wwPDB X-ray Structure Validation Summary Report (i)

Jun 22, 2024 – 09:14 PM 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)

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

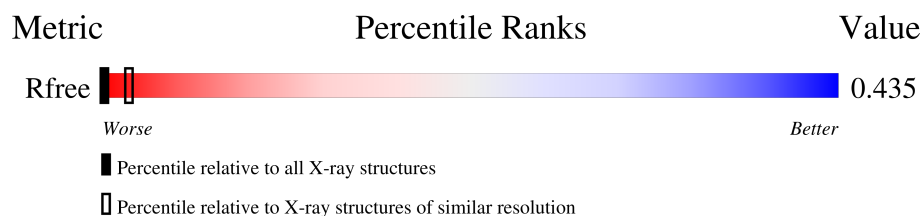|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 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.
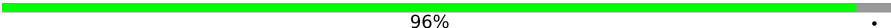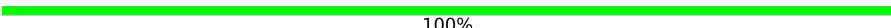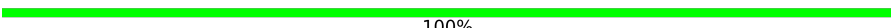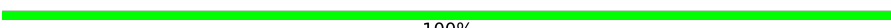
Metric	Percentile Ranks	Value
Rfree		0.435

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
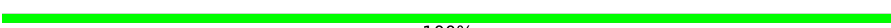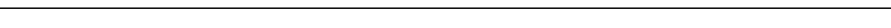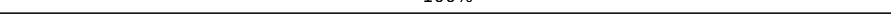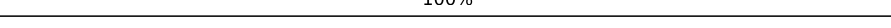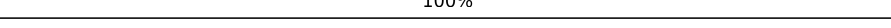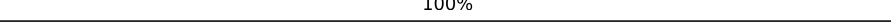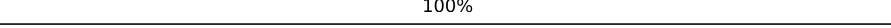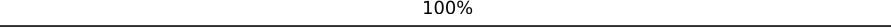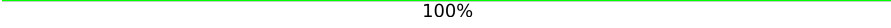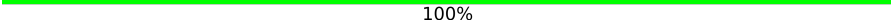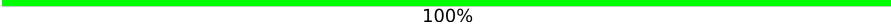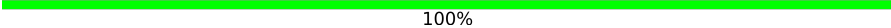
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1002 (9.50-3.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	L1	606	81% 19%
1	L2	606	81% 19%
1	L3	606	81% 19%
1	L4	606	81% 19%
1	L5	606	81% 19%
1	L6	606	81% 19%
2	M1	459	96% •
2	M2	459	96% •
2	M3	459	96% •
2	M4	459	96% •
2	M5	459	96% •
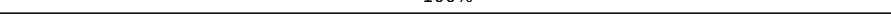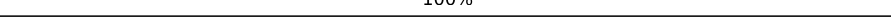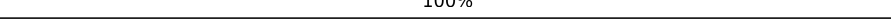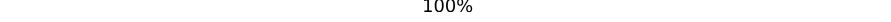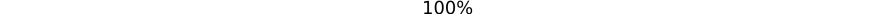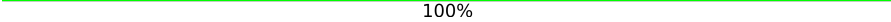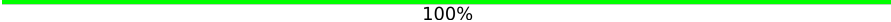
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Mol	Chain	Length	Quality of chain
2	M6	459	96% .
3	f1	30	100%
3	f2	30	100%
3	f3	30	100%
3	f4	30	100%
3	f5	30	100%
3	f6	30	100%
3	h1	30	100%
3	h2	30	100%
3	h3	30	100%
3	h4	30	100%
3	h5	30	100%
3	h6	30	100%
3	i1	30	100%
3	i2	30	100%
3	i3	30	100%
3	i4	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%
4	g5	22	100%
4	g6	22	100%
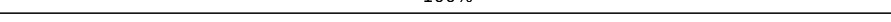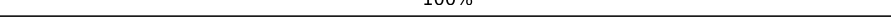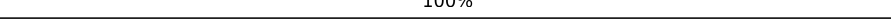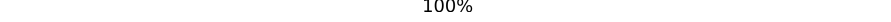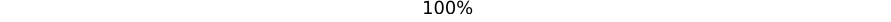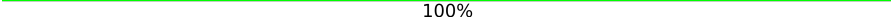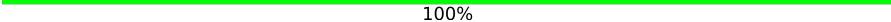
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Mol	Chain	Length	Quality of chain
5	j1	28	100%
5	j2	28	100%
5	j3	28	100%
5	j4	28	100%
5	j5	28	100%
5	j6	28	100%
5	k1	28	100%
5	k2	28	100%
5	k3	28	100%
5	k4	28	100%
5	k5	28	100%
5	k6	28	100%
5	p1	28	100%
5	p2	28	100%
5	p3	28	100%
5	p4	28	100%
5	p5	28	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%
5	s6	28	100%
6	l1	13	100%
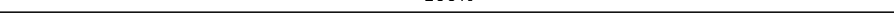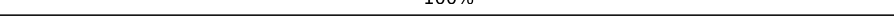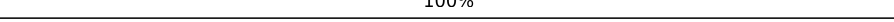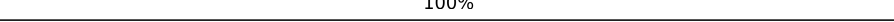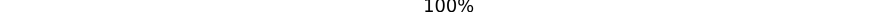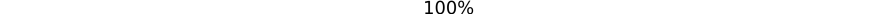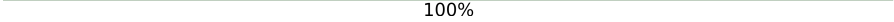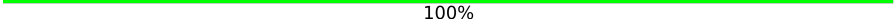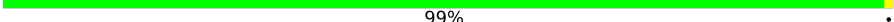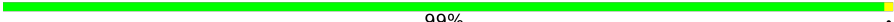
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Mol	Chain	Length	Quality of chain
6	l2	13	100%
6	l3	13	100%
6	l4	13	100%
6	l5	13	100%
6	l6	13	100%
7	U1	88	85% ... 15%
7	U2	88	85% ... 15%
7	U3	88	85% ... 15%
7	U4	88	85% ... 15%
7	U5	88	85% ... 15%
7	U6	88	85% ... 15%
8	n1	59	100%
8	n2	59	100%
8	n3	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%
10	t1	57	100%
10	t2	57	100%
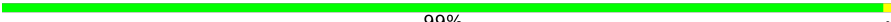
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Mol	Chain	Length	Quality of chain
10	t3	57	100%
10	t4	57	100%
10	t5	57	100%
10	t6	57	100%
11	u1	15	100%
11	u2	15	100%
11	u3	15	100%
11	u4	15	100%
11	u5	15	100%
11	u6	15	100%
12	v1	32	100%
12	v2	32	100%
12	v3	32	100%
12	v4	32	100%
12	v5	32	100%
12	v6	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	99%
14	BB	146	99%
14	BC	146	99%

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Mol	Chain	Length	Quality of chain
14	BD	146	99%
14	BE	146	99%
14	BF	146	99%

2 Entry composition ⓘ

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 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 140	C 84	N 28	O 28	0	0	0
5	j5	28	Total 140	C 84	N 28	O 28	0	0	0
5	k5	28	Total 140	C 84	N 28	O 28	0	0	0
5	p5	28	Total 140	C 84	N 28	O 28	0	0	0
5	s5	28	Total 140	C 84	N 28	O 28	0	0	0
5	j6	28	Total 140	C 84	N 28	O 28	0	0	0
5	k6	28	Total 140	C 84	N 28	O 28	0	0	0
5	p6	28	Total 140	C 84	N 28	O 28	0	0	0
5	s6	28	Total 140	C 84	N 28	O 28	0	0	0

- Molecule 6 is a protein called Unknown structure.

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

- Molecule 7 is a protein called SDAP.

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

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

- Molecule 8 is a protein called Unknown structure.

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

- Molecule 9 is a protein called Unknown structure.

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

- Molecule 10 is a protein called Unknown structure.

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

- Molecule 11 is a protein called Unknown structure.

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

- Molecule 12 is a protein called Unknown structure.

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

- Molecule 13 is a protein called Unknown structure.

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

- Molecule 14 is a protein called Unknown structure.

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

3 Residue-property plots ⓘ

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

• Molecule 1: NADH-ubiquinone oxidoreductase chain 5
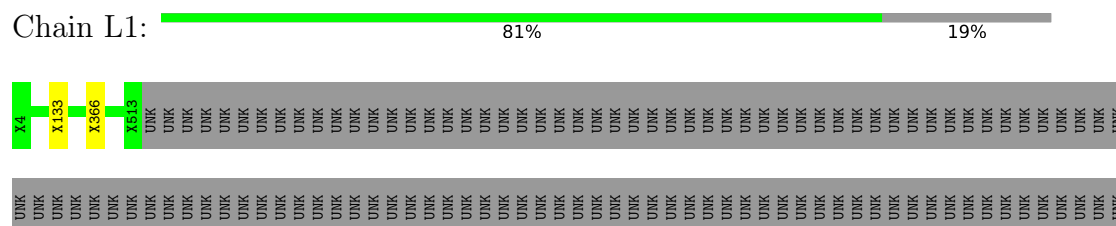
Chain L1:

• 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:

81%　　　　19%

X4　X133　X366　X513　UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

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

- Molecule 1: NADH-ubiquinone oxidoreductase chain 5

Chain L6:

81%　　　　19%

X4　X133　X366　X513　UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

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

- Molecule 2: NADH-ubiquinone oxidoreductase chain 4

Chain M1:

96%　　　　.

X3　X455　UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

- Molecule 2: NADH-ubiquinone oxidoreductase chain 4

Chain M2:

96%　　　　.

X3　X455　UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

- Molecule 2: NADH-ubiquinone oxidoreductase chain 4

Chain M3:

96%　　　　.

X3　X455　UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

- Molecule 2: NADH-ubiquinone oxidoreductase chain 4

Chain M4:

96%　　　　.

X3　X455　UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

- Molecule 2: NADH-ubiquinone oxidoreductase chain 4

Chain M5:

96%　　　　.

• Molecule 2: NADH-ubiquinone oxidoreductase chain 4

Chain M6:

• 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:

<center>100%</center>

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain i3:

<center>100%</center>

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain f4:

<center>100%</center>

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain h4:

<center>100%</center>

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain i4:

<center>100%</center>

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain f5:

<center>100%</center>

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain h5:

<center>100%</center>

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain i5:

<center>100%</center>

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain f6:

<center>100%</center>

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain h6:

<center>100%</center>

There are no outlier residues recorded for this chain.

• Molecule 3: Unknown structure

Chain i6:   100%

There are no outlier residues recorded for this chain.

• Molecule 4: Unknown structure

Chain g1:   100%

There are no outlier residues recorded for this chain.

• Molecule 4: Unknown structure

Chain g2:   100%

There are no outlier residues recorded for this chain.

• Molecule 4: Unknown structure

Chain g3:   100%

There are no outlier residues recorded for this chain.

• Molecule 4: Unknown structure

Chain g4:   100%

There are no outlier residues recorded for this chain.

• Molecule 4: Unknown structure

Chain g5:   100%

There are no outlier residues recorded for this chain.

• Molecule 4: Unknown structure

Chain g6:   100%

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain j1:   100%

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain k1:   100%

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain p1:
<!-- green bar, 100% -->

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain s1:
<!-- green bar, 100% -->

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain j2:
<!-- green bar, 100% -->

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain k2:
<!-- green bar, 100% -->

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain p2:
<!-- green bar, 100% -->

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain s2:
<!-- green bar, 100% -->

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain j3:
<!-- green bar, 100% -->

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain k3:
<!-- green bar, 100% -->

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain p3:
<!-- green bar, 100% -->

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain s3:
100%

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain j4:
100%

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain k4:
100%

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain p4:
100%

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain s4:
100%

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain j5:
100%

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain k5:
100%

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain p5:
100%

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain s5:
100%

There are no outlier residues recorded for this chain.

• Molecule 5: Unknown structure

Chain j6:
100%

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain k6:
100%

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain p6:
100%

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain s6:
100%

There are no outlier residues recorded for this chain.

- Molecule 6: Unknown structure

Chain l1:
100%

There are no outlier residues recorded for this chain.

- Molecule 6: Unknown structure

Chain l2:
100%

There are no outlier residues recorded for this chain.

- Molecule 6: Unknown structure

Chain l3:
100%

There are no outlier residues recorded for this chain.

- Molecule 6: Unknown structure

Chain l4:
100%

There are no outlier residues recorded for this chain.

- Molecule 6: Unknown structure

Chain l5:
100%

There are no outlier residues recorded for this chain.

- Molecule 6: Unknown structure

Chain l6:
100%

There are no outlier residues recorded for this chain.

• Molecule 7: SDAP

Chain U1:

85%   15%

• Molecule 7: SDAP

Chain U2:

85%   15%

• Molecule 7: SDAP

Chain U3:

85%   15%

• Molecule 7: SDAP

Chain U4:

85%   15%

• Molecule 7: SDAP

Chain U5:

85%   15%

• Molecule 7: SDAP

Chain U6:

85%   15%

• Molecule 8: Unknown structure

Chain n1:

100%

There are no outlier residues recorded for this chain.

• Molecule 8: Unknown structure

Chain n2:

100%

There are no outlier residues recorded for this chain.

• Molecule 8: Unknown structure

Chain n3:
100%

There are no outlier residues recorded for this chain.

• Molecule 8: Unknown structure

Chain n4:
100%

There are no outlier residues recorded for this chain.

• Molecule 8: Unknown structure

Chain n5:
100%

There are no outlier residues recorded for this chain.

• Molecule 8: Unknown structure

Chain n6:
100%

There are no outlier residues recorded for this chain.

• Molecule 9: Unknown structure

Chain o1:
100%

There are no outlier residues recorded for this chain.

• Molecule 9: Unknown structure

Chain o2:
100%

There are no outlier residues recorded for this chain.

• Molecule 9: Unknown structure

Chain o3:
100%

There are no outlier residues recorded for this chain.

• Molecule 9: Unknown structure

Chain o4:
100%

There are no outlier residues recorded for this chain.

• Molecule 9: Unknown structure

Chain o5:
100%

There are no outlier residues recorded for this chain.

• Molecule 9: Unknown structure

Chain o6:

100%

There are no outlier residues recorded for this chain.

• Molecule 10: Unknown structure

Chain t1:

100%

There are no outlier residues recorded for this chain.

• Molecule 10: Unknown structure

Chain t2:

100%

There are no outlier residues recorded for this chain.

• Molecule 10: Unknown structure

Chain t3:

100%

There are no outlier residues recorded for this chain.

• Molecule 10: Unknown structure

Chain t4:

100%

There are no outlier residues recorded for this chain.

• Molecule 10: Unknown structure

Chain t5:

100%

There are no outlier residues recorded for this chain.

• Molecule 10: Unknown structure

Chain t6:

100%

There are no outlier residues recorded for this chain.

• Molecule 11: Unknown structure

Chain u1:

100%

There are no outlier residues recorded for this chain.

• Molecule 11: Unknown structure

Chain u2:

100%

There are no outlier residues recorded for this chain.

• Molecule 11: Unknown structure

Chain u3:

100%

There are no outlier residues recorded for this chain.

• Molecule 11: Unknown structure

Chain u4:

100%

There are no outlier residues recorded for this chain.

• Molecule 11: Unknown structure

Chain u5:

100%

There are no outlier residues recorded for this chain.

• Molecule 11: Unknown structure

Chain u6:

100%

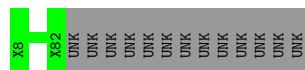There are no outlier residues recorded for this chain.

• Molecule 12: Unknown structure

Chain v1:

100%

There are no outlier residues recorded for this chain.

• Molecule 12: Unknown structure

Chain v2:

100%

There are no outlier residues recorded for this chain.

• Molecule 12: Unknown structure

Chain v3:

100%

There are no outlier residues recorded for this chain.

• Molecule 12: Unknown structure

Chain v4:

100%

There are no outlier residues recorded for this chain.

• Molecule 12: Unknown structure

Chain v5:

100%

There are no outlier residues recorded for this chain.

• Molecule 12: Unknown structure

Chain v6:

100%

There are no outlier residues recorded for this chain.

• Molecule 13: Unknown structure

Chain w1: 100%

There are no outlier residues recorded for this chain.

• Molecule 13: Unknown structure

Chain w2: 100%

There are no outlier residues recorded for this chain.

• Molecule 13: Unknown structure

Chain w3: 100%

There are no outlier residues recorded for this chain.

• Molecule 13: Unknown structure

Chain w4: 100%

There are no outlier residues recorded for this chain.

• Molecule 13: Unknown structure

Chain w5: 100%

There are no outlier residues recorded for this chain.

• Molecule 13: Unknown structure

Chain w6: 100%

There are no outlier residues recorded for this chain.

• Molecule 14: Unknown structure

Chain BA: 99%

X528 X533 X586 X1688

• Molecule 14: Unknown structure

Chain BB: 99%

X528 X533 X586 X1688
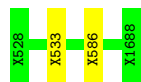
• Molecule 14: Unknown structure

Chain BC:

99%

X528 X533 X586 X1688

• Molecule 14: Unknown structure

Chain BD:

99%

X528 X533 X586 X1688

• Molecule 14: Unknown structure

Chain BE:

99%

X528 X533 X586 X1688

• Molecule 14: Unknown structure

Chain BF:

99%

X528 X533 X586 X1688
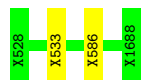
4　Data and refinement statistics　ⓘ

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	Peptide,Mainchain
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 ⓘ

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

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 monosaccharides 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	BA	9
14	BB	9
14	BC	9
14	BD	9
14	BE	9
14	BF	9
1	L4	4
1	L1	4
1	L2	4
1	L3	4
1	L5	4
1	L6	4
2	M1	1
2	M2	1
2	M3	1
2	M4	1
2	M5	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.