	sR	2007	-	0,6,6	-	-	-		
82	OHX	DL	103	-	0,6,6	-	-	-		
82	OHX	AR	3630	-	0,6,6	-	-	-		
82	OHX	AR	3461	-	0,6,6	-	-	-		
82	OHX	1	3587	-	0,6,6	-	-	-		
82	OHX	1	4135	-	0,6,6	-	-	-		
82	OHX	1	4144	1	0,5,6	-	-	-		
82	OHX	AR	3597	-	0,6,6	-	-	-		
82	OHX	1	4118	-	0,6,6	-	-	-		
82	OHX	AS	204	-	0,6,6	-	-	-		
82	OHX	3	201	-	0,6,6	-	-	-		
82	OHX	AR	3505	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3429	-	0,6,6	-	-	-		
82	OHX	1	3422	-	0,6,6	-	-	-		
82	OHX	1	3595	-	0,6,6	-	-	-		
82	OHX	AR	4137	-	0,6,6	-	-	-		
82	OHX	AR	3411	-	0,6,6	-	-	-		
82	OHX	1	4080	-	0,6,6	-	-	-		
82	OHX	CE	401	-	0,6,6	-	-	-		
82	OHX	3	202	-	0,6,6	-	-	-		
82	OHX	AR	3663	-	0,6,6	-	-	-		
82	OHX	AR	3517	-	0,6,6	-	-	-		
82	OHX	A	1925	-	0,6,6	-	-	-		
82	OHX	1	4074	-	0,6,6	-	-	-		
82	OHX	sR	1946	-	0,6,6	-	-	-		
82	OHX	A	1965	-	0,6,6	-	-	-		
82	OHX	1	3490	-	0,6,6	-	-	-		
82	OHX	AR	3545	-	0,6,6	-	-	-		
82	OHX	AR	3536	-	0,6,6	-	-	-		
82	OHX	AR	3657	-	0,6,6	-	-	-		
82	OHX	A	2134	-	0,6,6	-	-	-		
82	OHX	A	2102	-	0,6,6	-	-	-		
82	OHX	1	3504	-	0,6,6	-	-	-		
82	OHX	AR	3477	-	0,6,6	-	-	-		
82	OHX	sR	1907	-	0,6,6	-	-	-		
82	OHX	sR	1916[A]	-	0,6,6	-	-	-		
82	OHX	sR	1959	-	0,6,6	-	-	-		
82	OHX	1	3423	-	0,6,6	-	-	-		
82	OHX	AR	3521	-	0,6,6	-	-	-		
82	OHX	1	4089	-	0,6,6	-	-	-		
82	OHX	AR	3524	-	0,6,6	-	-	-		
82	OHX	AR	3484	-	0,6,6	-	-	-		
82	OHX	AR	3487	-	0,6,6	-	-	-		
82	OHX	1	3562	-	0,6,6	-	-	-		
82	OHX	1	3430	-	0,6,6	-	-	-		
82	OHX	1	3528	-	0,6,6	-	-	-		
82	OHX	1	3526	-	0,6,6	-	-	-		
82	OHX	AR	3592	-	0,6,6	-	-	-		
82	OHX	AR	3611	-	0,6,6	-	-	-		
82	OHX	sR	1906	-	0,6,6	-	-	-		
82	OHX	AR	3601	-	0,6,6	-	-	-		
82	OHX	1	3405	-	0,6,6	-	-	-		
82	OHX	Rb	401	-	0,6,6	-	-	-		
82	OHX	4	213	-	0,6,6	-	-	-		
82	OHX	1	3473	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3455	-	0,6,6	-	-	-		
82	OHX	AR	3436	-	0,6,6	-	-	-		
82	OHX	sR	1918	-	0,6,6	-	-	-		
82	OHX	AR	3594	-	0,6,6	-	-	-		
82	OHX	AP	502	-	0,6,6	-	-	-		
82	OHX	1	3543	-	0,6,6	-	-	-		
82	OHX	AR	3443	-	0,6,6	-	-	-		
82	OHX	A	1911	-	0,6,6	-	-	-		
82	OHX	AR	3639	-	0,6,6	-	-	-		
82	OHX	AR	3658	-	0,6,6	-	-	-		
82	OHX	sR	1920	-	0,6,6	-	-	-		
82	OHX	sR	1939	-	0,6,6	-	-	-		
82	OHX	AR	3549	-	0,6,6	-	-	-		
82	OHX	1	3434	-	0,6,6	-	-	-		
82	OHX	1	3451	-	0,6,6	-	-	-		
82	OHX	1	4153	-	0,6,6	-	-	-		
82	OHX	AR	3621	-	0,6,6	-	-	-		
82	OHX	sR	1982	-	0,6,6	-	-	-		
82	OHX	1	3542	-	0,6,6	-	-	-		
82	OHX	1	3588	-	0,6,6	-	-	-		
82	OHX	sR	1969	-	0,6,6	-	-	-		
82	OHX	AR	3499	-	0,6,6	-	-	-		
82	OHX	AR	4163	-	0,6,6	-	-	-		
82	OHX	AR	3546	-	0,6,6	-	-	-		
82	OHX	1	3576	-	0,6,6	-	-	-		
82	OHX	1	4143	-	0,6,6	-	-	-		
82	OHX	1	4108	-	0,6,6	-	-	-		
82	OHX	sR	2023	-	0,6,6	-	-	-		
82	OHX	AT	215	-	0,6,6	-	-	-		
82	OHX	1	4082	-	0,6,6	-	-	-		
82	OHX	AR	3591	-	0,6,6	-	-	-		
82	OHX	1	3491	-	0,6,6	-	-	-		
82	OHX	1	4127	-	0,6,6	-	-	-		
82	OHX	AR	3573	-	0,6,6	-	-	-		
82	OHX	c7	201	-	0,6,6	-	-	-		
82	OHX	sR	2001	-	0,6,6	-	-	-		
82	OHX	1	3492	-	0,6,6	-	-	-		
82	OHX	AR	3494	-	0,6,6	-	-	-		
82	OHX	AR	3561	-	0,6,6	-	-	-		
82	OHX	sR	1916[B]	-	0,6,6	-	-	-		
82	OHX	sR	2018	-	0,6,6	-	-	-		
82	OHX	sR	2179	-	0,6,6	-	-	-		
82	OHX	AR	3582	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	AR	3652	-	0,6,6	-	-	-		
82	OHX	A	2146	-	0,6,6	-	-	-		
82	OHX	A	1936	-	0,6,6	-	-	-		
82	OHX	A	1976	-	0,6,6	-	-	-		
82	OHX	1	4128	-	0,6,6	-	-	-		
82	OHX	A	1958	-	0,6,6	-	-	-		
82	OHX	AR	3610	-	0,6,6	-	-	-		
82	OHX	A	1914	-	0,6,6	-	-	-		
82	OHX	AR	3460	-	0,6,6	-	-	-		
82	OHX	A	2129	-	0,6,6	-	-	-		
82	OHX	CV	201	-	0,6,6	-	-	-		
82	OHX	sR	2177	-	0,6,6	-	-	-		
82	OHX	AR	3619	-	0,6,6	-	-	-		
82	OHX	1	3569	-	0,6,6	-	-	-		
82	OHX	sR	2013	-	0,6,6	-	-	-		
82	OHX	A	2147	-	0,6,6	-	-	-		
82	OHX	A	1939	-	0,6,6	-	-	-		
82	OHX	sR	1917	-	0,6,6	-	-	-		
82	OHX	AR	4145	-	0,6,6	-	-	-		
82	OHX	1	3553	-	0,6,6	-	-	-		
82	OHX	1	3591	-	0,6,6	-	-	-		
82	OHX	AR	3417	-	0,6,6	-	-	-		
82	OHX	AR	3492	-	0,6,6	-	-	-		
82	OHX	sR	1925	-	0,6,6	-	-	-		
82	OHX	1	3486	-	0,6,6	-	-	-		
82	OHX	AR	3624	-	0,6,6	-	-	-		
82	OHX	A	1961	-	0,6,6	-	-	-		
82	OHX	A	1969	-	0,6,6	-	-	-		
82	OHX	h	401	-	0,6,6	-	-	-		
82	OHX	1	3558	-	0,6,6	-	-	-		
82	OHX	A	1950	-	0,6,6	-	-	-		
82	OHX	AR	3463	-	0,6,6	-	-	-		
82	OHX	sR	1987	-	0,6,6	-	-	-		
82	OHX	sR	2174	-	0,6,6	-	-	-		
82	OHX	AR	3626	-	0,6,6	-	-	-		
82	OHX	A	2115	-	0,6,6	-	-	-		
82	OHX	AR	3529	-	0,6,6	-	-	-		
82	OHX	1	4104	-	0,6,6	-	-	-		
82	OHX	DD	102	-	0,6,6	-	-	-		
82	OHX	AR	3523	-	0,6,6	-	-	-		
82	OHX	AS	208	-	0,6,6	-	-	-		
82	OHX	AT	235	-	0,6,6	-	-	-		
82	OHX	1	3483	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3560	-	0,6,6	-	-	-		
82	OHX	AR	3519	-	0,6,6	-	-	-		
82	OHX	sR	1971	-	0,6,6	-	-	-		
82	OHX	1	3415	-	0,6,6	-	-	-		
82	OHX	1	3549	-	0,6,6	-	-	-		
82	OHX	1	3428	-	0,6,6	-	-	-		
82	OHX	1	3563	-	0,6,6	-	-	-		
82	OHX	A	1927	-	0,6,6	-	-	-		
82	OHX	1	3453	-	0,6,6	-	-	-		
82	OHX	1	4136	-	0,6,6	-	-	-		
82	OHX	AR	3489	-	0,6,6	-	-	-		
82	OHX	1	3603	-	0,6,6	-	-	-		
82	OHX	AR	3446	-	0,6,6	-	-	-		
82	OHX	1	4056	-	0,6,6	-	-	-		
82	OHX	AR	3493	-	0,6,6	-	-	-		
82	OHX	AR	3654	-	0,5,6	-	-	-		
82	OHX	1	3531	-	0,6,6	-	-	-		
82	OHX	sR	1912	-	0,6,6	-	-	-		
82	OHX	sR	1923	-	0,6,6	-	-	-		
82	OHX	1	3470	-	0,6,6	-	-	-		
82	OHX	AR	3514	-	0,6,6	-	-	-		
82	OHX	1	4138	-	0,6,6	-	-	-		
82	OHX	sR	1934	-	0,6,6	-	-	-		
82	OHX	A	2103	-	0,6,6	-	-	-		
82	OHX	AR	3502	-	0,6,6	-	-	-		
82	OHX	AR	3570	-	0,6,6	-	-	-		
82	OHX	AR	3474	-	0,6,6	-	-	-		
82	OHX	AR	3589	-	0,6,6	-	-	-		
82	OHX	CX	201	-	0,6,6	-	-	-		
82	OHX	c8	201	-	0,6,6	-	-	-		
82	OHX	sR	2008	-	0,6,6	-	-	-		
82	OHX	A	1947	-	0,6,6	-	-	-		
82	OHX	AR	3649	-	0,6,6	-	-	-		
82	OHX	AR	3498	-	0,6,6	-	-	-		
82	OHX	AS	209	-	0,6,6	-	-	-		
82	OHX	sR	1938	-	0,6,6	-	-	-		
82	OHX	1	4095	-	0,6,6	-	-	-		
82	OHX	AR	3418	-	0,6,6	-	-	-		
82	OHX	A	1905	-	0,6,6	-	-	-		
82	OHX	A	1916	-	0,6,6	-	-	-		
82	OHX	1	3575	-	0,6,6	-	-	-		
82	OHX	1	3419	-	0,6,6	-	-	-		
82	OHX	1	3450	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	3439	-	0,6,6	-	-	-		
82	OHX	AS	202	-	0,6,6	-	-	-		
82	OHX	1	3601	-	0,6,6	-	-	-		
82	OHX	1	3522	-	0,6,6	-	-	-		
82	OHX	AR	3541	-	0,6,6	-	-	-		
82	OHX	1	3481	-	0,6,6	-	-	-		
82	OHX	A	2139	-	0,6,6	-	-	-		
82	OHX	1	3574	-	0,6,6	-	-	-		
82	OHX	T	201	-	0,6,6	-	-	-		
82	OHX	A	1956	-	0,6,6	-	-	-		
82	OHX	AT	207	-	0,6,6	-	-	-		
82	OHX	sR	1983	-	0,6,6	-	-	-		
82	OHX	1	3402	-	0,6,6	-	-	-		
82	OHX	A	2133	-	0,6,6	-	-	-		
82	OHX	AR	3599	-	0,6,6	-	-	-		
82	OHX	1	3464	-	0,6,6	-	-	-		
82	OHX	2	201	-	0,6,6	-	-	-		
82	OHX	A	1955	-	0,6,6	-	-	-		
82	OHX	1	3459	-	0,6,6	-	-	-		
82	OHX	1	3443	-	0,6,6	-	-	-		
82	OHX	sR	1954	-	0,6,6	-	-	-		
82	OHX	1	4102	-	0,6,6	-	-	-		
82	OHX	A	1952	-	0,6,6	-	-	-		
82	OHX	sR	1930	-	0,6,6	-	-	-		
82	OHX	1	4113	-	0,6,6	-	-	-		
82	OHX	1	4137	-	0,6,6	-	-	-		
82	OHX	A	2128	-	0,6,6	-	-	-		
82	OHX	A	1915	-	0,6,6	-	-	-		
82	OHX	sR	2019	-	0,6,6	-	-	-		
82	OHX	1	3478	-	0,6,6	-	-	-		
82	OHX	sR	1948	-	0,6,6	-	-	-		
82	OHX	A	2131	-	0,6,6	-	-	-		
82	OHX	1	4099	-	0,5,6	-	-	-		
82	OHX	3	219	-	0,6,6	-	-	-		
82	OHX	AR	3669	-	0,5,6	-	-	-		
82	OHX	1	4154	-	0,6,6	-	-	-		
82	OHX	1	3432	-	0,6,6	-	-	-		
82	OHX	1	3536	-	0,6,6	-	-	-		
82	OHX	1	3584	-	0,6,6	-	-	-		
82	OHX	1	3556	-	0,6,6	-	-	-		
82	OHX	1	3466	-	0,6,6	-	-	-		
82	OHX	A	1972	-	0,6,6	-	-	-		
82	OHX	AR	3537	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	1	4083	-	0,6,6	-	-	-		
82	OHX	AR	3605	-	0,6,6	-	-	-		
82	OHX	AK	102	-	0,6,6	-	-	-		
82	OHX	A	1935	-	0,6,6	-	-	-		
82	OHX	AR	3511	-	0,6,6	-	-	-		
82	OHX	4	201	-	0,6,6	-	-	-		
82	OHX	sR	1909	-	0,6,6	-	-	-		
82	OHX	1	4124	-	0,6,6	-	-	-		
82	OHX	sR	2020	-	0,6,6	-	-	-		
82	OHX	1	3515	-	0,6,6	-	-	-		
82	OHX	1	3568	-	0,6,6	-	-	-		
82	OHX	4	207	-	0,6,6	-	-	-		
82	OHX	AR	3565	-	0,6,6	-	-	-		
82	OHX	A	1967	-	0,6,6	-	-	-		
82	OHX	sR	1935	-	0,6,6	-	-	-		
82	OHX	AR	3532	-	0,6,6	-	-	-		
82	OHX	1	4114[A]	-	0,6,6	-	-	-		
82	OHX	AR	4151	-	0,6,6	-	-	-		
82	OHX	1	3498	-	0,6,6	-	-	-		
82	OHX	AR	3403	-	0,6,6	-	-	-		
82	OHX	1	3506	-	0,6,6	-	-	-		
82	OHX	s1	301	-	0,6,6	-	-	-		
82	OHX	sR	1967	-	0,6,6	-	-	-		
82	OHX	sR	1991	-	0,6,6	-	-	-		
82	OHX	A	1963	-	0,6,6	-	-	-		
82	OHX	AR	3440	-	0,6,6	-	-	-		
82	OHX	A	1945	-	0,6,6	-	-	-		
82	OHX	sR	1962	-	0,6,6	-	-	-		
82	OHX	1	3538	-	0,6,6	-	-	-		
82	OHX	1	4112	-	0,6,6	-	-	-		
82	OHX	1	4145	-	0,6,6	-	-	-		
82	OHX	AR	3431	-	0,6,6	-	-	-		
82	OHX	1	4076	-	0,6,6	-	-	-		
82	OHX	AR	3606	-	0,6,6	-	-	-		
82	OHX	1	3414	-	0,6,6	-	-	-		
82	OHX	AR	3408	-	0,6,6	-	-	-		
82	OHX	1	3444	-	0,6,6	-	-	-		
82	OHX	1	3501	-	0,6,6	-	-	-		
82	OHX	sR	1976	-	0,6,6	-	-	-		
82	OHX	AR	3661	-	0,6,6	-	-	-		
82	OHX	1	3458	-	0,6,6	-	-	-		
82	OHX	1	3604	-	0,6,6	-	-	-		
82	OHX	sR	2173	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	OHX	AR	3559	-	0,6,6	-	-	-		
82	OHX	1	4093	-	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	X1K	1	4181	-	-	2/8/58/58	0/3/3/3
85	SPD	1	4180	-	-	2/7/7/7	-
85	SPD	AR	4204	-	-	2/7/7/7	-
86	X1K	AR	4205	-	-	0/8/58/58	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	AR	4205	X1K	C1-C10	-2.61	1.52	1.56
86	AR	4205	X1K	C5-C10	2.19	1.59	1.56
86	1	4181	X1K	C5-C10	2.12	1.59	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	1	4181	X1K	C1-C10-C5	-8.36	107.86	116.76
86	1	4181	X1K	C20-C1-C2	-5.75	97.05	109.01
86	AR	4205	X1K	C1-C10-C5	-5.56	110.83	116.76
86	1	4181	X1K	C20-C1-C	-4.56	101.24	107.87
86	AR	4205	X1K	C20-C1-C	-4.26	101.68	107.87

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	1	4181	X1K	C13-C14-C15-C16
85	AR	4204	SPD	C3-C4-C5-N6
85	1	4180	SPD	C3-C4-C5-N6
86	1	4181	X1K	C6-C13-C14-C15
85	AR	4204	SPD	N1-C2-C3-C4

There are no ring outliers.

516 monomers are involved in 741 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	AR	3510	OHX	1	0
82	CL	302	OHX	2	0
82	sR	1901	OHX	2	0
82	A	1907	OHX	2	0
82	1	3533	OHX	1	0
82	AR	3413	OHX	2	0
82	1	3502	OHX	1	0
82	AR	3407	OHX	2	0
82	A	2105	OHX	1	0
82	1	3539	OHX	1	0
82	1	4088	OHX	1	0
82	AR	4139	OHX	1	0
82	1	4152	OHX	2	0
82	1	3420	OHX	2	0
82	AR	3437	OHX	1	0
82	CG	304	OHX	0	1
82	A	1977	OHX	2	0
82	AT	211	OHX	1	0
82	AR	3427	OHX	1	0
82	1	4115	OHX	1	0
82	A	1918	OHX	2	0
82	sR	1928	OHX	2	0
82	AR	3425	OHX	3	0
82	1	3404	OHX	3	0
82	A	1940[A]	OHX	1	0
82	1	4081	OHX	2	0
82	A	2137	OHX	2	0
82	sR	1957	OHX	2	0
82	sR	1958	OHX	2	0
82	sR	1941	OHX	1	0
82	AT	214	OHX	1	0
82	AR	3448	OHX	2	0
82	A	2123	OHX	3	0
82	1	4109	OHX	1	0
82	AR	3642	OHX	4	0
82	AT	206	OHX	1	0
82	AS	203	OHX	1	0
82	1	3552	OHX	1	0
82	4	212	OHX	1	0
82	AR	3587	OHX	2	0
82	AR	4144	OHX	1	0
82	AR	3490	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	A	2104	OHX	3	0
82	sR	2017	OHX	1	0
82	1	3411	OHX	2	0
82	1	3500	OHX	1	0
82	AR	3571	OHX	1	0
82	1	4105	OHX	2	0
82	AR	3423	OHX	1	0
82	1	4140	OHX	1	0
82	AR	3506	OHX	1	0
82	CG	303	OHX	1	0
82	1	3476	OHX	1	0
82	sR	1964	OHX	2	0
82	A	2117	OHX	3	0
82	sR	1990	OHX	4	0
82	1	3600	OHX	1	0
82	sR	1965	OHX	1	0
82	sR	1995	OHX	2	0
82	A	2130	OHX	2	0
82	AR	3410	OHX	1	0
82	AR	3414	OHX	1	0
82	J	301	OHX	1	0
82	1	3592	OHX	2	0
82	AR	3478	OHX	3	0
82	AR	3507	OHX	1	0
82	sR	2003	OHX	2	0
82	A	2120	OHX	3	0
82	1	4091	OHX	1	0
82	AR	3434	OHX	1	0
82	AR	3671	OHX	1	0
82	AR	4148	OHX	2	0
82	A	1922	OHX	2	0
82	AR	3622	OHX	1	0
82	AR	4161	OHX	1	0
82	sR	2175	OHX	1	0
82	DQ	502	OHX	3	0
82	1	4077	OHX	3	0
82	AR	4156	OHX	1	0
82	AR	4150	OHX	2	0
82	1	4098	OHX	2	0
82	A	1934	OHX	1	0
82	A	2141	OHX	1	0
82	1	3567	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	A	1960	OHX	1	0
82	AR	3472	OHX	2	0
82	sR	1933	OHX	1	0
82	AR	3515	OHX	1	0
82	sR	1915	OHX	1	0
82	sR	1908	OHX	1	0
82	AR	3528	OHX	1	0
82	AS	201	OHX	1	0
82	DH	202	OHX	1	0
82	A	2144	OHX	1	0
82	A	1973	OHX	1	0
82	1	3581	OHX	1	0
82	4	204	OHX	1	0
82	AR	3419	OHX	2	0
82	A	2121	OHX	4	0
82	A	2127	OHX	4	0
82	sR	1975	OHX	1	0
82	sR	2176	OHX	1	0
82	1	3593	OHX	1	0
82	AR	3572	OHX	1	0
82	AR	3535	OHX	1	0
82	sR	1903	OHX	1	0
82	1	4149	OHX	1	0
82	AR	3548	OHX	1	0
82	A	2143	OHX	1	0
82	AR	3428	OHX	1	0
82	A	2136	OHX	1	0
82	sR	1988	OHX	2	0
82	sR	1931	OHX	1	0
82	AR	3453	OHX	2	0
82	A	2140	OHX	1	0
82	1	3446	OHX	1	0
82	AR	3420	OHX	1	0
82	1	4103	OHX	2	0
82	1	3521	OHX	1	0
82	A	1926	OHX	2	0
82	1	4139	OHX	1	0
82	A	2132	OHX	1	0
82	1	3406	OHX	1	0
82	sR	1927	OHX	1	0
82	AR	3421	OHX	1	0
82	AR	4160	OHX	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	A	2108	OHX	2	0
82	sR	2000	OHX	2	0
82	4	210	OHX	1	0
82	AR	3444	OHX	1	0
82	AR	4116	OHX	1	0
82	A	2118	OHX	1	0
82	1	3418	OHX	1	0
82	AR	3602	OHX	1	0
82	A	2114	OHX	3	0
82	1	4092	OHX	1	0
82	1	4147	OHX	1	0
82	AR	3450	OHX	1	0
82	1	3457	OHX	2	0
82	1	3497	OHX	1	0
82	AR	3629	OHX	2	0
82	AR	3441	OHX	1	0
82	1	3482	OHX	1	0
82	AS	205	OHX	1	0
82	sR	1940	OHX	1	0
82	A	1901	OHX	1	0
82	1	3445	OHX	1	0
82	AR	3604	OHX	4	0
82	AR	4136	OHX	1	0
82	AR	3464	OHX	1	0
82	AR	3655	OHX	1	0
82	AR	3459	OHX	2	0
82	AR	3656	OHX	1	0
82	sR	2181	OHX	1	0
82	1	3566	OHX	3	0
82	sR	1952	OHX	1	0
82	1	3435	OHX	1	0
82	1	4058	OHX	1	0
82	AR	4143	OHX	1	0
82	A	2116	OHX	1	0
82	AR	3618	OHX	1	0
82	AR	3651	OHX	2	0
82	4	228	OHX	2	0
82	1	4121	OHX	1	0
82	k	404	OHX	2	0
82	c3	202	OHX	1	0
82	1	4120	OHX	1	0
82	sR	2005	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	1	4151	OHX	3	0
82	1	4097	OHX	1	0
82	1	3527	OHX	1	0
82	1	3540	OHX	1	0
82	sR	2172	OHX	1	0
82	AT	209	OHX	1	0
82	1	3449	OHX	1	0
82	AR	3501	OHX	2	0
82	AR	3567	OHX	1	0
82	1	3465	OHX	2	0
82	A	2119	OHX	1	0
82	1	4101	OHX	2	0
82	3	220	OHX	1	0
82	sR	2015	OHX	1	0
82	1	4094	OHX	1	0
82	AR	3555	OHX	1	0
82	AR	3568	OHX	2	0
82	AR	3469	OHX	2	0
82	A	1971	OHX	2	0
82	A	1920	OHX	1	0
82	sR	2025	OHX	1	0
82	AR	3409	OHX	1	0
82	1	3487	OHX	2	0
82	AR	3485	OHX	1	0
82	A	1948	OHX	2	0
82	AR	3635	OHX	1	0
82	AR	3462	OHX	3	0
82	4	205	OHX	2	0
82	sR	1922	OHX	3	0
82	A	1938	OHX	1	0
82	sR	2170	OHX	1	0
82	sR	1914	OHX	2	0
82	AR	3583	OHX	2	0
82	AR	3653	OHX	2	0
82	1	4078	OHX	1	0
82	AR	4146	OHX	1	0
82	AR	3500	OHX	1	0
82	1	3520	OHX	1	0
82	1	3477	OHX	1	0
82	AR	3504	OHX	2	0
82	A	1942	OHX	2	0
82	c5	201	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	AR	3664	OHX	1	0
82	1	4125	OHX	3	0
82	1	3557	OHX	1	0
82	sR	1943	OHX	1	0
82	AR	3416	OHX	1	0
82	AT	213	OHX	1	0
82	1	4100	OHX	1	0
82	sR	1950	OHX	1	0
82	A	1940[B]	OHX	1	0
82	AR	4152	OHX	2	0
82	A	2125	OHX	2	0
82	1	4131	OHX	2	0
82	AR	3553	OHX	1	0
82	A	1937	OHX	1	0
82	1	4060	OHX	1	0
82	1	4107	OHX	3	0
82	1	4075	OHX	3	0
82	AR	3404	OHX	1	0
82	1	3480	OHX	1	0
82	sR	1994	OHX	1	0
82	AR	3442	OHX	2	0
82	A	2107	OHX	2	0
82	sR	1929	OHX	2	0
82	sR	1984	OHX	2	0
82	1	3546	OHX	1	0
82	A	2113	OHX	2	0
82	AG	202	OHX	1	0
82	1	3462	OHX	1	0
82	AC	102	OHX	2	0
82	AR	4141	OHX	1	0
82	1	3452	OHX	1	0
82	A	1906	OHX	2	0
82	A	2106	OHX	2	0
82	1	3594	OHX	1	0
82	z	202	OHX	2	0
82	AR	3412	OHX	1	0
82	AR	3666	OHX	1	0
82	AR	3631	OHX	1	0
82	1	4062	OHX	1	0
82	AR	3607	OHX	3	0
82	sR	1981	OHX	1	0
82	l	405	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	1	3474	OHX	1	0
82	1	4072	OHX	2	0
82	AR	3600	OHX	1	0
82	A	1908	OHX	3	0
82	1	4084	OHX	2	0
82	1	4085	OHX	1	0
82	A	1910	OHX	1	0
86	AR	4205	X1K	4	0
82	AR	3633	OHX	1	0
82	AR	3497	OHX	1	0
82	sR	2006	OHX	1	0
82	sR	1955	OHX	1	0
82	AR	3650	OHX	1	0
82	AR	3438	OHX	1	0
82	sR	1949	OHX	1	0
82	AR	3581	OHX	1	0
82	Q	201	OHX	1	0
82	AR	3451	OHX	1	0
82	A	1932	OHX	2	0
82	A	1975	OHX	1	0
82	1	3417	OHX	1	0
82	1	4079	OHX	1	0
82	AR	3465	OHX	1	0
82	AR	3637	OHX	1	0
82	A	2111	OHX	2	0
82	sR	1996	OHX	1	0
82	AR	3457	OHX	1	0
82	A	1912	OHX	2	0
82	sR	1953	OHX	1	0
82	sR	1911	OHX	1	0
82	AT	201	OHX	2	0
82	k	403	OHX	1	0
82	1	3535[A]	OHX	1	0
82	1	3586	OHX	1	0
82	1	4126	OHX	1	0
82	3	222	OHX	1	0
82	sR	2171	OHX	1	0
82	AR	3566	OHX	1	0
82	A	1919	OHX	1	0
82	1	4086	OHX	2	0
82	3	204	OHX	1	0
82	sR	1989	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	1	3426	OHX	1	0
82	1	3537	OHX	2	0
82	AR	3454	OHX	2	0
82	1	3472	OHX	1	0
82	AR	3525	OHX	1	0
82	A	1929	OHX	1	0
82	sR	1913	OHX	2	0
82	sR	1947	OHX	1	0
82	AR	3406	OHX	1	0
82	A	1944	OHX	1	0
82	1	3403	OHX	1	0
82	AR	3452	OHX	1	0
82	sR	1904	OHX	2	0
82	AR	3422	OHX	2	0
82	AR	4162	OHX	1	0
82	1	3408	OHX	1	0
82	1	3535[B]	OHX	1	0
82	AR	3433	OHX	1	0
82	AR	3588	OHX	1	0
82	sR	1970	OHX	1	0
82	AR	3467	OHX	1	0
82	sR	1956	OHX	1	0
82	CH	201	OHX	3	0
82	sR	1985	OHX	1	0
82	sR	2180	OHX	3	0
82	A	2126[A]	OHX	1	0
82	1	3505	OHX	2	0
82	sR	2010	OHX	1	0
82	1	3413	OHX	2	0
82	AR	3512	OHX	1	0
82	1	3407	OHX	2	0
82	1	3590	OHX	1	0
82	1	4073	OHX	1	0
82	1	3479	OHX	1	0
82	AR	3577	OHX	3	0
82	AR	3544	OHX	1	0
82	AR	3516	OHX	1	0
82	1	3493	OHX	1	0
82	AT	234	OHX	1	0
82	A	2135	OHX	2	0
82	1	4087	OHX	1	0
82	AR	3538	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	AR	3401	OHX	4	0
82	AR	3455	OHX	1	0
82	1	4096	OHX	1	0
82	1	3509	OHX	1	0
82	AR	3449	OHX	1	0
82	r	303	OHX	1	0
82	AR	3475	OHX	2	0
82	AR	4155	OHX	2	0
82	AR	3445	OHX	1	0
82	A	2142	OHX	1	0
82	A	2112	OHX	1	0
82	AR	3466	OHX	1	0
86	1	4181	X1K	1	0
82	1	4117	OHX	2	0
82	AR	3471	OHX	1	0
82	1	4116	OHX	1	0
82	A	1917	OHX	1	0
82	1	3510	OHX	1	0
82	1	3596	OHX	1	0
82	AT	202	OHX	1	0
82	AR	3550	OHX	2	0
82	1	3427	OHX	1	0
82	1	3512	OHX	1	0
82	A	2110	OHX	1	0
82	AR	3488	OHX	1	0
82	A	2124	OHX	1	0
82	AR	4159	OHX	1	0
82	AR	3667	OHX	1	0
82	1	3431	OHX	1	0
82	sR	2004	OHX	1	0
82	sR	1910	OHX	1	0
82	AR	4153	OHX	1	0
82	sR	1960	OHX	2	0
82	4	206	OHX	1	0
82	1	3508	OHX	1	0
82	1	4144	OHX	1	0
82	1	4118	OHX	3	0
82	AR	3505	OHX	1	0
82	AR	4137	OHX	1	0
82	AR	3411	OHX	1	0
82	1	4080	OHX	6	0
82	CE	401	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	AR	3517	OHX	2	0
82	A	1925	OHX	1	0
82	1	4074	OHX	3	0
82	1	3490	OHX	1	0
82	AR	3545	OHX	1	0
82	A	2102	OHX	1	0
82	1	3504	OHX	3	0
82	sR	1907	OHX	2	0
82	sR	1916[A]	OHX	1	0
82	sR	1959	OHX	3	0
82	1	3423	OHX	1	0
82	1	4089	OHX	1	0
82	AR	3524	OHX	2	0
82	AR	3484	OHX	1	0
82	1	3430	OHX	1	0
82	1	3526	OHX	2	0
82	AR	3592	OHX	1	0
82	sR	1906	OHX	1	0
82	1	3405	OHX	2	0
82	Rb	401	OHX	1	0
82	4	213	OHX	2	0
82	1	3455	OHX	4	0
82	sR	1918	OHX	3	0
82	AP	502	OHX	3	0
82	A	1911	OHX	1	0
82	sR	1920	OHX	1	0
82	AR	3549	OHX	1	0
82	1	3434	OHX	2	0
82	1	3451	OHX	1	0
82	sR	1969	OHX	3	0
82	AR	4163	OHX	1	0
82	AR	3546	OHX	2	0
82	1	4143	OHX	1	0
82	1	4108	OHX	2	0
82	sR	2023	OHX	2	0
82	1	4082	OHX	1	0
82	AR	3591	OHX	2	0
82	1	4127	OHX	2	0
82	AR	3573	OHX	1	0
82	c7	201	OHX	1	0
82	AR	3494	OHX	1	0
82	sR	1916[B]	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	sR	2179	OHX	1	0
82	1	4128	OHX	1	0
82	A	1958	OHX	1	0
82	AR	3460	OHX	1	0
82	CV	201	OHX	1	0
82	sR	2177	OHX	1	0
82	sR	2013	OHX	1	0
82	AR	4145	OHX	1	0
82	AR	3417	OHX	2	0
82	sR	1925	OHX	1	0
82	AR	3624	OHX	1	0
82	A	1969	OHX	1	0
82	1	3558	OHX	1	0
82	A	1950	OHX	1	0
82	AR	3463	OHX	1	0
82	sR	2174	OHX	1	0
82	AR	3529	OHX	1	0
82	1	4104	OHX	1	0
82	DD	102	OHX	1	0
82	AR	3523	OHX	1	0
82	AT	235	OHX	1	0
82	AR	3519	OHX	1	0
82	1	3415	OHX	1	0
82	1	3549	OHX	1	0
82	1	3453	OHX	1	0
82	1	4136	OHX	2	0
82	AR	3489	OHX	1	0
82	AR	3654	OHX	1	0
82	sR	1912	OHX	1	0
82	sR	1923	OHX	3	0
82	1	3470	OHX	2	0
82	AR	3514	OHX	1	0
82	1	4138	OHX	1	0
82	sR	1934	OHX	1	0
82	A	2103	OHX	1	0
82	CX	201	OHX	1	0
82	c8	201	OHX	1	0
82	AR	3498	OHX	1	0
82	sR	1938	OHX	1	0
82	AR	3418	OHX	1	0
82	A	1916	OHX	1	0
82	1	3419	OHX	3	0

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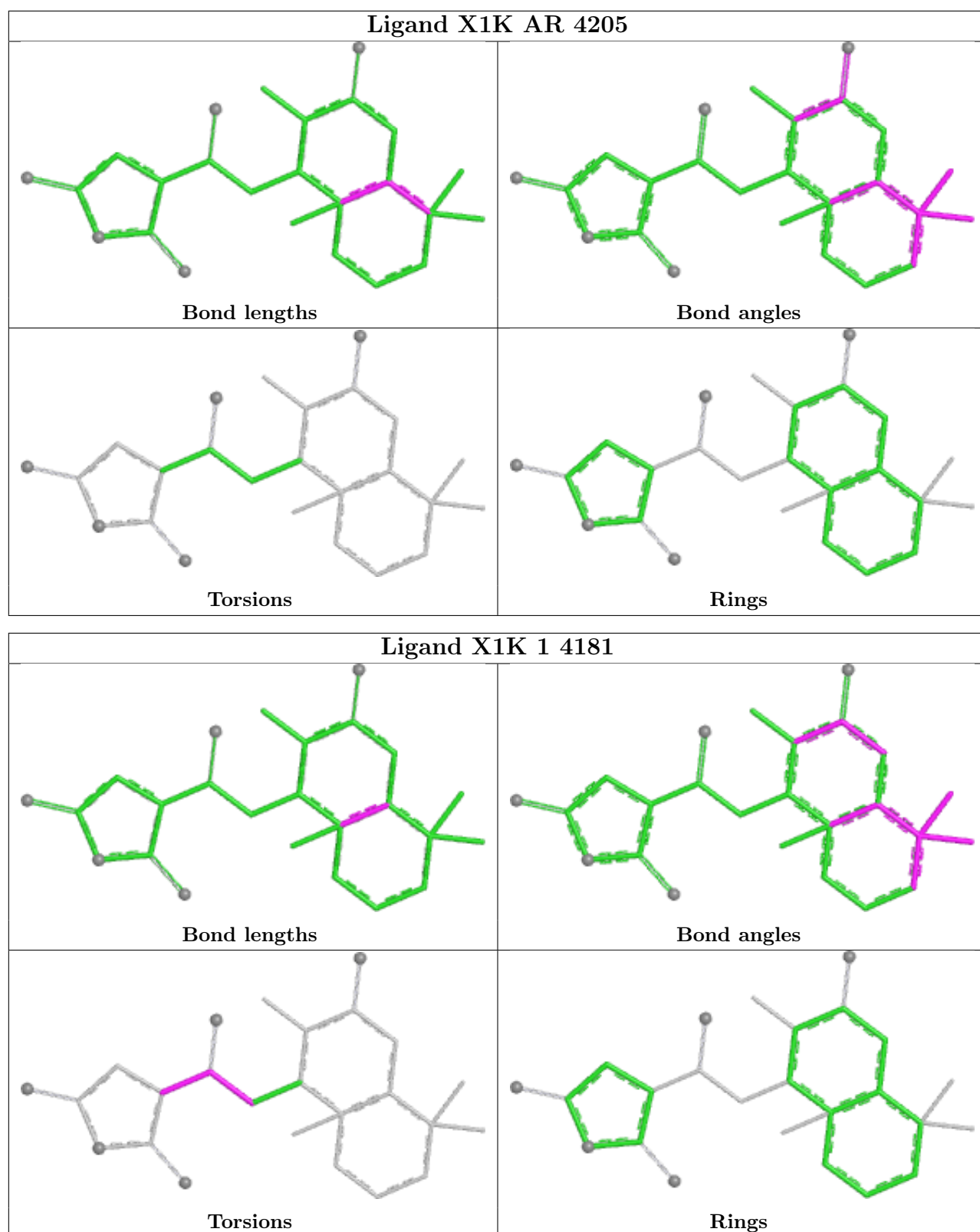
Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	1	3450	OHX	2	0
82	AS	202	OHX	1	0
82	1	3601	OHX	1	0
82	1	3522	OHX	1	0
82	AR	3541	OHX	1	0
82	1	3481	OHX	1	0
82	A	2139	OHX	1	0
82	T	201	OHX	2	0
82	AT	207	OHX	1	0
82	sR	1983	OHX	1	0
82	2	201	OHX	1	0
82	sR	1954	OHX	1	0
82	1	4102	OHX	3	0
82	A	1952	OHX	2	0
82	sR	1930	OHX	2	0
82	1	4113	OHX	2	0
82	1	4137	OHX	1	0
82	1	3478	OHX	1	0
82	A	2131	OHX	3	0
82	1	4099	OHX	1	0
82	3	219	OHX	1	0
82	1	4154	OHX	2	0
82	1	3584	OHX	2	0
82	A	1972	OHX	1	0
82	1	4083	OHX	1	0
82	AK	102	OHX	6	0
82	A	1935	OHX	1	0
82	AR	3511	OHX	1	0
82	1	4124	OHX	1	0
82	sR	2020	OHX	1	0
82	1	3515	OHX	1	0
82	4	207	OHX	1	0
82	AR	3565	OHX	2	0
82	A	1967	OHX	1	0
82	AR	3532	OHX	1	0
82	1	4114[A]	OHX	1	0
82	AR	3403	OHX	1	0
82	1	3506	OHX	1	0
82	s1	301	OHX	3	0
82	sR	1967	OHX	1	0
82	AR	3440	OHX	1	1
82	sR	1962	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	1	3538	OHX	1	0
82	1	4145	OHX	1	0
82	1	4076	OHX	2	0
82	AR	3408	OHX	3	0
82	1	3501	OHX	2	0
82	sR	1976	OHX	2	0
82	AR	3661	OHX	1	0
82	1	3458	OHX	1	0
82	1	3604	OHX	1	0
82	sR	2173	OHX	1	0
82	AR	3559	OHX	1	0
82	1	4093	OHX	2	0

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



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
58	c0	1
47	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	c0	84:GLU	C	87:HIS	N	9.31
1	A	1716:C	O3'	1717:G	P	4.49

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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