



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 01:46 pm GMT

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

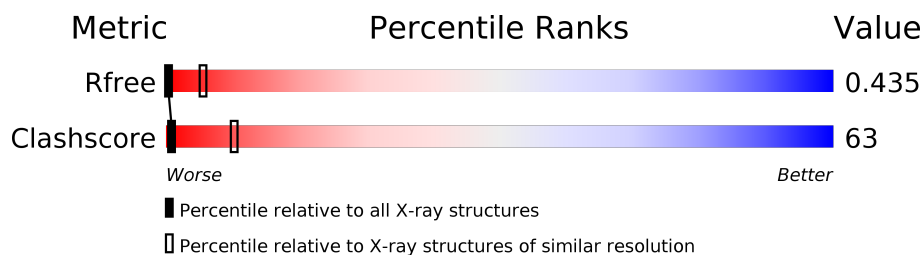
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

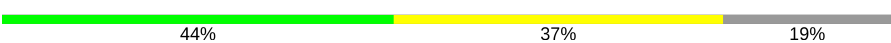



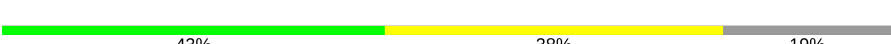
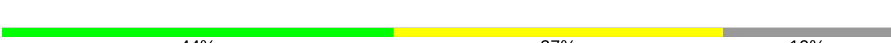

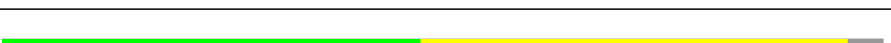
The reported resolution of this entry is 6.74 Å.

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.






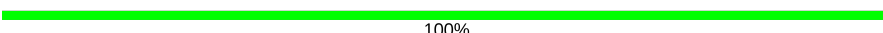
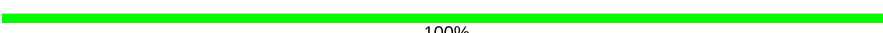
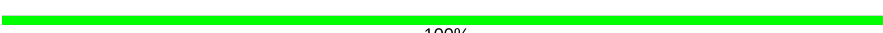








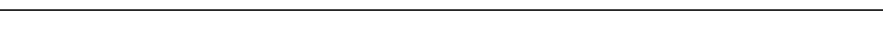
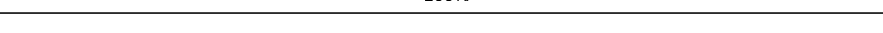
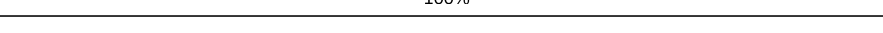
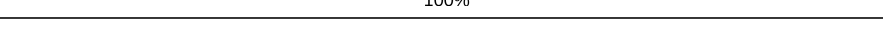
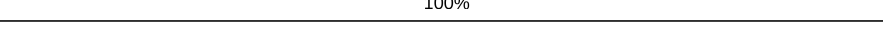
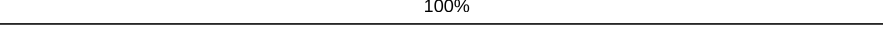
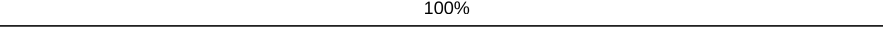
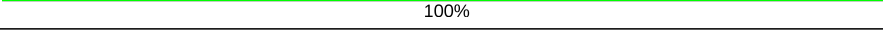
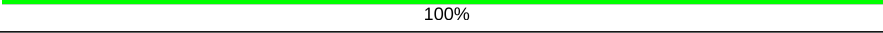
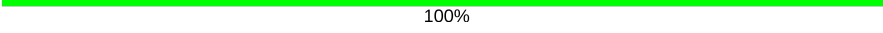
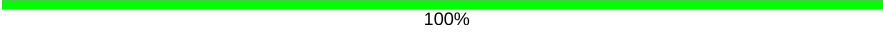
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	111664	1066 (9.50-3.80)
Clashscore	122126	1144 (9.50-3.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

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	
















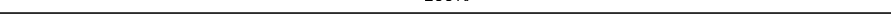
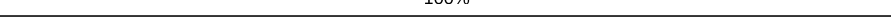
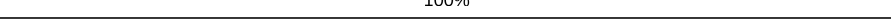
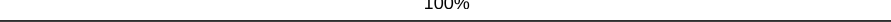
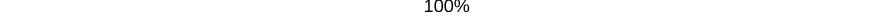
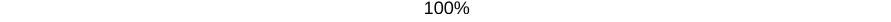
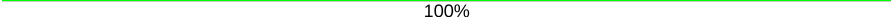
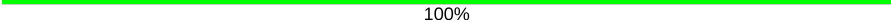

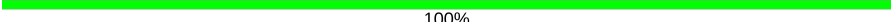
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Mol	Chain	Length	Quality of chain
2	M5	459	 48% 47%
2	M6	459	 48% 47%
3	f1	30	 100%
3	f2	30	 100%
3	f3	30	 100%
3	f4	30	 100%
3	f5	30	 100%
3	f6	30	 100%
3	h1	30	 100%
3	h2	30	 100%
3	h3	30	 100%
3	h4	30	 100%
3	h5	30	 100%
3	h6	30	 100%
3	i1	30	 100%
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%
4	g5	22	 100%
















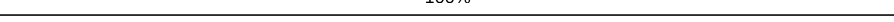
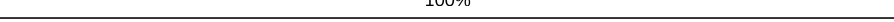
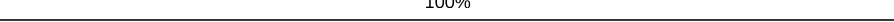
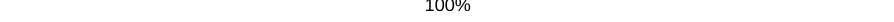
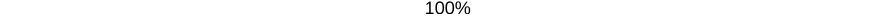
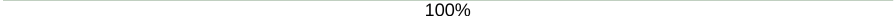
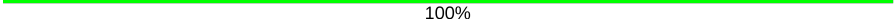

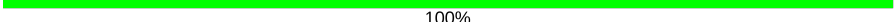
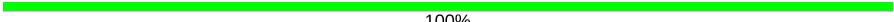
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Mol	Chain	Length	Quality of chain
4	g6	22	 100%
5	j1	28	 100%
5	j2	28	 100%
5	j3	28	 100%
5	j4	28	 100%
5	j5	28	 100%
5	j6	28	 100%
5	k1	28	 100%
5	k2	28	 100%
5	k3	28	 100%
5	k4	28	 100%
5	k5	28	 100%
5	k6	28	 100%
5	p1	28	 100%
5	p2	28	 100%
5	p3	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%
5	s6	28	 100%
















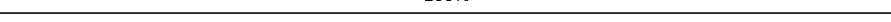
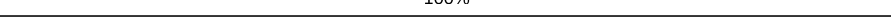
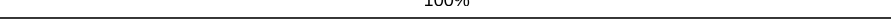
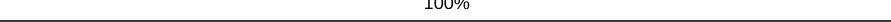
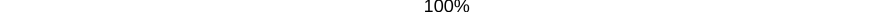
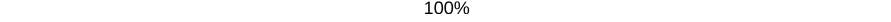
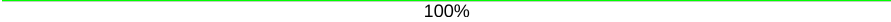
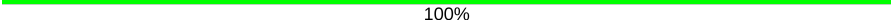


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Mol	Chain	Length	Quality of chain
6	l1	13	 100%
6	l2	13	 100%
6	l3	13	 100%
6	l4	13	 100%
6	l5	13	 100%
6	l6	13	 100%
7	U1	88	 55% 31% 15%
7	U2	88	 57% 28% 15%
7	U3	88	 55% 31% 15%
7	U4	88	 57% 28% 15%
7	U5	88	 55% 31% 15%
7	U6	88	 57% 28% 15%
8	n1	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%
10	t1	57	 100%





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Mol	Chain	Length	Quality of chain
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% •
14	BB	146	 86% 13% •

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Mol	Chain	Length	Quality of chain
14	BC	146	 84% 15% •
14	BD	146	 84% 15% •
14	BE	146	 83% 16% •
14	BF	146	 86% 14% •

## 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	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			

*Continued on next page...*

*Continued from previous page...*

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			

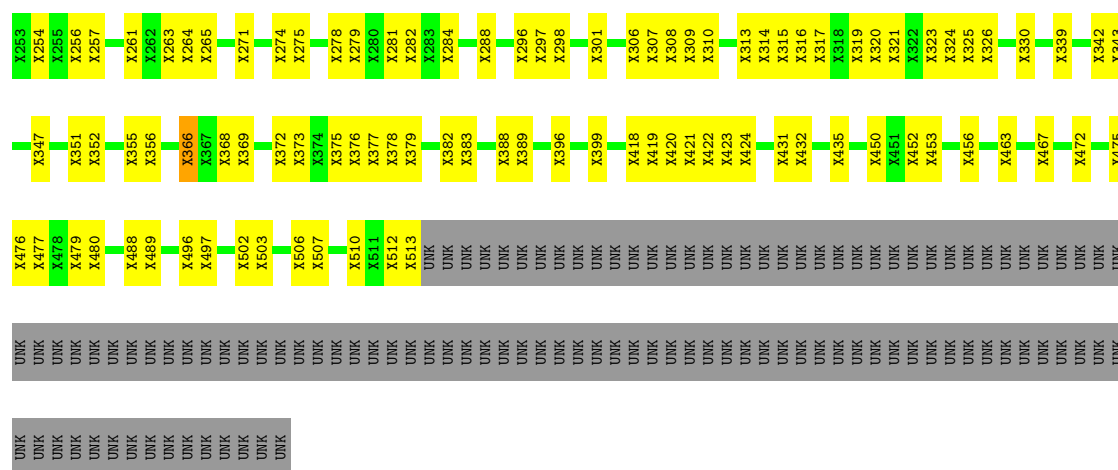
- Molecule 13 is a protein called Unknown structure.

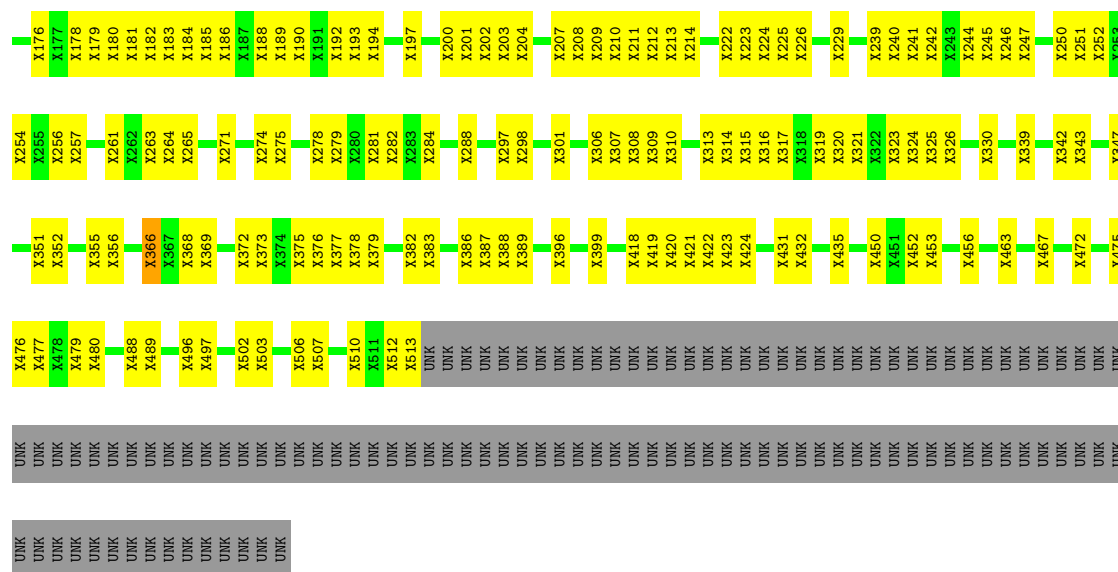
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	w1	27	Total	C	N	O	0	0	0
			135	81	27	27			
13	w2	27	Total	C	N	O	0	0	0
			135	81	27	27			
13	w3	27	Total	C	N	O	0	0	0
			135	81	27	27			
13	w4	27	Total	C	N	O	0	0	0
			135	81	27	27			
13	w5	27	Total	C	N	O	0	0	0
			135	81	27	27			
13	w6	27	Total	C	N	O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

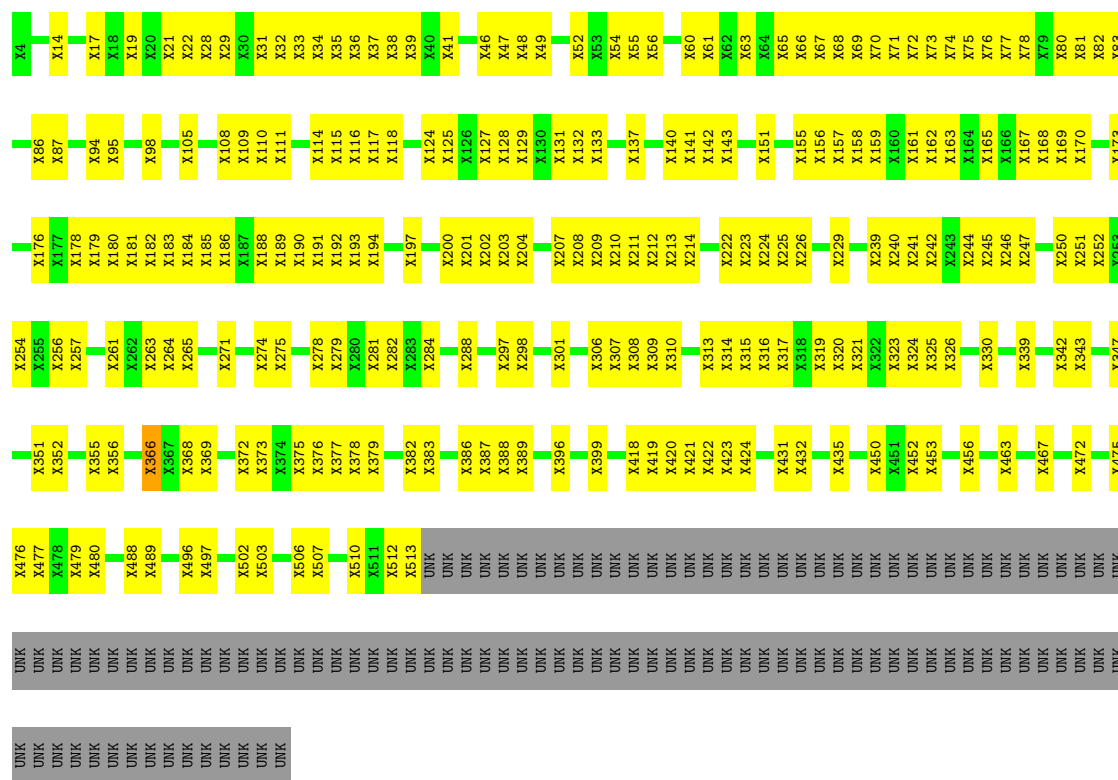






• Molecule 1: NADH-ubiquinone oxidoreductase chain 5

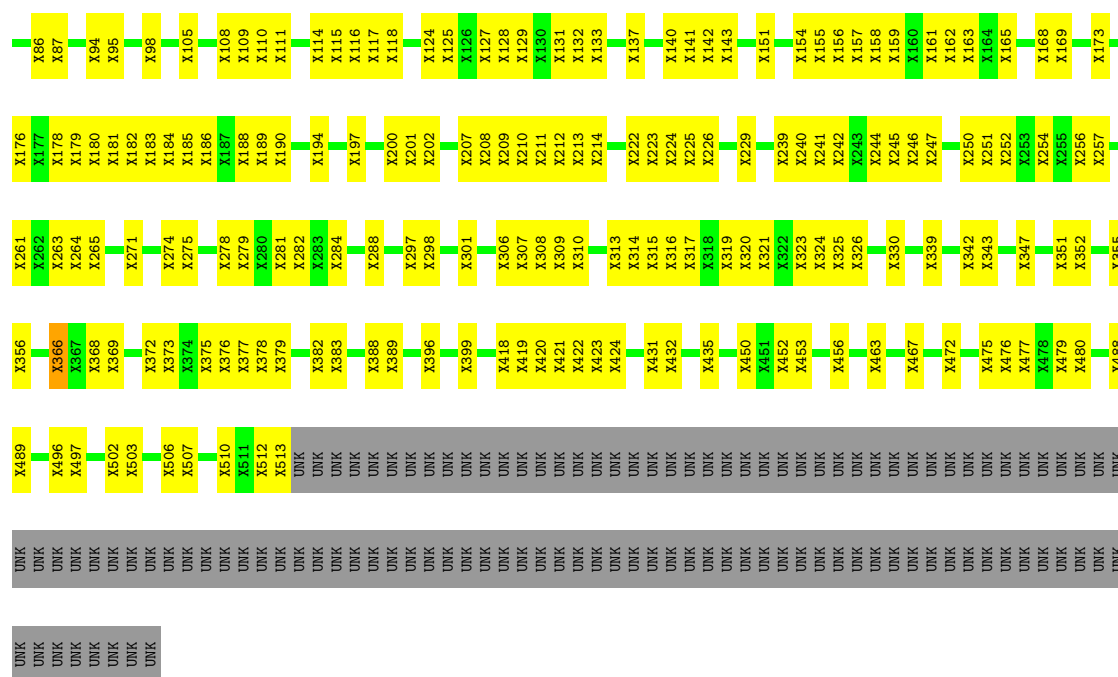
Chain L5: 43% 38% 19%



• Molecule 1: NADH-ubiquinone oxidoreductase chain 5

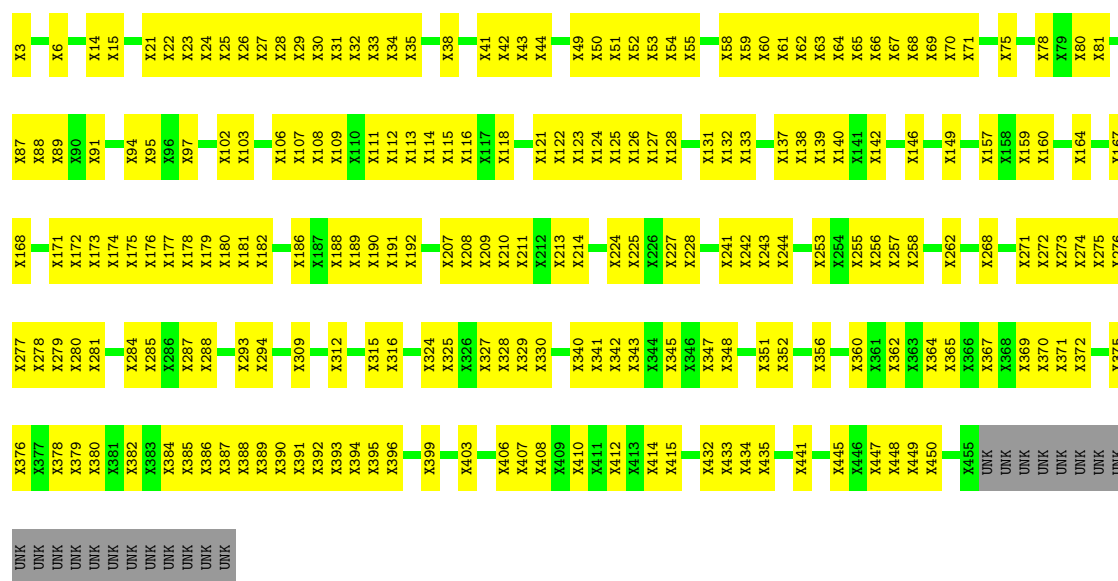
Chain L6: 44% 37% 19%





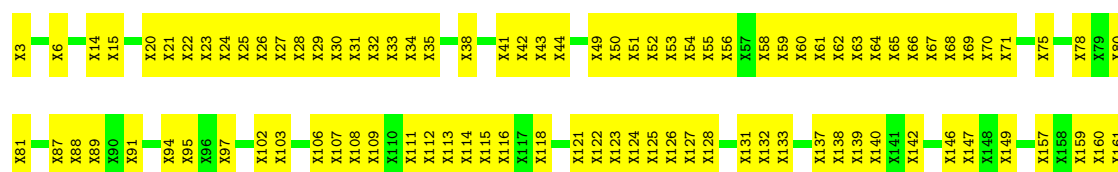
• Molecule 2: NADH-ubiquinone oxidoreductase chain 4

Chain M1: 48% 47%



• Molecule 2: NADH-ubiquinone oxidoreductase chain 4

Chain M2: 47% 49%





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

• Molecule 2: NADH-ubiquinone oxidoreductase chain 4

Chain M5:  48% 47%

X3 X6 X14 X15 X20 X21 X22 X23 X24 X25 X26 X27 X28 X29 X30 X31 X32 X33 X34 X35 X38 X41 X42 X43 X44 X49 X50 X51 X52 X53 X54 X55 X56 X57 X58 X59 X60 X61 X62 X63 X64 X65 X66 X67 X68 X69 X70 X71 X75 X78 X79 X80 X81 X87 X88 X89 X90 X91 X94 X95 X96 X97 X102 X103 X106 X107 X108 X109 X110 X111 X112 X113 X114 X115 X116 X117 X118 X121 X122 X123 X124 X125 X126 X127 X128 X131 X132 X133 X137 X138 X139 X140 X141 X142 X146 X149 X157 X158 X159 X160 X164 X167 X168 X171 X174 X175 X176 X177 X178 X179 X180 X181 X182 X186 X187 X188 X189 X190 X191 X192 X207 X208 X209 X210 X211 X224 X225 X226 X227 X228 X241 X242 X243 X244 X251 X252 X253 X254 X255 X256 X257 X258 X262 X268 X271 X272 X273 X274 X275 X276 X277 X278 X279 X280 X281 X284 X285 X286 X287 X288 X293 X294 X309 X312 X315 X316 X322 X323 X324 X325 X326 X327 X328 X329 X330 X340 X341 X342 X343 X344 X345 X346 X347 X348 X351 X352 X356 X360 X361 X362 X363 X364 X365 X366 X367 X368 X369 X370 X371 X372 X375 X376 X377 X378 X379 X380 X381 X382 X383 X384 X385 X386 X387 X388 X389 X390 X391 X392 X393 X394 X395 X396 X399 X403 X408 X409 X410 X411 X412 X413 X414 X415 X432 X433 X434 X435 X441 X445 X446 X447 X448 X449 X450 X455 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 M6:  48% 47%

X3 X6 X7 X8 X14 X15 X20 X21 X22 X23 X24 X25 X26 X27 X28 X29 X30 X31 X32 X33 X34 X35 X38 X41 X42 X43 X44 X49 X50 X51 X54 X55 X56 X57 X58 X59 X60 X61 X62 X63 X64 X65 X66 X67 X68 X69 X70 X71 X75 X78 X79 X80 X81 X87 X88 X89 X90 X91 X94 X95 X96 X97 X102 X103 X106 X107 X108 X109 X110 X111 X112 X113 X114 X115 X116 X117 X118 X121 X122 X123 X124 X125 X126 X127 X128 X131 X132 X133 X137 X138 X139 X140 X141 X142 X146 X149 X157 X158 X159 X160 X164 X167 X168 X171 X172 X173 X174 X175 X176 X177 X178 X179 X180 X181 X182 X188 X189 X190 X191 X192 X207 X208 X209 X210 X211 X224 X225 X226 X227 X228 X241 X242 X243 X244 X251 X252 X255 X256 X257 X258 X262 X268 X271 X272 X273 X274 X275 X276 X277 X278 X279 X280 X281 X284 X285 X286 X287 X288 X293 X294 X309 X312 X315 X316 X324 X325 X326 X327 X328 X329 X330 X340 X341 X342 X343 X344 X345 X346 X347 X348 X351 X352 X356 X360 X361 X362 X363 X364 X365 X366 X367 X368 X369 X370 X371 X372 X375 X376 X377 X378 X379 X380 X381 X382 X383 X384 X385 X386 X387 X388 X389 X390 X391 X392 X393 X394 X395 X396 X399 X403 X406 X407 X408 X409 X410 X411 X412 X413 X414 X415 X432 X433 X434 X435 X441 X445 X446 X447 X448 X449 X450 X455 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

UNK  
UNK  
UNK  
UNK  
UNK  
UNK  
UNK  
UNK

• Molecule 3: Unknown structure

Chain f1:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain h1:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain i1:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain f2:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain h2:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain i2:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain f3:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain h3:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain i3:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain f4:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain h4:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain i4:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain f5:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain h5:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain i5:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain f6:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Unknown structure

Chain h6:  100%

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:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain s1:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain j2:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain k2:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain p2:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain s2:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain j3:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain k3:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Unknown structure

Chain p3:  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 11:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: Unknown structure

Chain 12:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: Unknown structure

Chain 13:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: Unknown structure

Chain 14:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: Unknown structure

Chain 15:  100%

There are no outlier residues recorded for this chain.

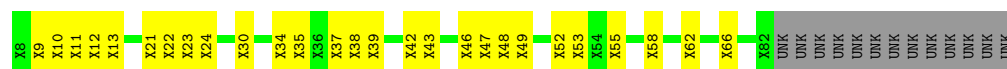
- Molecule 6: Unknown structure

Chain 16:  100%

There are no outlier residues recorded for this chain.

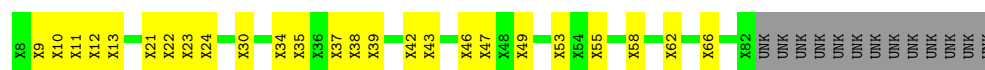
- Molecule 7: SDAP

Chain U1: 



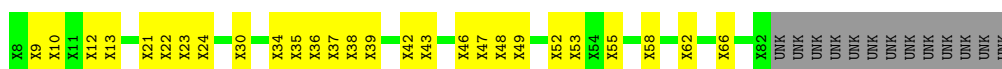
- Molecule 7: SDAP

Chain U2: 



- Molecule 7: SDAP

Chain U3: 



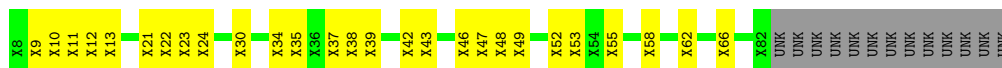
- Molecule 7: SDAP

Chain U4: 57% 28% 15%



- Molecule 7: SDAP

Chain U5: 55% 31% 15%



- Molecule 7: SDAP

Chain U6: 57% 28% 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.

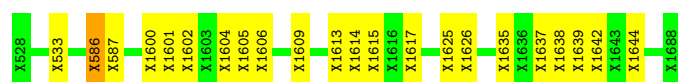
- Molecule 13: Unknown structure

Chain w6:  100%


There are no outlier residues recorded for this chain.

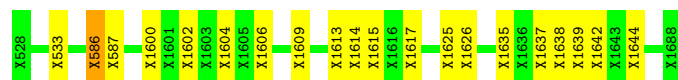
- Molecule 14: Unknown structure

Chain BA:  85% 14%




- Molecule 14: Unknown structure

Chain BB:  86% 13%




- Molecule 14: Unknown structure

Chain BC:  84% 15%




- Molecule 14: Unknown structure

Chain BD:  84% 15%




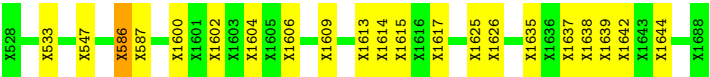
- Molecule 14: Unknown structure

Chain BE:  83% 16%



- Molecule 14: Unknown structure

Chain BF:  86% 14%



## 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 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 <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> )	0.36 , 102.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	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 <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.

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

## 5 Model quality

### 5.1 Standard geometry

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

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 [i](#)

#### 5.3.1 Protein backbone [i](#)

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

#### 5.3.2 Protein sidechains [i](#)

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

#### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
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.