



# wwPDB X-ray Structure Validation Summary Report

Oct 1, 2015 – 05:28 AM EDT

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 validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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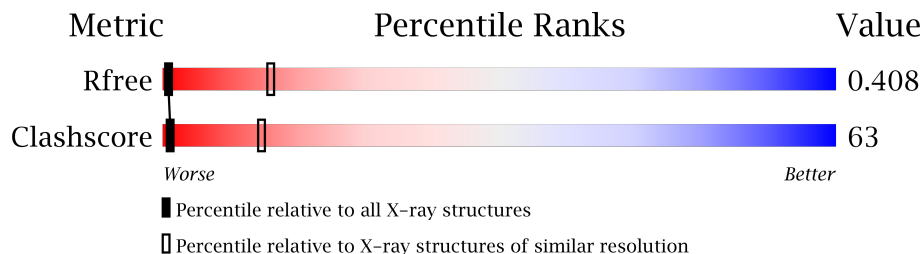
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.17 November 2013  
Xtriage (Phenix) : 1.9-1692  
EDS : stable25041  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.1.3  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable25041

# 1 Overall quality at a glance




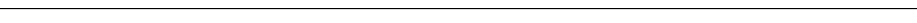


The reported resolution of this entry is 6.74 Å.

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.









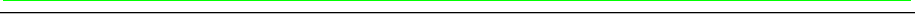

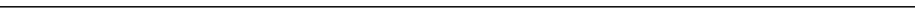
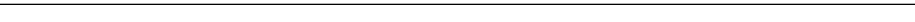












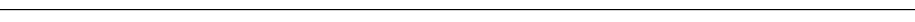

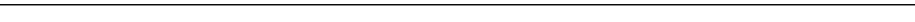











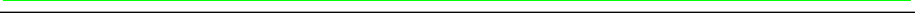

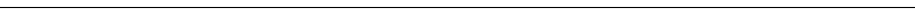



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1097 (9.50-3.50)
Clashscore	79885	1036 (9.50-3.52)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	L1	606	
1	L2	606	
1	L3	606	
1	L4	606	
1	L5	606	
1	L6	606	
2	M1	459	
2	M2	459	
2	M3	459	
2	M4	459	
2	M5	459	
2	M6	459	
3	f1	30	
3	f2	30	
3	f3	30	
3	f4	30	
3	f5	30	
3	f6	30	
3	h1	30	







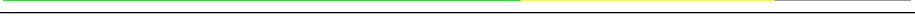

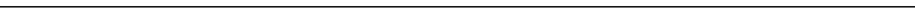
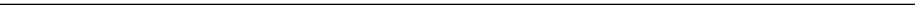












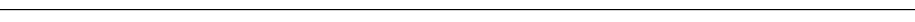

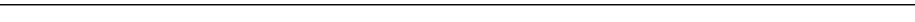











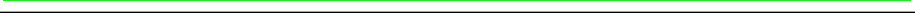

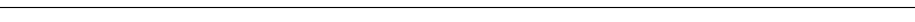



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Mol	Chain	Length	Quality of chain
3	h2	30	
3	h3	30	
3	h4	30	
3	h5	30	
3	h6	30	
3	i1	30	
3	i2	30	
3	i3	30	
3	i4	30	
3	i5	30	
3	i6	30	
4	g1	22	
4	g2	22	
4	g3	22	
4	g4	22	
4	g5	22	
4	g6	22	
5	j1	28	
5	j2	28	
5	j3	28	
5	j4	28	
5	j5	28	
5	j6	28	
5	k1	28	
5	k2	28	
5	k3	28	
5	k4	28	
5	k5	28	
5	k6	28	
5	p1	28	
5	p2	28	
5	p3	28	
5	p4	28	
5	p5	28	
5	p6	28	
5	s1	28	
5	s2	28	
5	s3	28	
5	s4	28	
5	s5	28	
5	s6	28	
6	l1	13	










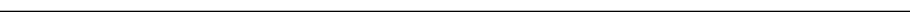

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Mol	Chain	Length	Quality of chain
6	l2	13	
6	l3	13	
6	l4	13	
6	l5	13	
6	l6	13	
7	U1	88	
7	U2	88	
7	U3	88	
7	U4	88	
7	U5	88	
7	U6	88	
8	n1	59	
8	n2	59	
8	n3	59	
8	n4	59	
8	n5	59	
8	n6	59	
9	o1	21	
9	o2	21	
9	o3	21	
9	o4	21	
9	o5	21	
9	o6	21	
10	t1	57	
10	t2	57	
10	t3	57	
10	t4	57	
10	t5	57	
10	t6	57	
11	u1	15	
11	u2	15	
11	u3	15	
11	u4	15	
11	u5	15	
11	u6	15	
12	v1	32	
12	v2	32	
12	v3	32	
12	v4	32	
12	v5	32	
12	v6	32	
13	w1	27	

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Mol	Chain	Length	Quality of chain
13	w2	27	
13	w3	27	
13	w4	27	
13	w5	27	
13	w6	27	
14	BA	146	
14	BB	146	
14	BC	146	
14	BD	146	
14	BE	146	
14	BF	146	

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 48030 atoms, of which 0 are hydrogen and 0 are deuterium.

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 150	C 90	N 30	O 30	0	0	0
3	h1	30	Total 150	C 90	N 30	O 30	0	0	0
3	i1	30	Total 150	C 90	N 30	O 30	0	0	0
3	f2	30	Total 150	C 90	N 30	O 30	0	0	0
3	h2	30	Total 150	C 90	N 30	O 30	0	0	0
3	i2	30	Total 150	C 90	N 30	O 30	0	0	0
3	f3	30	Total 150	C 90	N 30	O 30	0	0	0
3	h3	30	Total 150	C 90	N 30	O 30	0	0	0
3	i3	30	Total 150	C 90	N 30	O 30	0	0	0
3	f4	30	Total 150	C 90	N 30	O 30	0	0	0
3	h4	30	Total 150	C 90	N 30	O 30	0	0	0
3	i4	30	Total 150	C 90	N 30	O 30	0	0	0
3	f5	30	Total 150	C 90	N 30	O 30	0	0	0
3	h5	30	Total 150	C 90	N 30	O 30	0	0	0
3	i5	30	Total 150	C 90	N 30	O 30	0	0	0
3	f6	30	Total 150	C 90	N 30	O 30	0	0	0
3	h6	30	Total 150	C 90	N 30	O 30	0	0	0
3	i6	30	Total 150	C 90	N 30	O 30	0	0	0

- Molecule 4 is a protein called Unknown structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	g1	22	Total 110	C 66	N 22	O 22	0	0	0
4	g2	22	Total 110	C 66	N 22	O 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	0	0	0
			140	84	28	28			
5	j5	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	k5	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	p5	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	s5	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	j6	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	k6	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	p6	28	Total	C	N	O	0	0	0
			140	84	28	28			
5	s6	28	Total	C	N	O	0	0	0
			140	84	28	28			

- Molecule 6 is a protein called Unknown structure.

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

- Molecule 7 is a protein called SDAP.

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

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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	0	0	0
			285	171	57	57			
10	t2	57	Total	C	N	O	0	0	0
			285	171	57	57			
10	t3	57	Total	C	N	O	0	0	0
			285	171	57	57			
10	t4	57	Total	C	N	O	0	0	0
			285	171	57	57			
10	t5	57	Total	C	N	O	0	0	0
			285	171	57	57			
10	t6	57	Total	C	N	O	0	0	0
			285	171	57	57			

- Molecule 11 is a protein called Unknown structure.

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

- Molecule 12 is a protein called Unknown structure.

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

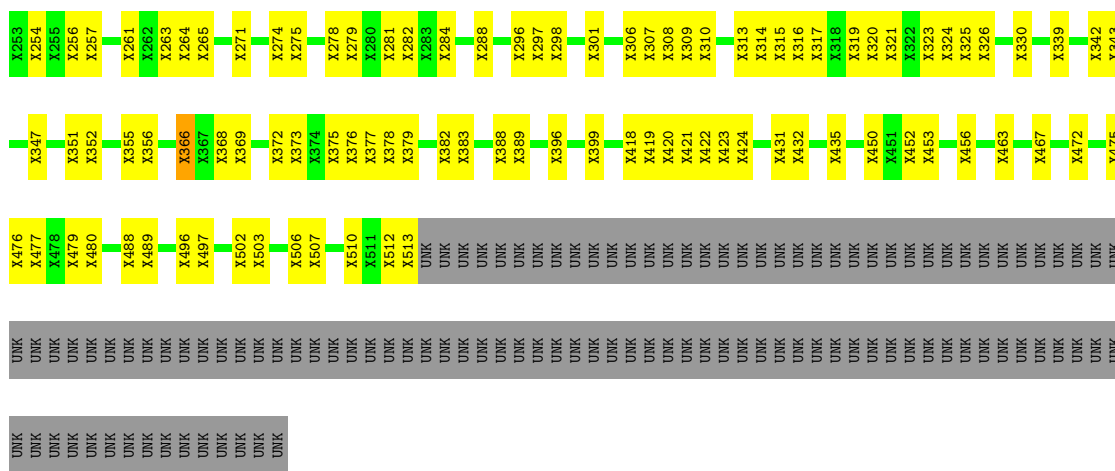
- Molecule 13 is a protein called Unknown structure.

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.

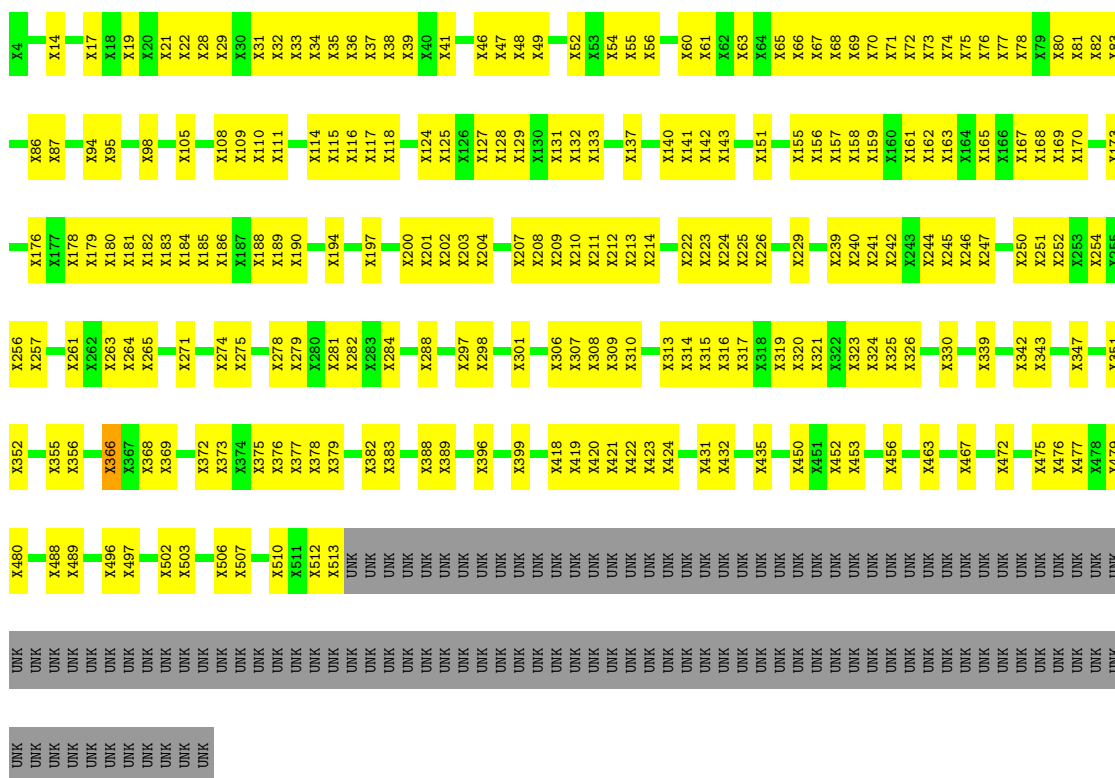
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	BA	146	Total	C	N	O	0	0	0
			730	438	146	146			
14	BB	146	Total	C	N	O	0	0	0
			730	438	146	146			
14	BC	146	Total	C	N	O	0	0	0
			730	438	146	146			
14	BD	146	Total	C	N	O	0	0	0
			730	438	146	146			
14	BE	146	Total	C	N	O	0	0	0
			730	438	146	146			
14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





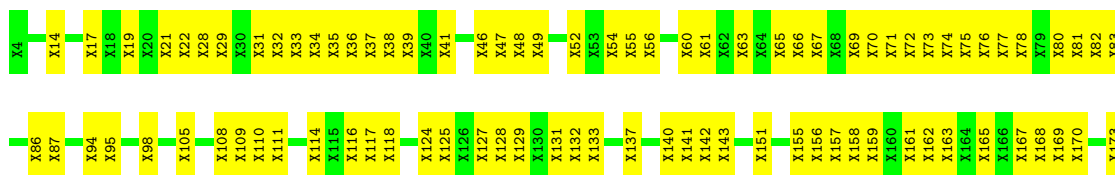
- Molecule 1: NADH-ubiquinone oxidoreductase chain 5

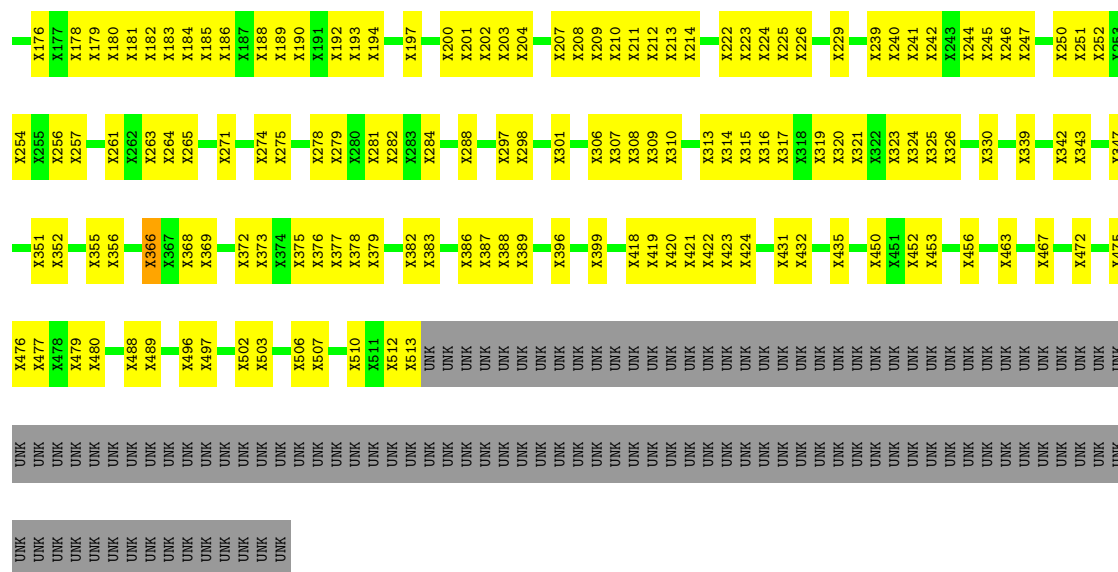
Chain L3:



- Molecule 1: NADH-ubiquinone oxidoreductase chain 5

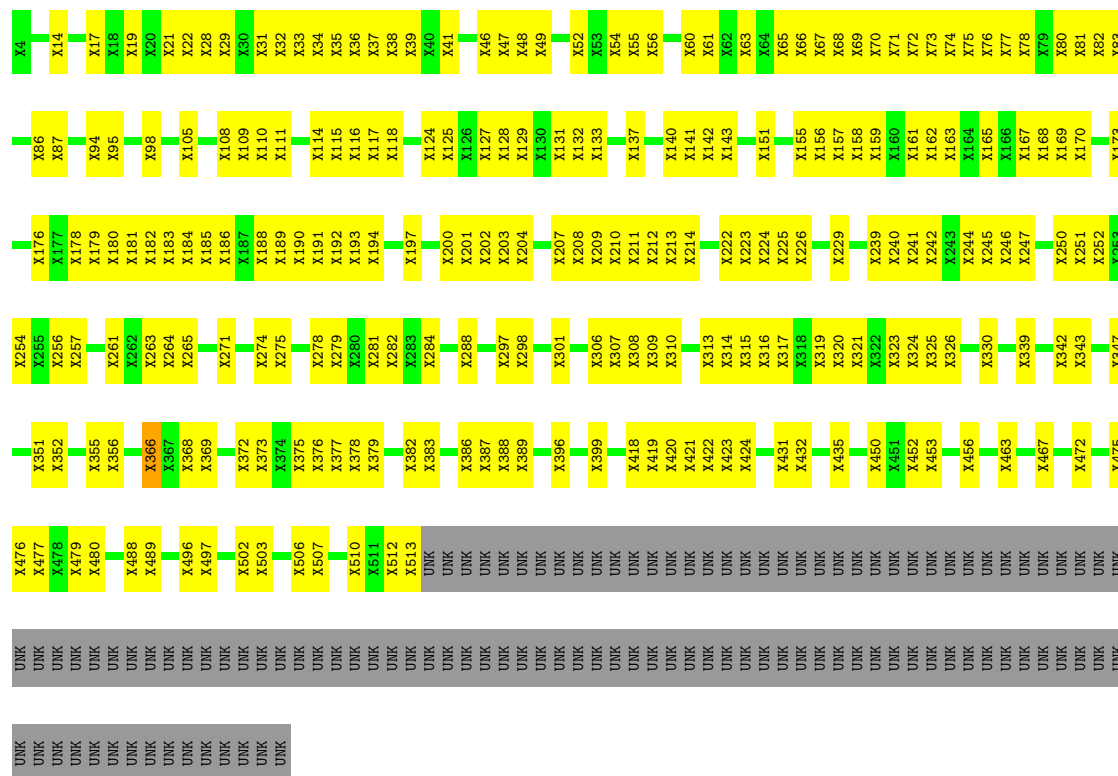
Chain L4:





• Molecule 1: NADH-ubiquinone oxidoreductase chain 5

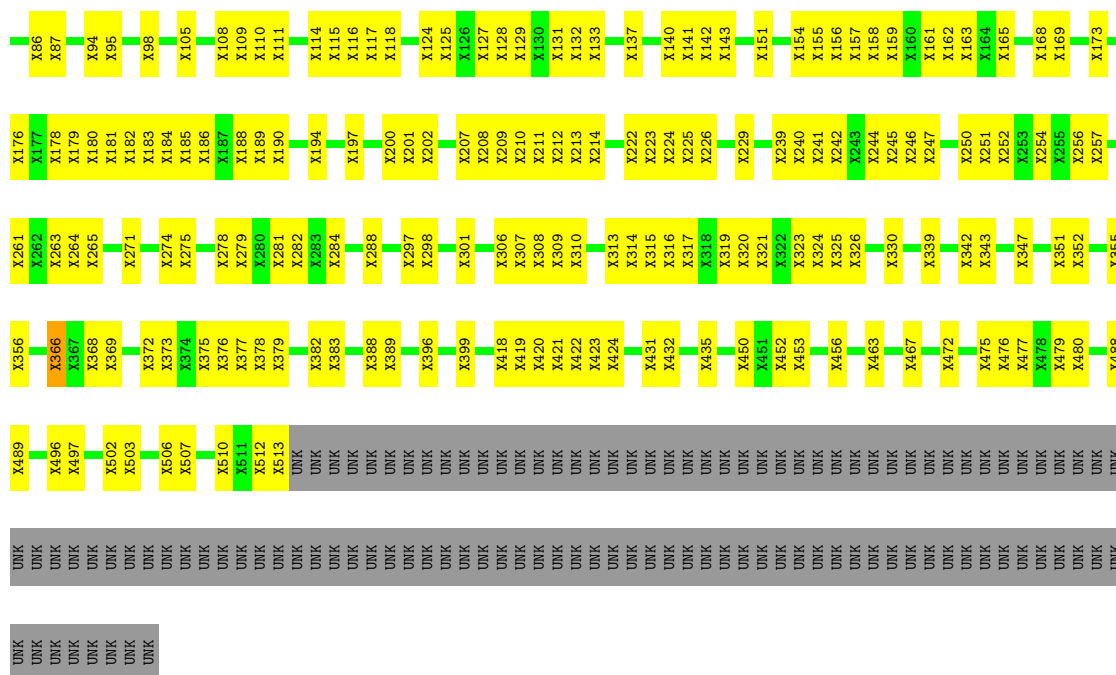
Chain L5:



• Molecule 1: NADH-ubiquinone oxidoreductase chain 5

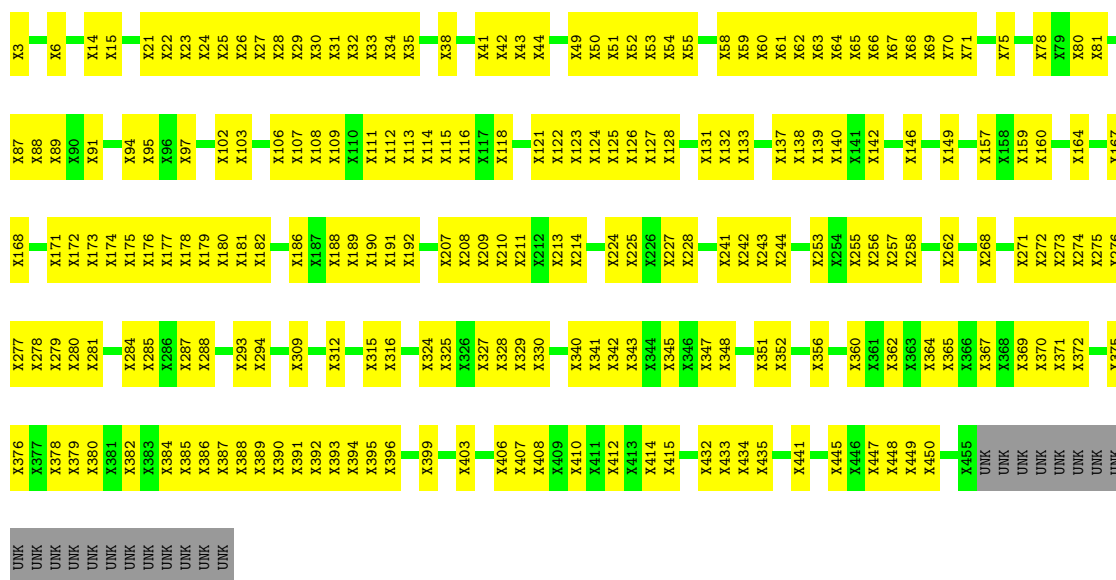
Chain L6:





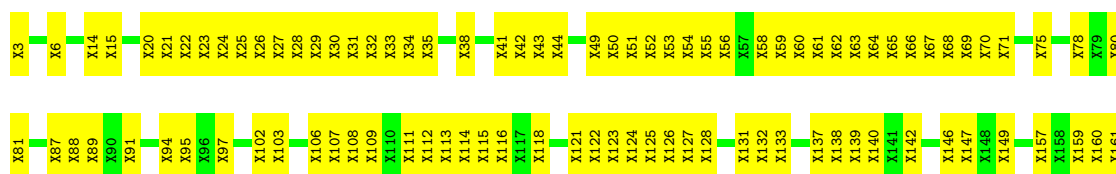
• Molecule 2: NADH-ubiquinone oxidoreductase chain 4

Chain M1:



• Molecule 2: NADH-ubiquinone oxidoreductase chain 4

Chain M2:

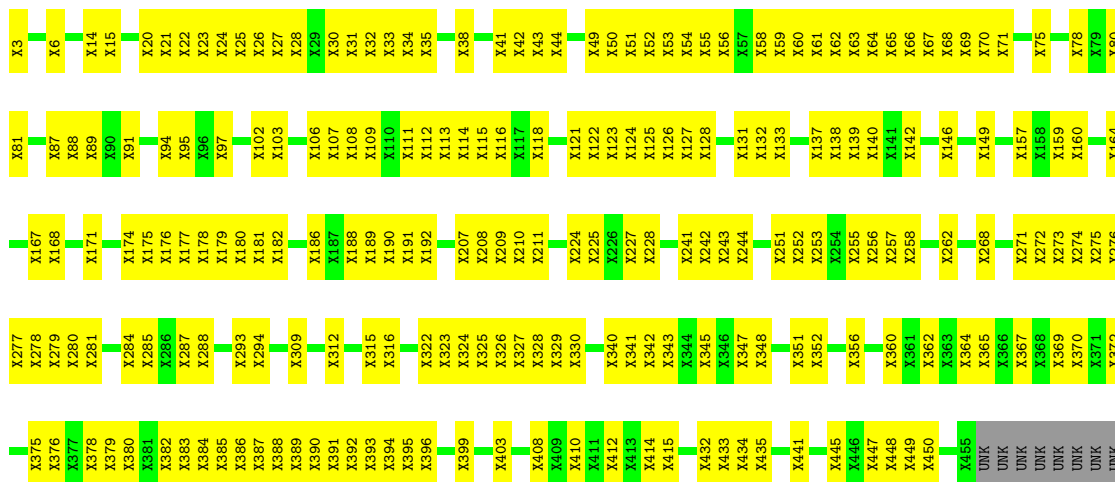




UNK  
UNK  
UNK  
UNK  
UNK  
UNK  
UNK  
UNK  
UNK  
UNK  
UNK  
UNK

• Molecule 2: NADH-ubiquinone oxidoreductase chain 4

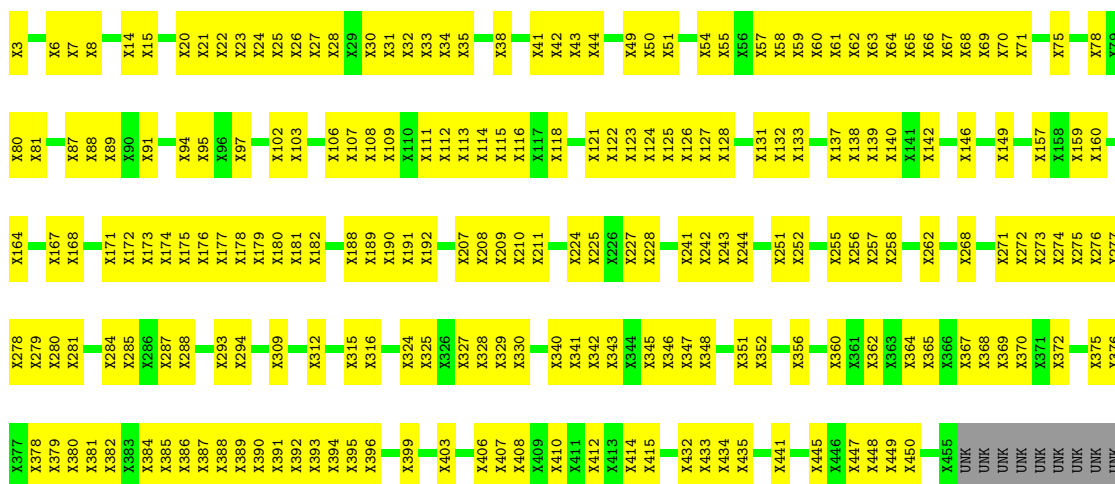
Chain M5:



UNK  
UNK  
UNK  
UNK  
UNK  
UNK  
UNK  
UNK  
UNK  
UNK  
UNK  
UNK

• Molecule 2: NADH-ubiquinone oxidoreductase chain 4

Chain M6:



UNK  
UNK  
UNK  
UNK  
UNK  
UNK  
UNK  
UNK  
UNK  
UNK  
UNK  
UNK

• Molecule 3: Unknown structure

Chain f1:

There are no outlier residues recorded for this chain.

• Molecule 3: Unknown structure

Chain h1: 

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain i1: 

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain f2: 

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain h2: 

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain i2: 

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain f3: 

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain h3: 

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain i3: 

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain f4: 

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain h4: 

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain i4: 

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain f5: 

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain h5: 

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain i5: 

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain f6: 

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain h6: 

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain i6: 

There are no outlier residues recorded for this chain.

- Molecule 4: Unknown structure

Chain g1: 

There are no outlier residues recorded for this chain.

- Molecule 4: Unknown structure

Chain g2: 

There are no outlier residues recorded for this chain.

- Molecule 4: Unknown structure

Chain g3: 

There are no outlier residues recorded for this chain.

- Molecule 4: Unknown structure

Chain g4: 

There are no outlier residues recorded for this chain.

- Molecule 4: Unknown structure

Chain g5: 

There are no outlier residues recorded for this chain.

- Molecule 4: Unknown structure

Chain g6: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain j1: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain k1: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain p1: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain s1: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain j2: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain k2: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain p2: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain s2: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain j3: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain k3: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain p3: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain s3: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain j4: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain k4: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain p4: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain s4: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain j5: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain k5: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain p5: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain s5: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain j6: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain k6: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain p6: 

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain s6: 

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

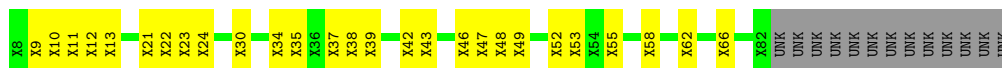
Chain l5: 

There are no outlier residues recorded for this chain.

- Chain 16:
- 

- Molecule 7: SDAP

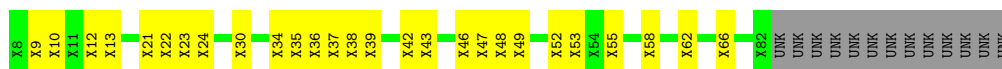
Chain U1: 



- Chain U2:



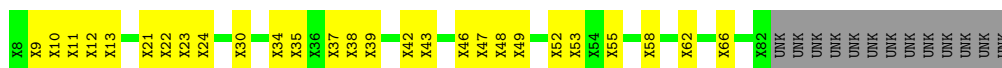
- Chain U3: 



- Chain U4:



- Chain U5: 



- Chain U6:



- Chain n1:
- 1

- 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: 

There are no outlier residues recorded for this chain.

- 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

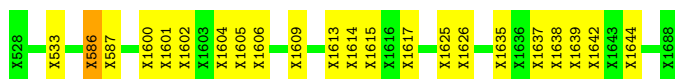
Chain w6:



There are no outlier residues recorded for this chain.

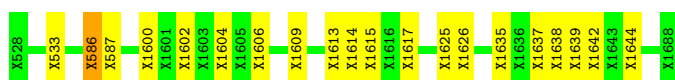
- Molecule 14: Unknown structure

Chain BA:



- Molecule 14: Unknown structure

Chain BB:



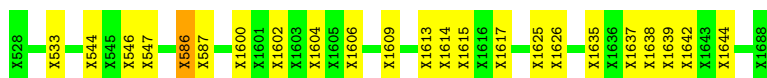
- Molecule 14: Unknown structure

Chain BC:



- Molecule 14: Unknown structure

Chain BD:



- Molecule 14: Unknown structure

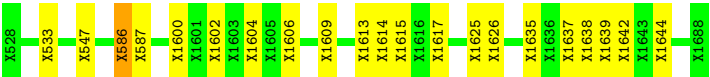
Chain BE:



- Molecule 14: Unknown structure

Chain BF:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 6.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.425 , 0.435 0.401 , 0.408	Depositor DCC
$R_{free}$ test set	2227 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	495.7	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 261.9	EDS
Estimated twinning fraction	0.037 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	1 of 44280 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.47	EDS
Total number of atoms	48030	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	g6	110	0	24	0	0
5	j1	140	0	33	0	0
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	n6	295	0	61	0	0
9	o1	105	0	23	0	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 63.

The worst 5 of 2873 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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 chains 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 ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	L1	0/606	-	-	-	-
1	L2	0/606	-	-	-	-
1	L3	0/606	-	-	-	-
1	L4	0/606	-	-	-	-
1	L5	0/606	-	-	-	-
1	L6	0/606	-	-	-	-
2	M1	0/459	-	-	-	-
2	M2	0/459	-	-	-	-
2	M3	0/459	-	-	-	-
2	M4	0/459	-	-	-	-
2	M5	0/459	-	-	-	-
2	M6	0/459	-	-	-	-
3	f1	0/30	-	-	-	-
3	f2	0/30	-	-	-	-
3	f3	0/30	-	-	-	-
3	f4	0/30	-	-	-	-
3	f5	0/30	-	-	-	-
3	f6	0/30	-	-	-	-
3	h1	0/30	-	-	-	-
3	h2	0/30	-	-	-	-
3	h3	0/30	-	-	-	-
3	h4	0/30	-	-	-	-
3	h5	0/30	-	-	-	-
3	h6	0/30	-	-	-	-
3	i1	0/30	-	-	-	-
3	i2	0/30	-	-	-	-
3	i3	0/30	-	-	-	-
3	i4	0/30	-	-	-	-
3	i5	0/30	-	-	-	-
3	i6	0/30	-	-	-	-
4	g1	0/22	-	-	-	-
4	g2	0/22	-	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
4	g3	0/22	-	-	-	-
4	g4	0/22	-	-	-	-
4	g5	0/22	-	-	-	-
4	g6	0/22	-	-	-	-
5	j1	0/28	-	-	-	-
5	j2	0/28	-	-	-	-
5	j3	0/28	-	-	-	-
5	j4	0/28	-	-	-	-
5	j5	0/28	-	-	-	-
5	j6	0/28	-	-	-	-
5	k1	0/28	-	-	-	-
5	k2	0/28	-	-	-	-
5	k3	0/28	-	-	-	-
5	k4	0/28	-	-	-	-
5	k5	0/28	-	-	-	-
5	k6	0/28	-	-	-	-
5	p1	0/28	-	-	-	-
5	p2	0/28	-	-	-	-
5	p3	0/28	-	-	-	-
5	p4	0/28	-	-	-	-
5	p5	0/28	-	-	-	-
5	p6	0/28	-	-	-	-
5	s1	0/28	-	-	-	-
5	s2	0/28	-	-	-	-
5	s3	0/28	-	-	-	-
5	s4	0/28	-	-	-	-
5	s5	0/28	-	-	-	-
5	s6	0/28	-	-	-	-
6	l1	0/13	-	-	-	-
6	l2	0/13	-	-	-	-
6	l3	0/13	-	-	-	-
6	l4	0/13	-	-	-	-
6	l5	0/13	-	-	-	-
6	l6	0/13	-	-	-	-
7	U1	0/88	-	-	-	-
7	U2	0/88	-	-	-	-
7	U3	0/88	-	-	-	-
7	U4	0/88	-	-	-	-
7	U5	0/88	-	-	-	-
7	U6	0/88	-	-	-	-
8	n1	0/59	-	-	-	-
8	n2	0/59	-	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
8	n3	0/59	-	-	-	-
8	n4	0/59	-	-	-	-
8	n5	0/59	-	-	-	-
8	n6	0/59	-	-	-	-
9	o1	0/21	-	-	-	-
9	o2	0/21	-	-	-	-
9	o3	0/21	-	-	-	-
9	o4	0/21	-	-	-	-
9	o5	0/21	-	-	-	-
9	o6	0/21	-	-	-	-
10	t1	0/57	-	-	-	-
10	t2	0/57	-	-	-	-
10	t3	0/57	-	-	-	-
10	t4	0/57	-	-	-	-
10	t5	0/57	-	-	-	-
10	t6	0/57	-	-	-	-
11	u1	0/15	-	-	-	-
11	u2	0/15	-	-	-	-
11	u3	0/15	-	-	-	-
11	u4	0/15	-	-	-	-
11	u5	0/15	-	-	-	-
11	u6	0/15	-	-	-	-
12	v1	0/32	-	-	-	-
12	v2	0/32	-	-	-	-
12	v3	0/32	-	-	-	-
12	v4	0/32	-	-	-	-
12	v5	0/32	-	-	-	-
12	v6	0/32	-	-	-	-
13	w1	0/27	-	-	-	-
13	w2	0/27	-	-	-	-
13	w3	0/27	-	-	-	-
13	w4	0/27	-	-	-	-
13	w5	0/27	-	-	-	-
13	w6	0/27	-	-	-	-
14	BA	0/146	-	-	-	-
14	BB	0/146	-	-	-	-
14	BC	0/146	-	-	-	-
14	BD	0/146	-	-	-	-
14	BE	0/146	-	-	-	-
14	BF	0/146	-	-	-	-
All	All	0/10482	-	-	-	-

There are no RSRZ outliers to report.

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.