wwPDB X-ray Structure Validation Summary Report (i)

Feb 23, 2024 – 02:35 AM EST

PDB ID	:	4V7R
Title	:	Yeast 80S ribosome.
Authors	:	Ben-Shem, A.; Jenner, L.; Yusupova, G.; Yusupov, M.
Deposited on	:	2010-07-23
Resolution	:	4.00 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

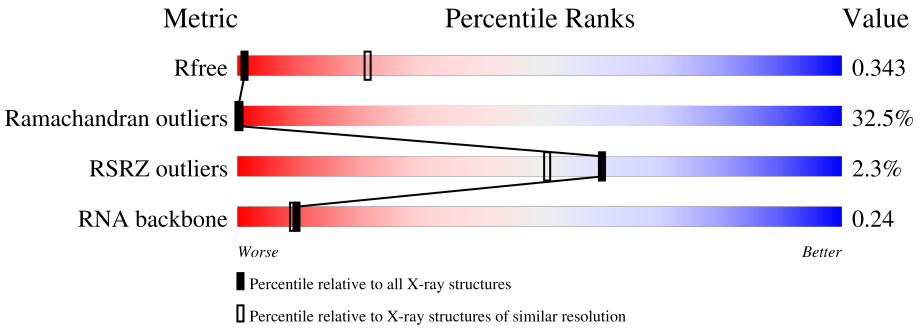
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1087 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)
RNA backbone	3102	1048 (5.00-3.00)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A1	1800	3% 36% 54% 9% ·
1	C1	1800	3% 36% 54% 10% ·
2	AA	252	2% 56% 26% 5% 13%
2	CA	252	% 56% 27% 5% 13%
3	AB	254	% 55% 27% · 14%
3	CB	254	% 56% 27% · 14%
4	AC	240	% 54% 24% · 21%

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Mol	Chain	Length	Quality of chain
4	CC	240	52% 25% 21%
5	AD	225	46% 28% 25%
5	CD	225	46% 28% 25%
6	AE	197	3% 54% 24% 20%
6	CE	197	51% 27% 20%
7	AF	156	33% 14% 51%
7	CF	156	4% 33% 14% 51%
8	AG	151	57% 17% 23%
8	CG	151	56% 19% 23%
9	AH	137	4% 66% 26% 7%
9	CH	137	4% 66% 26% 7%
10	AI	142	55% 26% 15%
10	CI	142	55% 27% 15%
11	AJ	143	63% 29% 6%
11	CJ	143	62% 29% 6%
12	AK	136	33% 15% 51%
12	CK	136	4% 34% 14% 51%
13	AL	146	59% 22% 18%
13	CL	146	3% 58% 23% 18%
14	AM	144	49% 24% 26%
14	CM	144	46% 27% 26%
15	AN	121	65% 24% 8%
15	CN	121	64% 25% 8%
16	AO	130	69% 26%
16	CO	130	67% 28%

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Mol	Chain	Length	Quality of chain
17	AP	145	51% 26% 20%
17	CP	145	51% 26% 20%
18	AQ	108	46% 14% 38%
18	CQ	108	43% 15% 42%
19	AR	67	6% 45% 25% 30%
19	CR	67	7% 43% 27% 30%
20	AS	56	43% 27% 30%
20	CS	56	41% 29% 30%
21	AT	319	4% 78% 19%
21	CT	319	4% 78% 19%
22	Aa	20	100%
22	Bo	20	95% 5%
22	Ca	20	100%
23	Ab	105	99%
23	Cb	105	99%
24	Ac	93	99%
24	Cc	93	100%
25	Ad	35	100%
25	Cd	35	100%
26	Ae	21	100%
26	Bj	21	100%
26	Dj	21	100%
27	Af	11	100%
28	Ah	41	100%
28	Ch	41	100%

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Mol	Chain	Length	Quality of chain
29	B1	3396	2% 29% 47% 19% 6%
29	D1	3396	3% 30% 47% 18% 6%
30	B2	121	32% 47% 21%
30	D2	121	% 32% 45% 22%
31	B3	158	4% 39% 50% 11%
31	D3	158	% 42% 51% 6%
32	BA	217	15% 66% 29%
32	DA	217	19% 71% 24%
33	BB	254	% 54% 35% 8%
33	DB	254	2% 56% 33% 8%
34	BC	387	54% 38% 6%
34	DC	387	53% 39% 6%
35	BD	362	51% 22% 26%
35	DD	362	% 50% 23% 26%
36	BE	297	% 63% 31%
36	DE	297	2% 61% 33%
37	BF	176	% 57% 40%
37	DF	176	% 56% 40% 5%
38	BG	244	61% 24% 12%
38	DG	244	62% 23% 12%
39	BH	256	2% 46% 20% 32%
39	DH	256	2% 47% 19% 32%
40	BI	191	% 72% 27%
40	DI	191	71% 27%
41	BJ	221	61% 31% 6%

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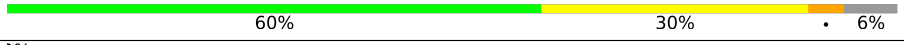
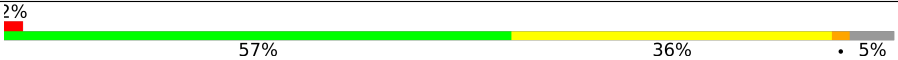
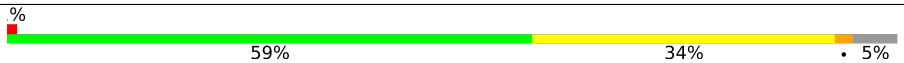
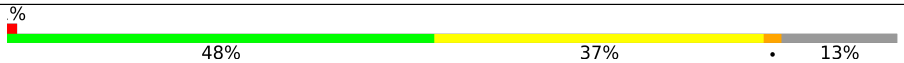
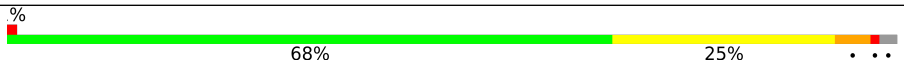
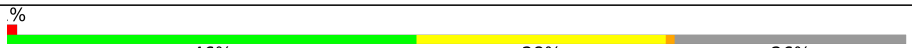
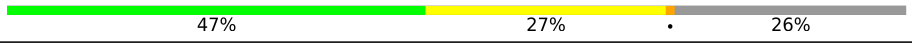
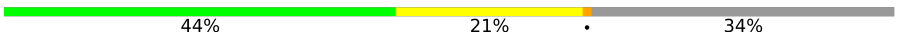
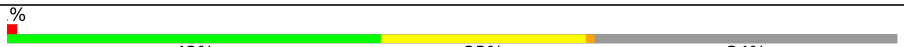
Mol	Chain	Length	Quality of chain
41	DJ	221	
42	BK	174	
42	DK	174	
43	BN	138	
43	DN	138	
44	BO	204	
44	DO	204	
45	BP	199	
45	DP	199	
46	BQ	184	
46	DQ	184	
47	BR	186	
47	DR	186	
48	BS	189	
48	DS	189	
49	BT	160	
49	DT	160	
50	BU	137	
50	DU	137	
51	BV	155	
51	DV	155	
52	BW	142	
52	DW	142	
53	BX	127	
53	DX	127	

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Mol	Chain	Length	Quality of chain
54	BY	149	2% 55% 40% 5%
54	DY	149	% 57% 39%
55	BZ	105	2% 73% 20% 7%
55	DZ	105	3% 76% 17% 7%
56	Ba	113	46% 30% 24%
56	Da	113	45% 31% 24%
57	Bb	130	52% 39% 5%
57	Db	130	% 56% 36%
58	Bc	120	44% 11% 43%
58	Dc	120	% 47% 8% 43%
59	Bd	88	45% 35% 18%
59	Dd	88	47% 35% 18%
60	Be	51	65% 29% 6%
60	De	51	67% 27% 6%
61	Bf	106	3% 63% 25% 10%
61	Df	106	9% 63% 25% 10%
62	Bg	92	% 64% 26% 10%
62	Dg	92	63% 27% 10%
63	Bh	44	100%
63	Dh	44	100%
64	Bi	12	100%
64	Di	12	100%
65	Bk	16	100%
65	Dk	16	100%
66	Bl	19	100%

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Mol	Chain	Length	Quality of chain
67	Bm	9	100%
68	Bn	27	100%
69	Bp	8	100%
70	Bq	17	100%
71	Br	23	100%
72	DL	165	% 50% 31% 16%
73	DM	312	% 26% 15% 58%

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
74	OHX	A1	1930	-	-	-	X
74	OHX	A1	1983	-	-	-	X
74	OHX	B1	3548	-	-	-	X
74	OHX	B1	3571	-	-	-	X
74	OHX	B1	3602	-	-	-	X
74	OHX	D1	3573	-	-	-	X
74	OHX	D1	3586	-	-	-	X
74	OHX	D1	3593	-	-	-	X
74	OHX	D1	3605	-	-	-	X
74	OHX	D3	211	-	-	-	X

2 Entry composition (i)

There are 74 unique types of molecules in this entry. The entry contains 309610 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A1	1789	Total 38107	C 17037	N 6732	O 12549	P 1789	0	0	0
1	C1	1789	Total 38107	C 17037	N 6732	O 12549	P 1789	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	AA	220	Total 1090	C 650	N 220	O 220	0	0	0
2	CA	220	Total 1090	C 650	N 220	O 220	0	0	0

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	AB	219	Total 1074	C 636	N 219	O 219	0	0	0
3	CB	219	Total 1074	C 636	N 219	O 219	0	0	0

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	AC	189	Total 928	C 550	N 189	O 189	0	0	0
4	CC	189	Total 928	C 550	N 189	O 189	0	0	0

- Molecule 5 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	AD	169	Total 836	C 498	N 169	O 169	0	0	0
5	CD	169	Total 836	C 498	N 169	O 169	0	0	0

- Molecule 6 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	AE	157	Total 777	C 463	N 157	O 157	0	0	0
6	CE	157	Total 777	C 463	N 157	O 157	0	0	0

- Molecule 7 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	AF	77	Total 382	C 228	N 77	O 77	0	0	0
7	CF	77	Total 382	C 228	N 77	O 77	0	0	0

- Molecule 8 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	AG	117	Total 580	C 346	N 117	O 117	0	0	0
8	CG	117	Total 580	C 346	N 117	O 117	0	0	0

- Molecule 9 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AH	128	Total 627	C 371	N 128	O 128	0	0	0
9	CH	128	Total 627	C 371	N 128	O 128	0	0	0

- Molecule 10 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	AI	121	Total 596	C 354	N 121	O 121	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CI	121	Total 596	C 354	N 121	O 121	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	AJ	134	Total 658	C 390	N 134	O 134	0	0	0
11	CJ	134	Total 658	C 390	N 134	O 134	0	0	0

- Molecule 12 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	AK	67	Total 332	C 198	N 67	O 67	0	0	0
12	CK	67	Total 332	C 198	N 67	O 67	0	0	0

- Molecule 13 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	AL	120	Total 591	C 351	N 120	O 120	0	0	0
13	CL	120	Total 591	C 351	N 120	O 120	0	0	0

- Molecule 14 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AM	106	Total 521	C 309	N 106	O 106	0	0	0
14	CM	106	Total 521	C 309	N 106	O 106	0	0	0

- Molecule 15 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	AN	111	Total 551	C 329	N 111	O 111	0	0	0
15	CN	111	Total 551	C 329	N 111	O 111	0	0	0

- Molecule 16 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	AO	127	Total	C	N	O	0	0	0
			622	368	127	127			
16	CO	127	Total	C	N	O	0	0	0
			622	368	127	127			

- Molecule 17 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	AP	116	Total	C	N	O	0	0	0
			566	334	116	116			
17	CP	116	Total	C	N	O	0	0	0
			566	334	116	116			

- Molecule 18 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AQ	67	Total	C	N	O	0	0	0
			332	198	67	67			
18	CQ	63	Total	C	N	O	0	0	0
			312	186	63	63			

- Molecule 19 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	AR	47	Total	C	N	O	0	0	0
			230	136	47	47			
19	CR	47	Total	C	N	O	0	0	0
			230	136	47	47			

- Molecule 20 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	AS	39	Total	C	N	O	0	0	0
			190	112	39	39			
20	CS	39	Total	C	N	O	0	0	0
			190	112	39	39			

- Molecule 21 is a protein called Guanine nucleotide-binding protein subunit beta-like protein; RACK-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AT	313	Total 1543	C 917	N 313	O 313	0	0	0
21	CT	313	Total 1543	C 917	N 313	O 313	0	0	0

- Molecule 22 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	Aa	20	Total 100	C 60	N 20	O 20	0	0	0
22	Bo	20	Total 100	C 60	N 20	O 20	0	0	0
22	Ca	20	Total 100	C 60	N 20	O 20	0	0	0

- Molecule 23 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	Ab	105	Total 525	C 315	N 105	O 105	0	0	0
23	Cb	105	Total 525	C 315	N 105	O 105	0	0	0

- Molecule 24 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	Ac	93	Total 465	C 279	N 93	O 93	0	0	0
24	Cc	93	Total 465	C 279	N 93	O 93	0	0	0

- Molecule 25 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	Ad	35	Total 175	C 105	N 35	O 35	0	0	0
25	Cd	35	Total 175	C 105	N 35	O 35	0	0	0

- Molecule 26 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	Ae	21	Total	C	N	O	0	0	0
			105	63	21	21			
26	Bj	21	Total	C	N	O	0	0	0
			105	63	21	21			
26	Dj	21	Total	C	N	O	0	0	0
			105	63	21	21			

- Molecule 27 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	Af	11	Total	C	N	O	0	0	0
			55	33	11	11			

- Molecule 28 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	Ah	41	Total	C	N	O	0	0	0
			205	123	41	41			
28	Ch	41	Total	C	N	O	0	0	0
			205	123	41	41			

- Molecule 29 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B1	3206	Total	C	N	O	P	0	0	0
			68577	30632	12365	22374	3206			
29	D1	3206	Total	C	N	O	P	0	0	0
			68577	30632	12365	22374	3206			

- Molecule 30 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B2	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
30	D2	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 31 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B3	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D3	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 32 is a protein called 60S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
32	BA	213	Total	C	N	O	0	0	0
			1055	629	213	213			
32	DA	213	Total	C	N	O	0	0	0
			1055	629	213	213			

- Molecule 33 is a protein called 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
33	BB	234	Total	C	N	O	0	0	0
			1106	638	234	234			
33	DB	234	Total	C	N	O	0	0	0
			1106	638	234	234			

- Molecule 34 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
34	BC	364	Total	C	N	O	0	0	0
			1791	1063	364	364			
34	DC	364	Total	C	N	O	0	0	0
			1791	1063	364	364			

- Molecule 35 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	BD	268	Total	C	N	O	0	0	0
			1312	776	268	268			
35	DD	268	Total	C	N	O	0	0	0
			1312	776	268	268			

- Molecule 36 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BE	287	Total	C	N	O	0	0	0
			1412	838	287	287			
36	DE	287	Total	C	N	O	0	0	0
			1412	838	287	287			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BE	112	ARG	LYS	conflict	UNP P26321
DE	112	ARG	LYS	conflict	UNP P26321

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BF	176	Total	C	N	O	0	0	0
			873	521	176	176			
37	DF	176	Total	C	N	O	0	0	0
			873	521	176	176			

- Molecule 38 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	BG	215	Total	C	N	O	0	0	0
			1061	631	215	215			
38	DG	215	Total	C	N	O	0	0	0
			1061	631	215	215			

- Molecule 39 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	BH	173	Total	C	N	O	0	0	0
			856	510	173	173			
39	DH	173	Total	C	N	O	0	0	0
			856	510	173	173			

- Molecule 40 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	BI	191	Total	C	N	O	0	0	0
			942	560	191	191			
40	DI	191	Total	C	N	O	0	0	0
			942	560	191	191			

- Molecule 41 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	BJ	208	Total	C	N	O	0	0	0
			1027	611	208	208			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	DJ	208	Total 1027	C 611	N 208	O 208	0	0	0

- Molecule 42 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	BK	165	Total 810	C 480	N 165	O 165	0	0	0
42	DK	165	Total 810	C 480	N 165	O 165	0	0	0

- Molecule 43 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BN	120	Total 593	C 353	N 120	O 120	0	0	0
43	DN	120	Total 593	C 353	N 120	O 120	0	0	0

- Molecule 44 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BO	187	Total 923	C 549	N 187	O 187	0	0	0
44	DO	187	Total 923	C 549	N 187	O 187	0	0	0

- Molecule 45 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BP	196	Total 967	C 575	N 196	O 196	0	0	0
45	DP	196	Total 967	C 575	N 196	O 196	0	0	0

- Molecule 46 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BQ	154	Total 761	C 453	N 154	O 154	0	0	0
46	DQ	154	Total 761	C 453	N 154	O 154	0	0	0

- Molecule 47 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	BR	143	Total	C	N	O	0	0	0
			706	420	143	143			
47	DR	143	Total	C	N	O	0	0	0
			706	420	143	143			

- Molecule 48 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	BS	188	Total	C	N	O	0	0	0
			931	555	188	188			
48	DS	188	Total	C	N	O	0	0	0
			931	555	188	188			

- Molecule 49 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	BT	119	Total	C	N	O	0	0	0
			586	348	119	119			
49	DT	119	Total	C	N	O	0	0	0
			586	348	119	119			

- Molecule 50 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	BU	129	Total	C	N	O	0	0	0
			631	373	129	129			
50	DU	129	Total	C	N	O	0	0	0
			631	373	129	129			

- Molecule 51 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BV	59	Total	C	N	O	0	0	0
			291	173	59	59			
51	DV	59	Total	C	N	O	0	0	0
			291	173	59	59			

- Molecule 52 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	BW	94	Total 468	C 280	N 94	O 94	0	0	0
52	DW	94	Total 468	C 280	N 94	O 94	0	0	0

- Molecule 53 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	BX	107	Total 530	C 316	N 107	O 107	0	0	0
53	DX	107	Total 530	C 316	N 107	O 107	0	0	0

- Molecule 54 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	BY	149	Total 727	C 429	N 149	O 149	0	0	0
54	DY	149	Total 727	C 429	N 149	O 149	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BY	38	GLU	GLN	conflict	UNP P02406
DY	38	GLU	GLN	conflict	UNP P02406

- Molecule 55 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	BZ	98	Total 481	C 285	N 98	O 98	0	0	0
55	DZ	98	Total 481	C 285	N 98	O 98	0	0	0

- Molecule 56 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	Ba	86	Total 425	C 253	N 86	O 86	0	0	0
56	Da	86	Total 425	C 253	N 86	O 86	0	0	0

- Molecule 57 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
57	Bb	125	Total	C	N	O	0	0	0
			618	368	125	125			
57	Db	125	Total	C	N	O	0	0	0
			618	368	125	125			

- Molecule 58 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	Bc	68	Total	C	N	O	0	0	0
			339	203	68	68			
58	Dc	68	Total	C	N	O	0	0	0
			339	203	68	68			

- Molecule 59 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
59	Bd	72	Total	C	N	O	0	0	0
			352	208	72	72			
59	Dd	72	Total	C	N	O	0	0	0
			352	208	72	72			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
60	Be	48	Total	C	N	O	0	0	0
			240	144	48	48			
60	De	48	Total	C	N	O	0	0	0
			240	144	48	48			

- Molecule 61 is a protein called 60S ribosomal protein L42.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
61	Bf	95	Total	C	N	O	0	0	0
			467	277	95	95			
61	Df	95	Total	C	N	O	0	0	0
			467	277	95	95			

- Molecule 62 is a protein called 60S ribosomal protein L43.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
62	Bg	83	Total 407	C 241	N 83	O 83	0	0	0
62	Dg	83	Total 407	C 241	N 83	O 83	0	0	0

- Molecule 63 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
63	Bh	44	Total 220	C 132	N 44	O 44	0	0	0
63	Dh	44	Total 220	C 132	N 44	O 44	0	0	0

- Molecule 64 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
64	Bi	12	Total 60	C 36	N 12	O 12	0	0	0
64	Di	12	Total 60	C 36	N 12	O 12	0	0	0

- Molecule 65 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
65	Bk	16	Total 80	C 48	N 16	O 16	0	0	0
65	Dk	16	Total 80	C 48	N 16	O 16	0	0	0

- Molecule 66 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
66	Bl	19	Total 95	C 57	N 19	O 19	0	0	0

- Molecule 67 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
67	Bm	9	Total 45	C 27	N 9	O 9	0	0	0

- Molecule 68 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
68	Bn	27	Total	C	N	O	0	0	0
			135	81	27	27			

- Molecule 69 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
69	Bp	8	Total	C	N	O	0	0	0
			40	24	8	8			

- Molecule 70 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
70	Bq	17	Total	C	N	O	0	0	0
			85	51	17	17			

- Molecule 71 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
71	Br	23	Total	C	N	O	0	0	0
			115	69	23	23			

- Molecule 72 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
72	DL	138	Total	C	N	O	0	0	0
			679	403	138	138			

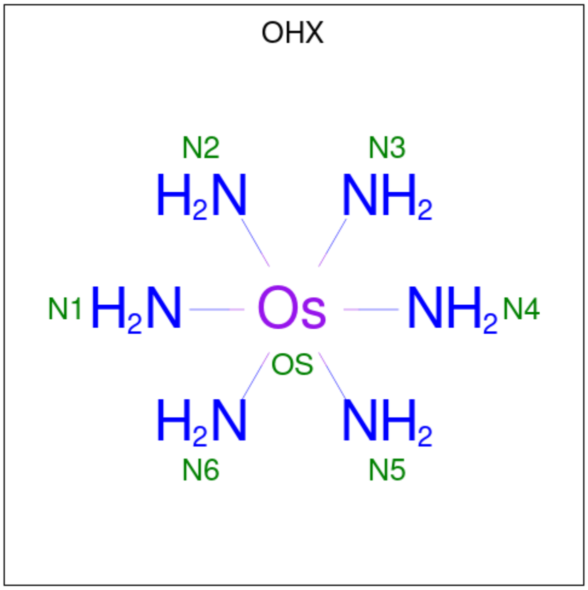
- Molecule 73 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
73	DM	130	Total	C	N	O	0	0	0
			641	381	130	130			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DM	83	TYR	ASN	conflict	UNP P05317

- Molecule 74 is osmium (III) hexammine (three-letter code: OHX) (formula: $H_{12}N_6Os$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
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74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
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74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
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74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	A1	1	Total N Os 7 6 1	0	0
74	AL	1	Total N Os 7 6 1	0	0
74	AS	1	Total N Os 7 6 1	0	0
74	AT	1	Total N Os 7 6 1	0	0
74	Ac	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
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74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
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74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
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74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
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74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
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74	B1	1	Total N Os 7 6 1	0	0
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B1	1	Total N Os 7 6 1	0	0
74	B2	1	Total N Os 7 6 1	0	0
74	B2	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	B2	1	Total N Os 7 6 1	0	0
74	B2	1	Total N Os 7 6 1	0	0
74	B2	1	Total N Os 7 6 1	0	0
74	B2	1	Total N Os 7 6 1	0	0
74	B2	1	Total N Os 7 6 1	0	0
74	B2	1	Total N Os 7 6 1	0	0
74	B2	1	Total N Os 7 6 1	0	0
74	B2	1	Total N Os 7 6 1	0	0
74	B3	1	Total N Os 7 6 1	0	0
74	B3	1	Total N Os 7 6 1	0	0
74	B3	1	Total N Os 7 6 1	0	0
74	B3	1	Total N Os 7 6 1	0	0
74	B3	1	Total N Os 7 6 1	0	0
74	B3	1	Total N Os 7 6 1	0	0
74	B3	1	Total N Os 7 6 1	0	0
74	B3	1	Total N Os 7 6 1	0	0
74	B3	1	Total N Os 7 6 1	0	0
74	B3	1	Total N Os 7 6 1	0	0
74	B3	1	Total N Os 7 6 1	0	0
74	B3	1	Total N Os 7 6 1	0	0
74	BC	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	BO	1	Total N Os 7 6 1	0	0
74	BT	1	Total N Os 7 6 1	0	0
74	Bd	1	Total N Os 7 6 1	0	0
74	Bd	1	Total N Os 7 6 1	0	0
74	Bg	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0
74	C1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	C1	1	Total N Os 7 6 1	0	0
74	CI	1	Total N Os 7 6 1	0	0
74	CS	1	Total N Os 7 6 1	0	0
74	CS	1	Total N Os 7 6 1	0	0
74	CT	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D1	1	Total N Os 7 6 1	0	0
74	D2	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
74	D2	1	Total N Os 7 6 1	0	0
74	D2	1	Total N Os 7 6 1	0	0
74	D2	1	Total N Os 7 6 1	0	0
74	D2	1	Total N Os 7 6 1	0	0
74	D2	1	Total N Os 7 6 1	0	0
74	D2	1	Total N Os 7 6 1	0	0
74	D2	1	Total N Os 7 6 1	0	0
74	D2	1	Total N Os 7 6 1	0	0
74	D3	1	Total N Os 7 6 1	0	0
74	D3	1	Total N Os 7 6 1	0	0
74	D3	1	Total N Os 7 6 1	0	0
74	D3	1	Total N Os 7 6 1	0	0
74	D3	1	Total N Os 7 6 1	0	0
74	D3	1	Total N Os 7 6 1	0	0
74	D3	1	Total N Os 7 6 1	0	0
74	D3	1	Total N Os 7 6 1	0	0
74	D3	1	Total N Os 7 6 1	0	0
74	D3	1	Total N Os 7 6 1	0	0
74	D3	1	Total N Os 7 6 1	0	0
74	D3	1	Total N Os 7 6 1	0	0
74	DC	1	Total N Os 7 6 1	0	0

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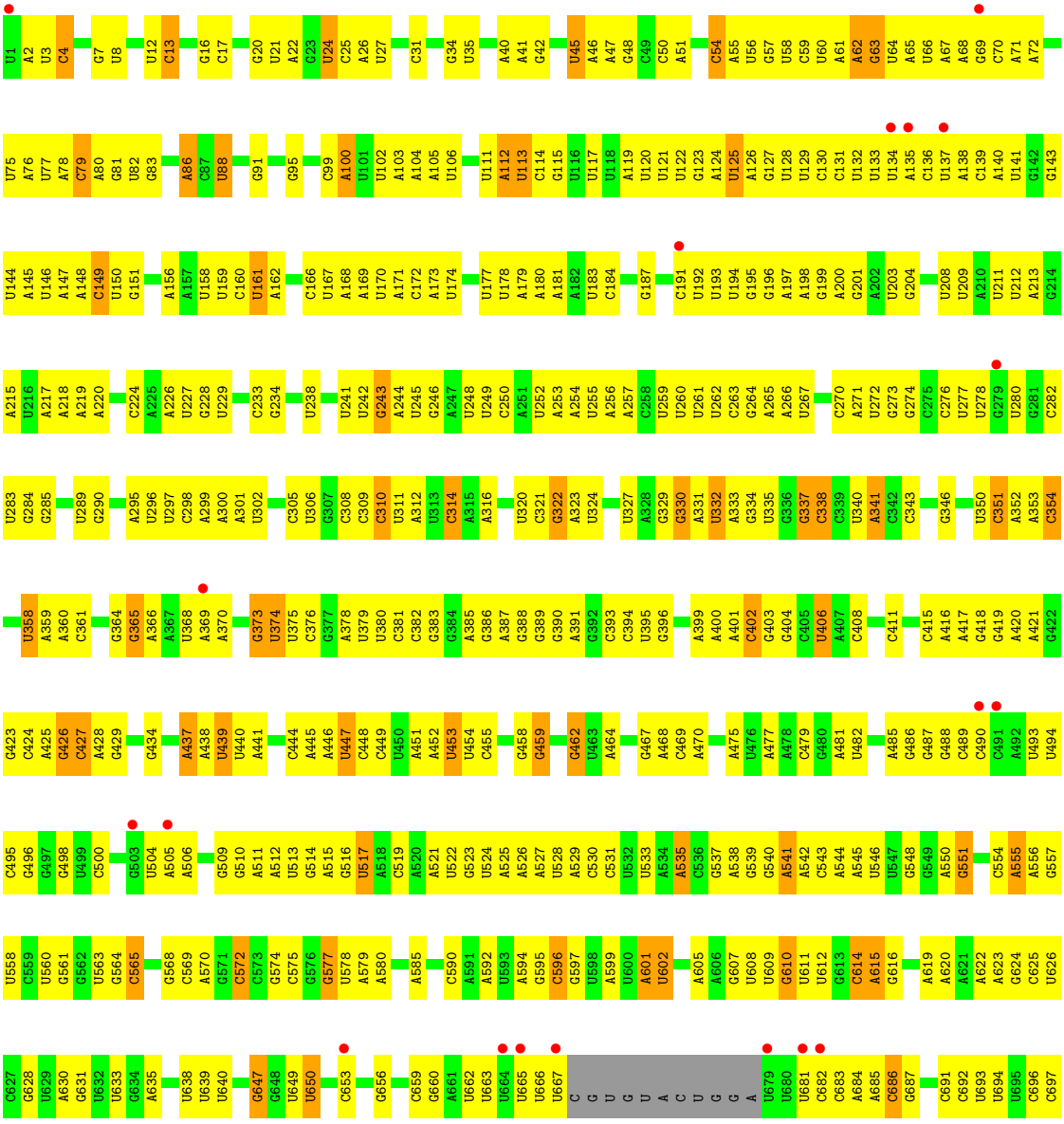
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	DE	1	Total	N	Os	0	0
			7	6	1		
74	DJ	1	Total	N	Os	0	0
			7	6	1		
74	DO	1	Total	N	Os	0	0
			7	6	1		
74	DO	1	Total	N	Os	0	0
			7	6	1		
74	DT	1	Total	N	Os	0	0
			7	6	1		
74	Dd	1	Total	N	Os	0	0
			7	6	1		
74	Dd	1	Total	N	Os	0	0
			7	6	1		
74	Dg	1	Total	N	Os	0	0
			7	6	1		

3 Residue-property plots (i)

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

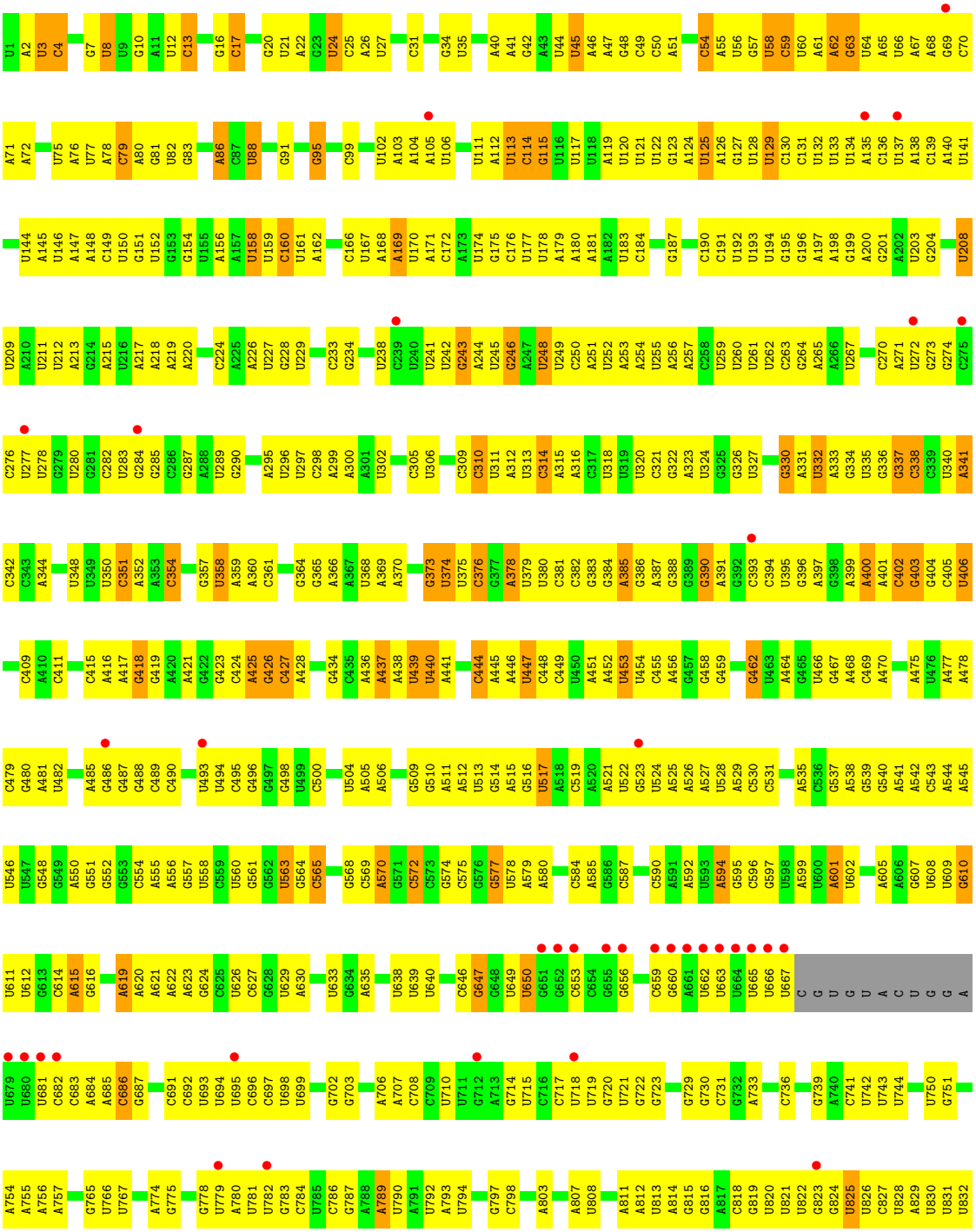
- Molecule 1: 18S ribosomal RNA

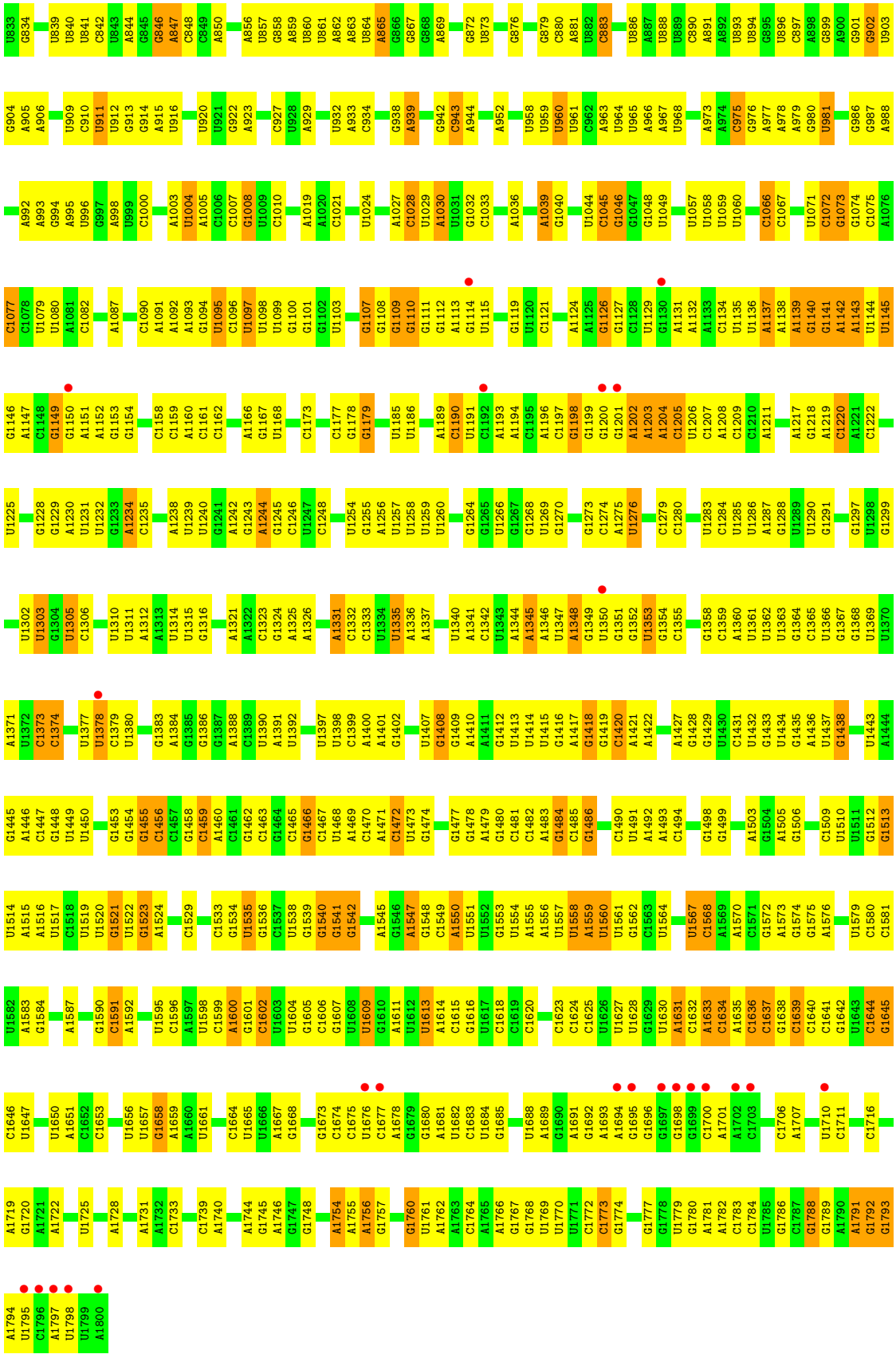
Chain A1:



• Molecule 1: 18S ribosomal RNA

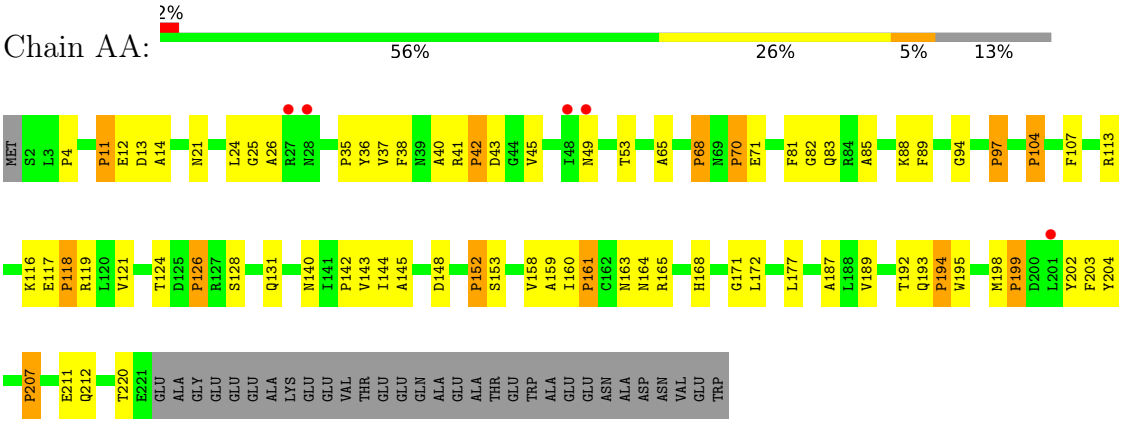
Chain C1:





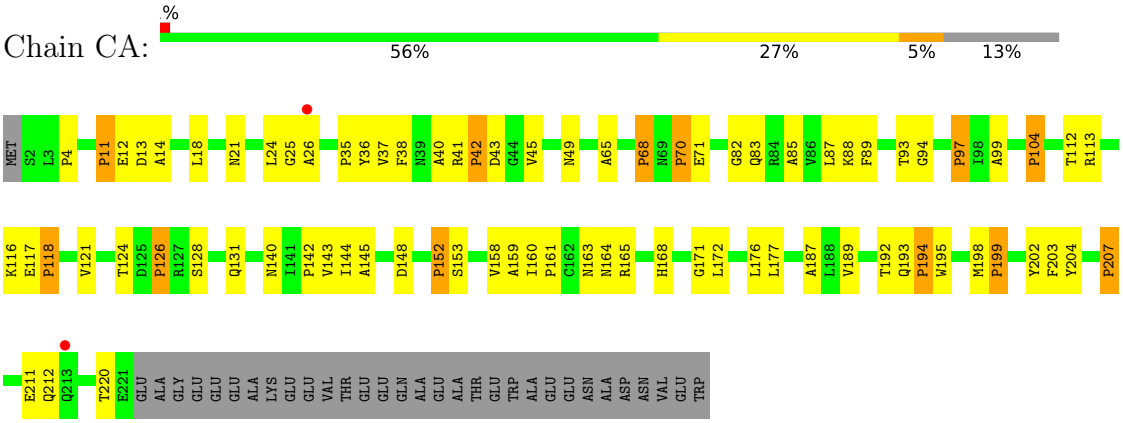
• Molecule 2: 40S ribosomal protein S0-A

Chain AA:



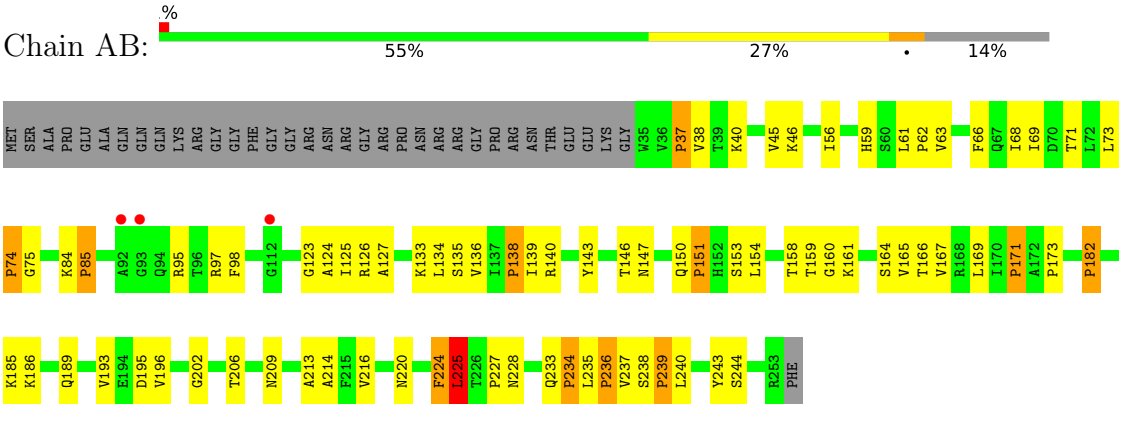
• Molecule 2: 40S ribosomal protein S0-A

Chain CA:



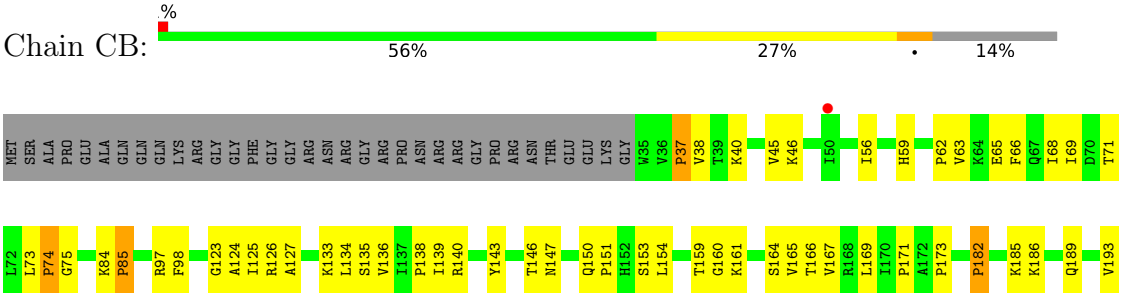
• Molecule 3: 40S ribosomal protein S2

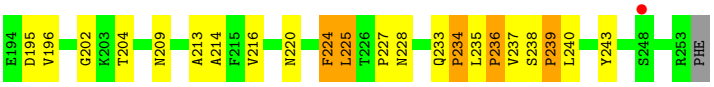
Chain AB:



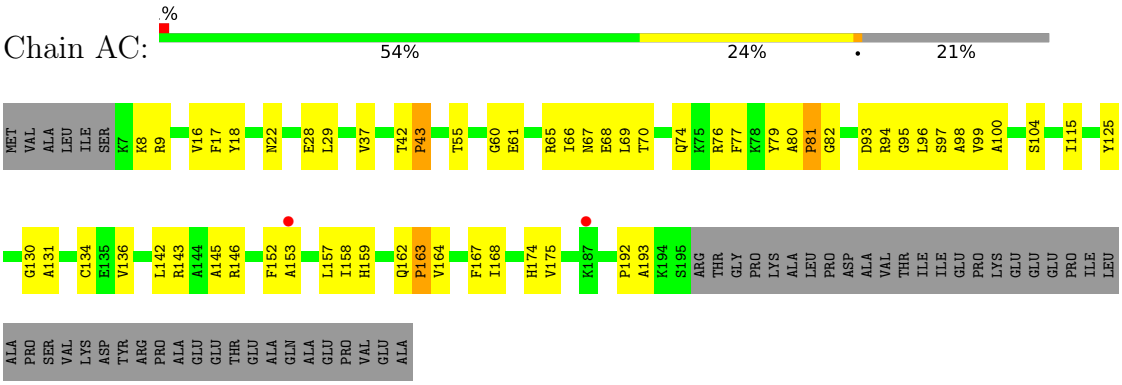
• Molecule 3: 40S ribosomal protein S2

Chain CB:

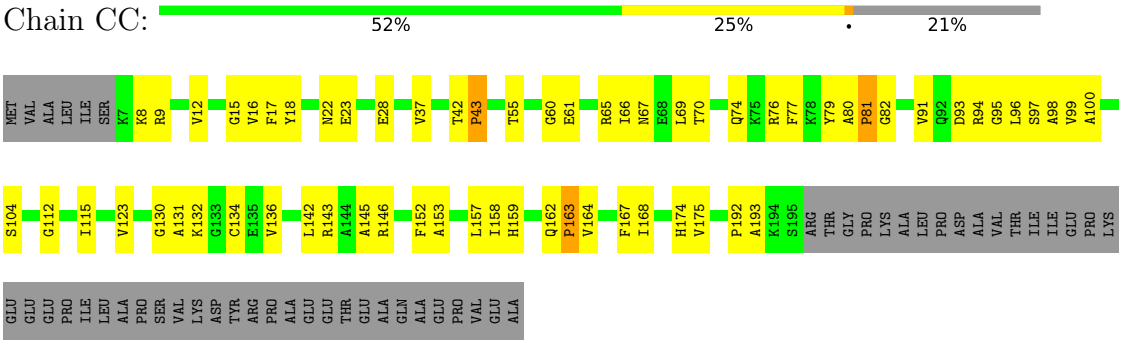




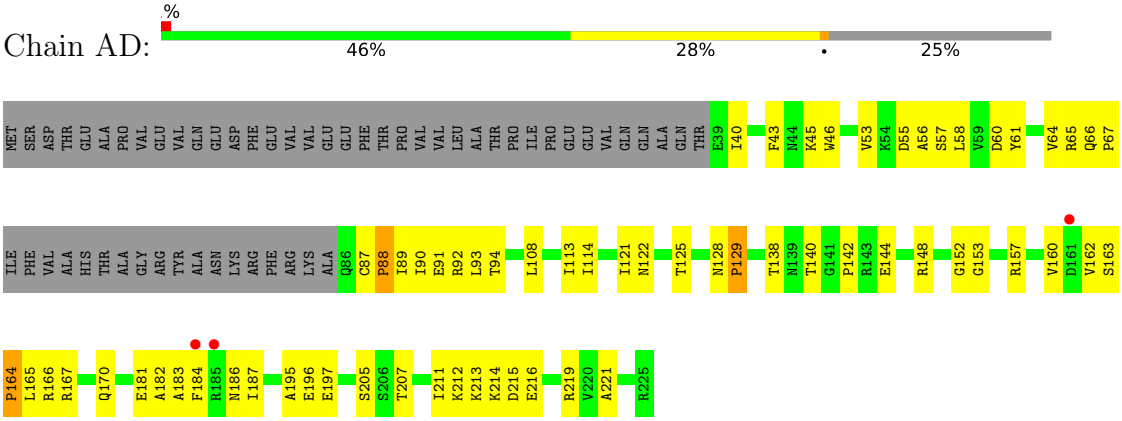
• Molecule 4: 40S ribosomal protein S3



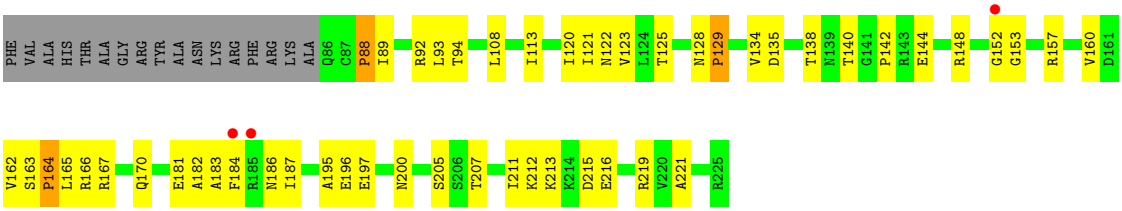
• Molecule 4: 40S ribosomal protein S3



• Molecule 5: 40S ribosomal protein S5

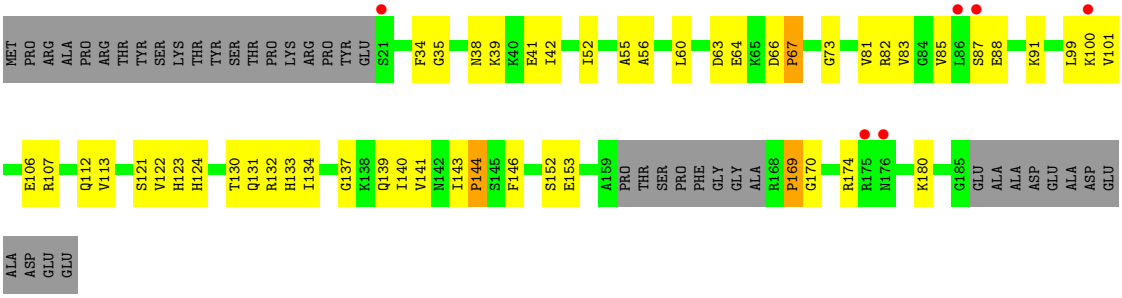


• Molecule 5: 40S ribosomal protein S5



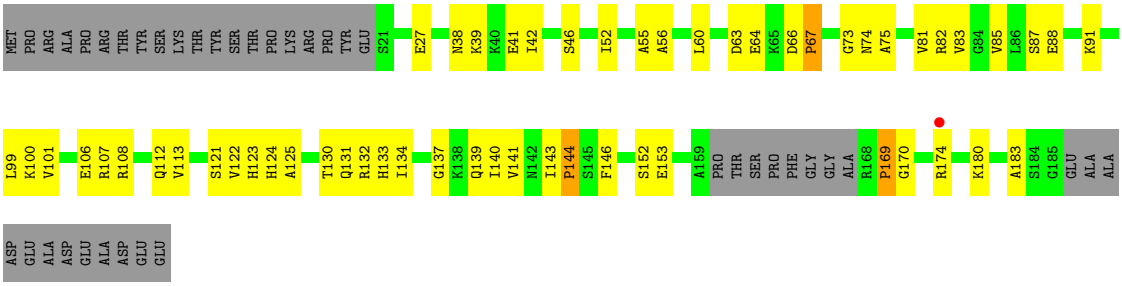
• Molecule 6: 40S ribosomal protein S9-A

Chain AE:



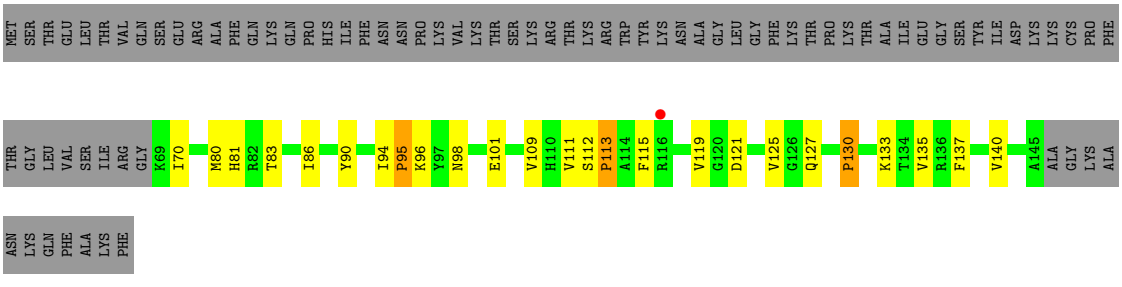
• Molecule 6: 40S ribosomal protein S9-A

Chain CE:



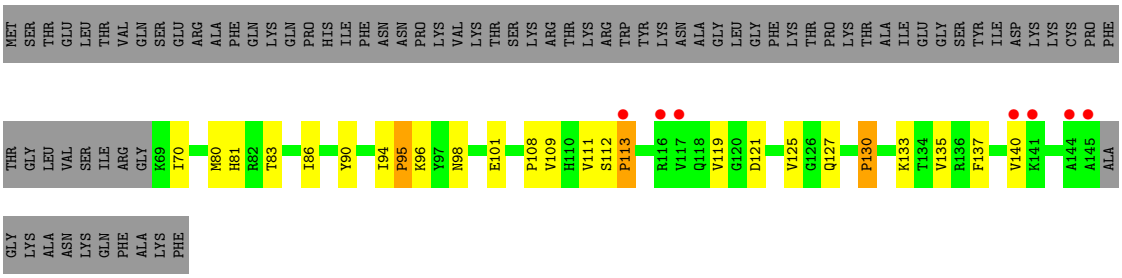
• Molecule 7: 40S ribosomal protein S11

Chain AF:



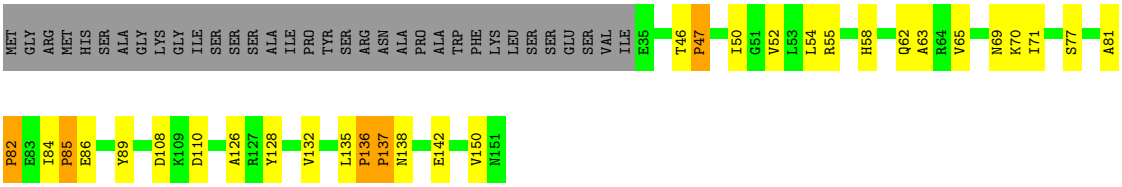
• Molecule 7: 40S ribosomal protein S11

Chain CF:



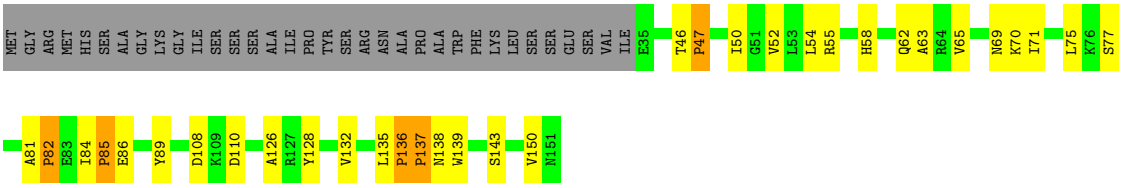
• Molecule 8: 40S ribosomal protein S13

Chain AG:



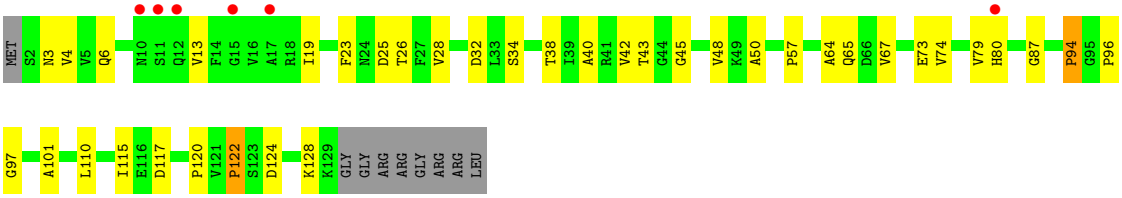
• Molecule 8: 40S ribosomal protein S13

Chain CG:



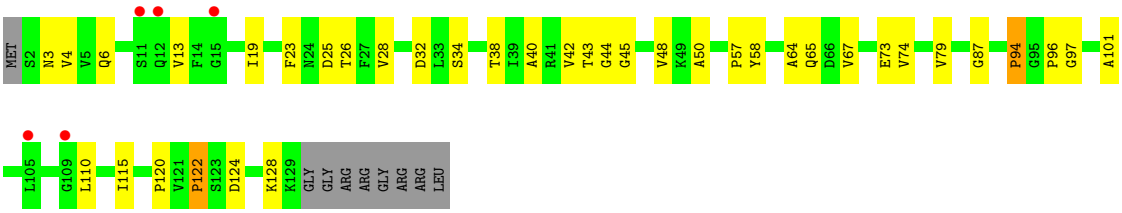
• Molecule 9: 40S ribosomal protein S14-A

Chain AH:



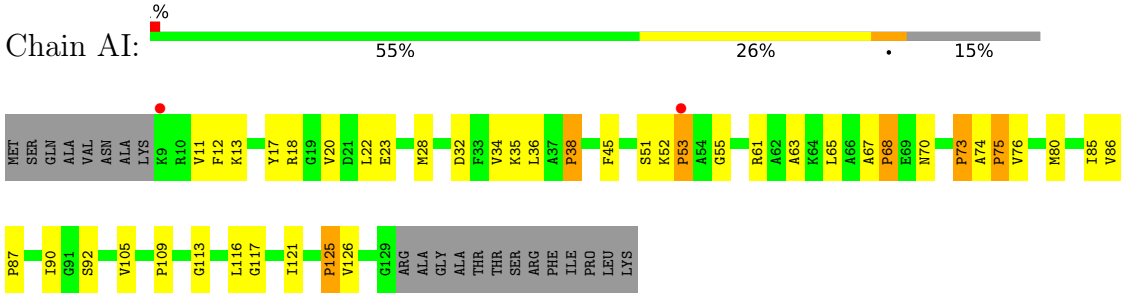
• Molecule 9: 40S ribosomal protein S14-A

Chain CH:



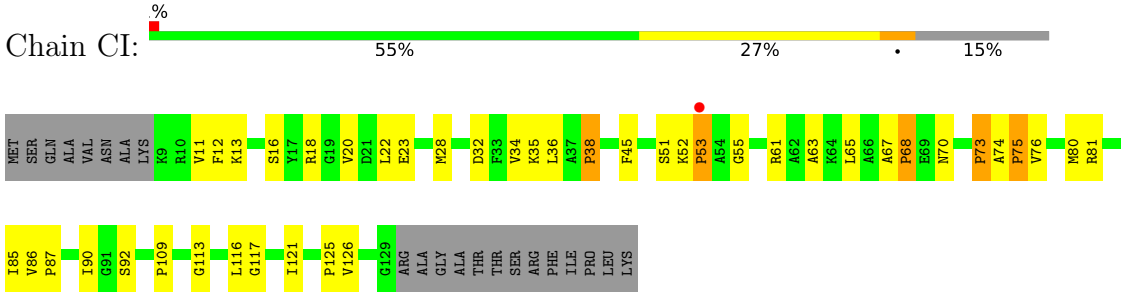
• Molecule 10: 40S ribosomal protein S15

Chain AI:



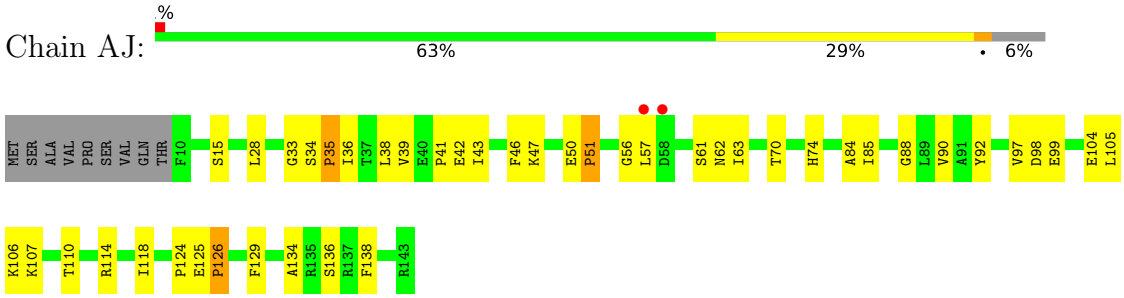
• Molecule 10: 40S ribosomal protein S15

Chain CI:



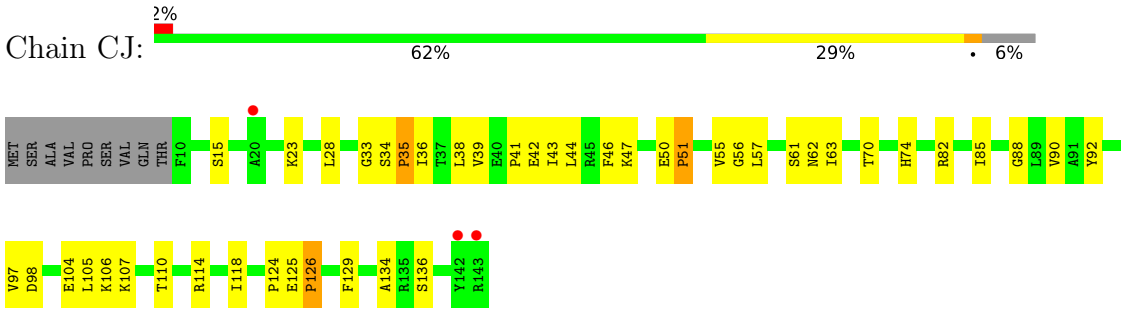
• Molecule 11: 40S ribosomal protein S16

Chain AJ:



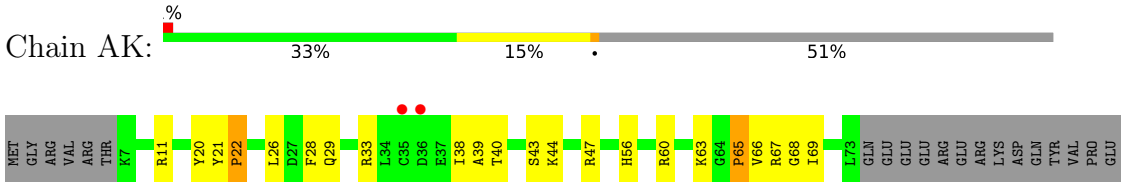
• Molecule 11: 40S ribosomal protein S16

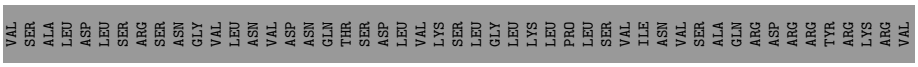
Chain CJ:



• Molecule 12: 40S ribosomal protein S17-A

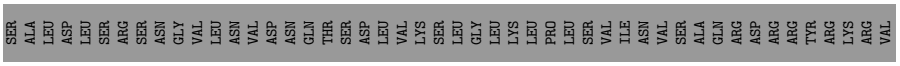
Chain AK:





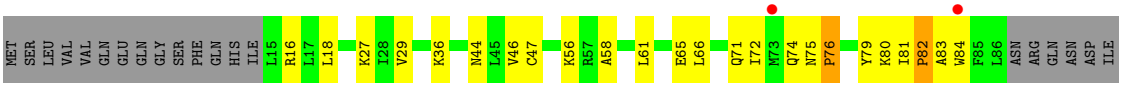
• Molecule 12: 40S ribosomal protein S17-A

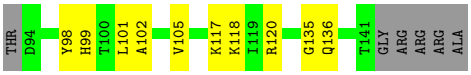
Chain CK:



• Molecule 13: 40S ribosomal protein S18

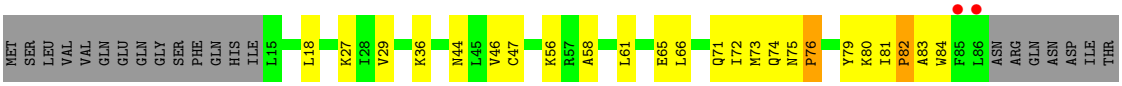
Chain AL:





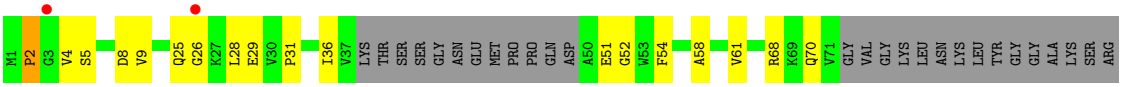
• Molecule 13: 40S ribosomal protein S18

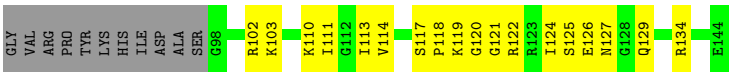
Chain CL:



• Molecule 14: 40S ribosomal protein S19-A

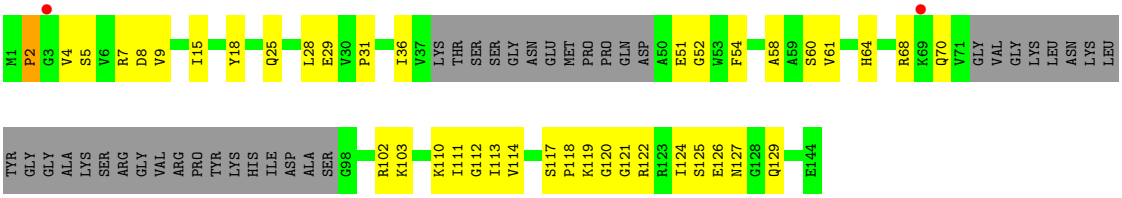
Chain AM:



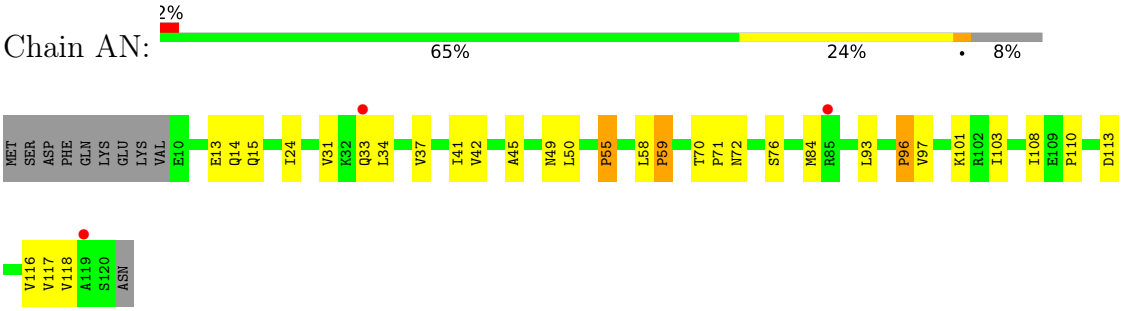


• Molecule 14: 40S ribosomal protein S19-A

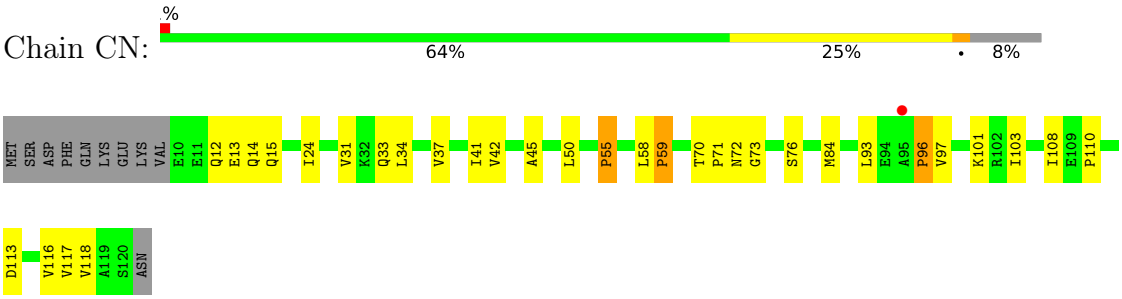
Chain CM:



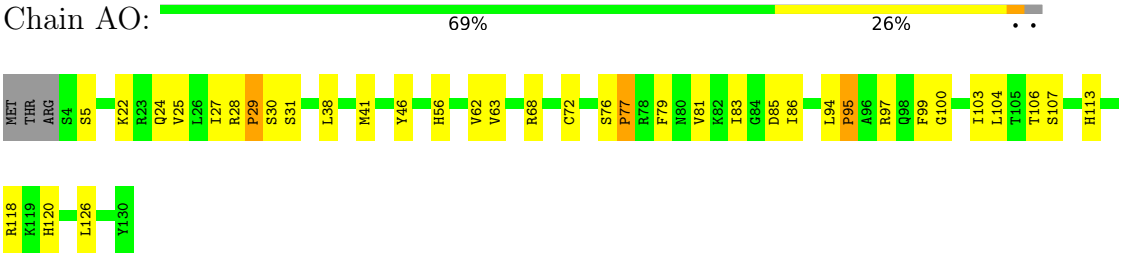
• Molecule 15: 40S ribosomal protein S20



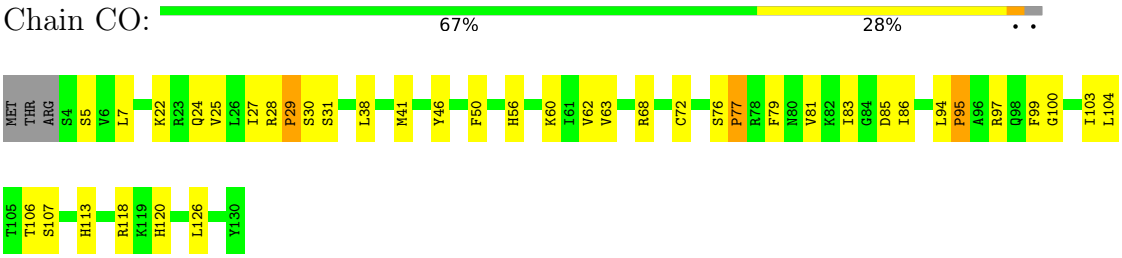
• Molecule 15: 40S ribosomal protein S20



• Molecule 16: 40S ribosomal protein S22-A

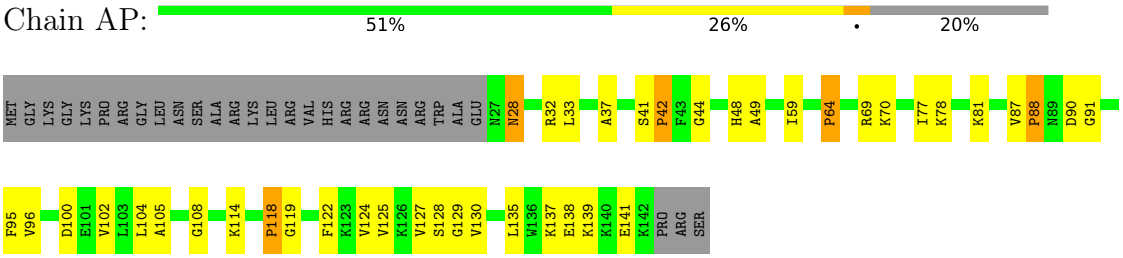


• Molecule 16: 40S ribosomal protein S22-A



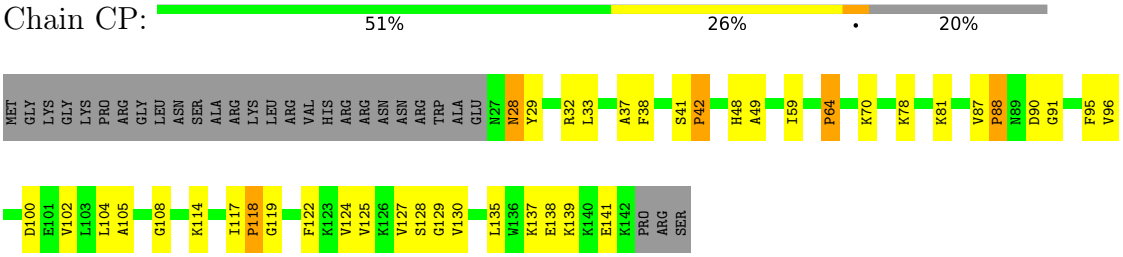
• Molecule 17: 40S ribosomal protein S23

Chain AP:



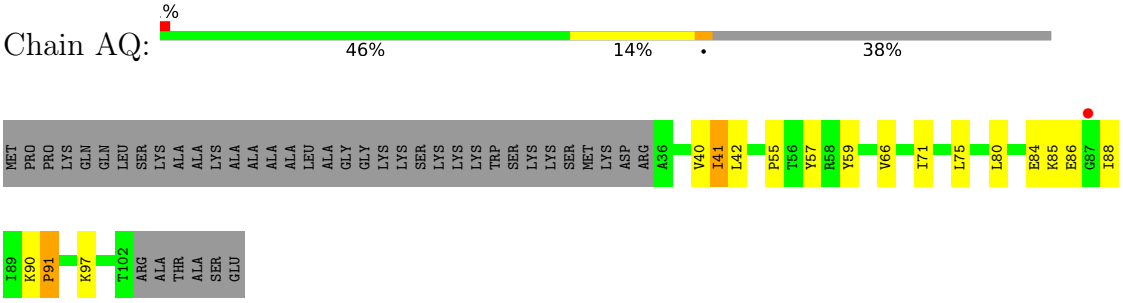
• Molecule 17: 40S ribosomal protein S23

Chain CP:



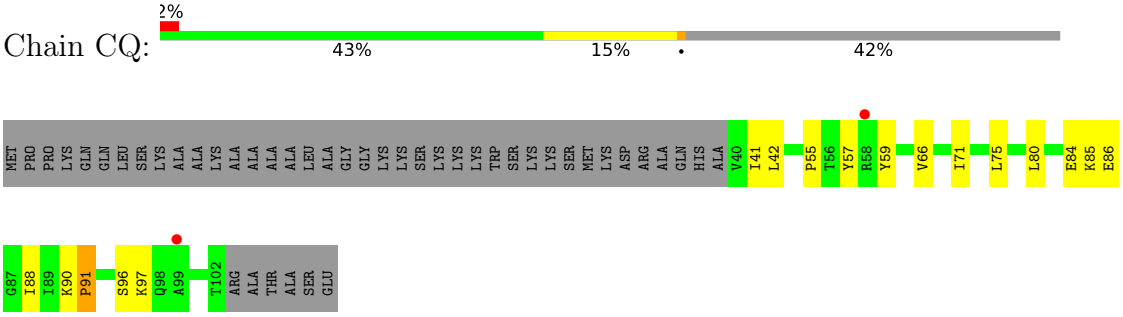
• Molecule 18: 40S ribosomal protein S25-A

Chain AQ:



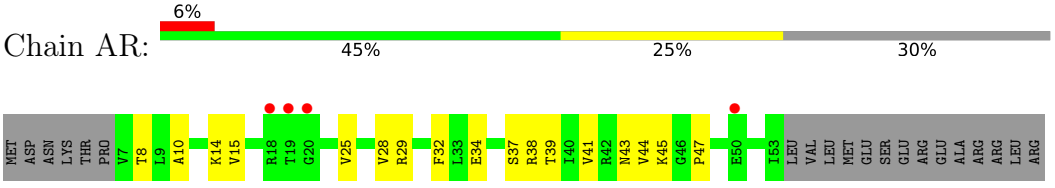
• Molecule 18: 40S ribosomal protein S25-A

Chain CQ:



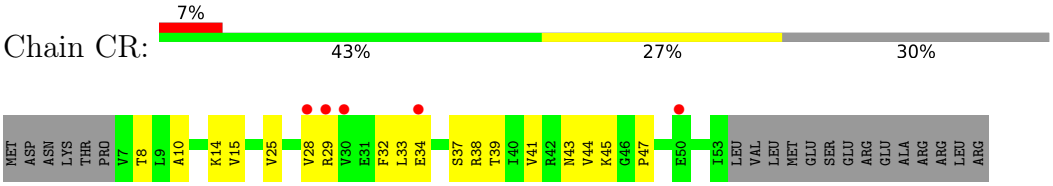
• Molecule 19: 40S ribosomal protein S28-A

Chain AR:



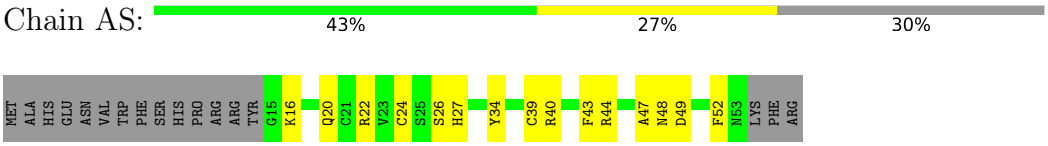
• Molecule 19: 40S ribosomal protein S28-A

Chain CR:



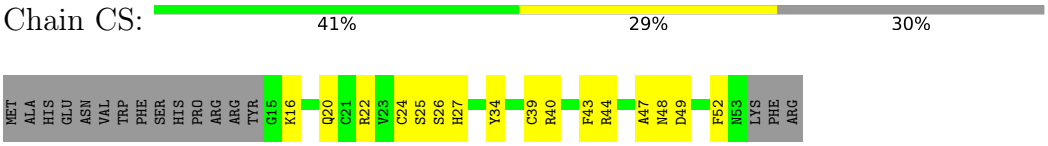
• Molecule 20: 40S ribosomal protein S29-A

Chain AS:



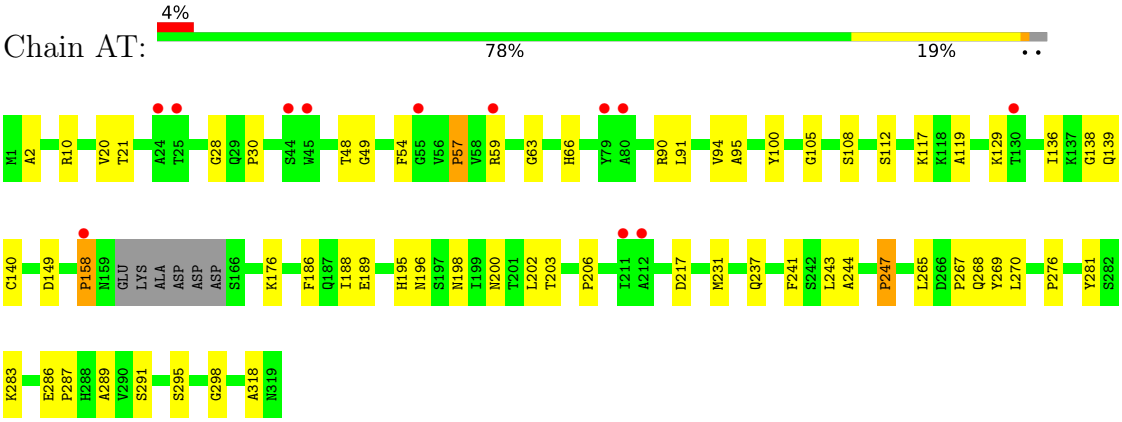
• Molecule 20: 40S ribosomal protein S29-A

Chain CS:



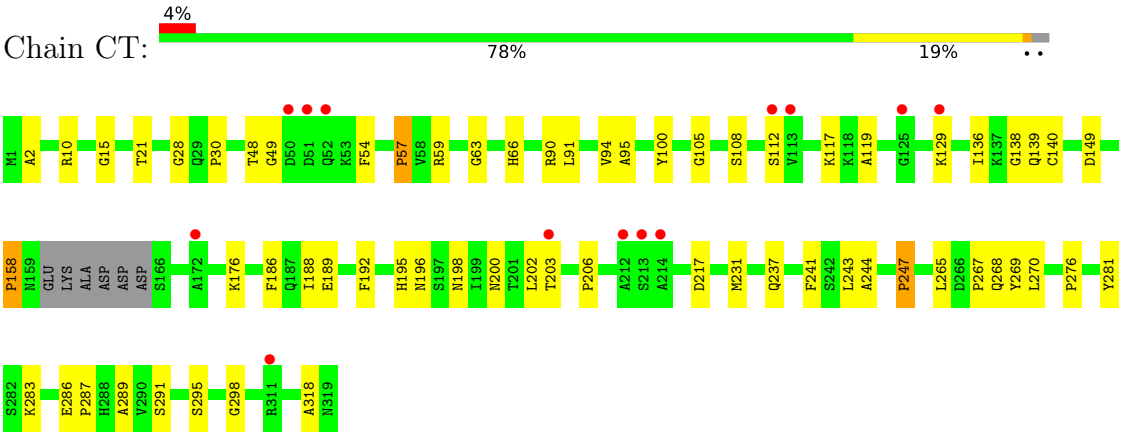
• Molecule 21: Guanine nucleotide-binding protein subunit beta-like protein; RACK-1

Chain AT:



• Molecule 21: Guanine nucleotide-binding protein subunit beta-like protein; RACK-1

Chain CT:

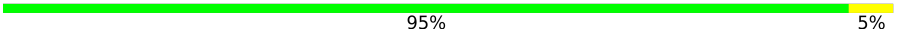


• Molecule 22: Unassigned secondary structure

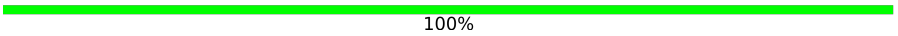
Chain Aa: 

There are no outlier residues recorded for this chain.

• Molecule 22: Unassigned secondary structure

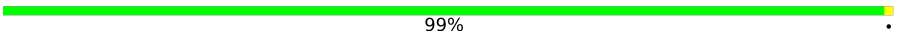
Chain Bo: 

• Molecule 22: Unassigned secondary structure

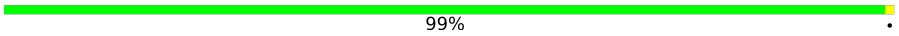
Chain Ca: 

There are no outlier residues recorded for this chain.

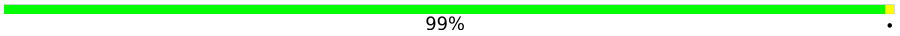
• Molecule 23: Unassigned secondary structure

Chain Ab: 

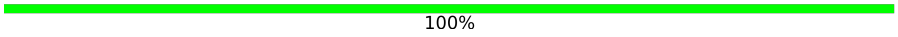
• Molecule 23: Unassigned secondary structure

Chain Cb: 

• Molecule 24: Unassigned secondary structure

Chain Ac: 

• Molecule 24: Unassigned secondary structure

Chain Cc: 

There are no outlier residues recorded for this chain.

• Molecule 25: Unassigned secondary structure

Chain Ad: 

There are no outlier residues recorded for this chain.

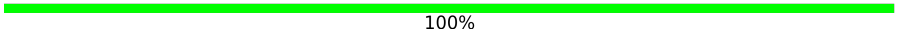
• Molecule 25: Unassigned secondary structure

Chain Cd:

There are no outlier residues recorded for this chain.

• Molecule 26: Unassigned secondary structure

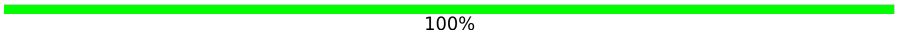
Chain Ae:



There are no outlier residues recorded for this chain.

• Molecule 26: Unassigned secondary structure

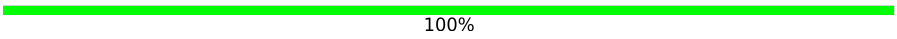
Chain Bj:



There are no outlier residues recorded for this chain.

• Molecule 26: Unassigned secondary structure

Chain Dj:



There are no outlier residues recorded for this chain.

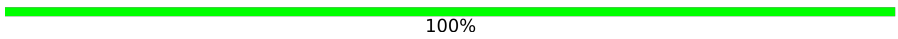
• Molecule 27: Unassigned secondary structure

Chain Af:

There are no outlier residues recorded for this chain.

• Molecule 28: Unassigned secondary structure

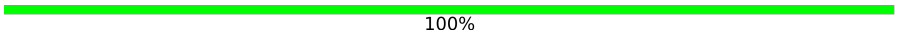
Chain Ah:



There are no outlier residues recorded for this chain.

• Molecule 28: Unassigned secondary structure

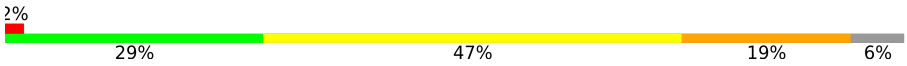
Chain Ch:

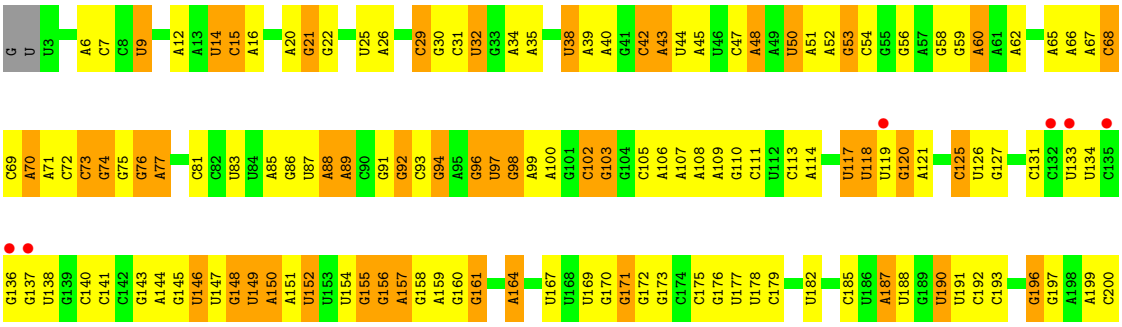


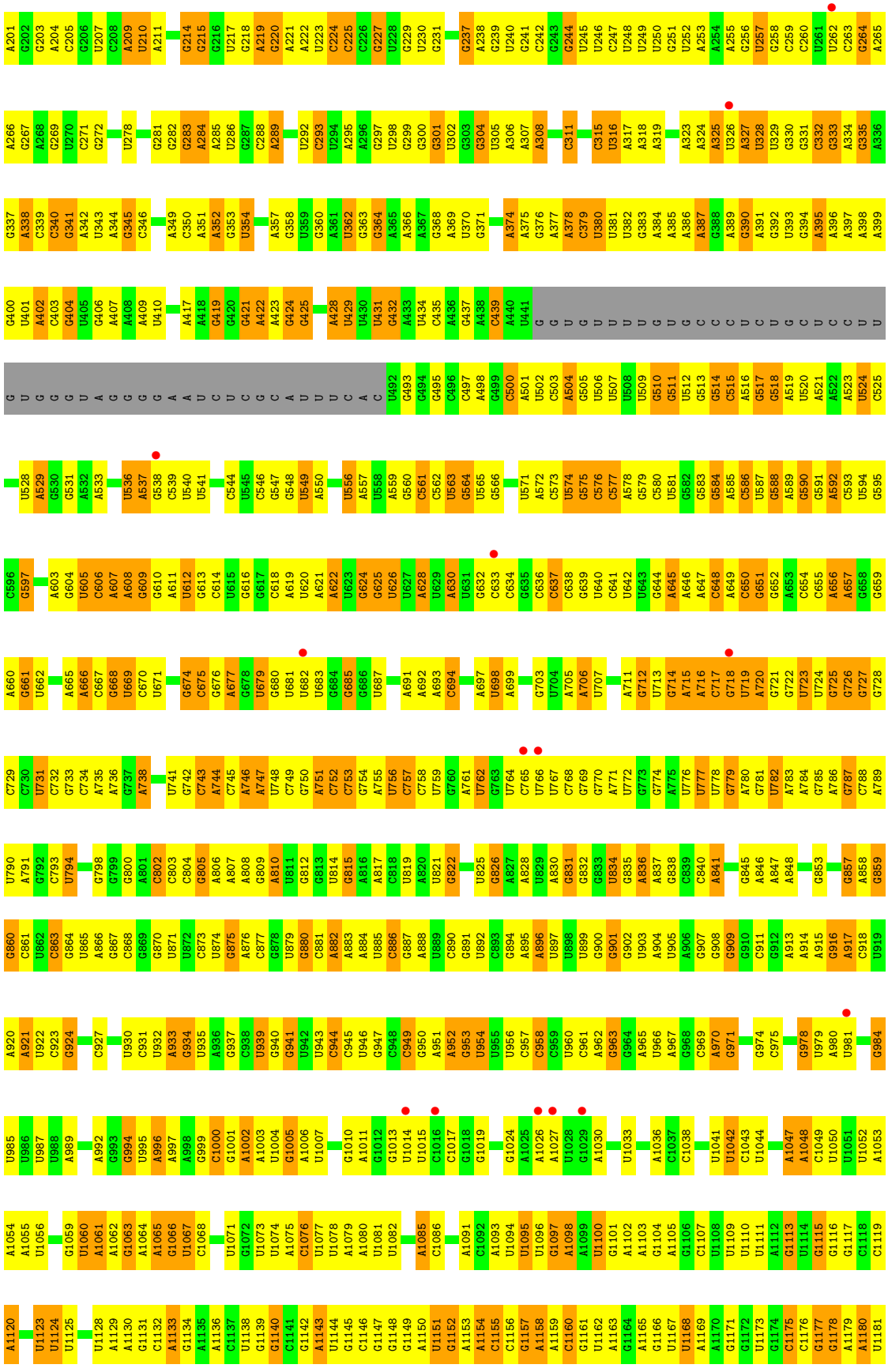
There are no outlier residues recorded for this chain.

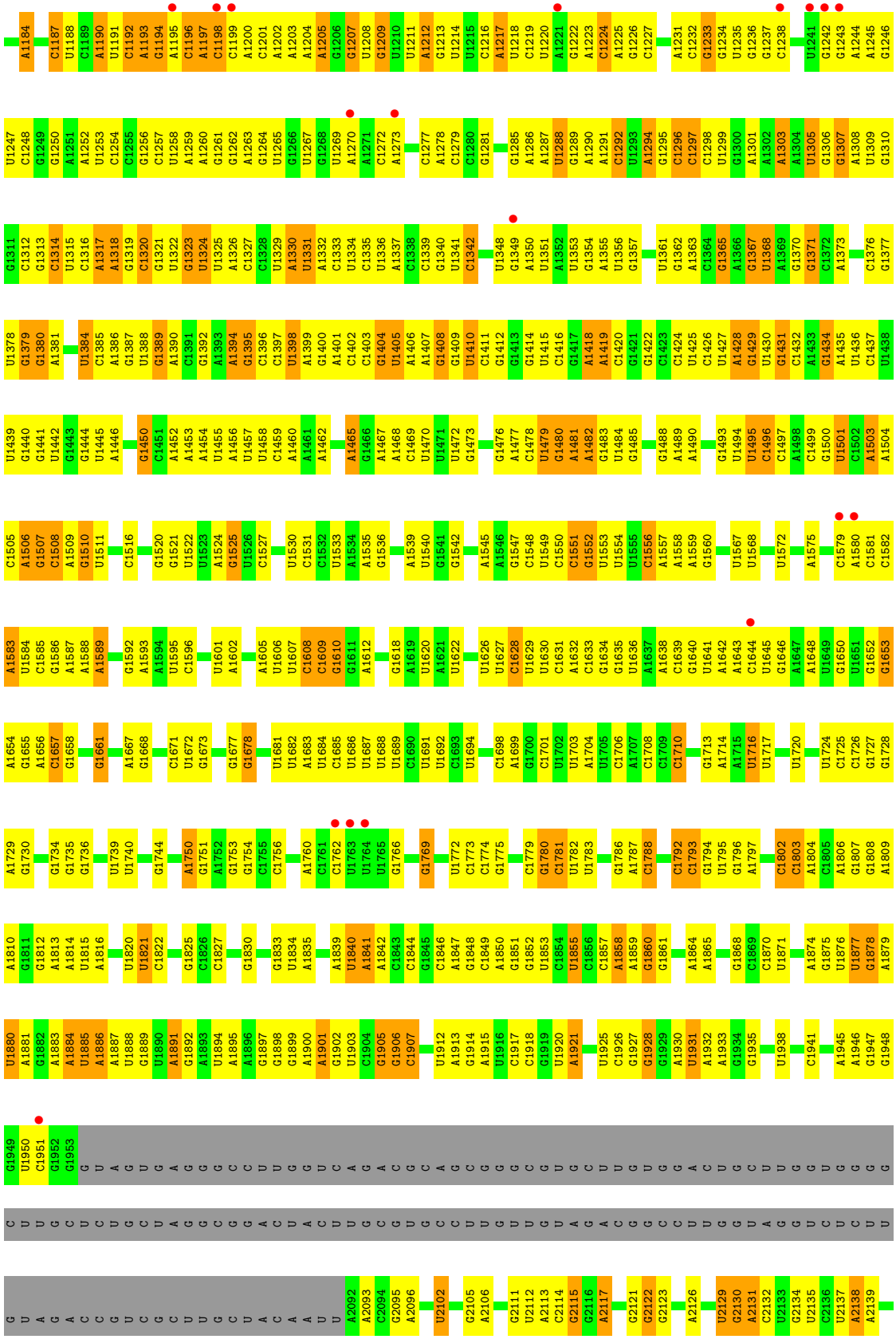
• Molecule 29: 25S ribosomal RNA

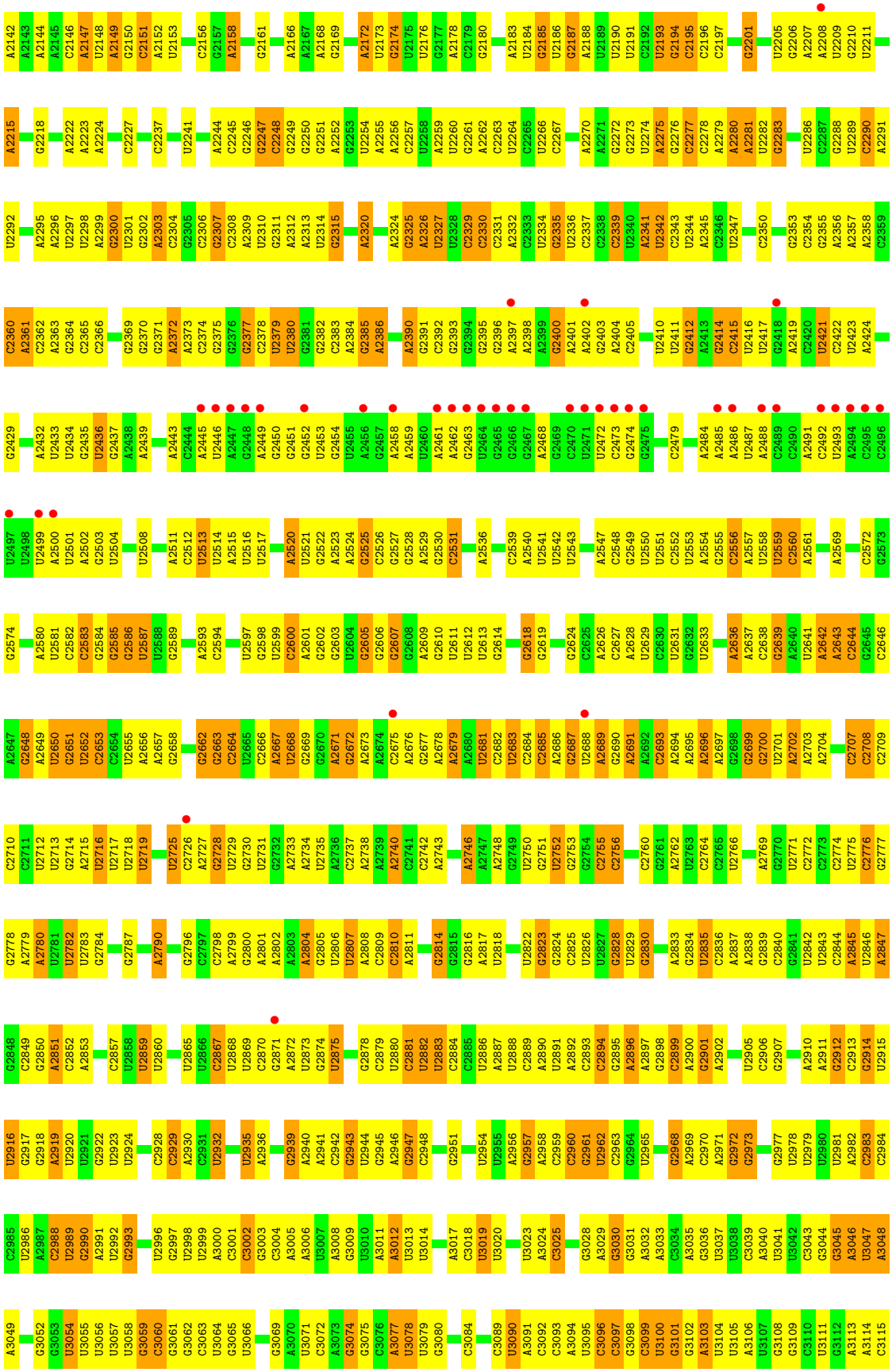
Chain B1:

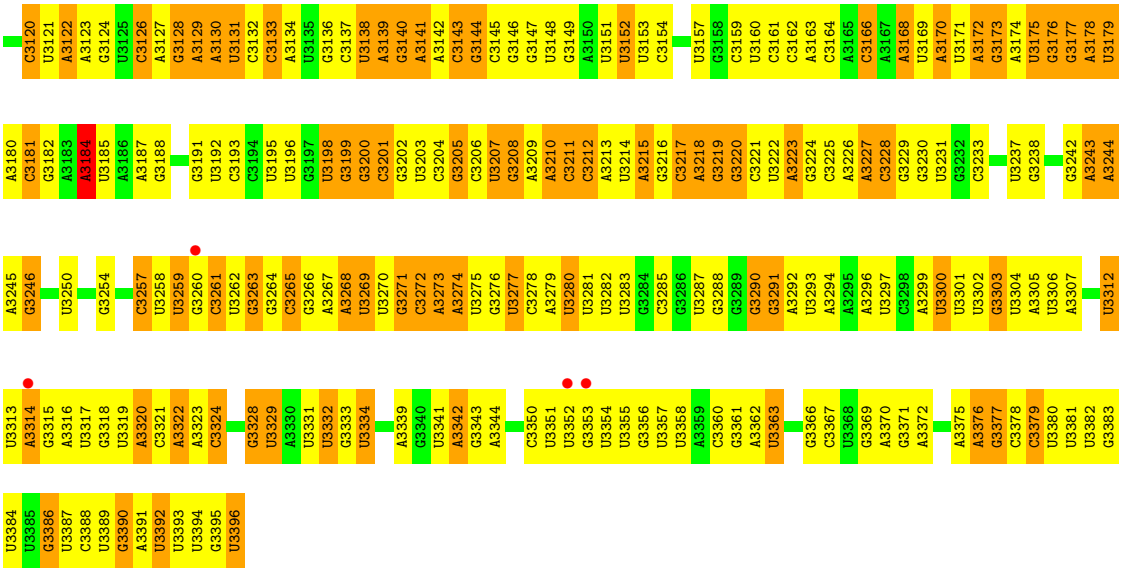






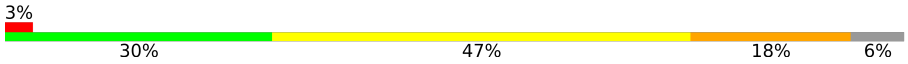


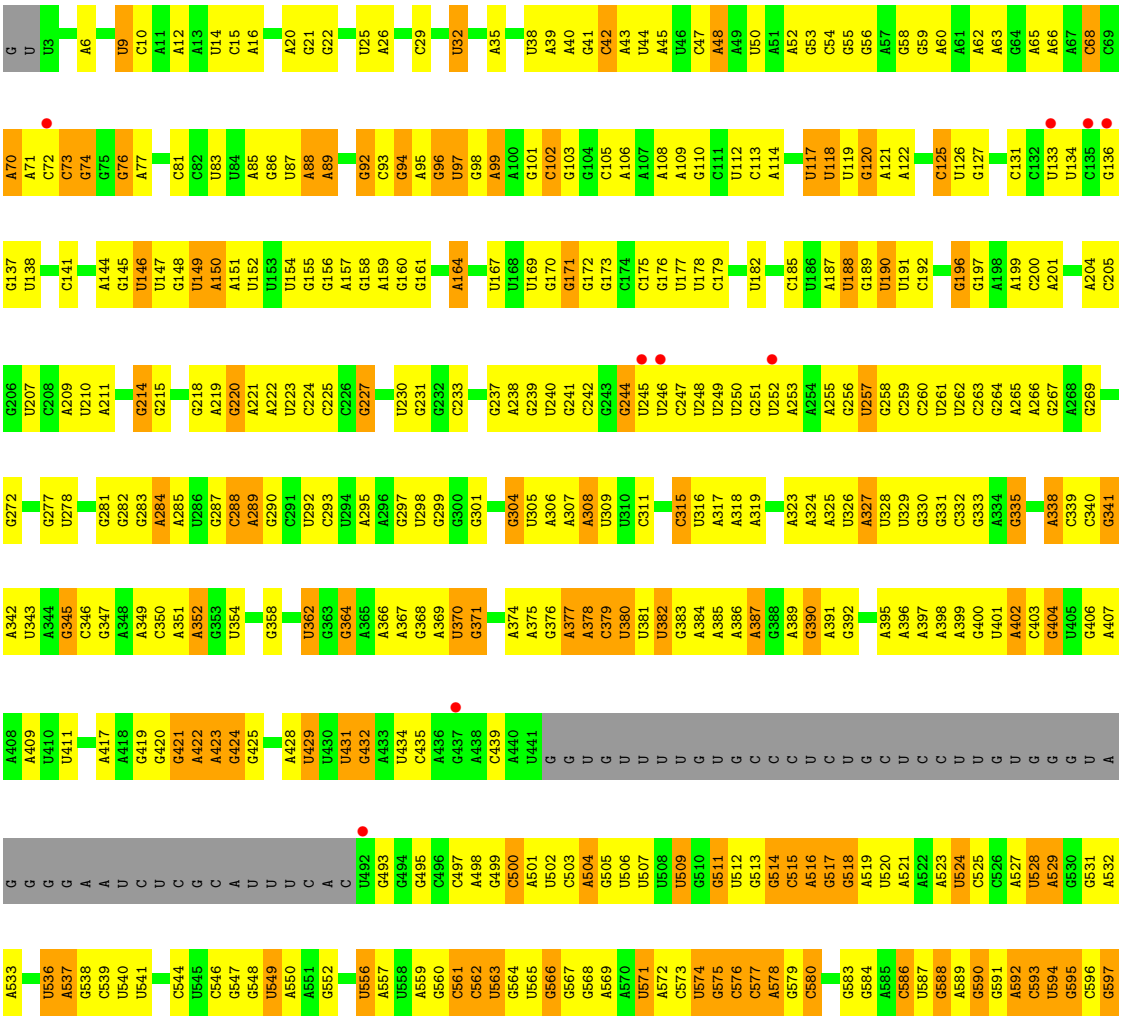


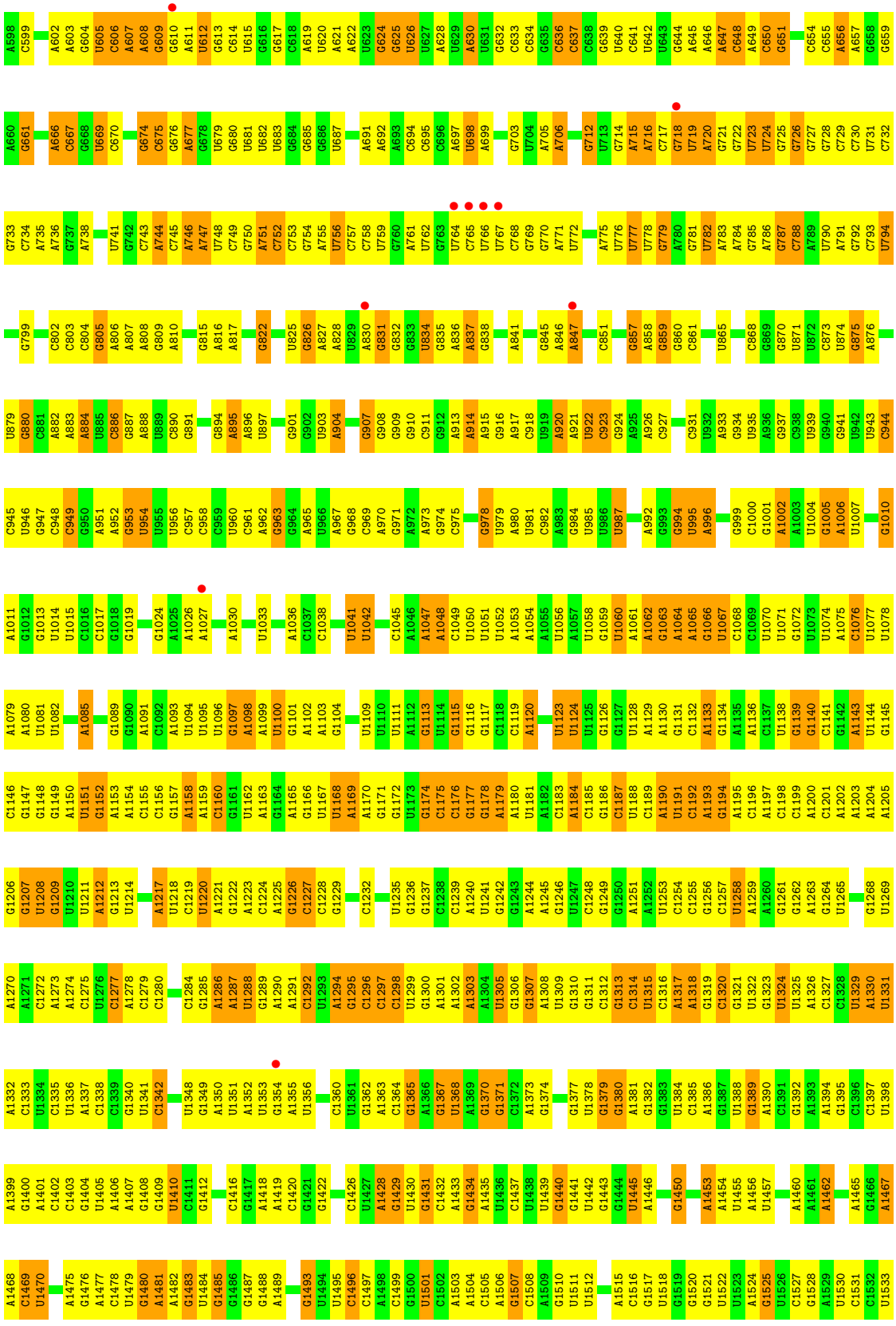


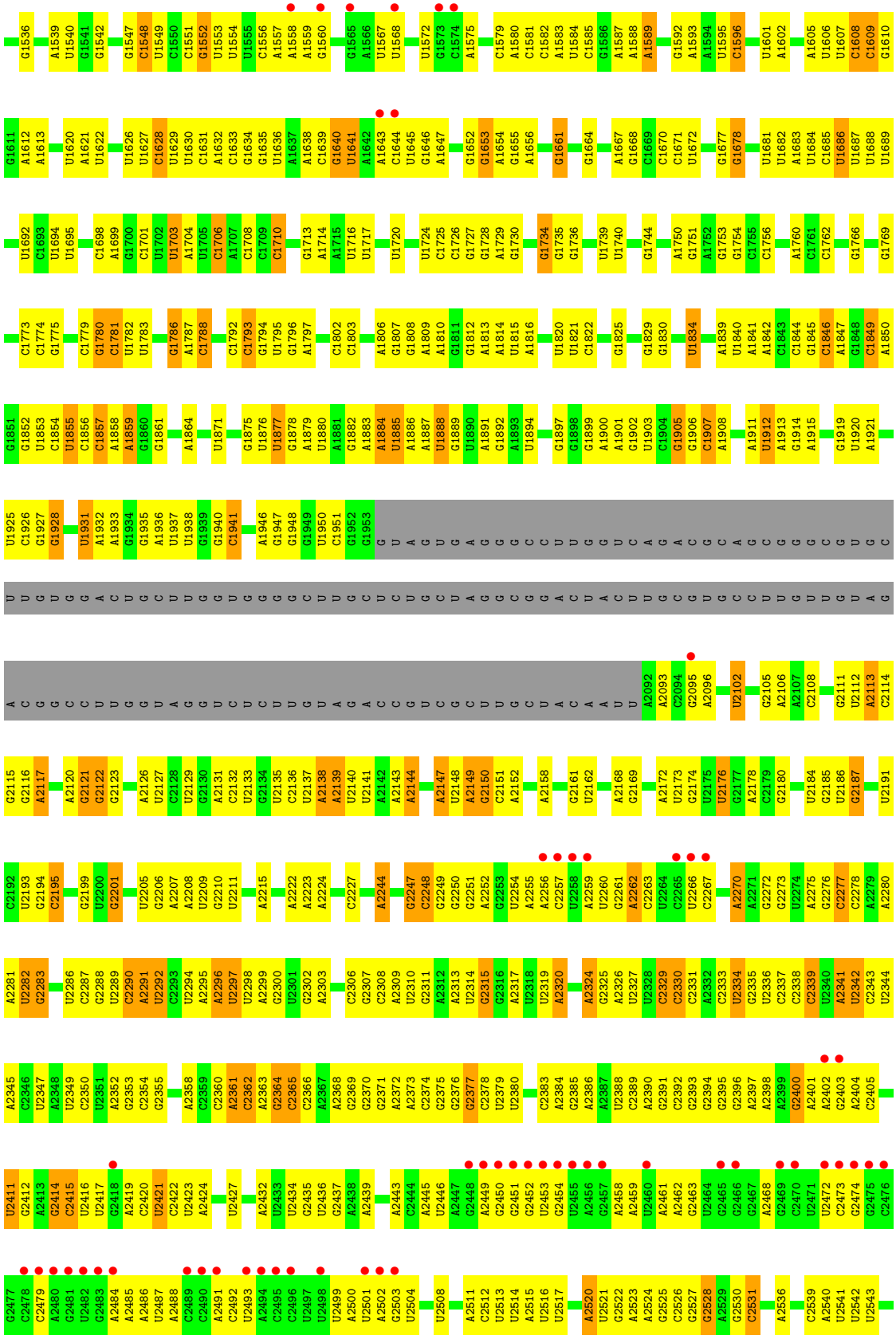
• Molecule 29: 25S ribosomal RNA

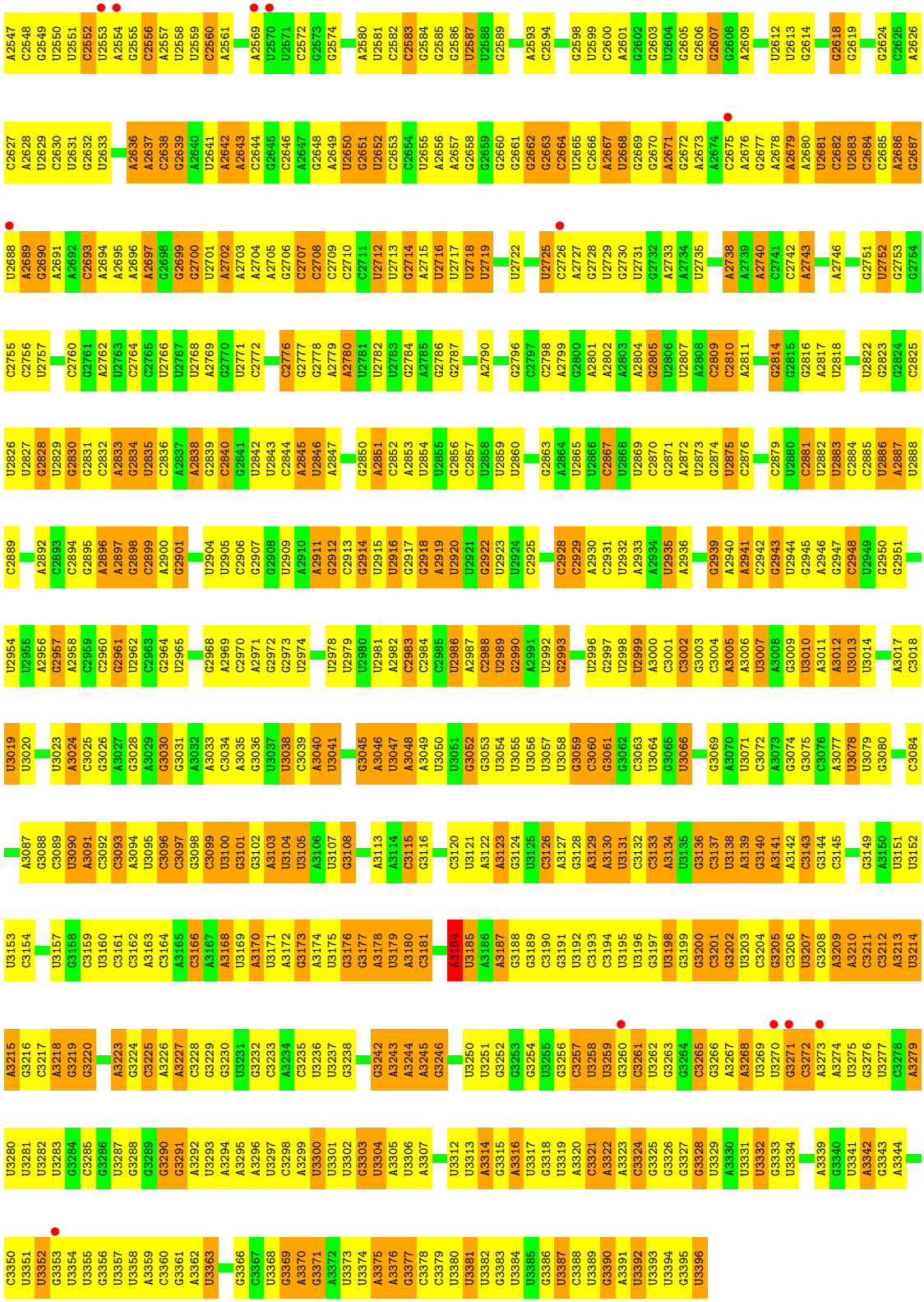
Chain D1:





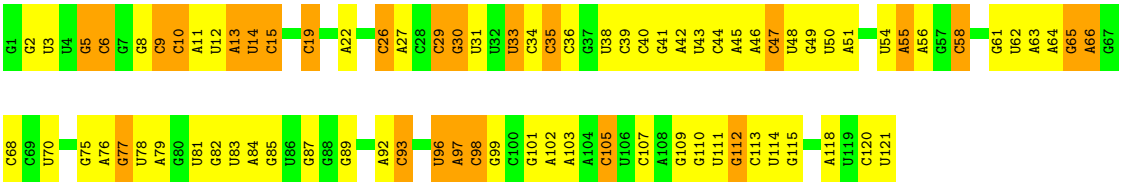






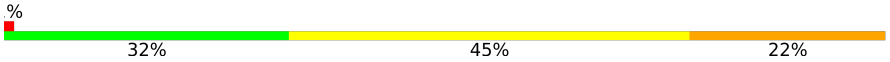
• Molecule 30: 5S ribosomal RNA

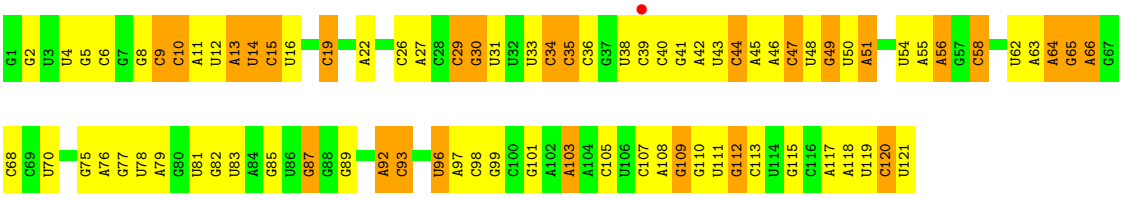
Chain B2:



• Molecule 30: 5S ribosomal RNA

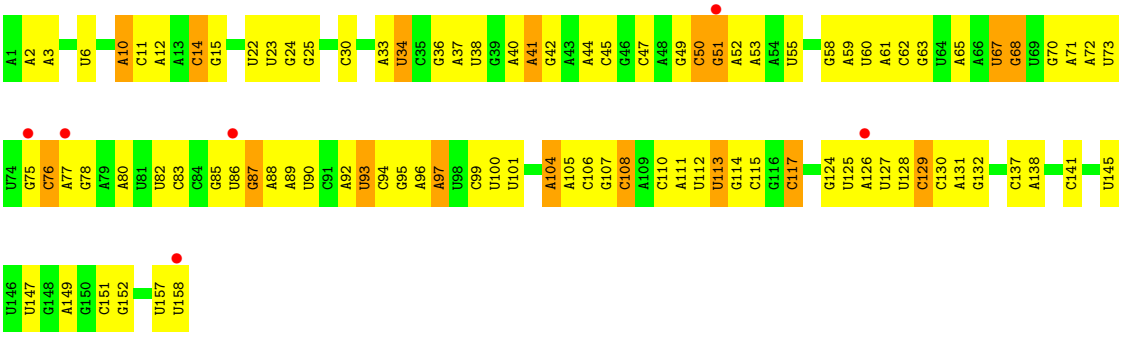
Chain D2:





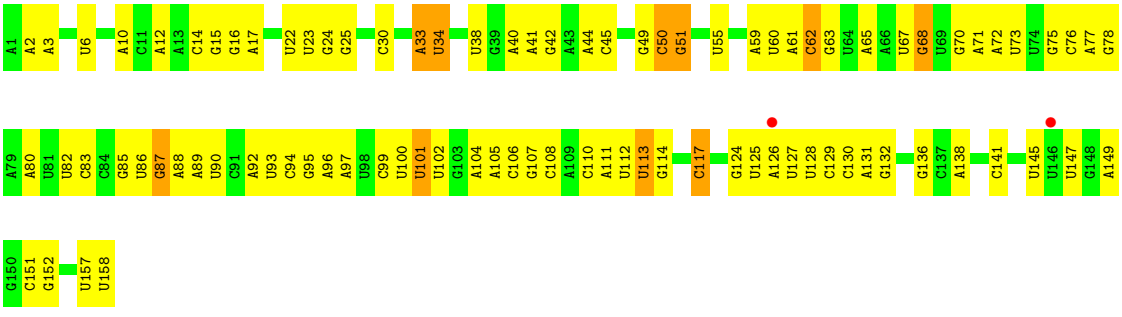
• Molecule 31: 5.8S ribosomal RNA

Chain B3:



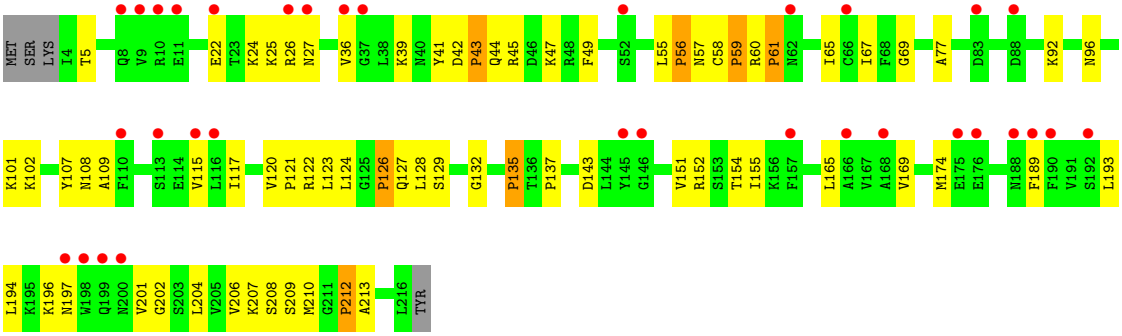
• Molecule 31: 5.8S ribosomal RNA

Chain D3:



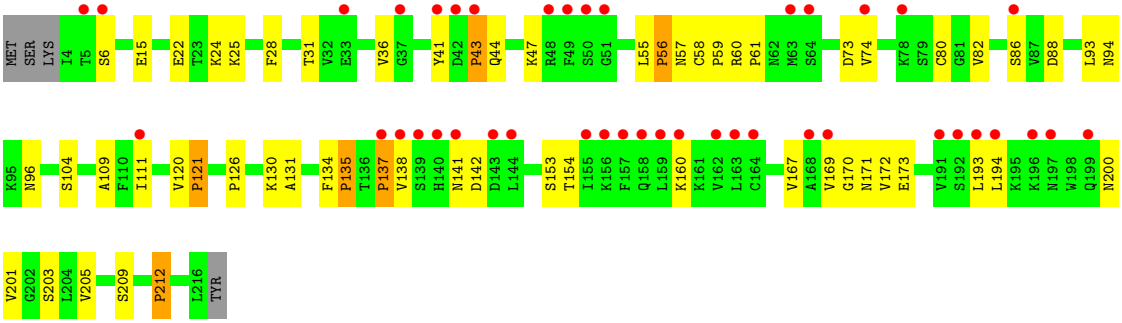
• Molecule 32: 60S ribosomal protein L1

Chain BA:



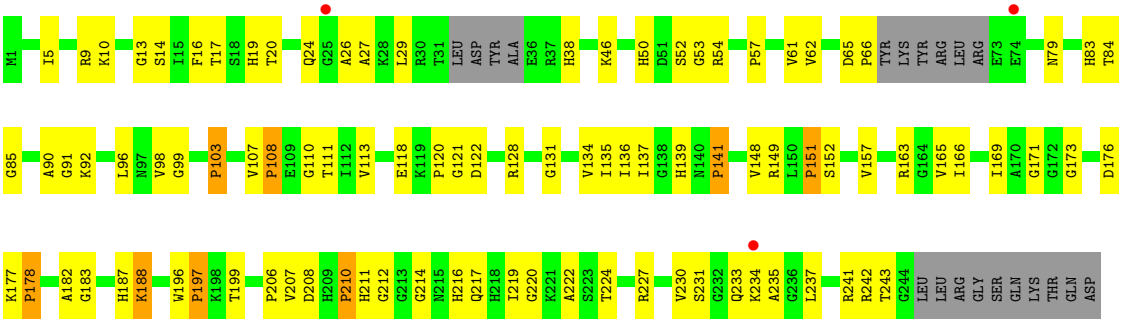
• Molecule 32: 60S ribosomal protein L1

Chain DA:



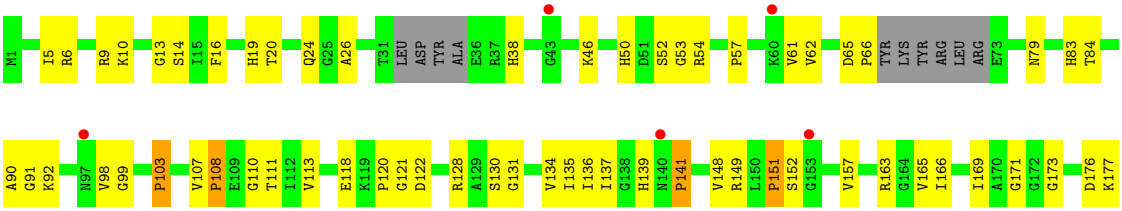
• Molecule 33: 60S ribosomal protein L2

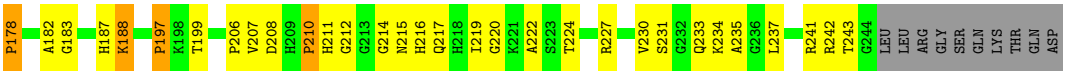
Chain BB:



• Molecule 33: 60S ribosomal protein L2

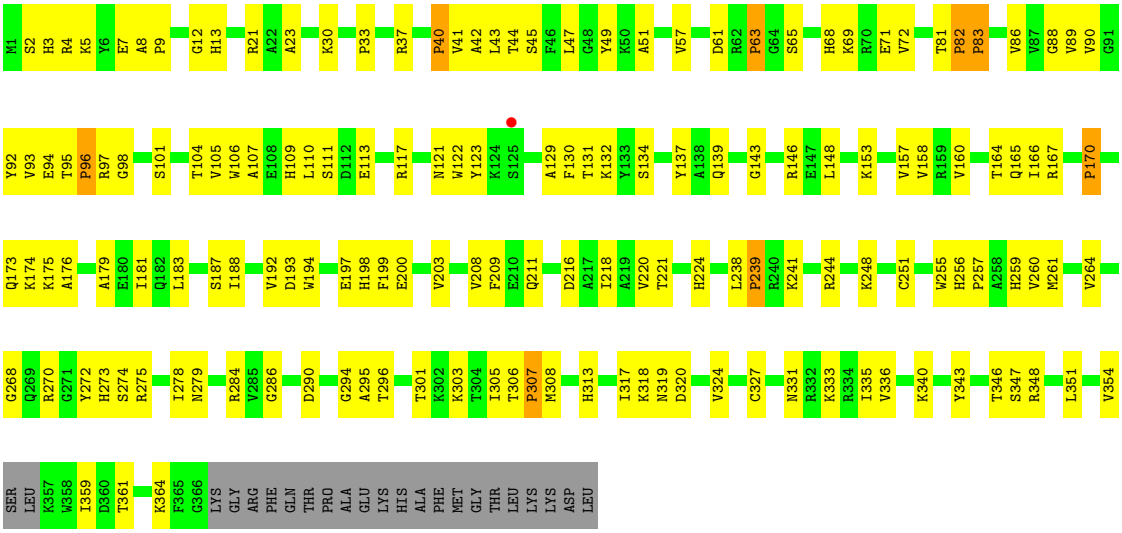
Chain DB:





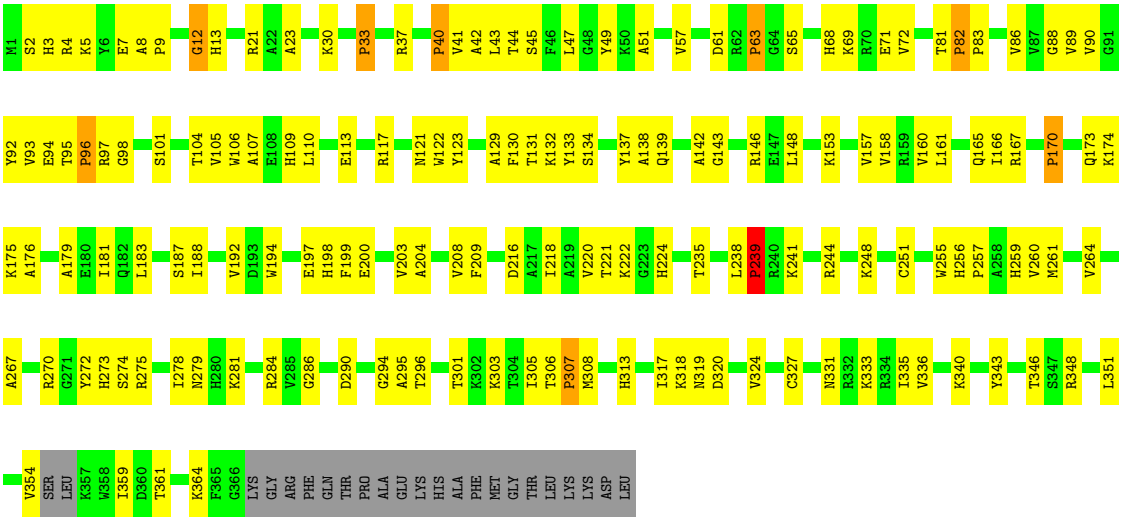
• Molecule 34: 60S ribosomal protein L3

Chain BC:



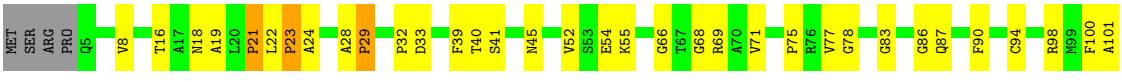
• Molecule 34: 60S ribosomal protein L3

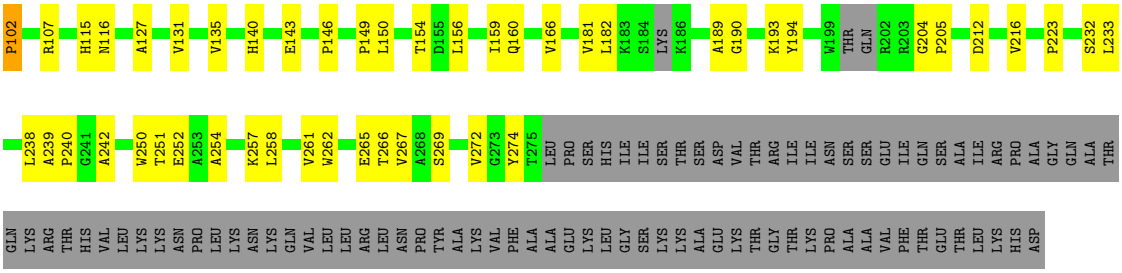
Chain DC:



• Molecule 35: 60S ribosomal protein L4-A

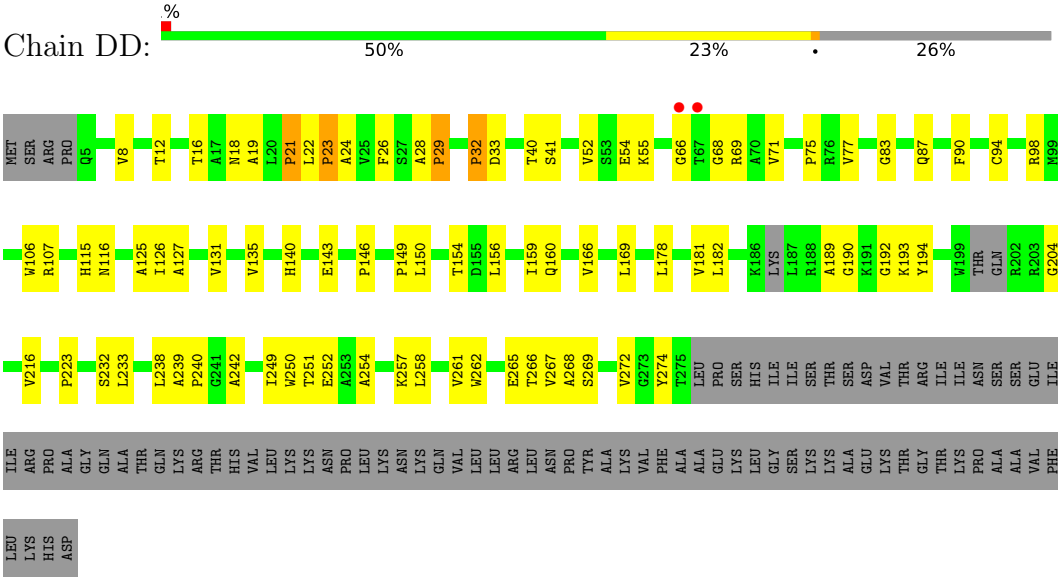
Chain BD:





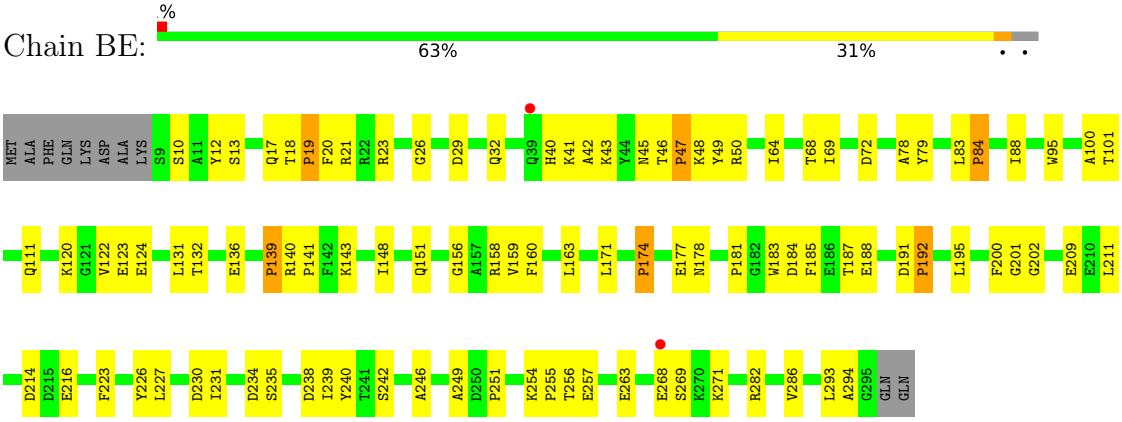
• Molecule 35: 60S ribosomal protein L4-A

Chain DD:



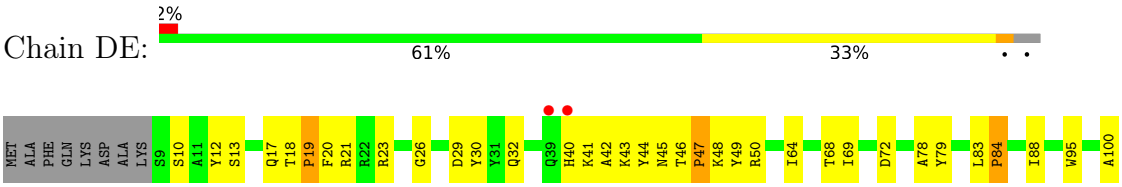
• Molecule 36: 60S ribosomal protein L5

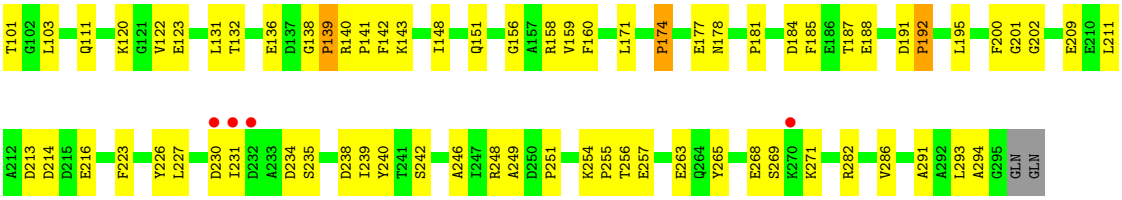
Chain BE:



• Molecule 36: 60S ribosomal protein L5

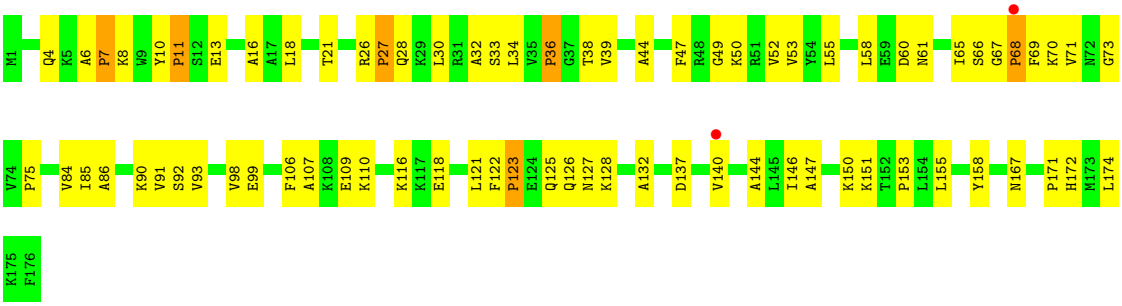
Chain DE:





• Molecule 37: 60S ribosomal protein L6-A

Chain BF:

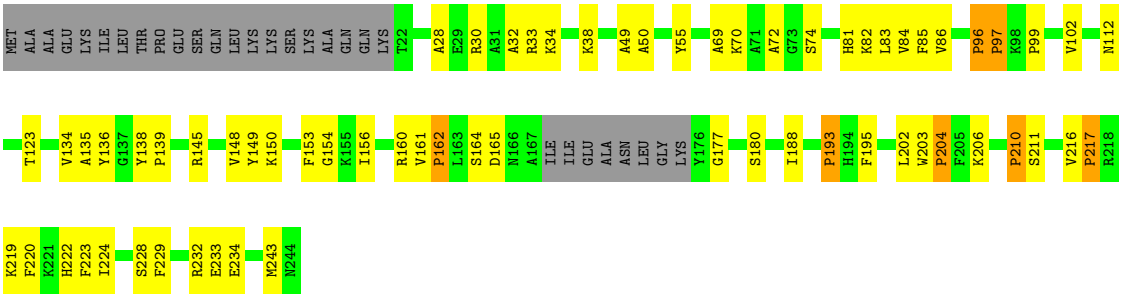


• Molecule 37: 60S ribosomal protein L6-A

Chain DF:

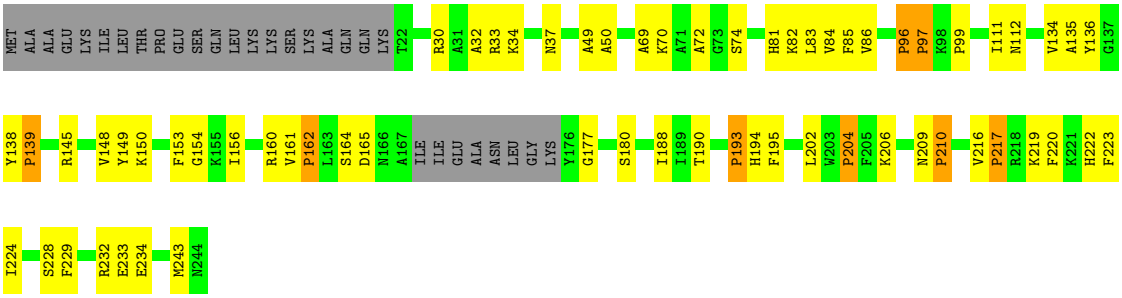
• Molecule 38: 60S ribosomal protein L7-A

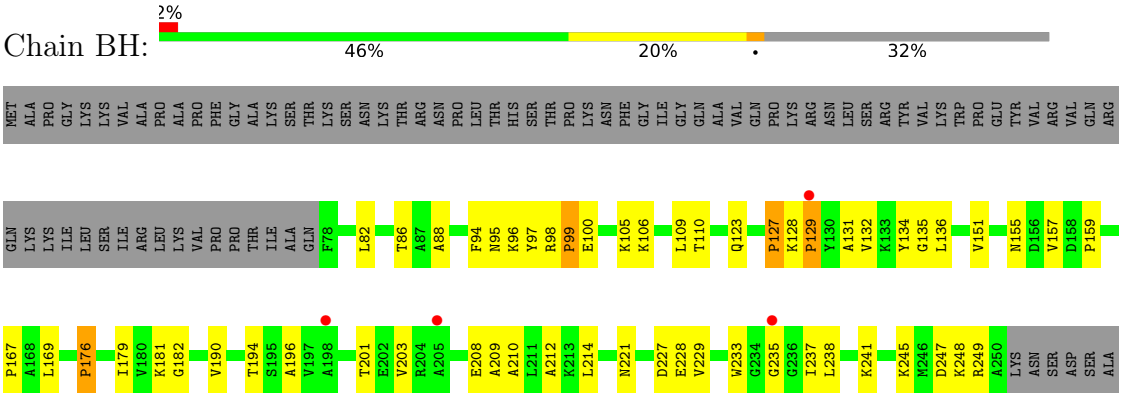
Chain BG:



• Molecule 38: 60S ribosomal protein L7-A

Chain DG:



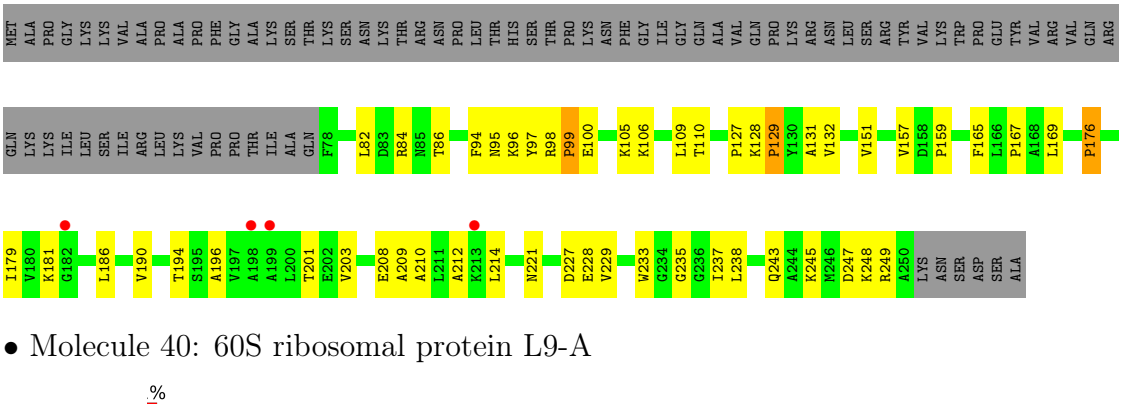


• Molecule 39: 60S ribosomal protein L8-A

Chain BH:

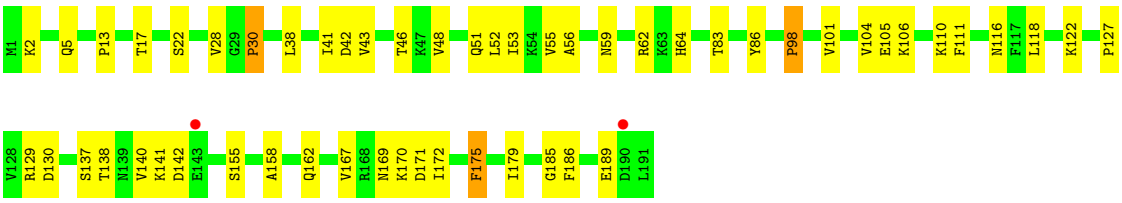
• Molecule 39: 60S ribosomal protein L8-A

Chain DH:



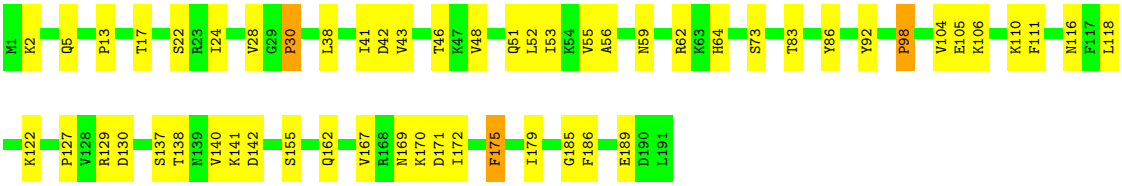
• Molecule 40: 60S ribosomal protein L9-A

Chain BI:

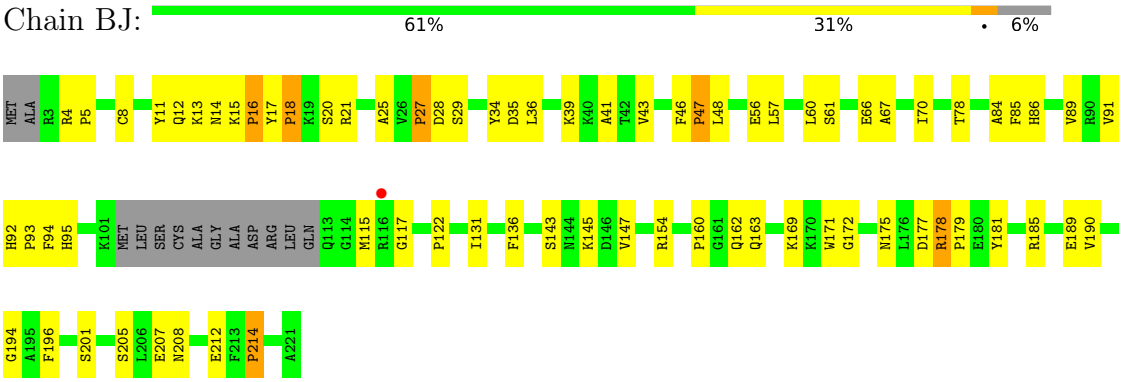


• Molecule 40: 60S ribosomal protein L9-A

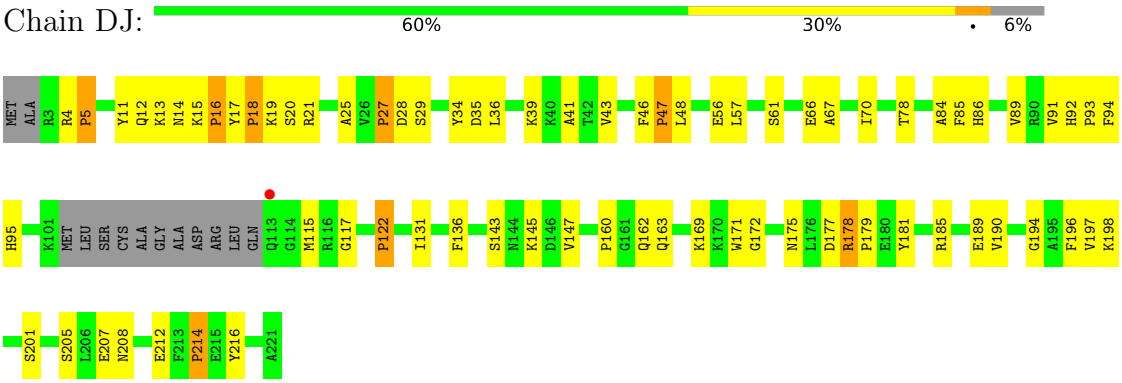
Chain DI:



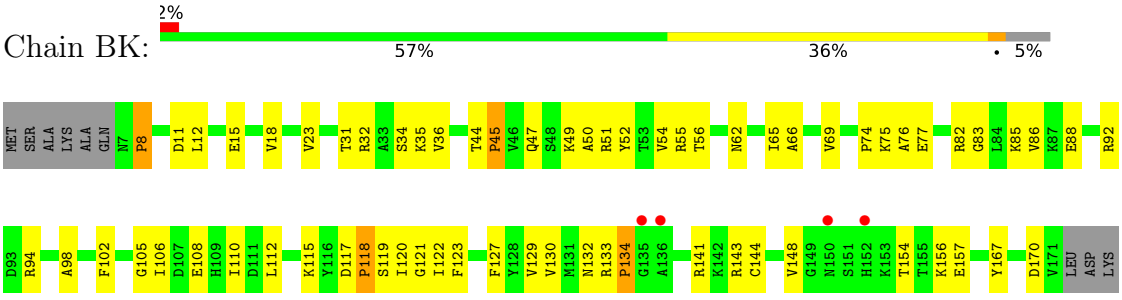
• Molecule 41: 60S ribosomal protein L10



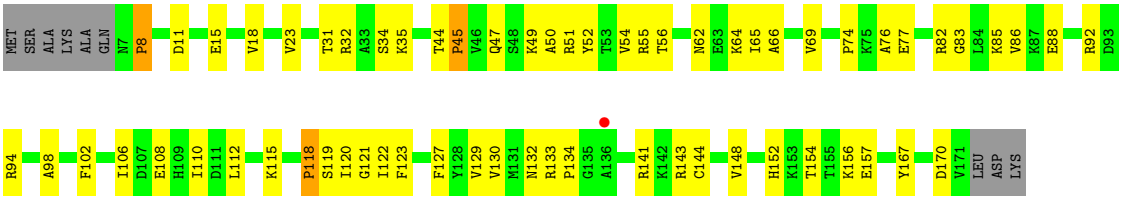
• Molecule 41: 60S ribosomal protein L10



• Molecule 42: 60S ribosomal protein L11-A

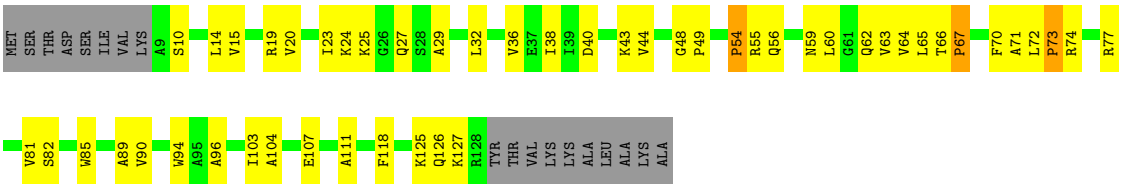


• Molecule 42: 60S ribosomal protein L11-A



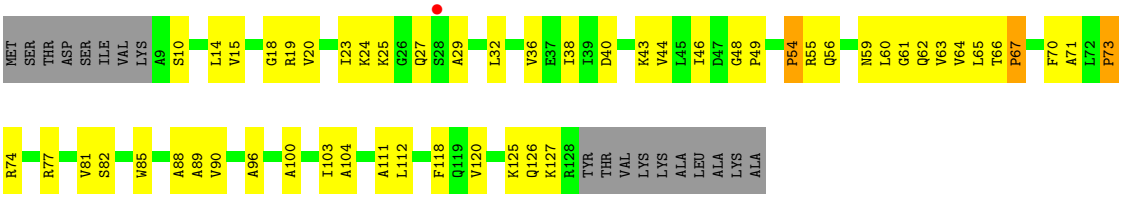
• Molecule 43: 60S ribosomal protein L14-A

Chain BN:



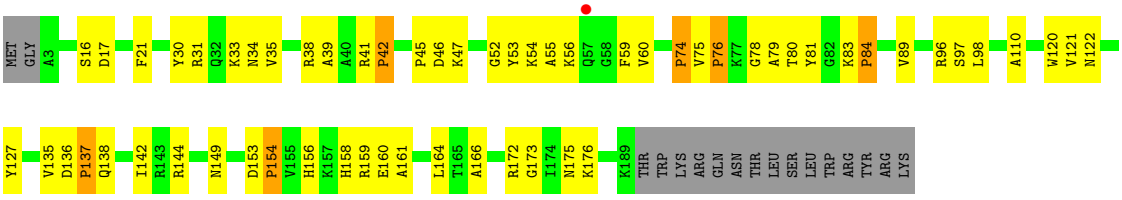
• Molecule 43: 60S ribosomal protein L14-A

Chain DN:



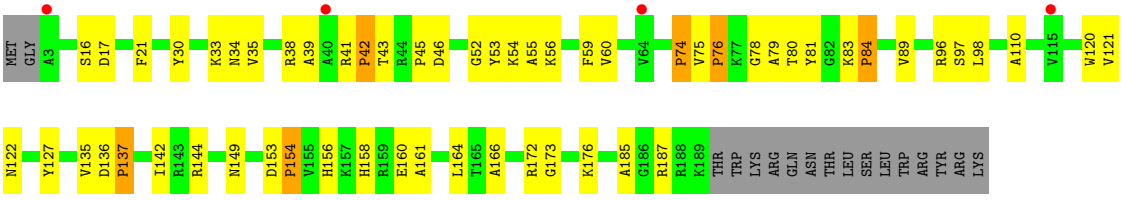
• Molecule 44: 60S ribosomal protein L15-A

Chain BO:



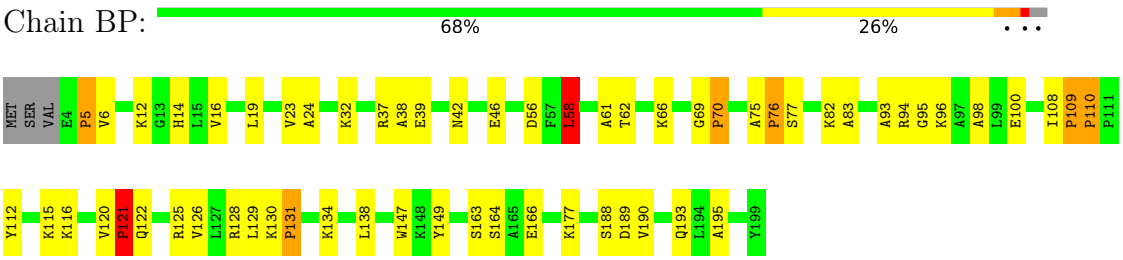
• Molecule 44: 60S ribosomal protein L15-A

Chain DO:



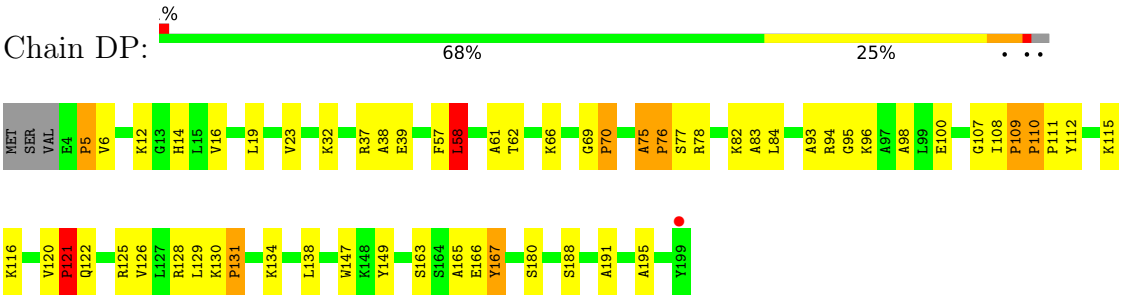
• Molecule 45: 60S ribosomal protein L16-A

Chain BP:



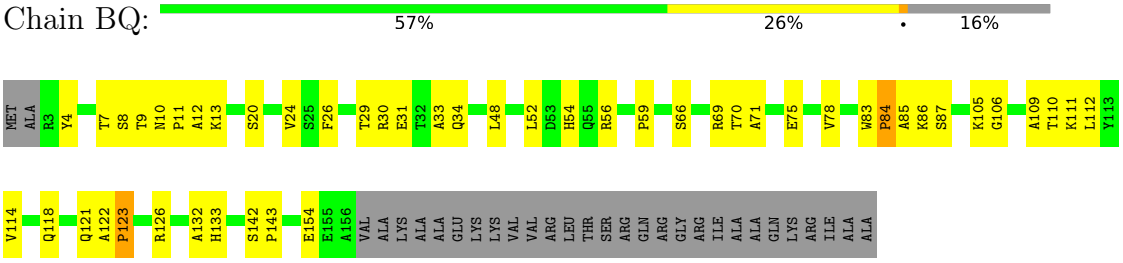
• Molecule 45: 60S ribosomal protein L16-A

Chain DP:



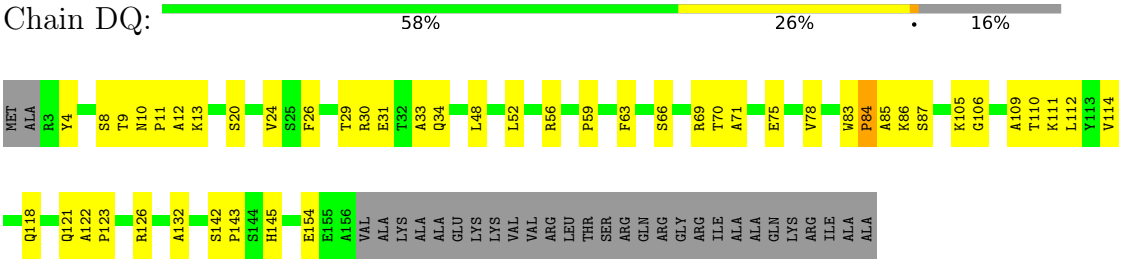
• Molecule 46: 60S ribosomal protein L17-A

Chain BQ:



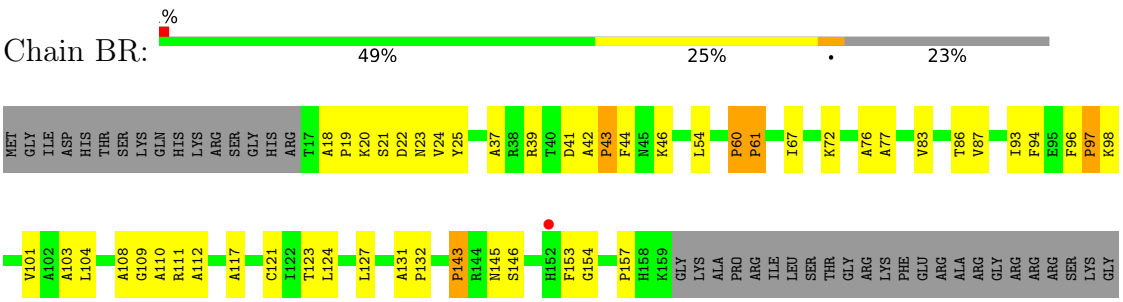
• Molecule 46: 60S ribosomal protein L17-A

Chain DQ:



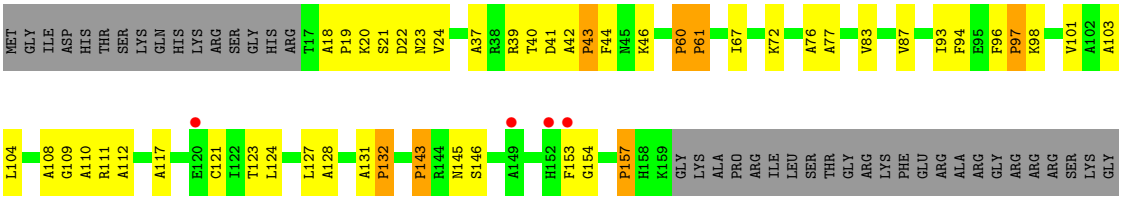
• Molecule 47: 60S ribosomal protein L18

Chain BR:



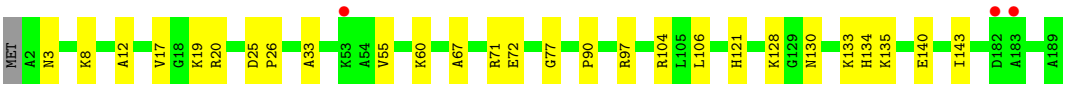
• Molecule 47: 60S ribosomal protein L18

Chain DR:



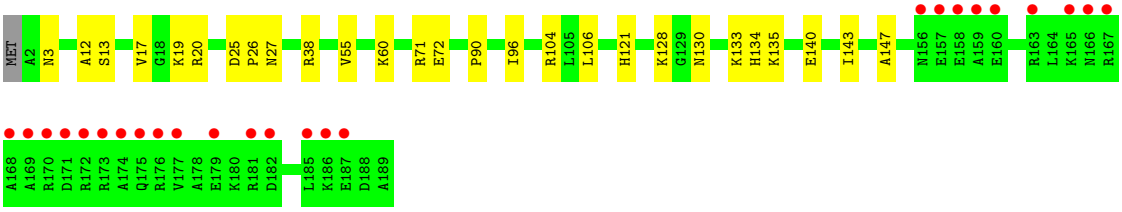
• Molecule 48: 60S ribosomal protein L19

Chain BS:



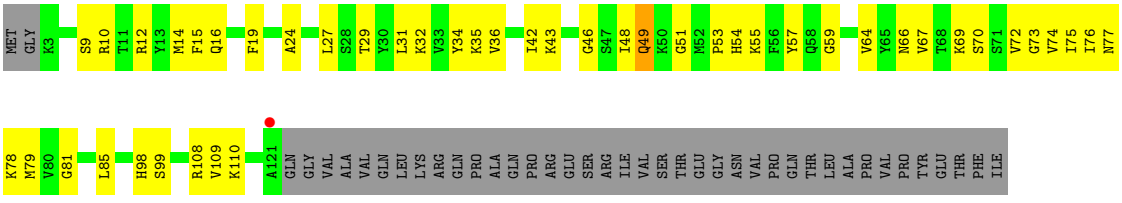
• Molecule 48: 60S ribosomal protein L19

Chain DS:



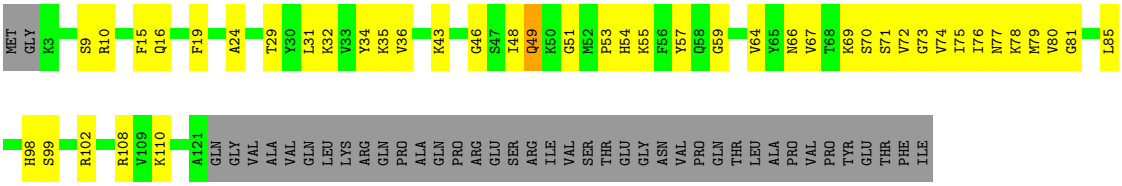
• Molecule 49: 60S ribosomal protein L21-A

Chain BT:



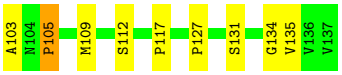
• Molecule 49: 60S ribosomal protein L21-A

Chain DT:



• Molecule 50: 60S ribosomal protein L23

Chain BU:

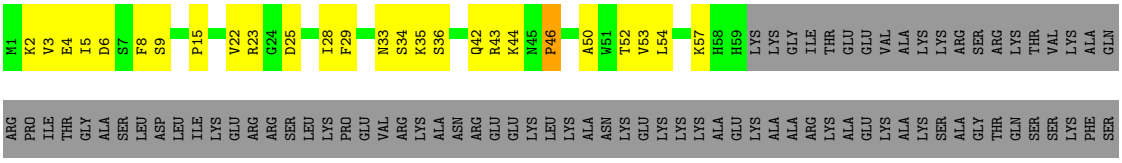


• Molecule 50: 60S ribosomal protein L23

Chain DU:

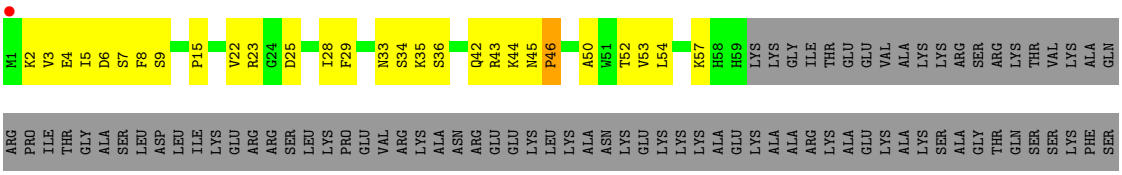
• Molecule 51: 60S ribosomal protein L24-A

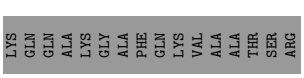
Chain BV:



• Molecule 51: 60S ribosomal protein L24-A

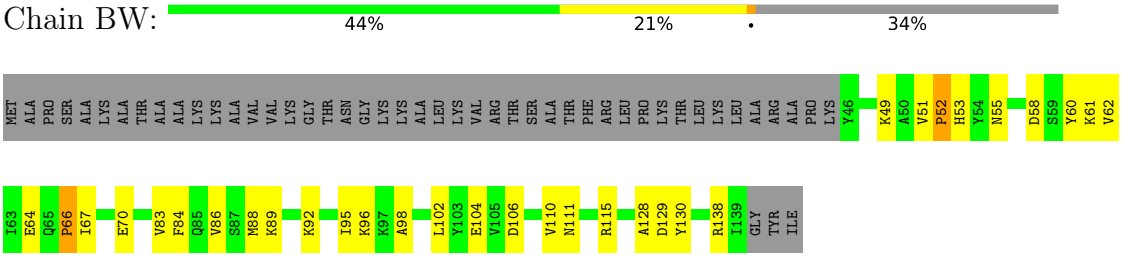
Chain DV:





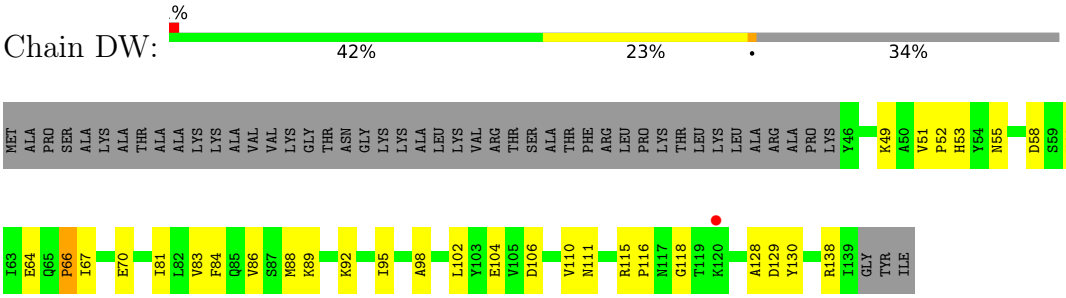
• Molecule 52: 60S ribosomal protein L25

Chain BW:



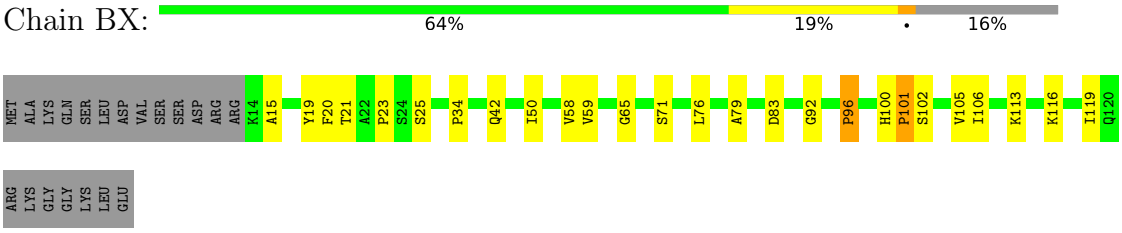
• Molecule 52: 60S ribosomal protein L25

Chain DW:



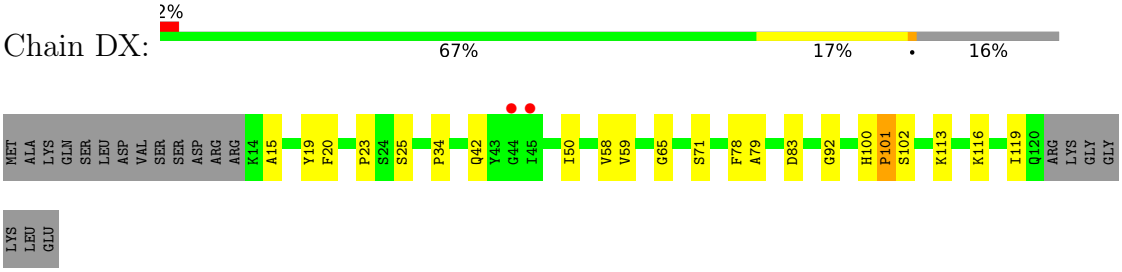
• Molecule 53: 60S ribosomal protein L26-A

Chain BX:



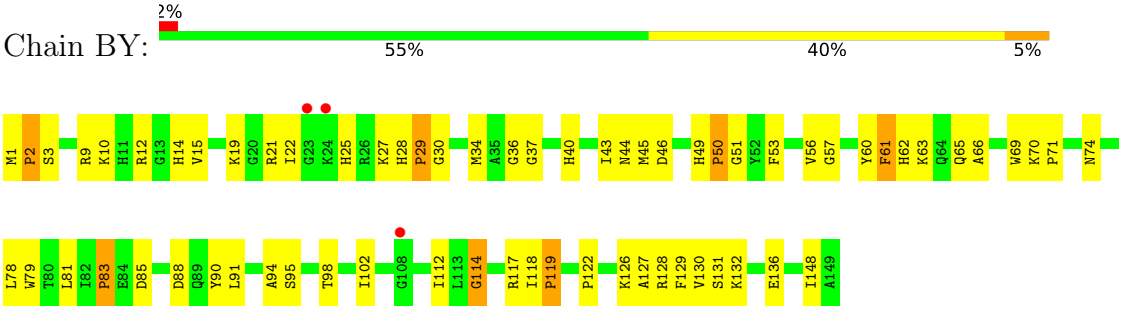
• Molecule 53: 60S ribosomal protein L26-A

Chain DX:



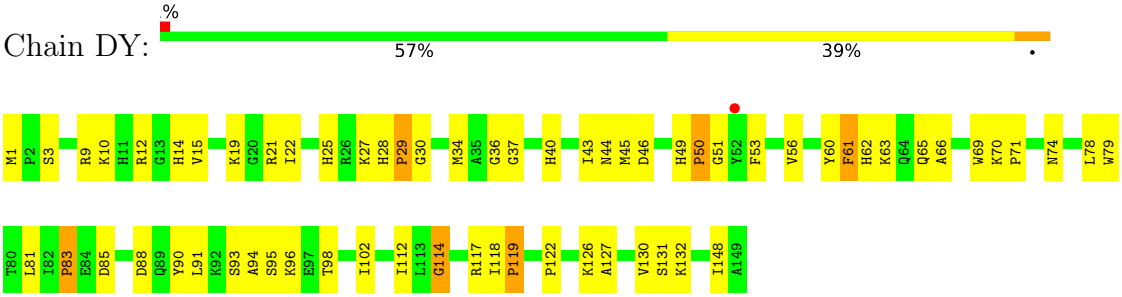
• Molecule 54: 60S ribosomal protein L28

Chain BY:



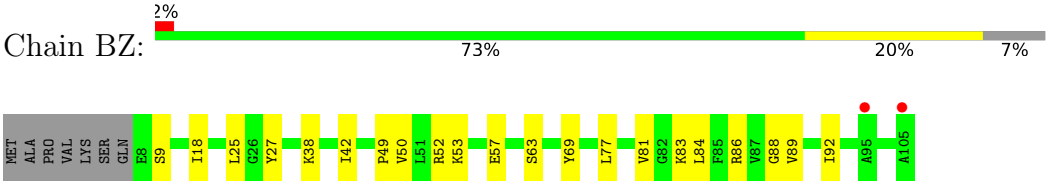
• Molecule 54: 60S ribosomal protein L28

Chain DY:



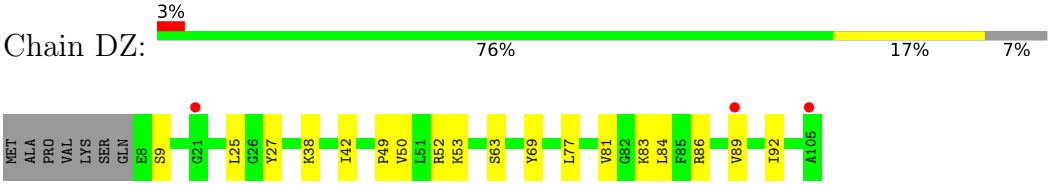
• Molecule 55: 60S ribosomal protein L30

Chain BZ:



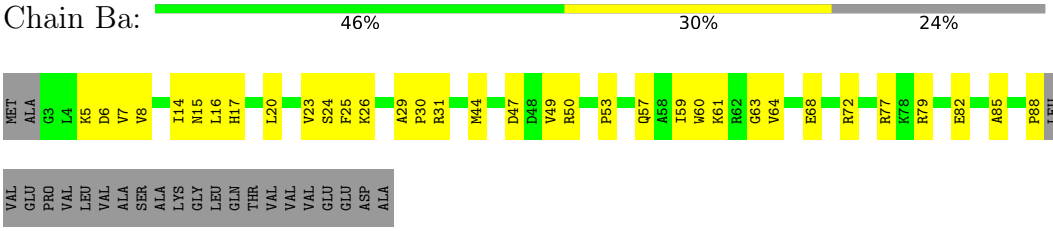
• Molecule 55: 60S ribosomal protein L30

Chain DZ:



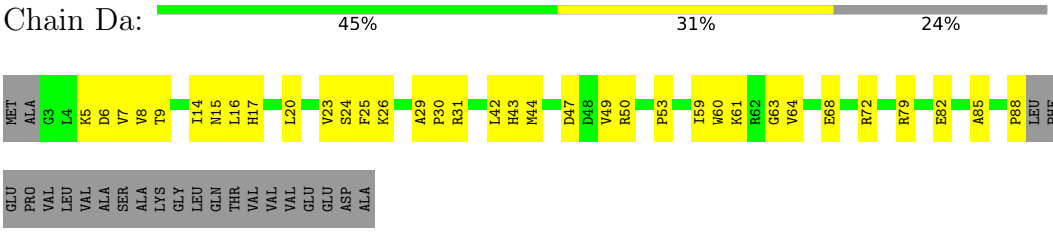
• Molecule 56: 60S ribosomal protein L31-A

Chain Ba:



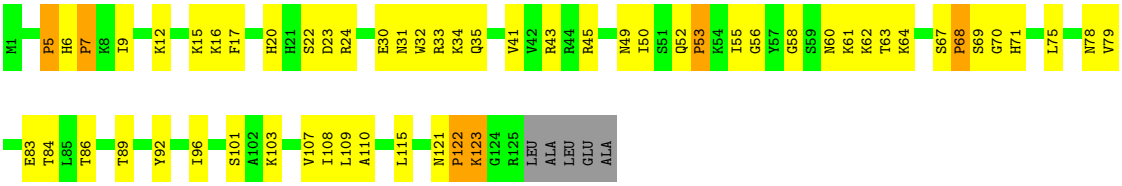
• Molecule 56: 60S ribosomal protein L31-A

Chain Da:



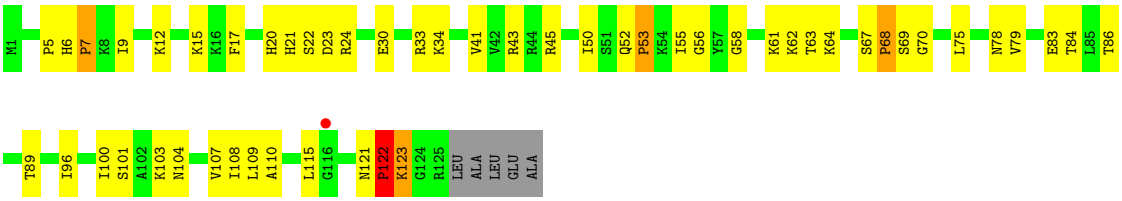
• Molecule 57: 60S ribosomal protein L32

Chain Bb:



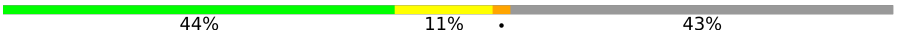
• Molecule 57: 60S ribosomal protein L32

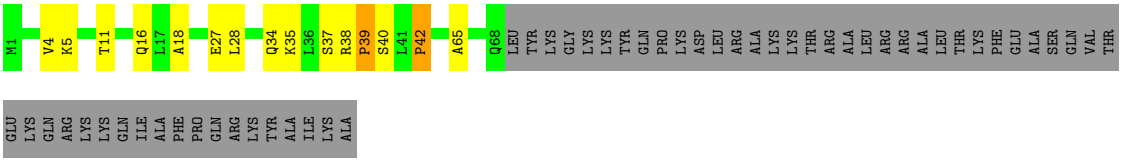
Chain Db:



• Molecule 58: 60S ribosomal protein L35

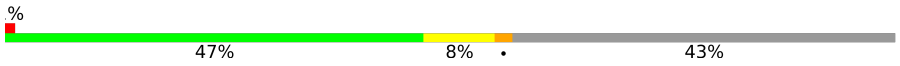
Chain Bc:

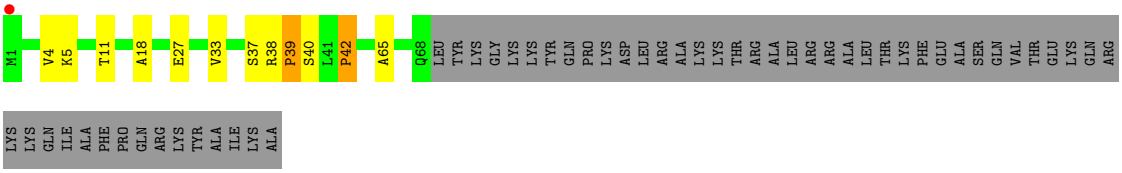




• Molecule 58: 60S ribosomal protein L35

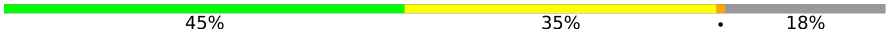
Chain Dc:

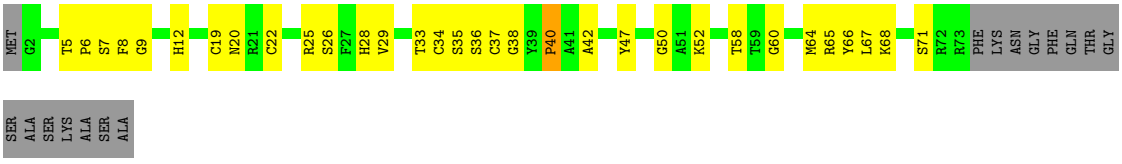




• Molecule 59: 60S ribosomal protein L37-A

Chain Bd:

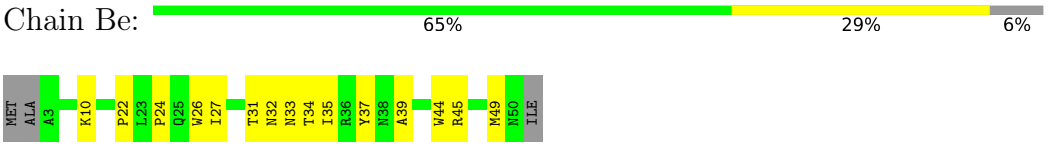




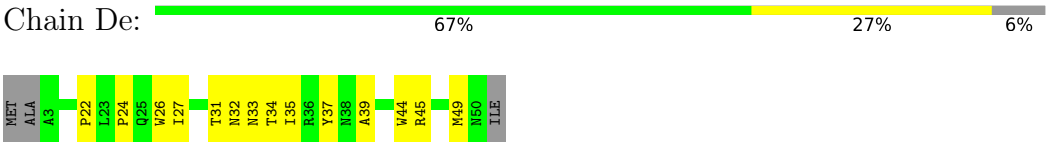
• Molecule 59: 60S ribosomal protein L37-A

Chain Dd:

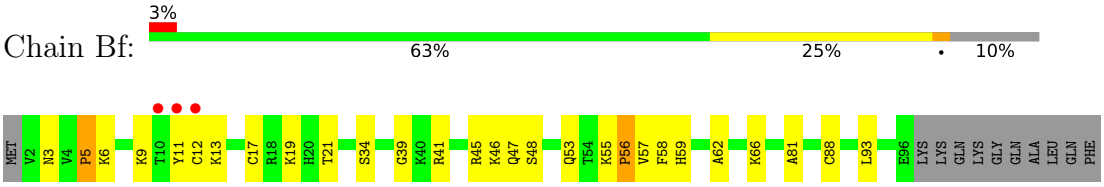
• Molecule 60: 60S ribosomal protein L39



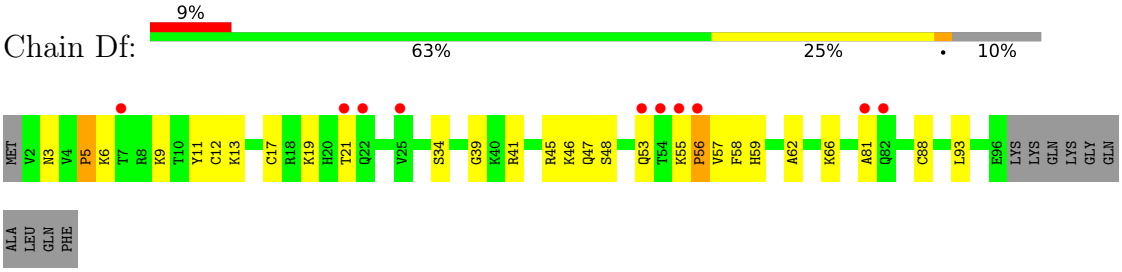
• Molecule 60: 60S ribosomal protein L39



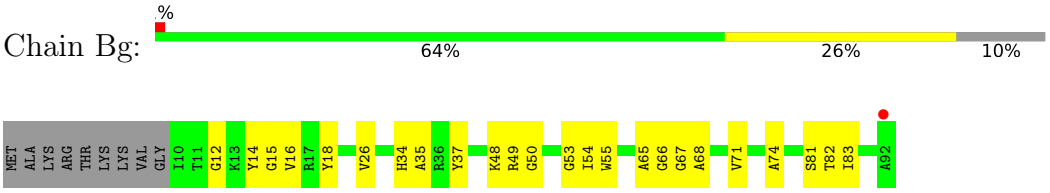
• Molecule 61: 60S ribosomal protein L42



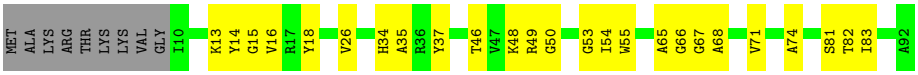
• Molecule 61: 60S ribosomal protein L42



• Molecule 62: 60S ribosomal protein L43



• Molecule 62: 60S ribosomal protein L43



• Molecule 63: Unassigned secondary structure

Chain Bh: 100%

There are no outlier residues recorded for this chain.

• Molecule 63: Unassigned secondary structure

Chain Dh: 100%

There are no outlier residues recorded for this chain.

• Molecule 64: Unassigned secondary structure

Chain Bi: 100%

There are no outlier residues recorded for this chain.

• Molecule 64: Unassigned secondary structure

Chain Di: 100%

There are no outlier residues recorded for this chain.

• Molecule 65: Unassigned secondary structure

Chain Bk: 100%

There are no outlier residues recorded for this chain.

• Molecule 65: Unassigned secondary structure

Chain Dk: 100%

There are no outlier residues recorded for this chain.

• Molecule 66: Unassigned secondary structure

Chain Bl: 100%

There are no outlier residues recorded for this chain.

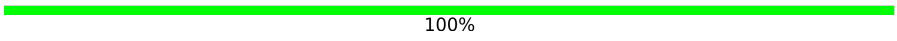
• Molecule 67: Unassigned secondary structure

Chain Bm: 100%

There are no outlier residues recorded for this chain.

• Molecule 68: Unassigned secondary structure

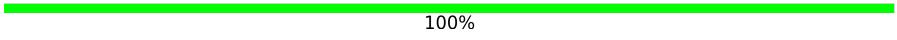
Chain Bn:



There are no outlier residues recorded for this chain.

• Molecule 69: Unassigned secondary structure

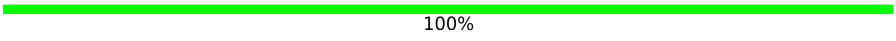
Chain Bp:



There are no outlier residues recorded for this chain.

• Molecule 70: Unassigned secondary structure

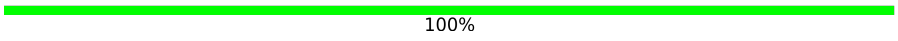
Chain Bq:



There are no outlier residues recorded for this chain.

• Molecule 71: Unassigned secondary structure

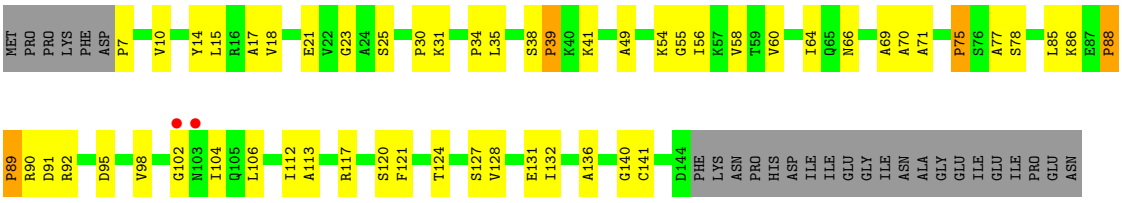
Chain Br:



There are no outlier residues recorded for this chain.

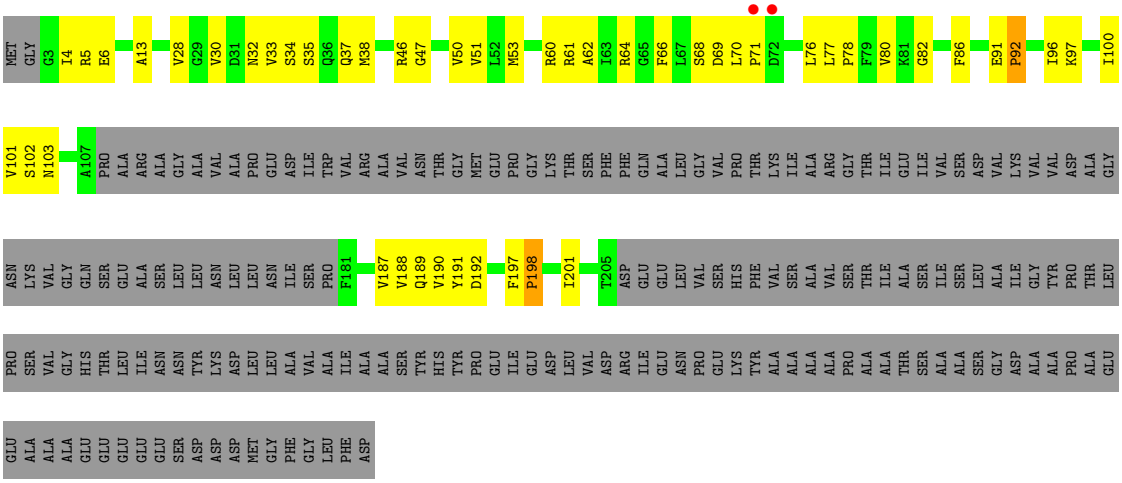
• Molecule 72: 60S ribosomal protein L12

Chain DL:



• Molecule 73: 60S acidic ribosomal protein P0

Chain DM:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	437.11Å 288.38Å 306.56Å 90.00° 99.13° 90.00°	Depositor
Resolution (Å)	268.00 – 4.00 268.66 – 4.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (268.00-4.00) 97.9 (268.66-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 4.02Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.278 , 0.341 0.283 , 0.343	Depositor DCC
R_{free} test set	12353 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	147.1	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.16 , 252.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	309610	wwPDB-VP
Average B, all atoms (Å^2)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OHX

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	A1	0.77	20/42619 (0.0%)	1.32	552/66408 (0.8%)
1	C1	0.83	25/42619 (0.1%)	1.37	627/66408 (0.9%)
2	AA	0.45	0/1089	0.86	16/1517 (1.1%)
2	CA	0.50	0/1089	0.87	15/1517 (1.0%)
3	AB	0.54	0/1073	0.91	13/1488 (0.9%)
3	CB	0.56	0/1073	0.91	10/1488 (0.7%)
4	AC	0.50	0/927	0.68	4/1286 (0.3%)
4	CC	0.47	0/927	0.67	4/1286 (0.3%)
5	AD	0.45	0/834	0.71	5/1159 (0.4%)
5	CD	0.50	0/834	0.79	5/1159 (0.4%)
6	AE	0.49	0/775	0.70	3/1077 (0.3%)
6	CE	0.53	0/775	0.73	3/1077 (0.3%)
7	AF	0.60	0/381	0.88	3/530 (0.6%)
7	CF	0.59	0/381	0.90	4/530 (0.8%)
8	AG	0.51	0/579	0.78	5/806 (0.6%)
8	CG	0.52	0/579	0.79	5/806 (0.6%)
9	AH	0.43	0/626	0.71	4/867 (0.5%)
9	CH	0.44	0/626	0.72	4/867 (0.5%)
10	AI	0.45	0/595	0.90	8/826 (1.0%)
10	CI	0.52	0/595	0.91	7/826 (0.8%)
11	AJ	0.49	0/657	0.78	5/911 (0.5%)
11	CJ	0.55	0/657	0.81	5/911 (0.5%)
12	AK	0.44	0/331	0.74	2/460 (0.4%)
12	CK	0.41	0/331	0.70	2/460 (0.4%)
13	AL	0.47	0/589	0.70	2/816 (0.2%)
13	CL	0.50	0/589	0.72	2/816 (0.2%)
14	AM	0.54	0/518	0.83	3/715 (0.4%)
14	CM	0.68	1/518 (0.2%)	0.89	3/715 (0.4%)
15	AN	0.51	0/550	0.84	5/766 (0.7%)
15	CN	0.52	0/550	0.86	5/766 (0.7%)
16	AO	0.53	0/621	0.83	3/860 (0.3%)
16	CO	0.56	0/621	0.85	3/860 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AP	0.61	0/565	0.92	4/781 (0.5%)
17	CP	0.68	0/565	0.97	5/781 (0.6%)
18	AQ	0.41	0/331	0.68	2/460 (0.4%)
18	CQ	0.44	0/311	0.74	2/432 (0.5%)
19	AR	0.40	0/229	0.63	1/316 (0.3%)
19	CR	0.42	0/229	0.68	1/316 (0.3%)
20	AS	0.54	0/189	0.70	0/260
20	CS	0.58	0/189	0.73	0/260
21	AT	0.43	0/1541	0.61	8/2141 (0.4%)
21	CT	0.45	0/1541	0.61	8/2141 (0.4%)
29	B1	1.11	229/76764 (0.3%)	1.79	2866/119684 (2.4%)
29	D1	1.08	218/76764 (0.3%)	1.75	2607/119684 (2.2%)
30	B2	1.06	8/2883 (0.3%)	1.70	90/4491 (2.0%)
30	D2	1.17	10/2883 (0.3%)	1.84	112/4491 (2.5%)
31	B3	0.91	6/3746 (0.2%)	1.41	64/5832 (1.1%)
31	D3	0.79	1/3746 (0.0%)	1.28	40/5832 (0.7%)
32	BA	0.34	0/1054	0.63	9/1468 (0.6%)
32	DA	0.33	0/1054	0.61	9/1468 (0.6%)
33	BB	0.62	0/1103	0.92	11/1501 (0.7%)
33	DB	0.53	0/1103	0.87	11/1501 (0.7%)
34	BC	0.70	0/1790	1.05	9/2487 (0.4%)
34	DC	0.76	0/1790	1.08	12/2487 (0.5%)
35	BD	0.67	0/1311	0.95	9/1817 (0.5%)
35	DD	0.55	0/1311	0.90	12/1817 (0.7%)
36	BE	0.53	0/1411	0.93	9/1960 (0.5%)
36	DE	0.59	0/1411	0.97	9/1960 (0.5%)
37	BF	0.76	0/872	1.20	10/1215 (0.8%)
37	DF	0.85	0/872	1.21	12/1215 (1.0%)
38	BG	0.73	0/1059	1.06	8/1471 (0.5%)
38	DG	0.75	0/1059	1.05	9/1471 (0.6%)
39	BH	0.48	0/855	0.79	6/1190 (0.5%)
39	DH	0.45	0/855	0.76	6/1190 (0.5%)
40	BI	0.64	0/941	0.86	4/1308 (0.3%)
40	DI	0.73	0/941	0.92	5/1308 (0.4%)
41	BJ	0.66	0/1025	0.89	8/1424 (0.6%)
41	DJ	0.71	0/1025	0.91	9/1424 (0.6%)
42	BK	0.56	0/809	0.86	5/1122 (0.4%)
42	DK	0.61	0/809	0.87	4/1122 (0.4%)
43	BN	0.71	0/592	1.05	6/823 (0.7%)
43	DN	0.82	0/592	1.14	6/823 (0.7%)
44	BO	0.59	0/922	0.88	7/1282 (0.5%)
44	DO	0.51	0/922	0.86	7/1282 (0.5%)
45	BP	0.80	0/966	1.12	10/1343 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
45	DP	0.84	1/966 (0.1%)	1.14	12/1343 (0.9%)
46	BQ	0.72	0/760	0.94	5/1057 (0.5%)
46	DQ	0.65	0/760	0.87	4/1057 (0.4%)
47	BR	0.70	0/705	1.00	6/980 (0.6%)
47	DR	0.60	0/705	0.94	7/980 (0.7%)
48	BS	0.52	0/930	0.63	2/1295 (0.2%)
48	DS	0.48	0/930	0.58	2/1295 (0.2%)
49	BT	0.68	0/585	0.85	0/812
49	DT	0.70	0/585	0.87	0/812
50	BU	0.63	0/630	0.86	5/872 (0.6%)
50	DU	0.75	0/630	0.93	5/872 (0.6%)
51	BV	0.54	0/290	0.84	2/402 (0.5%)
51	DV	0.58	0/290	0.85	2/402 (0.5%)
52	BW	0.55	0/467	0.84	2/651 (0.3%)
52	DW	0.49	0/467	0.81	3/651 (0.5%)
53	BX	0.55	0/529	0.78	4/736 (0.5%)
53	DX	0.49	0/529	0.74	3/736 (0.4%)
54	BY	0.70	0/726	1.10	9/1004 (0.9%)
54	DY	0.62	0/726	1.03	8/1004 (0.8%)
55	BZ	0.49	0/480	0.62	1/665 (0.2%)
55	DZ	0.46	0/480	0.62	1/665 (0.2%)
56	Ba	0.62	0/424	0.94	3/589 (0.5%)
56	Da	0.59	0/424	0.92	3/589 (0.5%)
57	Bb	0.72	0/617	1.13	6/858 (0.7%)
57	Db	0.61	0/617	1.07	6/858 (0.7%)
58	Bc	0.53	0/338	0.82	2/471 (0.4%)
58	Dc	0.45	0/338	0.74	2/471 (0.4%)
59	Bd	0.63	0/351	0.97	2/485 (0.4%)
59	Dd	0.54	0/351	0.89	2/485 (0.4%)
60	Be	0.59	0/239	0.85	2/333 (0.6%)
60	De	0.46	0/239	0.79	2/333 (0.6%)
61	Bf	0.47	0/466	0.68	2/646 (0.3%)
61	Df	0.39	0/466	0.66	2/646 (0.3%)
62	Bg	0.53	0/406	0.74	1/562 (0.2%)
62	Dg	0.49	0/406	0.67	0/562
72	DL	0.42	0/678	0.75	7/941 (0.7%)
73	DM	0.48	0/639	0.76	4/886 (0.5%)
All	All	0.92	519/326627 (0.2%)	1.50	7498/496371 (1.5%)

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
3	AB	0	2
3	CB	0	2
17	AP	0	1
17	CP	0	1
18	AQ	0	1
18	CQ	0	1
22	Bo	0	1
23	Ab	0	1
23	Cb	0	1
24	Ac	0	1
29	B1	0	3
29	D1	0	3
34	BC	0	5
34	DC	0	6
35	BD	0	1
35	DD	0	2
36	BE	0	1
36	DE	0	1
37	BF	0	4
37	DF	0	4
38	BG	0	1
38	DG	0	1
42	BK	0	1
42	DK	0	1
44	DO	0	1
45	BP	0	4
45	DP	0	5
49	BT	0	1
49	DT	0	1
51	BV	0	1
51	DV	0	1
54	BY	0	2
54	DY	0	2
56	Ba	0	1
56	Da	0	1
57	Bb	0	1
57	Db	0	1
All	All	0	68

The worst 5 of 519 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D1	3243	A	N9-C4	13.96	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D1	308	A	C6-N1	-13.36	1.26	1.35
29	B1	3184	A	C6-N1	-12.55	1.26	1.35
29	B1	308	A	C6-N1	-11.80	1.27	1.35
29	D1	2845	A	C6-N1	-11.64	1.27	1.35

The worst 5 of 7498 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	D1	244	G	N1-C6-O6	43.40	145.94	119.90
29	B1	244	G	N1-C6-O6	41.87	145.02	119.90
29	D1	2845	A	N1-C6-N6	40.75	143.05	118.60
29	D1	2845	A	C6-N1-C2	39.78	142.47	118.60
29	B1	2845	A	N1-C6-N6	39.33	142.20	118.60

There are no chirality outliers.

5 of 68 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AB	224	PHE	Peptide
3	AB	225	LEU	Peptide
17	AP	28	ASN	Peptide
18	AQ	41	ILE	Peptide
23	Ab	14	UNK	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AA	218/252 (86%)	75 (34%)	68 (31%)	75 (34%)	0	0
2	CA	218/252 (86%)	78 (36%)	63 (29%)	77 (35%)	0	0
3	AB	217/254 (85%)	85 (39%)	54 (25%)	78 (36%)	0	0
3	CB	217/254 (85%)	81 (37%)	62 (29%)	74 (34%)	0	0
4	AC	187/240 (78%)	72 (38%)	56 (30%)	59 (32%)	0	0
4	CC	187/240 (78%)	69 (37%)	55 (29%)	63 (34%)	0	0
5	AD	165/225 (73%)	55 (33%)	46 (28%)	64 (39%)	0	0
5	CD	165/225 (73%)	58 (35%)	44 (27%)	63 (38%)	0	0
6	AE	153/197 (78%)	48 (31%)	54 (35%)	51 (33%)	0	0
6	CE	153/197 (78%)	48 (31%)	49 (32%)	56 (37%)	0	0
7	AF	75/156 (48%)	32 (43%)	18 (24%)	25 (33%)	0	0
7	CF	75/156 (48%)	31 (41%)	20 (27%)	24 (32%)	0	0
8	AG	115/151 (76%)	46 (40%)	38 (33%)	31 (27%)	0	0
8	CG	115/151 (76%)	49 (43%)	33 (29%)	33 (29%)	0	0
9	AH	126/137 (92%)	52 (41%)	38 (30%)	36 (29%)	0	0
9	CH	126/137 (92%)	51 (40%)	39 (31%)	36 (29%)	0	0
10	AI	119/142 (84%)	38 (32%)	40 (34%)	41 (34%)	0	0
10	CI	119/142 (84%)	43 (36%)	35 (29%)	41 (34%)	0	0
11	AJ	132/143 (92%)	57 (43%)	33 (25%)	42 (32%)	0	0
11	CJ	132/143 (92%)	52 (39%)	37 (28%)	43 (33%)	0	0
12	AK	65/136 (48%)	27 (42%)	16 (25%)	22 (34%)	0	0
12	CK	65/136 (48%)	28 (43%)	16 (25%)	21 (32%)	0	0
13	AL	116/146 (80%)	48 (41%)	34 (29%)	34 (29%)	0	0
13	CL	116/146 (80%)	48 (41%)	33 (28%)	35 (30%)	0	0
14	AM	100/144 (69%)	38 (38%)	28 (28%)	34 (34%)	0	0
14	CM	100/144 (69%)	36 (36%)	27 (27%)	37 (37%)	0	0
15	AN	109/121 (90%)	49 (45%)	30 (28%)	30 (28%)	0	0
15	CN	109/121 (90%)	49 (45%)	29 (27%)	31 (28%)	0	0
16	AO	125/130 (96%)	48 (38%)	40 (32%)	37 (30%)	0	0
16	CO	125/130 (96%)	49 (39%)	36 (29%)	40 (32%)	0	0
17	AP	114/145 (79%)	48 (42%)	24 (21%)	42 (37%)	0	0
17	CP	114/145 (79%)	45 (40%)	28 (25%)	41 (36%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AQ	65/108 (60%)	28 (43%)	21 (32%)	16 (25%)	0	1
18	CQ	61/108 (56%)	28 (46%)	18 (30%)	15 (25%)	0	1
19	AR	45/67 (67%)	17 (38%)	12 (27%)	16 (36%)	0	0
19	CR	45/67 (67%)	17 (38%)	11 (24%)	17 (38%)	0	0
20	AS	37/56 (66%)	8 (22%)	14 (38%)	15 (40%)	0	0
20	CS	37/56 (66%)	8 (22%)	13 (35%)	16 (43%)	0	0
21	AT	309/319 (97%)	180 (58%)	71 (23%)	58 (19%)	0	2
21	CT	309/319 (97%)	184 (60%)	66 (21%)	59 (19%)	0	2
32	BA	211/217 (97%)	76 (36%)	67 (32%)	68 (32%)	0	0
32	DA	211/217 (97%)	76 (36%)	79 (37%)	56 (26%)	0	0
33	BB	228/254 (90%)	80 (35%)	55 (24%)	93 (41%)	0	0
33	DB	228/254 (90%)	83 (36%)	55 (24%)	90 (40%)	0	0
34	BC	362/387 (94%)	112 (31%)	100 (28%)	150 (41%)	0	0
34	DC	362/387 (94%)	109 (30%)	102 (28%)	151 (42%)	0	0
35	BD	266/362 (74%)	111 (42%)	79 (30%)	76 (29%)	0	0
35	DD	266/362 (74%)	109 (41%)	78 (29%)	79 (30%)	0	0
36	BE	285/297 (96%)	108 (38%)	82 (29%)	95 (33%)	0	0
36	DE	285/297 (96%)	105 (37%)	79 (28%)	101 (35%)	0	0
37	BF	174/176 (99%)	44 (25%)	62 (36%)	68 (39%)	0	0
37	DF	174/176 (99%)	43 (25%)	61 (35%)	70 (40%)	0	0
38	BG	211/244 (86%)	85 (40%)	62 (29%)	64 (30%)	0	0
38	DG	211/244 (86%)	89 (42%)	60 (28%)	62 (29%)	0	0
39	BH	171/256 (67%)	59 (34%)	58 (34%)	54 (32%)	0	0
39	DH	171/256 (67%)	60 (35%)	62 (36%)	49 (29%)	0	0
40	BI	189/191 (99%)	76 (40%)	60 (32%)	53 (28%)	0	0
40	DI	189/191 (99%)	79 (42%)	57 (30%)	53 (28%)	0	0
41	BJ	204/221 (92%)	80 (39%)	52 (26%)	72 (35%)	0	0
41	DJ	204/221 (92%)	75 (37%)	55 (27%)	74 (36%)	0	0
42	BK	163/174 (94%)	57 (35%)	42 (26%)	64 (39%)	0	0
42	DK	163/174 (94%)	56 (34%)	46 (28%)	61 (37%)	0	0
43	BN	118/138 (86%)	27 (23%)	44 (37%)	47 (40%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	DN	118/138 (86%)	28 (24%)	39 (33%)	51 (43%)	0	0
44	BO	185/204 (91%)	77 (42%)	49 (26%)	59 (32%)	0	0
44	DO	185/204 (91%)	76 (41%)	53 (29%)	56 (30%)	0	0
45	BP	194/199 (98%)	81 (42%)	56 (29%)	57 (29%)	0	0
45	DP	194/199 (98%)	77 (40%)	62 (32%)	55 (28%)	0	0
46	BQ	152/184 (83%)	62 (41%)	44 (29%)	46 (30%)	0	0
46	DQ	152/184 (83%)	62 (41%)	45 (30%)	45 (30%)	0	0
47	BR	141/186 (76%)	63 (45%)	28 (20%)	50 (36%)	0	0
47	DR	141/186 (76%)	59 (42%)	32 (23%)	50 (36%)	0	0
48	BS	186/189 (98%)	104 (56%)	57 (31%)	25 (13%)	0	4
48	DS	186/189 (98%)	101 (54%)	60 (32%)	25 (13%)	0	4
49	BT	117/160 (73%)	53 (45%)	18 (15%)	46 (39%)	0	0
49	DT	117/160 (73%)	50 (43%)	23 (20%)	44 (38%)	0	0
50	BU	127/137 (93%)	64 (50%)	28 (22%)	35 (28%)	0	0
50	DU	127/137 (93%)	70 (55%)	21 (16%)	36 (28%)	0	0
51	BV	57/155 (37%)	14 (25%)	19 (33%)	24 (42%)	0	0
51	DV	57/155 (37%)	15 (26%)	16 (28%)	26 (46%)	0	0
52	BW	92/142 (65%)	30 (33%)	30 (33%)	32 (35%)	0	0
52	DW	92/142 (65%)	32 (35%)	28 (30%)	32 (35%)	0	0
53	BX	105/127 (83%)	53 (50%)	28 (27%)	24 (23%)	0	1
53	DX	105/127 (83%)	55 (52%)	30 (29%)	20 (19%)	0	2
54	BY	147/149 (99%)	37 (25%)	47 (32%)	63 (43%)	0	0
54	DY	147/149 (99%)	36 (24%)	51 (35%)	60 (41%)	0	0
55	BZ	96/105 (91%)	48 (50%)	28 (29%)	20 (21%)	0	1
55	DZ	96/105 (91%)	51 (53%)	28 (29%)	17 (18%)	0	2
56	Ba	84/113 (74%)	27 (32%)	27 (32%)	30 (36%)	0	0
56	Da	84/113 (74%)	25 (30%)	28 (33%)	31 (37%)	0	0
57	Bb	123/130 (95%)	39 (32%)	28 (23%)	56 (46%)	0	0
57	Db	123/130 (95%)	41 (33%)	31 (25%)	51 (42%)	0	0
58	Bc	66/120 (55%)	28 (42%)	23 (35%)	15 (23%)	0	1
58	Dc	66/120 (55%)	28 (42%)	26 (39%)	12 (18%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	Bd	70/88 (80%)	19 (27%)	20 (29%)	31 (44%)	0	0
59	Dd	70/88 (80%)	17 (24%)	24 (34%)	29 (41%)	0	0
60	Be	46/51 (90%)	25 (54%)	8 (17%)	13 (28%)	0	0
60	De	46/51 (90%)	22 (48%)	12 (26%)	12 (26%)	0	1
61	Bf	93/106 (88%)	37 (40%)	28 (30%)	28 (30%)	0	0
61	Df	93/106 (88%)	37 (40%)	28 (30%)	28 (30%)	0	0
62	Bg	81/92 (88%)	31 (38%)	27 (33%)	23 (28%)	0	0
62	Dg	81/92 (88%)	32 (40%)	24 (30%)	25 (31%)	0	0
72	DL	136/165 (82%)	42 (31%)	42 (31%)	52 (38%)	0	0
73	DM	126/312 (40%)	48 (38%)	31 (25%)	47 (37%)	0	0
All	All	14930/18123 (82%)	5798 (39%)	4273 (29%)	4859 (32%)	0	0

5 of 4859 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AA	11	PRO
2	AA	13	ASP
2	AA	14	ALA
2	AA	21	ASN
2	AA	24	LEU

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	1787/1800 (99%)	1003 (56%)	148 (8%)
1	C1	1787/1800 (99%)	990 (55%)	150 (8%)
29	B1	3203/3396 (94%)	1725 (53%)	259 (8%)
29	D1	3203/3396 (94%)	1714 (53%)	257 (8%)
30	B2	120/121 (99%)	70 (58%)	12 (10%)
30	D2	120/121 (99%)	66 (55%)	12 (10%)
31	B3	157/158 (99%)	80 (50%)	9 (5%)
31	D3	157/158 (99%)	79 (50%)	9 (5%)
All	All	10534/10950 (96%)	5727 (54%)	856 (8%)

5 of 5727 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	2	A
1	A1	3	U
1	A1	4	C
1	A1	7	G
1	A1	8	U

5 of 856 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	262	U
1	C1	1761	U
29	D1	3093	C
1	C1	380	U
1	C1	254	A

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

715 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
74	OHX	D1	3475	-	0,6,6	-	-	-		
74	OHX	A1	1938	-	0,6,6	-	-	-		
74	OHX	A1	1907	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
74	OHX	B1	3448	-	0,6,6	-	-	-		
74	OHX	C1	1970	-	0,6,6	-	-	-		
74	OHX	D1	3432	-	0,6,6	-	-	-		
74	OHX	D1	3579	-	0,6,6	-	-	-		
74	OHX	D1	3424	-	0,6,6	-	-	-		
74	OHX	D2	207	-	0,6,6	-	-	-		
74	OHX	B1	3523	-	0,6,6	-	-	-		
74	OHX	D1	3408	-	0,6,6	-	-	-		
74	OHX	B1	3616	-	0,6,6	-	-	-		
74	OHX	B1	3420	-	0,6,6	-	-	-		
74	OHX	D1	3421	-	0,6,6	-	-	-		
74	OHX	B1	3557	-	0,6,6	-	-	-		
74	OHX	D1	3517	-	0,6,6	-	-	-		
74	OHX	D1	3510	-	0,6,6	-	-	-		
74	OHX	Dg	101	-	0,6,6	-	-	-		
74	OHX	A1	1910	-	0,6,6	-	-	-		
74	OHX	A1	1944	-	0,6,6	-	-	-		
74	OHX	D1	3574	-	0,6,6	-	-	-		
74	OHX	B1	3521	-	0,6,6	-	-	-		
74	OHX	B3	206	-	0,6,6	-	-	-		
74	OHX	A1	1926	-	0,6,6	-	-	-		
74	OHX	B3	201	-	0,6,6	-	-	-		
74	OHX	A1	1999	-	0,6,6	-	-	-		
74	OHX	B1	3609	-	0,6,6	-	-	-		
74	OHX	D1	3591	-	0,6,6	-	-	-		
74	OHX	B1	3493	-	0,6,6	-	-	-		
74	OHX	Ac	100	-	0,6,6	-	-	-		
74	OHX	C1	1909	-	0,6,6	-	-	-		
74	OHX	C1	1971	-	0,6,6	-	-	-		
74	OHX	A1	1931	1	0,6,6	-	-	-		
74	OHX	C1	1981	-	0,6,6	-	-	-		
74	OHX	B1	3491	-	0,6,6	-	-	-		
74	OHX	A1	1967	-	0,6,6	-	-	-		
74	OHX	C1	1963	-	0,6,6	-	-	-		
74	OHX	D1	3406	-	0,6,6	-	-	-		
74	OHX	D1	3422	-	0,6,6	-	-	-		
74	OHX	D1	3429	-	0,6,6	-	-	-		
74	OHX	B1	3403	-	0,6,6	-	-	-		
74	OHX	C1	1949	-	0,6,6	-	-	-		
74	OHX	A1	1957	-	0,6,6	-	-	-		
74	OHX	C1	1926	-	0,6,6	-	-	-		
74	OHX	C1	1920	-	0,6,6	-	-	-		
74	OHX	D1	3573	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
74	OHX	A1	1968	-	0,6,6	-	-	-		
74	OHX	B3	211	-	0,6,6	-	-	-		
74	OHX	B1	3614	-	0,6,6	-	-	-		
74	OHX	D3	208	-	0,6,6	-	-	-		
74	OHX	D1	3419	-	0,6,6	-	-	-		
74	OHX	A1	1922	-	0,6,6	-	-	-		
74	OHX	B1	3428	-	0,6,6	-	-	-		
74	OHX	C1	1998	-	0,6,6	-	-	-		
74	OHX	B1	3483	-	0,6,6	-	-	-		
74	OHX	D3	205	-	0,6,6	-	-	-		
74	OHX	A1	1962	-	0,6,6	-	-	-		
74	OHX	D1	3590	-	0,6,6	-	-	-		
74	OHX	C1	1910	-	0,6,6	-	-	-		
74	OHX	D1	3472	-	0,6,6	-	-	-		
74	OHX	D1	3580	-	0,6,6	-	-	-		
74	OHX	C1	1912	-	0,6,6	-	-	-		
74	OHX	D2	206	-	0,6,6	-	-	-		
74	OHX	B1	3464	-	0,6,6	-	-	-		
74	OHX	B1	3458	-	0,6,6	-	-	-		
74	OHX	D1	3512	-	0,6,6	-	-	-		
74	OHX	B1	3567	-	0,6,6	-	-	-		
74	OHX	A1	1936	-	0,6,6	-	-	-		
74	OHX	B1	3526	-	0,6,6	-	-	-		
74	OHX	D2	201	-	0,6,6	-	-	-		
74	OHX	B1	3544	-	0,6,6	-	-	-		
74	OHX	A1	1921	-	0,6,6	-	-	-		
74	OHX	C1	1972	-	0,6,6	-	-	-		
74	OHX	B1	3434	-	0,6,6	-	-	-		
74	OHX	A1	1961	-	0,6,6	-	-	-		
74	OHX	B1	3409	-	0,6,6	-	-	-		
74	OHX	B1	3572	-	0,6,6	-	-	-		
74	OHX	C1	1958	-	0,6,6	-	-	-		
74	OHX	D1	3528	-	0,6,6	-	-	-		
74	OHX	D1	3586	-	0,6,6	-	-	-		
74	OHX	B1	3549	-	0,6,6	-	-	-		
74	OHX	A1	1977	-	0,6,6	-	-	-		
74	OHX	A1	1997	-	0,6,6	-	-	-		
74	OHX	B1	3556	-	0,6,6	-	-	-		
74	OHX	D1	3523	-	0,6,6	-	-	-		
74	OHX	B1	3518	-	0,6,6	-	-	-		
74	OHX	D1	3583	-	0,6,6	-	-	-		
74	OHX	A1	1973	-	0,6,6	-	-	-		
74	OHX	D1	3572	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
74	OHX	C1	1945	-	0,6,6	-	-	-		
74	OHX	D1	3588	-	0,6,6	-	-	-		
74	OHX	D1	3433	-	0,6,6	-	-	-		
74	OHX	D1	3606	-	0,6,6	-	-	-		
74	OHX	C1	2001	-	0,6,6	-	-	-		
74	OHX	B1	3580	-	0,6,6	-	-	-		
74	OHX	B1	3401	-	0,6,6	-	-	-		
74	OHX	A1	1917	-	0,6,6	-	-	-		
74	OHX	D1	3560	-	0,6,6	-	-	-		
74	OHX	C1	1925	-	0,6,6	-	-	-		
74	OHX	D1	3504	-	0,6,6	-	-	-		
74	OHX	D1	3463	-	0,6,6	-	-	-		
74	OHX	B1	3418	-	0,6,6	-	-	-		
74	OHX	B1	3430	-	0,6,6	-	-	-		
74	OHX	DE	301	-	0,6,6	-	-	-		
74	OHX	C1	1984	-	0,6,6	-	-	-		
74	OHX	A1	1914	-	0,6,6	-	-	-		
74	OHX	B1	3565	-	0,6,6	-	-	-		
74	OHX	C1	1953	-	0,6,6	-	-	-		
74	OHX	C1	1915	-	0,6,6	-	-	-		
74	OHX	B1	3422	-	0,6,6	-	-	-		
74	OHX	B1	3606	-	0,6,6	-	-	-		
74	OHX	B1	3426	-	0,6,6	-	-	-		
74	OHX	B1	3473	-	0,6,6	-	-	-		
74	OHX	D1	3439	-	0,6,6	-	-	-		
74	OHX	B1	3449	-	0,6,6	-	-	-		
74	OHX	C1	1968	-	0,6,6	-	-	-		
74	OHX	A1	1986	-	0,6,6	-	-	-		
74	OHX	B1	3506	-	0,6,6	-	-	-		
74	OHX	D1	3413	-	0,6,6	-	-	-		
74	OHX	C1	1922	-	0,6,6	-	-	-		
74	OHX	B1	3476	-	0,6,6	-	-	-		
74	OHX	C1	1967	-	0,6,6	-	-	-		
74	OHX	D1	3506	-	0,6,6	-	-	-		
74	OHX	A1	1974	-	0,6,6	-	-	-		
74	OHX	D2	203	-	0,6,6	-	-	-		
74	OHX	C1	1962	-	0,6,6	-	-	-		
74	OHX	D1	3533	-	0,6,6	-	-	-		
74	OHX	A1	1942	-	0,6,6	-	-	-		
74	OHX	D1	3487	-	0,6,6	-	-	-		
74	OHX	B1	3504	-	0,6,6	-	-	-		
74	OHX	B1	3463	-	0,6,6	-	-	-		
74	OHX	B1	3615	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
74	OHX	D1	3401	-	0,6,6	-	-	-		
74	OHX	D1	3470	-	0,6,6	-	-	-		
74	OHX	C1	1936	-	0,6,6	-	-	-		
74	OHX	D1	3494	-	0,6,6	-	-	-		
74	OHX	D1	3496	-	0,6,6	-	-	-		
74	OHX	D1	3534	-	0,6,6	-	-	-		
74	OHX	B1	3550	-	0,6,6	-	-	-		
74	OHX	A1	1941	-	0,6,6	-	-	-		
74	OHX	B1	3545	-	0,6,6	-	-	-		
74	OHX	C1	1961	-	0,6,6	-	-	-		
74	OHX	D1	3411	-	0,6,6	-	-	-		
74	OHX	B1	3584	-	0,6,6	-	-	-		
74	OHX	D3	201	-	0,6,6	-	-	-		
74	OHX	D1	3535	-	0,6,6	-	-	-		
74	OHX	A1	1935	-	0,6,6	-	-	-		
74	OHX	A1	1954	-	0,6,6	-	-	-		
74	OHX	A1	1960	-	0,6,6	-	-	-		
74	OHX	B1	3570	-	0,6,6	-	-	-		
74	OHX	B2	210	-	0,6,6	-	-	-		
74	OHX	C1	1982	-	0,6,6	-	-	-		
74	OHX	D2	205	-	0,6,6	-	-	-		
74	OHX	C1	1940	-	0,6,6	-	-	-		
74	OHX	AT	401	-	0,6,6	-	-	-		
74	OHX	D1	3436	-	0,6,6	-	-	-		
74	OHX	B1	3537	-	0,6,6	-	-	-		
74	OHX	A1	1951	-	0,6,6	-	-	-		
74	OHX	C1	1956	-	0,6,6	-	-	-		
74	OHX	D1	3415	-	0,6,6	-	-	-		
74	OHX	B1	3407	-	0,6,6	-	-	-		
74	OHX	D1	3508	-	0,6,6	-	-	-		
74	OHX	A1	1965	-	0,6,6	-	-	-		
74	OHX	D1	3538	-	0,6,6	-	-	-		
74	OHX	C1	2000	-	0,6,6	-	-	-		
74	OHX	Bd	101	-	0,6,6	-	-	-		
74	OHX	D1	3445	-	0,6,6	-	-	-		
74	OHX	B1	3425	-	0,6,6	-	-	-		
74	OHX	B1	3507	-	0,6,6	-	-	-		
74	OHX	A1	1927	-	0,6,6	-	-	-		
74	OHX	C1	1996	-	0,6,6	-	-	-		
74	OHX	A1	1918	-	0,6,6	-	-	-		
74	OHX	B1	3501	-	0,6,6	-	-	-		
74	OHX	B1	3543	-	0,6,6	-	-	-		
74	OHX	D1	3427	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
74	OHX	D1	3479	-	0,6,6	-	-	-		
74	OHX	A1	1948	-	0,6,6	-	-	-		
74	OHX	D2	204	-	0,6,6	-	-	-		
74	OHX	D1	3581	-	0,6,6	-	-	-		
74	OHX	B1	3522	-	0,6,6	-	-	-		
74	OHX	D1	3426	-	0,6,6	-	-	-		
74	OHX	C1	1954	-	0,6,6	-	-	-		
74	OHX	D1	3549	-	0,6,6	-	-	-		
74	OHX	A1	1915	-	0,6,6	-	-	-		
74	OHX	B1	3602	-	0,6,6	-	-	-		
74	OHX	B1	3411	-	0,6,6	-	-	-		
74	OHX	D3	211	-	0,6,6	-	-	-		
74	OHX	C1	1983	1	0,6,6	-	-	-		
74	OHX	D1	3536	-	0,6,6	-	-	-		
74	OHX	C1	1942	-	0,6,6	-	-	-		
74	OHX	A1	1987	-	0,6,6	-	-	-		
74	OHX	D1	3452	-	0,6,6	-	-	-		
74	OHX	D1	3562	-	0,6,6	-	-	-		
74	OHX	B1	3404	-	0,6,6	-	-	-		
74	OHX	D1	3611	-	0,6,6	-	-	-		
74	OHX	A1	1929	-	0,6,6	-	-	-		
74	OHX	C1	1927	-	0,6,6	-	-	-		
74	OHX	B1	3462	-	0,6,6	-	-	-		
74	OHX	D1	3428	-	0,6,6	-	-	-		
74	OHX	D1	3582	-	0,6,6	-	-	-		
74	OHX	D1	3483	-	0,6,6	-	-	-		
74	OHX	C1	1941	-	0,6,6	-	-	-		
74	OHX	A1	1933	-	0,6,6	-	-	-		
74	OHX	D1	3531	-	0,6,6	-	-	-		
74	OHX	D1	3585	-	0,6,6	-	-	-		
74	OHX	A1	1946	-	0,6,6	-	-	-		
74	OHX	C1	1950	-	0,6,6	-	-	-		
74	OHX	D1	3525	-	0,6,6	-	-	-		
74	OHX	B1	3447	-	0,6,6	-	-	-		
74	OHX	C1	1964	-	0,6,6	-	-	-		
74	OHX	B1	3435	-	0,6,6	-	-	-		
74	OHX	B1	3485	-	0,6,6	-	-	-		
74	OHX	B1	3499	-	0,6,6	-	-	-		
74	OHX	A1	1932	-	0,6,6	-	-	-		
74	OHX	D1	3464	-	0,6,6	-	-	-		
74	OHX	D1	3503	-	0,6,6	-	-	-		
74	OHX	C1	1960	-	0,6,6	-	-	-		
74	OHX	D1	3620	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
74	OHX	A1	1949	-	0,6,6	-	-	-		
74	OHX	C1	1933	-	0,6,6	-	-	-		
74	OHX	B2	209	-	0,6,6	-	-	-		
74	OHX	B1	3477	-	0,6,6	-	-	-		
74	OHX	C1	1930	1	0,6,6	-	-	-		
74	OHX	D1	3500	-	0,6,6	-	-	-		
74	OHX	D1	3537	-	0,6,6	-	-	-		
74	OHX	B1	3486	-	0,6,6	-	-	-		
74	OHX	D3	206	-	0,6,6	-	-	-		
74	OHX	C1	1995	-	0,6,6	-	-	-		
74	OHX	Dd	101	-	0,6,6	-	-	-		
74	OHX	D1	3481	-	0,6,6	-	-	-		
74	OHX	B1	3469	-	0,6,6	-	-	-		
74	OHX	D1	3453	-	0,6,6	-	-	-		
74	OHX	D1	3604	-	0,6,6	-	-	-		
74	OHX	D1	3556	-	0,6,6	-	-	-		
74	OHX	B1	3558	-	0,6,6	-	-	-		
74	OHX	A1	1904	-	0,6,6	-	-	-		
74	OHX	CT	401	-	0,6,6	-	-	-		
74	OHX	D1	3559	-	0,6,6	-	-	-		
74	OHX	D1	3550	-	0,6,6	-	-	-		
74	OHX	B3	204	-	0,6,6	-	-	-		
74	OHX	C1	1948	-	0,6,6	-	-	-		
74	OHX	D1	3468	-	0,6,6	-	-	-		
74	OHX	A1	1952	-	0,6,6	-	-	-		
74	OHX	C1	1937	-	0,6,6	-	-	-		
74	OHX	D1	3599	-	0,6,6	-	-	-		
74	OHX	DT	201	-	0,6,6	-	-	-		
74	OHX	B1	3586	-	0,6,6	-	-	-		
74	OHX	C1	1932	-	0,6,6	-	-	-		
74	OHX	A1	1990	-	0,6,6	-	-	-		
74	OHX	D1	3501	-	0,6,6	-	-	-		
74	OHX	D1	3462	-	0,6,6	-	-	-		
74	OHX	C1	1911	-	0,6,6	-	-	-		
74	OHX	D1	3612	-	0,6,6	-	-	-		
74	OHX	D1	3451	-	0,6,6	-	-	-		
74	OHX	A1	1909	-	0,6,6	-	-	-		
74	OHX	D1	3489	-	0,6,6	-	-	-		
74	OHX	D1	3605	-	0,6,6	-	-	-		
74	OHX	D1	3566	-	0,6,6	-	-	-		
74	OHX	A1	1994	-	0,6,6	-	-	-		
74	OHX	Dd	102	-	0,6,6	-	-	-		
74	OHX	A1	1920	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
74	OHX	A1	1991	-	0,6,6	-	-	-		
74	OHX	B1	3525	-	0,6,6	-	-	-		
74	OHX	B1	3509	-	0,6,6	-	-	-		
74	OHX	D1	3473	-	0,6,6	-	-	-		
74	OHX	D1	3540	-	0,6,6	-	-	-		
74	OHX	B1	3551	-	0,6,6	-	-	-		
74	OHX	A1	2001	-	0,6,6	-	-	-		
74	OHX	B1	3601	-	0,6,6	-	-	-		
74	OHX	B2	208	-	0,6,6	-	-	-		
74	OHX	D1	3480	-	0,6,6	-	-	-		
74	OHX	D1	3418	-	0,6,6	-	-	-		
74	OHX	B1	3414	-	0,6,6	-	-	-		
74	OHX	B1	3577	-	0,6,6	-	-	-		
74	OHX	C1	1952	-	0,6,6	-	-	-		
74	OHX	A1	1912	-	0,6,6	-	-	-		
74	OHX	B1	3466	-	0,6,6	-	-	-		
74	OHX	C1	1959	-	0,6,6	-	-	-		
74	OHX	A1	1924	-	0,6,6	-	-	-		
74	OHX	D1	3519	-	0,6,6	-	-	-		
74	OHX	B1	3528	-	0,6,6	-	-	-		
74	OHX	C1	1993	-	0,6,6	-	-	-		
74	OHX	D1	3522	-	0,6,6	-	-	-		
74	OHX	A1	1972	-	0,6,6	-	-	-		
74	OHX	D1	3589	-	0,6,6	-	-	-		
74	OHX	B1	3541	-	0,6,6	-	-	-		
74	OHX	D1	3513	-	0,6,6	-	-	-		
74	OHX	A1	1903	-	0,6,6	-	-	-		
74	OHX	B3	210	-	0,6,6	-	-	-		
74	OHX	DO	302	-	0,6,6	-	-	-		
74	OHX	B1	3619	-	0,6,6	-	-	-		
74	OHX	B1	3461	-	0,6,6	-	-	-		
74	OHX	D1	3498	-	0,6,6	-	-	-		
74	OHX	CI	201	-	0,6,6	-	-	-		
74	OHX	A1	1978	-	0,6,6	-	-	-		
74	OHX	B1	3505	-	0,6,6	-	-	-		
74	OHX	B1	3600	-	0,6,6	-	-	-		
74	OHX	B1	3502	-	0,6,6	-	-	-		
74	OHX	B1	3532	-	0,6,6	-	-	-		
74	OHX	B1	3423	-	0,6,6	-	-	-		
74	OHX	B1	3576	-	0,6,6	-	-	-		
74	OHX	D1	3603	-	0,6,6	-	-	-		
74	OHX	C1	1924	-	0,6,6	-	-	-		
74	OHX	B1	3481	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
74	OHX	B1	3440	-	0,6,6	-	-	-		
74	OHX	B1	3408	-	0,6,6	-	-	-		
74	OHX	A1	1925	-	0,6,6	-	-	-		
74	OHX	A1	1911	-	0,6,6	-	-	-		
74	OHX	D1	3564	-	0,6,6	-	-	-		
74	OHX	D2	202	-	0,6,6	-	-	-		
74	OHX	C1	1987	-	0,6,6	-	-	-		
74	OHX	B1	3546	-	0,6,6	-	-	-		
74	OHX	C1	1990	-	0,6,6	-	-	-		
74	OHX	D1	3610	-	0,6,6	-	-	-		
74	OHX	D1	3423	-	0,6,6	-	-	-		
74	OHX	C1	1938	-	0,6,6	-	-	-		
74	OHX	B1	3419	-	0,6,6	-	-	-		
74	OHX	D1	3416	-	0,6,6	-	-	-		
74	OHX	A1	1947	-	0,6,6	-	-	-		
74	OHX	AL	201	-	0,6,6	-	-	-		
74	OHX	D1	3596	-	0,6,6	-	-	-		
74	OHX	B1	3605	-	0,6,6	-	-	-		
74	OHX	D1	3568	-	0,6,6	-	-	-		
74	OHX	C1	1946	-	0,6,6	-	-	-		
74	OHX	B1	3607	-	0,6,6	-	-	-		
74	OHX	B1	3470	-	0,6,6	-	-	-		
74	OHX	B1	3595	-	0,6,6	-	-	-		
74	OHX	B1	3489	-	0,6,6	-	-	-		
74	OHX	D1	3595	-	0,6,6	-	-	-		
74	OHX	C1	1992	-	0,6,6	-	-	-		
74	OHX	B1	3540	-	0,6,6	-	-	-		
74	OHX	B1	3421	-	0,6,6	-	-	-		
74	OHX	CS	102	-	0,6,6	-	-	-		
74	OHX	B1	3417	-	0,6,6	-	-	-		
74	OHX	D1	3403	-	0,6,6	-	-	-		
74	OHX	D1	3484	-	0,6,6	-	-	-		
74	OHX	B1	3548	-	0,6,6	-	-	-		
74	OHX	B1	3514	-	0,6,6	-	-	-		
74	OHX	D1	3444	-	0,6,6	-	-	-		
74	OHX	A1	1976	-	0,6,6	-	-	-		
74	OHX	A1	1963	-	0,6,6	-	-	-		
74	OHX	A1	1966	-	0,6,6	-	-	-		
74	OHX	D1	3555	-	0,6,6	-	-	-		
74	OHX	C1	1974	-	0,6,6	-	-	-		
74	OHX	B1	3529	-	0,6,6	-	-	-		
74	OHX	B1	3534	-	0,6,6	-	-	-		
74	OHX	D1	3624	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
74	OHX	D1	3530	-	0,6,6	-	-	-		
74	OHX	B1	3578	-	0,6,6	-	-	-		
74	OHX	A1	1913	-	0,6,6	-	-	-		
74	OHX	B1	3416	-	0,6,6	-	-	-		
74	OHX	B1	3542	-	0,6,6	-	-	-		
74	OHX	D1	3471	-	0,6,6	-	-	-		
74	OHX	B1	3510	-	0,6,6	-	-	-		
74	OHX	C1	1947	-	0,6,6	-	-	-		
74	OHX	A1	1989	-	0,6,6	-	-	-		
74	OHX	A1	1916	-	0,6,6	-	-	-		
74	OHX	B1	3441	-	0,6,6	-	-	-		
74	OHX	B1	3513	-	0,6,6	-	-	-		
74	OHX	B1	3589	-	0,6,6	-	-	-		
74	OHX	D1	3495	-	0,6,6	-	-	-		
74	OHX	C1	1975	-	0,6,6	-	-	-		
74	OHX	D1	3497	-	0,6,6	-	-	-		
74	OHX	C1	1957	-	0,6,6	-	-	-		
74	OHX	B1	3520	-	0,6,6	-	-	-		
74	OHX	A1	1982	-	0,6,6	-	-	-		
74	OHX	C1	1989	-	0,6,6	-	-	-		
74	OHX	D1	3505	-	0,6,6	-	-	-		
74	OHX	D1	3526	-	0,6,6	-	-	-		
74	OHX	C1	1978	-	0,6,6	-	-	-		
74	OHX	A1	1940	-	0,6,6	-	-	-		
74	OHX	D1	3455	-	0,6,6	-	-	-		
74	OHX	B1	3406	-	0,6,6	-	-	-		
74	OHX	B1	3590	-	0,6,6	-	-	-		
74	OHX	B1	3566	-	0,6,6	-	-	-		
74	OHX	B1	3497	-	0,6,6	-	-	-		
74	OHX	D1	3608	-	0,6,6	-	-	-		
74	OHX	C1	1919	-	0,6,6	-	-	-		
74	OHX	D1	3622	-	0,6,6	-	-	-		
74	OHX	A1	2000	-	0,6,6	-	-	-		
74	OHX	D1	3474	-	0,6,6	-	-	-		
74	OHX	D1	3569	-	0,6,6	-	-	-		
74	OHX	C1	1997	-	0,6,6	-	-	-		
74	OHX	C1	1903	-	0,6,6	-	-	-		
74	OHX	A1	1996	-	0,6,6	-	-	-		
74	OHX	D2	208	-	0,6,6	-	-	-		
74	OHX	B2	203	-	0,6,6	-	-	-		
74	OHX	B1	3582	-	0,6,6	-	-	-		
74	OHX	C1	1994	-	0,6,6	-	-	-		
74	OHX	A1	1964	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
74	OHX	C1	1973	-	0,6,6	-	-	-		
74	OHX	B1	3585	-	0,6,6	-	-	-		
74	OHX	B1	3552	-	0,6,6	-	-	-		
74	OHX	C1	1918	-	0,6,6	-	-	-		
74	OHX	A1	1992	-	0,6,6	-	-	-		
74	OHX	D3	209	-	0,6,6	-	-	-		
74	OHX	C1	1969	-	0,6,6	-	-	-		
74	OHX	CS	101	-	0,6,6	-	-	-		
74	OHX	B1	3487	-	0,6,6	-	-	-		
74	OHX	D1	3467	-	0,6,6	-	-	-		
74	OHX	B1	3459	-	0,6,6	-	-	-		
74	OHX	B1	3620	-	0,6,6	-	-	-		
74	OHX	D1	3557	-	0,6,6	-	-	-		
74	OHX	B1	3517	-	0,6,6	-	-	-		
74	OHX	D1	3509	-	0,6,6	-	-	-		
74	OHX	D1	3532	-	0,6,6	-	-	-		
74	OHX	A1	1983	-	0,6,6	-	-	-		
74	OHX	D1	3548	-	0,6,6	-	-	-		
74	OHX	B1	3547	-	0,6,6	-	-	-		
74	OHX	D1	3435	-	0,6,6	-	-	-		
74	OHX	D1	3551	-	0,6,6	-	-	-		
74	OHX	C1	1904	-	0,6,6	-	-	-		
74	OHX	D1	3592	-	0,6,6	-	-	-		
74	OHX	C1	1966	-	0,6,6	-	-	-		
74	OHX	D1	3520	-	0,6,6	-	-	-		
74	OHX	B1	3431	-	0,6,6	-	-	-		
74	OHX	C1	1928	-	0,6,6	-	-	-		
74	OHX	D1	3420	-	0,6,6	-	-	-		
74	OHX	D1	3477	-	0,6,6	-	-	-		
74	OHX	B1	3474	-	0,6,6	-	-	-		
74	OHX	A1	2002	-	0,6,6	-	-	-		
74	OHX	A1	1995	-	0,6,6	-	-	-		
74	OHX	C1	1913	-	0,6,6	-	-	-		
74	OHX	C1	1914	-	0,6,6	-	-	-		
74	OHX	B1	3456	-	0,6,6	-	-	-		
74	OHX	B1	3405	-	0,6,6	-	-	-		
74	OHX	A1	1939	-	0,6,6	-	-	-		
74	OHX	C1	1916	-	0,6,6	-	-	-		
74	OHX	D1	3600	-	0,6,6	-	-	-		
74	OHX	B1	3516	-	0,6,6	-	-	-		
74	OHX	B1	3442	-	0,6,6	-	-	-		
74	OHX	B1	3415	-	0,6,6	-	-	-		
74	OHX	B2	205	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
74	OHX	B1	3575	-	0,6,6	-	-	-		
74	OHX	DO	301	-	0,6,6	-	-	-		
74	OHX	B1	3451	-	0,6,6	-	-	-		
74	OHX	Bg	101	-	0,6,6	-	-	-		
74	OHX	DC	401	-	0,6,6	-	-	-		
74	OHX	D1	3561	-	0,6,6	-	-	-		
74	OHX	B2	204	-	0,6,6	-	-	-		
74	OHX	C1	1980	-	0,6,6	-	-	-		
74	OHX	D1	3593	-	0,6,6	-	-	-		
74	OHX	D1	3545	-	0,6,6	-	-	-		
74	OHX	B1	3553	-	0,6,6	-	-	-		
74	OHX	D1	3448	-	0,6,6	-	-	-		
74	OHX	D1	3502	-	0,6,6	-	-	-		
74	OHX	D1	3516	-	0,6,6	-	-	-		
74	OHX	B1	3482	-	0,6,6	-	-	-		
74	OHX	B1	3592	-	0,6,6	-	-	-		
74	OHX	B1	3433	-	0,6,6	-	-	-		
74	OHX	D1	3544	-	0,6,6	-	-	-		
74	OHX	C1	1939	-	0,6,6	-	-	-		
74	OHX	B3	208	-	0,6,6	-	-	-		
74	OHX	D1	3465	-	0,6,6	-	-	-		
74	OHX	A1	1937	-	0,6,6	-	-	-		
74	OHX	D1	3570	-	0,6,6	-	-	-		
74	OHX	B1	3490	-	0,6,6	-	-	-		
74	OHX	B2	202	-	0,6,6	-	-	-		
74	OHX	D1	3594	-	0,6,6	-	-	-		
74	OHX	B1	3561	-	0,6,6	-	-	-		
74	OHX	A1	1923	-	0,6,6	-	-	-		
74	OHX	D1	3607	-	0,6,6	-	-	-		
74	OHX	C1	1955	-	0,6,6	-	-	-		
74	OHX	A1	1905	-	0,6,6	-	-	-		
74	OHX	B3	209	-	0,6,6	-	-	-		
74	OHX	D1	3431	-	0,6,6	-	-	-		
74	OHX	D3	210	-	0,6,6	-	-	-		
74	OHX	B1	3508	-	0,6,6	-	-	-		
74	OHX	B1	3457	-	0,6,6	-	-	-		
74	OHX	B1	3471	-	0,6,6	-	-	-		
74	OHX	B1	3617	-	0,6,6	-	-	-		
74	OHX	D1	3417	-	0,6,6	-	-	-		
74	OHX	AS	101	-	0,6,6	-	-	-		
74	OHX	B1	3591	-	0,6,6	-	-	-		
74	OHX	D1	3486	-	0,6,6	-	-	-		
74	OHX	D1	3546	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
74	OHX	C1	1901	-	0,6,6	-	-	-		
74	OHX	D1	3553	-	0,6,6	-	-	-		
74	OHX	A1	1959	-	0,6,6	-	-	-		
74	OHX	A1	1971	-	0,6,6	-	-	-		
74	OHX	B1	3439	-	0,6,6	-	-	-		
74	OHX	A1	1993	-	0,6,6	-	-	-		
74	OHX	D1	3602	-	0,6,6	-	-	-		
74	OHX	D1	3615	-	0,6,6	-	-	-		
74	OHX	D1	3410	-	0,6,6	-	-	-		
74	OHX	D1	3529	-	0,6,6	-	-	-		
74	OHX	B1	3598	-	0,6,6	-	-	-		
74	OHX	C1	1923	-	0,6,6	-	-	-		
74	OHX	DJ	301	-	0,6,6	-	-	-		
74	OHX	BC	401	-	0,6,6	-	-	-		
74	OHX	BT	201	-	0,6,6	-	-	-		
74	OHX	C1	1905	-	0,6,6	-	-	-		
74	OHX	B1	3594	-	0,6,6	-	-	-		
74	OHX	A1	1984	-	0,6,6	-	-	-		
74	OHX	D1	3616	-	0,6,6	-	-	-		
74	OHX	C1	1907	-	0,6,6	-	-	-		
74	OHX	A1	1988	-	0,6,6	-	-	-		
74	OHX	B1	3581	-	0,6,6	-	-	-		
74	OHX	B1	3621	-	0,6,6	-	-	-		
74	OHX	A1	1906	-	0,6,6	-	-	-		
74	OHX	B1	3500	-	0,6,6	-	-	-		
74	OHX	B1	3535	-	0,6,6	-	-	-		
74	OHX	B1	3452	-	0,6,6	-	-	-		
74	OHX	C1	1908	-	0,6,6	-	-	-		
74	OHX	B1	3562	-	0,6,6	-	-	-		
74	OHX	B2	207	-	0,6,6	-	-	-		
74	OHX	D1	3450	-	0,6,6	-	-	-		
74	OHX	C1	1906	-	0,6,6	-	-	-		
74	OHX	D1	3437	-	0,6,6	-	-	-		
74	OHX	D1	3402	-	0,6,6	-	-	-		
74	OHX	B1	3453	-	0,6,6	-	-	-		
74	OHX	B1	3531	-	0,6,6	-	-	-		
74	OHX	C1	1991	-	0,6,6	-	-	-		
74	OHX	C1	1999	-	0,6,6	-	-	-		
74	OHX	D1	3430	-	0,6,6	-	-	-		
74	OHX	B1	3443	-	0,6,6	-	-	-		
74	OHX	D1	3614	-	0,6,6	-	-	-		
74	OHX	B1	3579	-	0,6,6	-	-	-		
74	OHX	D3	203	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
74	OHX	B1	3587	-	0,6,6	-	-	-		
74	OHX	B1	3564	-	0,6,6	-	-	-		
74	OHX	C1	1931	-	0,6,6	-	-	-		
74	OHX	D1	3514	-	0,6,6	-	-	-		
74	OHX	B1	3496	-	0,6,6	-	-	-		
74	OHX	D1	3521	-	0,6,6	-	-	-		
74	OHX	D1	3476	-	0,6,6	-	-	-		
74	OHX	D1	3613	-	0,6,6	-	-	-		
74	OHX	B1	3488	-	0,6,6	-	-	-		
74	OHX	D1	3565	-	0,6,6	-	-	-		
74	OHX	C1	1979	-	0,6,6	-	-	-		
74	OHX	D3	204	-	0,6,6	-	-	-		
74	OHX	B1	3533	-	0,6,6	-	-	-		
74	OHX	B1	3484	-	0,6,6	-	-	-		
74	OHX	B1	3460	-	0,6,6	-	-	-		
74	OHX	B1	3503	-	0,6,6	-	-	-		
74	OHX	B1	3538	-	0,6,6	-	-	-		
74	OHX	B1	3568	-	0,6,6	-	-	-		
74	OHX	B1	3468	-	0,6,6	-	-	-		
74	OHX	D1	3412	-	0,6,6	-	-	-		
74	OHX	D1	3625	-	0,6,6	-	-	-		
74	OHX	B1	3479	-	0,6,6	-	-	-		
74	OHX	B3	207	-	0,6,6	-	-	-		
74	OHX	A1	1902	-	0,6,6	-	-	-		
74	OHX	B1	3511	-	0,6,6	-	-	-		
74	OHX	C1	1944	-	0,6,6	-	-	-		
74	OHX	A1	1919	-	0,6,6	-	-	-		
74	OHX	D1	3409	-	0,6,6	-	-	-		
74	OHX	D1	3438	-	0,6,6	-	-	-		
74	OHX	D1	3488	-	0,6,6	-	-	-		
74	OHX	B1	3539	-	0,6,6	-	-	-		
74	OHX	D1	3571	-	0,6,6	-	-	-		
74	OHX	B3	203	-	0,6,6	-	-	-		
74	OHX	C1	1921	-	0,6,6	-	-	-		
74	OHX	B1	3455	-	0,6,6	-	-	-		
74	OHX	D1	3405	-	0,6,6	-	-	-		
74	OHX	D1	3491	-	0,6,6	-	-	-		
74	OHX	D3	212	-	0,6,6	-	-	-		
74	OHX	B1	3613	-	0,6,6	-	-	-		
74	OHX	B3	205	-	0,6,6	-	-	-		
74	OHX	D1	3601	-	0,6,6	-	-	-		
74	OHX	D1	3527	-	0,6,6	-	-	-		
74	OHX	B1	3530	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
74	OHX	B1	3480	-	0,6,6	-	-	-		
74	OHX	C1	1977	-	0,6,6	-	-	-		
74	OHX	B1	3498	-	0,6,6	-	-	-		
74	OHX	A1	1975	-	0,6,6	-	-	-		
74	OHX	B1	3410	-	0,6,6	-	-	-		
74	OHX	B1	3555	-	0,6,6	-	-	-		
74	OHX	B1	3604	-	0,6,6	-	-	-		
74	OHX	BO	301	-	0,6,6	-	-	-		
74	OHX	D1	3407	-	0,6,6	-	-	-		
74	OHX	D1	3456	-	0,6,6	-	-	-		
74	OHX	B1	3512	-	0,6,6	-	-	-		
74	OHX	D1	3554	-	0,6,6	-	-	-		
74	OHX	B1	3424	-	0,6,6	-	-	-		
74	OHX	D1	3524	-	0,6,6	-	-	-		
74	OHX	A1	1979	-	0,6,6	-	-	-		
74	OHX	A1	1955	-	0,6,6	-	-	-		
74	OHX	D1	3575	-	0,6,6	-	-	-		
74	OHX	B1	3427	-	0,6,6	-	-	-		
74	OHX	D1	3482	-	0,6,6	-	-	-		
74	OHX	C1	1917	-	0,6,6	-	-	-		
74	OHX	D1	3404	-	0,6,6	-	-	-		
74	OHX	B1	3450	-	0,6,6	-	-	-		
74	OHX	D1	3499	-	0,6,6	-	-	-		
74	OHX	B1	3519	-	0,6,6	-	-	-		
74	OHX	B1	3559	-	0,6,6	-	-	-		
74	OHX	B1	3573	-	0,6,6	-	-	-		
74	OHX	B1	3402	-	0,6,6	-	-	-		
74	OHX	B1	3515	-	0,6,6	-	-	-		
74	OHX	B3	212	-	0,6,6	-	-	-		
74	OHX	D2	209	-	0,6,6	-	-	-		
74	OHX	D1	3441	-	0,6,6	-	-	-		
74	OHX	B1	3437	-	0,6,6	-	-	-		
74	OHX	B1	3583	-	0,6,6	-	-	-		
74	OHX	A1	1970	-	0,6,6	-	-	-		
74	OHX	D1	3466	-	0,6,6	-	-	-		
74	OHX	B2	206	-	0,6,6	-	-	-		
74	OHX	B1	3618	-	0,6,6	-	-	-		
74	OHX	D1	3440	-	0,6,6	-	-	-		
74	OHX	B1	3454	-	0,6,6	-	-	-		
74	OHX	B1	3438	-	0,6,6	-	-	-		
74	OHX	D1	3447	-	0,6,6	-	-	-		
74	OHX	D1	3425	-	0,6,6	-	-	-		
74	OHX	B1	3593	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
74	OHX	A1	1934	-	0,6,6	-	-	-		
74	OHX	D1	3543	-	0,6,6	-	-	-		
74	OHX	C1	1986	-	0,6,6	-	-	-		
74	OHX	D1	3578	-	0,6,6	-	-	-		
74	OHX	A1	1956	-	0,6,6	-	-	-		
74	OHX	A1	1969	-	0,6,6	-	-	-		
74	OHX	D3	202	-	0,6,6	-	-	-		
74	OHX	B1	3554	-	0,6,6	-	-	-		
74	OHX	D1	3515	-	0,6,6	-	-	-		
74	OHX	B1	3524	-	0,6,6	-	-	-		
74	OHX	B1	3432	-	0,6,6	-	-	-		
74	OHX	B1	3596	-	0,6,6	-	-	-		
74	OHX	D1	3597	-	0,6,6	-	-	-		
74	OHX	D1	3518	-	0,6,6	-	-	-		
74	OHX	D1	3442	-	0,6,6	-	-	-		
74	OHX	D1	3492	-	0,6,6	-	-	-		
74	OHX	D1	3623	-	0,6,6	-	-	-		
74	OHX	D1	3454	-	0,6,6	-	-	-		
74	OHX	B1	3603	-	0,6,6	-	-	-		
74	OHX	C1	1902	-	0,6,6	-	-	-		
74	OHX	B1	3472	-	0,6,6	-	-	-		
74	OHX	B1	3412	-	0,6,6	-	-	-		
74	OHX	A1	1985	-	0,6,6	-	-	-		
74	OHX	Bd	102	-	0,6,6	-	-	-		
74	OHX	D1	3469	-	0,6,6	-	-	-		
74	OHX	D3	207	-	0,6,6	-	-	-		
74	OHX	A1	1928	-	0,6,6	-	-	-		
74	OHX	A1	1953	-	0,6,6	-	-	-		
74	OHX	A1	1981	-	0,6,6	-	-	-		
74	OHX	A1	1943	-	0,6,6	-	-	-		
74	OHX	B1	3612	-	0,6,6	-	-	-		
74	OHX	B1	3413	-	0,6,6	-	-	-		
74	OHX	D1	3563	-	0,6,6	-	-	-		
74	OHX	D1	3617	-	0,6,6	-	-	-		
74	OHX	D1	3587	-	0,6,6	-	-	-		
74	OHX	C1	1934	-	0,6,6	-	-	-		
74	OHX	C1	1943	-	0,6,6	-	-	-		
74	OHX	B1	3465	-	0,6,6	-	-	-		
74	OHX	C1	1935	-	0,6,6	-	-	-		
74	OHX	D1	3449	-	0,6,6	-	-	-		
74	OHX	B3	202	-	0,6,6	-	-	-		
74	OHX	B1	3588	-	0,6,6	-	-	-		
74	OHX	B1	3611	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
74	OHX	B1	3446	-	0,6,6	-	-	-		
74	OHX	D1	3460	-	0,6,6	-	-	-		
74	OHX	C1	1951	-	0,6,6	-	-	-		
74	OHX	D1	3621	-	0,6,6	-	-	-		
74	OHX	D1	3609	-	0,6,6	-	-	-		
74	OHX	A1	1950	-	0,6,6	-	-	-		
74	OHX	D1	3598	-	0,6,6	-	-	-		
74	OHX	A1	1980	-	0,6,6	-	-	-		
74	OHX	B1	3599	-	0,6,6	-	-	-		
74	OHX	B1	3444	-	0,6,6	-	-	-		
74	OHX	D1	3490	-	0,6,6	-	-	-		
74	OHX	A1	1958	-	0,6,6	-	-	-		
74	OHX	D1	3434	-	0,6,6	-	-	-		
74	OHX	D1	3618	-	0,6,6	-	-	-		
74	OHX	A1	1901	-	0,6,6	-	-	-		
74	OHX	D1	3478	-	0,6,6	-	-	-		
74	OHX	D1	3542	-	0,6,6	-	-	-		
74	OHX	D1	3558	-	0,6,6	-	-	-		
74	OHX	B1	3527	-	0,6,6	-	-	-		
74	OHX	D1	3493	-	0,6,6	-	-	-		
74	OHX	B1	3436	-	0,6,6	-	-	-		
74	OHX	D1	3507	-	0,6,6	-	-	-		
74	OHX	D1	3443	-	0,6,6	-	-	-		
74	OHX	B1	3429	-	0,6,6	-	-	-		
74	OHX	D1	3457	-	0,6,6	-	-	-		
74	OHX	A1	1930	-	0,6,6	-	-	-		
74	OHX	B1	3495	-	0,6,6	-	-	-		
74	OHX	A1	1945	-	0,6,6	-	-	-		
74	OHX	C1	1965	-	0,6,6	-	-	-		
74	OHX	C1	1988	-	0,6,6	-	-	-		
74	OHX	B1	3571	-	0,6,6	-	-	-		
74	OHX	D1	3576	-	0,6,6	-	-	-		
74	OHX	B1	3574	-	0,6,6	-	-	-		
74	OHX	B1	3445	-	0,6,6	-	-	-		
74	OHX	D1	3584	-	0,6,6	-	-	-		
74	OHX	D1	3446	-	0,6,6	-	-	-		
74	OHX	D1	3619	-	0,6,6	-	-	-		
74	OHX	C1	1976	-	0,6,6	-	-	-		
74	OHX	B1	3478	-	0,6,6	-	-	-		
74	OHX	D1	3414	-	0,6,6	-	-	-		
74	OHX	D1	3539	-	0,6,6	-	-	-		
74	OHX	B1	3597	-	0,6,6	-	-	-		
74	OHX	D1	3577	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
74	OHX	B1	3467	-	0,6,6	-	-	-		
74	OHX	A1	1998	-	0,6,6	-	-	-		
74	OHX	B1	3608	-	0,6,6	-	-	-		
74	OHX	A1	1908	-	0,6,6	-	-	-		
74	OHX	C1	1929	-	0,6,6	-	-	-		
74	OHX	C1	1985	-	0,6,6	-	-	-		
74	OHX	D1	3459	-	0,6,6	-	-	-		
74	OHX	D1	3552	-	0,6,6	-	-	-		
74	OHX	D1	3511	-	0,6,6	-	-	-		
74	OHX	B1	3610	-	0,6,6	-	-	-		
74	OHX	B1	3560	-	0,6,6	-	-	-		
74	OHX	B1	3536	-	0,6,6	-	-	-		
74	OHX	B1	3492	-	0,6,6	-	-	-		
74	OHX	D1	3458	-	0,6,6	-	-	-		
74	OHX	B1	3475	-	0,6,6	-	-	-		
74	OHX	D1	3541	-	0,6,6	-	-	-		
74	OHX	B1	3494	-	0,6,6	-	-	-		
74	OHX	D1	3567	-	0,6,6	-	-	-		
74	OHX	B1	3563	-	0,6,6	-	-	-		
74	OHX	D1	3547	-	0,6,6	-	-	-		
74	OHX	B2	201	-	0,6,6	-	-	-		
74	OHX	D1	3461	-	0,6,6	-	-	-		
74	OHX	B1	3569	-	0,6,6	-	-	-		
74	OHX	D1	3485	-	0,6,6	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

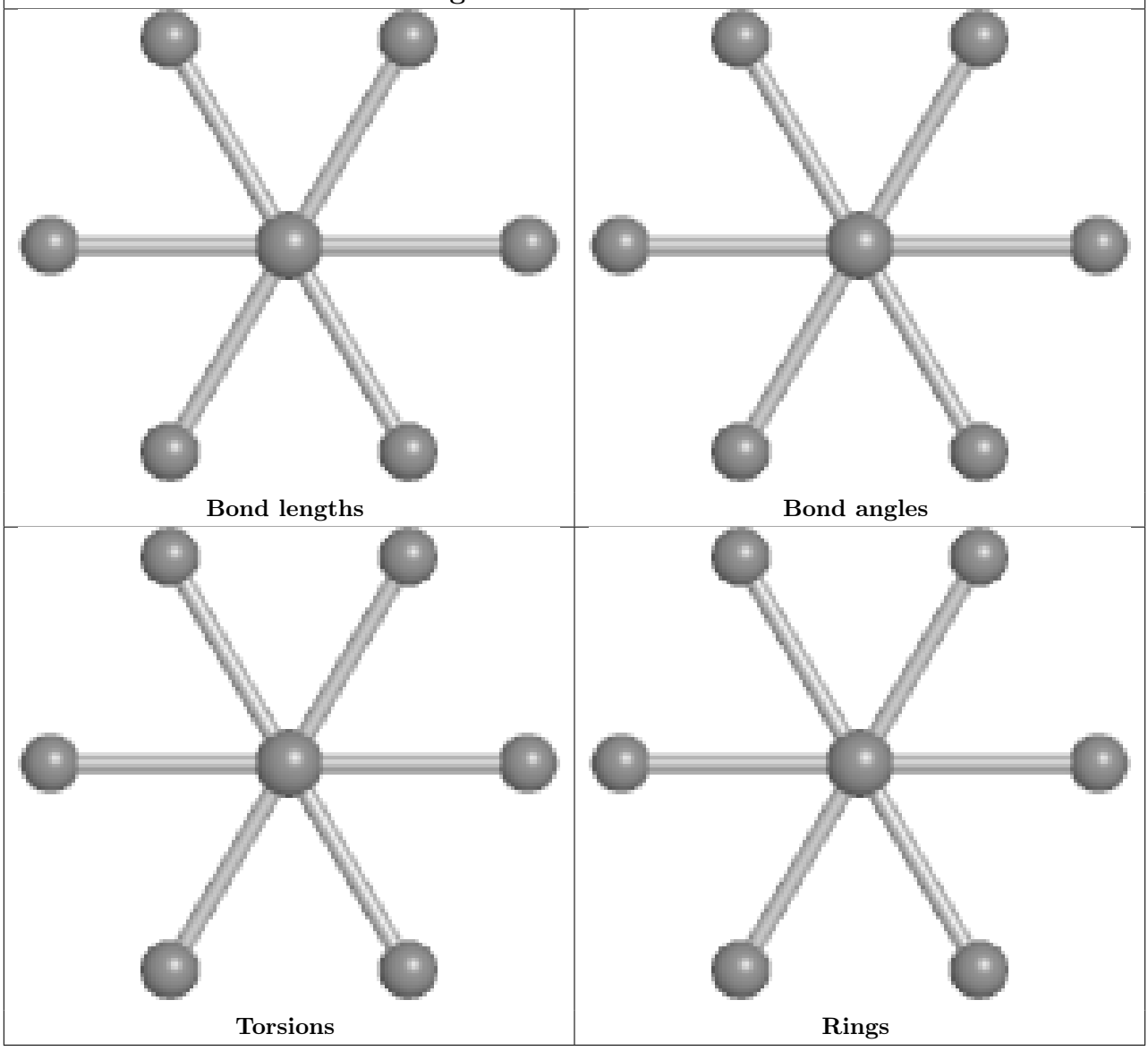
There are no ring outliers.

No monomer is involved in short contacts.

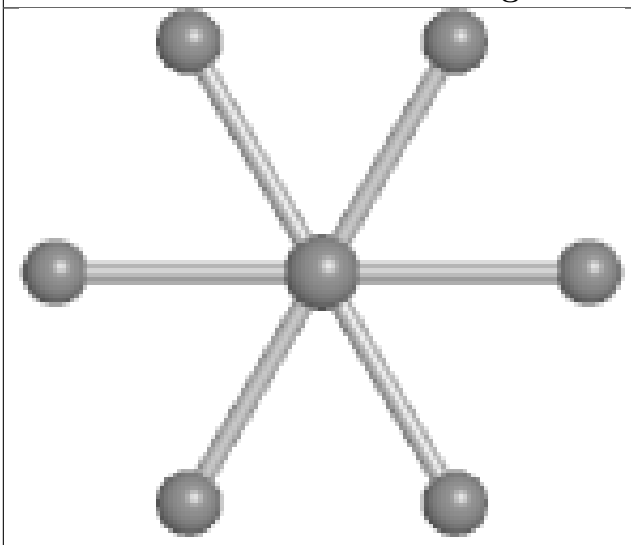
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

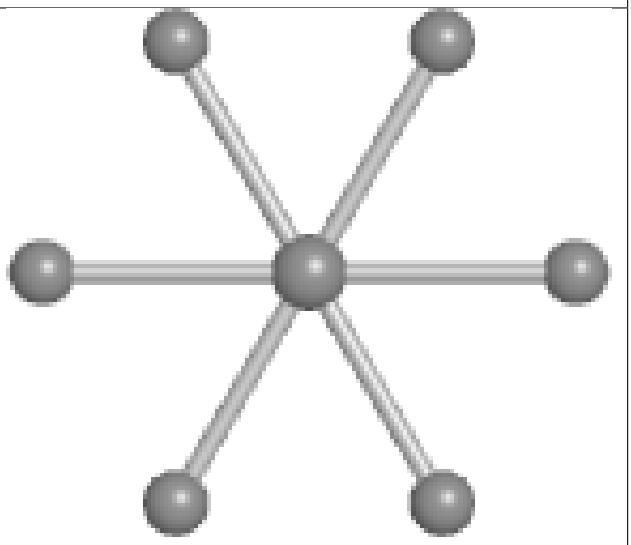
Ligand OHX D1 3573



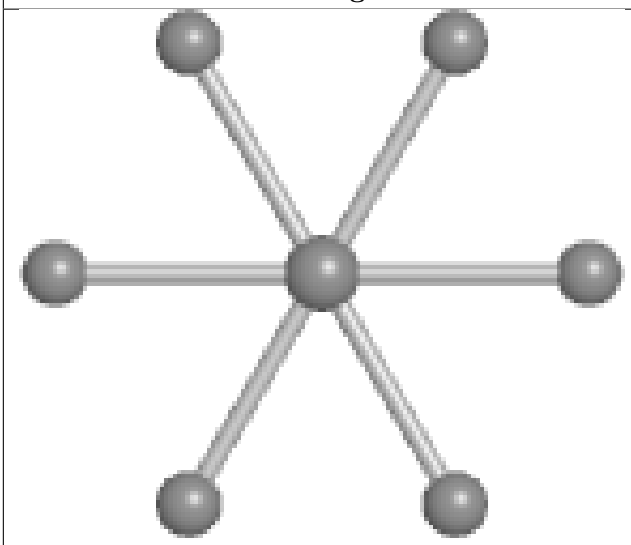
Ligand OHX D1 3586



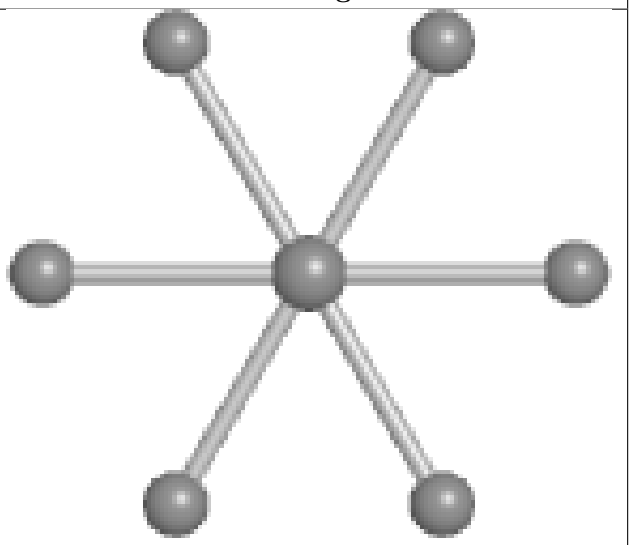
Bond lengths



Bond angles

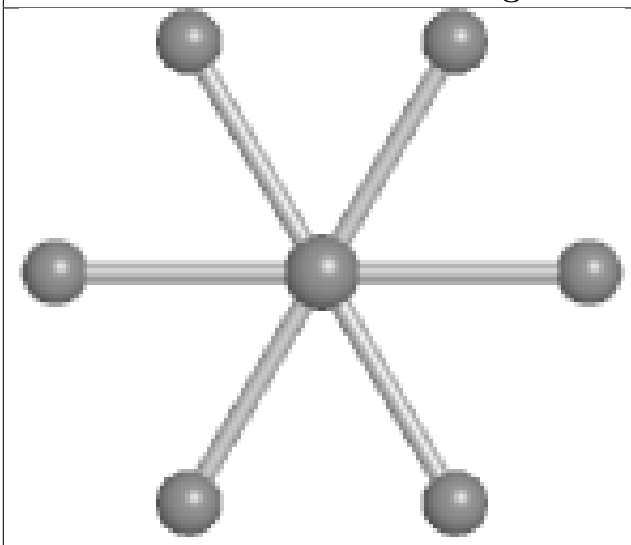


Torsions

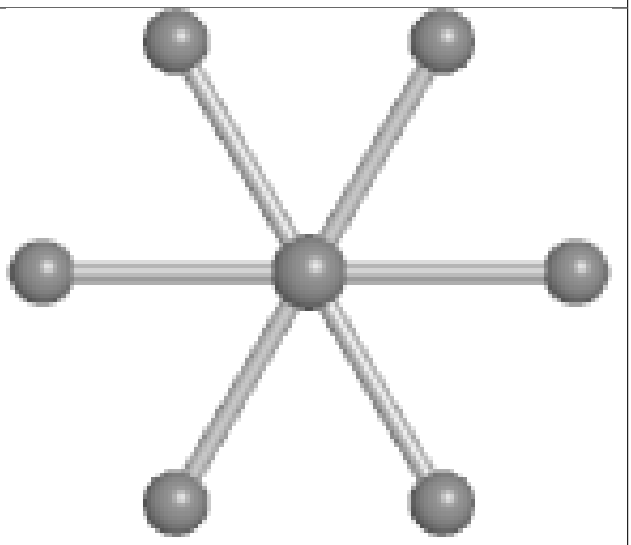


Rings

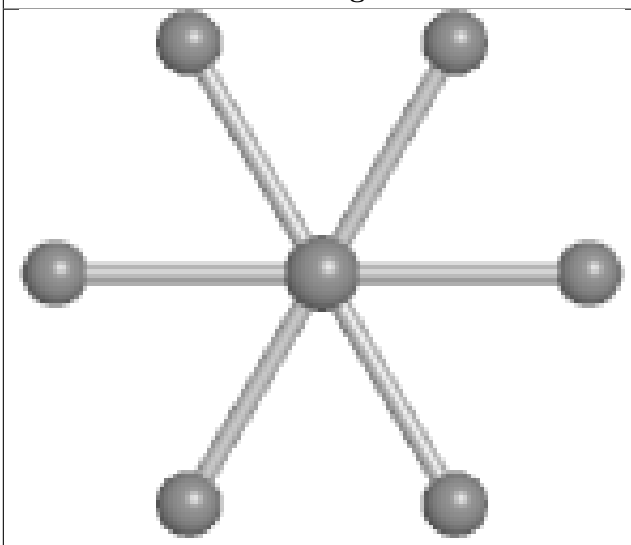
Ligand OHX B1 3602



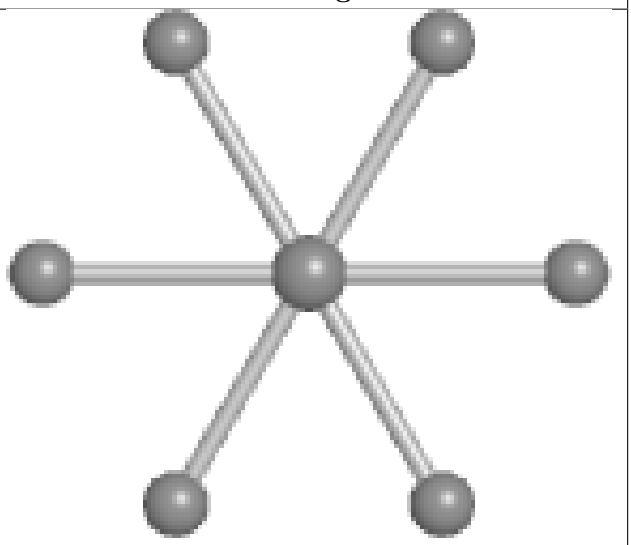
Bond lengths



Bond angles

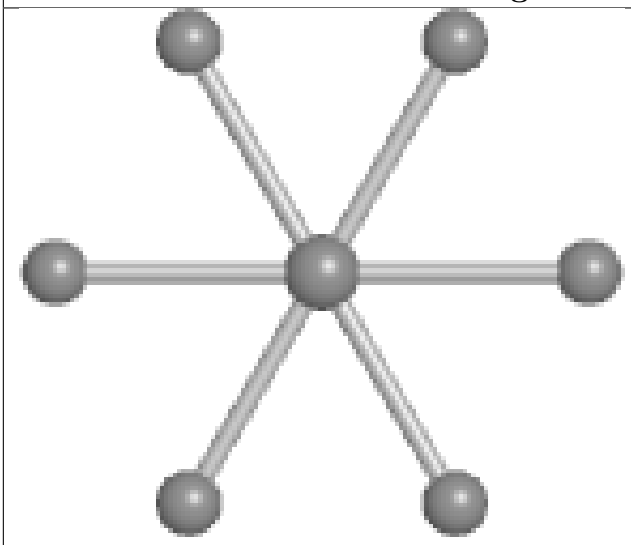


Torsions

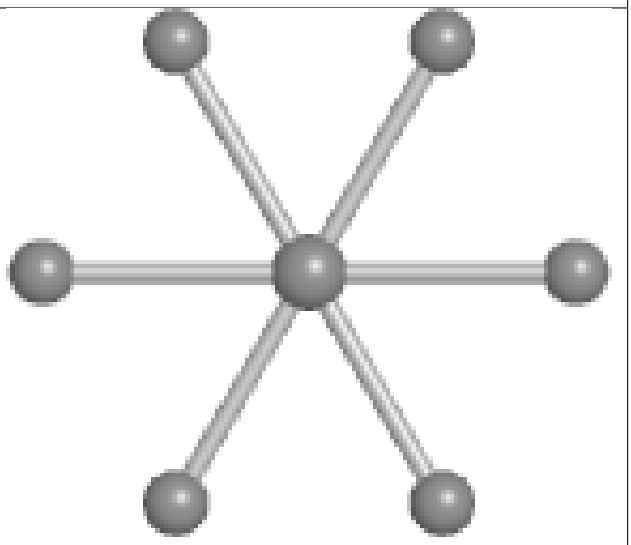


Rings

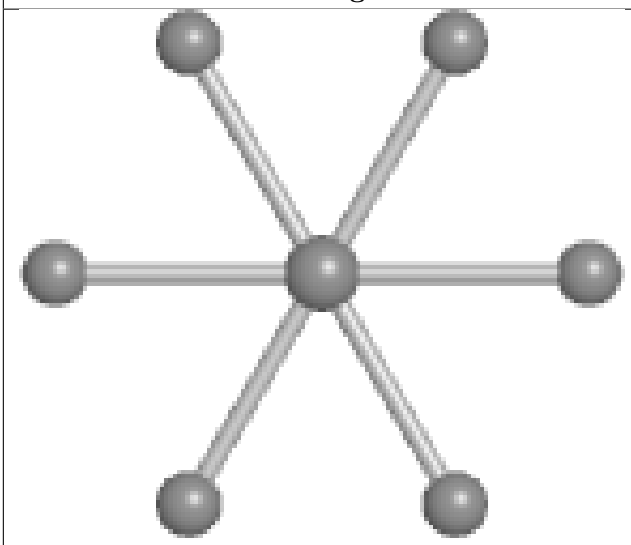
Ligand OHX D3 211



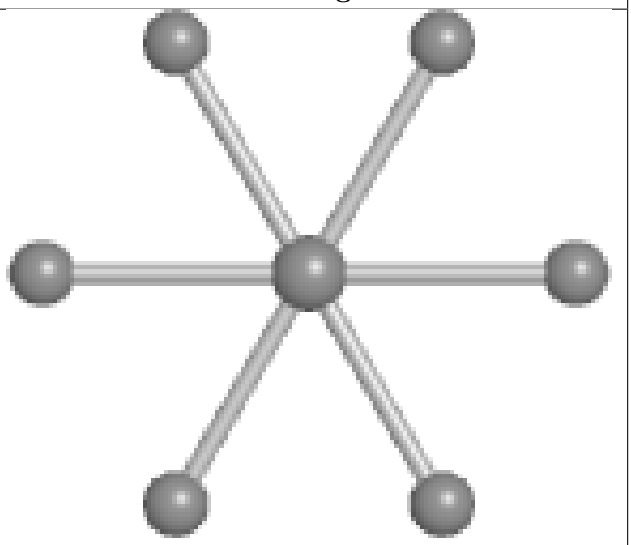
Bond lengths



Bond angles

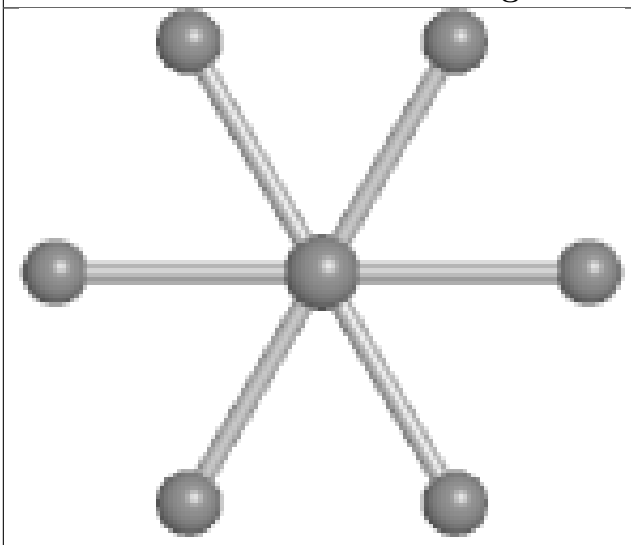


Torsions

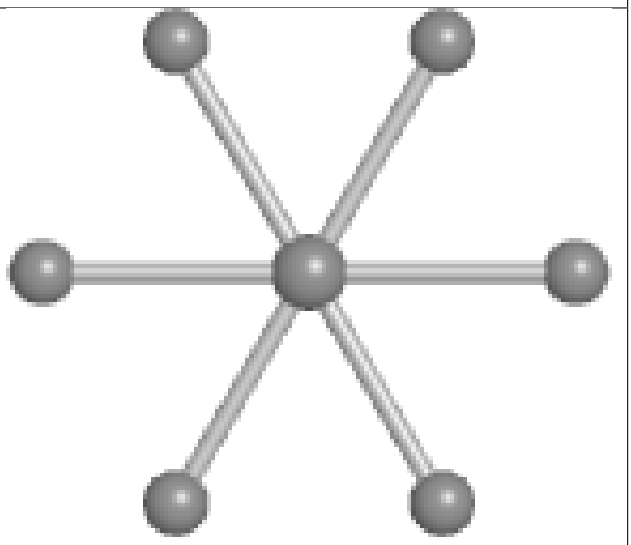


Rings

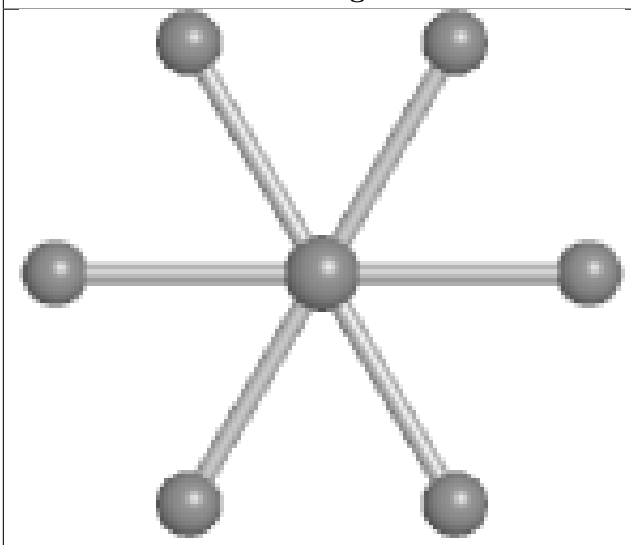
Ligand OHX D1 3605



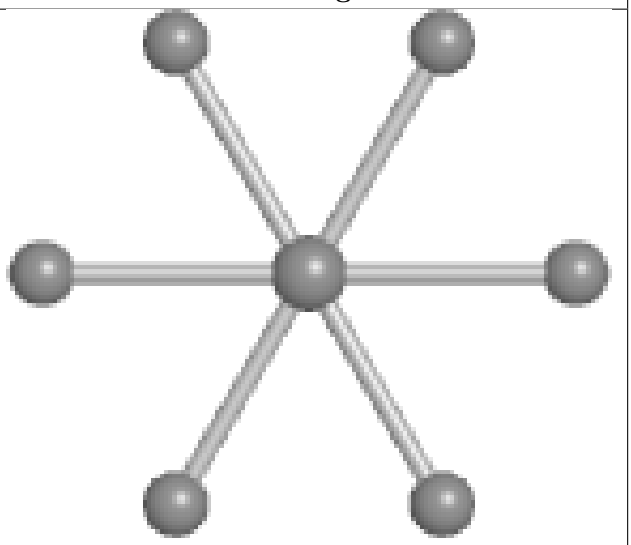
Bond lengths



Bond angles

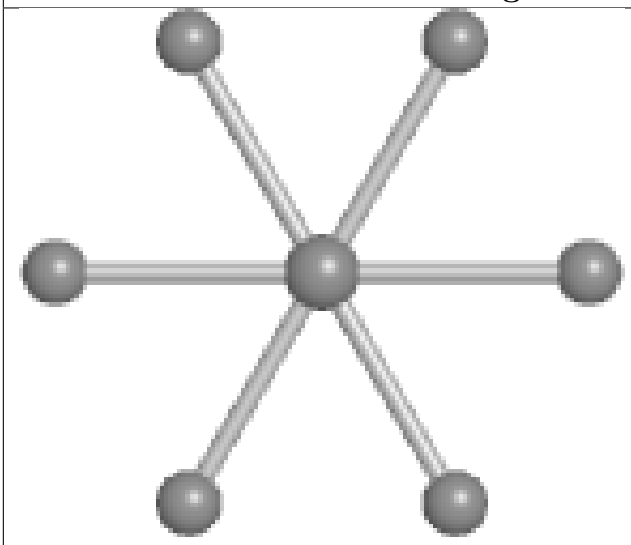


Torsions

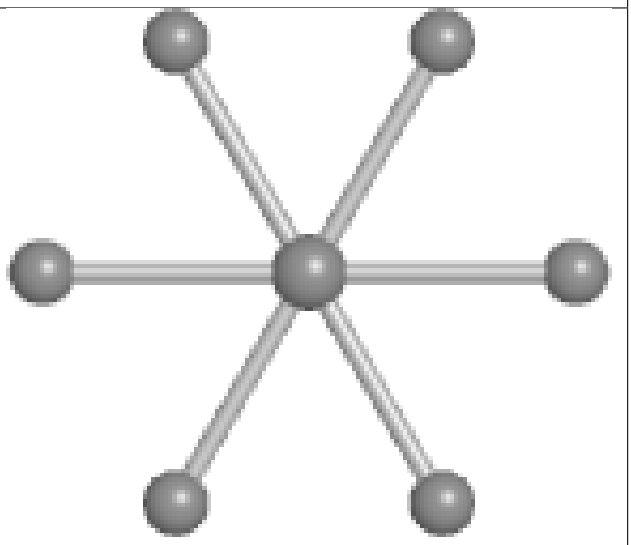


Rings

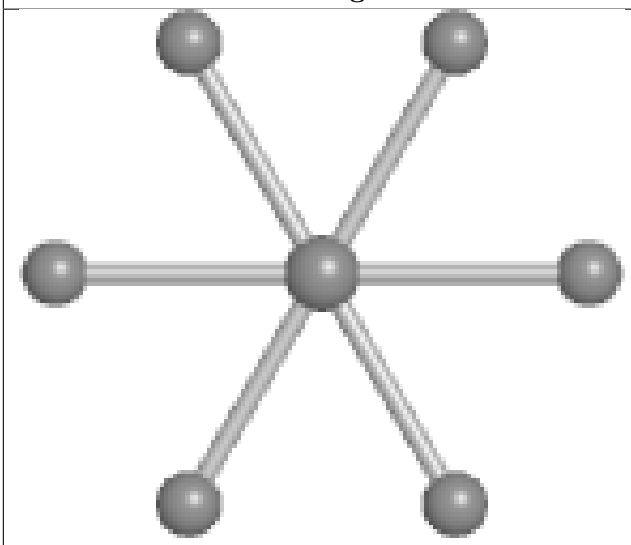
Ligand OHX B1 3548



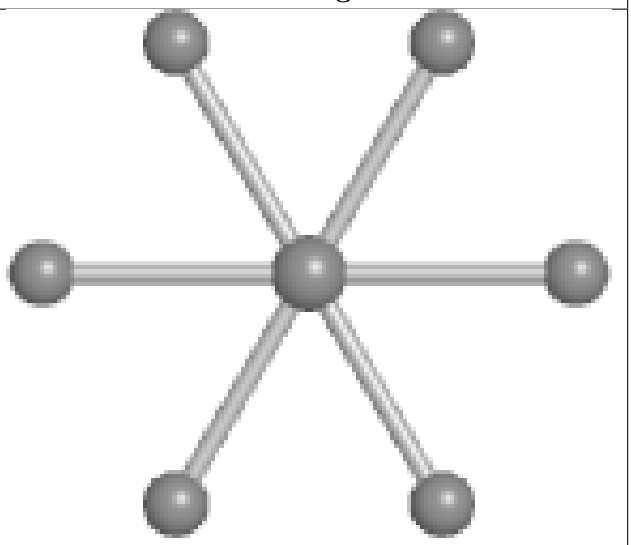
Bond lengths



Bond angles

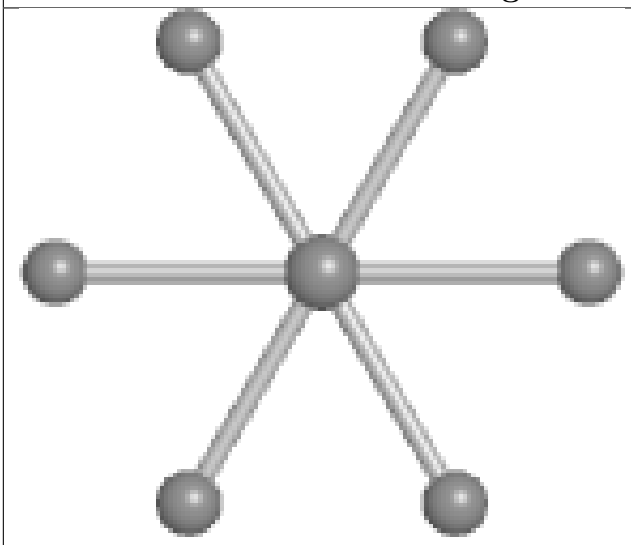


Torsions

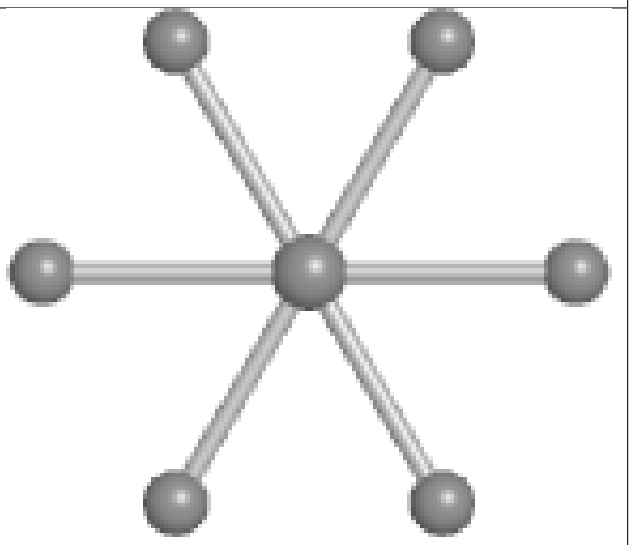


Rings

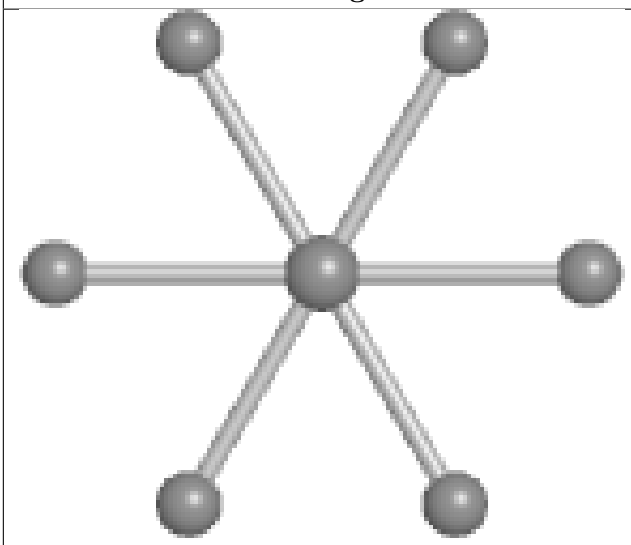
Ligand OHX A1 1983



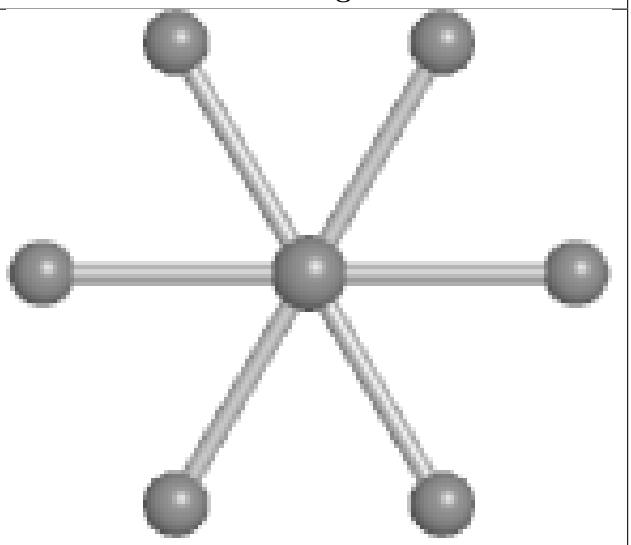
Bond lengths



Bond angles

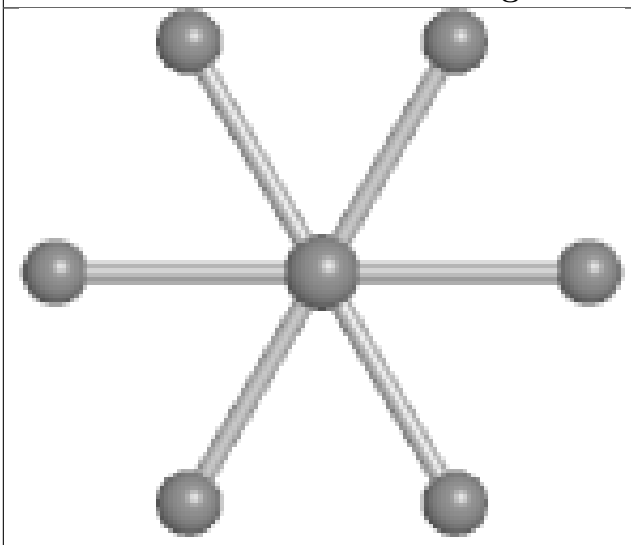


Torsions

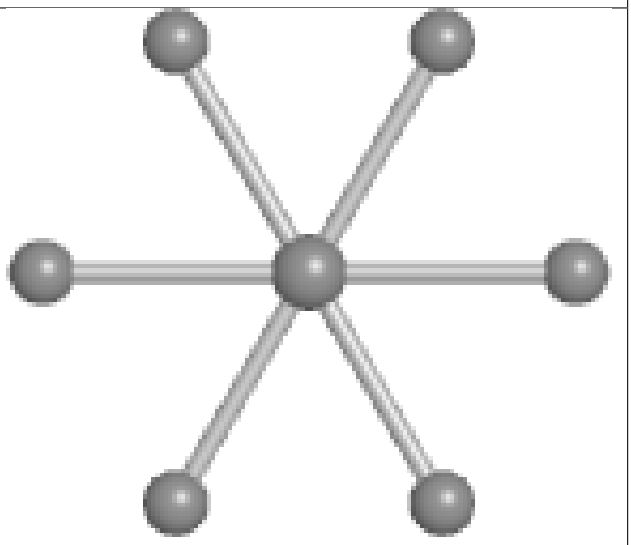


Rings

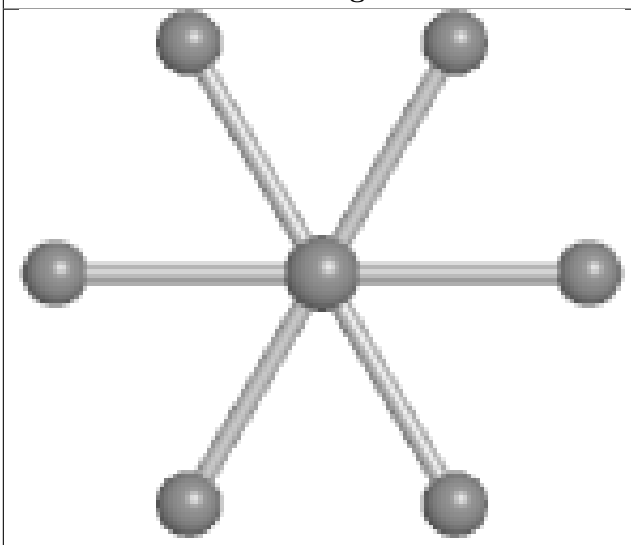
Ligand OHX D1 3593



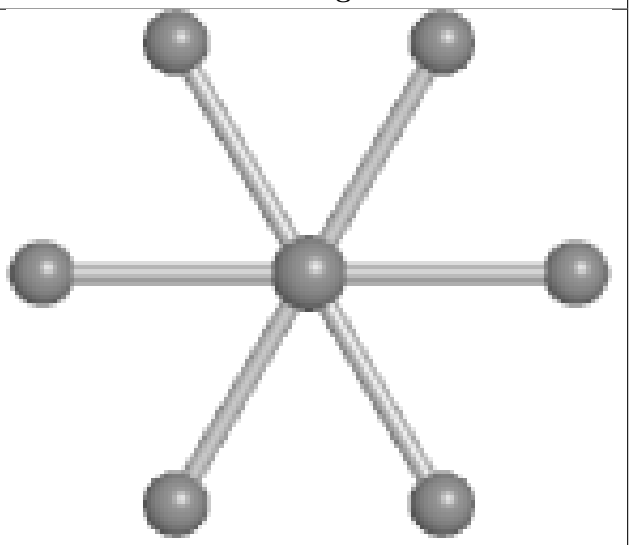
Bond lengths



Bond angles

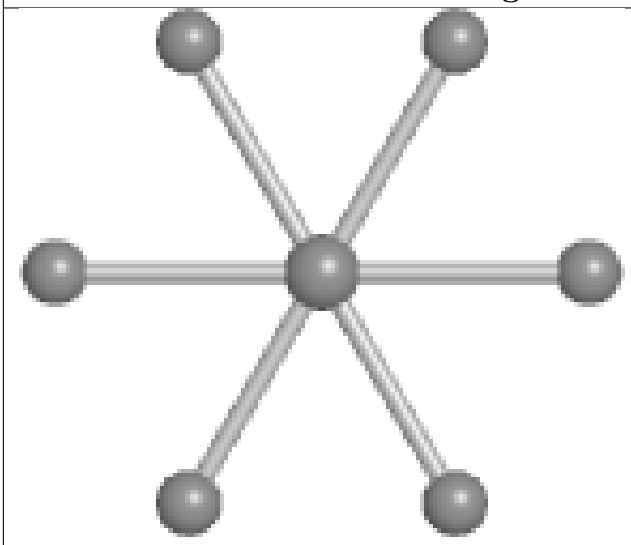


Torsions

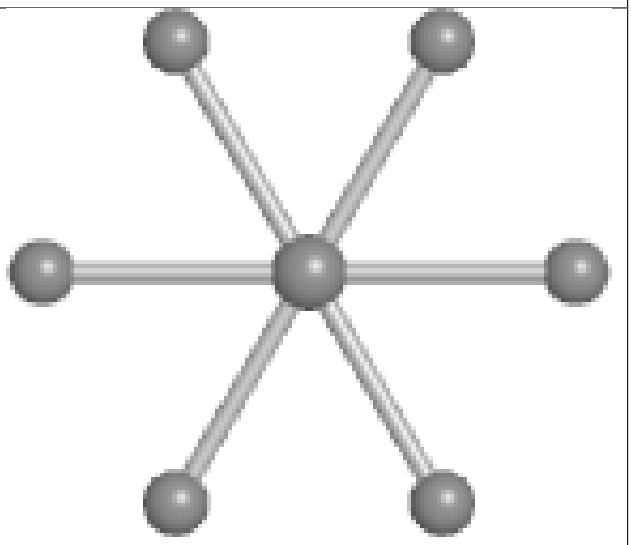


Rings

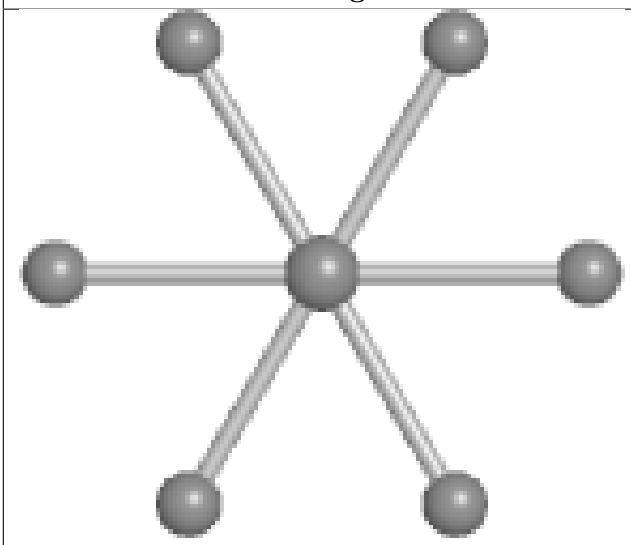
Ligand OHX A1 1930



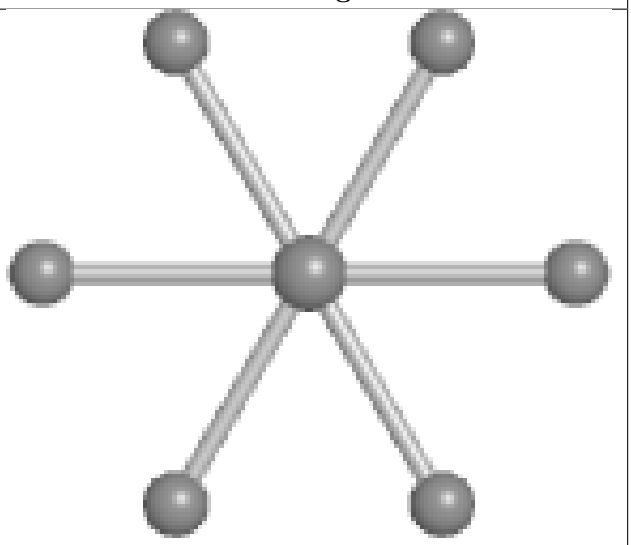
Bond lengths



Bond angles

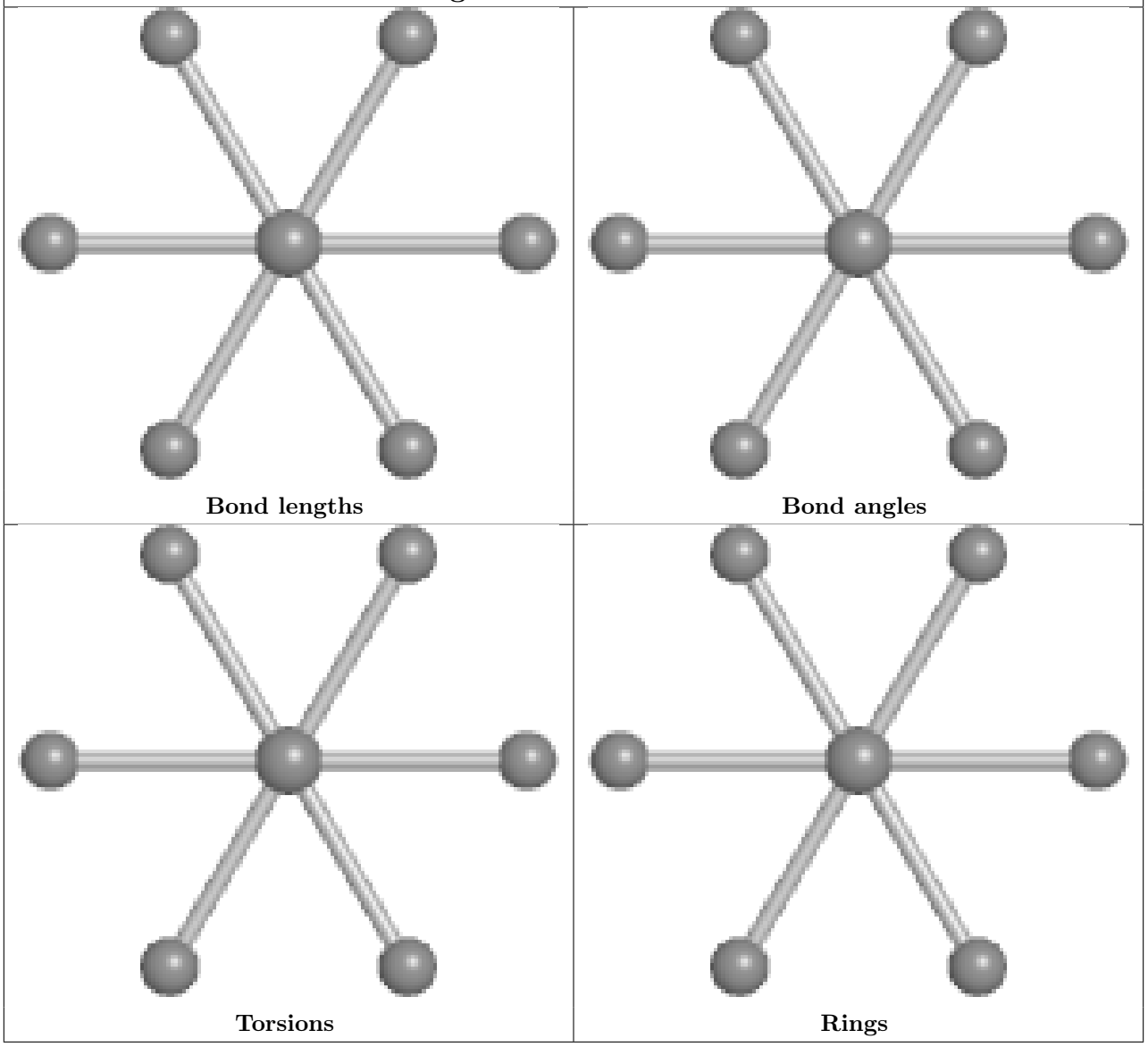


Torsions



Rings

Ligand OHX B1 3571



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	Ab	4
23	Cb	4
63	Bh	1

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Mol	Chain	Number of breaks
63	Dh	1
28	Ch	1
68	Bn	1
28	Ah	1
24	Cc	1
24	Ac	1

The worst 5 of 15 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Bh	23:UNK	C	34:UNK	N	29.25
1	Dh	23:UNK	C	34:UNK	N	28.80
1	Ch	25:UNK	C	50:UNK	N	22.77
1	Ab	19:UNK	C	21:UNK	N	20.41
1	Bn	19:UNK	C	27:UNK	N	20.28

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A1	1789/1800 (99%)	0.04	50 (2%) 53 42	45, 138, 429, 753	0
1	C1	1789/1800 (99%)	0.14	61 (3%) 45 36	42, 120, 419, 674	0
2	AA	220/252 (87%)	-0.53	5 (2%) 60 51	64, 150, 323, 474	0
2	CA	220/252 (87%)	-0.54	2 (0%) 84 77	66, 119, 336, 538	0
3	AB	219/254 (86%)	-0.38	3 (1%) 75 65	42, 117, 298, 500	0
3	CB	219/254 (86%)	-0.55	2 (0%) 84 77	50, 108, 288, 386	0
4	AC	189/240 (78%)	-0.35	2 (1%) 80 72	52, 120, 278, 403	0
4	CC	189/240 (78%)	-0.54	0 100 100	41, 120, 262, 460	0
5	AD	169/225 (75%)	-0.58	3 (1%) 68 59	58, 150, 355, 516	0
5	CD	169/225 (75%)	-0.63	3 (1%) 68 59	33, 108, 269, 383	0
6	AE	157/197 (79%)	-0.47	6 (3%) 40 32	44, 140, 362, 438	0
6	CE	157/197 (79%)	-0.46	1 (0%) 89 84	31, 99, 330, 482	0
7	AF	77/156 (49%)	-0.56	1 (1%) 77 68	45, 95, 205, 412	0
7	CF	77/156 (49%)	0.09	7 (9%) 9 8	56, 91, 267, 342	0
8	AG	117/151 (77%)	-0.78	0 100 100	35, 108, 284, 362	0
8	CG	117/151 (77%)	-0.76	0 100 100	46, 97, 263, 458	0
9	AH	128/137 (93%)	-0.21	6 (4%) 31 26	53, 186, 349, 436	0
9	CH	128/137 (93%)	-0.21	5 (3%) 39 31	39, 132, 354, 482	0
10	AI	121/142 (85%)	-0.51	2 (1%) 70 60	55, 140, 329, 419	0
10	CI	121/142 (85%)	-0.44	1 (0%) 86 79	46, 116, 273, 447	0
11	AJ	134/143 (93%)	-0.56	2 (1%) 73 64	74, 144, 302, 340	0
11	CJ	134/143 (93%)	-0.46	3 (2%) 62 52	44, 99, 288, 381	0
12	AK	67/136 (49%)	-0.43	2 (2%) 50 39	52, 142, 319, 407	0
12	CK	67/136 (49%)	0.19	5 (7%) 14 12	64, 199, 350, 401	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AL	120/146 (82%)	-0.46	2 (1%) 70 60	55, 146, 298, 514	0
13	CL	120/146 (82%)	-0.41	5 (4%) 36 29	52, 96, 293, 519	0
14	AM	106/144 (73%)	-0.53	2 (1%) 66 58	71, 138, 348, 425	0
14	CM	106/144 (73%)	-0.57	2 (1%) 66 58	42, 81, 260, 338	0
15	AN	111/121 (91%)	-0.34	3 (2%) 54 44	68, 129, 336, 412	0
15	CN	111/121 (91%)	-0.34	1 (0%) 84 77	32, 111, 286, 424	0
16	AO	127/130 (97%)	-0.39	0 100 100	53, 95, 256, 411	0
16	CO	127/130 (97%)	-0.75	0 100 100	54, 91, 229, 441	0
17	AP	116/145 (80%)	-0.63	0 100 100	29, 95, 247, 384	0
17	CP	116/145 (80%)	-0.63	0 100 100	29, 71, 190, 418	0
18	AQ	67/108 (62%)	-0.42	1 (1%) 73 64	94, 210, 332, 355	0
18	CQ	63/108 (58%)	-0.33	2 (3%) 47 37	68, 150, 282, 307	0
19	AR	47/67 (70%)	0.11	4 (8%) 10 9	107, 245, 393, 457	0
19	CR	47/67 (70%)	0.37	5 (10%) 6 6	51, 221, 381, 425	0
20	AS	39/56 (69%)	-0.48	0 100 100	58, 108, 181, 260	0
20	CS	39/56 (69%)	-0.49	0 100 100	37, 95, 140, 292	0
21	AT	313/319 (98%)	-0.23	12 (3%) 40 32	106, 195, 286, 348	0
21	CT	313/319 (98%)	-0.20	13 (4%) 36 29	67, 158, 257, 328	0
22	Aa	0/20	-	-	-	-
22	Bo	0/20	-	-	-	-
22	Ca	0/20	-	-	-	-
23	Ab	0/105	-	-	-	-
23	Cb	0/105	-	-	-	-
24	Ac	0/93	-	-	-	-
24	Cc	0/93	-	-	-	-
25	Ad	0/35	-	-	-	-
25	Cd	0/35	-	-	-	-
26	Ae	0/21	-	-	-	-
26	Bj	0/21	-	-	-	-
26	Dj	0/21	-	-	-	-
27	Af	0/11	-	-	-	-
28	Ah	0/41	-	-	-	-
28	Ch	0/41	-	-	-	-
29	B1	3206/3396 (94%)	0.04	83 (2%) 56 46	33, 86, 395, 634	0
29	D1	3206/3396 (94%)	0.09	88 (2%) 54 44	30, 94, 427, 674	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
30	B2	121/121 (100%)	-0.09	0 100 100	46, 118, 189, 323	0
30	D2	121/121 (100%)	-0.06	1 (0%) 86 79	36, 95, 180, 349	0
31	B3	158/158 (100%)	0.00	6 (3%) 40 32	46, 108, 258, 619	0
31	D3	158/158 (100%)	-0.02	2 (1%) 77 68	59, 136, 358, 586	0
32	BA	213/217 (98%)	0.51	33 (15%) 2 2	137, 327, 441, 483	0
32	DA	213/217 (98%)	0.73	42 (19%) 1 1	159, 354, 442, 484	0
33	BB	234/254 (92%)	-0.46	3 (1%) 77 68	25, 83, 246, 419	0
33	DB	234/254 (92%)	-0.24	5 (2%) 63 54	54, 108, 254, 417	0
34	BC	364/387 (94%)	-0.61	1 (0%) 94 90	20, 66, 216, 560	0
34	DC	364/387 (94%)	-0.69	0 100 100	29, 58, 208, 543	0
35	BD	268/362 (74%)	-0.71	0 100 100	34, 70, 207, 500	0
35	DD	268/362 (74%)	-0.52	2 (0%) 87 82	50, 102, 274, 463	0
36	BE	287/297 (96%)	-0.46	2 (0%) 87 82	58, 119, 355, 497	0
36	DE	287/297 (96%)	-0.60	6 (2%) 63 54	38, 91, 302, 478	0
37	BF	176/176 (100%)	-0.61	2 (1%) 80 72	25, 81, 305, 519	0
37	DF	176/176 (100%)	-0.50	1 (0%) 89 84	31, 69, 342, 518	0
38	BG	215/244 (88%)	-0.85	0 100 100	21, 59, 226, 486	0
38	DG	215/244 (88%)	-0.89	0 100 100	25, 49, 167, 330	0
39	BH	173/256 (67%)	-0.45	4 (2%) 60 51	45, 110, 297, 429	0
39	DH	173/256 (67%)	-0.38	4 (2%) 60 51	70, 146, 316, 422	0
40	BI	191/191 (100%)	-0.51	2 (1%) 82 74	27, 83, 237, 347	0
40	DI	191/191 (100%)	-0.89	0 100 100	22, 49, 164, 286	0
41	BJ	208/221 (94%)	-0.64	1 (0%) 91 85	39, 93, 251, 452	0
41	DJ	208/221 (94%)	-0.73	1 (0%) 91 85	25, 64, 257, 456	0
42	BK	165/174 (94%)	-0.48	4 (2%) 59 49	56, 125, 348, 497	0
42	DK	165/174 (94%)	-0.60	1 (0%) 89 84	45, 97, 330, 532	0
43	BN	120/138 (86%)	-0.58	0 100 100	34, 77, 260, 387	0
43	DN	120/138 (86%)	-0.69	1 (0%) 86 79	33, 60, 262, 325	0
44	BO	187/204 (91%)	-0.55	1 (0%) 91 85	38, 86, 178, 383	0
44	DO	187/204 (91%)	-0.36	4 (2%) 63 54	57, 119, 255, 327	0
45	BP	196/199 (98%)	-0.84	0 100 100	23, 48, 152, 409	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
45	DP	196/199 (98%)	-0.74	1 (0%) 91 85	23, 45, 111, 424	0
46	BQ	154/184 (83%)	-0.73	0 100 100	30, 55, 144, 337	0
46	DQ	154/184 (83%)	-0.78	0 100 100	37, 77, 243, 373	0
47	BR	143/186 (76%)	-0.71	1 (0%) 87 82	38, 70, 200, 421	0
47	DR	143/186 (76%)	-0.30	4 (2%) 53 42	60, 87, 244, 378	0
48	BS	188/189 (99%)	-0.49	3 (1%) 72 62	52, 101, 419, 569	0
48	DS	188/189 (99%)	0.17	25 (13%) 3 4	59, 109, 589, 657	0
49	BT	119/160 (74%)	-0.57	1 (0%) 86 79	42, 73, 221, 310	0
49	DT	119/160 (74%)	-0.62	0 100 100	36, 72, 184, 282	0
50	BU	129/137 (94%)	-0.55	0 100 100	27, 70, 208, 391	0
50	DU	129/137 (94%)	-0.62	0 100 100	20, 48, 151, 235	0
51	BV	59/155 (38%)	-0.68	0 100 100	29, 84, 259, 363	0
51	DV	59/155 (38%)	-0.48	1 (1%) 70 60	53, 73, 197, 320	0
52	BW	94/142 (66%)	-0.44	0 100 100	53, 91, 211, 312	0
52	DW	94/142 (66%)	-0.45	1 (1%) 80 72	64, 124, 247, 337	0
53	BX	107/127 (84%)	-0.70	0 100 100	58, 91, 182, 233	0
53	DX	107/127 (84%)	-0.48	2 (1%) 66 58	56, 106, 248, 361	0
54	BY	149/149 (100%)	-0.46	3 (2%) 65 56	30, 76, 331, 456	0
54	DY	149/149 (100%)	-0.52	1 (0%) 87 82	49, 95, 277, 409	0
55	BZ	98/105 (93%)	-0.33	2 (2%) 65 56	52, 128, 269, 360	0
55	DZ	98/105 (93%)	-0.30	3 (3%) 49 38	56, 134, 272, 365	0
56	Ba	86/113 (76%)	-0.67	0 100 100	38, 83, 232, 396	0
56	Da	86/113 (76%)	-0.64	0 100 100	51, 82, 274, 430	0
57	Bb	125/130 (96%)	-0.78	0 100 100	26, 54, 138, 435	0
57	Db	125/130 (96%)	-0.48	1 (0%) 86 79	39, 77, 168, 380	0
58	Bc	68/120 (56%)	-0.66	0 100 100	46, 89, 202, 381	0
58	Dc	68/120 (56%)	-0.74	1 (1%) 73 64	50, 123, 270, 348	0
59	Bd	72/88 (81%)	-0.53	0 100 100	36, 79, 322, 434	0
59	Dd	72/88 (81%)	-0.62	0 100 100	30, 103, 268, 336	0
60	Be	48/51 (94%)	-0.65	0 100 100	30, 72, 159, 290	0
60	De	48/51 (94%)	-0.58	0 100 100	40, 118, 222, 333	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
61	Bf	95/106 (89%)	-0.19	3 (3%) 47 37	57, 145, 363, 475	0
61	Df	95/106 (89%)	0.22	10 (10%) 6 6	62, 195, 389, 486	0
62	Bg	83/92 (90%)	-0.68	1 (1%) 79 70	35, 98, 311, 431	0
62	Dg	83/92 (90%)	-0.63	0 100 100	42, 103, 241, 369	0
63	Bh	0/44	-	-	-	-
63	Dh	0/44	-	-	-	-
64	Bi	0/12	-	-	-	-
64	Di	0/12	-	-	-	-
65	Bk	0/16	-	-	-	-
65	Dk	0/16	-	-	-	-
66	Bl	0/19	-	-	-	-
67	Bm	0/9	-	-	-	-
68	Bn	0/27	-	-	-	-
69	Bp	0/8	-	-	-	-
70	Bq	0/17	-	-	-	-
71	Br	0/23	-	-	-	-
72	DL	138/165 (83%)	-0.58	2 (1%) 75 65	84, 172, 387, 465	0
73	DM	130/312 (41%)	-0.53	2 (1%) 73 64	47, 121, 305, 409	0
All	All	25728/30002 (85%)	-0.26	592 (2%) 60 51	20, 105, 353, 753	0

The worst 5 of 592 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	B1	136	G	14.9
1	C1	681	U	14.6
29	D1	2495	C	14.4
1	A1	1701	A	13.6
29	D1	2494	A	13.5

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
74	OHX	B2	209	7/7	0.66	0.34	148,148,148,148	7
74	OHX	C1	1972	7/7	0.66	0.30	216,216,216,216	7
74	OHX	D1	3593	7/7	0.69	0.53	99,99,99,99	7
74	OHX	D1	3542	7/7	0.70	0.38	198,198,198,198	7
74	OHX	D3	211	7/7	0.70	0.41	137,137,137,137	7
74	OHX	D1	3525	7/7	0.72	0.27	106,106,106,106	7
74	OHX	C1	1950	7/7	0.72	0.28	215,215,215,215	7
74	OHX	C1	1970	7/7	0.73	0.30	176,176,176,176	7
74	OHX	A1	1930	7/7	0.73	0.43	228,228,228,228	7
74	OHX	D3	206	7/7	0.73	0.36	77,77,77,77	7
74	OHX	B1	3602	7/7	0.73	0.44	75,75,75,75	7
74	OHX	D3	205	7/7	0.74	0.25	199,199,199,199	7
74	OHX	A1	1983	7/7	0.74	0.59	122,122,122,122	7
74	OHX	B1	3571	7/7	0.74	0.48	176,176,176,176	7
74	OHX	C1	1978	7/7	0.75	0.29	145,145,145,145	7
74	OHX	D1	3551	7/7	0.76	0.30	120,120,120,120	7
74	OHX	D1	3573	7/7	0.76	0.43	135,135,135,135	7
74	OHX	C1	1957	7/7	0.76	0.38	226,226,226,226	7
74	OHX	C1	1979	7/7	0.77	0.33	190,190,190,190	7
74	OHX	B1	3552	7/7	0.77	0.32	138,138,138,138	7
74	OHX	D1	3605	7/7	0.77	0.47	93,93,93,93	7
74	OHX	D1	3522	7/7	0.78	0.27	133,133,133,133	7
74	OHX	A1	1999	7/7	0.78	0.38	99,99,99,99	7
74	OHX	D3	208	7/7	0.78	0.28	135,135,135,135	7
74	OHX	D1	3566	7/7	0.78	0.36	88,88,88,88	7
74	OHX	D1	3618	7/7	0.79	0.34	62,62,62,62	7
74	OHX	D1	3556	7/7	0.79	0.24	146,146,146,146	7
74	OHX	D1	3586	7/7	0.79	0.62	115,115,115,115	7
74	OHX	D1	3564	7/7	0.79	0.38	85,85,85,85	7
74	OHX	B1	3548	7/7	0.79	0.60	153,153,153,153	7
74	OHX	DE	301	7/7	0.79	0.24	302,302,302,302	7
74	OHX	C1	1988	7/7	0.80	0.27	146,146,146,146	7
74	OHX	C1	1998	7/7	0.80	0.62	129,129,129,129	7
74	OHX	B3	206	7/7	0.80	0.37	201,201,201,201	7
74	OHX	C1	1976	7/7	0.80	0.37	118,118,118,118	7
74	OHX	D1	3535	7/7	0.80	0.32	142,142,142,142	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
74	OHX	B1	3535	7/7	0.81	0.28	170,170,170,170	7
74	OHX	D1	3578	7/7	0.81	0.70	222,222,222,222	7
74	OHX	C1	1958	7/7	0.81	0.23	153,153,153,153	7
74	OHX	D1	3589	7/7	0.81	0.32	56,56,56,56	7
74	OHX	A1	1974	7/7	0.81	0.40	136,136,136,136	7
74	OHX	CS	102	7/7	0.81	0.35	184,184,184,184	7
74	OHX	B1	3577	7/7	0.82	0.47	148,148,148,148	7
74	OHX	C1	1962	7/7	0.82	0.30	180,180,180,180	7
74	OHX	B2	208	7/7	0.82	0.48	152,152,152,152	7
74	OHX	C1	1974	7/7	0.83	0.34	118,118,118,118	7
74	OHX	A1	1953	7/7	0.83	0.39	122,122,122,122	7
74	OHX	D1	3609	7/7	0.83	0.45	73,73,73,73	7
74	OHX	B1	3554	7/7	0.83	0.69	156,156,156,156	7
74	OHX	A1	1962	7/7	0.83	0.49	193,193,193,193	7
74	OHX	D1	3541	7/7	0.83	0.31	141,141,141,141	7
74	OHX	A1	1998	7/7	0.83	0.32	125,125,125,125	7
74	OHX	D1	3587	7/7	0.83	0.58	111,111,111,111	7
74	OHX	B1	3599	7/7	0.83	0.28	87,87,87,87	7
74	OHX	D1	3590	7/7	0.84	0.40	55,55,55,55	7
74	OHX	B1	3601	7/7	0.84	0.36	158,158,158,158	7
74	OHX	D1	3599	7/7	0.84	0.36	93,93,93,93	7
74	OHX	C1	1952	7/7	0.84	0.21	239,239,239,239	7
74	OHX	B1	3568	7/7	0.84	0.22	94,94,94,94	7
74	OHX	A1	2000	7/7	0.84	0.45	75,75,75,75	7
74	OHX	D1	3580	7/7	0.84	0.29	114,114,114,114	7
74	OHX	D1	3583	7/7	0.84	0.28	88,88,88,88	7
74	OHX	B1	3514	7/7	0.84	0.30	123,123,123,123	7
74	OHX	B2	210	7/7	0.84	0.43	131,131,131,131	7
74	OHX	B1	3555	7/7	0.84	0.30	103,103,103,103	7
74	OHX	B1	3580	7/7	0.85	0.38	84,84,84,84	7
74	OHX	A1	1993	7/7	0.85	0.33	108,108,108,108	7
74	OHX	B1	3600	7/7	0.85	0.34	135,135,135,135	7
74	OHX	C1	1990	7/7	0.85	0.27	105,105,105,105	7
74	OHX	C1	1993	7/7	0.85	0.28	93,93,93,93	7
74	OHX	C1	1968	7/7	0.85	0.30	103,103,103,103	7
74	OHX	B1	3560	7/7	0.85	0.33	105,105,105,105	7
74	OHX	D1	3488	7/7	0.85	0.20	141,141,141,141	7
74	OHX	D1	3509	7/7	0.85	0.33	120,120,120,120	7
74	OHX	C1	1938	7/7	0.85	0.30	191,191,191,191	7
74	OHX	B1	3562	7/7	0.85	0.59	130,130,130,130	7
74	OHX	B1	3621	7/7	0.85	0.36	83,83,83,83	7
74	OHX	D1	3553	7/7	0.86	0.25	145,145,145,145	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
74	OHX	B1	3511	7/7	0.86	0.39	160,160,160,160	7
74	OHX	D1	3596	7/7	0.86	0.21	114,114,114,114	7
74	OHX	D1	3490	7/7	0.86	0.36	167,167,167,167	7
74	OHX	D1	3600	7/7	0.86	0.30	96,96,96,96	7
74	OHX	D1	3507	7/7	0.86	0.28	133,133,133,133	7
74	OHX	A1	1958	7/7	0.86	0.19	116,116,116,116	7
74	OHX	A1	1990	7/7	0.86	0.28	117,117,117,117	7
74	OHX	C1	1966	7/7	0.86	0.42	127,127,127,127	7
74	OHX	A1	2002	7/7	0.86	0.43	185,185,185,185	7
74	OHX	B1	3614	7/7	0.86	0.34	163,163,163,163	7
74	OHX	B1	3561	7/7	0.86	0.50	280,280,280,280	7
74	OHX	B2	206	7/7	0.86	0.21	128,128,128,128	7
74	OHX	DO	301	7/7	0.86	0.23	285,285,285,285	7
74	OHX	A1	1978	7/7	0.87	0.36	139,139,139,139	7
74	OHX	C1	1954	7/7	0.87	0.25	116,116,116,116	7
74	OHX	D1	3529	7/7	0.87	0.28	130,130,130,130	7
74	OHX	B1	3581	7/7	0.87	0.34	106,106,106,106	7
74	OHX	B1	3583	7/7	0.87	0.28	126,126,126,126	7
74	OHX	C1	1959	7/7	0.87	0.29	166,166,166,166	7
74	OHX	B1	3539	7/7	0.87	0.33	137,137,137,137	7
74	OHX	B1	3493	7/7	0.87	0.21	135,135,135,135	7
74	OHX	B1	3526	7/7	0.87	0.25	174,174,174,174	7
74	OHX	D1	3563	7/7	0.87	0.35	99,99,99,99	7
74	OHX	D1	3616	7/7	0.87	0.46	150,150,150,150	7
74	OHX	C1	1969	7/7	0.87	0.30	133,133,133,133	7
74	OHX	D2	208	7/7	0.87	0.39	105,105,105,105	7
74	OHX	D2	209	7/7	0.87	0.32	74,74,74,74	7
74	OHX	BO	301	7/7	0.87	0.38	110,110,110,110	7
74	OHX	B1	3529	7/7	0.87	0.14	171,171,171,171	7
74	OHX	B1	3533	7/7	0.87	0.34	149,149,149,149	7
74	OHX	D1	3515	7/7	0.87	0.25	173,173,173,173	7
74	OHX	D1	3521	7/7	0.87	0.24	163,163,163,163	7
74	OHX	D1	3585	7/7	0.87	0.24	102,102,102,102	7
74	OHX	C1	1945	7/7	0.88	0.24	122,122,122,122	7
74	OHX	A1	1985	7/7	0.88	0.33	86,86,86,86	7
74	OHX	D1	3550	7/7	0.88	0.45	100,100,100,100	7
74	OHX	D1	3481	7/7	0.88	0.29	137,137,137,137	7
74	OHX	D1	3485	7/7	0.88	0.29	90,90,90,90	7
74	OHX	D1	3555	7/7	0.88	0.31	150,150,150,150	7
74	OHX	B2	204	7/7	0.88	0.23	132,132,132,132	7
74	OHX	D1	3558	7/7	0.88	0.30	127,127,127,127	7
74	OHX	A1	1951	7/7	0.88	0.29	259,259,259,259	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
74	OHX	D1	3611	7/7	0.88	0.36	82,82,82,82	7
74	OHX	B1	3544	7/7	0.88	0.30	130,130,130,130	7
74	OHX	A1	1925	7/7	0.88	0.37	165,165,165,165	7
74	OHX	D1	3624	7/7	0.88	0.42	95,95,95,95	7
74	OHX	D1	3569	7/7	0.88	0.29	88,88,88,88	7
74	OHX	D1	3572	7/7	0.88	0.34	91,91,91,91	7
74	OHX	B1	3474	7/7	0.88	0.26	179,179,179,179	7
74	OHX	C1	1985	7/7	0.88	0.30	153,153,153,153	7
74	OHX	C1	1987	7/7	0.88	0.36	108,108,108,108	7
74	OHX	A1	1964	7/7	0.88	0.74	85,85,85,85	7
74	OHX	B1	3603	7/7	0.88	0.29	63,63,63,63	7
74	OHX	DJ	301	7/7	0.88	0.29	138,138,138,138	7
74	OHX	B1	3534	7/7	0.88	0.27	128,128,128,128	7
74	OHX	A1	1970	7/7	0.89	0.23	66,66,66,66	7
74	OHX	A1	1955	7/7	0.89	0.34	110,110,110,110	7
74	OHX	D1	3524	7/7	0.89	0.28	162,162,162,162	7
74	OHX	B1	3595	7/7	0.89	0.32	73,73,73,73	7
74	OHX	D1	3527	7/7	0.89	0.19	146,146,146,146	7
74	OHX	B1	3597	7/7	0.89	0.35	137,137,137,137	7
74	OHX	C1	1991	7/7	0.89	0.28	77,77,77,77	7
74	OHX	C1	1967	7/7	0.89	0.25	100,100,100,100	7
74	OHX	B1	3538	7/7	0.89	0.28	93,93,93,93	7
74	OHX	D1	3597	7/7	0.89	0.65	222,222,222,222	7
74	OHX	D1	3546	7/7	0.89	0.32	105,105,105,105	7
74	OHX	D1	3548	7/7	0.89	0.25	77,77,77,77	7
74	OHX	B1	3523	7/7	0.89	0.30	150,150,150,150	7
74	OHX	D1	3606	7/7	0.89	0.24	63,63,63,63	7
74	OHX	D1	3460	7/7	0.89	0.22	138,138,138,138	7
74	OHX	B1	3541	7/7	0.89	0.28	117,117,117,117	7
74	OHX	D1	3484	7/7	0.89	0.22	116,116,116,116	7
74	OHX	A1	1946	7/7	0.89	0.19	153,153,153,153	7
74	OHX	D1	3622	7/7	0.89	0.30	142,142,142,142	7
74	OHX	D1	3557	7/7	0.89	0.25	148,148,148,148	7
74	OHX	D1	3625	7/7	0.89	0.24	100,100,100,100	7
74	OHX	B1	3545	7/7	0.89	0.34	82,82,82,82	7
74	OHX	A1	1997	7/7	0.89	0.39	100,100,100,100	7
74	OHX	D1	3495	7/7	0.89	0.17	160,160,160,160	7
74	OHX	D1	3503	7/7	0.89	0.25	120,120,120,120	7
74	OHX	D1	3506	7/7	0.89	0.32	131,131,131,131	7
74	OHX	D3	210	7/7	0.89	0.22	74,74,74,74	7
74	OHX	B1	3579	7/7	0.89	0.30	47,47,47,47	7
74	OHX	A1	1966	7/7	0.89	0.42	120,120,120,120	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
74	OHX	D1	3577	7/7	0.89	0.25	198,198,198,198	7
74	OHX	C1	1980	7/7	0.89	0.34	162,162,162,162	7
74	OHX	D1	3499	7/7	0.90	0.24	114,114,114,114	7
74	OHX	A1	1989	7/7	0.90	0.26	70,70,70,70	7
74	OHX	B1	3610	7/7	0.90	0.28	68,68,68,68	7
74	OHX	B1	3565	7/7	0.90	0.26	120,120,120,120	7
74	OHX	D1	3508	7/7	0.90	0.22	88,88,88,88	7
74	OHX	B1	3487	7/7	0.90	0.23	116,116,116,116	7
74	OHX	B1	3490	7/7	0.90	0.24	109,109,109,109	7
74	OHX	C1	1973	7/7	0.90	0.21	95,95,95,95	7
74	OHX	B2	205	7/7	0.90	0.18	159,159,159,159	7
74	OHX	B1	3572	7/7	0.90	0.36	56,56,56,56	7
74	OHX	B2	207	7/7	0.90	0.49	104,104,104,104	7
74	OHX	D1	3595	7/7	0.90	0.35	90,90,90,90	7
74	OHX	B1	3575	7/7	0.90	0.35	123,123,123,123	7
74	OHX	A1	1947	7/7	0.90	0.30	143,143,143,143	7
74	OHX	D1	3531	7/7	0.90	0.32	136,136,136,136	7
74	OHX	A1	1968	7/7	0.90	0.29	180,180,180,180	7
74	OHX	D1	3536	7/7	0.90	0.25	140,140,140,140	7
74	OHX	A1	1943	7/7	0.90	0.19	176,176,176,176	7
74	OHX	B1	3515	7/7	0.90	0.39	119,119,119,119	7
74	OHX	B1	3518	7/7	0.90	0.22	105,105,105,105	7
74	OHX	C1	1939	7/7	0.90	0.28	103,103,103,103	7
74	OHX	D1	3617	7/7	0.90	0.26	50,50,50,50	7
74	OHX	B1	3584	7/7	0.90	0.48	99,99,99,99	7
74	OHX	D1	3620	7/7	0.90	0.27	78,78,78,78	7
74	OHX	B1	3591	7/7	0.90	0.30	55,55,55,55	7
74	OHX	D1	3552	7/7	0.90	0.39	115,115,115,115	7
74	OHX	B1	3592	7/7	0.90	0.40	106,106,106,106	7
74	OHX	D2	204	7/7	0.90	0.20	116,116,116,116	7
74	OHX	A1	1939	7/7	0.90	0.19	100,100,100,100	7
74	OHX	D1	3466	7/7	0.90	0.22	103,103,103,103	7
74	OHX	D1	3475	7/7	0.90	0.34	142,142,142,142	7
74	OHX	A1	1963	7/7	0.90	0.34	137,137,137,137	7
74	OHX	D1	3559	7/7	0.90	0.21	116,116,116,116	7
74	OHX	A1	1954	7/7	0.90	0.20	153,153,153,153	7
74	OHX	B1	3557	7/7	0.90	0.49	46,46,46,46	7
74	OHX	B1	3530	7/7	0.90	0.31	138,138,138,138	7
74	OHX	C1	1965	7/7	0.90	0.42	101,101,101,101	7
74	OHX	A1	1965	7/7	0.90	0.25	114,114,114,114	7
74	OHX	B1	3546	7/7	0.91	0.41	148,148,148,148	7
74	OHX	D1	3539	7/7	0.91	0.24	69,69,69,69	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
74	OHX	D1	3594	7/7	0.91	0.30	30,30,30,30	7
74	OHX	D1	3473	7/7	0.91	0.16	123,123,123,123	7
74	OHX	B1	3593	7/7	0.91	0.24	46,46,46,46	7
74	OHX	D1	3476	7/7	0.91	0.28	100,100,100,100	7
74	OHX	D1	3477	7/7	0.91	0.15	142,142,142,142	7
74	OHX	B1	3594	7/7	0.91	0.33	100,100,100,100	7
74	OHX	D1	3601	7/7	0.91	0.57	99,99,99,99	7
74	OHX	D1	3602	7/7	0.91	0.31	109,109,109,109	7
74	OHX	B1	3502	7/7	0.91	0.28	166,166,166,166	7
74	OHX	B1	3510	7/7	0.91	0.33	153,153,153,153	7
74	OHX	A1	1935	7/7	0.91	0.23	156,156,156,156	7
74	OHX	A1	1933	7/7	0.91	0.20	152,152,152,152	7
74	OHX	B1	3556	7/7	0.91	0.25	104,104,104,104	7
74	OHX	A1	1969	7/7	0.91	0.26	87,87,87,87	7
74	OHX	A1	1994	7/7	0.91	0.25	123,123,123,123	7
74	OHX	B1	3607	7/7	0.91	0.32	44,44,44,44	7
74	OHX	A1	1996	7/7	0.91	0.24	100,100,100,100	7
74	OHX	B1	3613	7/7	0.91	0.46	93,93,93,93	7
74	OHX	C1	1956	7/7	0.91	0.31	170,170,170,170	7
74	OHX	D1	3513	7/7	0.91	0.27	160,160,160,160	7
74	OHX	A1	1984	7/7	0.91	0.21	65,65,65,65	7
74	OHX	B1	3615	7/7	0.91	0.34	49,49,49,49	7
74	OHX	B1	3620	7/7	0.91	0.31	58,58,58,58	7
74	OHX	B1	3586	7/7	0.91	0.35	116,116,116,116	7
74	OHX	C1	1999	7/7	0.91	0.26	41,41,41,41	7
74	OHX	C1	2000	7/7	0.91	0.38	82,82,82,82	7
74	OHX	B1	3589	7/7	0.91	0.50	85,85,85,85	7
74	OHX	D1	3457	7/7	0.91	0.32	130,130,130,130	7
74	OHX	D1	3532	7/7	0.91	0.26	102,102,102,102	7
74	OHX	A1	1942	7/7	0.91	0.30	97,97,97,97	7
74	OHX	Dd	102	7/7	0.91	0.23	118,118,118,118	7
74	OHX	C1	1977	7/7	0.92	0.26	102,102,102,102	7
74	OHX	A1	1938	7/7	0.92	0.19	155,155,155,155	7
74	OHX	B1	3504	7/7	0.92	0.35	140,140,140,140	7
74	OHX	D1	3575	7/7	0.92	0.29	84,84,84,84	7
74	OHX	B1	3604	7/7	0.92	0.30	53,53,53,53	7
74	OHX	D1	3505	7/7	0.92	0.36	160,160,160,160	7
74	OHX	C1	1981	7/7	0.92	0.38	87,87,87,87	7
74	OHX	C1	1982	7/7	0.92	0.27	106,106,106,106	7
74	OHX	B1	3506	7/7	0.92	0.29	53,53,53,53	7
74	OHX	C1	1947	7/7	0.92	0.28	70,70,70,70	7
74	OHX	B1	3507	7/7	0.92	0.26	104,104,104,104	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
74	OHX	D1	3588	7/7	0.92	0.24	336,336,336,336	7
74	OHX	C1	1989	7/7	0.92	0.53	114,114,114,114	7
74	OHX	D1	3516	7/7	0.92	0.33	138,138,138,138	7
74	OHX	D1	3519	7/7	0.92	0.37	111,111,111,111	7
74	OHX	B1	3611	7/7	0.92	0.33	68,68,68,68	7
74	OHX	B1	3612	7/7	0.92	0.28	45,45,45,45	7
74	OHX	C1	1992	7/7	0.92	0.41	76,76,76,76	7
74	OHX	B1	3559	7/7	0.92	0.23	68,68,68,68	7
74	OHX	D1	3598	7/7	0.92	0.28	65,65,65,65	7
74	OHX	D1	3526	7/7	0.92	0.18	158,158,158,158	7
74	OHX	C1	1994	7/7	0.92	0.29	47,47,47,47	7
74	OHX	C1	1995	7/7	0.92	0.32	51,51,51,51	7
74	OHX	C1	1996	7/7	0.92	0.43	86,86,86,86	7
74	OHX	C1	1997	7/7	0.92	0.24	36,36,36,36	7
74	OHX	A1	1981	7/7	0.92	0.26	128,128,128,128	7
74	OHX	B1	3588	7/7	0.92	0.32	78,78,78,78	7
74	OHX	D1	3610	7/7	0.92	0.47	94,94,94,94	7
74	OHX	B1	3617	7/7	0.92	0.38	90,90,90,90	7
74	OHX	A1	1952	7/7	0.92	0.32	110,110,110,110	7
74	OHX	CT	401	7/7	0.92	0.23	117,117,117,117	7
74	OHX	A1	1995	7/7	0.92	0.35	80,80,80,80	7
74	OHX	B1	3563	7/7	0.92	0.19	152,152,152,152	7
74	OHX	D1	3621	7/7	0.92	0.25	67,67,67,67	7
74	OHX	A1	1971	7/7	0.92	0.21	94,94,94,94	7
74	OHX	D1	3469	7/7	0.92	0.23	152,152,152,152	7
74	OHX	D1	3471	7/7	0.92	0.28	260,260,260,260	7
74	OHX	B1	3566	7/7	0.92	0.26	107,107,107,107	7
74	OHX	D1	3554	7/7	0.92	0.26	122,122,122,122	7
74	OHX	A1	1932	7/7	0.92	0.20	142,142,142,142	7
74	OHX	B1	3520	7/7	0.92	0.34	109,109,109,109	7
74	OHX	C1	1971	7/7	0.92	0.29	131,131,131,131	7
74	OHX	A1	1977	7/7	0.92	0.30	119,119,119,119	7
74	OHX	D3	209	7/7	0.92	0.20	127,127,127,127	7
74	OHX	D1	3482	7/7	0.92	0.21	107,107,107,107	7
74	OHX	D1	3562	7/7	0.92	0.18	121,121,121,121	7
74	OHX	B1	3525	7/7	0.92	0.25	54,54,54,54	7
74	OHX	B1	3498	7/7	0.92	0.32	83,83,83,83	7
74	OHX	B3	209	7/7	0.92	0.30	99,99,99,99	7
74	OHX	D1	3568	7/7	0.92	0.35	92,92,92,92	7
74	OHX	D1	3498	7/7	0.93	0.28	103,103,103,103	7
74	OHX	B1	3608	7/7	0.93	0.58	75,75,75,75	7
74	OHX	D1	3500	7/7	0.93	0.30	139,139,139,139	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
74	OHX	B1	3609	7/7	0.93	0.35	80,80,80,80	7
74	OHX	B3	210	7/7	0.93	0.40	64,64,64,64	7
74	OHX	B3	212	7/7	0.93	0.21	98,98,98,98	7
74	OHX	B1	3469	7/7	0.93	0.33	169,169,169,169	7
74	OHX	C1	1934	7/7	0.93	0.20	141,141,141,141	7
74	OHX	A1	1940	7/7	0.93	0.34	166,166,166,166	7
74	OHX	D1	3433	7/7	0.93	0.23	128,128,128,128	7
74	OHX	B1	3550	7/7	0.93	0.19	137,137,137,137	7
74	OHX	C1	1942	7/7	0.93	0.20	112,112,112,112	7
74	OHX	D1	3613	7/7	0.93	0.33	57,57,57,57	7
74	OHX	B1	3476	7/7	0.93	0.20	102,102,102,102	7
74	OHX	D1	3467	7/7	0.93	0.28	129,129,129,129	7
74	OHX	B1	3532	7/7	0.93	0.43	172,172,172,172	7
74	OHX	B1	3573	7/7	0.93	0.23	111,111,111,111	7
74	OHX	A1	1988	7/7	0.93	0.36	25,25,25,25	7
74	OHX	B1	3576	7/7	0.93	0.21	86,86,86,86	7
74	OHX	A1	1924	7/7	0.93	0.21	150,150,150,150	7
74	OHX	B2	203	7/7	0.93	0.36	174,174,174,174	7
74	OHX	D2	202	7/7	0.93	0.25	106,106,106,106	7
74	OHX	D1	3480	7/7	0.93	0.19	127,127,127,127	7
74	OHX	D2	207	7/7	0.93	0.22	111,111,111,111	7
74	OHX	D1	3579	7/7	0.93	0.30	44,44,44,44	7
74	OHX	A1	1982	7/7	0.93	0.19	148,148,148,148	7
74	OHX	D1	3534	7/7	0.93	0.41	142,142,142,142	7
74	OHX	B1	3517	7/7	0.93	0.30	111,111,111,111	7
74	OHX	D1	3483	7/7	0.93	0.23	98,98,98,98	7
74	OHX	A1	1991	7/7	0.93	0.31	98,98,98,98	7
74	OHX	A1	1950	7/7	0.93	0.17	127,127,127,127	7
74	OHX	A1	1921	7/7	0.93	0.27	148,148,148,148	7
74	OHX	D1	3545	7/7	0.93	0.42	77,77,77,77	7
74	OHX	B1	3606	7/7	0.93	0.38	74,74,74,74	7
74	OHX	D1	3547	7/7	0.93	0.19	64,64,64,64	7
74	OHX	B1	3505	7/7	0.93	0.17	134,134,134,134	7
74	OHX	B1	3549	7/7	0.94	0.30	86,86,86,86	7
74	OHX	D1	3493	7/7	0.94	0.17	126,126,126,126	7
74	OHX	C1	1975	7/7	0.94	0.24	119,119,119,119	7
74	OHX	B1	3585	7/7	0.94	0.29	197,197,197,197	7
74	OHX	A1	1959	7/7	0.94	0.26	110,110,110,110	7
74	OHX	A1	1944	7/7	0.94	0.21	108,108,108,108	7
74	OHX	D1	3501	7/7	0.94	0.17	102,102,102,102	7
74	OHX	B1	3488	7/7	0.94	0.18	104,104,104,104	7
74	OHX	B1	3521	7/7	0.94	0.25	107,107,107,107	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
74	OHX	D1	3581	7/7	0.94	0.26	60,60,60,60	7
74	OHX	A1	1941	7/7	0.94	0.19	124,124,124,124	7
74	OHX	B3	208	7/7	0.94	0.19	79,79,79,79	7
74	OHX	C1	1984	7/7	0.94	0.27	78,78,78,78	7
74	OHX	B1	3524	7/7	0.94	0.24	97,97,97,97	7
74	OHX	D1	3510	7/7	0.94	0.23	108,108,108,108	7
74	OHX	C1	1986	7/7	0.94	0.20	169,169,169,169	7
74	OHX	D1	3514	7/7	0.94	0.30	173,173,173,173	7
74	OHX	D1	3591	7/7	0.94	0.22	43,43,43,43	7
74	OHX	B1	3558	7/7	0.94	0.21	130,130,130,130	7
74	OHX	B1	3491	7/7	0.94	0.31	99,99,99,99	7
74	OHX	BC	401	7/7	0.94	0.21	66,66,66,66	7
74	OHX	A1	1973	7/7	0.94	0.28	101,101,101,101	7
74	OHX	Bd	102	7/7	0.94	0.19	73,73,73,73	7
74	OHX	C1	1919	7/7	0.94	0.26	159,159,159,159	7
74	OHX	C1	1933	7/7	0.94	0.21	111,111,111,111	7
74	OHX	B1	3598	7/7	0.94	0.22	100,100,100,100	7
74	OHX	C1	1935	7/7	0.94	0.17	93,93,93,93	7
74	OHX	D1	3528	7/7	0.94	0.35	96,96,96,96	7
74	OHX	D1	3604	7/7	0.94	0.14	44,44,44,44	7
74	OHX	B1	3527	7/7	0.94	0.21	84,84,84,84	7
74	OHX	B1	3497	7/7	0.94	0.24	103,103,103,103	7
74	OHX	A1	1987	7/7	0.94	0.23	72,72,72,72	7
74	OHX	A1	1927	7/7	0.94	0.22	139,139,139,139	7
74	OHX	B1	3503	7/7	0.94	0.18	86,86,86,86	7
74	OHX	C1	1948	7/7	0.94	0.20	117,117,117,117	7
74	OHX	D1	3614	7/7	0.94	0.49	83,83,83,83	7
74	OHX	D1	3538	7/7	0.94	0.25	87,87,87,87	7
74	OHX	C1	1949	7/7	0.94	0.19	97,97,97,97	7
74	OHX	B1	3567	7/7	0.94	0.10	126,126,126,126	7
74	OHX	D1	3454	7/7	0.94	0.19	117,117,117,117	7
74	OHX	A1	1948	7/7	0.94	0.27	106,106,106,106	7
74	OHX	B1	3569	7/7	0.94	0.18	95,95,95,95	7
74	OHX	A1	1949	7/7	0.94	0.20	101,101,101,101	7
74	OHX	AT	401	7/7	0.94	0.36	207,207,207,207	7
74	OHX	B1	3437	7/7	0.94	0.24	156,156,156,156	7
74	OHX	D2	203	7/7	0.94	0.25	94,94,94,94	7
74	OHX	B1	3574	7/7	0.94	0.44	136,136,136,136	7
74	OHX	D2	205	7/7	0.94	0.22	84,84,84,84	7
74	OHX	B1	3509	7/7	0.94	0.23	124,124,124,124	7
74	OHX	C1	1963	7/7	0.94	0.27	94,94,94,94	7
74	OHX	B1	3543	7/7	0.94	0.15	102,102,102,102	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
74	OHX	B1	3438	7/7	0.94	0.17	168,168,168,168	7
74	OHX	B1	3578	7/7	0.94	0.24	112,112,112,112	7
74	OHX	D3	207	7/7	0.94	0.23	123,123,123,123	7
74	OHX	A1	1980	7/7	0.94	0.19	136,136,136,136	7
74	OHX	B1	3619	7/7	0.94	0.22	85,85,85,85	7
74	OHX	B1	3470	7/7	0.94	0.19	122,122,122,122	7
74	OHX	B1	3547	7/7	0.94	0.28	117,117,117,117	7
74	OHX	B1	3582	7/7	0.94	0.27	83,83,83,83	7
74	OHX	A1	1922	7/7	0.94	0.24	133,133,133,133	7
74	OHX	D1	3489	7/7	0.94	0.32	75,75,75,75	7
74	OHX	DO	302	7/7	0.94	0.24	77,77,77,77	7
74	OHX	D1	3567	7/7	0.94	0.14	106,106,106,106	7
74	OHX	D1	3512	7/7	0.95	0.20	108,108,108,108	7
74	OHX	A1	1926	7/7	0.95	0.24	87,87,87,87	7
74	OHX	A1	1960	7/7	0.95	0.38	70,70,70,70	7
74	OHX	A1	1915	7/7	0.95	0.18	129,129,129,129	7
74	OHX	CI	201	7/7	0.95	0.31	143,143,143,143	7
74	OHX	D1	3517	7/7	0.95	0.29	126,126,126,126	7
74	OHX	B1	3522	7/7	0.95	0.16	129,129,129,129	7
74	OHX	B1	3494	7/7	0.95	0.18	118,118,118,118	7
74	OHX	B3	203	7/7	0.95	0.21	140,140,140,140	7
74	OHX	D1	3523	7/7	0.95	0.19	106,106,106,106	7
74	OHX	B1	3446	7/7	0.95	0.23	113,113,113,113	7
74	OHX	B3	207	7/7	0.95	0.18	68,68,68,68	7
74	OHX	D1	3459	7/7	0.95	0.21	96,96,96,96	7
74	OHX	B1	3448	7/7	0.95	0.19	124,124,124,124	7
74	OHX	B1	3553	7/7	0.95	0.19	66,66,66,66	7
74	OHX	B1	3457	7/7	0.95	0.23	147,147,147,147	7
74	OHX	D1	3530	7/7	0.95	0.19	51,51,51,51	7
74	OHX	D1	3468	7/7	0.95	0.26	130,130,130,130	7
74	OHX	B1	3459	7/7	0.95	0.16	160,160,160,160	7
74	OHX	D1	3533	7/7	0.95	0.27	92,92,92,92	7
74	OHX	B1	3528	7/7	0.95	0.37	158,158,158,158	7
74	OHX	D1	3472	7/7	0.95	0.21	185,185,185,185	7
74	OHX	D1	3603	7/7	0.95	0.43	114,114,114,114	7
74	OHX	B1	3465	7/7	0.95	0.17	142,142,142,142	7
74	OHX	D1	3537	7/7	0.95	0.23	74,74,74,74	7
74	OHX	A1	1934	7/7	0.95	0.25	122,122,122,122	7
74	OHX	D1	3607	7/7	0.95	0.29	78,78,78,78	7
74	OHX	C1	1910	7/7	0.95	0.20	138,138,138,138	7
74	OHX	B1	3531	7/7	0.95	0.30	65,65,65,65	7
74	OHX	C1	1926	7/7	0.95	0.21	96,96,96,96	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
74	OHX	D1	3544	7/7	0.95	0.43	127,127,127,127	7
74	OHX	C1	1930	7/7	0.95	0.17	112,112,112,112	7
74	OHX	D1	3615	7/7	0.95	0.27	73,73,73,73	7
74	OHX	C1	1931	7/7	0.95	0.19	130,130,130,130	7
74	OHX	C1	1932	7/7	0.95	0.18	115,115,115,115	7
74	OHX	A1	1919	7/7	0.95	0.25	141,141,141,141	7
74	OHX	D1	3619	7/7	0.95	0.21	86,86,86,86	7
74	OHX	D1	3549	7/7	0.95	0.27	127,127,127,127	7
74	OHX	B1	3473	7/7	0.95	0.17	91,91,91,91	7
74	OHX	B1	3587	7/7	0.95	0.15	154,154,154,154	7
74	OHX	C1	1983	7/7	0.95	0.19	59,59,59,59	7
74	OHX	A1	1936	7/7	0.95	0.20	129,129,129,129	7
74	OHX	B1	3616	7/7	0.95	0.28	103,103,103,103	7
74	OHX	D1	3494	7/7	0.95	0.25	105,105,105,105	7
74	OHX	A1	2001	7/7	0.95	0.24	26,26,26,26	7
74	OHX	D1	3496	7/7	0.95	0.27	155,155,155,155	7
74	OHX	C1	1944	7/7	0.95	0.12	134,134,134,134	7
74	OHX	B1	3481	7/7	0.95	0.23	133,133,133,133	7
74	OHX	D1	3561	7/7	0.95	0.21	65,65,65,65	7
74	OHX	C1	1946	7/7	0.95	0.22	63,63,63,63	7
74	OHX	B1	3513	7/7	0.95	0.23	171,171,171,171	7
74	OHX	B1	3484	7/7	0.95	0.25	143,143,143,143	7
74	OHX	D1	3504	7/7	0.95	0.16	101,101,101,101	7
74	OHX	B2	202	7/7	0.95	0.19	106,106,106,106	7
74	OHX	A1	1937	7/7	0.95	0.15	158,158,158,158	7
74	OHX	C1	1951	7/7	0.95	0.15	152,152,152,152	7
74	OHX	AL	201	7/7	0.95	0.20	122,122,122,122	7
74	OHX	B1	3596	7/7	0.95	0.33	56,56,56,56	7
74	OHX	C1	1955	7/7	0.95	0.20	106,106,106,106	7
74	OHX	D1	3576	7/7	0.95	0.21	76,76,76,76	7
74	OHX	D1	3511	7/7	0.95	0.28	85,85,85,85	7
74	OHX	B1	3501	7/7	0.96	0.31	99,99,99,99	7
74	OHX	B1	3570	7/7	0.96	0.28	91,91,91,91	7
74	OHX	D1	3574	7/7	0.96	0.19	114,114,114,114	7
74	OHX	B1	3456	7/7	0.96	0.25	106,106,106,106	7
74	OHX	A1	1945	7/7	0.96	0.18	108,108,108,108	7
74	OHX	C1	1936	7/7	0.96	0.34	126,126,126,126	7
74	OHX	C1	1937	7/7	0.96	0.17	124,124,124,124	7
74	OHX	B1	3536	7/7	0.96	0.28	324,324,324,324	7
74	OHX	B1	3537	7/7	0.96	0.21	56,56,56,56	7
74	OHX	C1	1940	7/7	0.96	0.25	139,139,139,139	7
74	OHX	C1	1941	7/7	0.96	0.18	109,109,109,109	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
74	OHX	D1	3584	7/7	0.96	0.27	47,47,47,47	7
74	OHX	A1	1928	7/7	0.96	0.15	99,99,99,99	7
74	OHX	C1	1943	7/7	0.96	0.15	141,141,141,141	7
74	OHX	B1	3461	7/7	0.96	0.19	101,101,101,101	7
74	OHX	B1	3462	7/7	0.96	0.21	90,90,90,90	7
74	OHX	B1	3542	7/7	0.96	0.38	64,64,64,64	7
74	OHX	D1	3518	7/7	0.96	0.21	108,108,108,108	7
74	OHX	B1	3463	7/7	0.96	0.16	137,137,137,137	7
74	OHX	D1	3592	7/7	0.96	0.23	118,118,118,118	7
74	OHX	D1	3520	7/7	0.96	0.18	109,109,109,109	7
74	OHX	C1	2001	7/7	0.96	0.25	130,130,130,130	7
74	OHX	B1	3618	7/7	0.96	0.24	109,109,109,109	7
74	OHX	A1	1957	7/7	0.96	0.18	129,129,129,129	7
74	OHX	A1	1929	7/7	0.96	0.14	114,114,114,114	7
74	OHX	A1	1908	7/7	0.96	0.24	96,96,96,96	7
74	OHX	B1	3512	7/7	0.96	0.22	113,113,113,113	7
74	OHX	B1	3472	7/7	0.96	0.25	132,132,132,132	7
74	OHX	D1	3458	7/7	0.96	0.17	103,103,103,103	7
74	OHX	A1	1986	7/7	0.96	0.18	98,98,98,98	7
74	OHX	A1	1972	7/7	0.96	0.17	87,87,87,87	7
74	OHX	D1	3461	7/7	0.96	0.18	128,128,128,128	7
74	OHX	D1	3462	7/7	0.96	0.16	114,114,114,114	7
74	OHX	D1	3463	7/7	0.96	0.18	140,140,140,140	7
74	OHX	D1	3464	7/7	0.96	0.18	92,92,92,92	7
74	OHX	B1	3551	7/7	0.96	0.43	84,84,84,84	7
74	OHX	B1	3516	7/7	0.96	0.21	136,136,136,136	7
74	OHX	A1	1923	7/7	0.96	0.17	98,98,98,98	7
74	OHX	D1	3612	7/7	0.96	0.23	36,36,36,36	7
74	OHX	C1	1960	7/7	0.96	0.13	111,111,111,111	7
74	OHX	C1	1961	7/7	0.96	0.18	101,101,101,101	7
74	OHX	D1	3540	7/7	0.96	0.20	85,85,85,85	7
74	OHX	B1	3590	7/7	0.96	0.21	69,69,69,69	7
74	OHX	B1	3479	7/7	0.96	0.35	145,145,145,145	7
74	OHX	A1	1917	7/7	0.96	0.14	130,130,130,130	7
74	OHX	B3	205	7/7	0.96	0.14	123,123,123,123	7
74	OHX	A1	1910	7/7	0.96	0.15	146,146,146,146	7
74	OHX	D1	3478	7/7	0.96	0.17	117,117,117,117	7
74	OHX	B1	3486	7/7	0.96	0.22	104,104,104,104	7
74	OHX	D1	3623	7/7	0.96	0.33	23,23,23,23	7
74	OHX	B1	3425	7/7	0.96	0.18	108,108,108,108	7
74	OHX	B1	3431	7/7	0.96	0.19	125,125,125,125	7
74	OHX	A1	1920	7/7	0.96	0.15	126,126,126,126	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
74	OHX	A1	1992	7/7	0.96	0.43	45,45,45,45	7
74	OHX	B1	3439	7/7	0.96	0.24	90,90,90,90	7
74	OHX	D1	3486	7/7	0.96	0.24	143,143,143,143	7
74	OHX	A1	1979	7/7	0.96	0.19	81,81,81,81	7
74	OHX	B1	3564	7/7	0.96	0.25	126,126,126,126	7
74	OHX	B1	3495	7/7	0.96	0.31	108,108,108,108	7
74	OHX	D1	3491	7/7	0.96	0.25	37,37,37,37	7
74	OHX	C1	1913	7/7	0.96	0.22	149,149,149,149	7
74	OHX	D1	3560	7/7	0.96	0.23	82,82,82,82	7
74	OHX	C1	1916	7/7	0.96	0.23	169,169,169,169	7
74	OHX	A1	1914	7/7	0.96	0.21	145,145,145,145	7
74	OHX	C1	1923	7/7	0.96	0.23	123,123,123,123	7
74	OHX	D1	3497	7/7	0.96	0.37	99,99,99,99	7
74	OHX	DC	401	7/7	0.96	0.23	93,93,93,93	7
74	OHX	B1	3455	7/7	0.96	0.20	134,134,134,134	7
74	OHX	C1	1927	7/7	0.96	0.14	149,149,149,149	7
74	OHX	B1	3605	7/7	0.96	0.26	52,52,52,52	7
74	OHX	B1	3500	7/7	0.96	0.15	116,116,116,116	7
74	OHX	D1	3570	7/7	0.96	0.30	49,49,49,49	7
74	OHX	Dg	101	7/7	0.96	0.16	69,69,69,69	7
74	OHX	B1	3483	7/7	0.97	0.28	71,71,71,71	7
74	OHX	D1	3406	7/7	0.97	0.13	107,107,107,107	0
74	OHX	D1	3413	7/7	0.97	0.23	114,114,114,114	7
74	OHX	D1	3416	7/7	0.97	0.16	108,108,108,108	7
74	OHX	D1	3425	7/7	0.97	0.16	126,126,126,126	7
74	OHX	B1	3443	7/7	0.97	0.21	134,134,134,134	7
74	OHX	D1	3435	7/7	0.97	0.18	92,92,92,92	7
74	OHX	D1	3439	7/7	0.97	0.23	107,107,107,107	7
74	OHX	D1	3443	7/7	0.97	0.16	96,96,96,96	7
74	OHX	D1	3447	7/7	0.97	0.20	142,142,142,142	7
74	OHX	D1	3448	7/7	0.97	0.21	107,107,107,107	7
74	OHX	D1	3451	7/7	0.97	0.22	112,112,112,112	7
74	OHX	D1	3453	7/7	0.97	0.24	124,124,124,124	7
74	OHX	B1	3485	7/7	0.97	0.23	110,110,110,110	7
74	OHX	B1	3444	7/7	0.97	0.15	111,111,111,111	7
74	OHX	A1	1911	7/7	0.97	0.20	112,112,112,112	7
74	OHX	A1	1975	7/7	0.97	0.17	67,67,67,67	7
74	OHX	C1	1905	7/7	0.97	0.13	114,114,114,114	7
74	OHX	C1	1908	7/7	0.97	0.15	104,104,104,104	7
74	OHX	C1	1909	7/7	0.97	0.14	130,130,130,130	7
74	OHX	B1	3489	7/7	0.97	0.11	129,129,129,129	7
74	OHX	C1	1912	7/7	0.97	0.15	117,117,117,117	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
74	OHX	D1	3465	7/7	0.97	0.16	101,101,101,101	7
74	OHX	B1	3449	7/7	0.97	0.18	105,105,105,105	7
74	OHX	C1	1915	7/7	0.97	0.21	120,120,120,120	7
74	OHX	B1	3451	7/7	0.97	0.17	86,86,86,86	7
74	OHX	B1	3492	7/7	0.97	0.14	70,70,70,70	7
74	OHX	D1	3470	7/7	0.97	0.15	84,84,84,84	7
74	OHX	C1	1921	7/7	0.97	0.09	145,145,145,145	7
74	OHX	C1	1922	7/7	0.97	0.18	142,142,142,142	7
74	OHX	D1	3608	7/7	0.97	0.23	14,14,14,14	7
74	OHX	B1	3453	7/7	0.97	0.24	127,127,127,127	7
74	OHX	D1	3474	7/7	0.97	0.30	118,118,118,118	7
74	OHX	C1	1924	7/7	0.97	0.14	82,82,82,82	7
74	OHX	B1	3454	7/7	0.97	0.33	123,123,123,123	7
74	OHX	D1	3543	7/7	0.97	0.19	45,45,45,45	7
74	OHX	A1	1976	7/7	0.97	0.19	51,51,51,51	7
74	OHX	C1	1928	7/7	0.97	0.17	165,165,165,165	7
74	OHX	D1	3479	7/7	0.97	0.24	99,99,99,99	7
74	OHX	B1	3496	7/7	0.97	0.15	122,122,122,122	7
74	OHX	A1	1956	7/7	0.97	0.12	159,159,159,159	7
74	OHX	A1	1912	7/7	0.97	0.16	125,125,125,125	7
74	OHX	B1	3499	7/7	0.97	0.16	123,123,123,123	7
74	OHX	A1	1967	7/7	0.97	0.30	96,96,96,96	7
74	OHX	A1	1905	7/7	0.97	0.17	118,118,118,118	0
74	OHX	B1	3410	7/7	0.97	0.19	111,111,111,111	0
74	OHX	D1	3487	7/7	0.97	0.24	103,103,103,103	7
74	OHX	A1	1909	7/7	0.97	0.16	115,115,115,115	7
74	OHX	B1	3426	7/7	0.97	0.17	111,111,111,111	7
74	OHX	B1	3467	7/7	0.97	0.15	119,119,119,119	7
74	OHX	B1	3468	7/7	0.97	0.28	89,89,89,89	7
74	OHX	B1	3429	7/7	0.97	0.17	93,93,93,93	7
74	OHX	D2	206	7/7	0.97	0.16	85,85,85,85	7
74	OHX	B1	3508	7/7	0.97	0.25	113,113,113,113	7
74	OHX	B1	3430	7/7	0.97	0.14	99,99,99,99	7
74	OHX	A1	1916	7/7	0.97	0.14	91,91,91,91	7
74	OHX	D3	203	7/7	0.97	0.17	86,86,86,86	7
74	OHX	D3	204	7/7	0.97	0.19	120,120,120,120	7
74	OHX	B1	3433	7/7	0.97	0.19	98,98,98,98	7
74	OHX	B1	3436	7/7	0.97	0.17	104,104,104,104	7
74	OHX	D1	3565	7/7	0.97	0.23	60,60,60,60	7
74	OHX	B1	3475	7/7	0.97	0.20	84,84,84,84	7
74	OHX	A1	1961	7/7	0.97	0.10	105,105,105,105	7
74	OHX	B1	3478	7/7	0.97	0.14	110,110,110,110	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
74	OHX	D1	3502	7/7	0.97	0.14	79,79,79,79	7
74	OHX	D3	212	7/7	0.97	0.27	71,71,71,71	7
74	OHX	A1	1906	7/7	0.97	0.15	97,97,97,97	7
74	OHX	D1	3571	7/7	0.97	0.17	77,77,77,77	7
74	OHX	B1	3480	7/7	0.97	0.18	85,85,85,85	7
74	OHX	A1	1918	7/7	0.97	0.18	94,94,94,94	7
74	OHX	B1	3519	7/7	0.97	0.28	115,115,115,115	7
74	OHX	CS	101	7/7	0.97	0.18	46,46,46,46	7
74	OHX	B1	3482	7/7	0.97	0.19	111,111,111,111	7
74	OHX	B1	3404	7/7	0.98	0.15	114,114,114,114	0
74	OHX	B1	3406	7/7	0.98	0.22	106,106,106,106	0
74	OHX	D1	3456	7/7	0.98	0.20	131,131,131,131	7
74	OHX	B3	211	7/7	0.98	0.16	67,67,67,67	7
74	OHX	B1	3407	7/7	0.98	0.14	105,105,105,105	0
74	OHX	B1	3409	7/7	0.98	0.18	122,122,122,122	0
74	OHX	B1	3471	7/7	0.98	0.11	130,130,130,130	7
74	OHX	B1	3440	7/7	0.98	0.19	105,105,105,105	7
74	OHX	Bg	101	7/7	0.98	0.17	79,79,79,79	7
74	OHX	C1	1903	7/7	0.98	0.17	115,115,115,115	0
74	OHX	C1	1904	7/7	0.98	0.16	113,113,113,113	0
74	OHX	B1	3441	7/7	0.98	0.20	129,129,129,129	7
74	OHX	A1	1907	7/7	0.98	0.22	111,111,111,111	7
74	OHX	B1	3411	7/7	0.98	0.15	105,105,105,105	0
74	OHX	B1	3414	7/7	0.98	0.14	106,106,106,106	0
74	OHX	B1	3477	7/7	0.98	0.19	101,101,101,101	7
74	OHX	C1	1953	7/7	0.98	0.13	56,56,56,56	7
74	OHX	B1	3417	7/7	0.98	0.12	102,102,102,102	0
74	OHX	C1	1914	7/7	0.98	0.12	128,128,128,128	7
74	OHX	B1	3418	7/7	0.98	0.16	106,106,106,106	0
74	OHX	B1	3419	7/7	0.98	0.17	109,109,109,109	7
74	OHX	B2	201	7/7	0.98	0.10	141,141,141,141	7
74	OHX	C1	1920	7/7	0.98	0.19	103,103,103,103	7
74	OHX	B1	3452	7/7	0.98	0.19	134,134,134,134	7
74	OHX	A1	1904	7/7	0.98	0.17	137,137,137,137	7
74	OHX	A1	1931	7/7	0.98	0.14	96,96,96,96	7
74	OHX	B1	3427	7/7	0.98	0.21	95,95,95,95	7
74	OHX	C1	1925	7/7	0.98	0.12	116,116,116,116	7
74	OHX	B1	3428	7/7	0.98	0.15	109,109,109,109	7
74	OHX	D1	3401	7/7	0.98	0.24	96,96,96,96	0
74	OHX	D1	3402	7/7	0.98	0.24	100,100,100,100	0
74	OHX	D1	3405	7/7	0.98	0.20	110,110,110,110	0
74	OHX	A1	1913	7/7	0.98	0.11	135,135,135,135	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
74	OHX	D1	3408	7/7	0.98	0.12	143,143,143,143	0
74	OHX	D1	3409	7/7	0.98	0.17	114,114,114,114	0
74	OHX	D1	3411	7/7	0.98	0.16	117,117,117,117	0
74	OHX	B1	3458	7/7	0.98	0.29	114,114,114,114	7
74	OHX	C1	1929	7/7	0.98	0.19	90,90,90,90	7
74	OHX	D1	3492	7/7	0.98	0.16	112,112,112,112	7
74	OHX	D1	3417	7/7	0.98	0.23	91,91,91,91	7
74	OHX	D1	3418	7/7	0.98	0.22	103,103,103,103	0
74	OHX	D1	3419	7/7	0.98	0.17	92,92,92,92	0
74	OHX	D1	3421	7/7	0.98	0.15	98,98,98,98	7
74	OHX	D1	3422	7/7	0.98	0.18	114,114,114,114	7
74	OHX	D1	3424	7/7	0.98	0.13	125,125,125,125	7
74	OHX	Ac	100	7/7	0.98	0.29	131,131,131,131	7
74	OHX	D1	3427	7/7	0.98	0.16	90,90,90,90	7
74	OHX	D1	3429	7/7	0.98	0.21	82,82,82,82	7
74	OHX	D1	3430	7/7	0.98	0.15	101,101,101,101	7
74	OHX	D1	3431	7/7	0.98	0.13	109,109,109,109	7
74	OHX	D1	3432	7/7	0.98	0.18	100,100,100,100	7
74	OHX	B1	3460	7/7	0.98	0.16	137,137,137,137	7
74	OHX	B3	202	7/7	0.98	0.15	116,116,116,116	0
74	OHX	B1	3402	7/7	0.98	0.18	99,99,99,99	0
74	OHX	D1	3440	7/7	0.98	0.18	137,137,137,137	7
74	OHX	D1	3441	7/7	0.98	0.20	124,124,124,124	7
74	OHX	D1	3442	7/7	0.98	0.16	126,126,126,126	7
74	OHX	B1	3432	7/7	0.98	0.19	79,79,79,79	7
74	OHX	D1	3445	7/7	0.98	0.20	101,101,101,101	7
74	OHX	D1	3446	7/7	0.98	0.15	83,83,83,83	7
74	OHX	B1	3403	7/7	0.98	0.25	126,126,126,126	0
74	OHX	B1	3435	7/7	0.98	0.28	130,130,130,130	7
74	OHX	D1	3450	7/7	0.98	0.21	112,112,112,112	7
74	OHX	D1	3582	7/7	0.98	0.13	71,71,71,71	7
74	OHX	B1	3466	7/7	0.98	0.17	120,120,120,120	7
74	OHX	D1	3452	7/7	0.98	0.09	94,94,94,94	7
74	OHX	B1	3408	7/7	0.99	0.20	98,98,98,98	0
74	OHX	B1	3420	7/7	0.99	0.19	93,93,93,93	7
74	OHX	B1	3421	7/7	0.99	0.18	141,141,141,141	0
74	OHX	B1	3422	7/7	0.99	0.12	93,93,93,93	7
74	OHX	B1	3423	7/7	0.99	0.21	91,91,91,91	7
74	OHX	D1	3444	7/7	0.99	0.18	72,72,72,72	7
74	OHX	C1	1964	7/7	0.99	0.15	88,88,88,88	7
74	OHX	B1	3424	7/7	0.99	0.14	105,105,105,105	7
74	OHX	BT	201	7/7	0.99	0.15	91,91,91,91	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
74	OHX	Bd	101	7/7	0.99	0.19	32,32,32,32	7
74	OHX	D1	3449	7/7	0.99	0.27	124,124,124,124	7
74	OHX	B1	3442	7/7	0.99	0.17	89,89,89,89	7
74	OHX	B1	3464	7/7	0.99	0.17	89,89,89,89	7
74	OHX	C1	1901	7/7	0.99	0.16	100,100,100,100	0
74	OHX	C1	1902	7/7	0.99	0.22	108,108,108,108	0
74	OHX	A1	1901	7/7	0.99	0.15	100,100,100,100	0
74	OHX	D1	3455	7/7	0.99	0.13	110,110,110,110	7
74	OHX	D1	3403	7/7	0.99	0.21	96,96,96,96	0
74	OHX	D1	3404	7/7	0.99	0.21	99,99,99,99	0
74	OHX	AS	101	7/7	0.99	0.14	29,29,29,29	7
74	OHX	B1	3445	7/7	0.99	0.12	113,113,113,113	7
74	OHX	D1	3407	7/7	0.99	0.13	113,113,113,113	0
74	OHX	C1	1906	7/7	0.99	0.17	101,101,101,101	7
74	OHX	C1	1907	7/7	0.99	0.14	123,123,123,123	7
74	OHX	D1	3410	7/7	0.99	0.21	96,96,96,96	0
74	OHX	A1	1902	7/7	0.99	0.14	112,112,112,112	0
74	OHX	D1	3412	7/7	0.99	0.18	126,126,126,126	0
74	OHX	B1	3447	7/7	0.99	0.16	126,126,126,126	7
74	OHX	D2	201	7/7	0.99	0.13	94,94,94,94	7
74	OHX	D1	3414	7/7	0.99	0.11	114,114,114,114	0
74	OHX	D1	3415	7/7	0.99	0.11	139,139,139,139	0
74	OHX	B1	3412	7/7	0.99	0.14	121,121,121,121	0
74	OHX	C1	1911	7/7	0.99	0.13	96,96,96,96	7
74	OHX	B1	3413	7/7	0.99	0.12	106,106,106,106	7
74	OHX	B1	3450	7/7	0.99	0.12	91,91,91,91	7
74	OHX	D1	3420	7/7	0.99	0.11	112,112,112,112	0
74	OHX	B1	3405	7/7	0.99	0.18	101,101,101,101	0
74	OHX	D3	201	7/7	0.99	0.14	93,93,93,93	0
74	OHX	D3	202	7/7	0.99	0.13	116,116,116,116	0
74	OHX	B3	201	7/7	0.99	0.19	117,117,117,117	0
74	OHX	D1	3423	7/7	0.99	0.12	88,88,88,88	7
74	OHX	B1	3540	7/7	0.99	0.18	58,58,58,58	7
74	OHX	C1	1917	7/7	0.99	0.15	130,130,130,130	7
74	OHX	D1	3426	7/7	0.99	0.17	112,112,112,112	7
74	OHX	C1	1918	7/7	0.99	0.14	123,123,123,123	7
74	OHX	D1	3428	7/7	0.99	0.15	80,80,80,80	7
74	OHX	B1	3415	7/7	0.99	0.14	93,93,93,93	7
74	OHX	B3	204	7/7	0.99	0.15	84,84,84,84	7
74	OHX	B1	3416	7/7	0.99	0.18	113,113,113,113	0
74	OHX	A1	1903	7/7	0.99	0.12	122,122,122,122	7
74	OHX	B1	3434	7/7	0.99	0.17	102,102,102,102	7

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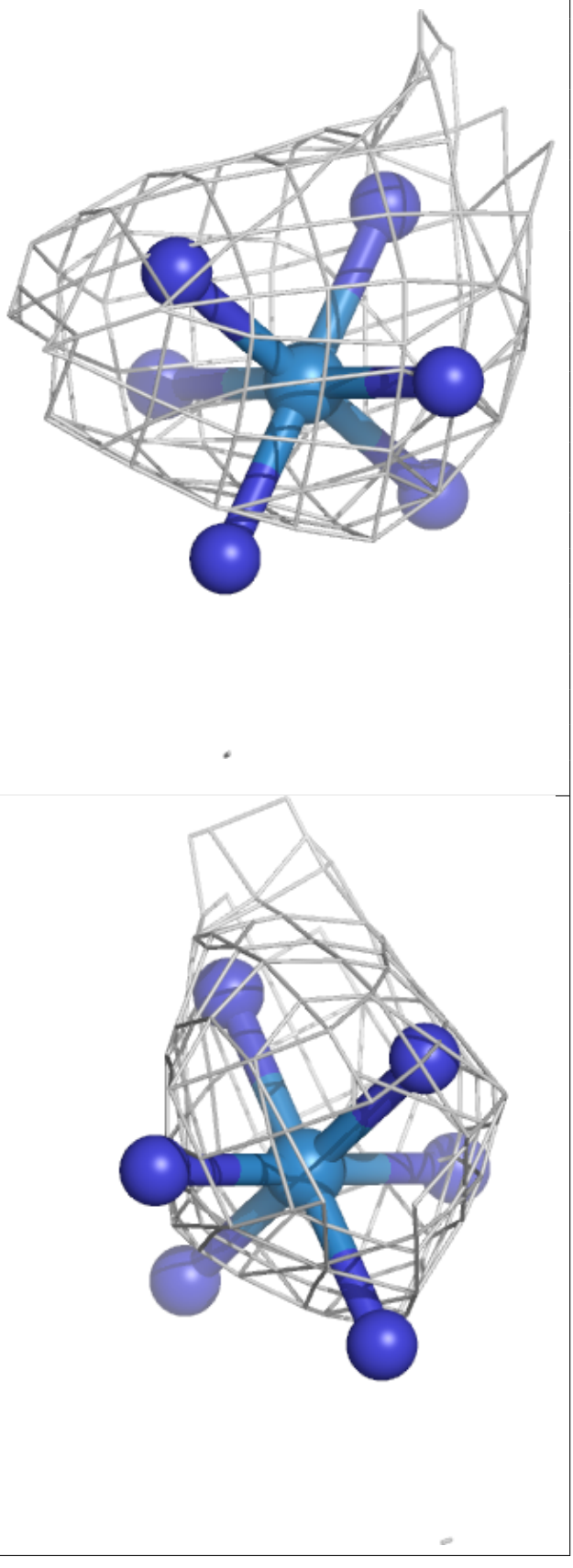
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
74	OHX	D1	3434	7/7	0.99	0.13	77,77,77,77	7
74	OHX	B1	3401	7/7	0.99	0.22	90,90,90,90	0
74	OHX	D1	3436	7/7	0.99	0.19	125,125,125,125	7
74	OHX	DT	201	7/7	0.99	0.18	100,100,100,100	0
74	OHX	Dd	101	7/7	0.99	0.15	32,32,32,32	7
74	OHX	D1	3437	7/7	0.99	0.24	103,103,103,103	7
74	OHX	D1	3438	7/7	0.99	0.12	98,98,98,98	7

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

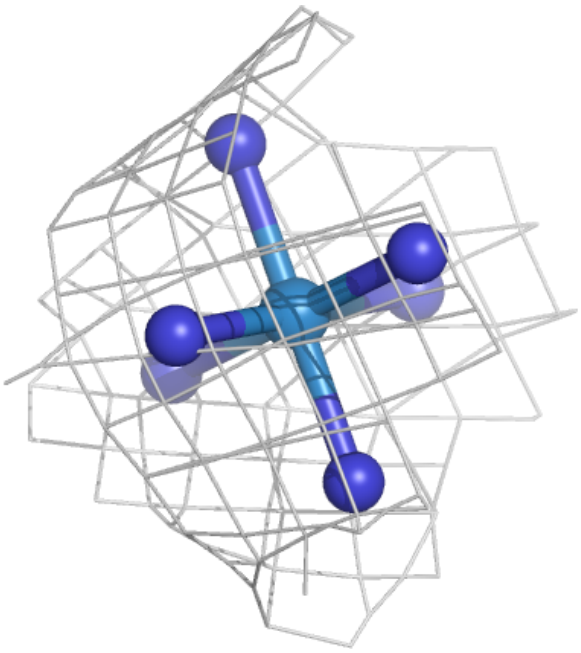
Electron density around OHX D1 3593:

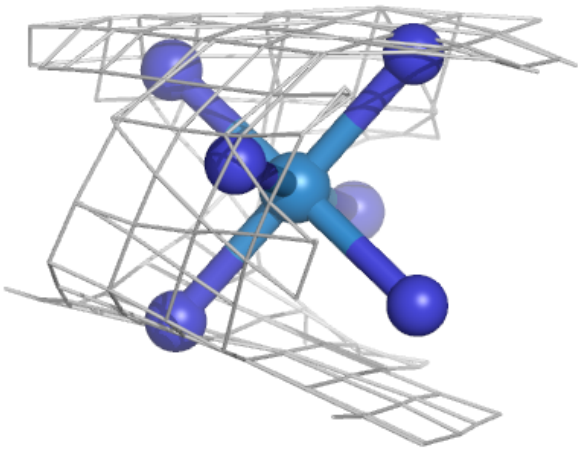
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

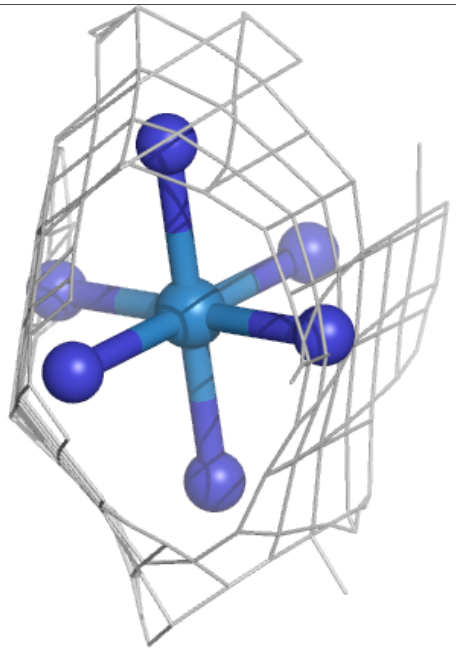


Electron density around OHX D3 211:

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

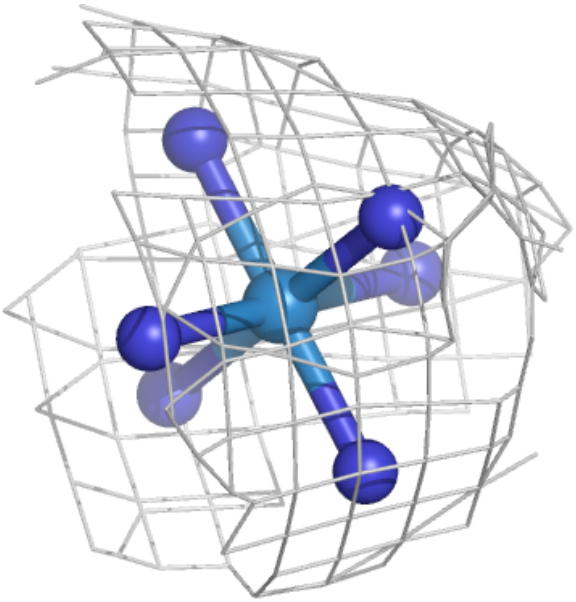


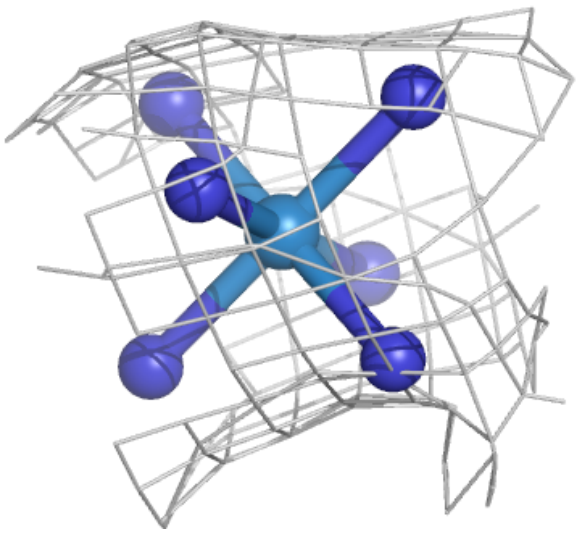


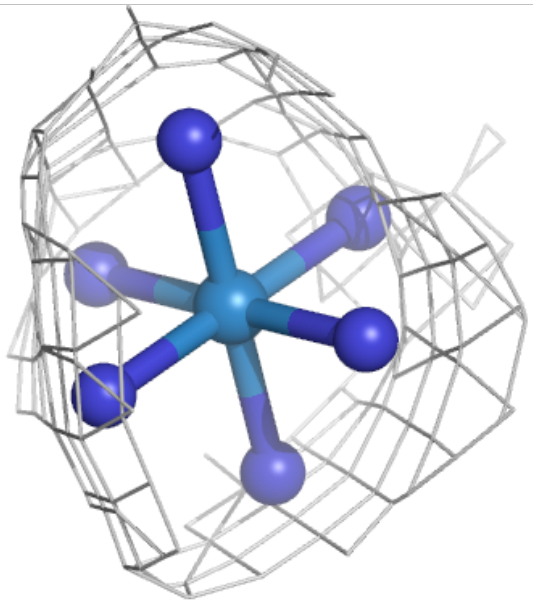


Electron density around OHX A1 1930:

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

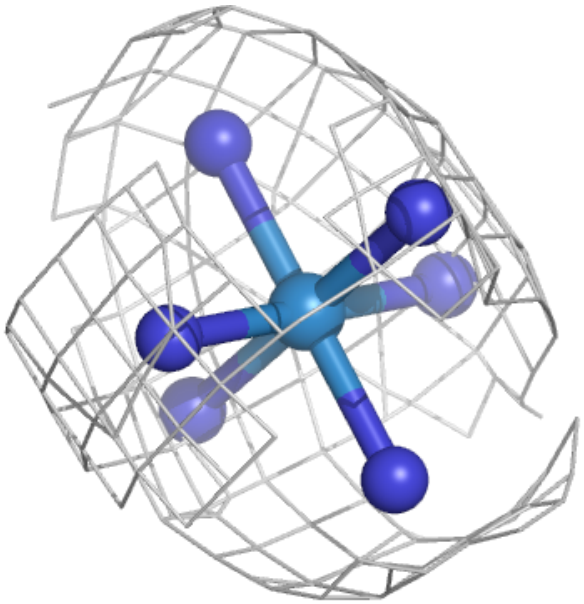


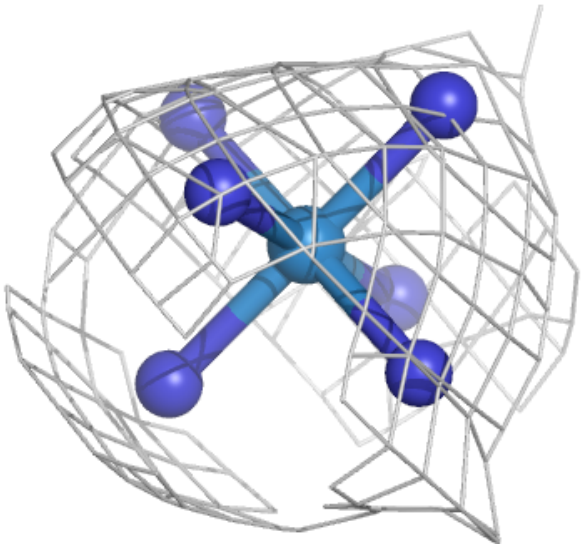


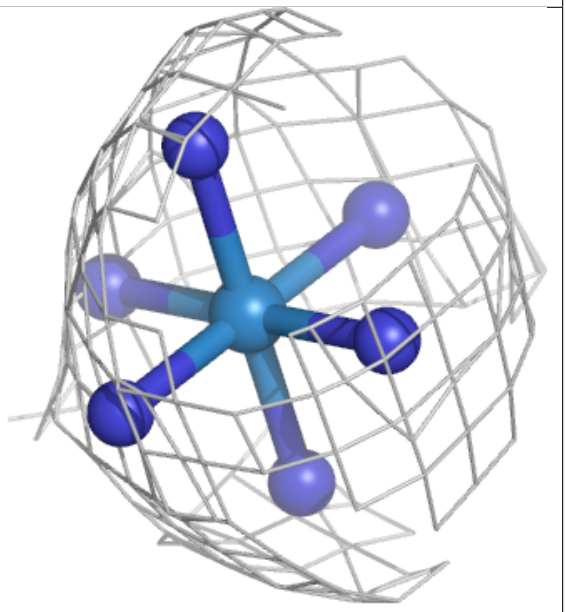


Electron density around OHX B1 3602:

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

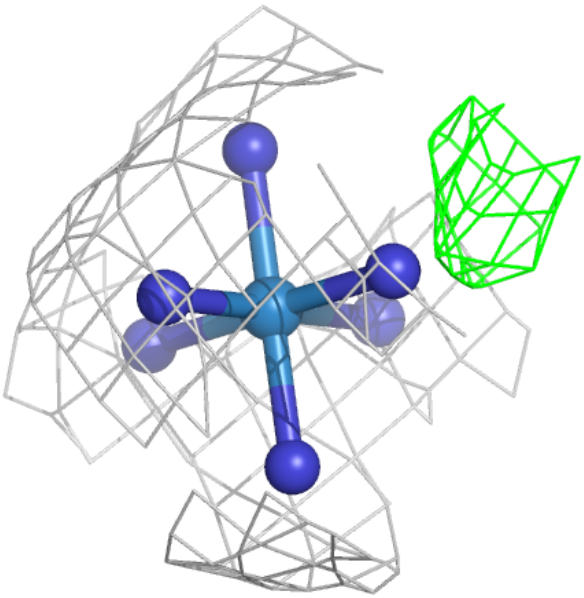


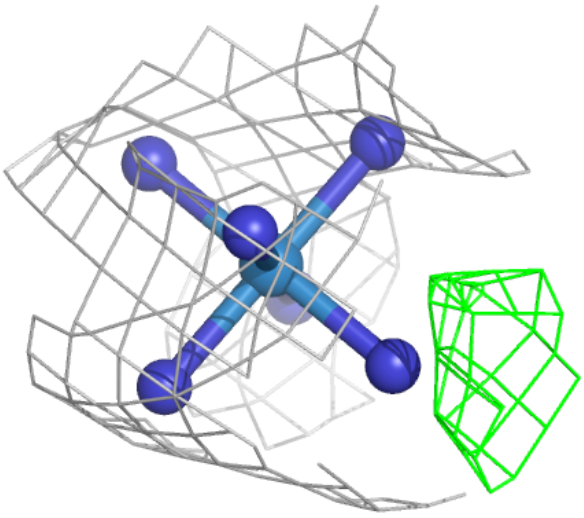


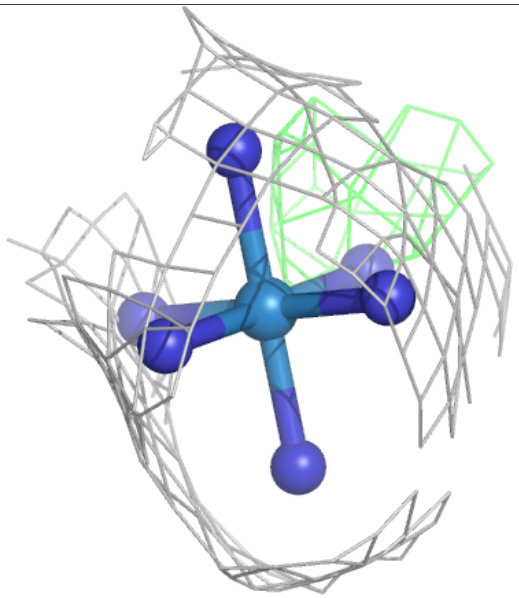


Electron density around OHX A1 1983:

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

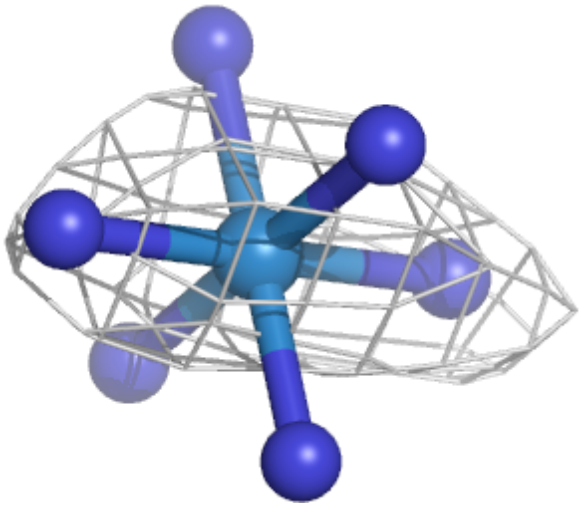


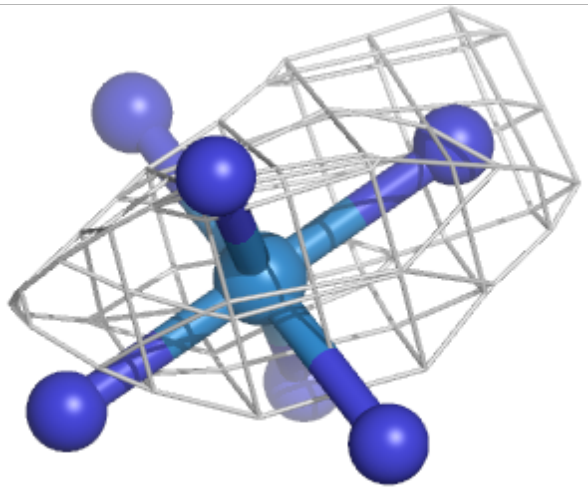


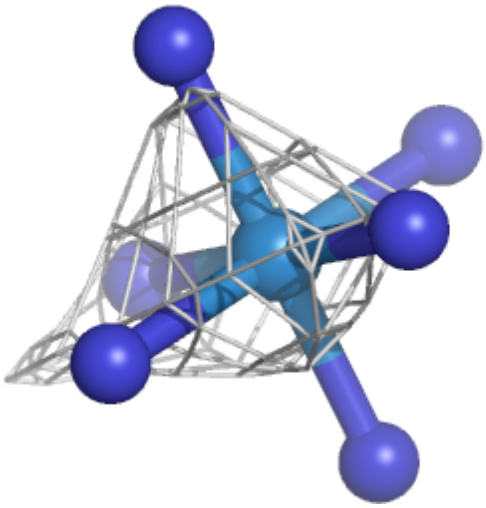


Electron density around OHX B1 3571:

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

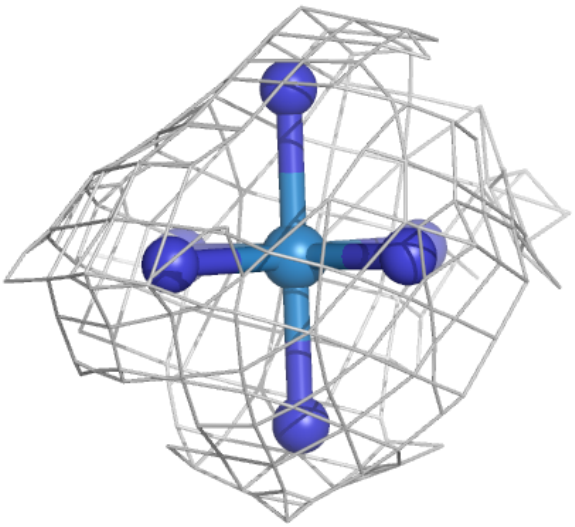


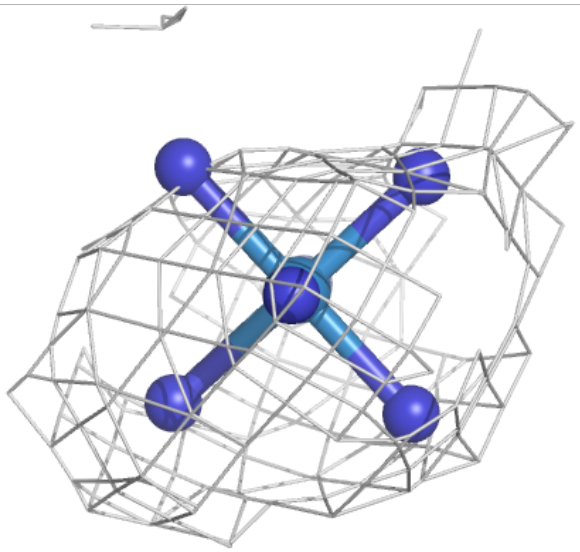


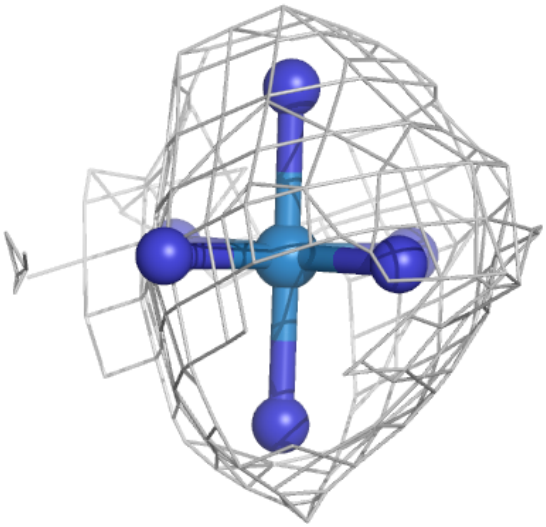


Electron density around OHX D1 3573:

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

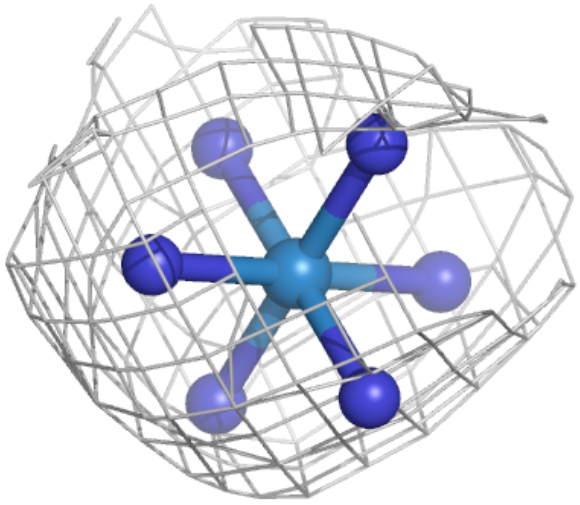


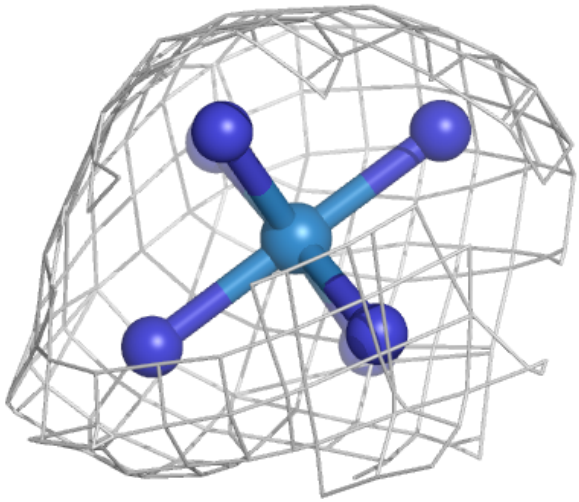


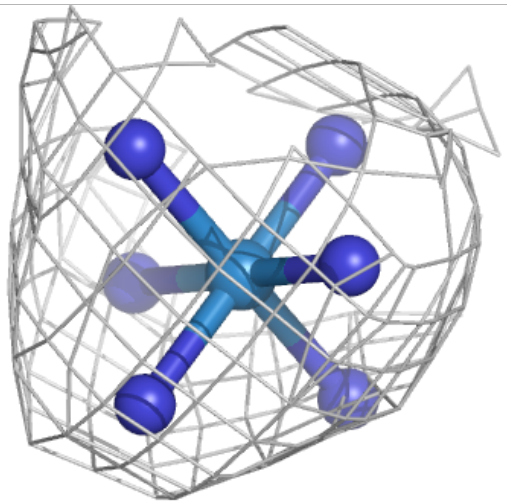


Electron density around OHX D1 3605:

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

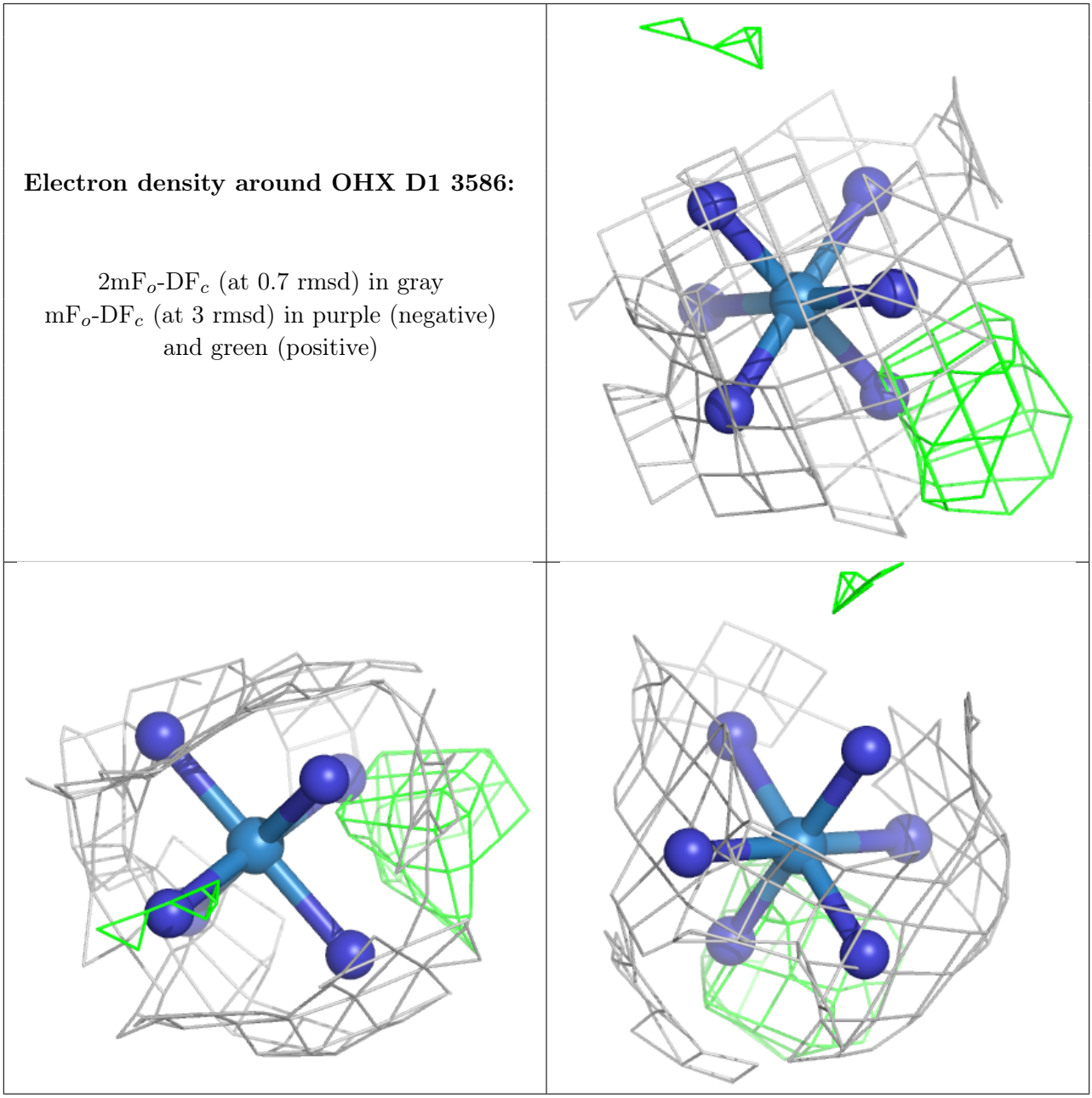






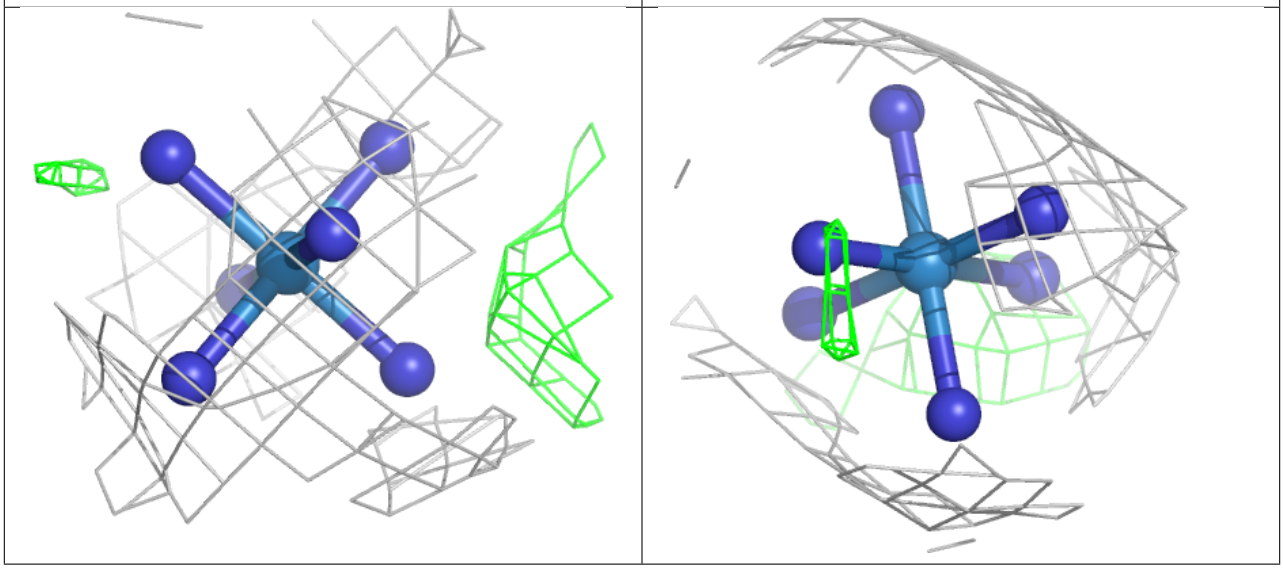
Electron density around OHX D1 3586:

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



Electron density around OHX B1 3548:

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



6.5 Other polymers

There are no such residues in this entry.