wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 05:02 am BST

PDB ID	:	5COD
Title	:	Bovine heart complex I membrane domain
Authors	:	Zhu, J.; Hirst, J.; King, M.S.; Yu, M.; Leslie, A.G.W.; Klipcan, L.
Deposited on	:	2015-07-20
Resolution	:	6.74 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 following versions of software and data (see references (1)) were used in the production of this report:

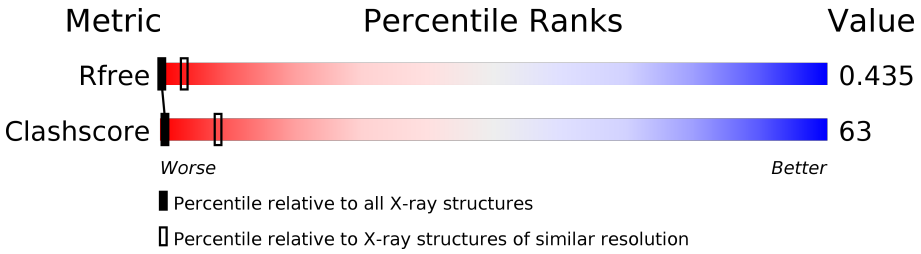
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 6.74 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	1002 (9.50-3.90)
Clashscore	141614	1066 (9.50-3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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%

Mol	Chain	Length	Quality of chain
1	L1	606	44% 37% 19%
1	L2	606	43% 38% 19%
1	L3	606	44% 37% 19%
1	L4	606	43% 38% 19%
1	L5	606	43% 38% 19%
1	L6	606	44% 37% 19%
2	M1	459	48% 47% .
2	M2	459	47% 49% .
2	M3	459	48% 48% .

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Mol	Chain	Length	Quality of chain
2	M4	459	47% 48%
2	M5	459	48% 47%
2	M6	459	48% 47%
3	f1	30	100%
3	f2	30	100%
3	f3	30	100%
3	f4	30	100%
3	f5	30	100%
3	f6	30	100%
3	h1	30	100%
3	h2	30	100%
3	h3	30	100%
3	h4	30	100%
3	h5	30	100%
3	h6	30	100%
3	i1	30	100%
3	i2	30	100%
3	i3	30	100%
3	i4	30	100%
3	i5	30	100%
3	i6	30	100%
4	g1	22	100%
4	g2	22	100%
4	g3	22	100%
4	g4	22	100%

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Mol	Chain	Length	Quality of chain
4	g5	22	100%
4	g6	22	100%
5	j1	28	100%
5	j2	28	100%
5	j3	28	100%
5	j4	28	100%
5	j5	28	100%
5	j6	28	100%
5	k1	28	100%
5	k2	28	100%
5	k3	28	100%
5	k4	28	100%
5	k5	28	100%
5	k6	28	100%
5	p1	28	100%
5	p2	28	100%
5	p3	28	100%
5	p4	28	100%
5	p5	28	100%
5	p6	28	100%
5	s1	28	100%
5	s2	28	100%
5	s3	28	100%
5	s4	28	100%
5	s5	28	100%

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Mol	Chain	Length	Quality of chain
5	s6	28	100%
6	l1	13	100%
6	l2	13	100%
6	l3	13	100%
6	l4	13	100%
6	l5	13	100%
6	l6	13	100%
7	U1	88	55% 31% 15%
7	U2	88	57% 28% 15%
7	U3	88	55% 31% 15%
7	U4	88	57% 28% 15%
7	U5	88	55% 31% 15%
7	U6	88	57% 28% 15%
8	n1	59	100%
8	n2	59	100%
8	n3	59	100%
8	n4	59	100%
8	n5	59	100%
8	n6	59	100%
9	o1	21	100%
9	o2	21	100%
9	o3	21	100%
9	o4	21	100%
9	o5	21	100%
9	o6	21	100%

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Mol	Chain	Length	Quality of chain
10	t1	57	100%
10	t2	57	100%
10	t3	57	100%
10	t4	57	100%
10	t5	57	100%
10	t6	57	100%
11	u1	15	100%
11	u2	15	100%
11	u3	15	100%
11	u4	15	100%
11	u5	15	100%
11	u6	15	100%
12	v1	32	100%
12	v2	32	100%
12	v3	32	100%
12	v4	32	100%
12	v5	32	100%
12	v6	32	100%
13	w1	27	100%
13	w2	27	100%
13	w3	27	100%
13	w4	27	100%
13	w5	27	100%
13	w6	27	100%
14	BA	146	85% 14%

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Mol	Chain	Length	Quality of chain
14	BB	146	
14	BC	146	
14	BD	146	
14	BE	146	
14	BF	146	

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 48030 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 protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	L1	493	Total	C	N	O	0	0	0
			2465	1479	493	493			
1	L2	493	Total	C	N	O	0	0	0
			2465	1479	493	493			
1	L3	493	Total	C	N	O	0	0	0
			2465	1479	493	493			
1	L4	493	Total	C	N	O	0	0	0
			2465	1479	493	493			
1	L5	493	Total	C	N	O	0	0	0
			2465	1479	493	493			
1	L6	493	Total	C	N	O	0	0	0
			2465	1479	493	493			

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M1	439	Total	C	N	O	0	0	0
			2195	1317	439	439			
2	M2	439	Total	C	N	O	0	0	0
			2195	1317	439	439			
2	M3	439	Total	C	N	O	0	0	0
			2195	1317	439	439			
2	M4	439	Total	C	N	O	0	0	0
			2195	1317	439	439			
2	M5	439	Total	C	N	O	0	0	0
			2195	1317	439	439			
2	M6	439	Total	C	N	O	0	0	0
			2195	1317	439	439			

- Molecule 3 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	f1	30	Total C N O 150 90 30 30	0	0	0
3	h1	30	Total C N O 150 90 30 30	0	0	0
3	i1	30	Total C N O 150 90 30 30	0	0	0
3	f2	30	Total C N O 150 90 30 30	0	0	0
3	h2	30	Total C N O 150 90 30 30	0	0	0
3	i2	30	Total C N O 150 90 30 30	0	0	0
3	f3	30	Total C N O 150 90 30 30	0	0	0
3	h3	30	Total C N O 150 90 30 30	0	0	0
3	i3	30	Total C N O 150 90 30 30	0	0	0
3	f4	30	Total C N O 150 90 30 30	0	0	0
3	h4	30	Total C N O 150 90 30 30	0	0	0
3	i4	30	Total C N O 150 90 30 30	0	0	0
3	f5	30	Total C N O 150 90 30 30	0	0	0
3	h5	30	Total C N O 150 90 30 30	0	0	0
3	i5	30	Total C N O 150 90 30 30	0	0	0
3	f6	30	Total C N O 150 90 30 30	0	0	0
3	h6	30	Total C N O 150 90 30 30	0	0	0
3	i6	30	Total C N O 150 90 30 30	0	0	0

- Molecule 4 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	g1	22	Total C N O 110 66 22 22	0	0	0
4	g2	22	Total C N O 110 66 22 22	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	g3	22	Total	C	N	O	0	0	0
			110	66	22	22			
4	g4	22	Total	C	N	O	0	0	0
			110	66	22	22			
4	g5	22	Total	C	N	O	0	0	0
			110	66	22	22			
4	g6	22	Total	C	N	O	0	0	0
			110	66	22	22			

- Molecule 5 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	j1	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	k1	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	p1	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	s1	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	j2	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	k2	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	p2	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	s2	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	j3	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	k3	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	p3	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	s3	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	j4	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	k4	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	p4	28	Total	C	N	O	0	0	0
			140	84	28	28			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	s4	28	Total C N O 140 84 28 28	0	0	0
5	j5	28	Total C N O 140 84 28 28	0	0	0
5	k5	28	Total C N O 140 84 28 28	0	0	0
5	p5	28	Total C N O 140 84 28 28	0	0	0
5	s5	28	Total C N O 140 84 28 28	0	0	0
5	j6	28	Total C N O 140 84 28 28	0	0	0
5	k6	28	Total C N O 140 84 28 28	0	0	0
5	p6	28	Total C N O 140 84 28 28	0	0	0
5	s6	28	Total C N O 140 84 28 28	0	0	0

- Molecule 6 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	l1	13	Total C N O 65 39 13 13	0	0	0
6	l2	13	Total C N O 65 39 13 13	0	0	0
6	l3	13	Total C N O 65 39 13 13	0	0	0
6	l4	13	Total C N O 65 39 13 13	0	0	0
6	l5	13	Total C N O 65 39 13 13	0	0	0
6	l6	13	Total C N O 65 39 13 13	0	0	0

- Molecule 7 is a protein called SDAP.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	U1	75	Total C N O 375 225 75 75	0	0	0
7	U2	75	Total C N O 375 225 75 75	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	U3	75	Total	C	N	O	0	0	0
			375	225	75	75			
7	U4	75	Total	C	N	O	0	0	0
			375	225	75	75			
7	U5	75	Total	C	N	O	0	0	0
			375	225	75	75			
7	U6	75	Total	C	N	O	0	0	0
			375	225	75	75			

- Molecule 8 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	n1	59	Total	C	N	O	0	0	0
			295	177	59	59			
8	n2	59	Total	C	N	O	0	0	0
			295	177	59	59			
8	n3	59	Total	C	N	O	0	0	0
			295	177	59	59			
8	n4	59	Total	C	N	O	0	0	0
			295	177	59	59			
8	n5	59	Total	C	N	O	0	0	0
			295	177	59	59			
8	n6	59	Total	C	N	O	0	0	0
			295	177	59	59			

- Molecule 9 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	o1	21	Total	C	N	O	0	0	0
			105	63	21	21			
9	o2	21	Total	C	N	O	0	0	0
			105	63	21	21			
9	o3	21	Total	C	N	O	0	0	0
			105	63	21	21			
9	o4	21	Total	C	N	O	0	0	0
			105	63	21	21			
9	o5	21	Total	C	N	O	0	0	0
			105	63	21	21			
9	o6	21	Total	C	N	O	0	0	0
			105	63	21	21			

- Molecule 10 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	t1	57	Total C N O 285 171 57 57	0	0	0
10	t2	57	Total C N O 285 171 57 57	0	0	0
10	t3	57	Total C N O 285 171 57 57	0	0	0
10	t4	57	Total C N O 285 171 57 57	0	0	0
10	t5	57	Total C N O 285 171 57 57	0	0	0
10	t6	57	Total C N O 285 171 57 57	0	0	0

- Molecule 11 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	u1	15	Total C N O 75 45 15 15	0	0	0
11	u2	15	Total C N O 75 45 15 15	0	0	0
11	u3	15	Total C N O 75 45 15 15	0	0	0
11	u4	15	Total C N O 75 45 15 15	0	0	0
11	u5	15	Total C N O 75 45 15 15	0	0	0
11	u6	15	Total C N O 75 45 15 15	0	0	0

- Molecule 12 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	v1	32	Total C N O 160 96 32 32	0	0	0
12	v2	32	Total C N O 160 96 32 32	0	0	0
12	v3	32	Total C N O 160 96 32 32	0	0	0
12	v4	32	Total C N O 160 96 32 32	0	0	0
12	v5	32	Total C N O 160 96 32 32	0	0	0
12	v6	32	Total C N O 160 96 32 32	0	0	0

- Molecule 13 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	w1	27	Total	C	N	O	0	0	0
			135	81	27	27			
13	w2	27	Total	C	N	O	0	0	0
			135	81	27	27			
13	w3	27	Total	C	N	O	0	0	0
			135	81	27	27			
13	w4	27	Total	C	N	O	0	0	0
			135	81	27	27			
13	w5	27	Total	C	N	O	0	0	0
			135	81	27	27			
13	w6	27	Total	C	N	O	0	0	0
			135	81	27	27			

- Molecule 14 is a protein called Unknown structure.

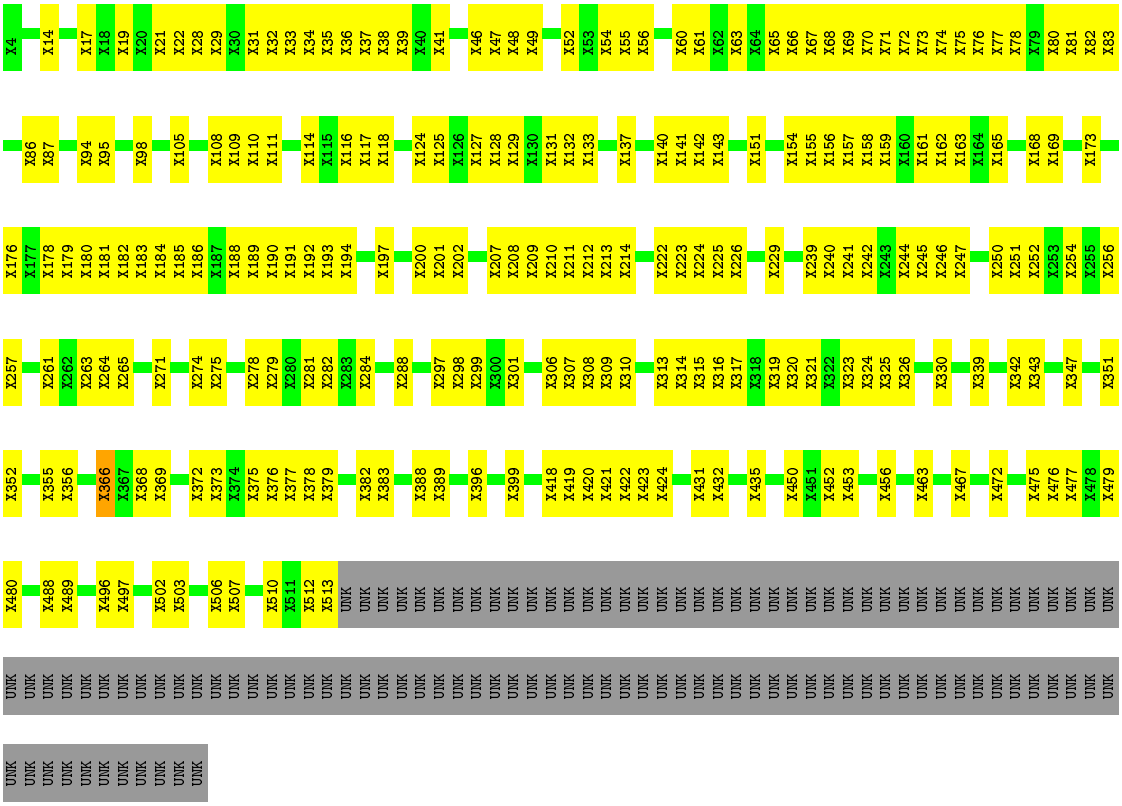
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	BA	146	Total	C	N	O	0	0	0
			730	438	146	146			
14	BB	146	Total	C	N	O	0	0	0
			730	438	146	146			
14	BC	146	Total	C	N	O	0	0	0
			730	438	146	146			
14	BD	146	Total	C	N	O	0	0	0
			730	438	146	146			
14	BE	146	Total	C	N	O	0	0	0
			730	438	146	146			
14	BF	146	Total	C	N	O	0	0	0
			730	438	146	146			

3 Residue-property plots (i)

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

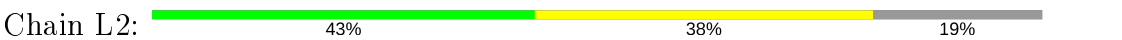
- Molecule 1: NADH-ubiquinone oxidoreductase chain 5

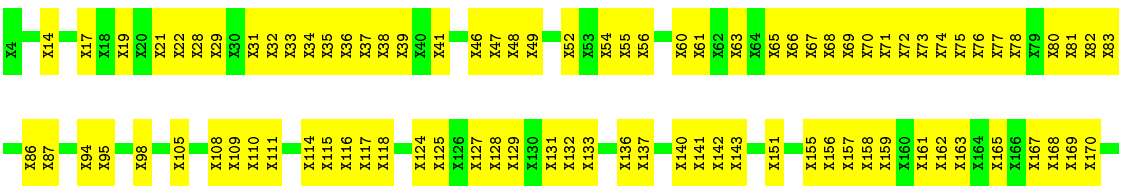
Chain L1:

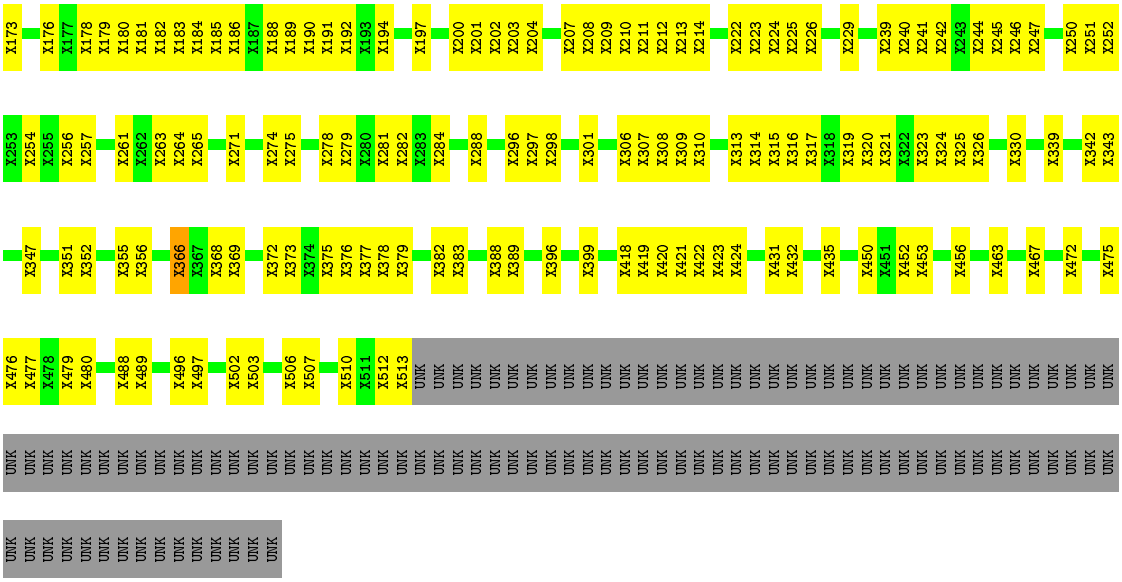


- Molecule 1: NADH-ubiquinone oxidoreductase chain 5

Chain L2:

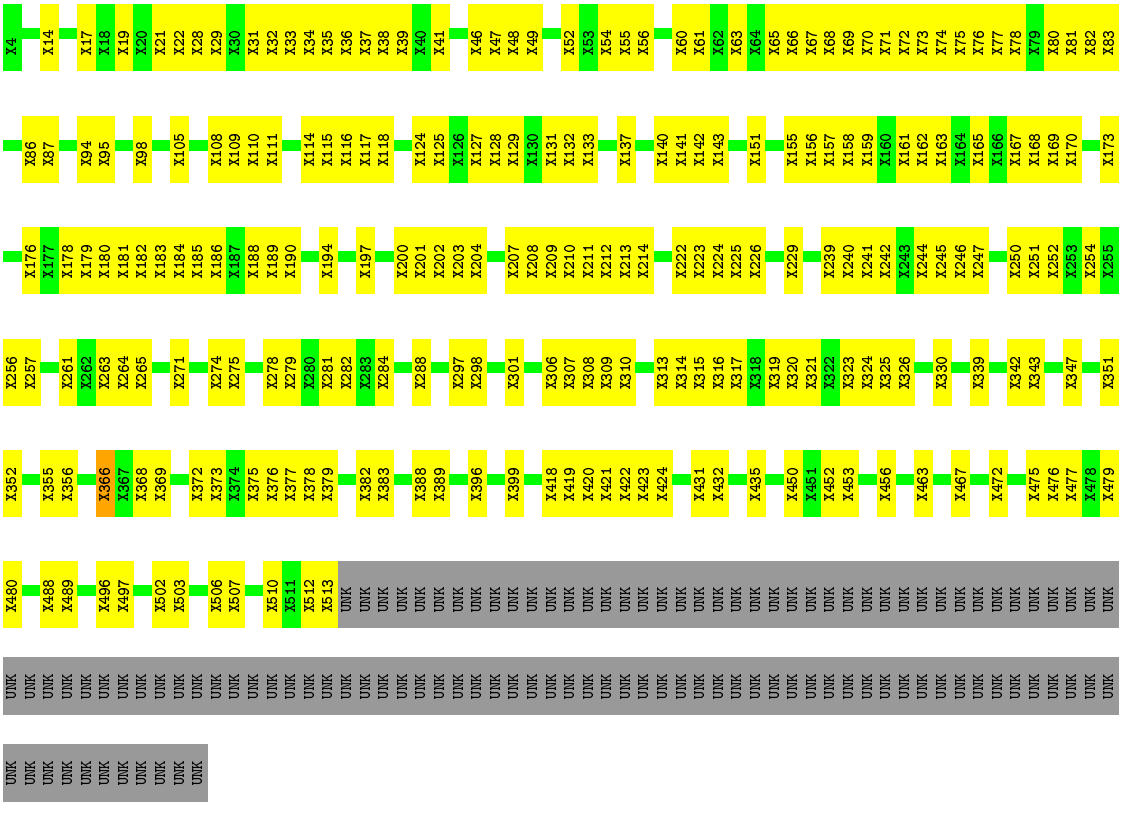






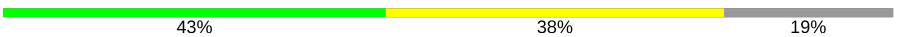
• Molecule 1: NADH-ubiquinone oxidoreductase chain 5

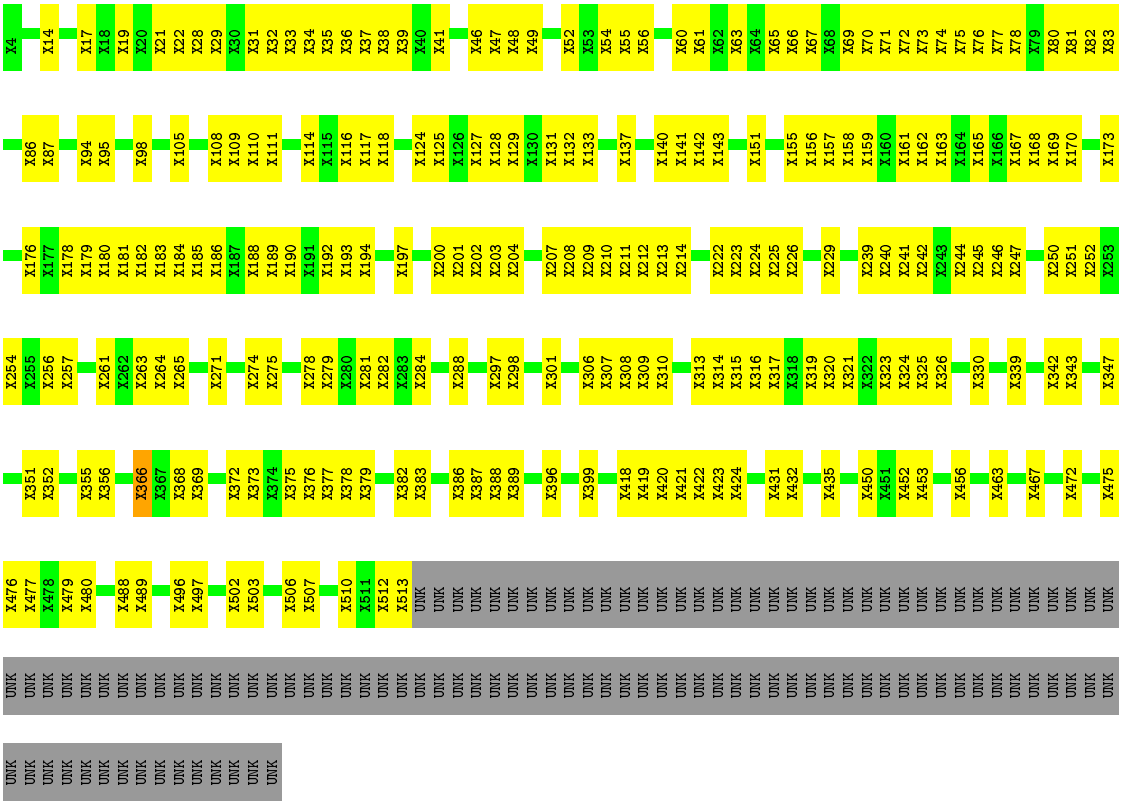
Chain L3:



• Molecule 1: NADH-ubiquinone oxidoreductase chain 5

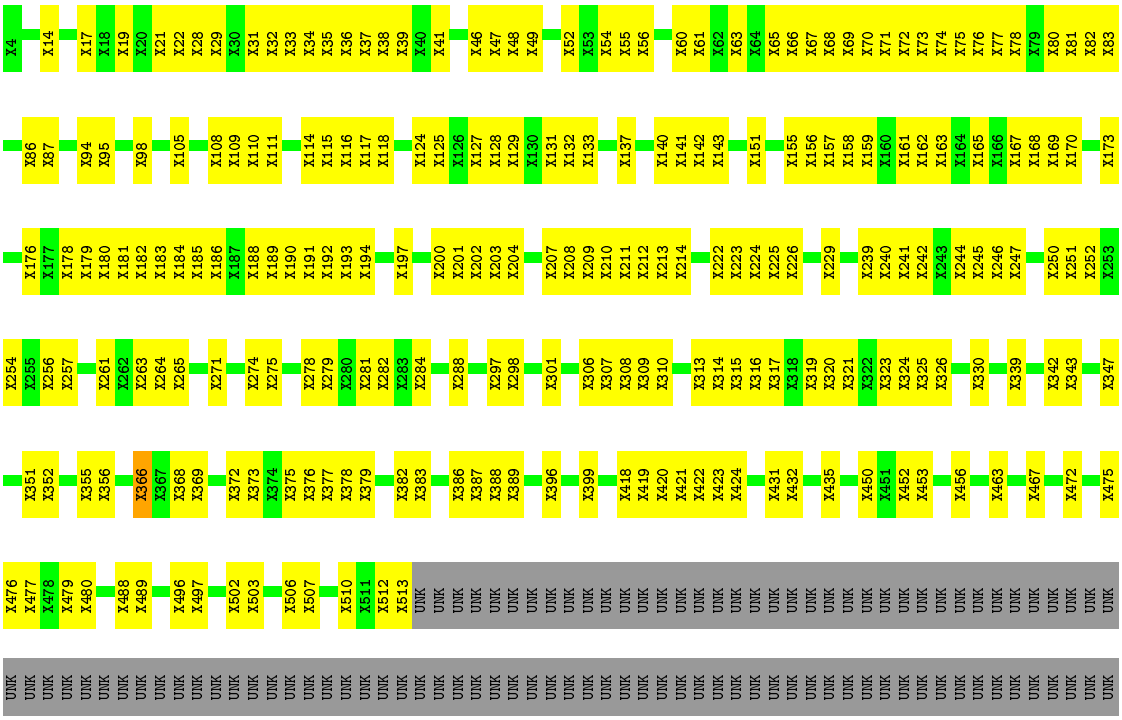
Chain L4:





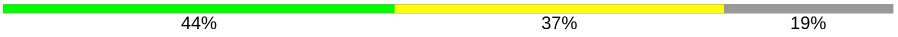
- Molecule 1: NADH-ubiquinone oxidoreductase chain 5

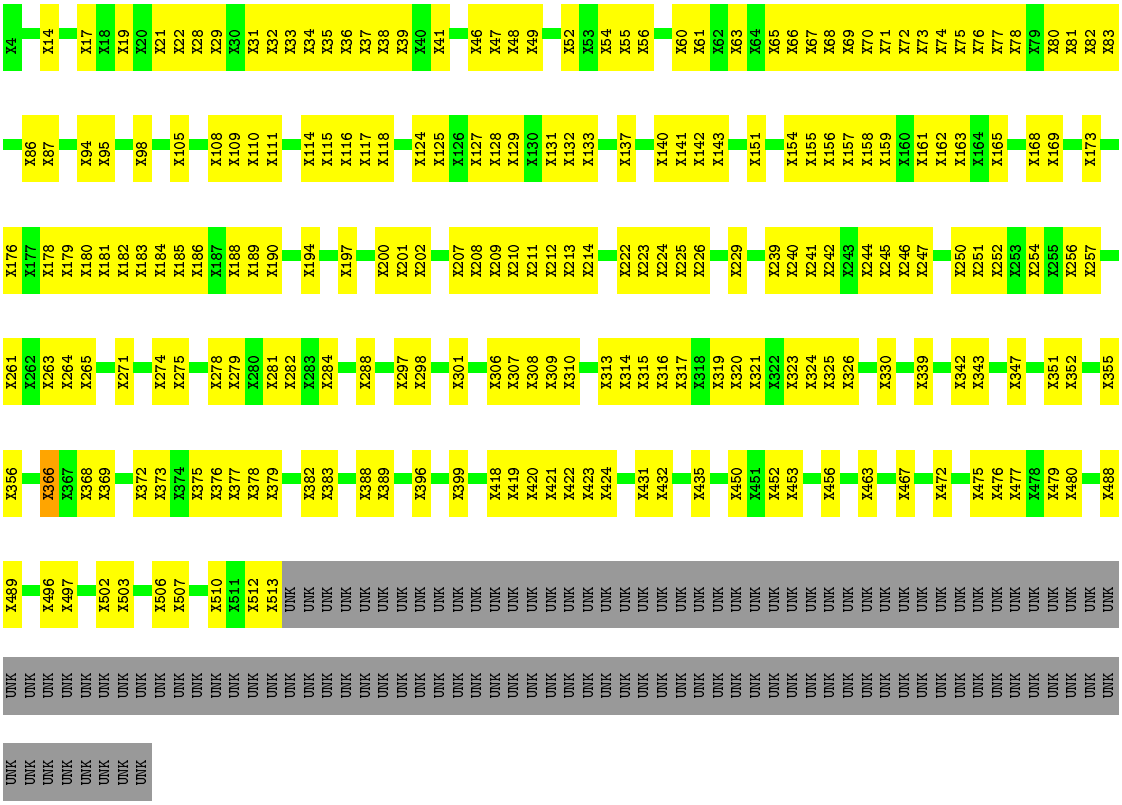
Chain L5:



- Molecule 1: NADH-ubiquinone oxidoreductase chain 5

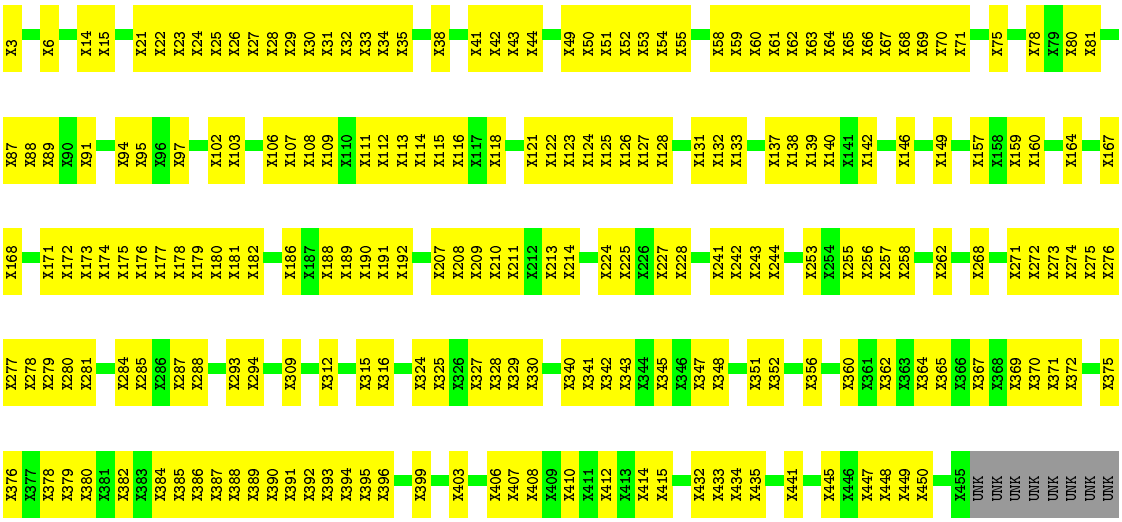
Chain L6:





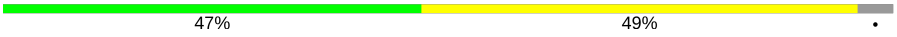
- Molecule 2: NADH-ubiquinone oxidoreductase chain 4

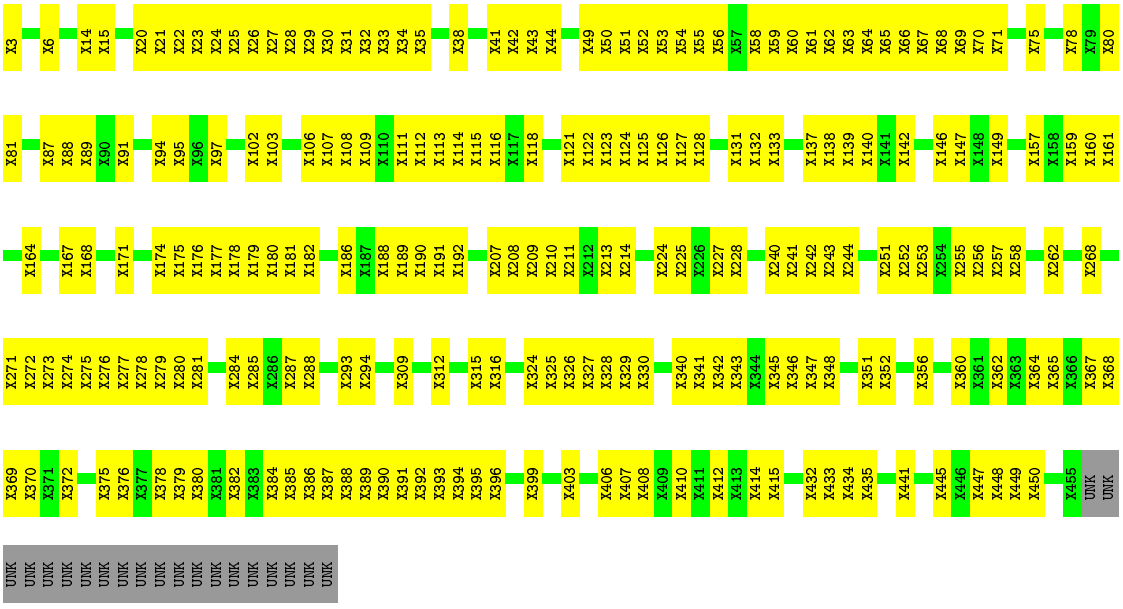
Chain M1:



- Molecule 2: NADH-ubiquinone oxidoreductase chain 4

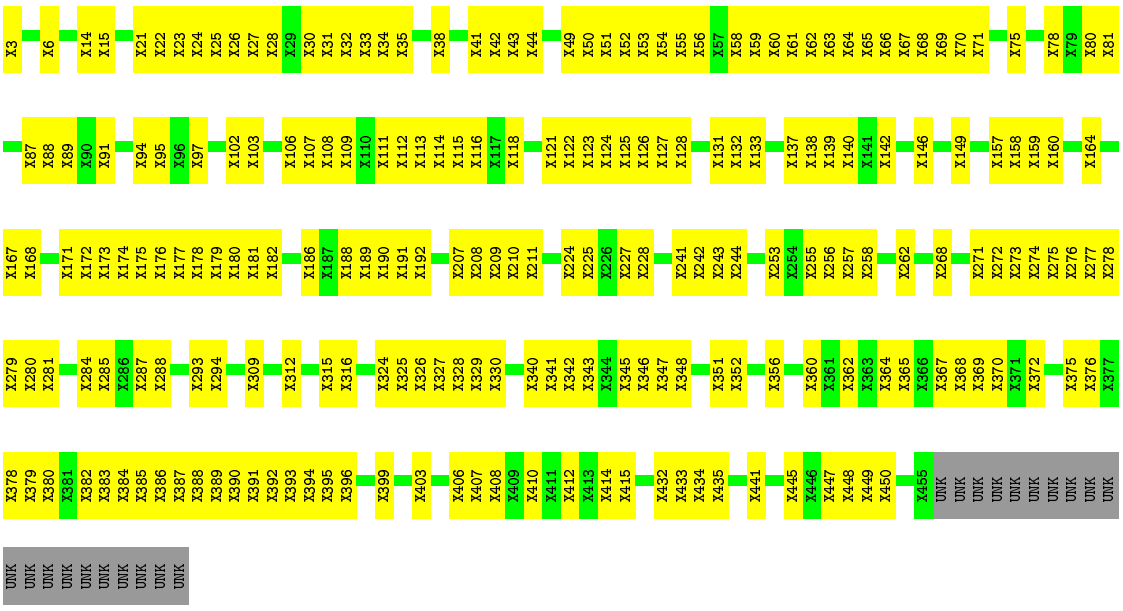
Chain M2:





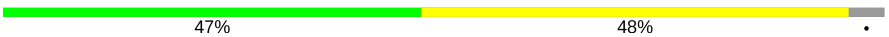
- Molecule 2: NADH-ubiquinone oxidoreductase chain 4

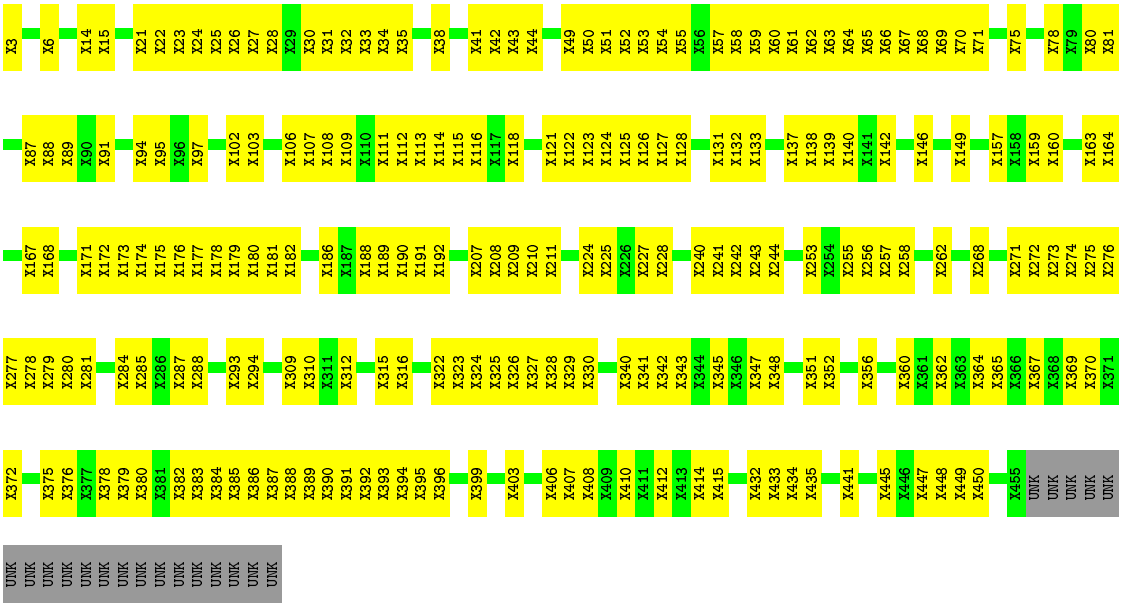
Chain M3:



- Molecule 2: NADH-ubiquinone oxidoreductase chain 4

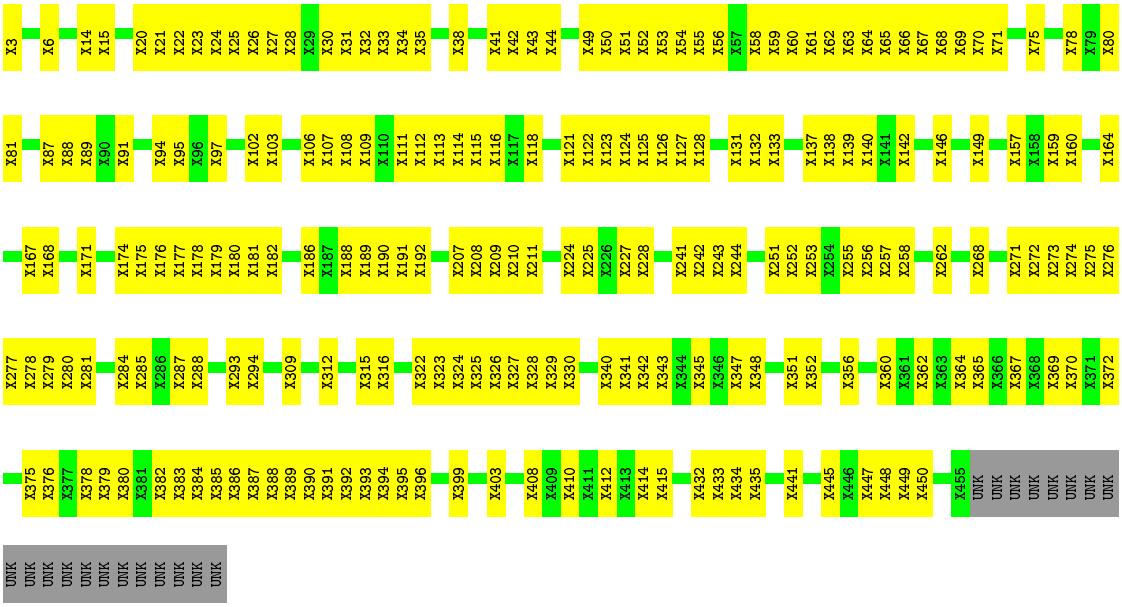
Chain M4:





• Molecule 2: NADH-ubiquinone oxidoreductase chain 4

Chain M5:



• Molecule 2: NADH-ubiquinone oxidoreductase chain 4

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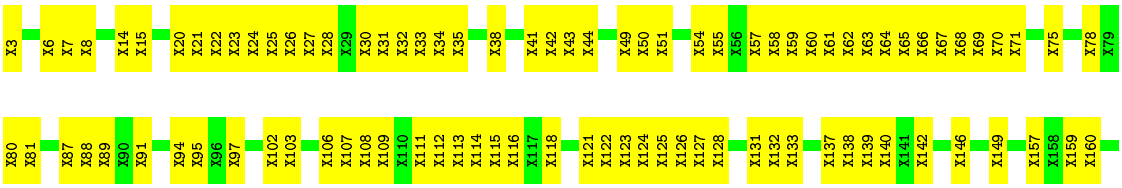

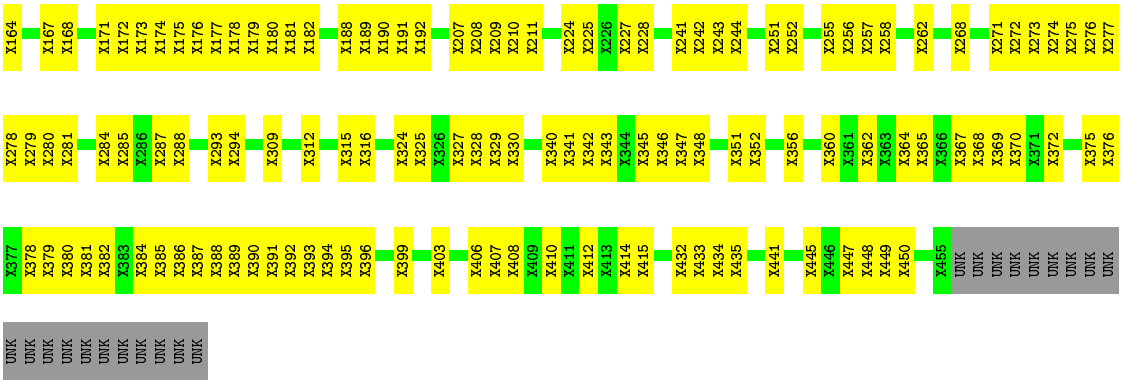

- Molecule 3: Unknown structure

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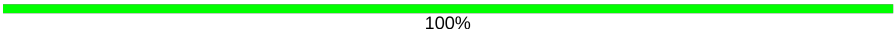

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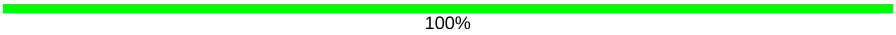
- Molecule 3: Unknown structure

Chain h1:



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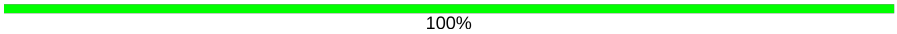
- Molecule 3: Unknown structure

Chain i1:



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- Molecule 3: Unknown structure

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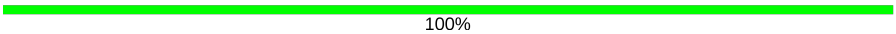

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- Molecule 3: Unknown structure

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- Molecule 3: Unknown structure

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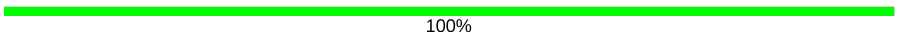

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- Molecule 3: Unknown structure

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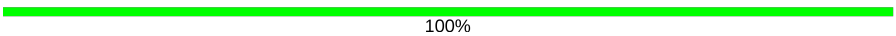

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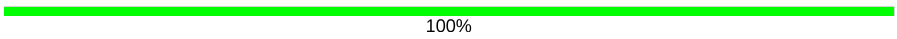
Chain i3: 

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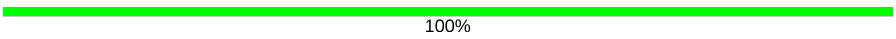
Chain f4: 

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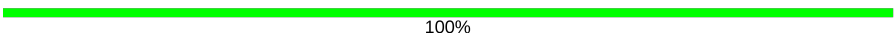
- Molecule 3: Unknown structure

Chain h4: 

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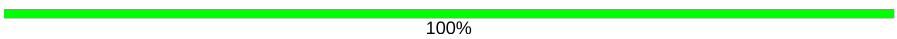
- Molecule 3: Unknown structure

Chain i4: 

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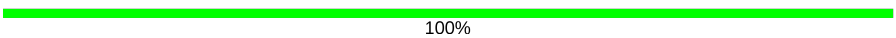
- Molecule 3: Unknown structure

Chain f5: 

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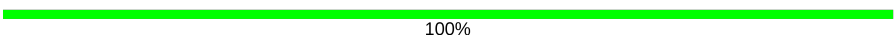
- Molecule 3: Unknown structure

Chain h5: 

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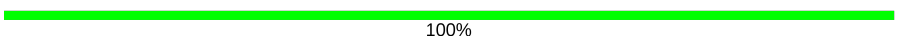
- Molecule 3: Unknown structure

Chain i5: 

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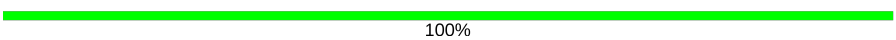
Chain f6: 

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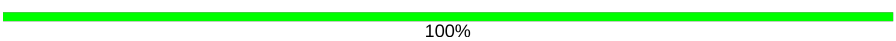
- Molecule 3: Unknown structure

Chain h6: 

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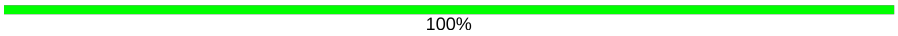
- Molecule 3: Unknown structure

Chain i6: 

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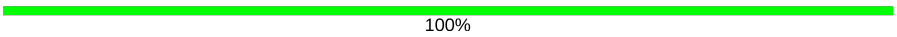
- Molecule 4: Unknown structure

Chain g1: 

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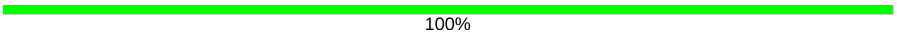
- Molecule 4: Unknown structure

Chain g2: 

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- Molecule 4: Unknown structure

Chain g3: 

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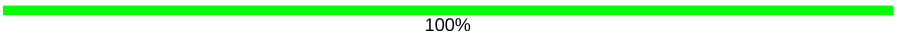
- Molecule 4: Unknown structure

Chain g4: 

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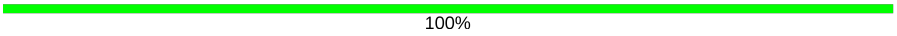
- Molecule 4: Unknown structure

Chain g5: 

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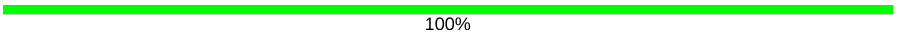
Chain g6: 

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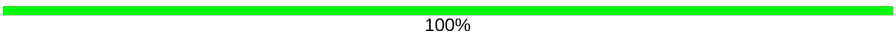
- Molecule 5: Unknown structure

Chain j1: 

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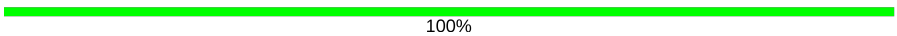
- Molecule 5: Unknown structure

Chain k1: 

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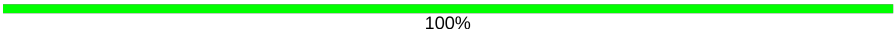
- Molecule 5: Unknown structure

Chain p1: 

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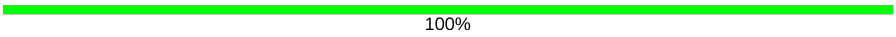
Chain s1: 

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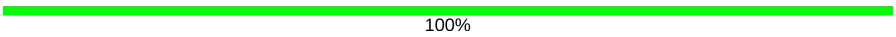
- Molecule 5: Unknown structure

Chain j2: 

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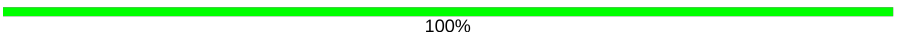
- Molecule 5: Unknown structure

Chain k2: 

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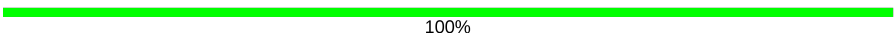
- Molecule 5: Unknown structure

Chain p2: 

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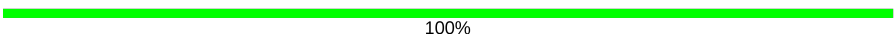
Chain s2: 

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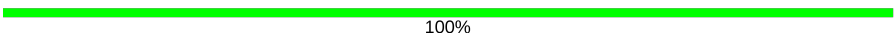
- Molecule 5: Unknown structure

Chain j3: 

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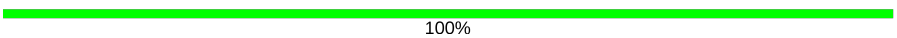
- Molecule 5: Unknown structure

Chain k3: 

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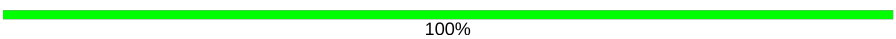
- Molecule 5: Unknown structure

Chain p3: 

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- Molecule 5: Unknown structure

Chain s3: 

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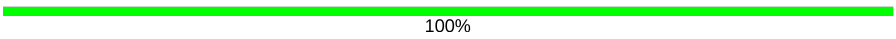
- Molecule 5: Unknown structure

Chain j4: 

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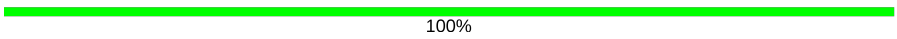
- Molecule 5: Unknown structure

Chain k4: 

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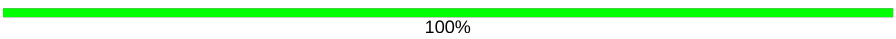
- Molecule 5: Unknown structure

Chain p4: 

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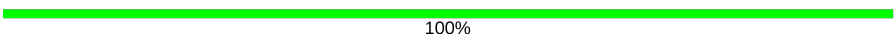
- Molecule 5: Unknown structure

Chain s4: 

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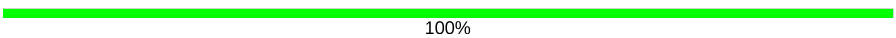
Chain j5: 

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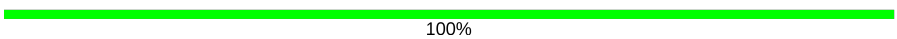
Chain k5: 

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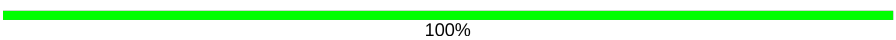
Chain p5: 

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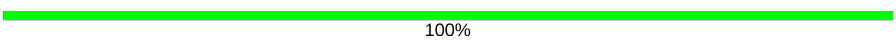
Chain s5: 

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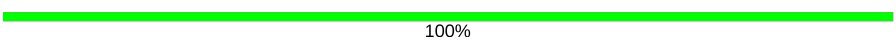
- Molecule 5: Unknown structure

Chain j6: 

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- Molecule 5: Unknown structure

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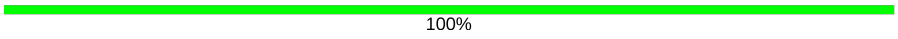

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- Molecule 5: Unknown structure

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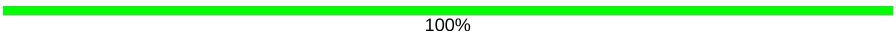

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- Molecule 5: Unknown structure

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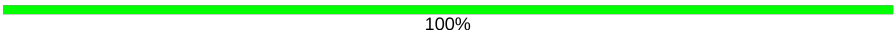


There are no outlier residues recorded for this chain.

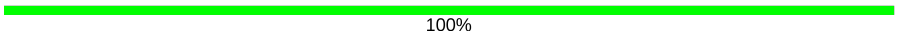
- Molecule 6: Unknown structure

Chain l1:

There are no outlier residues recorded for this chain.

- Molecule 6: Unknown structure

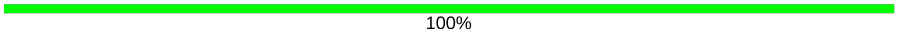
Chain l2:



There are no outlier residues recorded for this chain.

- Molecule 6: Unknown structure

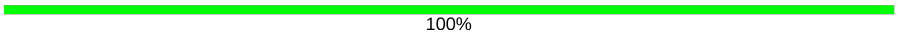
Chain l3:



There are no outlier residues recorded for this chain.

- Molecule 6: Unknown structure

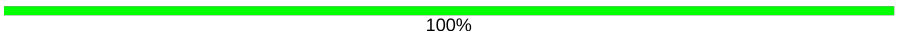
Chain l4:



There are no outlier residues recorded for this chain.

- Molecule 6: Unknown structure

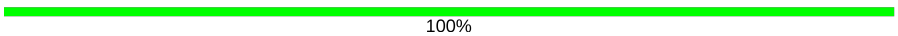
Chain l5:



There are no outlier residues recorded for this chain.

- Molecule 6: Unknown structure

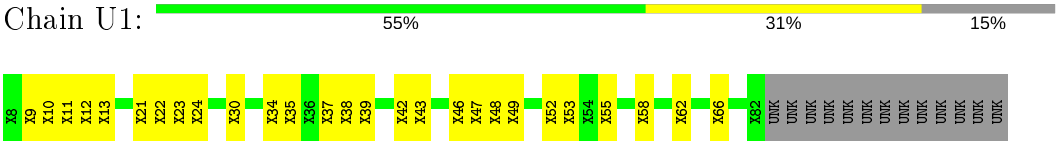
Chain l6:



There are no outlier residues recorded for this chain.

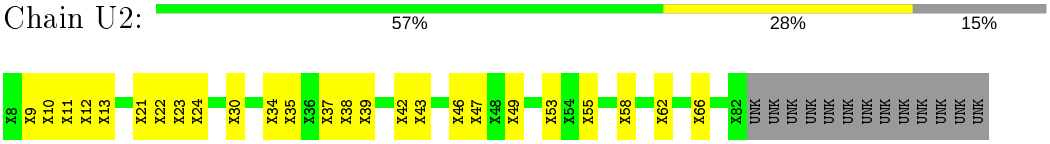
• Molecule 7: SDAP

Chain U1:



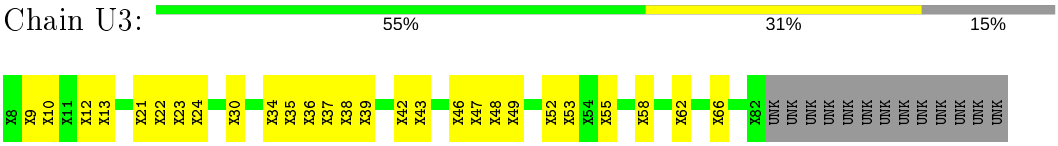
• Molecule 7: SDAP

Chain U2:



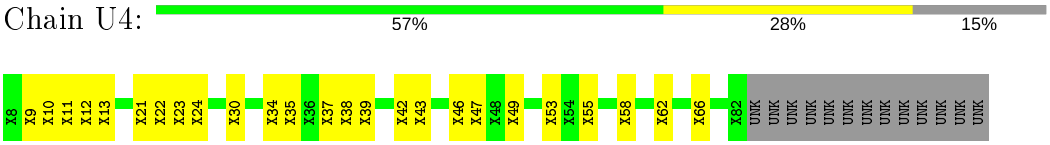
• Molecule 7: SDAP

Chain U3:



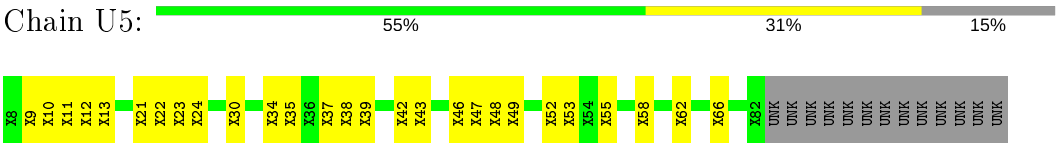
• Molecule 7: SDAP

Chain U4:



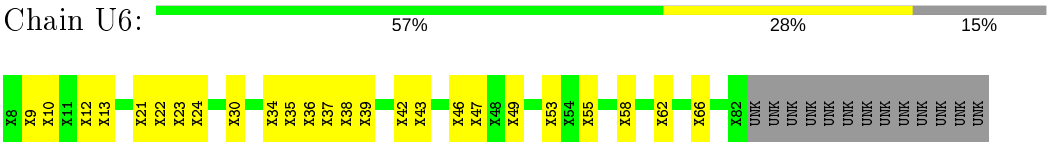
• Molecule 7: SDAP

Chain U5:



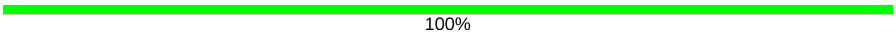
• Molecule 7: SDAP

Chain U6:



• Molecule 8: Unknown structure

Chain n1:



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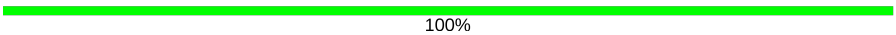
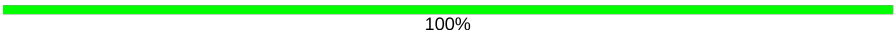
• Molecule 8: Unknown structure

Chain n2:



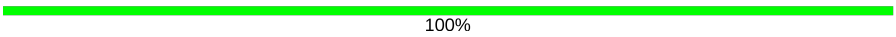
There are no outlier residues recorded for this chain.

- Molecule 8: Unknown structure

Chain n3: 

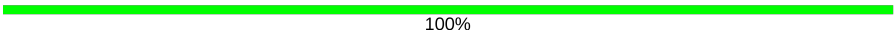
There are no outlier residues recorded for this chain.

- Molecule 8: Unknown structure

Chain n4: 

There are no outlier residues recorded for this chain.

- Molecule 8: Unknown structure

Chain n5: 

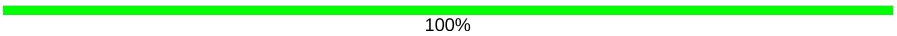
There are no outlier residues recorded for this chain.

- Molecule 8: Unknown structure

Chain n6: 

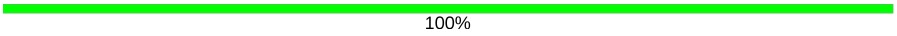
There are no outlier residues recorded for this chain.

- Molecule 9: Unknown structure

Chain o1: 

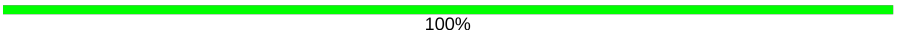
There are no outlier residues recorded for this chain.

- Molecule 9: Unknown structure

Chain o2: 

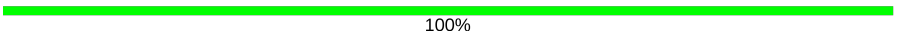
There are no outlier residues recorded for this chain.

- Molecule 9: Unknown structure

Chain o3: 

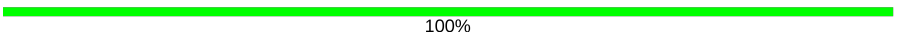
There are no outlier residues recorded for this chain.

- Molecule 9: Unknown structure

Chain o4: 

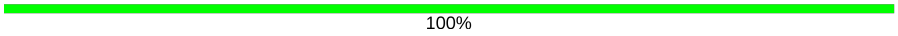
There are no outlier residues recorded for this chain.

- Molecule 9: Unknown structure

Chain o5: 

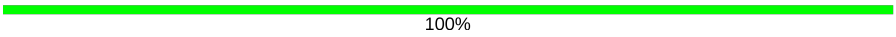
There are no outlier residues recorded for this chain.

• Molecule 9: Unknown structure

Chain o6: 

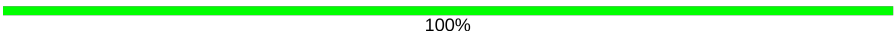
There are no outlier residues recorded for this chain.

• Molecule 10: Unknown structure

Chain t1: 

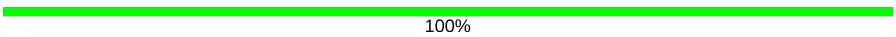
There are no outlier residues recorded for this chain.

• Molecule 10: Unknown structure

Chain t2: 

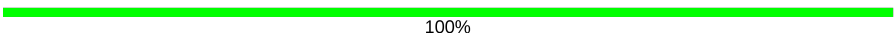
There are no outlier residues recorded for this chain.

• Molecule 10: Unknown structure

Chain t3: 

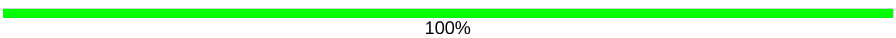
There are no outlier residues recorded for this chain.

• Molecule 10: Unknown structure

Chain t4: 

There are no outlier residues recorded for this chain.

• Molecule 10: Unknown structure

Chain t5: 

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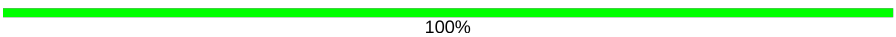
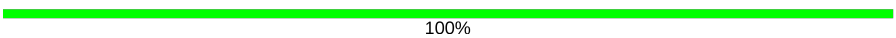
• Molecule 10: Unknown structure

Chain t6: 

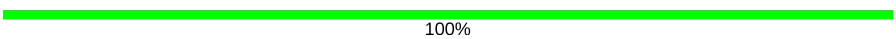
There are no outlier residues recorded for this chain.

• Molecule 11: Unknown structure

Chain u1: 

There are no outlier residues recorded for this chain.

• Molecule 11: Unknown structure

Chain u2: 

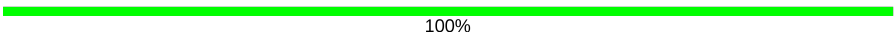
There are no outlier residues recorded for this chain.

• Molecule 11: Unknown structure

Chain u3: 

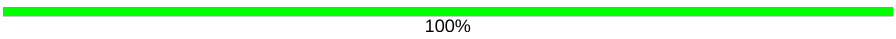
There are no outlier residues recorded for this chain.

- Molecule 11: Unknown structure

Chain u4: 

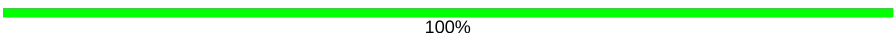
There are no outlier residues recorded for this chain.

- Molecule 11: Unknown structure

Chain u5: 

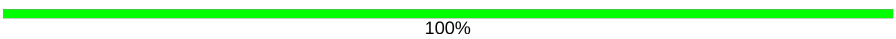
There are no outlier residues recorded for this chain.

- Molecule 11: Unknown structure

Chain u6: 

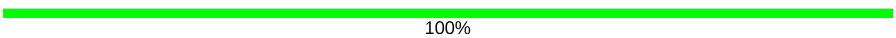
There are no outlier residues recorded for this chain.

- Molecule 12: Unknown structure

Chain v1: 

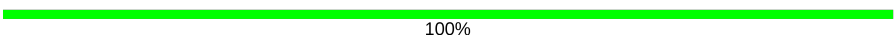
There are no outlier residues recorded for this chain.

- Molecule 12: Unknown structure

Chain v2: 

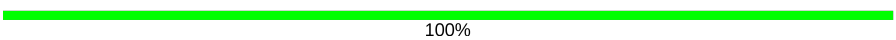
There are no outlier residues recorded for this chain.

- Molecule 12: Unknown structure

Chain v3: 

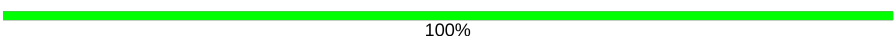
There are no outlier residues recorded for this chain.

- Molecule 12: Unknown structure

Chain v4: 

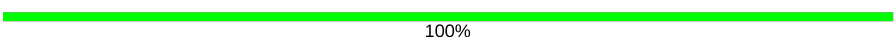
There are no outlier residues recorded for this chain.

- Molecule 12: Unknown structure

Chain v5: 

There are no outlier residues recorded for this chain.

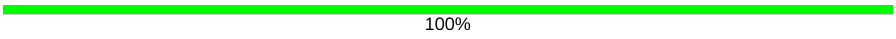
- Molecule 12: Unknown structure

Chain v6: 

There are no outlier residues recorded for this chain.

- Molecule 13: Unknown structure

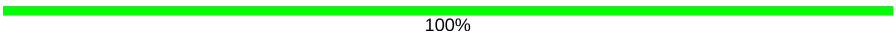
Chain w1:



There are no outlier residues recorded for this chain.

- Molecule 13: Unknown structure

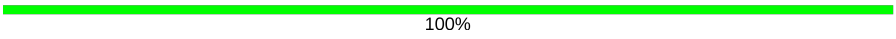
Chain w2:



There are no outlier residues recorded for this chain.

- Molecule 13: Unknown structure

Chain w3:



There are no outlier residues recorded for this chain.

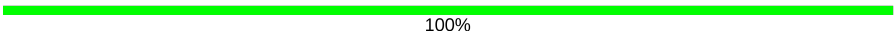
- Molecule 13: Unknown structure

Chain w4:

There are no outlier residues recorded for this chain.

- Molecule 13: Unknown structure

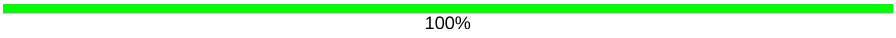
Chain w5:



There are no outlier residues recorded for this chain.

- Molecule 13: Unknown structure

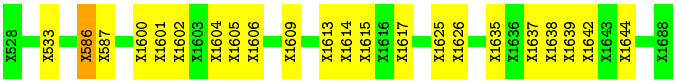
Chain w6:



There are no outlier residues recorded for this chain.

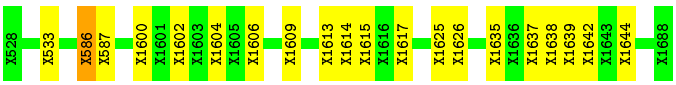
- Molecule 14: Unknown structure

Chain BA:



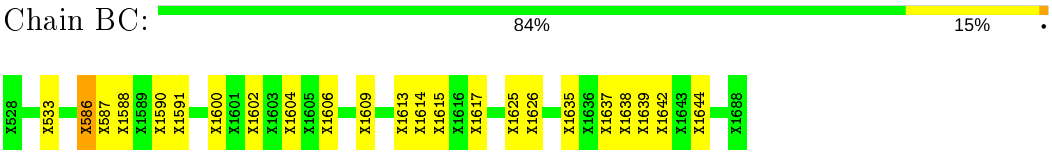
- Molecule 14: Unknown structure

Chain BB:



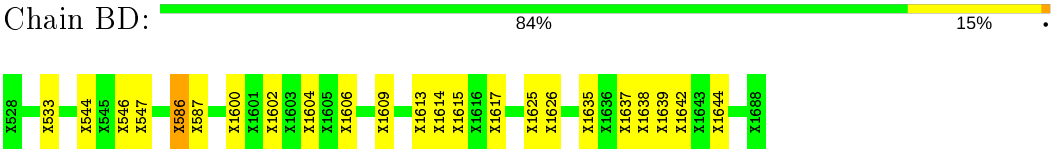
- Molecule 14: Unknown structure

Chain BC:



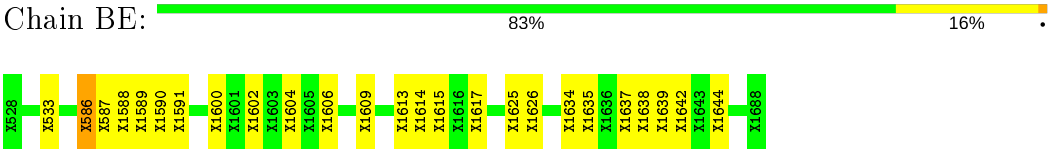
- Molecule 14: Unknown structure

Chain BD:



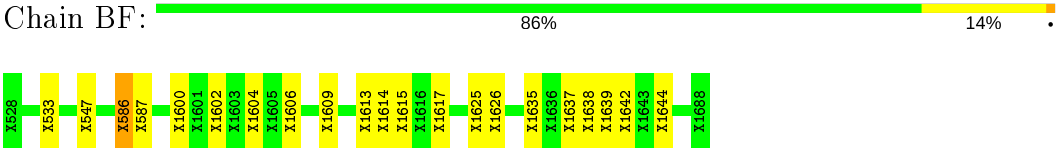
- Molecule 14: Unknown structure

Chain BE:



- Molecule 14: Unknown structure

Chain BF:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	244.83Å 251.41Å 412.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.69 – 6.74 49.44 – 6.74	Depositor EDS
% Data completeness (in resolution range)	97.2 (41.69-6.74) 90.7 (49.44-6.74)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 6.68Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.425 , 0.435 0.425 , 0.435	Depositor DCC
R_{free} test set	2228 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	495.7	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 102.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.037 for k,h,-l	Xtriage
F_o,F_c correlation	0.42	EDS
Total number of atoms	48030	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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

5.1 Standard geometry

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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
1	L1	0	2
1	L2	0	2
1	L3	0	2
1	L4	0	2
1	L5	0	2
1	L6	0	2
14	BA	0	3
14	BB	0	3
14	BC	0	3
14	BD	0	3
14	BE	0	3
14	BF	0	3
All	All	0	30

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	BA	533	UNK	Mainchain,Peptide
14	BA	586	UNK	Mainchain
1	L1	133	UNK	Peptide
1	L1	366	UNK	Peptide
1	L2	133	UNK	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L1	2465	0	517	226	0
1	L2	2465	0	517	228	0
1	L3	2465	0	517	227	0
1	L4	2465	0	517	227	0
1	L5	2465	0	517	227	0
1	L6	2465	0	517	221	0
2	M1	2195	0	455	202	0
2	M2	2195	0	455	209	0
2	M3	2195	0	455	206	0
2	M4	2195	0	455	205	0
2	M5	2195	0	455	201	0
2	M6	2195	0	455	206	0
3	f1	150	0	33	0	0
3	f2	150	0	33	0	0
3	f3	150	0	33	0	0
3	f4	150	0	33	0	0
3	f5	150	0	33	0	0
3	f6	150	0	33	0	0
3	h1	150	0	32	0	0
3	h2	150	0	32	0	0
3	h3	150	0	32	0	0
3	h4	150	0	32	0	0
3	h5	150	0	32	0	0
3	h6	150	0	32	0	0
3	i1	150	0	33	0	0
3	i2	150	0	33	0	0
3	i3	150	0	33	0	0
3	i4	150	0	33	0	0
3	i5	150	0	33	0	0
3	i6	150	0	33	0	0
4	g1	110	0	24	0	0
4	g2	110	0	24	0	0
4	g3	110	0	24	0	0
4	g4	110	0	24	0	0
4	g5	110	0	24	0	0
4	g6	110	0	24	0	0
5	j1	140	0	33	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	j2	140	0	33	0	0
5	j3	140	0	33	0	0
5	j4	140	0	33	0	0
5	j5	140	0	33	0	0
5	j6	140	0	33	0	0
5	k1	140	0	30	0	0
5	k2	140	0	30	0	0
5	k3	140	0	30	0	0
5	k4	140	0	30	0	0
5	k5	140	0	30	0	0
5	k6	140	0	30	0	0
5	p1	140	0	30	0	0
5	p2	140	0	30	0	0
5	p3	140	0	30	0	0
5	p4	140	0	30	0	0
5	p5	140	0	30	0	0
5	p6	140	0	30	0	0
5	s1	140	0	31	0	0
5	s2	140	0	31	0	0
5	s3	140	0	31	0	0
5	s4	140	0	31	0	0
5	s5	140	0	31	0	0
5	s6	140	0	31	0	0
6	l1	65	0	15	0	0
6	l2	65	0	15	0	0
6	l3	65	0	15	0	0
6	l4	65	0	15	0	0
6	l5	65	0	15	0	0
6	l6	65	0	15	0	0
7	U1	375	0	80	22	0
7	U2	375	0	80	21	0
7	U3	375	0	80	22	0
7	U4	375	0	80	21	0
7	U5	375	0	80	22	0
7	U6	375	0	80	21	0
8	n1	295	0	61	0	0
8	n2	295	0	61	0	0
8	n3	295	0	61	0	0
8	n4	295	0	61	0	0
8	n5	295	0	61	0	0
8	n6	295	0	61	0	0
9	o1	105	0	23	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	o2	105	0	23	0	0
9	o3	105	0	23	0	0
9	o4	105	0	23	0	0
9	o5	105	0	23	0	0
9	o6	105	0	23	0	0
10	t1	285	0	61	0	0
10	t2	285	0	61	0	0
10	t3	285	0	61	0	0
10	t4	285	0	61	0	0
10	t5	285	0	61	0	0
10	t6	285	0	61	0	0
11	u1	75	0	17	0	0
11	u2	75	0	17	0	0
11	u3	75	0	17	0	0
11	u4	75	0	17	0	0
11	u5	75	0	17	0	0
11	u6	75	0	17	0	0
12	v1	160	0	34	0	0
12	v2	160	0	34	0	0
12	v3	160	0	34	0	0
12	v4	160	0	34	0	0
12	v5	160	0	34	0	0
12	v6	160	0	34	0	0
13	w1	135	0	30	0	0
13	w2	135	0	29	0	0
13	w3	135	0	29	0	0
13	w4	135	0	29	0	0
13	w5	135	0	29	0	0
13	w6	135	0	29	0	0
14	BA	730	0	164	30	0
14	BB	730	0	164	29	0
14	BC	730	0	164	38	0
14	BD	730	0	164	39	0
14	BE	730	0	164	40	0
14	BF	730	0	164	39	0
All	All	48030	0	10213	2873	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 63.

The worst 5 of 2873 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:321:UNK:CB	1:L5:324:UNK:CB	1.91	1.48
14:BA:1609:UNK:CB	14:BA:1642:UNK:CB	1.92	1.47
1:L1:321:UNK:CB	1:L1:324:UNK:CB	1.91	1.47
1:L4:321:UNK:CB	1:L4:324:UNK:CB	1.91	1.47
14:BB:1609:UNK:CB	14:BB:1642:UNK:CB	1.92	1.46

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	BB	9
14	BA	9
14	BF	9
14	BE	9
14	BD	9
14	BC	9
1	L2	4
1	L3	4
1	L1	4
1	L6	4
1	L4	4
1	L5	4
2	M4	1
2	M5	1
2	M2	1
2	M3	1
2	M1	1
2	M6	1

The worst 5 of 84 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	563:UNK	C	571:UNK	N	83.40
1	BB	563:UNK	C	571:UNK	N	83.40
1	BC	563:UNK	C	571:UNK	N	83.40
1	BD	563:UNK	C	571:UNK	N	83.40
1	BE	563:UNK	C	571:UNK	N	83.40

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.